



Full wwPDB NMR Structure Validation Report ⓘ

Mar 26, 2026 – 02:29 AM UTC

PDB ID : 2MXA / pdb_00002mxa
BMRB ID : 19971
Title : Solution structure of the NDH-1 complex subunit CupS from *Thermosynechococcus elongatus*
Authors : Korste, A.; Wulfhorst, H.; Ikegami, T.; Nowaczyk, M.M.; Stoll, R.
Deposited on : 2014-12-17

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

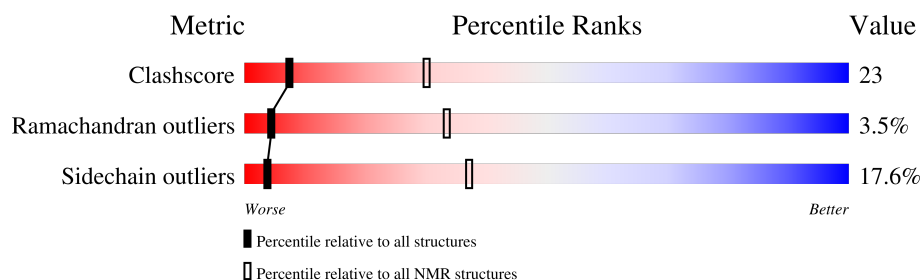
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 90%.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	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	159	

2 Ensemble composition and analysis

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

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:3-A:45, A:54-A:129 (119)	0.63	1

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

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

The models can be grouped into 2 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 2, 6, 8, 9
2	3, 4, 5, 7, 10

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1932 atoms, of which 981 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called NDH-1 complex sensory subunit CupS.

Mol	Chain	Residues	Atoms						Trace
1	A	129	Total	C	H	N	O	S	0
			1932	608	981	157	184	2	

There are 10 discrepancies between the modelled and reference sequences:

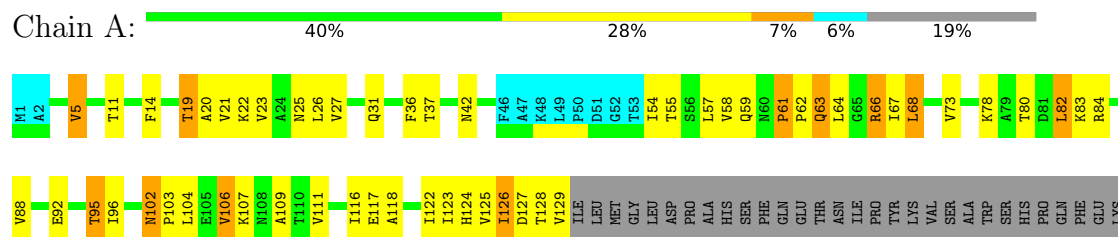
Chain	Residue	Modelled	Actual	Comment	Reference
A	150	SER	-	expression tag	UNP Q8DMA1
A	151	ALA	-	expression tag	UNP Q8DMA1
A	152	TRP	-	expression tag	UNP Q8DMA1
A	153	SER	-	expression tag	UNP Q8DMA1
A	154	HIS	-	expression tag	UNP Q8DMA1
A	155	PRO	-	expression tag	UNP Q8DMA1
A	156	GLN	-	expression tag	UNP Q8DMA1
A	157	PHE	-	expression tag	UNP Q8DMA1
A	158	GLU	-	expression tag	UNP Q8DMA1
A	159	LYS	-	expression tag	UNP Q8DMA1

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: NDH-1 complex sensory subunit CupS

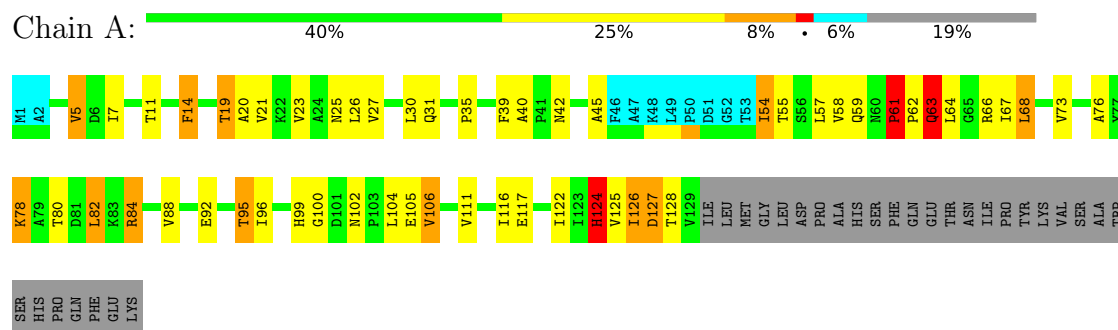


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

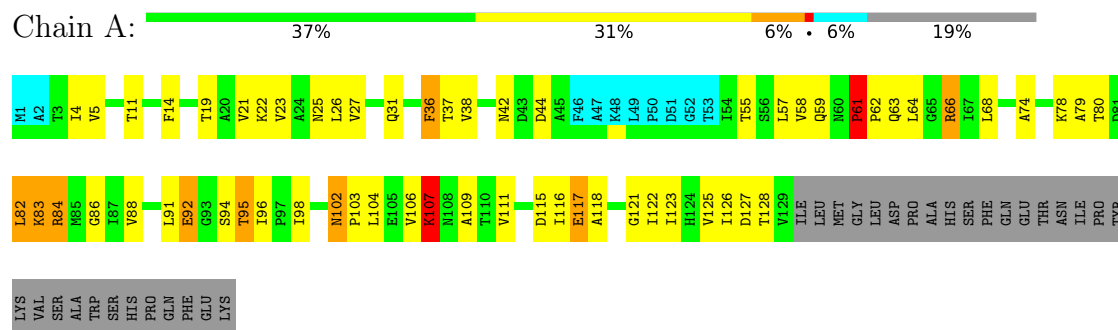
4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: NDH-1 complex sensory subunit CupS



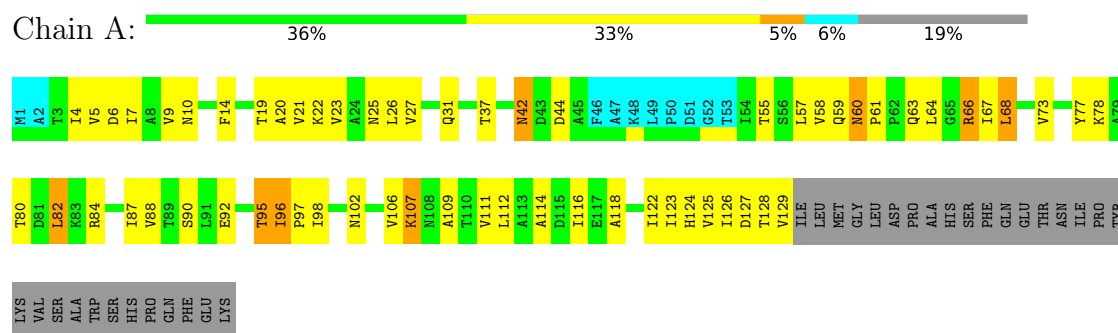
4.2.2 Score per residue for model 2

- Molecule 1: NDH-1 complex sensory subunit CupS



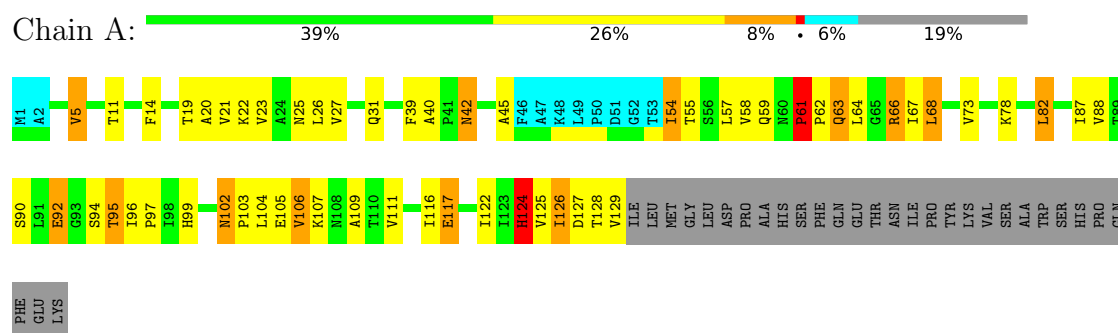
4.2.3 Score per residue for model 3

- Molecule 1: NDH-1 complex sensory subunit CupS



4.2.4 Score per residue for model 4

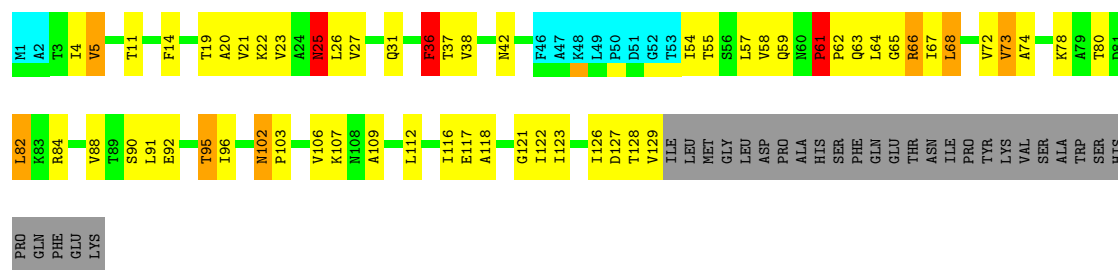
- Molecule 1: NDH-1 complex sensory subunit CupS



4.2.5 Score per residue for model 5

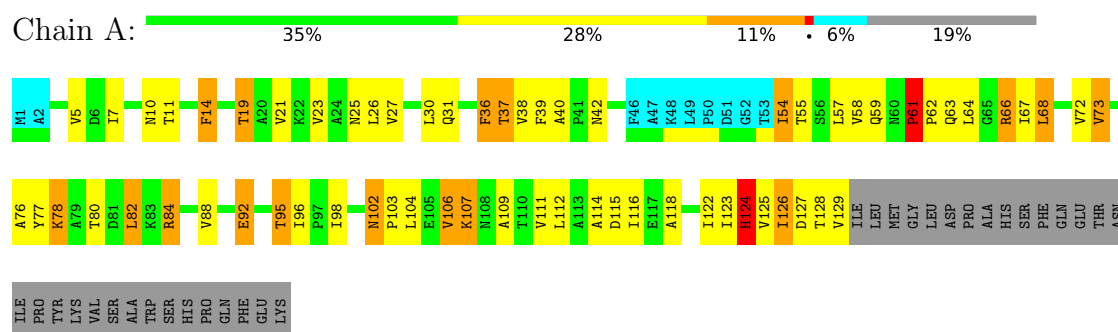
- Molecule 1: NDH-1 complex sensory subunit CupS





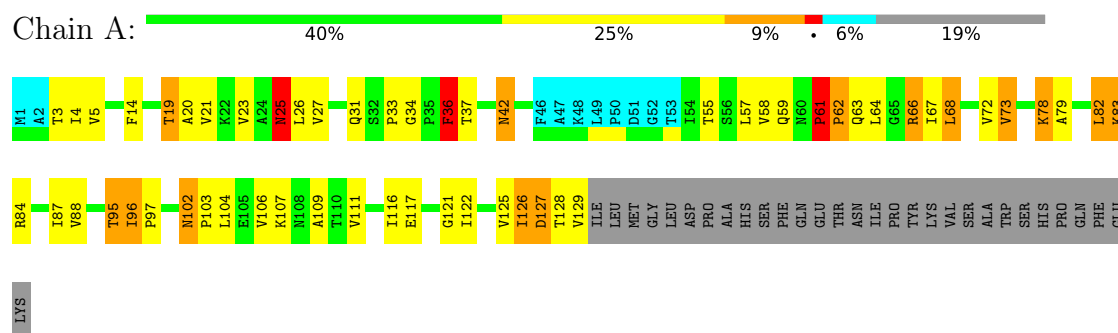
4.2.6 Score per residue for model 6

- Molecule 1: NDH-1 complex sensory subunit CupS



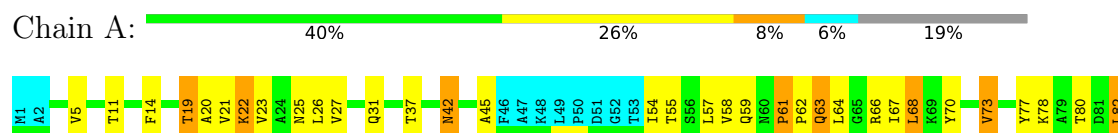
4.2.7 Score per residue for model 7

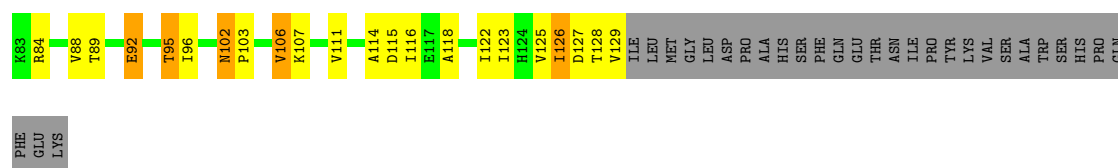
- Molecule 1: NDH-1 complex sensory subunit CupS



4.2.8 Score per residue for model 8

- Molecule 1: NDH-1 complex sensory subunit CupS

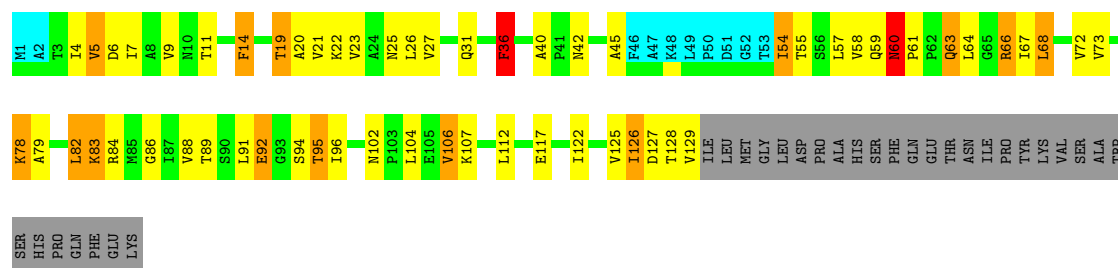




4.2.9 Score per residue for model 9

- Molecule 1: NDH-1 complex sensory subunit CupS

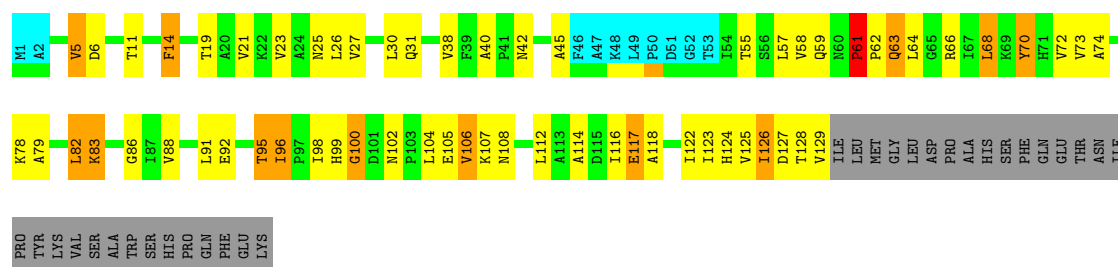
Chain A: 38% 27% 9% 6% 19%



4.2.10 Score per residue for model 10

- Molecule 1: NDH-1 complex sensory subunit CupS

Chain A: 36% 30% 8% 6% 19%



5 Refinement protocol and experimental data overview

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

Of the 40 calculated structures, 10 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
NMRPipe	structure solution	any
NMRPipe	structure solution	any
CNS	structure solution	
TALOS	structure solution	
TALOS	structure solution	
TALOS	structure solution	
TALOS	structure solution	
ARIA	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1866
Number of shifts mapped to atoms	1504
Number of unparsed shifts	0
Number of shifts with mapping errors	362
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	90%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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	0.61±0.01	0±0/894 (0.0± 0.0%)	0.92±0.03	2±1/1227 (0.2± 0.1%)
All	All	0.61	0/8940 (0.0%)	0.92	24/12270 (0.2%)

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	124	HIS	CA-CB-CG	8.28	122.08	113.80	4	3
1	A	61	PRO	CA-C-N	6.39	127.82	119.84	7	8
1	A	61	PRO	C-N-CA	6.39	127.82	119.84	7	8
1	A	36	PHE	CA-CB-CG	6.13	119.93	113.80	9	3
1	A	25	ASN	CA-CB-CG	5.73	118.33	112.60	7	2

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	879	906	903	41±6
All	All	8790	9060	9030	414

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 23.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:77:TYR:CG	1:A:82:LEU:HD21	0.89	2.03	6	1
1:A:42:ASN:ND2	1:A:127:ASP:HA	0.79	1.93	4	9
1:A:77:TYR:CD1	1:A:82:LEU:HD21	0.76	2.15	6	1
1:A:118:ALA:HB2	1:A:123:ILE:HG13	0.74	1.59	5	6
1:A:117:GLU:HA	1:A:122:ILE:HD13	0.70	1.63	2	7
1:A:64:LEU:HA	1:A:67:ILE:HD12	0.69	1.62	1	6
1:A:36:PHE:CD2	1:A:72:VAL:HG21	0.68	2.23	5	4
1:A:55:THR:O	1:A:58:VAL:HG12	0.68	1.88	9	10
1:A:5:VAL:HG13	1:A:31:GLN:NE2	0.67	2.04	2	10
1:A:112:LEU:HD11	1:A:127:ASP:HB2	0.66	1.67	10	5
1:A:104:LEU:HD23	1:A:111:VAL:HG21	0.66	1.65	6	3
1:A:78:LYS:HE3	1:A:122:ILE:HD11	0.65	1.68	10	2
1:A:92:GLU:OE1	1:A:94:SER:HB3	0.64	1.92	4	1
1:A:63:GLN:NE2	1:A:67:ILE:HD11	0.63	2.07	9	2
1:A:111:VAL:HG22	1:A:124:HIS:NE2	0.63	2.09	6	2
1:A:26:LEU:HD11	1:A:92:GLU:HB3	0.63	1.70	3	6
1:A:40:ALA:O	1:A:125:VAL:HA	0.63	1.93	1	5
1:A:78:LYS:CE	1:A:122:ILE:HD11	0.63	2.24	10	2
1:A:26:LEU:HD22	1:A:66:ARG:N	0.62	2.09	3	7
1:A:42:ASN:HD22	1:A:127:ASP:HA	0.62	1.52	3	9
1:A:78:LYS:O	1:A:82:LEU:HD22	0.61	1.96	3	10
1:A:83:LYS:HG2	1:A:104:LEU:CD1	0.61	2.26	7	4
1:A:37:THR:HG21	1:A:77:TYR:CG	0.60	2.31	6	1
1:A:106:VAL:O	1:A:107:LYS:HG2	0.60	1.96	8	2
1:A:55:THR:O	1:A:59:GLN:HG2	0.59	1.97	9	10
1:A:54:ILE:HD12	1:A:57:LEU:HD22	0.58	1.75	6	4
1:A:57:LEU:HD23	1:A:63:GLN:HE22	0.58	1.58	8	4
1:A:31:GLN:O	1:A:33:PRO:HD3	0.57	1.98	7	1
1:A:90:SER:HB2	1:A:92:GLU:OE2	0.57	2.00	4	1
1:A:63:GLN:HA	1:A:92:GLU:OE2	0.57	2.00	5	2
1:A:88:VAL:O	1:A:95:THR:HA	0.57	2.00	3	10
1:A:64:LEU:O	1:A:68:LEU:HD22	0.56	2.01	8	9
1:A:82:LEU:HD12	1:A:88:VAL:HG12	0.56	1.77	8	9
1:A:77:TYR:CB	1:A:82:LEU:HD21	0.55	2.31	6	1
1:A:70:TYR:CZ	1:A:72:VAL:HG11	0.55	2.35	10	1
1:A:92:GLU:CD	1:A:94:SER:HB3	0.55	2.27	4	1
1:A:78:LYS:HD3	1:A:122:ILE:HD12	0.55	1.78	2	3
1:A:39:PHE:HD1	1:A:124:HIS:NE2	0.55	1.99	4	1
1:A:111:VAL:HG22	1:A:124:HIS:CD2	0.55	2.37	6	2
1:A:77:TYR:CB	1:A:82:LEU:HD11	0.54	2.33	6	2
1:A:90:SER:HB3	1:A:92:GLU:OE1	0.54	2.03	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:126:ILE:HG13	1:A:128:THR:O	0.54	2.02	10	6
1:A:78:LYS:HD2	1:A:115:ASP:OD1	0.54	2.03	2	1
1:A:109:ALA:CB	1:A:128:THR:HB	0.53	2.33	7	2
1:A:39:PHE:HD1	1:A:124:HIS:CE1	0.53	2.20	6	1
1:A:78:LYS:HD2	1:A:115:ASP:CG	0.53	2.29	8	2
1:A:79:ALA:O	1:A:83:LYS:HG3	0.53	2.04	7	4
1:A:116:ILE:O	1:A:122:ILE:HA	0.53	2.04	6	9
1:A:77:TYR:HB2	1:A:82:LEU:HD21	0.52	1.81	6	1
1:A:111:VAL:HA	1:A:125:VAL:O	0.52	2.04	7	4
1:A:73:VAL:HG21	1:A:89:THR:O	0.52	2.04	9	2
1:A:60:ASN:H	1:A:61:PRO:HD3	0.52	1.65	3	2
1:A:19:THR:O	1:A:23:VAL:HG12	0.52	2.05	2	10
1:A:57:LEU:O	1:A:61:PRO:HD2	0.51	2.04	9	2
1:A:60:ASN:H	1:A:61:PRO:CD	0.51	2.17	3	2
1:A:78:LYS:HE3	1:A:122:ILE:CD1	0.51	2.34	10	2
1:A:54:ILE:HG13	1:A:67:ILE:HD13	0.51	1.82	6	3
1:A:7:ILE:O	1:A:11:THR:HG23	0.50	2.05	9	3
1:A:57:LEU:HD23	1:A:63:GLN:NE2	0.50	2.22	10	5
1:A:106:VAL:HG11	1:A:124:HIS:NE2	0.50	2.20	4	3
1:A:38:VAL:HG12	1:A:123:ILE:HG12	0.50	1.84	5	4
1:A:102:ASN:HB2	1:A:103:PRO:HD3	0.49	1.84	2	2
1:A:104:LEU:HB3	1:A:111:VAL:HG21	0.49	1.84	6	1
1:A:102:ASN:HB3	1:A:103:PRO:CD	0.49	2.37	4	1
1:A:99:HIS:C	1:A:105:GLU:HB2	0.49	2.32	1	2
1:A:63:GLN:O	1:A:67:ILE:HG13	0.49	2.08	7	4
1:A:61:PRO:O	1:A:63:GLN:N	0.49	2.45	10	7
1:A:6:ASP:O	1:A:9:VAL:HG12	0.49	2.07	9	2
1:A:77:TYR:HB2	1:A:82:LEU:CD2	0.49	2.38	6	1
1:A:78:LYS:HE3	1:A:122:ILE:HG13	0.48	1.85	6	3
1:A:37:THR:HA	1:A:122:ILE:O	0.48	2.09	7	5
1:A:26:LEU:O	1:A:30:LEU:HG	0.48	2.09	6	3
1:A:57:LEU:HB3	1:A:63:GLN:NE2	0.48	2.24	9	1
1:A:96:ILE:HG23	1:A:107:LYS:HB3	0.48	1.85	3	4
1:A:54:ILE:HA	1:A:57:LEU:HB2	0.47	1.85	1	6
1:A:88:VAL:HG22	1:A:96:ILE:O	0.47	2.09	4	10
1:A:58:VAL:HG23	1:A:64:LEU:HD13	0.47	1.86	3	4
1:A:80:THR:O	1:A:84:ARG:HB2	0.47	2.09	8	6
1:A:117:GLU:CA	1:A:122:ILE:HD13	0.47	2.38	4	3
1:A:88:VAL:HG13	1:A:98:ILE:CG1	0.47	2.39	2	4
1:A:4:ILE:HD12	1:A:5:VAL:N	0.47	2.25	9	5
1:A:124:HIS:CD2	1:A:124:HIS:O	0.47	2.67	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:7:ILE:HA	1:A:10:ASN:CB	0.47	2.40	6	1
1:A:45:ALA:HB2	1:A:127:ASP:C	0.46	2.35	1	1
1:A:37:THR:HG21	1:A:77:TYR:CD2	0.46	2.46	6	1
1:A:82:LEU:N	1:A:82:LEU:HD13	0.46	2.26	6	1
1:A:20:ALA:HB1	1:A:68:LEU:HD21	0.46	1.87	8	7
1:A:39:PHE:CD1	1:A:124:HIS:CE1	0.46	3.04	6	1
1:A:19:THR:HA	1:A:22:LYS:HE3	0.45	1.89	2	5
1:A:26:LEU:CD1	1:A:92:GLU:HB3	0.45	2.41	3	1
1:A:19:THR:HA	1:A:22:LYS:HB2	0.45	1.87	8	1
1:A:70:TYR:CE2	1:A:72:VAL:HG11	0.45	2.47	10	1
1:A:36:PHE:O	1:A:121:GLY:HA3	0.45	2.11	2	3
1:A:7:ILE:HA	1:A:10:ASN:HB3	0.45	1.88	6	2
1:A:99:HIS:HB2	1:A:105:GLU:HB2	0.45	1.87	1	1
1:A:106:VAL:HG22	1:A:107:LYS:HG2	0.45	1.87	10	1
1:A:6:ASP:CA	1:A:31:GLN:HE22	0.45	2.25	10	1
1:A:102:ASN:HB3	1:A:103:PRO:HD3	0.44	1.88	4	4
1:A:77:TYR:O	1:A:122:ILE:HG21	0.44	2.13	8	2
1:A:114:ALA:HB1	1:A:124:HIS:CD2	0.44	2.48	10	1
1:A:54:ILE:HD13	1:A:129:VAL:C	0.44	2.38	9	1
1:A:106:VAL:O	1:A:107:LYS:HG3	0.44	2.13	9	1
1:A:11:THR:HB	1:A:14:PHE:HB2	0.43	1.89	2	7
1:A:109:ALA:HA	1:A:128:THR:HB	0.43	1.88	5	2
1:A:114:ALA:HB1	1:A:124:HIS:ND1	0.43	2.28	3	1
1:A:106:VAL:HG11	1:A:124:HIS:CE1	0.43	2.48	4	1
1:A:109:ALA:HB2	1:A:128:THR:HB	0.43	1.90	7	1
1:A:74:ALA:HB3	1:A:91:LEU:HD13	0.43	1.90	5	1
1:A:40:ALA:N	1:A:124:HIS:O	0.42	2.48	4	1
1:A:38:VAL:CG1	1:A:123:ILE:HG12	0.42	2.44	6	1
1:A:104:LEU:HB3	1:A:111:VAL:CG2	0.42	2.44	6	1
1:A:58:VAL:CG2	1:A:64:LEU:HD13	0.42	2.43	9	1
1:A:90:SER:HB3	1:A:92:GLU:CD	0.42	2.40	5	1
1:A:25:ASN:HD22	1:A:25:ASN:C	0.42	2.22	7	1
1:A:87:ILE:HG13	1:A:97:PRO:HA	0.42	1.91	4	3
1:A:72:VAL:HG22	1:A:73:VAL:N	0.42	2.28	6	4
1:A:66:ARG:HD3	1:A:67:ILE:N	0.42	2.30	1	2
1:A:78:LYS:CD	1:A:122:ILE:HD12	0.42	2.45	2	1
1:A:109:ALA:HB1	1:A:126:ILE:HB	0.42	1.91	7	3
1:A:25:ASN:C	1:A:25:ASN:HD22	0.42	2.23	5	1
1:A:57:LEU:CD2	1:A:63:GLN:HE22	0.41	2.26	1	1
1:A:74:ALA:H	1:A:91:LEU:HD13	0.41	1.75	2	2
1:A:82:LEU:O	1:A:86:GLY:N	0.41	2.51	2	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:88:VAL:HG13	1:A:98:ILE:HG13	0.41	1.92	2	2
1:A:54:ILE:CD1	1:A:129:VAL:HG12	0.41	2.45	8	1
1:A:112:LEU:HD12	1:A:112:LEU:N	0.41	2.31	6	1
1:A:3:THR:HG22	1:A:5:VAL:HG12	0.41	1.91	7	1
1:A:114:ALA:O	1:A:115:ASP:HB3	0.41	2.16	6	1
1:A:35:PRO:HB2	1:A:76:ALA:HB2	0.41	1.93	1	1
1:A:39:PHE:HD1	1:A:124:HIS:CD2	0.41	2.34	4	1
1:A:45:ALA:O	1:A:129:VAL:HG23	0.41	2.16	9	3
1:A:61:PRO:HB3	1:A:62:PRO:HD2	0.40	1.93	7	1
1:A:26:LEU:HD22	1:A:65:GLY:C	0.40	2.41	5	1
1:A:54:ILE:HD11	1:A:129:VAL:HG12	0.40	1.94	8	1
1:A:63:GLN:O	1:A:63:GLN:HG2	0.40	2.16	9	1
1:A:100:GLY:HA2	1:A:105:GLU:HG3	0.40	1.94	10	1
1:A:111:VAL:HG11	1:A:114:ALA:CB	0.40	2.47	8	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	118/159 (74%)	104±2 (88±2%)	10±1 (8±1%)	4±1 (3±1%)	4	33
All	All	1180/1590 (74%)	1043 (88%)	96 (8%)	41 (3%)	4	33

All 10 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	102	ASN	10
1	A	61	PRO	8
1	A	62	PRO	8
1	A	107	LYS	4
1	A	63	GLN	3
1	A	100	GLY	2
1	A	60	ASN	2
1	A	14	PHE	2

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Mol	Chain	Res	Type	Models (Total)
1	A	76	ALA	1
1	A	34	GLY	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	98/132 (74%)	81±3 (82±3%)	17±3 (18±3%)	4	37
All	All	980/1320 (74%)	808 (82%)	172 (18%)	4	37

All 35 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	21	VAL	10
1	A	25	ASN	10
1	A	27	VAL	10
1	A	68	LEU	10
1	A	82	LEU	10
1	A	95	THR	10
1	A	106	VAL	10
1	A	126	ILE	10
1	A	66	ARG	9
1	A	73	VAL	8
1	A	92	GLU	7
1	A	5	VAL	5
1	A	14	PHE	5
1	A	19	THR	5
1	A	84	ARG	5
1	A	36	PHE	5
1	A	54	ILE	4
1	A	78	LYS	4
1	A	83	LYS	4
1	A	42	ASN	4
1	A	63	GLN	3
1	A	124	HIS	3
1	A	117	GLU	3

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Mol	Chain	Res	Type	Models (Total)
1	A	96	ILE	3
1	A	127	ASP	2
1	A	94	SER	2
1	A	107	LYS	2
1	A	70	TYR	2
1	A	39	PHE	1
1	A	37	THR	1
1	A	22	LYS	1
1	A	60	ASN	1
1	A	91	LEU	1
1	A	99	HIS	1
1	A	108	ASN	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 90% for the well-defined parts and 89% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list*

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	1866
Number of shifts mapped to atoms	1504
Number of unparsed shifts	0
Number of shifts with mapping errors	362
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	5

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

- No matching atom found in the structure. All 362 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	130	ILE	H	10.381	0.004	1
1	A	130	ILE	HA	4.108	0.005	1
1	A	130	ILE	HB	1.261	0.005	1
1	A	130	ILE	HD11	0.233	0.002	1
1	A	130	ILE	HD12	0.233	0.002	1
1	A	130	ILE	HD13	0.233	0.002	1
1	A	130	ILE	HG12	0.522	0.002	2
1	A	130	ILE	HG13	1.27	0.003	2
1	A	130	ILE	HG21	0.696	0.005	1
1	A	130	ILE	HG22	0.696	0.005	1
1	A	130	ILE	HG23	0.696	0.005	1
1	A	130	ILE	C	174.461	0.0	1
1	A	130	ILE	CA	62.651	0.074	1
1	A	130	ILE	CB	38.126	0.048	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	130	ILE	CD1	13.724	0.044	1
1	A	130	ILE	CG1	26.365	0.031	1
1	A	130	ILE	CG2	18.894	0.044	1
1	A	130	ILE	N	131.606	0.047	1
1	A	131	LEU	H	7.808	0.007	1
1	A	131	LEU	HA	4.542	0.004	1
1	A	131	LEU	HB2	1.474	0.008	2
1	A	131	LEU	HB3	1.475	0.008	2
1	A	131	LEU	HD11	0.794	0.008	2
1	A	131	LEU	HD12	0.794	0.008	2
1	A	131	LEU	HD13	0.794	0.008	2
1	A	131	LEU	HD21	0.808	0.003	2
1	A	131	LEU	HD22	0.808	0.003	2
1	A	131	LEU	HD23	0.808	0.003	2
1	A	131	LEU	HG	1.569	0.006	1
1	A	131	LEU	C	176.911	0.0	1
1	A	131	LEU	CA	53.828	0.03	1
1	A	131	LEU	CB	44.673	0.048	1
1	A	131	LEU	CD1	23.687	0.056	2
1	A	131	LEU	CD2	23.884	0.001	2
1	A	131	LEU	CG	26.239	0.002	1
1	A	131	LEU	N	121.996	0.047	1
1	A	132	MET	H	7.936	0.006	1
1	A	132	MET	HA	3.925	0.002	1
1	A	132	MET	HB2	1.645	0.002	2
1	A	132	MET	HB3	1.609	0.006	2
1	A	132	MET	HG2	1.904	0.001	2
1	A	132	MET	HG3	1.855	0.001	2
1	A	132	MET	CA	55.996	0.062	1
1	A	132	MET	CB	31.419	0.017	1
1	A	132	MET	CG	31.899	0.002	1
1	A	132	MET	N	119.785	0.026	1
1	A	133	GLY	H	8.129	0.002	1
1	A	133	GLY	HA2	3.841	0.001	2
1	A	133	GLY	HA3	3.841	0.001	2
1	A	133	GLY	C	173.744	0.0	1
1	A	133	GLY	CA	45.125	0.055	1
1	A	133	GLY	N	108.379	0.057	1
1	A	134	LEU	H	8.06	0.006	1
1	A	134	LEU	HA	4.287	0.003	1
1	A	134	LEU	HB2	1.502	0.002	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	134	LEU	HB3	1.563	0.003	2
1	A	134	LEU	HD11	0.842	0.004	2
1	A	134	LEU	HD12	0.842	0.004	2
1	A	134	LEU	HD13	0.842	0.004	2
1	A	134	LEU	HD21	0.788	0.004	2
1	A	134	LEU	HD22	0.788	0.004	2
1	A	134	LEU	HD23	0.788	0.004	2
1	A	134	LEU	HG	1.552	0.001	1
1	A	134	LEU	C	176.638	0.0	1
1	A	134	LEU	CA	54.93	0.075	1
1	A	134	LEU	CB	42.674	0.038	1
1	A	134	LEU	CD1	25.014	0.041	2
1	A	134	LEU	CD2	23.473	0.007	2
1	A	134	LEU	CG	27.032	0.042	1
1	A	134	LEU	N	121.379	0.061	1
1	A	135	ASP	H	8.312	0.006	1
1	A	135	ASP	HA	4.813	0.001	1
1	A	135	ASP	HB2	2.671	0.002	2
1	A	135	ASP	HB3	2.508	0.003	2
1	A	135	ASP	CA	51.902	0.064	1
1	A	135	ASP	CB	41.613	0.031	1
1	A	135	ASP	N	122.414	0.035	1
1	A	136	PRO	HA	4.259	0.002	1
1	A	136	PRO	HB2	2.236	0.004	2
1	A	136	PRO	HB3	1.9	0.003	2
1	A	136	PRO	HD2	3.814	0.004	1
1	A	136	PRO	HD3	3.814	0.004	1
1	A	136	PRO	HG2	1.955	0.006	1
1	A	136	PRO	HG3	1.955	0.006	1
1	A	136	PRO	C	176.933	0.0	1
1	A	136	PRO	CA	64.063	0.05	1
1	A	136	PRO	CB	32.112	0.032	1
1	A	136	PRO	CD	50.984	0.093	1
1	A	136	PRO	CG	27.309	0.068	1
1	A	137	ALA	H	8.343	0.003	1
1	A	137	ALA	HA	4.172	0.002	1
1	A	137	ALA	HB1	1.268	0.002	1
1	A	137	ALA	HB2	1.268	0.002	1
1	A	137	ALA	HB3	1.268	0.002	1
1	A	137	ALA	C	177.938	0.0	1
1	A	137	ALA	CA	53.03	0.031	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	137	ALA	CB	18.737	0.062	1
1	A	137	ALA	N	121.178	0.022	1
1	A	138	HIS	H	7.841	0.004	1
1	A	138	HIS	HA	4.566	0.003	1
1	A	138	HIS	HB2	3.128	0.006	2
1	A	138	HIS	HB3	2.983	0.006	2
1	A	138	HIS	C	175.404	0.0	1
1	A	138	HIS	CA	56.252	0.062	1
1	A	138	HIS	CB	30.972	0.059	1
1	A	138	HIS	N	117.273	0.109	1
1	A	139	SER	H	7.977	0.006	1
1	A	139	SER	HA	4.347	0.005	1
1	A	139	SER	HB2	3.726	0.001	2
1	A	139	SER	HB3	3.726	0.001	2
1	A	139	SER	C	174.169	0.0	1
1	A	139	SER	CA	58.681	0.043	1
1	A	139	SER	CB	63.855	0.085	1
1	A	139	SER	N	115.934	0.029	1
1	A	140	PHE	H	8.217	0.005	1
1	A	140	PHE	HA	4.558	0.004	1
1	A	140	PHE	HB2	3.141	0.007	2
1	A	140	PHE	HB3	3.024	0.015	2
1	A	140	PHE	HD1	7.233	0.004	3
1	A	140	PHE	HD2	7.233	0.004	3
1	A	140	PHE	C	175.476	0.0	1
1	A	140	PHE	CA	58.002	0.075	1
1	A	140	PHE	CB	39.124	0.072	1
1	A	140	PHE	CD1	131.813	0.001	3
1	A	140	PHE	CD2	131.813	0.001	3
1	A	140	PHE	N	121.295	0.015	1
1	A	141	GLN	H	8.094	0.004	1
1	A	141	GLN	HA	4.279	0.002	1
1	A	141	GLN	HB2	2.044	0.002	2
1	A	141	GLN	HB3	1.924	0.002	2
1	A	141	GLN	HE21	7.467	0.005	1
1	A	141	GLN	HE22	6.82	0.001	1
1	A	141	GLN	HG2	2.275	0.003	2
1	A	141	GLN	HG3	2.275	0.003	2
1	A	141	GLN	C	175.652	0.0	1
1	A	141	GLN	CA	55.898	0.023	1
1	A	141	GLN	CB	29.677	0.025	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	141	GLN	CD	180.381	0.002	1
1	A	141	GLN	CG	33.884	0.089	1
1	A	141	GLN	N	121.005	0.021	1
1	A	141	GLN	NE2	112.205	0.001	1
1	A	142	GLU	H	8.407	0.004	1
1	A	142	GLU	HA	4.272	0.002	1
1	A	142	GLU	HB2	2.061	0.006	2
1	A	142	GLU	HB3	1.95	0.006	2
1	A	142	GLU	HG2	2.255	0.008	2
1	A	142	GLU	HG3	2.255	0.008	2
1	A	142	GLU	C	176.569	0.0	1
1	A	142	GLU	CA	56.929	0.025	1
1	A	142	GLU	CB	30.321	0.028	1
1	A	142	GLU	CG	36.481	0.008	1
1	A	142	GLU	N	122.091	0.017	1
1	A	143	THR	H	8.135	0.005	1
1	A	143	THR	HA	4.33	0.004	1
1	A	143	THR	HB	4.212	0.003	1
1	A	143	THR	HG21	1.183	0.003	1
1	A	143	THR	HG22	1.183	0.003	1
1	A	143	THR	HG23	1.183	0.003	1
1	A	143	THR	C	174.131	0.0	1
1	A	143	THR	CA	61.908	0.021	1
1	A	143	THR	CB	69.791	0.053	1
1	A	143	THR	CG2	21.481	0.053	1
1	A	143	THR	N	114.211	0.022	1
1	A	144	ASN	H	8.455	0.007	1
1	A	144	ASN	HA	4.691	0.001	1
1	A	144	ASN	HB2	2.792	0.002	2
1	A	144	ASN	HB3	2.726	0.004	2
1	A	144	ASN	HD21	7.561	0.007	1
1	A	144	ASN	HD22	6.868	0.006	1
1	A	144	ASN	C	174.485	0.0	1
1	A	144	ASN	CA	53.27	0.05	1
1	A	144	ASN	CB	38.856	0.074	1
1	A	144	ASN	CG	177.138	0.0	1
1	A	144	ASN	N	120.943	0.066	1
1	A	144	ASN	ND2	112.698	0.004	1
1	A	145	ILE	H	8.002	0.004	1
1	A	145	ILE	HA	4.397	0.001	1
1	A	145	ILE	HB	1.806	0.002	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	145	ILE	HD11	0.829	0.002	1
1	A	145	ILE	HD12	0.829	0.002	1
1	A	145	ILE	HD13	0.829	0.002	1
1	A	145	ILE	HG12	1.458	0.002	2
1	A	145	ILE	HG13	1.114	0.004	2
1	A	145	ILE	HG21	0.84	0.006	1
1	A	145	ILE	HG22	0.84	0.006	1
1	A	145	ILE	HG23	0.84	0.006	1
1	A	145	ILE	CA	58.861	0.066	1
1	A	145	ILE	CB	38.719	0.048	1
1	A	145	ILE	CD1	12.648	0.067	1
1	A	145	ILE	CG1	26.932	0.065	1
1	A	145	ILE	CG2	17.246	0.082	1
1	A	145	ILE	N	122.46	0.074	1
1	A	146	PRO	HA	4.357	0.003	1
1	A	146	PRO	HB2	2.189	0.005	2
1	A	146	PRO	HB3	1.805	0.006	2
1	A	146	PRO	HD2	3.814	0.003	2
1	A	146	PRO	HD3	3.618	0.003	2
1	A	146	PRO	HG2	1.95	0.004	2
1	A	146	PRO	HG3	1.95	0.004	2
1	A	146	PRO	C	176.356	0.0	1
1	A	146	PRO	CA	63.362	0.025	1
1	A	146	PRO	CB	31.866	0.017	1
1	A	146	PRO	CD	50.973	0.052	1
1	A	146	PRO	CG	27.314	0.042	1
1	A	147	TYR	H	8.007	0.005	1
1	A	147	TYR	HA	4.488	0.004	1
1	A	147	TYR	HB2	2.968	0.008	2
1	A	147	TYR	HB3	2.969	0.008	2
1	A	147	TYR	HD1	7.072	0.006	3
1	A	147	TYR	HD2	7.072	0.006	3
1	A	147	TYR	HE1	6.795	0.006	3
1	A	147	TYR	HE2	6.795	0.006	3
1	A	147	TYR	C	175.324	0.0	1
1	A	147	TYR	CA	57.902	0.055	1
1	A	147	TYR	CB	38.816	0.073	1
1	A	147	TYR	CD1	133.201	0.022	3
1	A	147	TYR	CD2	133.201	0.022	3
1	A	147	TYR	CE1	118.216	0.028	3
1	A	147	TYR	CE2	118.216	0.028	3

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	147	TYR	N	120.291	0.019	1
1	A	148	LYS	H	8.042	0.004	1
1	A	148	LYS	HA	4.268	0.005	1
1	A	148	LYS	HB2	1.727	0.005	2
1	A	148	LYS	HB3	1.632	0.006	2
1	A	148	LYS	HD2	1.621	0.002	1
1	A	148	LYS	HD3	1.621	0.002	1
1	A	148	LYS	HE2	2.937	0.002	2
1	A	148	LYS	HE3	2.937	0.002	2
1	A	148	LYS	HG2	1.28	0.003	2
1	A	148	LYS	HG3	1.317	0.008	2
1	A	148	LYS	C	175.846	0.0	1
1	A	148	LYS	CA	55.986	0.047	1
1	A	148	LYS	CB	33.378	0.019	1
1	A	148	LYS	CD	29.113	0.053	1
1	A	148	LYS	CE	42.209	0.021	1
1	A	148	LYS	CG	24.636	0.019	1
1	A	148	LYS	N	123.461	0.017	1
1	A	149	VAL	H	8.069	0.004	1
1	A	149	VAL	HA	4.022	0.002	1
1	A	149	VAL	HB	2.012	0.002	1
1	A	149	VAL	HG11	0.894	0.004	2
1	A	149	VAL	HG12	0.894	0.004	2
1	A	149	VAL	HG13	0.894	0.004	2
1	A	149	VAL	HG21	0.914	0.007	2
1	A	149	VAL	HG22	0.914	0.007	2
1	A	149	VAL	HG23	0.914	0.007	2
1	A	149	VAL	C	176.103	0.0	1
1	A	149	VAL	CA	62.446	0.039	1
1	A	149	VAL	CB	32.756	0.049	1
1	A	149	VAL	CG1	20.893	0.033	2
1	A	149	VAL	CG2	20.441	0.0	2
1	A	149	VAL	N	121.671	0.032	1
1	A	150	SER	H	8.31	0.007	1
1	A	150	SER	HA	4.336	0.0	1
1	A	150	SER	HB2	3.718	0.0	1
1	A	150	SER	HB3	3.718	0.0	1
1	A	150	SER	C	174.259	0.0	1
1	A	150	SER	CA	58.184	0.064	1
1	A	150	SER	CB	63.956	0.022	1
1	A	150	SER	N	119.318	0.038	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	151	ALA	H	8.24	0.008	1
1	A	151	ALA	HA	4.212	0.003	1
1	A	151	ALA	HB1	1.228	0.003	1
1	A	151	ALA	HB2	1.228	0.003	1
1	A	151	ALA	HB3	1.228	0.003	1
1	A	151	ALA	C	177.197	0.0	1
1	A	151	ALA	CA	52.853	0.042	1
1	A	151	ALA	CB	19.099	0.026	1
1	A	151	ALA	N	125.7	0.018	1
1	A	152	TRP	H	7.934	0.005	1
1	A	152	TRP	HA	4.603	0.001	1
1	A	152	TRP	HB2	3.251	0.001	2
1	A	152	TRP	HB3	3.175	0.002	2
1	A	152	TRP	HE1	10.095	0.001	1
1	A	152	TRP	HH2	7.154	0.003	1
1	A	152	TRP	HZ2	7.429	0.004	1
1	A	152	TRP	HZ3	7.06	0.004	1
1	A	152	TRP	C	177.93	0.0	1
1	A	152	TRP	CA	57.27	0.031	1
1	A	152	TRP	CB	29.709	0.024	1
1	A	152	TRP	CH2	124.453	0.033	1
1	A	152	TRP	CZ2	114.499	0.063	1
1	A	152	TRP	CZ3	121.876	0.016	1
1	A	152	TRP	N	119.068	0.018	1
1	A	152	TRP	NE1	129.244	0.022	1
1	A	153	SER	H	7.824	0.012	1
1	A	153	SER	HA	4.318	0.001	1
1	A	153	SER	HB2	3.671	0.018	2
1	A	153	SER	HB3	3.64	0.001	2
1	A	153	SER	C	173.204	0.0	1
1	A	153	SER	CA	57.952	0.058	1
1	A	153	SER	CB	63.892	0.083	1
1	A	153	SER	N	116.976	0.034	1
1	A	154	HIS	H	8.04	0.004	1
1	A	154	HIS	HA	4.696	0.001	1
1	A	154	HIS	HB2	3.034	0.002	2
1	A	154	HIS	HB3	2.945	0.001	2
1	A	154	HIS	CA	54.713	0.043	1
1	A	154	HIS	CB	30.737	0.044	1
1	A	154	HIS	N	122.653	0.026	1
1	A	155	PRO	HA	4.324	0.005	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	155	PRO	HB2	2.2	0.006	2
1	A	155	PRO	HB3	1.763	0.006	2
1	A	155	PRO	HD2	3.685	0.006	2
1	A	155	PRO	HD3	3.362	0.006	2
1	A	155	PRO	HG2	1.943	0.004	2
1	A	155	PRO	HG3	1.944	0.003	2
1	A	155	PRO	C	176.829	0.0	1
1	A	155	PRO	CA	63.611	0.046	1
1	A	155	PRO	CB	32.106	0.102	1
1	A	155	PRO	CD	50.658	0.035	1
1	A	155	PRO	CG	27.481	0.045	1
1	A	156	GLN	H	8.714	0.005	1
1	A	156	GLN	HA	4.245	0.002	1
1	A	156	GLN	HB2	1.95	0.003	2
1	A	156	GLN	HB3	1.869	0.002	2
1	A	156	GLN	HE21	6.801	0.002	1
1	A	156	GLN	HE22	7.412	0.004	1
1	A	156	GLN	HG2	2.186	0.002	2
1	A	156	GLN	HG3	2.186	0.002	2
1	A	156	GLN	C	175.595	0.0	1
1	A	156	GLN	CA	55.898	0.025	1
1	A	156	GLN	CB	29.416	0.013	1
1	A	156	GLN	CD	180.437	0.006	1
1	A	156	GLN	CG	33.75	0.041	1
1	A	156	GLN	N	120.311	0.034	1
1	A	156	GLN	NE2	112.38	0.03	1
1	A	157	PHE	H	8.129	0.004	1
1	A	157	PHE	HA	4.658	0.002	1
1	A	157	PHE	HB2	2.984	0.005	2
1	A	157	PHE	HB3	3.192	0.004	2
1	A	157	PHE	C	175.397	0.0	1
1	A	157	PHE	CA	57.421	0.056	1
1	A	157	PHE	CB	39.784	0.041	1
1	A	157	PHE	N	120.408	0.015	1
1	A	158	GLU	H	8.268	0.004	1
1	A	158	GLU	HA	4.247	0.002	1
1	A	158	GLU	HB2	2.025	0.006	2
1	A	158	GLU	HB3	1.884	0.005	2
1	A	158	GLU	HG2	2.202	0.005	2
1	A	158	GLU	HG3	2.202	0.005	2
1	A	158	GLU	C	175.102	0.0	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	158	GLU	CA	56.603	0.03	1
1	A	158	GLU	CB	30.552	0.029	1
1	A	158	GLU	CG	36.354	0.04	1
1	A	158	GLU	N	122.621	0.008	1
1	A	159	LYS	H	7.869	0.004	1
1	A	159	LYS	HA	4.12	0.003	1
1	A	159	LYS	HB2	1.804	0.006	2
1	A	159	LYS	HB3	1.701	0.006	2
1	A	159	LYS	HD2	1.664	0.005	1
1	A	159	LYS	HD3	1.664	0.005	1
1	A	159	LYS	HE2	2.981	0.004	1
1	A	159	LYS	HE3	2.981	0.004	1
1	A	159	LYS	HG2	1.379	0.002	2
1	A	159	LYS	HG3	1.379	0.002	2
1	A	159	LYS	CA	57.755	0.034	1
1	A	159	LYS	CB	33.828	0.082	1
1	A	159	LYS	CD	29.299	0.054	1
1	A	159	LYS	CE	42.295	0.027	1
1	A	159	LYS	CG	24.711	0.006	1
1	A	159	LYS	N	127.136	0.009	1

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	157	-0.30 ± 0.12	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	147	0.08 ± 0.10	None needed (< 0.5 ppm)
$^{13}\text{C}'$	136	0.06 ± 0.16	None needed (< 0.5 ppm)
^{15}N	142	0.47 ± 0.44	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 90%, i.e. 1413 atoms were assigned a chemical shift out of a possible 1564. 0 out of 25 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	568/587 (97%)	235/238 (99%)	223/238 (94%)	110/111 (99%)

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	Total	¹ H	¹³ C	¹⁵ N
Sidechain	827/905 (91%)	562/600 (94%)	255/284 (90%)	10/21 (48%)
Aromatic	18/72 (25%)	9/35 (26%)	9/31 (29%)	0/6 (0%)
Overall	1413/1564 (90%)	806/873 (92%)	487/553 (88%)	120/138 (87%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 89%, i.e. 1502 atoms were assigned a chemical shift out of a possible 1689. 0 out of 26 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	603/636 (95%)	250/258 (97%)	238/258 (92%)	115/120 (96%)
Sidechain	881/971 (91%)	599/644 (93%)	272/305 (89%)	10/22 (45%)
Aromatic	18/82 (22%)	9/40 (22%)	9/36 (25%)	0/6 (0%)
Overall	1502/1689 (89%)	858/942 (91%)	519/599 (87%)	125/148 (84%)

7.1.4 Statistically unusual chemical shifts ⓘ

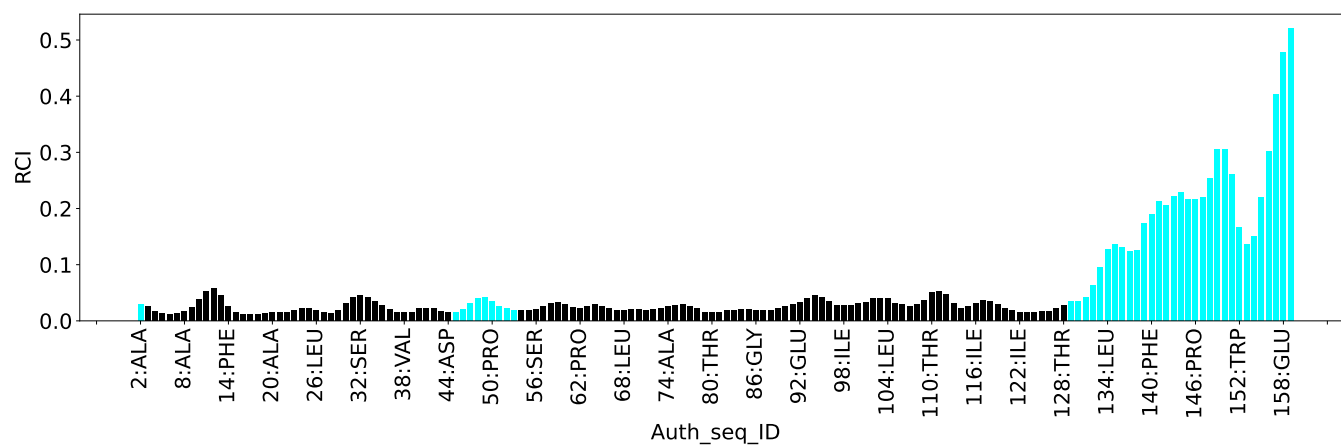
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	37	THR	HG1	6.10	0.08 – 2.19	23.5
1	A	11	THR	HG1	5.95	0.08 – 2.19	22.8
1	A	79	ALA	H	11.65	5.31 – 11.08	6.0
1	A	105	GLU	HB3	0.87	0.95 – 3.05	-5.4
1	A	121	GLY	HA3	5.76	2.08 – 5.71	5.1

7.1.5 Random Coil Index (RCI) plots ⓘ

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	2089
Intra-residue ($ i-j =0$)	929
Sequential ($ i-j =1$)	449
Medium range ($ i-j >1$ and $ i-j <5$)	283
Long range ($ i-j \geq 5$)	428
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	221
Number of unmapped restraints	0
Number of restraints per residue	14.5
Number of long range restraints per residue ¹	2.7

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)	54.6	0.2
0.2-0.5 (Medium)	72.3	0.5
>0.5 (Large)	154.3	3.71

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

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

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	19.9	9.2
10.0-20.0 (Medium)	0.2	12.71
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

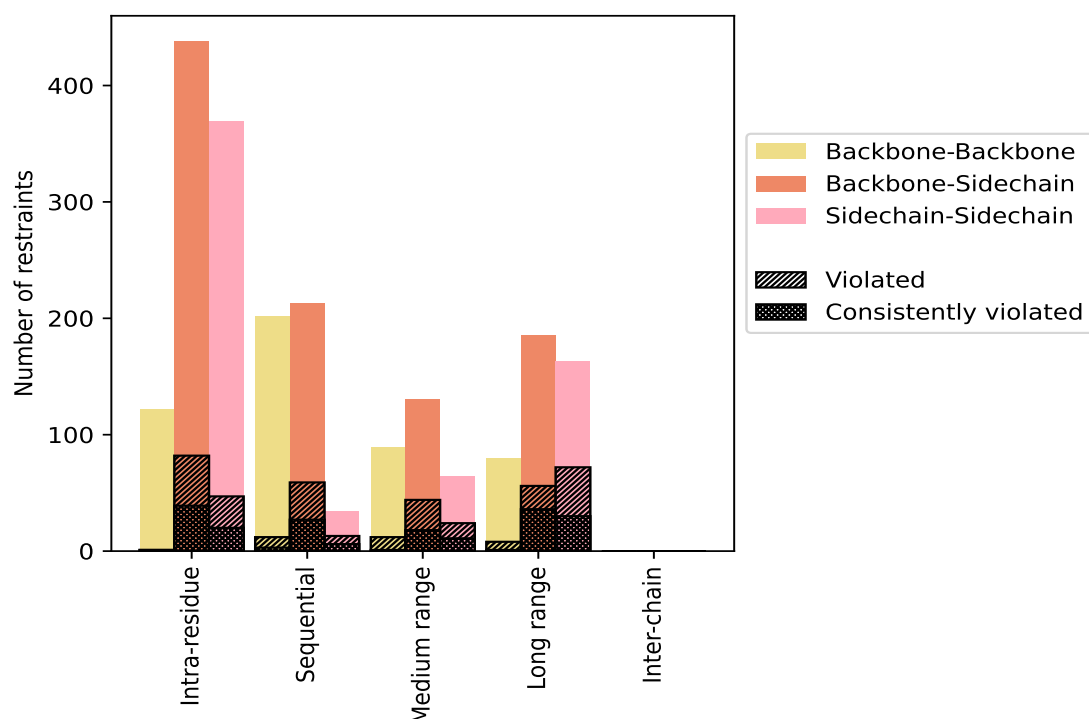
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue (i-j =0)	929	44.5	130	14.0	6.2	60	6.5	2.9
Backbone-Backbone	122	5.8	1	0.8	0.0	1	0.8	0.0
Backbone-Sidechain	438	21.0	82	18.7	3.9	39	8.9	1.9
Sidechain-Sidechain	369	17.7	47	12.7	2.2	20	5.4	1.0
Sequential (i-j =1)	449	21.5	84	18.7	4.0	36	8.0	1.7
Backbone-Backbone	202	9.7	12	5.9	0.6	3	1.5	0.1
Backbone-Sidechain	213	10.2	59	27.7	2.8	27	12.7	1.3
Sidechain-Sidechain	34	1.6	13	38.2	0.6	6	17.6	0.3
Medium range (i-j >1 & i-j <5)	283	13.5	80	28.3	3.8	30	10.6	1.4
Backbone-Backbone	89	4.3	12	13.5	0.6	1	1.1	0.0
Backbone-Sidechain	130	6.2	44	33.8	2.1	18	13.8	0.9
Sidechain-Sidechain	64	3.1	24	37.5	1.1	11	17.2	0.5
Long range (i-j ≥5)	428	20.5	136	31.8	6.5	67	15.7	3.2
Backbone-Backbone	80	3.8	8	10.0	0.4	1	1.2	0.0
Backbone-Sidechain	185	8.9	56	30.3	2.7	36	19.5	1.7
Sidechain-Sidechain	163	7.8	72	44.2	3.4	30	18.4	1.4
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	2089	100.0	430	20.6	20.6	193	9.2	9.2
Backbone-Backbone	493	23.6	33	6.7	1.6	6	1.2	0.3
Backbone-Sidechain	966	46.2	241	24.9	11.5	120	12.4	5.7
Sidechain-Sidechain	630	30.2	156	24.8	7.5	67	10.6	3.2

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

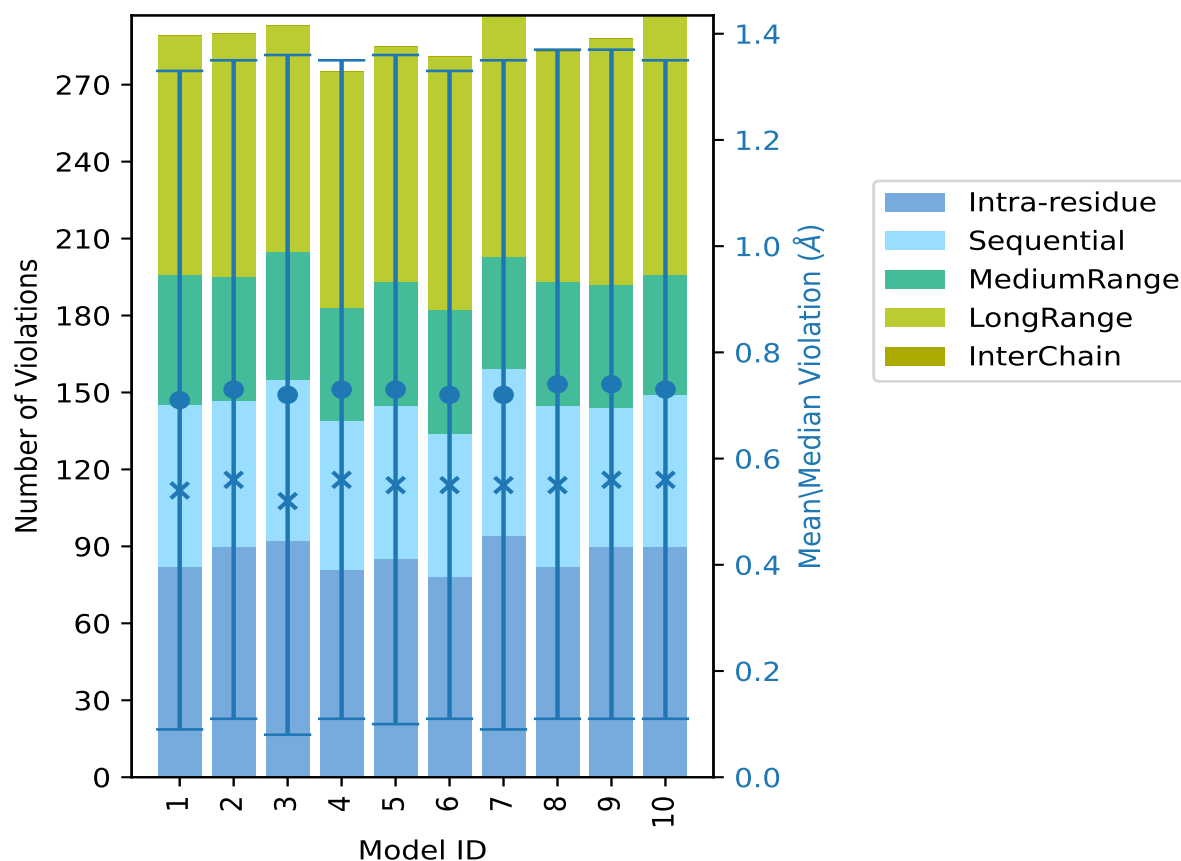
9.2 Distance violation statistics for each model [i](#)

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	82	63	51	93	0	289	0.71	3.57	0.62	0.54
2	90	57	48	95	0	290	0.73	3.2	0.62	0.56
3	92	63	50	88	0	293	0.72	3.71	0.64	0.52
4	81	58	44	92	0	275	0.73	2.7	0.62	0.56
5	85	60	48	92	0	285	0.73	3.57	0.63	0.55
6	78	56	48	99	0	281	0.72	2.71	0.61	0.55
7	94	65	44	94	0	297	0.72	3.25	0.63	0.55
8	82	63	48	90	0	283	0.74	2.9	0.63	0.55
9	90	54	48	96	0	288	0.74	3.19	0.63	0.56
10	90	59	47	101	0	297	0.73	3.17	0.62	0.56

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, 1659(IR:799, SQ:365, MR:203, LR:292, 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	%
22	9	11	20	0	62	1	10.0
8	8	13	8	0	37	2	20.0
12	6	3	7	0	28	3	30.0

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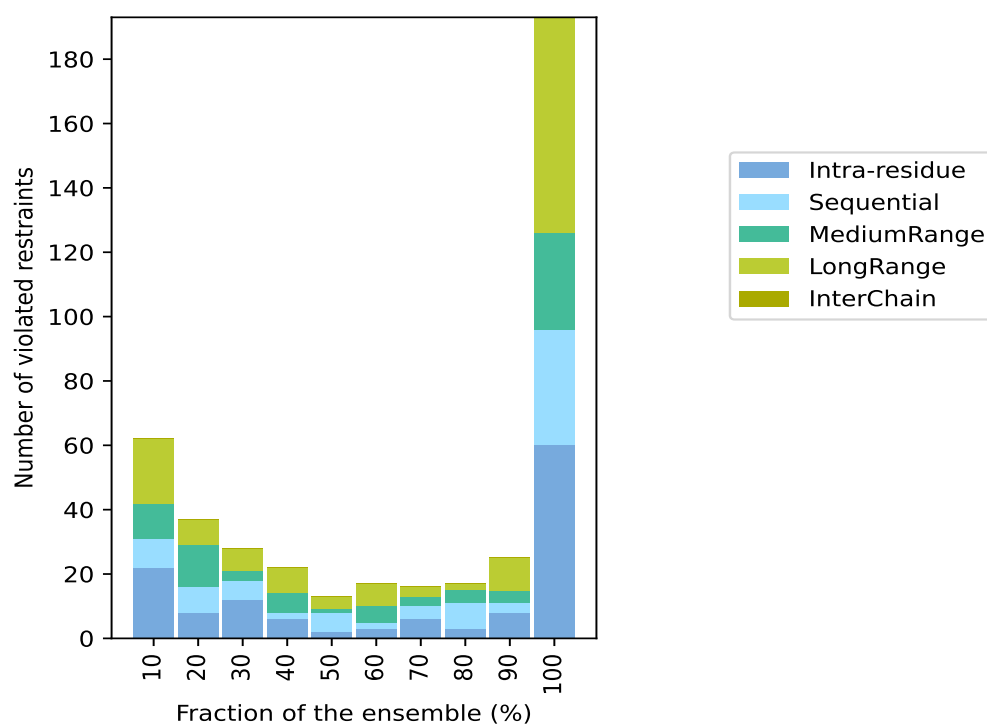
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
6	2	6	8	0	22	4	40.0
2	6	1	4	0	13	5	50.0
3	2	5	7	0	17	6	60.0
6	4	3	3	0	16	7	70.0
3	8	4	2	0	17	8	80.0
8	3	4	10	0	25	9	90.0
60	36	30	67	0	193	10	100.0

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

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

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

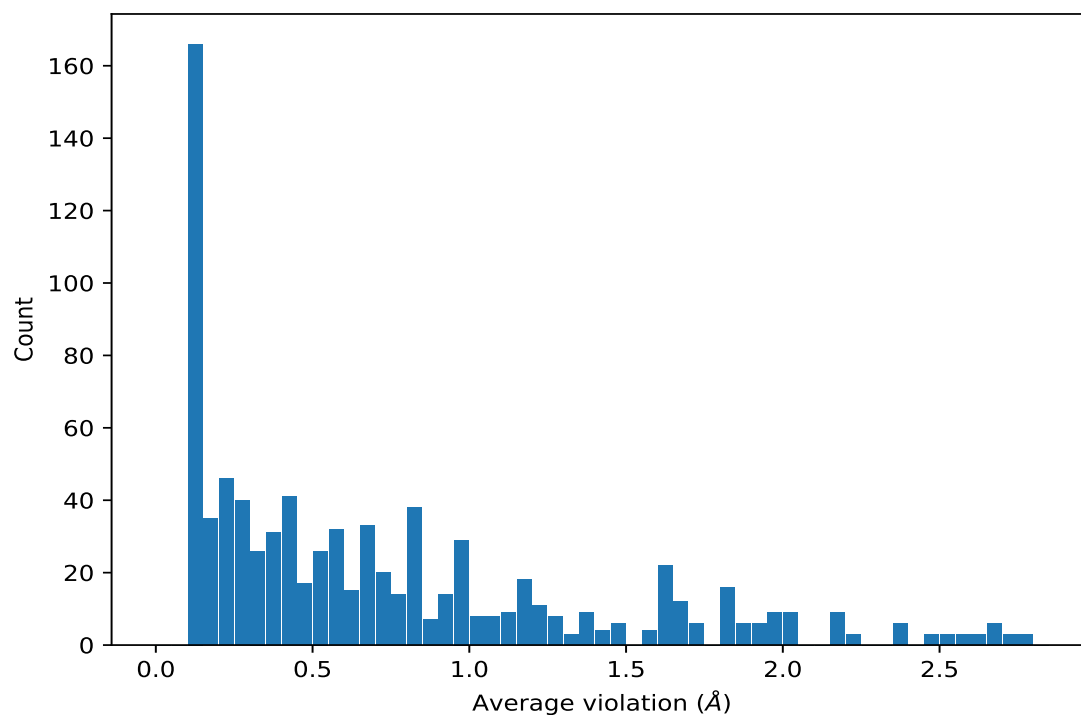


9.4 Most violated distance restraints in the ensemble [i](#)

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)
(1,1256)	1:83:A:LYS:HD3	1:104:A:LEU:HD21	10	2.79	0.74	2.87
(1,1256)	1:83:A:LYS:HD3	1:104:A:LEU:HD22	10	2.79	0.74	2.87
(1,1256)	1:83:A:LYS:HD3	1:104:A:LEU:HD23	10	2.79	0.74	2.87
(1,1411)	1:91:A:LEU:HA	1:73:A:VAL:HG11	10	2.71	0.03	2.71
(1,1411)	1:91:A:LEU:HA	1:73:A:VAL:HG12	10	2.71	0.03	2.71
(1,1411)	1:91:A:LEU:HA	1:73:A:VAL:HG13	10	2.71	0.03	2.71
(1,943)	1:64:A:LEU:HD11	1:24:A:ALA:HA	10	2.69	0.03	2.68
(1,943)	1:64:A:LEU:HD12	1:24:A:ALA:HA	10	2.69	0.03	2.68
(1,943)	1:64:A:LEU:HD13	1:24:A:ALA:HA	10	2.69	0.03	2.68
(1,1969)	1:124:A:HIS:HB2	1:104:A:LEU:HD11	10	2.68	0.25	2.62
(1,1969)	1:124:A:HIS:HB2	1:104:A:LEU:HD12	10	2.68	0.25	2.62
(1,1969)	1:124:A:HIS:HB2	1:104:A:LEU:HD13	10	2.68	0.25	2.62
(1,1023)	1:68:A:LEU:HD11	1:21:A:VAL:HA	10	2.61	0.1	2.64
(1,1023)	1:68:A:LEU:HD12	1:21:A:VAL:HA	10	2.61	0.1	2.64
(1,1023)	1:68:A:LEU:HD13	1:21:A:VAL:HA	10	2.61	0.1	2.64

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,204)	1:18:A:VAL:HG11	1:22:A:LYS:HE3	10	2.59	0.09	2.56
(1,204)	1:18:A:VAL:HG12	1:22:A:LYS:HE3	10	2.59	0.09	2.56
(1,204)	1:18:A:VAL:HG13	1:22:A:LYS:HE3	10	2.59	0.09	2.56
(1,958)	1:64:A:LEU:HD21	1:67:A:ILE:HB	10	2.51	0.04	2.51
(1,958)	1:64:A:LEU:HD22	1:67:A:ILE:HB	10	2.51	0.04	2.51
(1,958)	1:64:A:LEU:HD23	1:67:A:ILE:HB	10	2.51	0.04	2.51
(1,944)	1:64:A:LEU:HD11	1:24:A:ALA:H	10	2.45	0.05	2.46
(1,944)	1:64:A:LEU:HD12	1:24:A:ALA:H	10	2.45	0.05	2.46
(1,944)	1:64:A:LEU:HD13	1:24:A:ALA:H	10	2.45	0.05	2.46
(1,1082)	1:73:A:VAL:HG21	1:39:A:PHE:H	10	2.39	0.19	2.39
(1,1082)	1:73:A:VAL:HG22	1:39:A:PHE:H	10	2.39	0.19	2.39
(1,1082)	1:73:A:VAL:HG23	1:39:A:PHE:H	10	2.39	0.19	2.39
(1,1370)	1:88:A:VAL:HG11	1:96:A:ILE:HA	10	2.37	0.04	2.38
(1,1370)	1:88:A:VAL:HG12	1:96:A:ILE:HA	10	2.37	0.04	2.38
(1,1370)	1:88:A:VAL:HG13	1:96:A:ILE:HA	10	2.37	0.04	2.38
(1,1739)	1:111:A:VAL:HG11	1:106:A:VAL:H	10	2.24	0.11	2.21
(1,1739)	1:111:A:VAL:HG12	1:106:A:VAL:H	10	2.24	0.11	2.21
(1,1739)	1:111:A:VAL:HG13	1:106:A:VAL:H	10	2.24	0.11	2.21
(1,1985)	1:125:A:VAL:HG11	1:116:A:ILE:HD11	10	2.19	0.07	2.21
(1,1985)	1:125:A:VAL:HG11	1:116:A:ILE:HD12	10	2.19	0.07	2.21
(1,1985)	1:125:A:VAL:HG11	1:116:A:ILE:HD13	10	2.19	0.07	2.21
(1,1985)	1:125:A:VAL:HG12	1:116:A:ILE:HD11	10	2.19	0.07	2.21
(1,1985)	1:125:A:VAL:HG12	1:116:A:ILE:HD12	10	2.19	0.07	2.21
(1,1985)	1:125:A:VAL:HG12	1:116:A:ILE:HD13	10	2.19	0.07	2.21
(1,1985)	1:125:A:VAL:HG13	1:116:A:ILE:HD11	10	2.19	0.07	2.21
(1,1985)	1:125:A:VAL:HG13	1:116:A:ILE:HD12	10	2.19	0.07	2.21
(1,1985)	1:125:A:VAL:HG13	1:116:A:ILE:HD13	10	2.19	0.07	2.21
(1,187)	1:18:A:VAL:HG21	1:15:A:SER:HB3	10	2.04	0.03	2.04
(1,187)	1:18:A:VAL:HG22	1:15:A:SER:HB3	10	2.04	0.03	2.04
(1,187)	1:18:A:VAL:HG23	1:15:A:SER:HB3	10	2.04	0.03	2.04
(1,1077)	1:72:A:VAL:HA	1:73:A:VAL:HG21	10	2.04	0.02	2.04
(1,1077)	1:72:A:VAL:HA	1:73:A:VAL:HG22	10	2.04	0.02	2.04
(1,1077)	1:72:A:VAL:HA	1:73:A:VAL:HG23	10	2.04	0.02	2.04
(1,1258)	1:83:A:LYS:HB2	1:104:A:LEU:HD21	10	2.01	0.98	1.32
(1,1258)	1:83:A:LYS:HB2	1:104:A:LEU:HD22	10	2.01	0.98	1.32
(1,1258)	1:83:A:LYS:HB2	1:104:A:LEU:HD23	10	2.01	0.98	1.32
(1,432)	1:30:A:LEU:HD21	1:91:A:LEU:HD11	10	1.98	0.06	1.98
(1,432)	1:30:A:LEU:HD21	1:91:A:LEU:HD12	10	1.98	0.06	1.98
(1,432)	1:30:A:LEU:HD21	1:91:A:LEU:HD13	10	1.98	0.06	1.98
(1,432)	1:30:A:LEU:HD22	1:91:A:LEU:HD11	10	1.98	0.06	1.98
(1,432)	1:30:A:LEU:HD22	1:91:A:LEU:HD12	10	1.98	0.06	1.98
(1,432)	1:30:A:LEU:HD22	1:91:A:LEU:HD13	10	1.98	0.06	1.98

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,432)	1:30:A:LEU:HD23	1:91:A:LEU:HD11	10	1.98	0.06	1.98
(1,432)	1:30:A:LEU:HD23	1:91:A:LEU:HD12	10	1.98	0.06	1.98
(1,432)	1:30:A:LEU:HD23	1:91:A:LEU:HD13	10	1.98	0.06	1.98
(1,205)	1:18:A:VAL:HG11	1:22:A:LYS:HE2	10	1.92	0.24	1.85
(1,205)	1:18:A:VAL:HG12	1:22:A:LYS:HE2	10	1.92	0.24	1.85
(1,205)	1:18:A:VAL:HG13	1:22:A:LYS:HE2	10	1.92	0.24	1.85
(1,518)	1:36:A:PHE:HB2	1:72:A:VAL:HG11	10	1.91	0.39	2.08
(1,518)	1:36:A:PHE:HB2	1:72:A:VAL:HG12	10	1.91	0.39	2.08
(1,518)	1:36:A:PHE:HB2	1:72:A:VAL:HG13	10	1.91	0.39	2.08
(1,1235)	1:82:A:LEU:HA	1:88:A:VAL:HG21	10	1.86	0.09	1.86
(1,1235)	1:82:A:LEU:HA	1:88:A:VAL:HG22	10	1.86	0.09	1.86
(1,1235)	1:82:A:LEU:HA	1:88:A:VAL:HG23	10	1.86	0.09	1.86
(1,1028)	1:68:A:LEU:HD11	1:65:A:GLY:HA3	10	1.85	0.11	1.88
(1,1028)	1:68:A:LEU:HD12	1:65:A:GLY:HA3	10	1.85	0.11	1.88
(1,1028)	1:68:A:LEU:HD13	1:65:A:GLY:HA3	10	1.85	0.11	1.88
(1,1491)	1:96:A:ILE:HB	1:88:A:VAL:HG11	10	1.84	0.08	1.85
(1,1491)	1:96:A:ILE:HB	1:88:A:VAL:HG12	10	1.84	0.08	1.85
(1,1491)	1:96:A:ILE:HB	1:88:A:VAL:HG13	10	1.84	0.08	1.85
(1,1980)	1:124:A:HIS:HA	1:125:A:VAL:HG11	10	1.82	0.05	1.85
(1,1980)	1:124:A:HIS:HA	1:125:A:VAL:HG12	10	1.82	0.05	1.85
(1,1980)	1:124:A:HIS:HA	1:125:A:VAL:HG13	10	1.82	0.05	1.85
(1,1768)	1:112:A:LEU:HD11	1:125:A:VAL:HG21	10	1.81	0.11	1.77
(1,1768)	1:112:A:LEU:HD11	1:125:A:VAL:HG22	10	1.81	0.11	1.77
(1,1768)	1:112:A:LEU:HD11	1:125:A:VAL:HG23	10	1.81	0.11	1.77
(1,1768)	1:112:A:LEU:HD12	1:125:A:VAL:HG21	10	1.81	0.11	1.77
(1,1768)	1:112:A:LEU:HD12	1:125:A:VAL:HG22	10	1.81	0.11	1.77
(1,1768)	1:112:A:LEU:HD12	1:125:A:VAL:HG23	10	1.81	0.11	1.77
(1,1768)	1:112:A:LEU:HD13	1:125:A:VAL:HG21	10	1.81	0.11	1.77
(1,1768)	1:112:A:LEU:HD13	1:125:A:VAL:HG22	10	1.81	0.11	1.77
(1,1768)	1:112:A:LEU:HD13	1:125:A:VAL:HG23	10	1.81	0.11	1.77
(1,915)	1:62:A:PRO:HB3	1:92:A:GLU:HB3	10	1.8	0.19	1.87
(1,1769)	1:112:A:LEU:HB2	1:125:A:VAL:HG21	10	1.73	0.14	1.78
(1,1769)	1:112:A:LEU:HB2	1:125:A:VAL:HG22	10	1.73	0.14	1.78
(1,1769)	1:112:A:LEU:HB2	1:125:A:VAL:HG23	10	1.73	0.14	1.78
(1,1213)	1:82:A:LEU:HD11	1:79:A:ALA:HA	10	1.71	0.08	1.72
(1,1213)	1:82:A:LEU:HD12	1:79:A:ALA:HA	10	1.71	0.08	1.72
(1,1213)	1:82:A:LEU:HD13	1:79:A:ALA:HA	10	1.71	0.08	1.72
(1,229)	1:20:A:ALA:HA	1:64:A:LEU:HD11	10	1.69	0.09	1.72
(1,229)	1:20:A:ALA:HA	1:64:A:LEU:HD12	10	1.69	0.09	1.72
(1,229)	1:20:A:ALA:HA	1:64:A:LEU:HD13	10	1.69	0.09	1.72
(1,942)	1:64:A:LEU:HD11	1:24:A:ALA:HB1	10	1.66	0.04	1.66
(1,942)	1:64:A:LEU:HD11	1:24:A:ALA:HB2	10	1.66	0.04	1.66

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,942)	1:64:A:LEU:HD11	1:24:A:ALA:HB3	10	1.66	0.04	1.66
(1,942)	1:64:A:LEU:HD12	1:24:A:ALA:HB1	10	1.66	0.04	1.66
(1,942)	1:64:A:LEU:HD12	1:24:A:ALA:HB2	10	1.66	0.04	1.66
(1,942)	1:64:A:LEU:HD12	1:24:A:ALA:HB3	10	1.66	0.04	1.66
(1,942)	1:64:A:LEU:HD13	1:24:A:ALA:HB1	10	1.66	0.04	1.66
(1,942)	1:64:A:LEU:HD13	1:24:A:ALA:HB2	10	1.66	0.04	1.66
(1,942)	1:64:A:LEU:HD13	1:24:A:ALA:HB3	10	1.66	0.04	1.66
(1,430)	1:30:A:LEU:HD21	1:72:A:VAL:HG21	10	1.65	0.33	1.76
(1,430)	1:30:A:LEU:HD21	1:72:A:VAL:HG22	10	1.65	0.33	1.76
(1,430)	1:30:A:LEU:HD21	1:72:A:VAL:HG23	10	1.65	0.33	1.76
(1,430)	1:30:A:LEU:HD22	1:72:A:VAL:HG21	10	1.65	0.33	1.76
(1,430)	1:30:A:LEU:HD22	1:72:A:VAL:HG22	10	1.65	0.33	1.76
(1,430)	1:30:A:LEU:HD22	1:72:A:VAL:HG23	10	1.65	0.33	1.76
(1,430)	1:30:A:LEU:HD23	1:72:A:VAL:HG21	10	1.65	0.33	1.76
(1,430)	1:30:A:LEU:HD23	1:72:A:VAL:HG22	10	1.65	0.33	1.76
(1,430)	1:30:A:LEU:HD23	1:72:A:VAL:HG23	10	1.65	0.33	1.76
(1,1067)	1:72:A:VAL:HG21	1:71:A:HIS:H	10	1.64	0.07	1.62
(1,1067)	1:72:A:VAL:HG22	1:71:A:HIS:H	10	1.64	0.07	1.62
(1,1067)	1:72:A:VAL:HG23	1:71:A:HIS:H	10	1.64	0.07	1.62
(1,1647)	1:106:A:VAL:HG11	1:104:A:LEU:HD11	10	1.64	0.19	1.68
(1,1647)	1:106:A:VAL:HG11	1:104:A:LEU:HD12	10	1.64	0.19	1.68
(1,1647)	1:106:A:VAL:HG11	1:104:A:LEU:HD13	10	1.64	0.19	1.68
(1,1647)	1:106:A:VAL:HG12	1:104:A:LEU:HD11	10	1.64	0.19	1.68
(1,1647)	1:106:A:VAL:HG12	1:104:A:LEU:HD12	10	1.64	0.19	1.68
(1,1647)	1:106:A:VAL:HG12	1:104:A:LEU:HD13	10	1.64	0.19	1.68
(1,1647)	1:106:A:VAL:HG13	1:104:A:LEU:HD11	10	1.64	0.19	1.68
(1,1647)	1:106:A:VAL:HG13	1:104:A:LEU:HD12	10	1.64	0.19	1.68
(1,1647)	1:106:A:VAL:HG13	1:104:A:LEU:HD13	10	1.64	0.19	1.68
(1,67)	1:7:A:ILE:HG13	1:6:A:ASP:HB2	10	1.6	0.04	1.61
(1,804)	1:56:A:SER:H	1:57:A:LEU:HB3	10	1.56	0.04	1.58
(1,1373)	1:88:A:VAL:HG11	1:96:A:ILE:H	10	1.56	0.03	1.57
(1,1373)	1:88:A:VAL:HG12	1:96:A:ILE:H	10	1.56	0.03	1.57
(1,1373)	1:88:A:VAL:HG13	1:96:A:ILE:H	10	1.56	0.03	1.57
(1,1627)	1:104:A:LEU:HB2	1:111:A:VAL:H	10	1.48	0.06	1.5
(1,543)	1:37:A:THR:H	1:72:A:VAL:HG11	10	1.47	0.19	1.44
(1,543)	1:37:A:THR:H	1:72:A:VAL:HG12	10	1.47	0.19	1.44
(1,543)	1:37:A:THR:H	1:72:A:VAL:HG13	10	1.47	0.19	1.44
(1,167)	1:14:A:PHE:HB2	1:18:A:VAL:H	10	1.46	0.18	1.47
(1,955)	1:64:A:LEU:HD21	1:64:A:LEU:HA	10	1.42	0.02	1.42
(1,955)	1:64:A:LEU:HD22	1:64:A:LEU:HA	10	1.42	0.02	1.42
(1,955)	1:64:A:LEU:HD23	1:64:A:LEU:HA	10	1.42	0.02	1.42
(1,855)	1:59:A:GLN:HE22	1:56:A:SER:HA	10	1.39	0.06	1.4

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,232)	1:20:A:ALA:HA	1:68:A:LEU:HD11	10	1.38	0.09	1.36
(1,232)	1:20:A:ALA:HA	1:68:A:LEU:HD12	10	1.38	0.09	1.36
(1,232)	1:20:A:ALA:HA	1:68:A:LEU:HD13	10	1.38	0.09	1.36
(1,853)	1:58:A:VAL:HG21	1:64:A:LEU:HB3	10	1.37	0.15	1.43
(1,853)	1:58:A:VAL:HG22	1:64:A:LEU:HB3	10	1.37	0.15	1.43
(1,853)	1:58:A:VAL:HG23	1:64:A:LEU:HB3	10	1.37	0.15	1.43
(1,1923)	1:122:A:ILE:HG13	1:121:A:GLY:HA2	10	1.34	0.11	1.34
(1,4)	1:2:A:ALA:HB1	1:6:A:ASP:HB2	10	1.28	0.18	1.32
(1,4)	1:2:A:ALA:HB2	1:6:A:ASP:HB2	10	1.28	0.18	1.32
(1,4)	1:2:A:ALA:HB3	1:6:A:ASP:HB2	10	1.28	0.18	1.32
(1,709)	1:48:A:LYS:HD2	1:50:A:PRO:HD3	10	1.27	0.63	1.66
(1,709)	1:48:A:LYS:HD3	1:50:A:PRO:HD3	10	1.27	0.63	1.66
(1,1334)	1:87:A:ILE:H	1:88:A:VAL:HG21	10	1.25	0.03	1.25
(1,1334)	1:87:A:ILE:H	1:88:A:VAL:HG22	10	1.25	0.03	1.25
(1,1334)	1:87:A:ILE:H	1:88:A:VAL:HG23	10	1.25	0.03	1.25
(1,1774)	1:113:A:ALA:H	1:111:A:VAL:HG21	10	1.24	0.2	1.18
(1,1774)	1:113:A:ALA:H	1:111:A:VAL:HG22	10	1.24	0.2	1.18
(1,1774)	1:113:A:ALA:H	1:111:A:VAL:HG23	10	1.24	0.2	1.18
(1,1577)	1:101:A:ASP:H	1:103:A:PRO:HG3	10	1.23	0.09	1.23
(1,769)	1:54:A:ILE:HG12	1:57:A:LEU:HD21	10	1.22	0.15	1.23
(1,769)	1:54:A:ILE:HG12	1:57:A:LEU:HD22	10	1.22	0.15	1.23
(1,769)	1:54:A:ILE:HG12	1:57:A:LEU:HD23	10	1.22	0.15	1.23
(1,612)	1:42:A:ASN:HB3	1:125:A:VAL:HG21	10	1.2	0.15	1.19
(1,612)	1:42:A:ASN:HB3	1:125:A:VAL:HG22	10	1.2	0.15	1.19
(1,612)	1:42:A:ASN:HB3	1:125:A:VAL:HG23	10	1.2	0.15	1.19
(1,1938)	1:122:A:ILE:HG13	1:122:A:ILE:H	10	1.18	0.04	1.19
(1,711)	1:48:A:LYS:HG2	1:128:A:THR:HG21	10	1.16	0.19	1.16
(1,711)	1:48:A:LYS:HG2	1:128:A:THR:HG22	10	1.16	0.19	1.16
(1,711)	1:48:A:LYS:HG2	1:128:A:THR:HG23	10	1.16	0.19	1.16
(1,1629)	1:104:A:LEU:HD11	1:114:A:ALA:HB1	10	1.16	0.11	1.1
(1,1629)	1:104:A:LEU:HD11	1:114:A:ALA:HB2	10	1.16	0.11	1.1
(1,1629)	1:104:A:LEU:HD11	1:114:A:ALA:HB3	10	1.16	0.11	1.1
(1,1629)	1:104:A:LEU:HD12	1:114:A:ALA:HB1	10	1.16	0.11	1.1
(1,1629)	1:104:A:LEU:HD12	1:114:A:ALA:HB2	10	1.16	0.11	1.1
(1,1629)	1:104:A:LEU:HD12	1:114:A:ALA:HB3	10	1.16	0.11	1.1
(1,1629)	1:104:A:LEU:HD13	1:114:A:ALA:HB1	10	1.16	0.11	1.1
(1,1629)	1:104:A:LEU:HD13	1:114:A:ALA:HB2	10	1.16	0.11	1.1
(1,1629)	1:104:A:LEU:HD13	1:114:A:ALA:HB3	10	1.16	0.11	1.1
(1,1421)	1:91:A:LEU:HA	1:91:A:LEU:HD21	10	1.15	0.14	1.19
(1,1421)	1:91:A:LEU:HA	1:91:A:LEU:HD22	10	1.15	0.14	1.19
(1,1421)	1:91:A:LEU:HA	1:91:A:LEU:HD23	10	1.15	0.14	1.19
(1,773)	1:54:A:ILE:HG12	1:58:A:VAL:H	10	1.11	0.18	1.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,174)	1:15:A:SER:HB3	1:18:A:VAL:H	10	1.1	0.06	1.11
(1,1605)	1:104:A:LEU:HA	1:104:A:LEU:HD21	10	1.1	0.02	1.09
(1,1605)	1:104:A:LEU:HA	1:104:A:LEU:HD22	10	1.1	0.02	1.09
(1,1605)	1:104:A:LEU:HA	1:104:A:LEU:HD23	10	1.1	0.02	1.09
(1,313)	1:24:A:ALA:HB1	1:25:A:ASN:HB2	10	1.09	0.01	1.09
(1,313)	1:24:A:ALA:HB2	1:25:A:ASN:HB2	10	1.09	0.01	1.09
(1,313)	1:24:A:ALA:HB3	1:25:A:ASN:HB2	10	1.09	0.01	1.09
(1,914)	1:62:A:PRO:HB3	1:63:A:GLN:H	10	1.08	0.02	1.08
(1,807)	1:56:A:SER:HA	1:59:A:GLN:HB3	10	1.03	0.07	1.01
(1,1215)	1:104:A:LEU:HD12	1:79:A:ALA:H	10	1.02	0.09	1.02
(1,1215)	1:104:A:LEU:HD13	1:79:A:ALA:H	10	1.02	0.09	1.02
(1,1215)	1:104:A:LEU:HD11	1:79:A:ALA:H	10	1.02	0.09	1.02
(1,960)	1:64:A:LEU:HB3	1:67:A:ILE:HD11	10	0.98	0.04	0.99
(1,960)	1:64:A:LEU:HB3	1:67:A:ILE:HD12	10	0.98	0.04	0.99
(1,960)	1:64:A:LEU:HB3	1:67:A:ILE:HD13	10	0.98	0.04	0.99
(1,1441)	1:91:A:LEU:HD21	1:93:A:GLY:H	10	0.98	0.1	1.0
(1,1441)	1:91:A:LEU:HD22	1:93:A:GLY:H	10	0.98	0.1	1.0
(1,1441)	1:91:A:LEU:HD23	1:93:A:GLY:H	10	0.98	0.1	1.0
(1,775)	1:57:A:LEU:HD22	1:66:A:ARG:HD2	10	0.98	0.1	0.98
(1,775)	1:57:A:LEU:HD22	1:66:A:ARG:HD3	10	0.98	0.1	0.98
(1,775)	1:26:A:LEU:HD13	1:66:A:ARG:HD2	10	0.98	0.1	0.98
(1,775)	1:57:A:LEU:HD21	1:66:A:ARG:HD3	10	0.98	0.1	0.98
(1,775)	1:57:A:LEU:HD23	1:66:A:ARG:HD3	10	0.98	0.1	0.98
(1,1377)	1:88:A:VAL:HG11	1:98:A:ILE:H	10	0.97	0.04	0.96
(1,1377)	1:88:A:VAL:HG12	1:98:A:ILE:H	10	0.97	0.04	0.96
(1,1377)	1:88:A:VAL:HG13	1:98:A:ILE:H	10	0.97	0.04	0.96
(1,1091)	1:73:A:VAL:HG11	1:74:A:ALA:H	10	0.96	0.04	0.96
(1,1091)	1:73:A:VAL:HG12	1:74:A:ALA:H	10	0.96	0.04	0.96
(1,1091)	1:73:A:VAL:HG13	1:74:A:ALA:H	10	0.96	0.04	0.96
(1,1029)	1:68:A:LEU:HD21	1:67:A:ILE:HG21	10	0.96	0.05	0.96
(1,1029)	1:68:A:LEU:HD21	1:67:A:ILE:HG22	10	0.96	0.05	0.96
(1,1029)	1:68:A:LEU:HD21	1:67:A:ILE:HG23	10	0.96	0.05	0.96
(1,1029)	1:68:A:LEU:HD22	1:67:A:ILE:HG21	10	0.96	0.05	0.96
(1,1029)	1:68:A:LEU:HD22	1:67:A:ILE:HG22	10	0.96	0.05	0.96
(1,1029)	1:68:A:LEU:HD22	1:67:A:ILE:HG23	10	0.96	0.05	0.96
(1,1029)	1:68:A:LEU:HD23	1:67:A:ILE:HG21	10	0.96	0.05	0.96
(1,1029)	1:68:A:LEU:HD23	1:67:A:ILE:HG22	10	0.96	0.05	0.96
(1,1029)	1:68:A:LEU:HD23	1:67:A:ILE:HG23	10	0.96	0.05	0.96
(1,1600)	1:103:A:PRO:HG3	1:111:A:VAL:H	10	0.95	0.07	0.94
(1,1075)	1:72:A:VAL:HG21	1:72:A:VAL:H	10	0.94	0.03	0.94
(1,1075)	1:72:A:VAL:HG22	1:72:A:VAL:H	10	0.94	0.03	0.94
(1,1075)	1:72:A:VAL:HG23	1:72:A:VAL:H	10	0.94	0.03	0.94

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,272)	1:22:A:LYS:HB3	1:22:A:LYS:HE2	10	0.92	0.25	1.02
(1,582)	1:40:A:ALA:H	1:124:A:HIS:HB3	10	0.92	0.49	1.19
(1,898)	1:62:A:PRO:HB2	1:26:A:LEU:H	10	0.91	0.1	0.9
(1,169)	1:15:A:SER:HB3	1:15:A:SER:H	10	0.9	0.01	0.9
(1,874)	1:59:A:GLN:HE22	1:59:A:GLN:HB2	10	0.9	0.01	0.9
(1,186)	1:18:A:VAL:HG11	1:14:A:PHE:H	10	0.88	0.05	0.9
(1,186)	1:18:A:VAL:HG12	1:14:A:PHE:H	10	0.88	0.05	0.9
(1,186)	1:18:A:VAL:HG13	1:14:A:PHE:H	10	0.88	0.05	0.9
(1,1391)	1:89:A:THR:HG21	1:93:A:GLY:HA3	10	0.87	0.04	0.88
(1,1391)	1:89:A:THR:HG22	1:93:A:GLY:HA3	10	0.87	0.04	0.88
(1,1391)	1:89:A:THR:HG23	1:93:A:GLY:HA3	10	0.87	0.04	0.88
(1,1994)	1:125:A:VAL:HG11	1:125:A:VAL:H	10	0.84	0.01	0.84
(1,1994)	1:125:A:VAL:HG12	1:125:A:VAL:H	10	0.84	0.01	0.84
(1,1994)	1:125:A:VAL:HG13	1:125:A:VAL:H	10	0.84	0.01	0.84
(1,1327)	1:87:A:ILE:HG13	1:87:A:ILE:HG21	10	0.83	0.0	0.83
(1,1327)	1:87:A:ILE:HG13	1:87:A:ILE:HG22	10	0.83	0.0	0.83
(1,1327)	1:87:A:ILE:HG13	1:87:A:ILE:HG23	10	0.83	0.0	0.83
(1,1616)	1:104:A:LEU:HD21	1:105:A:GLU:H	10	0.82	0.02	0.82
(1,1616)	1:104:A:LEU:HD22	1:105:A:GLU:H	10	0.82	0.02	0.82
(1,1616)	1:104:A:LEU:HD23	1:105:A:GLU:H	10	0.82	0.02	0.82
(1,1983)	1:125:A:VAL:HG11	1:40:A:ALA:HB1	10	0.81	0.08	0.83
(1,1983)	1:125:A:VAL:HG11	1:40:A:ALA:HB2	10	0.81	0.08	0.83
(1,1983)	1:125:A:VAL:HG11	1:40:A:ALA:HB3	10	0.81	0.08	0.83
(1,1983)	1:125:A:VAL:HG12	1:40:A:ALA:HB1	10	0.81	0.08	0.83
(1,1983)	1:125:A:VAL:HG12	1:40:A:ALA:HB2	10	0.81	0.08	0.83
(1,1983)	1:125:A:VAL:HG12	1:40:A:ALA:HB3	10	0.81	0.08	0.83
(1,1983)	1:125:A:VAL:HG13	1:40:A:ALA:HB1	10	0.81	0.08	0.83
(1,1983)	1:125:A:VAL:HG13	1:40:A:ALA:HB2	10	0.81	0.08	0.83
(1,1983)	1:125:A:VAL:HG13	1:40:A:ALA:HB3	10	0.81	0.08	0.83
(1,322)	1:24:A:ALA:HB1	1:64:A:LEU:HB2	10	0.81	0.1	0.79
(1,322)	1:24:A:ALA:HB2	1:64:A:LEU:HB2	10	0.81	0.1	0.79
(1,322)	1:24:A:ALA:HB3	1:64:A:LEU:HB2	10	0.81	0.1	0.79
(1,1995)	1:125:A:VAL:HG21	1:126:A:ILE:H	10	0.81	0.03	0.82
(1,1995)	1:125:A:VAL:HG22	1:126:A:ILE:H	10	0.81	0.03	0.82
(1,1995)	1:125:A:VAL:HG23	1:126:A:ILE:H	10	0.81	0.03	0.82
(1,1040)	1:68:A:LEU:HD21	1:68:A:LEU:HA	10	0.81	0.02	0.8
(1,1040)	1:68:A:LEU:HD22	1:68:A:LEU:HA	10	0.81	0.02	0.8
(1,1040)	1:68:A:LEU:HD23	1:68:A:LEU:HA	10	0.81	0.02	0.8
(1,1641)	1:106:A:VAL:HG21	1:39:A:PHE:HB2	10	0.8	0.12	0.78
(1,1641)	1:106:A:VAL:HG22	1:39:A:PHE:HB2	10	0.8	0.12	0.78
(1,1641)	1:106:A:VAL:HG23	1:39:A:PHE:HB2	10	0.8	0.12	0.78
(1,1824)	1:116:A:ILE:HG21	1:116:A:ILE:HG13	10	0.8	0.0	0.8

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1824)	1:116:A:ILE:HG22	1:116:A:ILE:HG13	10	0.8	0.0	0.8
(1,1824)	1:116:A:ILE:HG23	1:116:A:ILE:HG13	10	0.8	0.0	0.8
(1,1094)	1:73:A:VAL:HG11	1:91:A:LEU:H	10	0.79	0.11	0.8
(1,1094)	1:73:A:VAL:HG12	1:91:A:LEU:H	10	0.79	0.11	0.8
(1,1094)	1:73:A:VAL:HG13	1:91:A:LEU:H	10	0.79	0.11	0.8
(1,1970)	1:124:A:HIS:HB2	1:113:A:ALA:H	10	0.78	0.4	0.98
(1,708)	1:48:A:LYS:HG3	1:49:A:LEU:H	10	0.78	0.16	0.85
(1,860)	1:59:A:GLN:H	1:59:A:GLN:HB3	10	0.78	0.01	0.78
(1,1300)	1:85:A:MET:HG2	1:86:A:GLY:H	10	0.78	0.02	0.78
(1,1848)	1:117:A:GLU:HB3	1:117:A:GLU:H	10	0.76	0.33	0.98
(1,1720)	1:110:A:THR:HG21	1:103:A:PRO:HB3	10	0.76	0.1	0.8
(1,1720)	1:110:A:THR:HG22	1:103:A:PRO:HB3	10	0.76	0.1	0.8
(1,1720)	1:110:A:THR:HG23	1:103:A:PRO:HB3	10	0.76	0.1	0.8
(1,476)	1:33:A:PRO:HB3	1:34:A:GLY:H	10	0.73	0.03	0.74
(1,1612)	1:104:A:LEU:HB3	1:104:A:LEU:HD11	10	0.73	0.01	0.73
(1,1612)	1:104:A:LEU:HB3	1:104:A:LEU:HD12	10	0.73	0.01	0.73
(1,1612)	1:104:A:LEU:HB3	1:104:A:LEU:HD13	10	0.73	0.01	0.73
(1,1076)	1:72:A:VAL:HG11	1:73:A:VAL:H	10	0.72	0.07	0.74
(1,1076)	1:72:A:VAL:HG12	1:73:A:VAL:H	10	0.72	0.07	0.74
(1,1076)	1:72:A:VAL:HG13	1:73:A:VAL:H	10	0.72	0.07	0.74
(1,448)	1:3:A:THR:HG22	1:31:A:GLN:HE21	10	0.72	0.05	0.71
(1,448)	1:3:A:THR:HG21	1:31:A:GLN:HE21	10	0.72	0.05	0.71
(1,448)	1:3:A:THR:HG23	1:31:A:GLN:HE21	10	0.72	0.05	0.71
(1,1566)	1:100:A:GLY:HA3	1:101:A:ASP:H	10	0.71	0.05	0.72
(1,631)	1:44:A:ASP:HB2	1:45:A:ALA:H	10	0.71	0.03	0.71
(1,680)	1:47:A:ALA:HB2	1:44:A:ASP:H	10	0.7	0.05	0.7
(1,680)	1:47:A:ALA:HB3	1:44:A:ASP:H	10	0.7	0.05	0.7
(1,680)	1:47:A:ALA:HB1	1:44:A:ASP:H	10	0.7	0.05	0.7
(1,1604)	1:104:A:LEU:H	1:103:A:PRO:HG3	10	0.7	0.01	0.7
(1,1414)	1:91:A:LEU:HD23	1:74:A:ALA:HB1	10	0.7	0.12	0.72
(1,1414)	1:91:A:LEU:HD22	1:74:A:ALA:HB1	10	0.7	0.12	0.72
(1,1414)	1:91:A:LEU:HD21	1:74:A:ALA:HB2	10	0.7	0.12	0.72
(1,1414)	1:91:A:LEU:HD23	1:74:A:ALA:HB2	10	0.7	0.12	0.72
(1,1414)	1:91:A:LEU:HD21	1:74:A:ALA:HB3	10	0.7	0.12	0.72
(1,370)	1:89:A:THR:HG23	1:92:A:GLU:H	10	0.7	0.1	0.7
(1,370)	1:89:A:THR:HG22	1:92:A:GLU:H	10	0.7	0.1	0.7
(1,370)	1:89:A:THR:HG21	1:92:A:GLU:H	10	0.7	0.1	0.7
(1,819)	1:57:A:LEU:HD11	1:57:A:LEU:HB3	10	0.7	0.0	0.7
(1,819)	1:57:A:LEU:HD12	1:57:A:LEU:HB3	10	0.7	0.0	0.7
(1,819)	1:57:A:LEU:HD13	1:57:A:LEU:HB3	10	0.7	0.0	0.7
(1,622)	1:44:A:ASP:HB2	1:42:A:ASN:HD21	10	0.67	0.24	0.66
(1,969)	1:65:A:GLY:HA2	1:26:A:LEU:HD11	10	0.66	0.18	0.72

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,969)	1:65:A:GLY:HA2	1:26:A:LEU:HD12	10	0.66	0.18	0.72
(1,969)	1:65:A:GLY:HA2	1:26:A:LEU:HD13	10	0.66	0.18	0.72
(1,726)	1:49:A:LEU:HB3	1:50:A:PRO:HD3	10	0.66	0.43	0.42
(1,1601)	1:104:A:LEU:HD11	1:79:A:ALA:H	10	0.66	0.08	0.68
(1,1601)	1:104:A:LEU:HD12	1:79:A:ALA:H	10	0.66	0.08	0.68
(1,1601)	1:104:A:LEU:HD13	1:79:A:ALA:H	10	0.66	0.08	0.68
(1,1921)	1:122:A:ILE:HG13	1:118:A:ALA:H	10	0.64	0.07	0.64
(1,342)	1:36:A:PHE:HB2	1:75:A:GLY:H	10	0.64	0.24	0.66
(1,601)	1:42:A:ASN:HA	1:42:A:ASN:HD22	10	0.64	0.08	0.64
(1,679)	1:44:A:ASP:HB3	1:47:A:ALA:H	10	0.64	0.05	0.62
(1,989)	1:66:A:ARG:HA	1:66:A:ARG:HB3	10	0.63	0.07	0.64
(1,270)	1:22:A:LYS:HG2	1:22:A:LYS:HE3	10	0.63	0.12	0.68
(1,1984)	1:125:A:VAL:HG21	1:112:A:LEU:H	10	0.62	0.05	0.64
(1,1984)	1:125:A:VAL:HG22	1:112:A:LEU:H	10	0.62	0.05	0.64
(1,1984)	1:125:A:VAL:HG23	1:112:A:LEU:H	10	0.62	0.05	0.64
(1,1423)	1:91:A:LEU:HB3	1:91:A:LEU:HD11	10	0.6	0.11	0.64
(1,1423)	1:91:A:LEU:HB3	1:91:A:LEU:HD12	10	0.6	0.11	0.64
(1,1423)	1:91:A:LEU:HB3	1:91:A:LEU:HD13	10	0.6	0.11	0.64
(1,856)	1:59:A:GLN:HA	1:59:A:GLN:HB2	10	0.6	0.01	0.6
(1,974)	1:65:A:GLY:H	1:64:A:LEU:HB2	10	0.59	0.02	0.6
(1,429)	1:30:A:LEU:HD13	1:70:A:TYR:H	10	0.57	0.19	0.66
(1,429)	1:30:A:LEU:HD11	1:70:A:TYR:H	10	0.57	0.19	0.66
(1,429)	1:30:A:LEU:HD12	1:70:A:TYR:H	10	0.57	0.19	0.66
(1,700)	1:48:A:LYS:HG3	1:48:A:LYS:HA	10	0.57	0.05	0.58
(1,1289)	1:85:A:MET:HB3	1:85:A:MET:H	10	0.57	0.01	0.57
(1,195)	1:18:A:VAL:HG21	1:18:A:VAL:HA	10	0.56	0.01	0.56
(1,195)	1:18:A:VAL:HG22	1:18:A:VAL:HA	10	0.56	0.01	0.56
(1,195)	1:18:A:VAL:HG23	1:18:A:VAL:HA	10	0.56	0.01	0.56
(1,520)	1:36:A:PHE:HA	1:72:A:VAL:HG11	10	0.56	0.22	0.53
(1,520)	1:36:A:PHE:HA	1:72:A:VAL:HG12	10	0.56	0.22	0.53
(1,520)	1:36:A:PHE:HA	1:72:A:VAL:HG13	10	0.56	0.22	0.53
(1,1113)	1:76:A:ALA:HB2	1:36:A:PHE:H	10	0.56	0.09	0.59
(1,1113)	1:76:A:ALA:HB3	1:36:A:PHE:H	10	0.56	0.09	0.59
(1,1113)	1:76:A:ALA:HB1	1:77:A:TYR:H	10	0.56	0.09	0.59
(1,1113)	1:76:A:ALA:HB2	1:77:A:TYR:H	10	0.56	0.09	0.59
(1,1894)	1:120:A:ASN:HB3	1:121:A:GLY:H	10	0.56	0.07	0.56
(1,723)	1:49:A:LEU:HB3	1:49:A:LEU:H	10	0.55	0.03	0.55
(1,393)	1:28:A:GLU:H	1:28:A:GLU:HB2	10	0.54	0.01	0.54
(1,1027)	1:68:A:LEU:HD11	1:65:A:GLY:HA2	10	0.53	0.13	0.57
(1,1027)	1:68:A:LEU:HD12	1:65:A:GLY:HA2	10	0.53	0.13	0.57
(1,1027)	1:68:A:LEU:HD13	1:65:A:GLY:HA2	10	0.53	0.13	0.57
(1,690)	1:48:A:LYS:HG2	1:48:A:LYS:HB3	10	0.53	0.03	0.55

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,772)	1:55:A:THR:HG21	1:58:A:VAL:H	10	0.53	0.08	0.55
(1,772)	1:55:A:THR:HG22	1:58:A:VAL:H	10	0.53	0.08	0.55
(1,772)	1:55:A:THR:HG23	1:58:A:VAL:H	10	0.53	0.08	0.55
(1,33)	1:5:A:VAL:HG11	1:6:A:ASP:HB3	10	0.53	0.04	0.54
(1,33)	1:5:A:VAL:HG12	1:6:A:ASP:HB3	10	0.53	0.04	0.54
(1,33)	1:5:A:VAL:HG13	1:6:A:ASP:HB3	10	0.53	0.04	0.54
(1,1358)	1:88:A:VAL:HA	1:88:A:VAL:HG21	10	0.52	0.0	0.52
(1,1358)	1:88:A:VAL:HA	1:88:A:VAL:HG22	10	0.52	0.0	0.52
(1,1358)	1:88:A:VAL:HA	1:88:A:VAL:HG23	10	0.52	0.0	0.52
(1,1408)	1:91:A:LEU:HD11	1:30:A:LEU:HA	10	0.51	0.12	0.5
(1,1408)	1:91:A:LEU:HD12	1:30:A:LEU:HA	10	0.51	0.12	0.5
(1,1408)	1:91:A:LEU:HD13	1:30:A:LEU:HA	10	0.51	0.12	0.5
(1,200)	1:18:A:VAL:HG11	1:19:A:THR:H	10	0.5	0.02	0.51
(1,200)	1:18:A:VAL:HG12	1:19:A:THR:H	10	0.5	0.02	0.51
(1,200)	1:18:A:VAL:HG13	1:19:A:THR:H	10	0.5	0.02	0.51
(1,1116)	1:76:A:ALA:H	1:75:A:GLY:HA3	10	0.5	0.02	0.49
(1,1596)	1:103:A:PRO:HB3	1:104:A:LEU:H	10	0.49	0.02	0.5
(1,1737)	1:20:A:ALA:HB1	1:64:A:LEU:HD13	10	0.48	0.15	0.52
(1,1737)	1:20:A:ALA:HB2	1:64:A:LEU:HD11	10	0.48	0.15	0.52
(1,1737)	1:20:A:ALA:HB2	1:64:A:LEU:HD12	10	0.48	0.15	0.52
(1,1737)	1:20:A:ALA:HB2	1:64:A:LEU:HD13	10	0.48	0.15	0.52
(1,1737)	1:20:A:ALA:HB1	1:64:A:LEU:HD11	10	0.48	0.15	0.52
(1,1737)	1:20:A:ALA:HB3	1:64:A:LEU:HD12	10	0.48	0.15	0.52
(1,1737)	1:20:A:ALA:HB3	1:64:A:LEU:HD11	10	0.48	0.15	0.52
(1,1070)	1:72:A:VAL:HG11	1:72:A:VAL:HA	10	0.46	0.01	0.46
(1,1070)	1:72:A:VAL:HG12	1:72:A:VAL:HA	10	0.46	0.01	0.46
(1,1070)	1:72:A:VAL:HG13	1:72:A:VAL:HA	10	0.46	0.01	0.46
(1,332)	1:25:A:ASN:HB3	1:25:A:ASN:HD22	10	0.45	0.0	0.45
(1,1176)	1:79:A:ALA:HA	1:104:A:LEU:HD11	10	0.44	0.11	0.45
(1,1176)	1:79:A:ALA:HA	1:104:A:LEU:HD12	10	0.44	0.11	0.45
(1,1176)	1:79:A:ALA:HA	1:104:A:LEU:HD13	10	0.44	0.11	0.45
(1,433)	1:31:A:GLN:HE21	1:6:A:ASP:HB3	10	0.44	0.09	0.44
(1,544)	1:37:A:THR:HB	1:73:A:VAL:HG21	10	0.43	0.02	0.43
(1,544)	1:37:A:THR:HB	1:73:A:VAL:HG22	10	0.43	0.02	0.43
(1,544)	1:37:A:THR:HB	1:73:A:VAL:HG23	10	0.43	0.02	0.43
(1,1981)	1:124:A:HIS:HB2	1:125:A:VAL:H	10	0.42	0.18	0.48
(1,331)	1:25:A:ASN:H	1:25:A:ASN:HB2	10	0.42	0.01	0.42
(1,157)	1:13:A:GLY:HA3	1:13:A:GLY:H	10	0.41	0.01	0.42
(1,981)	1:65:A:GLY:HA3	1:68:A:LEU:H	10	0.41	0.14	0.46
(1,1410)	1:58:A:VAL:HG12	1:59:A:GLN:HA	10	0.41	0.05	0.42
(1,1410)	1:58:A:VAL:HG13	1:59:A:GLN:HA	10	0.41	0.05	0.42
(1,1410)	1:58:A:VAL:HG11	1:59:A:GLN:HA	10	0.41	0.05	0.42

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1024)	1:68:A:LEU:HD21	1:64:A:LEU:HD21	10	0.41	0.03	0.39
(1,1024)	1:68:A:LEU:HD21	1:64:A:LEU:HD22	10	0.41	0.03	0.39
(1,1024)	1:68:A:LEU:HD21	1:64:A:LEU:HD23	10	0.41	0.03	0.39
(1,1024)	1:68:A:LEU:HD22	1:64:A:LEU:HD21	10	0.41	0.03	0.39
(1,1024)	1:68:A:LEU:HD22	1:64:A:LEU:HD22	10	0.41	0.03	0.39
(1,1024)	1:68:A:LEU:HD22	1:64:A:LEU:HD23	10	0.41	0.03	0.39
(1,1024)	1:68:A:LEU:HD23	1:64:A:LEU:HD21	10	0.41	0.03	0.39
(1,1024)	1:68:A:LEU:HD23	1:64:A:LEU:HD22	10	0.41	0.03	0.39
(1,1024)	1:68:A:LEU:HD23	1:64:A:LEU:HD23	10	0.41	0.03	0.39
(1,624)	1:44:A:ASP:HB3	1:44:A:ASP:HA	10	0.4	0.0	0.4
(1,1827)	1:116:A:ILE:H	1:116:A:ILE:HG12	10	0.39	0.01	0.4
(1,901)	1:62:A:PRO:HB2	1:62:A:PRO:HA	10	0.39	0.01	0.39
(1,553)	1:37:A:THR:HG21	1:82:A:LEU:HD11	10	0.38	0.19	0.34
(1,553)	1:37:A:THR:HG21	1:82:A:LEU:HD12	10	0.38	0.19	0.34
(1,553)	1:37:A:THR:HG21	1:82:A:LEU:HD13	10	0.38	0.19	0.34
(1,553)	1:37:A:THR:HG22	1:82:A:LEU:HD11	10	0.38	0.19	0.34
(1,553)	1:37:A:THR:HG22	1:82:A:LEU:HD12	10	0.38	0.19	0.34
(1,553)	1:37:A:THR:HG22	1:82:A:LEU:HD13	10	0.38	0.19	0.34
(1,553)	1:37:A:THR:HG23	1:82:A:LEU:HD11	10	0.38	0.19	0.34
(1,553)	1:37:A:THR:HG23	1:82:A:LEU:HD12	10	0.38	0.19	0.34
(1,553)	1:37:A:THR:HG23	1:82:A:LEU:HD13	10	0.38	0.19	0.34
(1,227)	1:20:A:ALA:HB1	1:64:A:LEU:HD11	10	0.38	0.13	0.4
(1,227)	1:20:A:ALA:HB1	1:64:A:LEU:HD12	10	0.38	0.13	0.4
(1,227)	1:20:A:ALA:HB1	1:64:A:LEU:HD13	10	0.38	0.13	0.4
(1,227)	1:20:A:ALA:HB2	1:64:A:LEU:HD11	10	0.38	0.13	0.4
(1,227)	1:20:A:ALA:HB2	1:64:A:LEU:HD12	10	0.38	0.13	0.4
(1,227)	1:20:A:ALA:HB2	1:64:A:LEU:HD13	10	0.38	0.13	0.4
(1,227)	1:20:A:ALA:HB3	1:64:A:LEU:HD11	10	0.38	0.13	0.4
(1,227)	1:20:A:ALA:HB3	1:64:A:LEU:HD12	10	0.38	0.13	0.4
(1,227)	1:20:A:ALA:HB3	1:64:A:LEU:HD13	10	0.38	0.13	0.4
(1,371)	1:91:A:LEU:HB2	1:93:A:GLY:H	10	0.38	0.07	0.39
(1,1740)	1:111:A:VAL:HG11	1:111:A:VAL:HA	10	0.37	0.09	0.4
(1,1740)	1:111:A:VAL:HG12	1:111:A:VAL:HA	10	0.37	0.09	0.4
(1,1740)	1:111:A:VAL:HG13	1:111:A:VAL:HA	10	0.37	0.09	0.4
(1,1303)	1:85:A:MET:HB3	1:86:A:GLY:H	10	0.36	0.01	0.36
(1,1345)	1:87:A:ILE:HG13	1:95:A:THR:HB	10	0.36	0.08	0.38
(1,1337)	1:87:A:ILE:HA	1:88:A:VAL:HG11	10	0.36	0.01	0.36
(1,1337)	1:87:A:ILE:HA	1:88:A:VAL:HG12	10	0.36	0.01	0.36
(1,1337)	1:87:A:ILE:HA	1:88:A:VAL:HG13	10	0.36	0.01	0.36
(1,180)	1:18:A:VAL:HG11	1:11:A:THR:HB	10	0.35	0.08	0.4
(1,180)	1:18:A:VAL:HG12	1:11:A:THR:HB	10	0.35	0.08	0.4
(1,180)	1:18:A:VAL:HG13	1:11:A:THR:HB	10	0.35	0.08	0.4

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1493)	1:96:A:ILE:HD12	1:90:A:SER:H	10	0.34	0.11	0.36
(1,1493)	1:96:A:ILE:HD13	1:90:A:SER:H	10	0.34	0.11	0.36
(1,1493)	1:96:A:ILE:HD11	1:90:A:SER:H	10	0.34	0.11	0.36
(1,1493)	1:98:A:ILE:HD12	1:106:A:VAL:H	10	0.34	0.11	0.36
(1,571)	1:39:A:PHE:HB3	1:39:A:PHE:H	10	0.34	0.03	0.34
(1,869)	1:59:A:GLN:HE22	1:59:A:GLN:HG3	10	0.33	0.01	0.32
(1,1277)	1:84:A:ARG:HD2	1:84:A:ARG:HG2	10	0.32	0.02	0.33
(1,391)	1:28:A:GLU:HA	1:28:A:GLU:HB2	10	0.32	0.02	0.32
(1,183)	1:18:A:VAL:HG11	1:11:A:THR:H	10	0.31	0.11	0.36
(1,183)	1:18:A:VAL:HG12	1:11:A:THR:H	10	0.31	0.11	0.36
(1,183)	1:18:A:VAL:HG13	1:11:A:THR:H	10	0.31	0.11	0.36
(1,1593)	1:103:A:PRO:HD3	1:103:A:PRO:HG2	10	0.31	0.01	0.31
(1,990)	1:66:A:ARG:H	1:66:A:ARG:HB2	10	0.3	0.15	0.3
(1,1148)	1:78:A:LYS:H	1:78:A:LYS:HD3	10	0.3	0.2	0.2
(1,825)	1:57:A:LEU:HB3	1:57:A:LEU:H	10	0.3	0.03	0.3
(1,758)	1:54:A:ILE:HG12	1:54:A:ILE:HA	10	0.3	0.04	0.3
(1,1453)	1:92:A:GLU:H	1:93:A:GLY:HA3	10	0.3	0.04	0.3
(1,1271)	1:84:A:ARG:HD3	1:84:A:ARG:HG3	10	0.28	0.01	0.29
(1,957)	1:64:A:LEU:HD11	1:65:A:GLY:H	10	0.27	0.05	0.28
(1,957)	1:64:A:LEU:HD12	1:65:A:GLY:H	10	0.27	0.05	0.28
(1,957)	1:64:A:LEU:HD13	1:65:A:GLY:H	10	0.27	0.05	0.28
(1,1583)	1:103:A:PRO:HD2	1:103:A:PRO:HB2	10	0.27	0.02	0.26
(1,1361)	1:88:A:VAL:H	1:88:A:VAL:HG11	10	0.27	0.02	0.27
(1,1361)	1:88:A:VAL:H	1:88:A:VAL:HG12	10	0.27	0.02	0.27
(1,1361)	1:88:A:VAL:H	1:88:A:VAL:HG13	10	0.27	0.02	0.27
(1,1231)	1:82:A:LEU:HD11	1:83:A:LYS:H	10	0.26	0.05	0.27
(1,1231)	1:82:A:LEU:HD12	1:83:A:LYS:H	10	0.26	0.05	0.27
(1,1231)	1:82:A:LEU:HD13	1:83:A:LYS:H	10	0.26	0.05	0.27
(1,1816)	1:116:A:ILE:HA	1:116:A:ILE:HG13	10	0.26	0.01	0.25
(1,830)	1:57:A:LEU:HB3	1:58:A:VAL:H	10	0.25	0.1	0.24
(1,762)	1:54:A:ILE:HG12	1:54:A:ILE:H	10	0.24	0.08	0.24
(1,909)	1:62:A:PRO:HB2	1:62:A:PRO:HG3	10	0.24	0.01	0.24
(1,1621)	1:104:A:LEU:HB2	1:105:A:GLU:H	10	0.22	0.02	0.22
(1,48)	1:5:A:VAL:HB	1:31:A:GLN:HE21	10	0.21	0.01	0.22
(1,1261)	1:84:A:ARG:HB3	1:84:A:ARG:H	10	0.21	0.03	0.22
(1,929)	1:63:A:GLN:HG2	1:63:A:GLN:HE22	10	0.2	0.08	0.18
(1,929)	1:63:A:GLN:HG3	1:63:A:GLN:HE22	10	0.2	0.08	0.18
(1,1351)	1:87:A:ILE:H	1:97:A:PRO:HA	10	0.2	0.01	0.2
(1,967)	1:65:A:GLY:HA2	1:26:A:LEU:HD21	10	0.17	0.02	0.16
(1,967)	1:65:A:GLY:HA2	1:26:A:LEU:HD22	10	0.17	0.02	0.16
(1,967)	1:65:A:GLY:HA2	1:26:A:LEU:HD23	10	0.17	0.02	0.16
(1,1571)	1:101:A:ASP:HB3	1:101:A:ASP:HA	10	0.17	0.01	0.17

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,280)	1:22:A:LYS:HG2	1:22:A:LYS:H	10	0.17	0.04	0.17
(1,1219)	1:82:A:LEU:HD11	1:82:A:LEU:HB2	10	0.17	0.02	0.16
(1,1219)	1:82:A:LEU:HD12	1:82:A:LEU:HB2	10	0.17	0.02	0.16
(1,1219)	1:82:A:LEU:HD13	1:82:A:LEU:HB2	10	0.17	0.02	0.16
(1,1364)	1:87:A:ILE:HG22	1:88:A:VAL:H	10	0.15	0.01	0.16
(1,1364)	1:87:A:ILE:HG21	1:88:A:VAL:H	10	0.15	0.01	0.16
(1,1364)	1:87:A:ILE:HG23	1:88:A:VAL:H	10	0.15	0.01	0.16
(1,730)	1:40:A:ALA:H	1:126:A:ILE:HG21	10	0.15	0.03	0.15
(1,730)	1:40:A:ALA:H	1:126:A:ILE:HG22	10	0.15	0.03	0.15
(1,730)	1:40:A:ALA:H	1:126:A:ILE:HG23	10	0.15	0.03	0.15
(1,2084)	1:129:A:VAL:HG11	1:129:A:VAL:H	10	0.15	0.01	0.15
(1,2084)	1:129:A:VAL:HG12	1:129:A:VAL:H	10	0.15	0.01	0.15
(1,2084)	1:129:A:VAL:HG13	1:129:A:VAL:H	10	0.15	0.01	0.15
(1,748)	1:54:A:ILE:HG13	1:54:A:ILE:HB	10	0.14	0.01	0.15
(1,1378)	1:88:A:VAL:H	1:98:A:ILE:HD11	10	0.12	0.01	0.12
(1,1378)	1:88:A:VAL:H	1:98:A:ILE:HD12	10	0.12	0.01	0.12
(1,1378)	1:88:A:VAL:H	1:98:A:ILE:HD13	10	0.12	0.01	0.12
(1,1823)	1:116:A:ILE:HG12	1:116:A:ILE:HB	10	0.11	0.0	0.11
(1,881)	1:59:A:GLN:HB3	1:60:A:ASN:HD21	9	1.43	0.37	1.31
(1,774)	1:54:A:ILE:HG12	1:63:A:GLN:HE22	9	1.22	0.42	1.37
(1,575)	1:39:A:PHE:HA	1:124:A:HIS:HB3	9	1.2	0.58	1.52
(1,1257)	1:96:A:ILE:HG13	1:107:A:LYS:HE2	9	1.07	0.39	1.11
(1,1257)	1:96:A:ILE:HG13	1:107:A:LYS:HE3	9	1.07	0.39	1.11
(1,340)	1:25:A:ASN:HD22	1:92:A:GLU:HB3	9	1.06	0.19	1.16
(1,611)	1:42:A:ASN:HB2	1:112:A:LEU:HD11	9	0.9	0.56	1.26
(1,611)	1:42:A:ASN:HB2	1:112:A:LEU:HD12	9	0.9	0.56	1.26
(1,611)	1:42:A:ASN:HB2	1:112:A:LEU:HD13	9	0.9	0.56	1.26
(1,1519)	1:96:A:ILE:HG13	1:107:A:LYS:HE2	9	0.84	0.32	0.89
(1,1519)	1:96:A:ILE:HG13	1:107:A:LYS:HE3	9	0.84	0.32	0.89
(1,262)	1:22:A:LYS:HE2	1:19:A:THR:HG21	9	0.68	0.01	0.68
(1,262)	1:22:A:LYS:HE2	1:19:A:THR:HG22	9	0.68	0.01	0.68
(1,262)	1:22:A:LYS:HE2	1:19:A:THR:HG23	9	0.68	0.01	0.68
(1,1516)	1:96:A:ILE:HG13	1:107:A:LYS:HB2	9	0.66	0.28	0.62
(1,1211)	1:82:A:LEU:HD21	1:77:A:TYR:HD1	9	0.62	0.08	0.63
(1,1211)	1:82:A:LEU:HD21	1:77:A:TYR:HD2	9	0.62	0.08	0.63
(1,1211)	1:82:A:LEU:HD22	1:77:A:TYR:HD1	9	0.62	0.08	0.63
(1,1211)	1:82:A:LEU:HD22	1:77:A:TYR:HD2	9	0.62	0.08	0.63
(1,1211)	1:82:A:LEU:HD23	1:77:A:TYR:HD1	9	0.62	0.08	0.63
(1,1211)	1:82:A:LEU:HD23	1:77:A:TYR:HD2	9	0.62	0.08	0.63
(1,344)	1:60:A:ASN:HB3	1:60:A:ASN:HD22	9	0.58	0.07	0.6
(1,344)	1:25:A:ASN:HD22	1:92:A:GLU:HB3	9	0.58	0.07	0.6
(1,1505)	1:96:A:ILE:HG13	1:96:A:ILE:HG21	9	0.55	0.03	0.54

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1505)	1:96:A:ILE:HG13	1:96:A:ILE:HG22	9	0.55	0.03	0.54
(1,1505)	1:96:A:ILE:HG13	1:96:A:ILE:HG23	9	0.55	0.03	0.54
(1,920)	1:54:A:ILE:HD13	1:63:A:GLN:HE21	9	0.48	0.09	0.48
(1,920)	1:54:A:ILE:HD12	1:63:A:GLN:HE21	9	0.48	0.09	0.48
(1,920)	1:54:A:ILE:HD11	1:63:A:GLN:HE21	9	0.48	0.09	0.48
(1,1435)	1:91:A:LEU:HD21	1:91:A:LEU:H	9	0.44	0.04	0.43
(1,1435)	1:91:A:LEU:HD22	1:91:A:LEU:H	9	0.44	0.04	0.43
(1,1435)	1:91:A:LEU:HD23	1:91:A:LEU:H	9	0.44	0.04	0.43
(1,276)	1:22:A:LYS:HG2	1:22:A:LYS:HE2	9	0.32	0.06	0.33
(1,435)	1:31:A:GLN:HE22	1:27:A:VAL:HG22	9	0.3	0.01	0.3
(1,435)	1:31:A:GLN:HE22	1:27:A:VAL:HG23	9	0.3	0.01	0.3
(1,435)	1:31:A:GLN:HE22	1:27:A:VAL:HG21	9	0.3	0.01	0.3
(1,1126)	1:77:A:TYR:HB3	1:77:A:TYR:H	9	0.25	0.02	0.25
(1,257)	1:21:A:VAL:HG21	1:65:A:GLY:HA2	9	0.24	0.08	0.24
(1,257)	1:21:A:VAL:HG22	1:65:A:GLY:HA2	9	0.24	0.08	0.24
(1,257)	1:21:A:VAL:HG23	1:65:A:GLY:HA2	9	0.24	0.08	0.24
(1,1275)	1:84:A:ARG:HB3	1:84:A:ARG:HG3	9	0.23	0.02	0.24
(1,1145)	1:78:A:LYS:HG2	1:78:A:LYS:HD2	9	0.23	0.04	0.24
(1,1859)	1:118:A:ALA:HB1	1:119:A:GLU:HG3	9	0.21	0.02	0.21
(1,1859)	1:118:A:ALA:HB2	1:119:A:GLU:HG3	9	0.21	0.02	0.21
(1,1859)	1:118:A:ALA:HB3	1:119:A:GLU:HG3	9	0.21	0.02	0.21
(1,1284)	1:85:A:MET:HA	1:85:A:MET:HG3	9	0.18	0.02	0.19
(1,32)	1:5:A:VAL:HG11	1:6:A:ASP:HA	9	0.15	0.02	0.14
(1,32)	1:5:A:VAL:HG12	1:6:A:ASP:HA	9	0.15	0.02	0.14
(1,32)	1:5:A:VAL:HG13	1:6:A:ASP:HA	9	0.15	0.02	0.14
(1,1115)	1:76:A:ALA:H	1:74:A:ALA:HA	9	0.13	0.01	0.13
(1,1224)	1:82:A:LEU:H	1:82:A:LEU:HG	9	0.13	0.01	0.13
(1,1662)	1:106:A:VAL:HG11	1:107:A:LYS:HG3	8	0.71	0.23	0.74
(1,1662)	1:106:A:VAL:HG12	1:107:A:LYS:HG3	8	0.71	0.23	0.74
(1,1662)	1:106:A:VAL:HG13	1:107:A:LYS:HG3	8	0.71	0.23	0.74
(1,1263)	1:84:A:ARG:HD3	1:84:A:ARG:HA	8	0.68	0.02	0.68
(1,1864)	1:118:A:ALA:HB3	1:121:A:GLY:HA2	8	0.42	0.13	0.4
(1,1864)	1:118:A:ALA:HB2	1:121:A:GLY:HA2	8	0.42	0.13	0.4
(1,1864)	1:118:A:ALA:HB1	1:121:A:GLY:HA2	8	0.42	0.13	0.4
(1,878)	1:59:A:GLN:HB3	1:60:A:ASN:H	8	0.38	0.02	0.38
(1,1273)	1:84:A:ARG:HB3	1:84:A:ARG:HD2	8	0.33	0.03	0.32
(1,1968)	1:124:A:HIS:HB3	1:39:A:PHE:HD1	8	0.29	0.14	0.26
(1,1968)	1:124:A:HIS:HB3	1:39:A:PHE:HD2	8	0.29	0.14	0.26
(1,992)	1:66:A:ARG:HG3	1:67:A:ILE:H	8	0.28	0.15	0.24
(1,652)	1:45:A:ALA:HB1	1:48:A:LYS:HG2	8	0.26	0.12	0.24
(1,652)	1:45:A:ALA:HB2	1:48:A:LYS:HG2	8	0.26	0.12	0.24
(1,652)	1:45:A:ALA:HB3	1:48:A:LYS:HG2	8	0.26	0.12	0.24

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1454)	1:92:A:GLU:HB3	1:93:A:GLY:H	8	0.25	0.14	0.17
(1,794)	1:55:A:THR:HG21	1:59:A:GLN:HE22	8	0.16	0.02	0.16
(1,794)	1:55:A:THR:HG22	1:59:A:GLN:HE22	8	0.16	0.02	0.16
(1,794)	1:55:A:THR:HG23	1:59:A:GLN:HE22	8	0.16	0.02	0.16
(1,845)	1:58:A:VAL:HG11	1:59:A:GLN:HA	8	0.13	0.01	0.13
(1,845)	1:58:A:VAL:HG12	1:59:A:GLN:HA	8	0.13	0.01	0.13
(1,845)	1:58:A:VAL:HG13	1:59:A:GLN:HA	8	0.13	0.01	0.13
(1,887)	1:60:A:ASN:HB3	1:60:A:ASN:H	8	0.13	0.02	0.12
(1,1840)	1:117:A:GLU:H	1:116:A:ILE:H	8	0.12	0.02	0.12
(1,1409)	1:91:A:LEU:HB3	1:30:A:LEU:H	8	0.12	0.01	0.12
(1,1122)	1:76:A:ALA:H	1:77:A:TYR:H	8	0.12	0.02	0.12
(1,1926)	1:122:A:ILE:H	1:121:A:GLY:HA2	8	0.12	0.01	0.12
(1,154)	1:12:A:PRO:HA	1:14:A:PHE:H	8	0.11	0.01	0.11
(1,1147)	1:78:A:LYS:HA	1:78:A:LYS:HD3	7	0.94	0.2	1.02
(1,1850)	1:117:A:GLU:HB2	1:118:A:ALA:H	7	0.74	0.01	0.75
(1,1518)	1:96:A:ILE:HG13	1:107:A:LYS:HD2	7	0.73	0.46	0.62
(1,1518)	1:96:A:ILE:HG13	1:107:A:LYS:HD3	7	0.73	0.46	0.62
(1,1684)	1:107:A:LYS:HG2	1:107:A:LYS:HE2	7	0.59	0.08	0.62
(1,1684)	1:107:A:LYS:HG2	1:107:A:LYS:HE3	7	0.59	0.08	0.62
(1,2029)	1:126:A:ILE:HA	1:127:A:ASP:HB3	7	0.47	0.08	0.48
(1,1979)	1:124:A:HIS:HB3	1:124:A:HIS:H	7	0.44	0.01	0.44
(1,1603)	1:104:A:LEU:H	1:103:A:PRO:HG3	7	0.44	0.13	0.51
(1,1603)	1:104:A:LEU:H	1:105:A:GLU:HG2	7	0.44	0.13	0.51
(1,1842)	1:117:A:GLU:HB2	1:117:A:GLU:HA	7	0.32	0.0	0.32
(1,1771)	1:112:A:LEU:HD11	1:127:A:ASP:HB3	7	0.29	0.06	0.29
(1,1771)	1:112:A:LEU:HD12	1:127:A:ASP:HB3	7	0.29	0.06	0.29
(1,1771)	1:112:A:LEU:HD13	1:127:A:ASP:HB3	7	0.29	0.06	0.29
(1,483)	1:35:A:PRO:HD2	1:35:A:PRO:HB2	7	0.28	0.04	0.26
(1,1177)	1:79:A:ALA:HB1	1:104:A:LEU:HD21	7	0.21	0.06	0.2
(1,1177)	1:79:A:ALA:HB1	1:104:A:LEU:HD22	7	0.21	0.06	0.2
(1,1177)	1:79:A:ALA:HB1	1:104:A:LEU:HD23	7	0.21	0.06	0.2
(1,1177)	1:79:A:ALA:HB2	1:104:A:LEU:HD21	7	0.21	0.06	0.2
(1,1177)	1:79:A:ALA:HB2	1:104:A:LEU:HD22	7	0.21	0.06	0.2
(1,1177)	1:79:A:ALA:HB2	1:104:A:LEU:HD23	7	0.21	0.06	0.2
(1,1177)	1:79:A:ALA:HB3	1:104:A:LEU:HD21	7	0.21	0.06	0.2
(1,1177)	1:79:A:ALA:HB3	1:104:A:LEU:HD22	7	0.21	0.06	0.2
(1,1177)	1:79:A:ALA:HB3	1:104:A:LEU:HD23	7	0.21	0.06	0.2
(1,1214)	1:78:A:LYS:HG2	1:79:A:ALA:H	7	0.21	0.07	0.2
(1,1296)	1:85:A:MET:H	1:85:A:MET:HG2	7	0.15	0.03	0.15
(1,998)	1:67:A:ILE:HG21	1:68:A:LEU:HA	7	0.15	0.02	0.14
(1,998)	1:67:A:ILE:HG22	1:68:A:LEU:HA	7	0.15	0.02	0.14
(1,998)	1:67:A:ILE:HG23	1:68:A:LEU:HA	7	0.15	0.02	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1163)	1:78:A:LYS:H	1:80:A:THR:H	7	0.14	0.03	0.14
(1,1731)	1:110:A:THR:H	1:111:A:VAL:H	7	0.11	0.0	0.11
(1,1615)	1:104:A:LEU:HA	1:105:A:GLU:HG2	6	1.0	0.41	1.19
(1,527)	1:36:A:PHE:HB2	1:120:A:ASN:HD22	6	0.73	0.27	0.84
(1,983)	1:66:A:ARG:HB2	1:66:A:ARG:HD2	6	0.44	0.08	0.44
(1,1238)	1:82:A:LEU:HB3	1:104:A:LEU:HD21	6	0.35	0.14	0.38
(1,1238)	1:82:A:LEU:HB3	1:104:A:LEU:HD22	6	0.35	0.14	0.38
(1,1238)	1:82:A:LEU:HB3	1:104:A:LEU:HD23	6	0.35	0.14	0.38
(1,380)	1:26:A:LEU:HD23	1:66:A:ARG:HA	6	0.22	0.07	0.24
(1,380)	1:26:A:LEU:HD21	1:66:A:ARG:HA	6	0.22	0.07	0.24
(1,380)	1:26:A:LEU:HD22	1:66:A:ARG:HA	6	0.22	0.07	0.24
(1,1155)	1:78:A:LYS:HA	1:78:A:LYS:HE2	6	0.19	0.06	0.2
(1,1155)	1:78:A:LYS:HA	1:78:A:LYS:HE3	6	0.19	0.06	0.2
(1,1598)	1:110:A:THR:H	1:111:A:VAL:HB	6	0.18	0.05	0.18
(1,1415)	1:91:A:LEU:HD21	1:74:A:ALA:HB1	6	0.18	0.05	0.15
(1,1415)	1:91:A:LEU:HD21	1:74:A:ALA:HB2	6	0.18	0.05	0.15
(1,1415)	1:91:A:LEU:HD21	1:74:A:ALA:HB3	6	0.18	0.05	0.15
(1,1415)	1:91:A:LEU:HD22	1:74:A:ALA:HB1	6	0.18	0.05	0.15
(1,1415)	1:91:A:LEU:HD22	1:74:A:ALA:HB2	6	0.18	0.05	0.15
(1,1415)	1:91:A:LEU:HD22	1:74:A:ALA:HB3	6	0.18	0.05	0.15
(1,1415)	1:91:A:LEU:HD23	1:74:A:ALA:HB1	6	0.18	0.05	0.15
(1,1415)	1:91:A:LEU:HD23	1:74:A:ALA:HB2	6	0.18	0.05	0.15
(1,1415)	1:91:A:LEU:HD23	1:74:A:ALA:HB3	6	0.18	0.05	0.15
(1,64)	1:6:A:ASP:HA	1:9:A:VAL:HB	6	0.17	0.04	0.16
(1,290)	1:22:A:LYS:HG3	1:27:A:VAL:HG21	6	0.15	0.03	0.14
(1,290)	1:22:A:LYS:HG3	1:27:A:VAL:HG22	6	0.15	0.03	0.14
(1,290)	1:22:A:LYS:HG3	1:27:A:VAL:HG23	6	0.15	0.03	0.14
(1,1272)	1:84:A:ARG:HB3	1:84:A:ARG:HD3	6	0.15	0.02	0.14
(1,1251)	1:83:A:LYS:HB3	1:86:A:GLY:H	6	0.12	0.01	0.13
(1,742)	1:53:A:THR:HB	1:55:A:THR:H	6	0.11	0.01	0.12
(1,252)	1:21:A:VAL:HG21	1:26:A:LEU:HA	6	0.11	0.01	0.11
(1,252)	1:21:A:VAL:HG22	1:26:A:LEU:HA	6	0.11	0.01	0.11
(1,252)	1:21:A:VAL:HG23	1:26:A:LEU:HA	6	0.11	0.01	0.11
(1,686)	1:47:A:ALA:H	1:49:A:LEU:H	6	0.11	0.01	0.11
(1,1416)	1:91:A:LEU:HA	1:74:A:ALA:HB1	6	0.11	0.01	0.11
(1,1416)	1:91:A:LEU:HA	1:74:A:ALA:HB2	6	0.11	0.01	0.11
(1,1416)	1:91:A:LEU:HA	1:74:A:ALA:HB3	6	0.11	0.01	0.11
(1,246)	1:21:A:VAL:HG21	1:23:A:VAL:H	6	0.11	0.01	0.11
(1,246)	1:21:A:VAL:HG22	1:23:A:VAL:H	6	0.11	0.01	0.11
(1,246)	1:21:A:VAL:HG23	1:23:A:VAL:H	6	0.11	0.01	0.11
(1,530)	1:36:A:PHE:HB3	1:121:A:GLY:H	5	1.31	0.08	1.28
(1,1578)	1:102:A:ASN:HB3	1:101:A:ASP:H	5	1.14	0.07	1.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1798)	1:114:A:ALA:H	1:115:A:ASP:HB3	5	1.08	0.79	1.73
(1,1639)	1:105:A:GLU:H	1:105:A:GLU:HG2	5	0.77	0.07	0.81
(1,517)	1:36:A:PHE:HB2	1:37:A:THR:H	5	0.54	0.03	0.55
(1,1579)	1:102:A:ASN:HB2	1:102:A:ASN:HA	5	0.25	0.02	0.26
(1,321)	1:24:A:ALA:HB1	1:62:A:PRO:HB2	5	0.21	0.06	0.21
(1,321)	1:24:A:ALA:HB2	1:62:A:PRO:HB2	5	0.21	0.06	0.21
(1,321)	1:24:A:ALA:HB3	1:62:A:PRO:HB2	5	0.21	0.06	0.21
(1,1208)	1:81:A:ASP:HA	1:84:A:ARG:HB3	5	0.21	0.04	0.22
(1,1205)	1:81:A:ASP:H	1:82:A:LEU:HD11	5	0.16	0.02	0.16
(1,1205)	1:81:A:ASP:H	1:82:A:LEU:HD12	5	0.16	0.02	0.16
(1,1205)	1:81:A:ASP:H	1:82:A:LEU:HD13	5	0.16	0.02	0.16
(1,547)	1:37:A:THR:H	1:73:A:VAL:HG21	5	0.14	0.03	0.15
(1,547)	1:37:A:THR:H	1:73:A:VAL:HG22	5	0.14	0.03	0.15
(1,547)	1:37:A:THR:H	1:73:A:VAL:HG23	5	0.14	0.03	0.15
(1,1942)	1:122:A:ILE:HD11	1:123:A:ILE:H	5	0.14	0.03	0.16
(1,1942)	1:122:A:ILE:HD12	1:123:A:ILE:H	5	0.14	0.03	0.16
(1,1942)	1:122:A:ILE:HD13	1:123:A:ILE:H	5	0.14	0.03	0.16
(1,1136)	1:77:A:TYR:H	1:121:A:GLY:HA3	5	0.12	0.02	0.12
(1,803)	1:56:A:SER:HA	1:57:A:LEU:H	5	0.1	0.0	0.1
(1,1186)	1:80:A:THR:HA	1:83:A:LYS:HB3	4	1.3	0.02	1.3
(1,1528)	1:98:A:ILE:HG21	1:83:A:LYS:HB2	4	1.21	0.01	1.2
(1,1528)	1:98:A:ILE:HG22	1:83:A:LYS:HB2	4	1.21	0.01	1.2
(1,1528)	1:98:A:ILE:HG23	1:83:A:LYS:HB2	4	1.21	0.01	1.2
(1,1253)	1:83:A:LYS:HG3	1:98:A:ILE:HG21	4	0.96	0.03	0.96
(1,1253)	1:83:A:LYS:HG3	1:98:A:ILE:HG22	4	0.96	0.03	0.96
(1,1253)	1:83:A:LYS:HG3	1:98:A:ILE:HG23	4	0.96	0.03	0.96
(1,735)	1:52:A:GLY:HA2	1:54:A:ILE:H	4	0.86	0.04	0.84
(1,1240)	1:83:A:LYS:HA	1:83:A:LYS:HG3	4	0.73	0.02	0.73
(1,563)	1:38:A:VAL:HG21	1:38:A:VAL:H	4	0.68	0.02	0.68
(1,563)	1:38:A:VAL:HG22	1:38:A:VAL:H	4	0.68	0.02	0.68
(1,563)	1:38:A:VAL:HG23	1:38:A:VAL:H	4	0.68	0.02	0.68
(1,1259)	1:84:A:ARG:H	1:83:A:LYS:HB3	4	0.59	0.02	0.59
(1,1149)	1:78:A:LYS:HG3	1:78:A:LYS:HE2	4	0.55	0.23	0.44
(1,1149)	1:78:A:LYS:HG3	1:78:A:LYS:HE3	4	0.55	0.23	0.44
(1,1168)	1:78:A:LYS:HG3	1:122:A:ILE:HD11	4	0.53	0.17	0.62
(1,1168)	1:78:A:LYS:HG3	1:122:A:ILE:HD12	4	0.53	0.17	0.62
(1,1168)	1:78:A:LYS:HG3	1:122:A:ILE:HD13	4	0.53	0.17	0.62
(1,776)	1:54:A:ILE:HG13	1:67:A:ILE:HG21	4	0.4	0.24	0.38
(1,776)	1:54:A:ILE:HG13	1:67:A:ILE:HG22	4	0.4	0.24	0.38
(1,776)	1:54:A:ILE:HG13	1:67:A:ILE:HG23	4	0.4	0.24	0.38
(1,1244)	1:83:A:LYS:HB3	1:83:A:LYS:H	4	0.32	0.01	0.32
(1,368)	1:26:A:LEU:HD21	1:66:A:ARG:HB3	4	0.32	0.05	0.33

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,368)	1:26:A:LEU:HD22	1:66:A:ARG:HB3	4	0.32	0.05	0.33
(1,368)	1:26:A:LEU:HD23	1:66:A:ARG:HB3	4	0.32	0.05	0.33
(1,1252)	1:83:A:LYS:HG2	1:86:A:GLY:H	4	0.3	0.01	0.3
(1,1252)	1:83:A:LYS:HG3	1:86:A:GLY:H	4	0.3	0.01	0.3
(1,1403)	1:90:A:SER:HB2	1:92:A:GLU:H	4	0.2	0.02	0.2
(1,1248)	1:83:A:LYS:HG2	1:83:A:LYS:H	4	0.19	0.01	0.2
(1,1248)	1:83:A:LYS:HG3	1:83:A:LYS:H	4	0.19	0.01	0.2
(1,107)	1:8:A:ALA:HA	1:18:A:VAL:HG21	4	0.18	0.08	0.16
(1,107)	1:8:A:ALA:HA	1:18:A:VAL:HG22	4	0.18	0.08	0.16
(1,107)	1:8:A:ALA:HA	1:18:A:VAL:HG23	4	0.18	0.08	0.16
(1,1234)	1:86:A:GLY:H	1:98:A:ILE:HG12	4	0.18	0.03	0.18
(1,230)	1:20:A:ALA:HB1	1:68:A:LEU:HD11	4	0.15	0.04	0.15
(1,230)	1:20:A:ALA:HB1	1:68:A:LEU:HD12	4	0.15	0.04	0.15
(1,230)	1:20:A:ALA:HB1	1:68:A:LEU:HD13	4	0.15	0.04	0.15
(1,230)	1:20:A:ALA:HB2	1:68:A:LEU:HD11	4	0.15	0.04	0.15
(1,230)	1:20:A:ALA:HB2	1:68:A:LEU:HD12	4	0.15	0.04	0.15
(1,230)	1:20:A:ALA:HB2	1:68:A:LEU:HD13	4	0.15	0.04	0.15
(1,230)	1:20:A:ALA:HB3	1:68:A:LEU:HD11	4	0.15	0.04	0.15
(1,230)	1:20:A:ALA:HB3	1:68:A:LEU:HD12	4	0.15	0.04	0.15
(1,230)	1:20:A:ALA:HB3	1:68:A:LEU:HD13	4	0.15	0.04	0.15
(1,1919)	1:122:A:ILE:HB	1:118:A:ALA:H	4	0.12	0.01	0.12
(1,642)	1:45:A:ALA:HB1	1:44:A:ASP:H	4	0.12	0.02	0.11
(1,642)	1:45:A:ALA:HB2	1:44:A:ASP:H	4	0.12	0.02	0.11
(1,642)	1:45:A:ALA:HB3	1:44:A:ASP:H	4	0.12	0.02	0.11
(1,1167)	1:78:A:LYS:HE2	1:122:A:ILE:HG21	4	0.12	0.0	0.12
(1,1167)	1:78:A:LYS:HE2	1:122:A:ILE:HG22	4	0.12	0.0	0.12
(1,1167)	1:78:A:LYS:HE2	1:122:A:ILE:HG23	4	0.12	0.0	0.12
(1,1167)	1:78:A:LYS:HE3	1:122:A:ILE:HG21	4	0.12	0.0	0.12
(1,1167)	1:78:A:LYS:HE3	1:122:A:ILE:HG22	4	0.12	0.0	0.12
(1,1167)	1:78:A:LYS:HE3	1:122:A:ILE:HG23	4	0.12	0.0	0.12
(1,911)	1:62:A:PRO:HB3	1:62:A:PRO:HG2	4	0.11	0.01	0.11
(1,727)	1:49:A:LEU:HB2	1:50:A:PRO:HD2	3	1.46	0.03	1.46
(1,1187)	1:80:A:THR:H	1:115:A:ASP:HB2	3	0.9	0.13	0.91
(1,525)	1:107:A:LYS:HB3	1:107:A:LYS:HE2	3	0.77	0.1	0.82
(1,525)	1:107:A:LYS:HB3	1:107:A:LYS:HE3	3	0.77	0.1	0.82
(1,728)	1:49:A:LEU:HB2	1:50:A:PRO:HD3	3	0.67	0.03	0.68
(1,1447)	1:92:A:GLU:HA	1:92:A:GLU:HG3	3	0.41	0.21	0.56
(1,1451)	1:92:A:GLU:H	1:92:A:GLU:HG3	3	0.37	0.03	0.36
(1,1052)	1:69:A:LYS:HB2	1:70:A:TYR:H	3	0.26	0.03	0.26
(1,1191)	1:81:A:ASP:H	1:78:A:LYS:HB3	3	0.24	0.11	0.18
(1,1845)	1:117:A:GLU:HA	1:117:A:GLU:HG3	3	0.22	0.02	0.22
(1,1999)	1:126:A:ILE:HG21	1:39:A:PHE:HD1	3	0.21	0.05	0.23

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1999)	1:126:A:ILE:HG21	1:39:A:PHE:HD2	3	0.21	0.05	0.23
(1,1999)	1:126:A:ILE:HG22	1:39:A:PHE:HD1	3	0.21	0.05	0.23
(1,1999)	1:126:A:ILE:HG22	1:39:A:PHE:HD2	3	0.21	0.05	0.23
(1,1999)	1:126:A:ILE:HG23	1:39:A:PHE:HD1	3	0.21	0.05	0.23
(1,1999)	1:126:A:ILE:HG23	1:39:A:PHE:HD2	3	0.21	0.05	0.23
(1,1809)	1:115:A:ASP:HB3	1:115:A:ASP:H	3	0.21	0.01	0.21
(1,1701)	1:108:A:ASN:HB3	1:108:A:ASN:HD22	3	0.2	0.01	0.19
(1,1475)	1:94:A:SER:HB3	1:94:A:SER:H	3	0.15	0.0	0.15
(1,692)	1:48:A:LYS:HA	1:48:A:LYS:HB3	3	0.13	0.01	0.13
(1,2046)	1:127:A:ASP:H	1:127:A:ASP:HB2	3	0.13	0.0	0.13
(1,596)	1:42:A:ASN:HB2	1:42:A:ASN:HD22	3	0.12	0.01	0.12
(1,2031)	1:126:A:ILE:H	1:127:A:ASP:HA	3	0.12	0.01	0.11
(1,2078)	1:129:A:VAL:HB	1:53:A:THR:H	3	0.12	0.01	0.12
(1,66)	1:7:A:ILE:HD11	1:5:A:VAL:H	3	0.12	0.0	0.12
(1,66)	1:7:A:ILE:HD12	1:5:A:VAL:H	3	0.12	0.0	0.12
(1,66)	1:7:A:ILE:HD13	1:5:A:VAL:H	3	0.12	0.0	0.12
(1,1095)	1:74:A:ALA:HA	1:36:A:PHE:H	3	0.12	0.01	0.12
(1,1146)	1:78:A:LYS:HB3	1:78:A:LYS:HD2	3	0.12	0.01	0.11
(1,1146)	1:78:A:LYS:HB3	1:78:A:LYS:HD3	3	0.12	0.01	0.11
(1,1169)	1:78:A:LYS:HG2	1:122:A:ILE:HD11	3	0.11	0.02	0.1
(1,1169)	1:78:A:LYS:HG2	1:122:A:ILE:HD12	3	0.11	0.02	0.1
(1,1169)	1:78:A:LYS:HG2	1:122:A:ILE:HD13	3	0.11	0.02	0.1
(1,1162)	1:78:A:LYS:HA	1:80:A:THR:H	3	0.11	0.0	0.11
(1,865)	1:59:A:GLN:HG3	1:59:A:GLN:H	3	0.11	0.0	0.11
(1,1394)	1:89:A:THR:HG21	1:95:A:THR:H	3	0.11	0.0	0.11
(1,1394)	1:89:A:THR:HG22	1:95:A:THR:H	3	0.11	0.0	0.11
(1,1394)	1:89:A:THR:HG23	1:95:A:THR:H	3	0.11	0.0	0.11
(1,1438)	1:91:A:LEU:HB2	1:92:A:GLU:H	3	0.11	0.01	0.1
(1,1793)	1:114:A:ALA:HB1	1:114:A:ALA:H	3	0.1	0.0	0.1
(1,1793)	1:114:A:ALA:HB2	1:114:A:ALA:H	3	0.1	0.0	0.1
(1,1793)	1:114:A:ALA:HB3	1:114:A:ALA:H	3	0.1	0.0	0.1
(1,1341)	1:87:A:ILE:HG21	1:88:A:VAL:H	3	0.1	0.0	0.1
(1,1341)	1:87:A:ILE:HG22	1:88:A:VAL:H	3	0.1	0.0	0.1
(1,1341)	1:87:A:ILE:HG23	1:88:A:VAL:H	3	0.1	0.0	0.1
(1,938)	1:3:A:THR:HG22	1:31:A:GLN:HG2	2	1.4	0.19	1.4
(1,938)	1:63:A:GLN:HG2	1:67:A:ILE:HG13	2	1.4	0.19	1.4
(1,936)	1:63:A:GLN:HG2	1:66:A:ARG:HD2	2	1.16	0.04	1.16
(1,111)	1:9:A:VAL:H	1:9:A:VAL:HG21	2	1.04	0.02	1.04
(1,111)	1:9:A:VAL:H	1:9:A:VAL:HG22	2	1.04	0.02	1.04
(1,111)	1:9:A:VAL:H	1:9:A:VAL:HG23	2	1.04	0.02	1.04
(1,109)	1:9:A:VAL:HG11	1:9:A:VAL:HA	2	0.82	0.01	0.82
(1,109)	1:9:A:VAL:HG12	1:9:A:VAL:HA	2	0.82	0.01	0.82

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,109)	1:9:A:VAL:HG13	1:9:A:VAL:HA	2	0.82	0.01	0.82
(1,1130)	1:77:A:TYR:HB3	1:81:A:ASP:HB3	2	0.68	0.45	0.68
(1,1464)	1:93:A:GLY:H	1:92:A:GLU:HG3	2	0.54	0.02	0.54
(1,343)	1:25:A:ASN:HD22	1:92:A:GLU:HB3	2	0.47	0.07	0.47
(1,113)	1:10:A:ASN:HB2	1:7:A:ILE:HG21	2	0.42	0.05	0.42
(1,113)	1:10:A:ASN:HB2	1:7:A:ILE:HG22	2	0.42	0.05	0.42
(1,113)	1:10:A:ASN:HB2	1:7:A:ILE:HG23	2	0.42	0.05	0.42
(1,1558)	1:99:A:HIS:HB2	1:100:A:GLY:H	2	0.34	0.01	0.34
(1,1567)	1:100:A:GLY:HA2	1:105:A:GLU:H	2	0.28	0.13	0.28
(1,923)	1:63:A:GLN:HE21	1:63:A:GLN:HB2	2	0.26	0.02	0.26
(1,923)	1:63:A:GLN:HE21	1:63:A:GLN:HB3	2	0.26	0.02	0.26
(1,120)	1:10:A:ASN:HB3	1:10:A:ASN:HD22	2	0.22	0.01	0.22
(1,879)	1:59:A:GLN:HA	1:60:A:ASN:H	2	0.22	0.02	0.22
(1,882)	1:60:A:ASN:HA	1:59:A:GLN:H	2	0.18	0.02	0.18
(1,1719)	1:110:A:THR:HG21	1:103:A:PRO:HG3	2	0.15	0.02	0.15
(1,1719)	1:110:A:THR:HG22	1:103:A:PRO:HG3	2	0.15	0.02	0.15
(1,1719)	1:110:A:THR:HG23	1:103:A:PRO:HG3	2	0.15	0.02	0.15
(1,179)	1:18:A:VAL:HG21	1:8:A:ALA:HB1	2	0.14	0.03	0.14
(1,179)	1:18:A:VAL:HG21	1:8:A:ALA:HB2	2	0.14	0.03	0.14
(1,179)	1:18:A:VAL:HG21	1:8:A:ALA:HB3	2	0.14	0.03	0.14
(1,179)	1:18:A:VAL:HG22	1:8:A:ALA:HB1	2	0.14	0.03	0.14
(1,179)	1:18:A:VAL:HG22	1:8:A:ALA:HB2	2	0.14	0.03	0.14
(1,179)	1:18:A:VAL:HG22	1:8:A:ALA:HB3	2	0.14	0.03	0.14
(1,179)	1:18:A:VAL:HG23	1:8:A:ALA:HB1	2	0.14	0.03	0.14
(1,179)	1:18:A:VAL:HG23	1:8:A:ALA:HB2	2	0.14	0.03	0.14
(1,179)	1:18:A:VAL:HG23	1:8:A:ALA:HB3	2	0.14	0.03	0.14
(1,852)	1:58:A:VAL:H	1:60:A:ASN:H	2	0.14	0.02	0.14
(1,1671)	1:106:A:VAL:HG11	1:111:A:VAL:HB	2	0.14	0.02	0.14
(1,1671)	1:106:A:VAL:HG12	1:111:A:VAL:HB	2	0.14	0.02	0.14
(1,1671)	1:106:A:VAL:HG13	1:111:A:VAL:HB	2	0.14	0.02	0.14
(1,538)	1:37:A:THR:HG21	1:37:A:THR:H	2	0.13	0.03	0.13
(1,538)	1:37:A:THR:HG22	1:37:A:THR:H	2	0.13	0.03	0.13
(1,538)	1:37:A:THR:HG23	1:37:A:THR:H	2	0.13	0.03	0.13
(1,427)	1:30:A:LEU:HD11	1:31:A:GLN:H	2	0.12	0.02	0.12
(1,427)	1:30:A:LEU:HD12	1:31:A:GLN:H	2	0.12	0.02	0.12
(1,427)	1:30:A:LEU:HD13	1:31:A:GLN:H	2	0.12	0.02	0.12
(1,809)	1:56:A:SER:H	1:59:A:GLN:H	2	0.12	0.01	0.12
(1,1971)	1:124:A:HIS:HB3	1:114:A:ALA:HB1	2	0.12	0.02	0.12
(1,1971)	1:124:A:HIS:HB3	1:114:A:ALA:HB2	2	0.12	0.02	0.12
(1,1971)	1:124:A:HIS:HB3	1:114:A:ALA:HB3	2	0.12	0.02	0.12
(1,163)	1:14:A:PHE:HB3	1:14:A:PHE:H	2	0.12	0.01	0.12
(1,793)	1:55:A:THR:HG21	1:59:A:GLN:H	2	0.12	0.0	0.12

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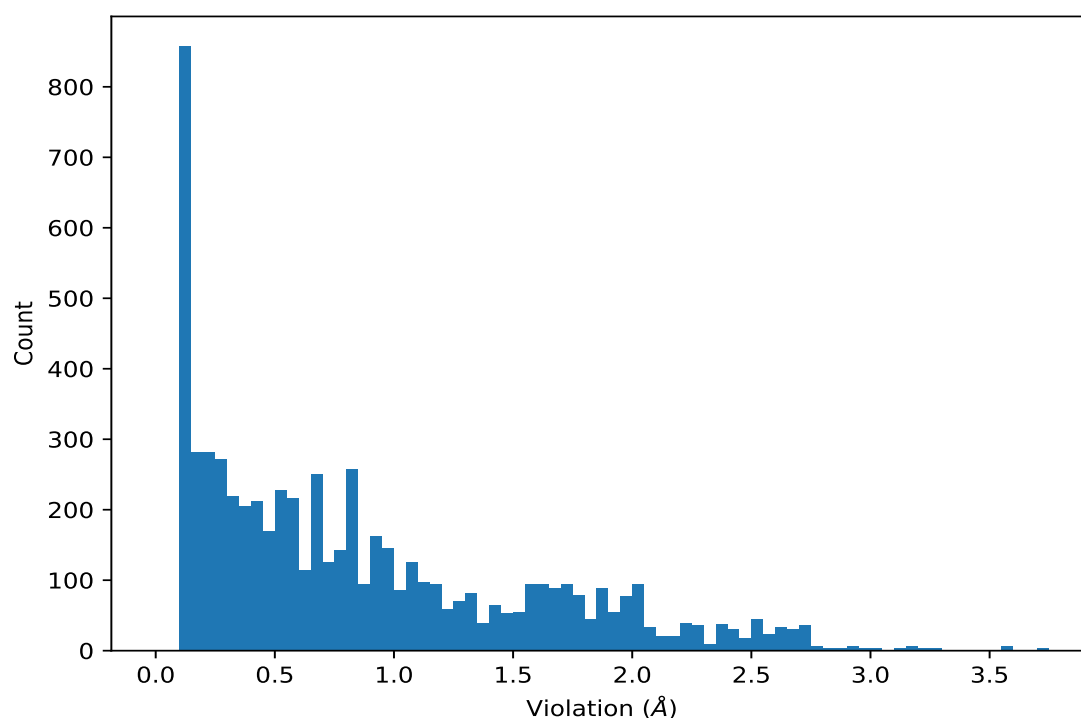
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,793)	1:55:A:THR:HG22	1:59:A:GLN:H	2	0.12	0.0	0.12
(1,793)	1:55:A:THR:HG23	1:59:A:GLN:H	2	0.12	0.0	0.12
(1,1407)	1:91:A:LEU:HD11	1:29:A:ALA:HB1	2	0.12	0.02	0.12
(1,1407)	1:91:A:LEU:HD11	1:29:A:ALA:HB2	2	0.12	0.02	0.12
(1,1407)	1:91:A:LEU:HD11	1:29:A:ALA:HB3	2	0.12	0.02	0.12
(1,1407)	1:91:A:LEU:HD12	1:29:A:ALA:HB1	2	0.12	0.02	0.12
(1,1407)	1:91:A:LEU:HD12	1:29:A:ALA:HB2	2	0.12	0.02	0.12
(1,1407)	1:91:A:LEU:HD12	1:29:A:ALA:HB3	2	0.12	0.02	0.12
(1,1407)	1:91:A:LEU:HD13	1:29:A:ALA:HB1	2	0.12	0.02	0.12
(1,1407)	1:91:A:LEU:HD13	1:29:A:ALA:HB2	2	0.12	0.02	0.12
(1,1407)	1:91:A:LEU:HD13	1:29:A:ALA:HB3	2	0.12	0.02	0.12
(1,1868)	1:118:A:ALA:HA	1:121:A:GLY:H	2	0.12	0.02	0.12
(1,835)	1:58:A:VAL:HG11	1:55:A:THR:H	2	0.12	0.0	0.12
(1,835)	1:58:A:VAL:HG12	1:55:A:THR:H	2	0.12	0.0	0.12
(1,835)	1:58:A:VAL:HG13	1:55:A:THR:H	2	0.12	0.0	0.12
(1,1190)	1:81:A:ASP:H	1:78:A:LYS:H	2	0.12	0.0	0.12
(1,1829)	1:116:A:ILE:HG21	1:118:A:ALA:H	2	0.11	0.0	0.11
(1,1829)	1:116:A:ILE:HG22	1:118:A:ALA:H	2	0.11	0.0	0.11
(1,1829)	1:116:A:ILE:HG23	1:118:A:ALA:H	2	0.11	0.0	0.11
(1,1966)	1:123:A:ILE:HG12	1:124:A:HIS:H	2	0.11	0.0	0.11
(1,2075)	1:129:A:VAL:HG11	1:49:A:LEU:HA	2	0.11	0.01	0.11
(1,2075)	1:129:A:VAL:HG12	1:49:A:LEU:HA	2	0.11	0.01	0.11
(1,2075)	1:129:A:VAL:HG13	1:49:A:LEU:HA	2	0.11	0.01	0.11
(1,189)	1:18:A:VAL:H	1:16:A:THR:HA	2	0.11	0.0	0.11
(1,779)	1:55:A:THR:HB	1:53:A:THR:H	2	0.11	0.0	0.11
(1,1762)	1:112:A:LEU:HD11	1:112:A:LEU:HA	2	0.11	0.0	0.11
(1,1762)	1:112:A:LEU:HD12	1:112:A:LEU:HA	2	0.11	0.0	0.11
(1,1762)	1:112:A:LEU:HD13	1:112:A:LEU:HA	2	0.11	0.0	0.11
(1,2033)	1:126:A:ILE:HG12	1:127:A:ASP:H	2	0.11	0.0	0.11
(1,1283)	1:84:A:ARG:HB2	1:85:A:MET:H	2	0.1	0.0	0.1
(1,1939)	1:122:A:ILE:H	1:122:A:ILE:HG21	2	0.1	0.0	0.1
(1,1939)	1:122:A:ILE:H	1:122:A:ILE:HG22	2	0.1	0.0	0.1
(1,1939)	1:122:A:ILE:H	1:122:A:ILE:HG23	2	0.1	0.0	0.1

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1256)	1:83:A:LYS:HD3	1:104:A:LEU:HD21	3	3.71
(1,1256)	1:83:A:LYS:HD3	1:104:A:LEU:HD22	3	3.71
(1,1256)	1:83:A:LYS:HD3	1:104:A:LEU:HD23	3	3.71
(1,1256)	1:83:A:LYS:HD3	1:104:A:LEU:HD21	1	3.57
(1,1256)	1:83:A:LYS:HD3	1:104:A:LEU:HD22	1	3.57
(1,1256)	1:83:A:LYS:HD3	1:104:A:LEU:HD23	1	3.57
(1,1256)	1:83:A:LYS:HD3	1:104:A:LEU:HD21	5	3.57
(1,1256)	1:83:A:LYS:HD3	1:104:A:LEU:HD22	5	3.57
(1,1256)	1:83:A:LYS:HD3	1:104:A:LEU:HD23	5	3.57
(1,1258)	1:83:A:LYS:HB2	1:104:A:LEU:HD21	7	3.25
(1,1258)	1:83:A:LYS:HB2	1:104:A:LEU:HD22	7	3.25
(1,1258)	1:83:A:LYS:HB2	1:104:A:LEU:HD23	7	3.25
(1,1258)	1:83:A:LYS:HB2	1:104:A:LEU:HD21	2	3.2
(1,1258)	1:83:A:LYS:HB2	1:104:A:LEU:HD22	2	3.2
(1,1258)	1:83:A:LYS:HB2	1:104:A:LEU:HD23	2	3.2
(1,1258)	1:83:A:LYS:HB2	1:104:A:LEU:HD21	9	3.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1258)	1:83:A:LYS:HB2	1:104:A:LEU:HD22	9	3.19
(1,1258)	1:83:A:LYS:HB2	1:104:A:LEU:HD23	9	3.19
(1,1258)	1:83:A:LYS:HB2	1:104:A:LEU:HD21	10	3.17
(1,1258)	1:83:A:LYS:HB2	1:104:A:LEU:HD22	10	3.17
(1,1258)	1:83:A:LYS:HB2	1:104:A:LEU:HD23	10	3.17
(1,1969)	1:124:A:HIS:HB2	1:104:A:LEU:HD11	3	3.1
(1,1969)	1:124:A:HIS:HB2	1:104:A:LEU:HD12	3	3.1
(1,1969)	1:124:A:HIS:HB2	1:104:A:LEU:HD13	3	3.1
(1,1256)	1:83:A:LYS:HD3	1:104:A:LEU:HD21	7	3.01
(1,1256)	1:83:A:LYS:HD3	1:104:A:LEU:HD22	7	3.01
(1,1256)	1:83:A:LYS:HD3	1:104:A:LEU:HD23	7	3.01
(1,1256)	1:83:A:LYS:HD3	1:104:A:LEU:HD21	9	2.99
(1,1256)	1:83:A:LYS:HD3	1:104:A:LEU:HD22	9	2.99
(1,1256)	1:83:A:LYS:HD3	1:104:A:LEU:HD23	9	2.99
(1,1969)	1:124:A:HIS:HB2	1:104:A:LEU:HD11	5	2.93
(1,1969)	1:124:A:HIS:HB2	1:104:A:LEU:HD12	5	2.93
(1,1969)	1:124:A:HIS:HB2	1:104:A:LEU:HD13	5	2.93
(1,1969)	1:124:A:HIS:HB2	1:104:A:LEU:HD11	10	2.92
(1,1969)	1:124:A:HIS:HB2	1:104:A:LEU:HD12	10	2.92
(1,1969)	1:124:A:HIS:HB2	1:104:A:LEU:HD13	10	2.92
(1,1969)	1:124:A:HIS:HB2	1:104:A:LEU:HD11	8	2.9
(1,1969)	1:124:A:HIS:HB2	1:104:A:LEU:HD12	8	2.9
(1,1969)	1:124:A:HIS:HB2	1:104:A:LEU:HD13	8	2.9
(1,204)	1:18:A:VAL:HG11	1:22:A:LYS:HE3	7	2.83
(1,204)	1:18:A:VAL:HG12	1:22:A:LYS:HE3	7	2.83
(1,204)	1:18:A:VAL:HG13	1:22:A:LYS:HE3	7	2.83
(1,1411)	1:91:A:LEU:HA	1:73:A:VAL:HG11	9	2.75
(1,1411)	1:91:A:LEU:HA	1:73:A:VAL:HG12	9	2.75
(1,1411)	1:91:A:LEU:HA	1:73:A:VAL:HG13	9	2.75
(1,1256)	1:83:A:LYS:HD3	1:104:A:LEU:HD21	8	2.75
(1,1256)	1:83:A:LYS:HD3	1:104:A:LEU:HD22	8	2.75
(1,1256)	1:83:A:LYS:HD3	1:104:A:LEU:HD23	8	2.75
(1,1411)	1:91:A:LEU:HA	1:73:A:VAL:HG11	5	2.74
(1,1411)	1:91:A:LEU:HA	1:73:A:VAL:HG12	5	2.74
(1,1411)	1:91:A:LEU:HA	1:73:A:VAL:HG13	5	2.74
(1,943)	1:64:A:LEU:HD11	1:24:A:ALA:HA	2	2.74
(1,943)	1:64:A:LEU:HD12	1:24:A:ALA:HA	2	2.74
(1,943)	1:64:A:LEU:HD13	1:24:A:ALA:HA	2	2.74
(1,1411)	1:91:A:LEU:HA	1:73:A:VAL:HG11	3	2.73
(1,1411)	1:91:A:LEU:HA	1:73:A:VAL:HG12	3	2.73
(1,1411)	1:91:A:LEU:HA	1:73:A:VAL:HG13	3	2.73
(1,943)	1:64:A:LEU:HD11	1:24:A:ALA:HA	8	2.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,943)	1:64:A:LEU:HD12	1:24:A:ALA:HA	8	2.73
(1,943)	1:64:A:LEU:HD13	1:24:A:ALA:HA	8	2.73
(1,1411)	1:91:A:LEU:HA	1:73:A:VAL:HG11	7	2.72
(1,1411)	1:91:A:LEU:HA	1:73:A:VAL:HG12	7	2.72
(1,1411)	1:91:A:LEU:HA	1:73:A:VAL:HG13	7	2.72
(1,1411)	1:91:A:LEU:HA	1:73:A:VAL:HG11	6	2.71
(1,1411)	1:91:A:LEU:HA	1:73:A:VAL:HG12	6	2.71
(1,1411)	1:91:A:LEU:HA	1:73:A:VAL:HG13	6	2.71
(1,1411)	1:91:A:LEU:HA	1:73:A:VAL:HG11	10	2.71
(1,1411)	1:91:A:LEU:HA	1:73:A:VAL:HG12	10	2.71
(1,1411)	1:91:A:LEU:HA	1:73:A:VAL:HG13	10	2.71
(1,1023)	1:68:A:LEU:HD11	1:21:A:VAL:HA	6	2.71
(1,1023)	1:68:A:LEU:HD12	1:21:A:VAL:HA	6	2.71
(1,1023)	1:68:A:LEU:HD13	1:21:A:VAL:HA	6	2.71
(1,1411)	1:91:A:LEU:HA	1:73:A:VAL:HG11	1	2.7
(1,1411)	1:91:A:LEU:HA	1:73:A:VAL:HG12	1	2.7
(1,1411)	1:91:A:LEU:HA	1:73:A:VAL:HG13	1	2.7
(1,1256)	1:83:A:LYS:HD3	1:104:A:LEU:HD21	4	2.7
(1,1256)	1:83:A:LYS:HD3	1:104:A:LEU:HD22	4	2.7
(1,1256)	1:83:A:LYS:HD3	1:104:A:LEU:HD23	4	2.7
(1,943)	1:64:A:LEU:HD11	1:24:A:ALA:HA	6	2.7
(1,943)	1:64:A:LEU:HD12	1:24:A:ALA:HA	6	2.7
(1,943)	1:64:A:LEU:HD13	1:24:A:ALA:HA	6	2.7
(1,943)	1:64:A:LEU:HD11	1:24:A:ALA:HA	10	2.7
(1,943)	1:64:A:LEU:HD12	1:24:A:ALA:HA	10	2.7
(1,943)	1:64:A:LEU:HD13	1:24:A:ALA:HA	10	2.7
(1,1411)	1:91:A:LEU:HA	1:73:A:VAL:HG11	2	2.69
(1,1411)	1:91:A:LEU:HA	1:73:A:VAL:HG12	2	2.69
(1,1411)	1:91:A:LEU:HA	1:73:A:VAL:HG13	2	2.69
(1,1023)	1:68:A:LEU:HD11	1:21:A:VAL:HA	7	2.69
(1,1023)	1:68:A:LEU:HD12	1:21:A:VAL:HA	7	2.69
(1,1023)	1:68:A:LEU:HD13	1:21:A:VAL:HA	7	2.69
(1,943)	1:64:A:LEU:HD11	1:24:A:ALA:HA	9	2.69
(1,943)	1:64:A:LEU:HD12	1:24:A:ALA:HA	9	2.69
(1,943)	1:64:A:LEU:HD13	1:24:A:ALA:HA	9	2.69
(1,1411)	1:91:A:LEU:HA	1:73:A:VAL:HG11	8	2.68
(1,1411)	1:91:A:LEU:HA	1:73:A:VAL:HG12	8	2.68
(1,1411)	1:91:A:LEU:HA	1:73:A:VAL:HG13	8	2.68
(1,1023)	1:68:A:LEU:HD11	1:21:A:VAL:HA	8	2.68
(1,1023)	1:68:A:LEU:HD12	1:21:A:VAL:HA	8	2.68
(1,1023)	1:68:A:LEU:HD13	1:21:A:VAL:HA	8	2.68
(1,943)	1:64:A:LEU:HD11	1:24:A:ALA:HA	1	2.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,943)	1:64:A:LEU:HD12	1:24:A:ALA:HA	1	2.68
(1,943)	1:64:A:LEU:HD13	1:24:A:ALA:HA	1	2.68
(1,943)	1:64:A:LEU:HD11	1:24:A:ALA:HA	3	2.67
(1,943)	1:64:A:LEU:HD12	1:24:A:ALA:HA	3	2.67
(1,943)	1:64:A:LEU:HD13	1:24:A:ALA:HA	3	2.67
(1,1969)	1:124:A:HIS:HB2	1:104:A:LEU:HD11	9	2.66
(1,1969)	1:124:A:HIS:HB2	1:104:A:LEU:HD12	9	2.66
(1,1969)	1:124:A:HIS:HB2	1:104:A:LEU:HD13	9	2.66
(1,1023)	1:68:A:LEU:HD11	1:21:A:VAL:HA	2	2.66
(1,1023)	1:68:A:LEU:HD12	1:21:A:VAL:HA	2	2.66
(1,1023)	1:68:A:LEU:HD13	1:21:A:VAL:HA	2	2.66
(1,943)	1:64:A:LEU:HD11	1:24:A:ALA:HA	5	2.66
(1,943)	1:64:A:LEU:HD12	1:24:A:ALA:HA	5	2.66
(1,943)	1:64:A:LEU:HD13	1:24:A:ALA:HA	5	2.66
(1,1411)	1:91:A:LEU:HA	1:73:A:VAL:HG11	4	2.65
(1,1411)	1:91:A:LEU:HA	1:73:A:VAL:HG12	4	2.65
(1,1411)	1:91:A:LEU:HA	1:73:A:VAL:HG13	4	2.65
(1,1023)	1:68:A:LEU:HD11	1:21:A:VAL:HA	9	2.65
(1,1023)	1:68:A:LEU:HD12	1:21:A:VAL:HA	9	2.65
(1,1023)	1:68:A:LEU:HD13	1:21:A:VAL:HA	9	2.65
(1,943)	1:64:A:LEU:HD11	1:24:A:ALA:HA	7	2.65
(1,943)	1:64:A:LEU:HD12	1:24:A:ALA:HA	7	2.65
(1,943)	1:64:A:LEU:HD13	1:24:A:ALA:HA	7	2.65
(1,204)	1:18:A:VAL:HG11	1:22:A:LYS:HE3	8	2.65
(1,204)	1:18:A:VAL:HG12	1:22:A:LYS:HE3	8	2.65
(1,204)	1:18:A:VAL:HG13	1:22:A:LYS:HE3	8	2.65
(1,1082)	1:73:A:VAL:HG21	1:39:A:PHE:H	5	2.64
(1,1082)	1:73:A:VAL:HG22	1:39:A:PHE:H	5	2.64
(1,1082)	1:73:A:VAL:HG23	1:39:A:PHE:H	5	2.64
(1,943)	1:64:A:LEU:HD11	1:24:A:ALA:HA	4	2.64
(1,943)	1:64:A:LEU:HD12	1:24:A:ALA:HA	4	2.64
(1,943)	1:64:A:LEU:HD13	1:24:A:ALA:HA	4	2.64
(1,1082)	1:73:A:VAL:HG21	1:39:A:PHE:H	2	2.63
(1,1082)	1:73:A:VAL:HG22	1:39:A:PHE:H	2	2.63
(1,1082)	1:73:A:VAL:HG23	1:39:A:PHE:H	2	2.63
(1,1023)	1:68:A:LEU:HD11	1:21:A:VAL:HA	4	2.63
(1,1023)	1:68:A:LEU:HD12	1:21:A:VAL:HA	4	2.63
(1,1023)	1:68:A:LEU:HD13	1:21:A:VAL:HA	4	2.63
(1,1256)	1:83:A:LYS:HD3	1:104:A:LEU:HD21	6	2.62
(1,1256)	1:83:A:LYS:HD3	1:104:A:LEU:HD22	6	2.62
(1,1256)	1:83:A:LYS:HD3	1:104:A:LEU:HD23	6	2.62
(1,1023)	1:68:A:LEU:HD11	1:21:A:VAL:HA	3	2.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1023)	1:68:A:LEU:HD12	1:21:A:VAL:HA	3	2.62
(1,1023)	1:68:A:LEU:HD13	1:21:A:VAL:HA	3	2.62
(1,205)	1:18:A:VAL:HG11	1:22:A:LYS:HE2	8	2.6
(1,205)	1:18:A:VAL:HG12	1:22:A:LYS:HE2	8	2.6
(1,205)	1:18:A:VAL:HG13	1:22:A:LYS:HE2	8	2.6
(1,1082)	1:73:A:VAL:HG21	1:39:A:PHE:H	9	2.59
(1,1082)	1:73:A:VAL:HG22	1:39:A:PHE:H	9	2.59
(1,1082)	1:73:A:VAL:HG23	1:39:A:PHE:H	9	2.59
(1,1969)	1:124:A:HIS:HB2	1:104:A:LEU:HD11	2	2.58
(1,1969)	1:124:A:HIS:HB2	1:104:A:LEU:HD12	2	2.58
(1,1969)	1:124:A:HIS:HB2	1:104:A:LEU:HD13	2	2.58
(1,1023)	1:68:A:LEU:HD11	1:21:A:VAL:HA	1	2.58
(1,1023)	1:68:A:LEU:HD12	1:21:A:VAL:HA	1	2.58
(1,1023)	1:68:A:LEU:HD13	1:21:A:VAL:HA	1	2.58
(1,958)	1:64:A:LEU:HD21	1:67:A:ILE:HB	9	2.58
(1,958)	1:64:A:LEU:HD22	1:67:A:ILE:HB	9	2.58
(1,958)	1:64:A:LEU:HD23	1:67:A:ILE:HB	9	2.58
(1,204)	1:18:A:VAL:HG11	1:22:A:LYS:HE3	3	2.57
(1,204)	1:18:A:VAL:HG12	1:22:A:LYS:HE3	3	2.57
(1,204)	1:18:A:VAL:HG13	1:22:A:LYS:HE3	3	2.57
(1,204)	1:18:A:VAL:HG11	1:22:A:LYS:HE3	9	2.57
(1,204)	1:18:A:VAL:HG12	1:22:A:LYS:HE3	9	2.57
(1,204)	1:18:A:VAL:HG13	1:22:A:LYS:HE3	9	2.57
(1,204)	1:18:A:VAL:HG11	1:22:A:LYS:HE3	10	2.57
(1,204)	1:18:A:VAL:HG12	1:22:A:LYS:HE3	10	2.57
(1,204)	1:18:A:VAL:HG13	1:22:A:LYS:HE3	10	2.57
(1,204)	1:18:A:VAL:HG11	1:22:A:LYS:HE3	1	2.56
(1,204)	1:18:A:VAL:HG12	1:22:A:LYS:HE3	1	2.56
(1,204)	1:18:A:VAL:HG13	1:22:A:LYS:HE3	1	2.56
(1,958)	1:64:A:LEU:HD21	1:67:A:ILE:HB	2	2.55
(1,958)	1:64:A:LEU:HD22	1:67:A:ILE:HB	2	2.55
(1,958)	1:64:A:LEU:HD23	1:67:A:ILE:HB	2	2.55
(1,204)	1:18:A:VAL:HG11	1:22:A:LYS:HE3	5	2.55
(1,204)	1:18:A:VAL:HG12	1:22:A:LYS:HE3	5	2.55
(1,204)	1:18:A:VAL:HG13	1:22:A:LYS:HE3	5	2.55
(1,204)	1:18:A:VAL:HG11	1:22:A:LYS:HE3	2	2.54
(1,204)	1:18:A:VAL:HG12	1:22:A:LYS:HE3	2	2.54
(1,204)	1:18:A:VAL:HG13	1:22:A:LYS:HE3	2	2.54
(1,204)	1:18:A:VAL:HG11	1:22:A:LYS:HE3	4	2.54
(1,204)	1:18:A:VAL:HG12	1:22:A:LYS:HE3	4	2.54
(1,204)	1:18:A:VAL:HG13	1:22:A:LYS:HE3	4	2.54
(1,958)	1:64:A:LEU:HD21	1:67:A:ILE:HB	6	2.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,958)	1:64:A:LEU:HD22	1:67:A:ILE:HB	6	2.53
(1,958)	1:64:A:LEU:HD23	1:67:A:ILE:HB	6	2.53
(1,958)	1:64:A:LEU:HD21	1:67:A:ILE:HB	7	2.53
(1,958)	1:64:A:LEU:HD22	1:67:A:ILE:HB	7	2.53
(1,958)	1:64:A:LEU:HD23	1:67:A:ILE:HB	7	2.53
(1,944)	1:64:A:LEU:HD11	1:24:A:ALA:H	8	2.53
(1,944)	1:64:A:LEU:HD12	1:24:A:ALA:H	8	2.53
(1,944)	1:64:A:LEU:HD13	1:24:A:ALA:H	8	2.53
(1,204)	1:18:A:VAL:HG11	1:22:A:LYS:HE3	6	2.53
(1,204)	1:18:A:VAL:HG12	1:22:A:LYS:HE3	6	2.53
(1,204)	1:18:A:VAL:HG13	1:22:A:LYS:HE3	6	2.53
(1,1023)	1:68:A:LEU:HD11	1:21:A:VAL:HA	5	2.52
(1,1023)	1:68:A:LEU:HD12	1:21:A:VAL:HA	5	2.52
(1,1023)	1:68:A:LEU:HD13	1:21:A:VAL:HA	5	2.52
(1,958)	1:64:A:LEU:HD21	1:67:A:ILE:HB	3	2.52
(1,958)	1:64:A:LEU:HD22	1:67:A:ILE:HB	3	2.52
(1,958)	1:64:A:LEU:HD23	1:67:A:ILE:HB	3	2.52
(1,944)	1:64:A:LEU:HD11	1:24:A:ALA:H	7	2.51
(1,944)	1:64:A:LEU:HD12	1:24:A:ALA:H	7	2.51
(1,944)	1:64:A:LEU:HD13	1:24:A:ALA:H	7	2.51
(1,958)	1:64:A:LEU:HD21	1:67:A:ILE:HB	4	2.5
(1,958)	1:64:A:LEU:HD22	1:67:A:ILE:HB	4	2.5
(1,958)	1:64:A:LEU:HD23	1:67:A:ILE:HB	4	2.5
(1,958)	1:64:A:LEU:HD21	1:67:A:ILE:HB	5	2.5
(1,958)	1:64:A:LEU:HD22	1:67:A:ILE:HB	5	2.5
(1,958)	1:64:A:LEU:HD23	1:67:A:ILE:HB	5	2.5
(1,958)	1:64:A:LEU:HD21	1:67:A:ILE:HB	8	2.5
(1,958)	1:64:A:LEU:HD22	1:67:A:ILE:HB	8	2.5
(1,958)	1:64:A:LEU:HD23	1:67:A:ILE:HB	8	2.5
(1,944)	1:64:A:LEU:HD11	1:24:A:ALA:H	1	2.5
(1,944)	1:64:A:LEU:HD12	1:24:A:ALA:H	1	2.5
(1,944)	1:64:A:LEU:HD13	1:24:A:ALA:H	1	2.5
(1,958)	1:64:A:LEU:HD21	1:67:A:ILE:HB	10	2.49
(1,958)	1:64:A:LEU:HD22	1:67:A:ILE:HB	10	2.49
(1,958)	1:64:A:LEU:HD23	1:67:A:ILE:HB	10	2.49
(1,944)	1:64:A:LEU:HD11	1:24:A:ALA:H	6	2.49
(1,944)	1:64:A:LEU:HD12	1:24:A:ALA:H	6	2.49
(1,944)	1:64:A:LEU:HD13	1:24:A:ALA:H	6	2.49
(1,944)	1:64:A:LEU:HD11	1:24:A:ALA:H	4	2.48
(1,944)	1:64:A:LEU:HD12	1:24:A:ALA:H	4	2.48
(1,944)	1:64:A:LEU:HD13	1:24:A:ALA:H	4	2.48
(1,1739)	1:111:A:VAL:HG11	1:106:A:VAL:H	3	2.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1739)	1:111:A:VAL:HG12	1:106:A:VAL:H	3	2.47
(1,1739)	1:111:A:VAL:HG13	1:106:A:VAL:H	3	2.47
(1,518)	1:36:A:PHE:HB2	1:72:A:VAL:HG11	10	2.47
(1,518)	1:36:A:PHE:HB2	1:72:A:VAL:HG12	10	2.47
(1,518)	1:36:A:PHE:HB2	1:72:A:VAL:HG13	10	2.47
(1,1969)	1:124:A:HIS:HB2	1:104:A:LEU:HD11	6	2.45
(1,1969)	1:124:A:HIS:HB2	1:104:A:LEU:HD12	6	2.45
(1,1969)	1:124:A:HIS:HB2	1:104:A:LEU:HD13	6	2.45
(1,1082)	1:73:A:VAL:HG21	1:39:A:PHE:H	7	2.44
(1,1082)	1:73:A:VAL:HG22	1:39:A:PHE:H	7	2.44
(1,1082)	1:73:A:VAL:HG23	1:39:A:PHE:H	7	2.44
(1,958)	1:64:A:LEU:HD21	1:67:A:ILE:HB	1	2.44
(1,958)	1:64:A:LEU:HD22	1:67:A:ILE:HB	1	2.44
(1,958)	1:64:A:LEU:HD23	1:67:A:ILE:HB	1	2.44
(1,944)	1:64:A:LEU:HD11	1:24:A:ALA:H	2	2.44
(1,944)	1:64:A:LEU:HD12	1:24:A:ALA:H	2	2.44
(1,944)	1:64:A:LEU:HD13	1:24:A:ALA:H	2	2.44
(1,944)	1:64:A:LEU:HD11	1:24:A:ALA:H	5	2.44
(1,944)	1:64:A:LEU:HD12	1:24:A:ALA:H	5	2.44
(1,944)	1:64:A:LEU:HD13	1:24:A:ALA:H	5	2.44
(1,1969)	1:124:A:HIS:HB2	1:104:A:LEU:HD11	4	2.43
(1,1969)	1:124:A:HIS:HB2	1:104:A:LEU:HD12	4	2.43
(1,1969)	1:124:A:HIS:HB2	1:104:A:LEU:HD13	4	2.43
(1,1969)	1:124:A:HIS:HB2	1:104:A:LEU:HD11	1	2.41
(1,1969)	1:124:A:HIS:HB2	1:104:A:LEU:HD12	1	2.41
(1,1969)	1:124:A:HIS:HB2	1:104:A:LEU:HD13	1	2.41
(1,1969)	1:124:A:HIS:HB2	1:104:A:LEU:HD11	7	2.41
(1,1969)	1:124:A:HIS:HB2	1:104:A:LEU:HD12	7	2.41
(1,1969)	1:124:A:HIS:HB2	1:104:A:LEU:HD13	7	2.41
(1,1370)	1:88:A:VAL:HG11	1:96:A:ILE:HA	1	2.41
(1,1370)	1:88:A:VAL:HG12	1:96:A:ILE:HA	1	2.41
(1,1370)	1:88:A:VAL:HG13	1:96:A:ILE:HA	1	2.41
(1,1370)	1:88:A:VAL:HG11	1:96:A:ILE:HA	8	2.41
(1,1370)	1:88:A:VAL:HG12	1:96:A:ILE:HA	8	2.41
(1,1370)	1:88:A:VAL:HG13	1:96:A:ILE:HA	8	2.41
(1,944)	1:64:A:LEU:HD11	1:24:A:ALA:H	10	2.41
(1,944)	1:64:A:LEU:HD12	1:24:A:ALA:H	10	2.41
(1,944)	1:64:A:LEU:HD13	1:24:A:ALA:H	10	2.41
(1,1370)	1:88:A:VAL:HG11	1:96:A:ILE:HA	4	2.4
(1,1370)	1:88:A:VAL:HG12	1:96:A:ILE:HA	4	2.4
(1,1370)	1:88:A:VAL:HG13	1:96:A:ILE:HA	4	2.4
(1,1370)	1:88:A:VAL:HG11	1:96:A:ILE:HA	9	2.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1370)	1:88:A:VAL:HG12	1:96:A:ILE:HA	9	2.4
(1,1370)	1:88:A:VAL:HG13	1:96:A:ILE:HA	9	2.4
(1,1082)	1:73:A:VAL:HG21	1:39:A:PHE:H	10	2.4
(1,1082)	1:73:A:VAL:HG22	1:39:A:PHE:H	10	2.4
(1,1082)	1:73:A:VAL:HG23	1:39:A:PHE:H	10	2.4
(1,881)	1:59:A:GLN:HB3	1:60:A:ASN:HD21	3	2.4
(1,1370)	1:88:A:VAL:HG11	1:96:A:ILE:HA	7	2.39
(1,1370)	1:88:A:VAL:HG12	1:96:A:ILE:HA	7	2.39
(1,1370)	1:88:A:VAL:HG13	1:96:A:ILE:HA	7	2.39
(1,944)	1:64:A:LEU:HD11	1:24:A:ALA:H	3	2.39
(1,944)	1:64:A:LEU:HD12	1:24:A:ALA:H	3	2.39
(1,944)	1:64:A:LEU:HD13	1:24:A:ALA:H	3	2.39
(1,1370)	1:88:A:VAL:HG11	1:96:A:ILE:HA	10	2.38
(1,1370)	1:88:A:VAL:HG12	1:96:A:ILE:HA	10	2.38
(1,1370)	1:88:A:VAL:HG13	1:96:A:ILE:HA	10	2.38
(1,1082)	1:73:A:VAL:HG21	1:39:A:PHE:H	3	2.38
(1,1082)	1:73:A:VAL:HG22	1:39:A:PHE:H	3	2.38
(1,1082)	1:73:A:VAL:HG23	1:39:A:PHE:H	3	2.38
(1,1739)	1:111:A:VAL:HG11	1:106:A:VAL:H	2	2.37
(1,1739)	1:111:A:VAL:HG12	1:106:A:VAL:H	2	2.37
(1,1739)	1:111:A:VAL:HG13	1:106:A:VAL:H	2	2.37
(1,1023)	1:68:A:LEU:HD11	1:21:A:VAL:HA	10	2.37
(1,1023)	1:68:A:LEU:HD12	1:21:A:VAL:HA	10	2.37
(1,1023)	1:68:A:LEU:HD13	1:21:A:VAL:HA	10	2.37
(1,1370)	1:88:A:VAL:HG11	1:96:A:ILE:HA	6	2.36
(1,1370)	1:88:A:VAL:HG12	1:96:A:ILE:HA	6	2.36
(1,1370)	1:88:A:VAL:HG13	1:96:A:ILE:HA	6	2.36
(1,944)	1:64:A:LEU:HD11	1:24:A:ALA:H	9	2.36
(1,944)	1:64:A:LEU:HD12	1:24:A:ALA:H	9	2.36
(1,944)	1:64:A:LEU:HD13	1:24:A:ALA:H	9	2.36
(1,1739)	1:111:A:VAL:HG11	1:106:A:VAL:H	4	2.35
(1,1739)	1:111:A:VAL:HG12	1:106:A:VAL:H	4	2.35
(1,1739)	1:111:A:VAL:HG13	1:106:A:VAL:H	4	2.35
(1,1370)	1:88:A:VAL:HG11	1:96:A:ILE:HA	2	2.34
(1,1370)	1:88:A:VAL:HG12	1:96:A:ILE:HA	2	2.34
(1,1370)	1:88:A:VAL:HG13	1:96:A:ILE:HA	2	2.34
(1,1370)	1:88:A:VAL:HG11	1:96:A:ILE:HA	5	2.34
(1,1370)	1:88:A:VAL:HG12	1:96:A:ILE:HA	5	2.34
(1,1370)	1:88:A:VAL:HG13	1:96:A:ILE:HA	5	2.34
(1,1082)	1:73:A:VAL:HG21	1:39:A:PHE:H	4	2.31
(1,1082)	1:73:A:VAL:HG22	1:39:A:PHE:H	4	2.31
(1,1082)	1:73:A:VAL:HG23	1:39:A:PHE:H	4	2.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1370)	1:88:A:VAL:HG11	1:96:A:ILE:HA	3	2.29
(1,1370)	1:88:A:VAL:HG12	1:96:A:ILE:HA	3	2.29
(1,1370)	1:88:A:VAL:HG13	1:96:A:ILE:HA	3	2.29
(1,1985)	1:125:A:VAL:HG11	1:116:A:ILE:HD11	4	2.28
(1,1985)	1:125:A:VAL:HG11	1:116:A:ILE:HD12	4	2.28
(1,1985)	1:125:A:VAL:HG11	1:116:A:ILE:HD13	4	2.28
(1,1985)	1:125:A:VAL:HG12	1:116:A:ILE:HD11	4	2.28
(1,1985)	1:125:A:VAL:HG12	1:116:A:ILE:HD12	4	2.28
(1,1985)	1:125:A:VAL:HG12	1:116:A:ILE:HD13	4	2.28
(1,1985)	1:125:A:VAL:HG13	1:116:A:ILE:HD11	4	2.28
(1,1985)	1:125:A:VAL:HG13	1:116:A:ILE:HD12	4	2.28
(1,1985)	1:125:A:VAL:HG13	1:116:A:ILE:HD13	4	2.28
(1,518)	1:36:A:PHE:HB2	1:72:A:VAL:HG11	8	2.27
(1,518)	1:36:A:PHE:HB2	1:72:A:VAL:HG12	8	2.27
(1,518)	1:36:A:PHE:HB2	1:72:A:VAL:HG13	8	2.27
(1,1985)	1:125:A:VAL:HG11	1:116:A:ILE:HD11	10	2.26
(1,1985)	1:125:A:VAL:HG11	1:116:A:ILE:HD12	10	2.26
(1,1985)	1:125:A:VAL:HG11	1:116:A:ILE:HD13	10	2.26
(1,1985)	1:125:A:VAL:HG12	1:116:A:ILE:HD11	10	2.26
(1,1985)	1:125:A:VAL:HG12	1:116:A:ILE:HD12	10	2.26
(1,1985)	1:125:A:VAL:HG12	1:116:A:ILE:HD13	10	2.26
(1,1985)	1:125:A:VAL:HG13	1:116:A:ILE:HD11	10	2.26
(1,1985)	1:125:A:VAL:HG13	1:116:A:ILE:HD12	10	2.26
(1,1985)	1:125:A:VAL:HG13	1:116:A:ILE:HD13	10	2.26
(1,1739)	1:111:A:VAL:HG11	1:106:A:VAL:H	7	2.26
(1,1739)	1:111:A:VAL:HG12	1:106:A:VAL:H	7	2.26
(1,1739)	1:111:A:VAL:HG13	1:106:A:VAL:H	7	2.26
(1,1985)	1:125:A:VAL:HG11	1:116:A:ILE:HD11	8	2.25
(1,1985)	1:125:A:VAL:HG11	1:116:A:ILE:HD12	8	2.25
(1,1985)	1:125:A:VAL:HG11	1:116:A:ILE:HD13	8	2.25
(1,1985)	1:125:A:VAL:HG12	1:116:A:ILE:HD11	8	2.25
(1,1985)	1:125:A:VAL:HG12	1:116:A:ILE:HD12	8	2.25
(1,1985)	1:125:A:VAL:HG12	1:116:A:ILE:HD13	8	2.25
(1,1985)	1:125:A:VAL:HG13	1:116:A:ILE:HD11	8	2.25
(1,1985)	1:125:A:VAL:HG13	1:116:A:ILE:HD12	8	2.25
(1,1985)	1:125:A:VAL:HG13	1:116:A:ILE:HD13	8	2.25
(1,1985)	1:125:A:VAL:HG11	1:116:A:ILE:HD11	2	2.24
(1,1985)	1:125:A:VAL:HG11	1:116:A:ILE:HD12	2	2.24
(1,1985)	1:125:A:VAL:HG11	1:116:A:ILE:HD13	2	2.24
(1,1985)	1:125:A:VAL:HG12	1:116:A:ILE:HD11	2	2.24
(1,1985)	1:125:A:VAL:HG12	1:116:A:ILE:HD12	2	2.24
(1,1985)	1:125:A:VAL:HG12	1:116:A:ILE:HD13	2	2.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1985)	1:125:A:VAL:HG13	1:116:A:ILE:HD11	2	2.24
(1,1985)	1:125:A:VAL:HG13	1:116:A:ILE:HD12	2	2.24
(1,1985)	1:125:A:VAL:HG13	1:116:A:ILE:HD13	2	2.24
(1,1985)	1:125:A:VAL:HG11	1:116:A:ILE:HD11	3	2.22
(1,1985)	1:125:A:VAL:HG11	1:116:A:ILE:HD12	3	2.22
(1,1985)	1:125:A:VAL:HG11	1:116:A:ILE:HD13	3	2.22
(1,1985)	1:125:A:VAL:HG12	1:116:A:ILE:HD11	3	2.22
(1,1985)	1:125:A:VAL:HG12	1:116:A:ILE:HD12	3	2.22
(1,1985)	1:125:A:VAL:HG12	1:116:A:ILE:HD13	3	2.22
(1,1985)	1:125:A:VAL:HG13	1:116:A:ILE:HD11	3	2.22
(1,1985)	1:125:A:VAL:HG13	1:116:A:ILE:HD12	3	2.22
(1,1985)	1:125:A:VAL:HG13	1:116:A:ILE:HD13	3	2.22
(1,1739)	1:111:A:VAL:HG11	1:106:A:VAL:H	8	2.22
(1,1739)	1:111:A:VAL:HG12	1:106:A:VAL:H	8	2.22
(1,1739)	1:111:A:VAL:HG13	1:106:A:VAL:H	8	2.22
(1,1082)	1:73:A:VAL:HG21	1:39:A:PHE:H	8	2.22
(1,1082)	1:73:A:VAL:HG22	1:39:A:PHE:H	8	2.22
(1,1082)	1:73:A:VAL:HG23	1:39:A:PHE:H	8	2.22
(1,1082)	1:73:A:VAL:HG21	1:39:A:PHE:H	6	2.21
(1,1082)	1:73:A:VAL:HG22	1:39:A:PHE:H	6	2.21
(1,1082)	1:73:A:VAL:HG23	1:39:A:PHE:H	6	2.21
(1,1985)	1:125:A:VAL:HG11	1:116:A:ILE:HD11	1	2.2
(1,1985)	1:125:A:VAL:HG11	1:116:A:ILE:HD12	1	2.2
(1,1985)	1:125:A:VAL:HG11	1:116:A:ILE:HD13	1	2.2
(1,1985)	1:125:A:VAL:HG12	1:116:A:ILE:HD11	1	2.2
(1,1985)	1:125:A:VAL:HG12	1:116:A:ILE:HD12	1	2.2
(1,1985)	1:125:A:VAL:HG12	1:116:A:ILE:HD13	1	2.2
(1,1985)	1:125:A:VAL:HG13	1:116:A:ILE:HD11	1	2.2
(1,1985)	1:125:A:VAL:HG13	1:116:A:ILE:HD12	1	2.2
(1,1985)	1:125:A:VAL:HG13	1:116:A:ILE:HD13	1	2.2
(1,1739)	1:111:A:VAL:HG11	1:106:A:VAL:H	10	2.2
(1,1739)	1:111:A:VAL:HG12	1:106:A:VAL:H	10	2.2
(1,1739)	1:111:A:VAL:HG13	1:106:A:VAL:H	10	2.2
(1,1739)	1:111:A:VAL:HG11	1:106:A:VAL:H	5	2.19
(1,1739)	1:111:A:VAL:HG12	1:106:A:VAL:H	5	2.19
(1,1739)	1:111:A:VAL:HG13	1:106:A:VAL:H	5	2.19
(1,518)	1:36:A:PHE:HB2	1:72:A:VAL:HG11	4	2.18
(1,518)	1:36:A:PHE:HB2	1:72:A:VAL:HG12	4	2.18
(1,518)	1:36:A:PHE:HB2	1:72:A:VAL:HG13	4	2.18
(1,518)	1:36:A:PHE:HB2	1:72:A:VAL:HG11	1	2.17
(1,518)	1:36:A:PHE:HB2	1:72:A:VAL:HG12	1	2.17
(1,518)	1:36:A:PHE:HB2	1:72:A:VAL:HG13	1	2.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1985)	1:125:A:VAL:HG11	1:116:A:ILE:HD11	5	2.16
(1,1985)	1:125:A:VAL:HG11	1:116:A:ILE:HD12	5	2.16
(1,1985)	1:125:A:VAL:HG11	1:116:A:ILE:HD13	5	2.16
(1,1985)	1:125:A:VAL:HG12	1:116:A:ILE:HD11	5	2.16
(1,1985)	1:125:A:VAL:HG12	1:116:A:ILE:HD12	5	2.16
(1,1985)	1:125:A:VAL:HG12	1:116:A:ILE:HD13	5	2.16
(1,1985)	1:125:A:VAL:HG13	1:116:A:ILE:HD11	5	2.16
(1,1985)	1:125:A:VAL:HG13	1:116:A:ILE:HD12	5	2.16
(1,1985)	1:125:A:VAL:HG13	1:116:A:ILE:HD13	5	2.16
(1,1739)	1:111:A:VAL:HG11	1:106:A:VAL:H	6	2.16
(1,1739)	1:111:A:VAL:HG12	1:106:A:VAL:H	6	2.16
(1,1739)	1:111:A:VAL:HG13	1:106:A:VAL:H	6	2.16
(1,187)	1:18:A:VAL:HG21	1:15:A:SER:HB3	5	2.13
(1,187)	1:18:A:VAL:HG22	1:15:A:SER:HB3	5	2.13
(1,187)	1:18:A:VAL:HG23	1:15:A:SER:HB3	5	2.13
(1,1985)	1:125:A:VAL:HG11	1:116:A:ILE:HD11	9	2.11
(1,1985)	1:125:A:VAL:HG11	1:116:A:ILE:HD12	9	2.11
(1,1985)	1:125:A:VAL:HG11	1:116:A:ILE:HD13	9	2.11
(1,1985)	1:125:A:VAL:HG12	1:116:A:ILE:HD11	9	2.11
(1,1985)	1:125:A:VAL:HG12	1:116:A:ILE:HD12	9	2.11
(1,1985)	1:125:A:VAL:HG12	1:116:A:ILE:HD13	9	2.11
(1,1985)	1:125:A:VAL:HG13	1:116:A:ILE:HD11	9	2.11
(1,1985)	1:125:A:VAL:HG13	1:116:A:ILE:HD12	9	2.11
(1,1985)	1:125:A:VAL:HG13	1:116:A:ILE:HD13	9	2.11
(1,1739)	1:111:A:VAL:HG11	1:106:A:VAL:H	1	2.11
(1,1739)	1:111:A:VAL:HG12	1:106:A:VAL:H	1	2.11
(1,1739)	1:111:A:VAL:HG13	1:106:A:VAL:H	1	2.11
(1,1739)	1:111:A:VAL:HG11	1:106:A:VAL:H	9	2.11
(1,1739)	1:111:A:VAL:HG12	1:106:A:VAL:H	9	2.11
(1,1739)	1:111:A:VAL:HG13	1:106:A:VAL:H	9	2.11
(1,518)	1:36:A:PHE:HB2	1:72:A:VAL:HG11	3	2.11
(1,518)	1:36:A:PHE:HB2	1:72:A:VAL:HG12	3	2.11
(1,518)	1:36:A:PHE:HB2	1:72:A:VAL:HG13	3	2.11
(1,1985)	1:125:A:VAL:HG11	1:116:A:ILE:HD11	6	2.08
(1,1985)	1:125:A:VAL:HG11	1:116:A:ILE:HD12	6	2.08
(1,1985)	1:125:A:VAL:HG11	1:116:A:ILE:HD13	6	2.08
(1,1985)	1:125:A:VAL:HG12	1:116:A:ILE:HD11	6	2.08
(1,1985)	1:125:A:VAL:HG12	1:116:A:ILE:HD12	6	2.08
(1,1985)	1:125:A:VAL:HG12	1:116:A:ILE:HD13	6	2.08
(1,1985)	1:125:A:VAL:HG13	1:116:A:ILE:HD11	6	2.08
(1,1985)	1:125:A:VAL:HG13	1:116:A:ILE:HD12	6	2.08
(1,1985)	1:125:A:VAL:HG13	1:116:A:ILE:HD13	6	2.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1985)	1:125:A:VAL:HG11	1:116:A:ILE:HD11	7	2.08
(1,1985)	1:125:A:VAL:HG11	1:116:A:ILE:HD12	7	2.08
(1,1985)	1:125:A:VAL:HG11	1:116:A:ILE:HD13	7	2.08
(1,1985)	1:125:A:VAL:HG12	1:116:A:ILE:HD11	7	2.08
(1,1985)	1:125:A:VAL:HG12	1:116:A:ILE:HD12	7	2.08
(1,1985)	1:125:A:VAL:HG12	1:116:A:ILE:HD13	7	2.08
(1,1985)	1:125:A:VAL:HG13	1:116:A:ILE:HD11	7	2.08
(1,1985)	1:125:A:VAL:HG13	1:116:A:ILE:HD12	7	2.08
(1,1985)	1:125:A:VAL:HG13	1:116:A:ILE:HD13	7	2.08
(1,432)	1:30:A:LEU:HD21	1:91:A:LEU:HD11	2	2.07
(1,432)	1:30:A:LEU:HD21	1:91:A:LEU:HD12	2	2.07
(1,432)	1:30:A:LEU:HD21	1:91:A:LEU:HD13	2	2.07
(1,432)	1:30:A:LEU:HD22	1:91:A:LEU:HD11	2	2.07
(1,432)	1:30:A:LEU:HD22	1:91:A:LEU:HD12	2	2.07
(1,432)	1:30:A:LEU:HD22	1:91:A:LEU:HD13	2	2.07
(1,432)	1:30:A:LEU:HD23	1:91:A:LEU:HD11	2	2.07
(1,432)	1:30:A:LEU:HD23	1:91:A:LEU:HD12	2	2.07
(1,432)	1:30:A:LEU:HD23	1:91:A:LEU:HD13	2	2.07
(1,1077)	1:72:A:VAL:HA	1:73:A:VAL:HG21	3	2.06
(1,1077)	1:72:A:VAL:HA	1:73:A:VAL:HG22	3	2.06
(1,1077)	1:72:A:VAL:HA	1:73:A:VAL:HG23	3	2.06
(1,187)	1:18:A:VAL:HG21	1:15:A:SER:HB3	1	2.06
(1,187)	1:18:A:VAL:HG22	1:15:A:SER:HB3	1	2.06
(1,187)	1:18:A:VAL:HG23	1:15:A:SER:HB3	1	2.06
(1,1082)	1:73:A:VAL:HG21	1:39:A:PHE:H	1	2.05
(1,1082)	1:73:A:VAL:HG22	1:39:A:PHE:H	1	2.05
(1,1082)	1:73:A:VAL:HG23	1:39:A:PHE:H	1	2.05
(1,1077)	1:72:A:VAL:HA	1:73:A:VAL:HG21	1	2.05
(1,1077)	1:72:A:VAL:HA	1:73:A:VAL:HG22	1	2.05
(1,1077)	1:72:A:VAL:HA	1:73:A:VAL:HG23	1	2.05
(1,1077)	1:72:A:VAL:HA	1:73:A:VAL:HG21	5	2.05
(1,1077)	1:72:A:VAL:HA	1:73:A:VAL:HG22	5	2.05
(1,1077)	1:72:A:VAL:HA	1:73:A:VAL:HG23	5	2.05
(1,1077)	1:72:A:VAL:HA	1:73:A:VAL:HG21	10	2.05
(1,1077)	1:72:A:VAL:HA	1:73:A:VAL:HG22	10	2.05
(1,1077)	1:72:A:VAL:HA	1:73:A:VAL:HG23	10	2.05
(1,915)	1:62:A:PRO:HB3	1:92:A:GLU:HB3	9	2.05
(1,187)	1:18:A:VAL:HG21	1:15:A:SER:HB3	4	2.05
(1,187)	1:18:A:VAL:HG22	1:15:A:SER:HB3	4	2.05
(1,187)	1:18:A:VAL:HG23	1:15:A:SER:HB3	4	2.05
(1,1077)	1:72:A:VAL:HA	1:73:A:VAL:HG21	4	2.04
(1,1077)	1:72:A:VAL:HA	1:73:A:VAL:HG22	4	2.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1077)	1:72:A:VAL:HA	1:73:A:VAL:HG23	4	2.04
(1,1077)	1:72:A:VAL:HA	1:73:A:VAL:HG21	7	2.04
(1,1077)	1:72:A:VAL:HA	1:73:A:VAL:HG22	7	2.04
(1,1077)	1:72:A:VAL:HA	1:73:A:VAL:HG23	7	2.04
(1,1077)	1:72:A:VAL:HA	1:73:A:VAL:HG21	9	2.04
(1,1077)	1:72:A:VAL:HA	1:73:A:VAL:HG22	9	2.04
(1,1077)	1:72:A:VAL:HA	1:73:A:VAL:HG23	9	2.04
(1,915)	1:62:A:PRO:HB3	1:92:A:GLU:HB3	8	2.04
(1,518)	1:36:A:PHE:HB2	1:72:A:VAL:HG11	2	2.04
(1,518)	1:36:A:PHE:HB2	1:72:A:VAL:HG12	2	2.04
(1,518)	1:36:A:PHE:HB2	1:72:A:VAL:HG13	2	2.04
(1,432)	1:30:A:LEU:HD21	1:91:A:LEU:HD11	3	2.04
(1,432)	1:30:A:LEU:HD21	1:91:A:LEU:HD12	3	2.04
(1,432)	1:30:A:LEU:HD21	1:91:A:LEU:HD13	3	2.04
(1,432)	1:30:A:LEU:HD22	1:91:A:LEU:HD11	3	2.04
(1,432)	1:30:A:LEU:HD22	1:91:A:LEU:HD12	3	2.04
(1,432)	1:30:A:LEU:HD22	1:91:A:LEU:HD13	3	2.04
(1,432)	1:30:A:LEU:HD23	1:91:A:LEU:HD11	3	2.04
(1,432)	1:30:A:LEU:HD23	1:91:A:LEU:HD12	3	2.04
(1,432)	1:30:A:LEU:HD23	1:91:A:LEU:HD13	3	2.04
(1,187)	1:18:A:VAL:HG21	1:15:A:SER:HB3	8	2.04
(1,187)	1:18:A:VAL:HG22	1:15:A:SER:HB3	8	2.04
(1,187)	1:18:A:VAL:HG23	1:15:A:SER:HB3	8	2.04
(1,187)	1:18:A:VAL:HG21	1:15:A:SER:HB3	10	2.04
(1,187)	1:18:A:VAL:HG22	1:15:A:SER:HB3	10	2.04
(1,187)	1:18:A:VAL:HG23	1:15:A:SER:HB3	10	2.04
(1,1077)	1:72:A:VAL:HA	1:73:A:VAL:HG21	8	2.03
(1,1077)	1:72:A:VAL:HA	1:73:A:VAL:HG22	8	2.03
(1,1077)	1:72:A:VAL:HA	1:73:A:VAL:HG23	8	2.03
(1,432)	1:30:A:LEU:HD21	1:91:A:LEU:HD11	5	2.03
(1,432)	1:30:A:LEU:HD21	1:91:A:LEU:HD12	5	2.03
(1,432)	1:30:A:LEU:HD21	1:91:A:LEU:HD13	5	2.03
(1,432)	1:30:A:LEU:HD22	1:91:A:LEU:HD11	5	2.03
(1,432)	1:30:A:LEU:HD22	1:91:A:LEU:HD12	5	2.03
(1,432)	1:30:A:LEU:HD22	1:91:A:LEU:HD13	5	2.03
(1,432)	1:30:A:LEU:HD23	1:91:A:LEU:HD11	5	2.03
(1,432)	1:30:A:LEU:HD23	1:91:A:LEU:HD12	5	2.03
(1,432)	1:30:A:LEU:HD23	1:91:A:LEU:HD13	5	2.03
(1,187)	1:18:A:VAL:HG21	1:15:A:SER:HB3	9	2.03
(1,187)	1:18:A:VAL:HG22	1:15:A:SER:HB3	9	2.03
(1,187)	1:18:A:VAL:HG23	1:15:A:SER:HB3	9	2.03
(1,1077)	1:72:A:VAL:HA	1:73:A:VAL:HG21	2	2.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1077)	1:72:A:VAL:HA	1:73:A:VAL:HG22	2	2.02
(1,1077)	1:72:A:VAL:HA	1:73:A:VAL:HG23	2	2.02
(1,432)	1:30:A:LEU:HD21	1:91:A:LEU:HD11	6	2.02
(1,432)	1:30:A:LEU:HD21	1:91:A:LEU:HD12	6	2.02
(1,432)	1:30:A:LEU:HD21	1:91:A:LEU:HD13	6	2.02
(1,432)	1:30:A:LEU:HD22	1:91:A:LEU:HD11	6	2.02
(1,432)	1:30:A:LEU:HD22	1:91:A:LEU:HD12	6	2.02
(1,432)	1:30:A:LEU:HD22	1:91:A:LEU:HD13	6	2.02
(1,432)	1:30:A:LEU:HD23	1:91:A:LEU:HD11	6	2.02
(1,432)	1:30:A:LEU:HD23	1:91:A:LEU:HD12	6	2.02
(1,432)	1:30:A:LEU:HD23	1:91:A:LEU:HD13	6	2.02
(1,430)	1:30:A:LEU:HD21	1:72:A:VAL:HG21	3	2.02
(1,430)	1:30:A:LEU:HD21	1:72:A:VAL:HG22	3	2.02
(1,430)	1:30:A:LEU:HD21	1:72:A:VAL:HG23	3	2.02
(1,430)	1:30:A:LEU:HD22	1:72:A:VAL:HG21	3	2.02
(1,430)	1:30:A:LEU:HD22	1:72:A:VAL:HG22	3	2.02
(1,430)	1:30:A:LEU:HD22	1:72:A:VAL:HG23	3	2.02
(1,430)	1:30:A:LEU:HD23	1:72:A:VAL:HG21	3	2.02
(1,430)	1:30:A:LEU:HD23	1:72:A:VAL:HG22	3	2.02
(1,430)	1:30:A:LEU:HD23	1:72:A:VAL:HG23	3	2.02
(1,187)	1:18:A:VAL:HG21	1:15:A:SER:HB3	3	2.02
(1,187)	1:18:A:VAL:HG22	1:15:A:SER:HB3	3	2.02
(1,187)	1:18:A:VAL:HG23	1:15:A:SER:HB3	3	2.02
(1,187)	1:18:A:VAL:HG21	1:15:A:SER:HB3	6	2.02
(1,187)	1:18:A:VAL:HG22	1:15:A:SER:HB3	6	2.02
(1,187)	1:18:A:VAL:HG23	1:15:A:SER:HB3	6	2.02
(1,187)	1:18:A:VAL:HG21	1:15:A:SER:HB3	7	2.02
(1,187)	1:18:A:VAL:HG22	1:15:A:SER:HB3	7	2.02
(1,187)	1:18:A:VAL:HG23	1:15:A:SER:HB3	7	2.02
(1,1077)	1:72:A:VAL:HA	1:73:A:VAL:HG21	6	2.0
(1,1077)	1:72:A:VAL:HA	1:73:A:VAL:HG22	6	2.0
(1,1077)	1:72:A:VAL:HA	1:73:A:VAL:HG23	6	2.0
(1,187)	1:18:A:VAL:HG21	1:15:A:SER:HB3	2	2.0
(1,187)	1:18:A:VAL:HG22	1:15:A:SER:HB3	2	2.0
(1,187)	1:18:A:VAL:HG23	1:15:A:SER:HB3	2	2.0
(1,430)	1:30:A:LEU:HD21	1:72:A:VAL:HG21	4	1.99
(1,430)	1:30:A:LEU:HD21	1:72:A:VAL:HG22	4	1.99
(1,430)	1:30:A:LEU:HD21	1:72:A:VAL:HG23	4	1.99
(1,430)	1:30:A:LEU:HD22	1:72:A:VAL:HG21	4	1.99
(1,430)	1:30:A:LEU:HD22	1:72:A:VAL:HG22	4	1.99
(1,430)	1:30:A:LEU:HD22	1:72:A:VAL:HG23	4	1.99
(1,430)	1:30:A:LEU:HD23	1:72:A:VAL:HG21	4	1.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,430)	1:30:A:LEU:HD23	1:72:A:VAL:HG22	4	1.99
(1,430)	1:30:A:LEU:HD23	1:72:A:VAL:HG23	4	1.99
(1,205)	1:18:A:VAL:HG11	1:22:A:LYS:HE2	9	1.99
(1,205)	1:18:A:VAL:HG12	1:22:A:LYS:HE2	9	1.99
(1,205)	1:18:A:VAL:HG13	1:22:A:LYS:HE2	9	1.99
(1,1235)	1:82:A:LEU:HA	1:88:A:VAL:HG21	6	1.98
(1,1235)	1:82:A:LEU:HA	1:88:A:VAL:HG22	6	1.98
(1,1235)	1:82:A:LEU:HA	1:88:A:VAL:HG23	6	1.98
(1,1235)	1:82:A:LEU:HA	1:88:A:VAL:HG21	7	1.98
(1,1235)	1:82:A:LEU:HA	1:88:A:VAL:HG22	7	1.98
(1,1235)	1:82:A:LEU:HA	1:88:A:VAL:HG23	7	1.98
(1,432)	1:30:A:LEU:HD21	1:91:A:LEU:HD11	4	1.98
(1,432)	1:30:A:LEU:HD21	1:91:A:LEU:HD12	4	1.98
(1,432)	1:30:A:LEU:HD21	1:91:A:LEU:HD13	4	1.98
(1,432)	1:30:A:LEU:HD22	1:91:A:LEU:HD11	4	1.98
(1,432)	1:30:A:LEU:HD22	1:91:A:LEU:HD12	4	1.98
(1,432)	1:30:A:LEU:HD22	1:91:A:LEU:HD13	4	1.98
(1,432)	1:30:A:LEU:HD23	1:91:A:LEU:HD11	4	1.98
(1,432)	1:30:A:LEU:HD23	1:91:A:LEU:HD12	4	1.98
(1,432)	1:30:A:LEU:HD23	1:91:A:LEU:HD13	4	1.98
(1,432)	1:30:A:LEU:HD21	1:91:A:LEU:HD11	10	1.98
(1,432)	1:30:A:LEU:HD21	1:91:A:LEU:HD12	10	1.98
(1,432)	1:30:A:LEU:HD21	1:91:A:LEU:HD13	10	1.98
(1,432)	1:30:A:LEU:HD22	1:91:A:LEU:HD11	10	1.98
(1,432)	1:30:A:LEU:HD22	1:91:A:LEU:HD12	10	1.98
(1,432)	1:30:A:LEU:HD22	1:91:A:LEU:HD13	10	1.98
(1,432)	1:30:A:LEU:HD23	1:91:A:LEU:HD11	10	1.98
(1,432)	1:30:A:LEU:HD23	1:91:A:LEU:HD12	10	1.98
(1,432)	1:30:A:LEU:HD23	1:91:A:LEU:HD13	10	1.98
(1,1028)	1:68:A:LEU:HD11	1:65:A:GLY:HA3	6	1.97
(1,1028)	1:68:A:LEU:HD12	1:65:A:GLY:HA3	6	1.97
(1,1028)	1:68:A:LEU:HD13	1:65:A:GLY:HA3	6	1.97
(1,1768)	1:112:A:LEU:HD11	1:125:A:VAL:HG21	8	1.96
(1,1768)	1:112:A:LEU:HD11	1:125:A:VAL:HG22	8	1.96
(1,1768)	1:112:A:LEU:HD11	1:125:A:VAL:HG23	8	1.96
(1,1768)	1:112:A:LEU:HD12	1:125:A:VAL:HG21	8	1.96
(1,1768)	1:112:A:LEU:HD12	1:125:A:VAL:HG22	8	1.96
(1,1768)	1:112:A:LEU:HD12	1:125:A:VAL:HG23	8	1.96
(1,1768)	1:112:A:LEU:HD13	1:125:A:VAL:HG21	8	1.96
(1,1768)	1:112:A:LEU:HD13	1:125:A:VAL:HG22	8	1.96
(1,1768)	1:112:A:LEU:HD13	1:125:A:VAL:HG23	8	1.96
(1,1768)	1:112:A:LEU:HD11	1:125:A:VAL:HG21	9	1.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1768)	1:112:A:LEU:HD11	1:125:A:VAL:HG22	9	1.96
(1,1768)	1:112:A:LEU:HD11	1:125:A:VAL:HG23	9	1.96
(1,1768)	1:112:A:LEU:HD12	1:125:A:VAL:HG21	9	1.96
(1,1768)	1:112:A:LEU:HD12	1:125:A:VAL:HG22	9	1.96
(1,1768)	1:112:A:LEU:HD12	1:125:A:VAL:HG23	9	1.96
(1,1768)	1:112:A:LEU:HD13	1:125:A:VAL:HG21	9	1.96
(1,1768)	1:112:A:LEU:HD13	1:125:A:VAL:HG22	9	1.96
(1,1768)	1:112:A:LEU:HD13	1:125:A:VAL:HG23	9	1.96
(1,1768)	1:112:A:LEU:HD11	1:125:A:VAL:HG21	10	1.96
(1,1768)	1:112:A:LEU:HD11	1:125:A:VAL:HG22	10	1.96
(1,1768)	1:112:A:LEU:HD11	1:125:A:VAL:HG23	10	1.96
(1,1768)	1:112:A:LEU:HD12	1:125:A:VAL:HG21	10	1.96
(1,1768)	1:112:A:LEU:HD12	1:125:A:VAL:HG22	10	1.96
(1,1768)	1:112:A:LEU:HD12	1:125:A:VAL:HG23	10	1.96
(1,1768)	1:112:A:LEU:HD13	1:125:A:VAL:HG21	10	1.96
(1,1768)	1:112:A:LEU:HD13	1:125:A:VAL:HG22	10	1.96
(1,1768)	1:112:A:LEU:HD13	1:125:A:VAL:HG23	10	1.96
(1,1028)	1:68:A:LEU:HD11	1:65:A:GLY:HA3	9	1.96
(1,1028)	1:68:A:LEU:HD12	1:65:A:GLY:HA3	9	1.96
(1,1028)	1:68:A:LEU:HD13	1:65:A:GLY:HA3	9	1.96
(1,432)	1:30:A:LEU:HD21	1:91:A:LEU:HD11	1	1.96
(1,432)	1:30:A:LEU:HD21	1:91:A:LEU:HD12	1	1.96
(1,432)	1:30:A:LEU:HD21	1:91:A:LEU:HD13	1	1.96
(1,432)	1:30:A:LEU:HD22	1:91:A:LEU:HD11	1	1.96
(1,432)	1:30:A:LEU:HD22	1:91:A:LEU:HD12	1	1.96
(1,432)	1:30:A:LEU:HD22	1:91:A:LEU:HD13	1	1.96
(1,432)	1:30:A:LEU:HD23	1:91:A:LEU:HD11	1	1.96
(1,432)	1:30:A:LEU:HD23	1:91:A:LEU:HD12	1	1.96
(1,432)	1:30:A:LEU:HD23	1:91:A:LEU:HD13	1	1.96
(1,205)	1:18:A:VAL:HG11	1:22:A:LYS:HE2	7	1.95
(1,205)	1:18:A:VAL:HG12	1:22:A:LYS:HE2	7	1.95
(1,205)	1:18:A:VAL:HG13	1:22:A:LYS:HE2	7	1.95
(1,1235)	1:82:A:LEU:HA	1:88:A:VAL:HG21	9	1.94
(1,1235)	1:82:A:LEU:HA	1:88:A:VAL:HG22	9	1.94
(1,1235)	1:82:A:LEU:HA	1:88:A:VAL:HG23	9	1.94
(1,432)	1:30:A:LEU:HD21	1:91:A:LEU:HD11	8	1.94
(1,432)	1:30:A:LEU:HD21	1:91:A:LEU:HD12	8	1.94
(1,432)	1:30:A:LEU:HD21	1:91:A:LEU:HD13	8	1.94
(1,432)	1:30:A:LEU:HD22	1:91:A:LEU:HD11	8	1.94
(1,432)	1:30:A:LEU:HD22	1:91:A:LEU:HD12	8	1.94
(1,432)	1:30:A:LEU:HD22	1:91:A:LEU:HD13	8	1.94
(1,432)	1:30:A:LEU:HD23	1:91:A:LEU:HD11	8	1.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,432)	1:30:A:LEU:HD23	1:91:A:LEU:HD12	8	1.94
(1,432)	1:30:A:LEU:HD23	1:91:A:LEU:HD13	8	1.94
(1,1491)	1:96:A:ILE:HB	1:88:A:VAL:HG11	7	1.93
(1,1491)	1:96:A:ILE:HB	1:88:A:VAL:HG12	7	1.93
(1,1491)	1:96:A:ILE:HB	1:88:A:VAL:HG13	7	1.93
(1,1491)	1:96:A:ILE:HB	1:88:A:VAL:HG11	10	1.93
(1,1491)	1:96:A:ILE:HB	1:88:A:VAL:HG12	10	1.93
(1,1491)	1:96:A:ILE:HB	1:88:A:VAL:HG13	10	1.93
(1,1028)	1:68:A:LEU:HD11	1:65:A:GLY:HA3	3	1.93
(1,1028)	1:68:A:LEU:HD12	1:65:A:GLY:HA3	3	1.93
(1,1028)	1:68:A:LEU:HD13	1:65:A:GLY:HA3	3	1.93
(1,543)	1:37:A:THR:H	1:72:A:VAL:HG11	2	1.93
(1,543)	1:37:A:THR:H	1:72:A:VAL:HG12	2	1.93
(1,543)	1:37:A:THR:H	1:72:A:VAL:HG13	2	1.93
(1,1647)	1:106:A:VAL:HG11	1:104:A:LEU:HD11	5	1.92
(1,1647)	1:106:A:VAL:HG11	1:104:A:LEU:HD12	5	1.92
(1,1647)	1:106:A:VAL:HG11	1:104:A:LEU:HD13	5	1.92
(1,1647)	1:106:A:VAL:HG12	1:104:A:LEU:HD11	5	1.92
(1,1647)	1:106:A:VAL:HG12	1:104:A:LEU:HD12	5	1.92
(1,1647)	1:106:A:VAL:HG12	1:104:A:LEU:HD13	5	1.92
(1,1647)	1:106:A:VAL:HG13	1:104:A:LEU:HD11	5	1.92
(1,1647)	1:106:A:VAL:HG13	1:104:A:LEU:HD12	5	1.92
(1,1647)	1:106:A:VAL:HG13	1:104:A:LEU:HD13	5	1.92
(1,915)	1:62:A:PRO:HB3	1:92:A:GLU:HB3	6	1.92
(1,1768)	1:112:A:LEU:HD11	1:125:A:VAL:HG21	2	1.91
(1,1768)	1:112:A:LEU:HD11	1:125:A:VAL:HG22	2	1.91
(1,1768)	1:112:A:LEU:HD11	1:125:A:VAL:HG23	2	1.91
(1,1768)	1:112:A:LEU:HD12	1:125:A:VAL:HG21	2	1.91
(1,1768)	1:112:A:LEU:HD12	1:125:A:VAL:HG22	2	1.91
(1,1768)	1:112:A:LEU:HD12	1:125:A:VAL:HG23	2	1.91
(1,1768)	1:112:A:LEU:HD13	1:125:A:VAL:HG21	2	1.91
(1,1768)	1:112:A:LEU:HD13	1:125:A:VAL:HG22	2	1.91
(1,1768)	1:112:A:LEU:HD13	1:125:A:VAL:HG23	2	1.91
(1,1491)	1:96:A:ILE:HB	1:88:A:VAL:HG11	8	1.91
(1,1491)	1:96:A:ILE:HB	1:88:A:VAL:HG12	8	1.91
(1,1491)	1:96:A:ILE:HB	1:88:A:VAL:HG13	8	1.91
(1,1235)	1:82:A:LEU:HA	1:88:A:VAL:HG21	2	1.91
(1,1235)	1:82:A:LEU:HA	1:88:A:VAL:HG22	2	1.91
(1,1235)	1:82:A:LEU:HA	1:88:A:VAL:HG23	2	1.91
(1,1028)	1:68:A:LEU:HD11	1:65:A:GLY:HA3	2	1.91
(1,1028)	1:68:A:LEU:HD12	1:65:A:GLY:HA3	2	1.91
(1,1028)	1:68:A:LEU:HD13	1:65:A:GLY:HA3	2	1.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,430)	1:30:A:LEU:HD21	1:72:A:VAL:HG21	5	1.9
(1,430)	1:30:A:LEU:HD21	1:72:A:VAL:HG22	5	1.9
(1,430)	1:30:A:LEU:HD21	1:72:A:VAL:HG23	5	1.9
(1,430)	1:30:A:LEU:HD22	1:72:A:VAL:HG21	5	1.9
(1,430)	1:30:A:LEU:HD22	1:72:A:VAL:HG22	5	1.9
(1,430)	1:30:A:LEU:HD22	1:72:A:VAL:HG23	5	1.9
(1,430)	1:30:A:LEU:HD23	1:72:A:VAL:HG21	5	1.9
(1,430)	1:30:A:LEU:HD23	1:72:A:VAL:HG22	5	1.9
(1,430)	1:30:A:LEU:HD23	1:72:A:VAL:HG23	5	1.9
(1,1769)	1:112:A:LEU:HB2	1:125:A:VAL:HG21	8	1.89
(1,1769)	1:112:A:LEU:HB2	1:125:A:VAL:HG22	8	1.89
(1,1769)	1:112:A:LEU:HB2	1:125:A:VAL:HG23	8	1.89
(1,1491)	1:96:A:ILE:HB	1:88:A:VAL:HG11	9	1.89
(1,1491)	1:96:A:ILE:HB	1:88:A:VAL:HG12	9	1.89
(1,1491)	1:96:A:ILE:HB	1:88:A:VAL:HG13	9	1.89
(1,1028)	1:68:A:LEU:HD11	1:65:A:GLY:HA3	7	1.89
(1,1028)	1:68:A:LEU:HD12	1:65:A:GLY:HA3	7	1.89
(1,1028)	1:68:A:LEU:HD13	1:65:A:GLY:HA3	7	1.89
(1,915)	1:62:A:PRO:HB3	1:92:A:GLU:HB3	1	1.89
(1,432)	1:30:A:LEU:HD21	1:91:A:LEU:HD11	9	1.88
(1,432)	1:30:A:LEU:HD21	1:91:A:LEU:HD12	9	1.88
(1,432)	1:30:A:LEU:HD21	1:91:A:LEU:HD13	9	1.88
(1,432)	1:30:A:LEU:HD22	1:91:A:LEU:HD11	9	1.88
(1,432)	1:30:A:LEU:HD22	1:91:A:LEU:HD12	9	1.88
(1,432)	1:30:A:LEU:HD22	1:91:A:LEU:HD13	9	1.88
(1,432)	1:30:A:LEU:HD23	1:91:A:LEU:HD11	9	1.88
(1,432)	1:30:A:LEU:HD23	1:91:A:LEU:HD12	9	1.88
(1,432)	1:30:A:LEU:HD23	1:91:A:LEU:HD13	9	1.88
(1,205)	1:18:A:VAL:HG11	1:22:A:LYS:HE2	6	1.88
(1,205)	1:18:A:VAL:HG12	1:22:A:LYS:HE2	6	1.88
(1,205)	1:18:A:VAL:HG13	1:22:A:LYS:HE2	6	1.88
(1,1980)	1:124:A:HIS:HA	1:125:A:VAL:HG11	10	1.87
(1,1980)	1:124:A:HIS:HA	1:125:A:VAL:HG12	10	1.87
(1,1980)	1:124:A:HIS:HA	1:125:A:VAL:HG13	10	1.87
(1,1769)	1:112:A:LEU:HB2	1:125:A:VAL:HG21	9	1.87
(1,1769)	1:112:A:LEU:HB2	1:125:A:VAL:HG22	9	1.87
(1,1769)	1:112:A:LEU:HB2	1:125:A:VAL:HG23	9	1.87
(1,1491)	1:96:A:ILE:HB	1:88:A:VAL:HG11	2	1.87
(1,1491)	1:96:A:ILE:HB	1:88:A:VAL:HG12	2	1.87
(1,1491)	1:96:A:ILE:HB	1:88:A:VAL:HG13	2	1.87
(1,1235)	1:82:A:LEU:HA	1:88:A:VAL:HG21	4	1.87
(1,1235)	1:82:A:LEU:HA	1:88:A:VAL:HG22	4	1.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1235)	1:82:A:LEU:HA	1:88:A:VAL:HG23	4	1.87
(1,1028)	1:68:A:LEU:HD11	1:65:A:GLY:HA3	5	1.87
(1,1028)	1:68:A:LEU:HD12	1:65:A:GLY:HA3	5	1.87
(1,1028)	1:68:A:LEU:HD13	1:65:A:GLY:HA3	5	1.87
(1,1028)	1:68:A:LEU:HD11	1:65:A:GLY:HA3	8	1.87
(1,1028)	1:68:A:LEU:HD12	1:65:A:GLY:HA3	8	1.87
(1,1028)	1:68:A:LEU:HD13	1:65:A:GLY:HA3	8	1.87
(1,915)	1:62:A:PRO:HB3	1:92:A:GLU:HB3	7	1.87
(1,430)	1:30:A:LEU:HD21	1:72:A:VAL:HG21	10	1.87
(1,430)	1:30:A:LEU:HD21	1:72:A:VAL:HG22	10	1.87
(1,430)	1:30:A:LEU:HD21	1:72:A:VAL:HG23	10	1.87
(1,430)	1:30:A:LEU:HD22	1:72:A:VAL:HG21	10	1.87
(1,430)	1:30:A:LEU:HD22	1:72:A:VAL:HG22	10	1.87
(1,430)	1:30:A:LEU:HD22	1:72:A:VAL:HG23	10	1.87
(1,430)	1:30:A:LEU:HD23	1:72:A:VAL:HG21	10	1.87
(1,430)	1:30:A:LEU:HD23	1:72:A:VAL:HG22	10	1.87
(1,430)	1:30:A:LEU:HD23	1:72:A:VAL:HG23	10	1.87
(1,1980)	1:124:A:HIS:HA	1:125:A:VAL:HG11	2	1.86
(1,1980)	1:124:A:HIS:HA	1:125:A:VAL:HG12	2	1.86
(1,1980)	1:124:A:HIS:HA	1:125:A:VAL:HG13	2	1.86
(1,1980)	1:124:A:HIS:HA	1:125:A:VAL:HG11	8	1.86
(1,1980)	1:124:A:HIS:HA	1:125:A:VAL:HG12	8	1.86
(1,1980)	1:124:A:HIS:HA	1:125:A:VAL:HG13	8	1.86
(1,1980)	1:124:A:HIS:HA	1:125:A:VAL:HG11	9	1.86
(1,1980)	1:124:A:HIS:HA	1:125:A:VAL:HG12	9	1.86
(1,1980)	1:124:A:HIS:HA	1:125:A:VAL:HG13	9	1.86
(1,1455)	1:92:A:GLU:HG2	1:94:A:SER:HB2	4	1.86
(1,915)	1:62:A:PRO:HB3	1:92:A:GLU:HB3	3	1.86
(1,432)	1:30:A:LEU:HD21	1:91:A:LEU:HD11	7	1.86
(1,432)	1:30:A:LEU:HD21	1:91:A:LEU:HD12	7	1.86
(1,432)	1:30:A:LEU:HD21	1:91:A:LEU:HD13	7	1.86
(1,432)	1:30:A:LEU:HD22	1:91:A:LEU:HD11	7	1.86
(1,432)	1:30:A:LEU:HD22	1:91:A:LEU:HD12	7	1.86
(1,432)	1:30:A:LEU:HD22	1:91:A:LEU:HD13	7	1.86
(1,432)	1:30:A:LEU:HD23	1:91:A:LEU:HD11	7	1.86
(1,432)	1:30:A:LEU:HD23	1:91:A:LEU:HD12	7	1.86
(1,432)	1:30:A:LEU:HD23	1:91:A:LEU:HD13	7	1.86
(1,205)	1:18:A:VAL:HG11	1:22:A:LYS:HE2	1	1.86
(1,205)	1:18:A:VAL:HG12	1:22:A:LYS:HE2	1	1.86
(1,205)	1:18:A:VAL:HG13	1:22:A:LYS:HE2	1	1.86
(1,1980)	1:124:A:HIS:HA	1:125:A:VAL:HG11	3	1.85
(1,1980)	1:124:A:HIS:HA	1:125:A:VAL:HG12	3	1.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1980)	1:124:A:HIS:HA	1:125:A:VAL:HG13	3	1.85
(1,1235)	1:82:A:LEU:HA	1:88:A:VAL:HG21	3	1.85
(1,1235)	1:82:A:LEU:HA	1:88:A:VAL:HG22	3	1.85
(1,1235)	1:82:A:LEU:HA	1:88:A:VAL:HG23	3	1.85
(1,1980)	1:124:A:HIS:HA	1:125:A:VAL:HG11	5	1.84
(1,1980)	1:124:A:HIS:HA	1:125:A:VAL:HG12	5	1.84
(1,1980)	1:124:A:HIS:HA	1:125:A:VAL:HG13	5	1.84
(1,1980)	1:124:A:HIS:HA	1:125:A:VAL:HG11	7	1.84
(1,1980)	1:124:A:HIS:HA	1:125:A:VAL:HG12	7	1.84
(1,1980)	1:124:A:HIS:HA	1:125:A:VAL:HG13	7	1.84
(1,1769)	1:112:A:LEU:HB2	1:125:A:VAL:HG21	10	1.84
(1,1769)	1:112:A:LEU:HB2	1:125:A:VAL:HG22	10	1.84
(1,1769)	1:112:A:LEU:HB2	1:125:A:VAL:HG23	10	1.84
(1,205)	1:18:A:VAL:HG11	1:22:A:LYS:HE2	10	1.84
(1,205)	1:18:A:VAL:HG12	1:22:A:LYS:HE2	10	1.84
(1,205)	1:18:A:VAL:HG13	1:22:A:LYS:HE2	10	1.84
(1,1769)	1:112:A:LEU:HB2	1:125:A:VAL:HG21	2	1.83
(1,1769)	1:112:A:LEU:HB2	1:125:A:VAL:HG22	2	1.83
(1,1769)	1:112:A:LEU:HB2	1:125:A:VAL:HG23	2	1.83
(1,1491)	1:96:A:ILE:HB	1:88:A:VAL:HG11	1	1.83
(1,1491)	1:96:A:ILE:HB	1:88:A:VAL:HG12	1	1.83
(1,1491)	1:96:A:ILE:HB	1:88:A:VAL:HG13	1	1.83
(1,1491)	1:96:A:ILE:HB	1:88:A:VAL:HG11	6	1.83
(1,1491)	1:96:A:ILE:HB	1:88:A:VAL:HG12	6	1.83
(1,1491)	1:96:A:ILE:HB	1:88:A:VAL:HG13	6	1.83
(1,1235)	1:82:A:LEU:HA	1:88:A:VAL:HG21	1	1.83
(1,1235)	1:82:A:LEU:HA	1:88:A:VAL:HG22	1	1.83
(1,1235)	1:82:A:LEU:HA	1:88:A:VAL:HG23	1	1.83
(1,205)	1:18:A:VAL:HG11	1:22:A:LYS:HE2	3	1.83
(1,205)	1:18:A:VAL:HG12	1:22:A:LYS:HE2	3	1.83
(1,205)	1:18:A:VAL:HG13	1:22:A:LYS:HE2	3	1.83
(1,1213)	1:82:A:LEU:HD11	1:79:A:ALA:HA	1	1.82
(1,1213)	1:82:A:LEU:HD12	1:79:A:ALA:HA	1	1.82
(1,1213)	1:82:A:LEU:HD13	1:79:A:ALA:HA	1	1.82
(1,1213)	1:82:A:LEU:HD11	1:79:A:ALA:HA	2	1.82
(1,1213)	1:82:A:LEU:HD12	1:79:A:ALA:HA	2	1.82
(1,1213)	1:82:A:LEU:HD13	1:79:A:ALA:HA	2	1.82
(1,1235)	1:82:A:LEU:HA	1:88:A:VAL:HG21	10	1.81
(1,1235)	1:82:A:LEU:HA	1:88:A:VAL:HG22	10	1.81
(1,1235)	1:82:A:LEU:HA	1:88:A:VAL:HG23	10	1.81
(1,1769)	1:112:A:LEU:HB2	1:125:A:VAL:HG21	7	1.8
(1,1769)	1:112:A:LEU:HB2	1:125:A:VAL:HG22	7	1.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1769)	1:112:A:LEU:HB2	1:125:A:VAL:HG23	7	1.8
(1,229)	1:20:A:ALA:HA	1:64:A:LEU:HD11	7	1.8
(1,229)	1:20:A:ALA:HA	1:64:A:LEU:HD12	7	1.8
(1,229)	1:20:A:ALA:HA	1:64:A:LEU:HD13	7	1.8
(1,205)	1:18:A:VAL:HG11	1:22:A:LYS:HE2	5	1.8
(1,205)	1:18:A:VAL:HG12	1:22:A:LYS:HE2	5	1.8
(1,205)	1:18:A:VAL:HG13	1:22:A:LYS:HE2	5	1.8
(1,430)	1:30:A:LEU:HD21	1:72:A:VAL:HG21	1	1.79
(1,430)	1:30:A:LEU:HD21	1:72:A:VAL:HG22	1	1.79
(1,430)	1:30:A:LEU:HD21	1:72:A:VAL:HG23	1	1.79
(1,430)	1:30:A:LEU:HD22	1:72:A:VAL:HG21	1	1.79
(1,430)	1:30:A:LEU:HD22	1:72:A:VAL:HG22	1	1.79
(1,430)	1:30:A:LEU:HD22	1:72:A:VAL:HG23	1	1.79
(1,430)	1:30:A:LEU:HD23	1:72:A:VAL:HG21	1	1.79
(1,430)	1:30:A:LEU:HD23	1:72:A:VAL:HG22	1	1.79
(1,430)	1:30:A:LEU:HD23	1:72:A:VAL:HG23	1	1.79
(1,229)	1:20:A:ALA:HA	1:64:A:LEU:HD11	4	1.79
(1,229)	1:20:A:ALA:HA	1:64:A:LEU:HD12	4	1.79
(1,229)	1:20:A:ALA:HA	1:64:A:LEU:HD13	4	1.79
(1,205)	1:18:A:VAL:HG11	1:22:A:LYS:HE2	4	1.79
(1,205)	1:18:A:VAL:HG12	1:22:A:LYS:HE2	4	1.79
(1,205)	1:18:A:VAL:HG13	1:22:A:LYS:HE2	4	1.79
(1,1768)	1:112:A:LEU:HD11	1:125:A:VAL:HG21	3	1.78
(1,1768)	1:112:A:LEU:HD11	1:125:A:VAL:HG22	3	1.78
(1,1768)	1:112:A:LEU:HD11	1:125:A:VAL:HG23	3	1.78
(1,1768)	1:112:A:LEU:HD12	1:125:A:VAL:HG21	3	1.78
(1,1768)	1:112:A:LEU:HD12	1:125:A:VAL:HG22	3	1.78
(1,1768)	1:112:A:LEU:HD12	1:125:A:VAL:HG23	3	1.78
(1,1768)	1:112:A:LEU:HD13	1:125:A:VAL:HG21	3	1.78
(1,1768)	1:112:A:LEU:HD13	1:125:A:VAL:HG22	3	1.78
(1,1768)	1:112:A:LEU:HD13	1:125:A:VAL:HG23	3	1.78
(1,1647)	1:106:A:VAL:HG11	1:104:A:LEU:HD11	1	1.78
(1,1647)	1:106:A:VAL:HG11	1:104:A:LEU:HD12	1	1.78
(1,1647)	1:106:A:VAL:HG11	1:104:A:LEU:HD13	1	1.78
(1,1647)	1:106:A:VAL:HG12	1:104:A:LEU:HD11	1	1.78
(1,1647)	1:106:A:VAL:HG12	1:104:A:LEU:HD12	1	1.78
(1,1647)	1:106:A:VAL:HG12	1:104:A:LEU:HD13	1	1.78
(1,1647)	1:106:A:VAL:HG13	1:104:A:LEU:HD11	1	1.78
(1,1647)	1:106:A:VAL:HG13	1:104:A:LEU:HD12	1	1.78
(1,1647)	1:106:A:VAL:HG13	1:104:A:LEU:HD13	1	1.78
(1,1491)	1:96:A:ILE:HB	1:88:A:VAL:HG11	4	1.78
(1,1491)	1:96:A:ILE:HB	1:88:A:VAL:HG12	4	1.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1491)	1:96:A:ILE:HB	1:88:A:VAL:HG13	4	1.78
(1,1067)	1:72:A:VAL:HG21	1:71:A:HIS:H	1	1.78
(1,1067)	1:72:A:VAL:HG22	1:71:A:HIS:H	1	1.78
(1,1067)	1:72:A:VAL:HG23	1:71:A:HIS:H	1	1.78
(1,1769)	1:112:A:LEU:HB2	1:125:A:VAL:HG21	3	1.77
(1,1769)	1:112:A:LEU:HB2	1:125:A:VAL:HG22	3	1.77
(1,1769)	1:112:A:LEU:HB2	1:125:A:VAL:HG23	3	1.77
(1,1213)	1:82:A:LEU:HD11	1:79:A:ALA:HA	6	1.77
(1,1213)	1:82:A:LEU:HD12	1:79:A:ALA:HA	6	1.77
(1,1213)	1:82:A:LEU:HD13	1:79:A:ALA:HA	6	1.77
(1,1768)	1:112:A:LEU:HD11	1:125:A:VAL:HG21	7	1.76
(1,1768)	1:112:A:LEU:HD11	1:125:A:VAL:HG22	7	1.76
(1,1768)	1:112:A:LEU:HD11	1:125:A:VAL:HG23	7	1.76
(1,1768)	1:112:A:LEU:HD12	1:125:A:VAL:HG21	7	1.76
(1,1768)	1:112:A:LEU:HD12	1:125:A:VAL:HG22	7	1.76
(1,1768)	1:112:A:LEU:HD12	1:125:A:VAL:HG23	7	1.76
(1,1768)	1:112:A:LEU:HD13	1:125:A:VAL:HG21	7	1.76
(1,1768)	1:112:A:LEU:HD13	1:125:A:VAL:HG22	7	1.76
(1,1768)	1:112:A:LEU:HD13	1:125:A:VAL:HG23	7	1.76
(1,1647)	1:106:A:VAL:HG11	1:104:A:LEU:HD11	6	1.76
(1,1647)	1:106:A:VAL:HG11	1:104:A:LEU:HD12	6	1.76
(1,1647)	1:106:A:VAL:HG11	1:104:A:LEU:HD13	6	1.76
(1,1647)	1:106:A:VAL:HG12	1:104:A:LEU:HD11	6	1.76
(1,1647)	1:106:A:VAL:HG12	1:104:A:LEU:HD12	6	1.76
(1,1647)	1:106:A:VAL:HG12	1:104:A:LEU:HD13	6	1.76
(1,1647)	1:106:A:VAL:HG13	1:104:A:LEU:HD11	6	1.76
(1,1647)	1:106:A:VAL:HG13	1:104:A:LEU:HD12	6	1.76
(1,1647)	1:106:A:VAL:HG13	1:104:A:LEU:HD13	6	1.76
(1,915)	1:62:A:PRO:HB3	1:92:A:GLU:HB3	5	1.76
(1,229)	1:20:A:ALA:HA	1:64:A:LEU:HD11	1	1.76
(1,229)	1:20:A:ALA:HA	1:64:A:LEU:HD12	1	1.76
(1,229)	1:20:A:ALA:HA	1:64:A:LEU:HD13	1	1.76
(1,229)	1:20:A:ALA:HA	1:64:A:LEU:HD11	6	1.76
(1,229)	1:20:A:ALA:HA	1:64:A:LEU:HD12	6	1.76
(1,229)	1:20:A:ALA:HA	1:64:A:LEU:HD13	6	1.76
(1,1980)	1:124:A:HIS:HA	1:125:A:VAL:HG11	1	1.75
(1,1980)	1:124:A:HIS:HA	1:125:A:VAL:HG12	1	1.75
(1,1980)	1:124:A:HIS:HA	1:125:A:VAL:HG13	1	1.75
(1,1213)	1:82:A:LEU:HD11	1:79:A:ALA:HA	9	1.75
(1,1213)	1:82:A:LEU:HD12	1:79:A:ALA:HA	9	1.75
(1,1213)	1:82:A:LEU:HD13	1:79:A:ALA:HA	9	1.75
(1,1028)	1:68:A:LEU:HD11	1:65:A:GLY:HA3	1	1.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1028)	1:68:A:LEU:HD12	1:65:A:GLY:HA3	1	1.75
(1,1028)	1:68:A:LEU:HD13	1:65:A:GLY:HA3	1	1.75
(1,1980)	1:124:A:HIS:HA	1:125:A:VAL:HG11	4	1.74
(1,1980)	1:124:A:HIS:HA	1:125:A:VAL:HG12	4	1.74
(1,1980)	1:124:A:HIS:HA	1:125:A:VAL:HG13	4	1.74
(1,1980)	1:124:A:HIS:HA	1:125:A:VAL:HG11	6	1.74
(1,1980)	1:124:A:HIS:HA	1:125:A:VAL:HG12	6	1.74
(1,1980)	1:124:A:HIS:HA	1:125:A:VAL:HG13	6	1.74
(1,1768)	1:112:A:LEU:HD11	1:125:A:VAL:HG21	4	1.74
(1,1768)	1:112:A:LEU:HD11	1:125:A:VAL:HG22	4	1.74
(1,1768)	1:112:A:LEU:HD11	1:125:A:VAL:HG23	4	1.74
(1,1768)	1:112:A:LEU:HD12	1:125:A:VAL:HG21	4	1.74
(1,1768)	1:112:A:LEU:HD12	1:125:A:VAL:HG22	4	1.74
(1,1768)	1:112:A:LEU:HD12	1:125:A:VAL:HG23	4	1.74
(1,1768)	1:112:A:LEU:HD13	1:125:A:VAL:HG21	4	1.74
(1,1768)	1:112:A:LEU:HD13	1:125:A:VAL:HG22	4	1.74
(1,1768)	1:112:A:LEU:HD13	1:125:A:VAL:HG23	4	1.74
(1,1647)	1:106:A:VAL:HG11	1:104:A:LEU:HD11	3	1.74
(1,1647)	1:106:A:VAL:HG11	1:104:A:LEU:HD12	3	1.74
(1,1647)	1:106:A:VAL:HG11	1:104:A:LEU:HD13	3	1.74
(1,1647)	1:106:A:VAL:HG12	1:104:A:LEU:HD11	3	1.74
(1,1647)	1:106:A:VAL:HG12	1:104:A:LEU:HD12	3	1.74
(1,1647)	1:106:A:VAL:HG12	1:104:A:LEU:HD13	3	1.74
(1,1647)	1:106:A:VAL:HG13	1:104:A:LEU:HD11	3	1.74
(1,1647)	1:106:A:VAL:HG13	1:104:A:LEU:HD12	3	1.74
(1,1647)	1:106:A:VAL:HG13	1:104:A:LEU:HD13	3	1.74
(1,1067)	1:72:A:VAL:HG21	1:71:A:HIS:H	3	1.74
(1,1067)	1:72:A:VAL:HG22	1:71:A:HIS:H	3	1.74
(1,1067)	1:72:A:VAL:HG23	1:71:A:HIS:H	3	1.74
(1,1798)	1:114:A:ALA:H	1:115:A:ASP:HB3	3	1.73
(1,1798)	1:114:A:ALA:H	1:115:A:ASP:HB3	5	1.73
(1,1798)	1:114:A:ALA:H	1:115:A:ASP:HB3	7	1.73
(1,1647)	1:106:A:VAL:HG11	1:104:A:LEU:HD11	4	1.73
(1,1647)	1:106:A:VAL:HG11	1:104:A:LEU:HD12	4	1.73
(1,1647)	1:106:A:VAL:HG11	1:104:A:LEU:HD13	4	1.73
(1,1647)	1:106:A:VAL:HG12	1:104:A:LEU:HD11	4	1.73
(1,1647)	1:106:A:VAL:HG12	1:104:A:LEU:HD12	4	1.73
(1,1647)	1:106:A:VAL:HG12	1:104:A:LEU:HD13	4	1.73
(1,1647)	1:106:A:VAL:HG13	1:104:A:LEU:HD11	4	1.73
(1,1647)	1:106:A:VAL:HG13	1:104:A:LEU:HD12	4	1.73
(1,1647)	1:106:A:VAL:HG13	1:104:A:LEU:HD13	4	1.73
(1,1491)	1:96:A:ILE:HB	1:88:A:VAL:HG11	3	1.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1491)	1:96:A:ILE:HB	1:88:A:VAL:HG12	3	1.73
(1,1491)	1:96:A:ILE:HB	1:88:A:VAL:HG13	3	1.73
(1,1235)	1:82:A:LEU:HA	1:88:A:VAL:HG21	8	1.73
(1,1235)	1:82:A:LEU:HA	1:88:A:VAL:HG22	8	1.73
(1,1235)	1:82:A:LEU:HA	1:88:A:VAL:HG23	8	1.73
(1,1213)	1:82:A:LEU:HD11	1:79:A:ALA:HA	8	1.73
(1,1213)	1:82:A:LEU:HD12	1:79:A:ALA:HA	8	1.73
(1,1213)	1:82:A:LEU:HD13	1:79:A:ALA:HA	8	1.73
(1,709)	1:48:A:LYS:HD2	1:50:A:PRO:HD3	2	1.73
(1,709)	1:48:A:LYS:HD3	1:50:A:PRO:HD3	2	1.73
(1,430)	1:30:A:LEU:HD21	1:72:A:VAL:HG21	8	1.73
(1,430)	1:30:A:LEU:HD21	1:72:A:VAL:HG22	8	1.73
(1,430)	1:30:A:LEU:HD21	1:72:A:VAL:HG23	8	1.73
(1,430)	1:30:A:LEU:HD22	1:72:A:VAL:HG21	8	1.73
(1,430)	1:30:A:LEU:HD22	1:72:A:VAL:HG22	8	1.73
(1,430)	1:30:A:LEU:HD22	1:72:A:VAL:HG23	8	1.73
(1,430)	1:30:A:LEU:HD23	1:72:A:VAL:HG21	8	1.73
(1,430)	1:30:A:LEU:HD23	1:72:A:VAL:HG22	8	1.73
(1,430)	1:30:A:LEU:HD23	1:72:A:VAL:HG23	8	1.73
(1,229)	1:20:A:ALA:HA	1:64:A:LEU:HD11	5	1.73
(1,229)	1:20:A:ALA:HA	1:64:A:LEU:HD12	5	1.73
(1,229)	1:20:A:ALA:HA	1:64:A:LEU:HD13	5	1.73
(1,1768)	1:112:A:LEU:HD11	1:125:A:VAL:HG21	5	1.72
(1,1768)	1:112:A:LEU:HD11	1:125:A:VAL:HG22	5	1.72
(1,1768)	1:112:A:LEU:HD11	1:125:A:VAL:HG23	5	1.72
(1,1768)	1:112:A:LEU:HD12	1:125:A:VAL:HG21	5	1.72
(1,1768)	1:112:A:LEU:HD12	1:125:A:VAL:HG22	5	1.72
(1,1768)	1:112:A:LEU:HD12	1:125:A:VAL:HG23	5	1.72
(1,1768)	1:112:A:LEU:HD13	1:125:A:VAL:HG21	5	1.72
(1,1768)	1:112:A:LEU:HD13	1:125:A:VAL:HG22	5	1.72
(1,1768)	1:112:A:LEU:HD13	1:125:A:VAL:HG23	5	1.72
(1,942)	1:64:A:LEU:HD11	1:24:A:ALA:HB1	8	1.72
(1,942)	1:64:A:LEU:HD11	1:24:A:ALA:HB2	8	1.72
(1,942)	1:64:A:LEU:HD11	1:24:A:ALA:HB3	8	1.72
(1,942)	1:64:A:LEU:HD12	1:24:A:ALA:HB1	8	1.72
(1,942)	1:64:A:LEU:HD12	1:24:A:ALA:HB2	8	1.72
(1,942)	1:64:A:LEU:HD12	1:24:A:ALA:HB3	8	1.72
(1,942)	1:64:A:LEU:HD13	1:24:A:ALA:HB1	8	1.72
(1,942)	1:64:A:LEU:HD13	1:24:A:ALA:HB2	8	1.72
(1,942)	1:64:A:LEU:HD13	1:24:A:ALA:HB3	8	1.72
(1,1769)	1:112:A:LEU:HB2	1:125:A:VAL:HG21	5	1.71
(1,1769)	1:112:A:LEU:HB2	1:125:A:VAL:HG22	5	1.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1769)	1:112:A:LEU:HB2	1:125:A:VAL:HG23	5	1.71
(1,1491)	1:96:A:ILE:HB	1:88:A:VAL:HG11	5	1.71
(1,1491)	1:96:A:ILE:HB	1:88:A:VAL:HG12	5	1.71
(1,1491)	1:96:A:ILE:HB	1:88:A:VAL:HG13	5	1.71
(1,1213)	1:82:A:LEU:HD11	1:79:A:ALA:HA	7	1.71
(1,1213)	1:82:A:LEU:HD12	1:79:A:ALA:HA	7	1.71
(1,1213)	1:82:A:LEU:HD13	1:79:A:ALA:HA	7	1.71
(1,709)	1:48:A:LYS:HD2	1:50:A:PRO:HD3	8	1.71
(1,709)	1:48:A:LYS:HD3	1:50:A:PRO:HD3	8	1.71
(1,229)	1:20:A:ALA:HA	1:64:A:LEU:HD11	8	1.71
(1,229)	1:20:A:ALA:HA	1:64:A:LEU:HD12	8	1.71
(1,229)	1:20:A:ALA:HA	1:64:A:LEU:HD13	8	1.71
(1,1235)	1:82:A:LEU:HA	1:88:A:VAL:HG21	5	1.7
(1,1235)	1:82:A:LEU:HA	1:88:A:VAL:HG22	5	1.7
(1,1235)	1:82:A:LEU:HA	1:88:A:VAL:HG23	5	1.7
(1,205)	1:18:A:VAL:HG11	1:22:A:LYS:HE2	2	1.7
(1,205)	1:18:A:VAL:HG12	1:22:A:LYS:HE2	2	1.7
(1,205)	1:18:A:VAL:HG13	1:22:A:LYS:HE2	2	1.7
(1,1213)	1:82:A:LEU:HD11	1:79:A:ALA:HA	4	1.69
(1,1213)	1:82:A:LEU:HD12	1:79:A:ALA:HA	4	1.69
(1,1213)	1:82:A:LEU:HD13	1:79:A:ALA:HA	4	1.69
(1,709)	1:48:A:LYS:HD2	1:50:A:PRO:HD3	6	1.69
(1,709)	1:48:A:LYS:HD3	1:50:A:PRO:HD3	6	1.69
(1,1768)	1:112:A:LEU:HD11	1:125:A:VAL:HG21	6	1.68
(1,1768)	1:112:A:LEU:HD11	1:125:A:VAL:HG22	6	1.68
(1,1768)	1:112:A:LEU:HD11	1:125:A:VAL:HG23	6	1.68
(1,1768)	1:112:A:LEU:HD12	1:125:A:VAL:HG21	6	1.68
(1,1768)	1:112:A:LEU:HD12	1:125:A:VAL:HG22	6	1.68
(1,1768)	1:112:A:LEU:HD12	1:125:A:VAL:HG23	6	1.68
(1,1768)	1:112:A:LEU:HD13	1:125:A:VAL:HG21	6	1.68
(1,1768)	1:112:A:LEU:HD13	1:125:A:VAL:HG22	6	1.68
(1,1768)	1:112:A:LEU:HD13	1:125:A:VAL:HG23	6	1.68
(1,1067)	1:72:A:VAL:HG21	1:71:A:HIS:H	10	1.68
(1,1067)	1:72:A:VAL:HG22	1:71:A:HIS:H	10	1.68
(1,1067)	1:72:A:VAL:HG23	1:71:A:HIS:H	10	1.68
(1,1028)	1:68:A:LEU:HD11	1:65:A:GLY:HA3	10	1.68
(1,1028)	1:68:A:LEU:HD12	1:65:A:GLY:HA3	10	1.68
(1,1028)	1:68:A:LEU:HD13	1:65:A:GLY:HA3	10	1.68
(1,942)	1:64:A:LEU:HD11	1:24:A:ALA:HB1	1	1.68
(1,942)	1:64:A:LEU:HD11	1:24:A:ALA:HB2	1	1.68
(1,942)	1:64:A:LEU:HD11	1:24:A:ALA:HB3	1	1.68
(1,942)	1:64:A:LEU:HD12	1:24:A:ALA:HB1	1	1.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,942)	1:64:A:LEU:HD12	1:24:A:ALA:HB2	1	1.68
(1,942)	1:64:A:LEU:HD12	1:24:A:ALA:HB3	1	1.68
(1,942)	1:64:A:LEU:HD13	1:24:A:ALA:HB1	1	1.68
(1,942)	1:64:A:LEU:HD13	1:24:A:ALA:HB2	1	1.68
(1,942)	1:64:A:LEU:HD13	1:24:A:ALA:HB3	1	1.68
(1,942)	1:64:A:LEU:HD11	1:24:A:ALA:HB1	2	1.68
(1,942)	1:64:A:LEU:HD11	1:24:A:ALA:HB2	2	1.68
(1,942)	1:64:A:LEU:HD11	1:24:A:ALA:HB3	2	1.68
(1,942)	1:64:A:LEU:HD12	1:24:A:ALA:HB1	2	1.68
(1,942)	1:64:A:LEU:HD12	1:24:A:ALA:HB2	2	1.68
(1,942)	1:64:A:LEU:HD12	1:24:A:ALA:HB3	2	1.68
(1,942)	1:64:A:LEU:HD13	1:24:A:ALA:HB1	2	1.68
(1,942)	1:64:A:LEU:HD13	1:24:A:ALA:HB2	2	1.68
(1,942)	1:64:A:LEU:HD13	1:24:A:ALA:HB3	2	1.68
(1,942)	1:64:A:LEU:HD11	1:24:A:ALA:HB1	7	1.68
(1,942)	1:64:A:LEU:HD11	1:24:A:ALA:HB2	7	1.68
(1,942)	1:64:A:LEU:HD11	1:24:A:ALA:HB3	7	1.68
(1,942)	1:64:A:LEU:HD12	1:24:A:ALA:HB1	7	1.68
(1,942)	1:64:A:LEU:HD12	1:24:A:ALA:HB2	7	1.68
(1,942)	1:64:A:LEU:HD12	1:24:A:ALA:HB3	7	1.68
(1,942)	1:64:A:LEU:HD13	1:24:A:ALA:HB1	7	1.68
(1,942)	1:64:A:LEU:HD13	1:24:A:ALA:HB2	7	1.68
(1,942)	1:64:A:LEU:HD13	1:24:A:ALA:HB3	7	1.68
(1,709)	1:48:A:LYS:HD2	1:50:A:PRO:HD3	1	1.68
(1,709)	1:48:A:LYS:HD3	1:50:A:PRO:HD3	1	1.68
(1,709)	1:48:A:LYS:HD2	1:50:A:PRO:HD3	4	1.68
(1,709)	1:48:A:LYS:HD3	1:50:A:PRO:HD3	4	1.68
(1,1768)	1:112:A:LEU:HD11	1:125:A:VAL:HG21	1	1.67
(1,1768)	1:112:A:LEU:HD11	1:125:A:VAL:HG22	1	1.67
(1,1768)	1:112:A:LEU:HD11	1:125:A:VAL:HG23	1	1.67
(1,1768)	1:112:A:LEU:HD12	1:125:A:VAL:HG21	1	1.67
(1,1768)	1:112:A:LEU:HD12	1:125:A:VAL:HG22	1	1.67
(1,1768)	1:112:A:LEU:HD12	1:125:A:VAL:HG23	1	1.67
(1,1768)	1:112:A:LEU:HD13	1:125:A:VAL:HG21	1	1.67
(1,1768)	1:112:A:LEU:HD13	1:125:A:VAL:HG22	1	1.67
(1,1768)	1:112:A:LEU:HD13	1:125:A:VAL:HG23	1	1.67
(1,942)	1:64:A:LEU:HD11	1:24:A:ALA:HB1	6	1.67
(1,942)	1:64:A:LEU:HD11	1:24:A:ALA:HB2	6	1.67
(1,942)	1:64:A:LEU:HD11	1:24:A:ALA:HB3	6	1.67
(1,942)	1:64:A:LEU:HD12	1:24:A:ALA:HB1	6	1.67
(1,942)	1:64:A:LEU:HD12	1:24:A:ALA:HB2	6	1.67
(1,942)	1:64:A:LEU:HD12	1:24:A:ALA:HB3	6	1.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,942)	1:64:A:LEU:HD13	1:24:A:ALA:HB1	6	1.67
(1,942)	1:64:A:LEU:HD13	1:24:A:ALA:HB2	6	1.67
(1,942)	1:64:A:LEU:HD13	1:24:A:ALA:HB3	6	1.67
(1,167)	1:14:A:PHE:HB2	1:18:A:VAL:H	2	1.67
(1,1257)	1:96:A:ILE:HG13	1:107:A:LYS:HE2	9	1.66
(1,1028)	1:68:A:LEU:HD11	1:65:A:GLY:HA3	4	1.66
(1,1028)	1:68:A:LEU:HD12	1:65:A:GLY:HA3	4	1.66
(1,1028)	1:68:A:LEU:HD13	1:65:A:GLY:HA3	4	1.66
(1,942)	1:64:A:LEU:HD11	1:24:A:ALA:HB1	4	1.66
(1,942)	1:64:A:LEU:HD11	1:24:A:ALA:HB2	4	1.66
(1,942)	1:64:A:LEU:HD11	1:24:A:ALA:HB3	4	1.66
(1,942)	1:64:A:LEU:HD12	1:24:A:ALA:HB1	4	1.66
(1,942)	1:64:A:LEU:HD12	1:24:A:ALA:HB2	4	1.66
(1,942)	1:64:A:LEU:HD12	1:24:A:ALA:HB3	4	1.66
(1,942)	1:64:A:LEU:HD13	1:24:A:ALA:HB1	4	1.66
(1,942)	1:64:A:LEU:HD13	1:24:A:ALA:HB2	4	1.66
(1,942)	1:64:A:LEU:HD13	1:24:A:ALA:HB3	4	1.66
(1,1213)	1:82:A:LEU:HD11	1:79:A:ALA:HA	3	1.65
(1,1213)	1:82:A:LEU:HD12	1:79:A:ALA:HA	3	1.65
(1,1213)	1:82:A:LEU:HD13	1:79:A:ALA:HA	3	1.65
(1,1213)	1:82:A:LEU:HD11	1:79:A:ALA:HA	10	1.65
(1,1213)	1:82:A:LEU:HD12	1:79:A:ALA:HA	10	1.65
(1,1213)	1:82:A:LEU:HD13	1:79:A:ALA:HA	10	1.65
(1,1067)	1:72:A:VAL:HG21	1:71:A:HIS:H	4	1.65
(1,1067)	1:72:A:VAL:HG22	1:71:A:HIS:H	4	1.65
(1,1067)	1:72:A:VAL:HG23	1:71:A:HIS:H	4	1.65
(1,942)	1:64:A:LEU:HD11	1:24:A:ALA:HB1	10	1.65
(1,942)	1:64:A:LEU:HD11	1:24:A:ALA:HB2	10	1.65
(1,942)	1:64:A:LEU:HD11	1:24:A:ALA:HB3	10	1.65
(1,942)	1:64:A:LEU:HD12	1:24:A:ALA:HB1	10	1.65
(1,942)	1:64:A:LEU:HD12	1:24:A:ALA:HB2	10	1.65
(1,942)	1:64:A:LEU:HD12	1:24:A:ALA:HB3	10	1.65
(1,942)	1:64:A:LEU:HD13	1:24:A:ALA:HB1	10	1.65
(1,942)	1:64:A:LEU:HD13	1:24:A:ALA:HB2	10	1.65
(1,942)	1:64:A:LEU:HD13	1:24:A:ALA:HB3	10	1.65
(1,709)	1:48:A:LYS:HD2	1:50:A:PRO:HD3	10	1.65
(1,709)	1:48:A:LYS:HD3	1:50:A:PRO:HD3	10	1.65
(1,67)	1:7:A:ILE:HG13	1:6:A:ASP:HB2	2	1.65
(1,942)	1:64:A:LEU:HD11	1:24:A:ALA:HB1	5	1.64
(1,942)	1:64:A:LEU:HD11	1:24:A:ALA:HB2	5	1.64
(1,942)	1:64:A:LEU:HD11	1:24:A:ALA:HB3	5	1.64
(1,942)	1:64:A:LEU:HD12	1:24:A:ALA:HB1	5	1.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,942)	1:64:A:LEU:HD12	1:24:A:ALA:HB2	5	1.64
(1,942)	1:64:A:LEU:HD12	1:24:A:ALA:HB3	5	1.64
(1,942)	1:64:A:LEU:HD13	1:24:A:ALA:HB1	5	1.64
(1,942)	1:64:A:LEU:HD13	1:24:A:ALA:HB2	5	1.64
(1,942)	1:64:A:LEU:HD13	1:24:A:ALA:HB3	5	1.64
(1,229)	1:20:A:ALA:HA	1:64:A:LEU:HD11	10	1.64
(1,229)	1:20:A:ALA:HA	1:64:A:LEU:HD12	10	1.64
(1,229)	1:20:A:ALA:HA	1:64:A:LEU:HD13	10	1.64
(1,67)	1:7:A:ILE:HG13	1:6:A:ASP:HB2	1	1.64
(1,1647)	1:106:A:VAL:HG11	1:104:A:LEU:HD11	8	1.63
(1,1647)	1:106:A:VAL:HG11	1:104:A:LEU:HD12	8	1.63
(1,1647)	1:106:A:VAL:HG11	1:104:A:LEU:HD13	8	1.63
(1,1647)	1:106:A:VAL:HG12	1:104:A:LEU:HD11	8	1.63
(1,1647)	1:106:A:VAL:HG12	1:104:A:LEU:HD12	8	1.63
(1,1647)	1:106:A:VAL:HG12	1:104:A:LEU:HD13	8	1.63
(1,1647)	1:106:A:VAL:HG13	1:104:A:LEU:HD11	8	1.63
(1,1647)	1:106:A:VAL:HG13	1:104:A:LEU:HD12	8	1.63
(1,1647)	1:106:A:VAL:HG13	1:104:A:LEU:HD13	8	1.63
(1,1067)	1:72:A:VAL:HG21	1:71:A:HIS:H	6	1.63
(1,1067)	1:72:A:VAL:HG22	1:71:A:HIS:H	6	1.63
(1,1067)	1:72:A:VAL:HG23	1:71:A:HIS:H	6	1.63
(1,167)	1:14:A:PHE:HB2	1:18:A:VAL:H	4	1.63
(1,1647)	1:106:A:VAL:HG11	1:104:A:LEU:HD11	9	1.62
(1,1647)	1:106:A:VAL:HG11	1:104:A:LEU:HD12	9	1.62
(1,1647)	1:106:A:VAL:HG11	1:104:A:LEU:HD13	9	1.62
(1,1647)	1:106:A:VAL:HG12	1:104:A:LEU:HD11	9	1.62
(1,1647)	1:106:A:VAL:HG12	1:104:A:LEU:HD12	9	1.62
(1,1647)	1:106:A:VAL:HG12	1:104:A:LEU:HD13	9	1.62
(1,1647)	1:106:A:VAL:HG13	1:104:A:LEU:HD11	9	1.62
(1,1647)	1:106:A:VAL:HG13	1:104:A:LEU:HD12	9	1.62
(1,1647)	1:106:A:VAL:HG13	1:104:A:LEU:HD13	9	1.62
(1,1092)	1:73:A:VAL:HG21	1:77:A:TYR:HE1	6	1.62
(1,1092)	1:73:A:VAL:HG21	1:77:A:TYR:HE2	6	1.62
(1,1092)	1:73:A:VAL:HG22	1:77:A:TYR:HE1	6	1.62
(1,1092)	1:73:A:VAL:HG22	1:77:A:TYR:HE2	6	1.62
(1,1092)	1:73:A:VAL:HG23	1:77:A:TYR:HE1	6	1.62
(1,1092)	1:73:A:VAL:HG23	1:77:A:TYR:HE2	6	1.62
(1,1067)	1:72:A:VAL:HG21	1:71:A:HIS:H	7	1.62
(1,1067)	1:72:A:VAL:HG22	1:71:A:HIS:H	7	1.62
(1,1067)	1:72:A:VAL:HG23	1:71:A:HIS:H	7	1.62
(1,942)	1:64:A:LEU:HD11	1:24:A:ALA:HB1	3	1.62
(1,942)	1:64:A:LEU:HD11	1:24:A:ALA:HB2	3	1.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,942)	1:64:A:LEU:HD11	1:24:A:ALA:HB3	3	1.62
(1,942)	1:64:A:LEU:HD12	1:24:A:ALA:HB1	3	1.62
(1,942)	1:64:A:LEU:HD12	1:24:A:ALA:HB2	3	1.62
(1,942)	1:64:A:LEU:HD12	1:24:A:ALA:HB3	3	1.62
(1,942)	1:64:A:LEU:HD13	1:24:A:ALA:HB1	3	1.62
(1,942)	1:64:A:LEU:HD13	1:24:A:ALA:HB2	3	1.62
(1,942)	1:64:A:LEU:HD13	1:24:A:ALA:HB3	3	1.62
(1,774)	1:54:A:ILE:HG12	1:63:A:GLN:HE22	4	1.62
(1,709)	1:48:A:LYS:HD2	1:50:A:PRO:HD3	9	1.62
(1,709)	1:48:A:LYS:HD3	1:50:A:PRO:HD3	9	1.62
(1,575)	1:39:A:PHE:HA	1:124:A:HIS:HB3	5	1.62
(1,67)	1:7:A:ILE:HG13	1:6:A:ASP:HB2	4	1.62
(1,67)	1:7:A:ILE:HG13	1:6:A:ASP:HB2	9	1.62
(1,67)	1:7:A:ILE:HG13	1:6:A:ASP:HB2	10	1.62
(1,1373)	1:88:A:VAL:HG11	1:96:A:ILE:H	9	1.61
(1,1373)	1:88:A:VAL:HG12	1:96:A:ILE:H	9	1.61
(1,1373)	1:88:A:VAL:HG13	1:96:A:ILE:H	9	1.61
(1,229)	1:20:A:ALA:HA	1:64:A:LEU:HD11	2	1.61
(1,229)	1:20:A:ALA:HA	1:64:A:LEU:HD12	2	1.61
(1,229)	1:20:A:ALA:HA	1:64:A:LEU:HD13	2	1.61
(1,167)	1:14:A:PHE:HB2	1:18:A:VAL:H	5	1.61
(1,167)	1:14:A:PHE:HB2	1:18:A:VAL:H	8	1.61
(1,1774)	1:113:A:ALA:H	1:111:A:VAL:HG21	1	1.6
(1,1774)	1:113:A:ALA:H	1:111:A:VAL:HG22	1	1.6
(1,1774)	1:113:A:ALA:H	1:111:A:VAL:HG23	1	1.6
(1,804)	1:56:A:SER:H	1:57:A:LEU:HB3	6	1.6
(1,804)	1:56:A:SER:H	1:57:A:LEU:HB3	7	1.6
(1,67)	1:7:A:ILE:HG13	1:6:A:ASP:HB2	5	1.6
(1,1373)	1:88:A:VAL:HG11	1:96:A:ILE:H	8	1.59
(1,1373)	1:88:A:VAL:HG12	1:96:A:ILE:H	8	1.59
(1,1373)	1:88:A:VAL:HG13	1:96:A:ILE:H	8	1.59
(1,1067)	1:72:A:VAL:HG21	1:71:A:HIS:H	2	1.59
(1,1067)	1:72:A:VAL:HG22	1:71:A:HIS:H	2	1.59
(1,1067)	1:72:A:VAL:HG23	1:71:A:HIS:H	2	1.59
(1,938)	1:3:A:THR:HG22	1:31:A:GLN:HG2	2	1.59
(1,915)	1:62:A:PRO:HB3	1:92:A:GLU:HB3	4	1.59
(1,575)	1:39:A:PHE:HA	1:124:A:HIS:HB3	2	1.59
(1,229)	1:20:A:ALA:HA	1:64:A:LEU:HD11	3	1.59
(1,229)	1:20:A:ALA:HA	1:64:A:LEU:HD12	3	1.59
(1,229)	1:20:A:ALA:HA	1:64:A:LEU:HD13	3	1.59
(1,1067)	1:72:A:VAL:HG21	1:71:A:HIS:H	8	1.58
(1,1067)	1:72:A:VAL:HG22	1:71:A:HIS:H	8	1.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1067)	1:72:A:VAL:HG23	1:71:A:HIS:H	8	1.58
(1,1067)	1:72:A:VAL:HG21	1:71:A:HIS:H	9	1.58
(1,1067)	1:72:A:VAL:HG22	1:71:A:HIS:H	9	1.58
(1,1067)	1:72:A:VAL:HG23	1:71:A:HIS:H	9	1.58
(1,942)	1:64:A:LEU:HD11	1:24:A:ALA:HB1	9	1.58
(1,942)	1:64:A:LEU:HD11	1:24:A:ALA:HB2	9	1.58
(1,942)	1:64:A:LEU:HD11	1:24:A:ALA:HB3	9	1.58
(1,942)	1:64:A:LEU:HD12	1:24:A:ALA:HB1	9	1.58
(1,942)	1:64:A:LEU:HD12	1:24:A:ALA:HB2	9	1.58
(1,942)	1:64:A:LEU:HD12	1:24:A:ALA:HB3	9	1.58
(1,942)	1:64:A:LEU:HD13	1:24:A:ALA:HB1	9	1.58
(1,942)	1:64:A:LEU:HD13	1:24:A:ALA:HB2	9	1.58
(1,942)	1:64:A:LEU:HD13	1:24:A:ALA:HB3	9	1.58
(1,915)	1:62:A:PRO:HB3	1:92:A:GLU:HB3	2	1.58
(1,804)	1:56:A:SER:H	1:57:A:LEU:HB3	2	1.58
(1,804)	1:56:A:SER:H	1:57:A:LEU:HB3	4	1.58
(1,804)	1:56:A:SER:H	1:57:A:LEU:HB3	8	1.58
(1,67)	1:7:A:ILE:HG13	1:6:A:ASP:HB2	3	1.58
(1,67)	1:7:A:ILE:HG13	1:6:A:ASP:HB2	8	1.58
(1,1769)	1:112:A:LEU:HB2	1:125:A:VAL:HG21	4	1.57
(1,1769)	1:112:A:LEU:HB2	1:125:A:VAL:HG22	4	1.57
(1,1769)	1:112:A:LEU:HB2	1:125:A:VAL:HG23	4	1.57
(1,1647)	1:106:A:VAL:HG11	1:104:A:LEU:HD11	2	1.57
(1,1647)	1:106:A:VAL:HG11	1:104:A:LEU:HD12	2	1.57
(1,1647)	1:106:A:VAL:HG11	1:104:A:LEU:HD13	2	1.57
(1,1647)	1:106:A:VAL:HG12	1:104:A:LEU:HD11	2	1.57
(1,1647)	1:106:A:VAL:HG12	1:104:A:LEU:HD12	2	1.57
(1,1647)	1:106:A:VAL:HG12	1:104:A:LEU:HD13	2	1.57
(1,1647)	1:106:A:VAL:HG13	1:104:A:LEU:HD11	2	1.57
(1,1647)	1:106:A:VAL:HG13	1:104:A:LEU:HD12	2	1.57
(1,1647)	1:106:A:VAL:HG13	1:104:A:LEU:HD13	2	1.57
(1,1373)	1:88:A:VAL:HG11	1:96:A:ILE:H	1	1.57
(1,1373)	1:88:A:VAL:HG12	1:96:A:ILE:H	1	1.57
(1,1373)	1:88:A:VAL:HG13	1:96:A:ILE:H	1	1.57
(1,1373)	1:88:A:VAL:HG11	1:96:A:ILE:H	4	1.57
(1,1373)	1:88:A:VAL:HG12	1:96:A:ILE:H	4	1.57
(1,1373)	1:88:A:VAL:HG13	1:96:A:ILE:H	4	1.57
(1,1373)	1:88:A:VAL:HG11	1:96:A:ILE:H	6	1.57
(1,1373)	1:88:A:VAL:HG12	1:96:A:ILE:H	6	1.57
(1,1373)	1:88:A:VAL:HG13	1:96:A:ILE:H	6	1.57
(1,1373)	1:88:A:VAL:HG11	1:96:A:ILE:H	10	1.57
(1,1373)	1:88:A:VAL:HG12	1:96:A:ILE:H	10	1.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1373)	1:88:A:VAL:HG13	1:96:A:ILE:H	10	1.57
(1,853)	1:58:A:VAL:HG21	1:64:A:LEU:HB3	9	1.57
(1,853)	1:58:A:VAL:HG22	1:64:A:LEU:HB3	9	1.57
(1,853)	1:58:A:VAL:HG23	1:64:A:LEU:HB3	9	1.57
(1,804)	1:56:A:SER:H	1:57:A:LEU:HB3	5	1.57
(1,804)	1:56:A:SER:H	1:57:A:LEU:HB3	9	1.57
(1,543)	1:37:A:THR:H	1:72:A:VAL:HG11	1	1.57
(1,543)	1:37:A:THR:H	1:72:A:VAL:HG12	1	1.57
(1,543)	1:37:A:THR:H	1:72:A:VAL:HG13	1	1.57
(1,543)	1:37:A:THR:H	1:72:A:VAL:HG11	3	1.57
(1,543)	1:37:A:THR:H	1:72:A:VAL:HG12	3	1.57
(1,543)	1:37:A:THR:H	1:72:A:VAL:HG13	3	1.57
(1,1373)	1:88:A:VAL:HG11	1:96:A:ILE:H	7	1.56
(1,1373)	1:88:A:VAL:HG12	1:96:A:ILE:H	7	1.56
(1,1373)	1:88:A:VAL:HG13	1:96:A:ILE:H	7	1.56
(1,1067)	1:72:A:VAL:HG21	1:71:A:HIS:H	5	1.56
(1,1067)	1:72:A:VAL:HG22	1:71:A:HIS:H	5	1.56
(1,1067)	1:72:A:VAL:HG23	1:71:A:HIS:H	5	1.56
(1,804)	1:56:A:SER:H	1:57:A:LEU:HB3	10	1.56
(1,774)	1:54:A:ILE:HG12	1:63:A:GLN:HE22	1	1.56
(1,774)	1:54:A:ILE:HG12	1:63:A:GLN:HE22	8	1.56
(1,575)	1:39:A:PHE:HA	1:124:A:HIS:HB3	7	1.56
(1,518)	1:36:A:PHE:HB2	1:72:A:VAL:HG11	9	1.56
(1,518)	1:36:A:PHE:HB2	1:72:A:VAL:HG12	9	1.56
(1,518)	1:36:A:PHE:HB2	1:72:A:VAL:HG13	9	1.56
(1,67)	1:7:A:ILE:HG13	1:6:A:ASP:HB2	6	1.56
(1,1256)	1:83:A:LYS:HD3	1:104:A:LEU:HD21	2	1.55
(1,1256)	1:83:A:LYS:HD3	1:104:A:LEU:HD22	2	1.55
(1,1256)	1:83:A:LYS:HD3	1:104:A:LEU:HD23	2	1.55
(1,1213)	1:82:A:LEU:HD11	1:79:A:ALA:HA	5	1.55
(1,1213)	1:82:A:LEU:HD12	1:79:A:ALA:HA	5	1.55
(1,1213)	1:82:A:LEU:HD13	1:79:A:ALA:HA	5	1.55
(1,881)	1:59:A:GLN:HB3	1:60:A:ASN:HD21	6	1.55
(1,711)	1:48:A:LYS:HG2	1:128:A:THR:HG21	7	1.55
(1,711)	1:48:A:LYS:HG2	1:128:A:THR:HG22	7	1.55
(1,711)	1:48:A:LYS:HG2	1:128:A:THR:HG23	7	1.55
(1,543)	1:37:A:THR:H	1:72:A:VAL:HG11	10	1.55
(1,543)	1:37:A:THR:H	1:72:A:VAL:HG12	10	1.55
(1,543)	1:37:A:THR:H	1:72:A:VAL:HG13	10	1.55
(1,1627)	1:104:A:LEU:HB2	1:111:A:VAL:H	1	1.54
(1,1373)	1:88:A:VAL:HG11	1:96:A:ILE:H	5	1.54
(1,1373)	1:88:A:VAL:HG12	1:96:A:ILE:H	5	1.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1373)	1:88:A:VAL:HG13	1:96:A:ILE:H	5	1.54
(1,1923)	1:122:A:ILE:HG13	1:121:A:GLY:HA2	8	1.53
(1,1774)	1:113:A:ALA:H	1:111:A:VAL:HG21	6	1.53
(1,1774)	1:113:A:ALA:H	1:111:A:VAL:HG22	6	1.53
(1,1774)	1:113:A:ALA:H	1:111:A:VAL:HG23	6	1.53
(1,1373)	1:88:A:VAL:HG11	1:96:A:ILE:H	2	1.53
(1,1373)	1:88:A:VAL:HG12	1:96:A:ILE:H	2	1.53
(1,1373)	1:88:A:VAL:HG13	1:96:A:ILE:H	2	1.53
(1,804)	1:56:A:SER:H	1:57:A:LEU:HB3	3	1.53
(1,1627)	1:104:A:LEU:HB2	1:111:A:VAL:H	6	1.52
(1,575)	1:39:A:PHE:HA	1:124:A:HIS:HB3	8	1.52
(1,575)	1:39:A:PHE:HA	1:124:A:HIS:HB3	9	1.52
(1,518)	1:36:A:PHE:HB2	1:72:A:VAL:HG11	6	1.52
(1,518)	1:36:A:PHE:HB2	1:72:A:VAL:HG12	6	1.52
(1,518)	1:36:A:PHE:HB2	1:72:A:VAL:HG13	6	1.52
(1,67)	1:7:A:ILE:HG13	1:6:A:ASP:HB2	7	1.52
(1,1627)	1:104:A:LEU:HB2	1:111:A:VAL:H	4	1.51
(1,1627)	1:104:A:LEU:HB2	1:111:A:VAL:H	10	1.51
(1,1373)	1:88:A:VAL:HG11	1:96:A:ILE:H	3	1.51
(1,1373)	1:88:A:VAL:HG12	1:96:A:ILE:H	3	1.51
(1,1373)	1:88:A:VAL:HG13	1:96:A:ILE:H	3	1.51
(1,853)	1:58:A:VAL:HG21	1:64:A:LEU:HB3	8	1.51
(1,853)	1:58:A:VAL:HG22	1:64:A:LEU:HB3	8	1.51
(1,853)	1:58:A:VAL:HG23	1:64:A:LEU:HB3	8	1.51
(1,232)	1:20:A:ALA:HA	1:68:A:LEU:HD11	4	1.51
(1,232)	1:20:A:ALA:HA	1:68:A:LEU:HD12	4	1.51
(1,232)	1:20:A:ALA:HA	1:68:A:LEU:HD13	4	1.51
(1,232)	1:20:A:ALA:HA	1:68:A:LEU:HD11	6	1.51
(1,232)	1:20:A:ALA:HA	1:68:A:LEU:HD12	6	1.51
(1,232)	1:20:A:ALA:HA	1:68:A:LEU:HD13	6	1.51
(1,229)	1:20:A:ALA:HA	1:64:A:LEU:HD11	9	1.51
(1,229)	1:20:A:ALA:HA	1:64:A:LEU:HD12	9	1.51
(1,229)	1:20:A:ALA:HA	1:64:A:LEU:HD13	9	1.51
(1,1769)	1:112:A:LEU:HB2	1:125:A:VAL:HG21	1	1.5
(1,1769)	1:112:A:LEU:HB2	1:125:A:VAL:HG22	1	1.5
(1,1769)	1:112:A:LEU:HB2	1:125:A:VAL:HG23	1	1.5
(1,1769)	1:112:A:LEU:HB2	1:125:A:VAL:HG21	6	1.5
(1,1769)	1:112:A:LEU:HB2	1:125:A:VAL:HG22	6	1.5
(1,1769)	1:112:A:LEU:HB2	1:125:A:VAL:HG23	6	1.5
(1,1627)	1:104:A:LEU:HB2	1:111:A:VAL:H	9	1.5
(1,543)	1:37:A:THR:H	1:72:A:VAL:HG11	8	1.5
(1,543)	1:37:A:THR:H	1:72:A:VAL:HG12	8	1.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,543)	1:37:A:THR:H	1:72:A:VAL:HG13	8	1.5
(1,430)	1:30:A:LEU:HD21	1:72:A:VAL:HG21	7	1.5
(1,430)	1:30:A:LEU:HD21	1:72:A:VAL:HG22	7	1.5
(1,430)	1:30:A:LEU:HD21	1:72:A:VAL:HG23	7	1.5
(1,430)	1:30:A:LEU:HD22	1:72:A:VAL:HG21	7	1.5
(1,430)	1:30:A:LEU:HD22	1:72:A:VAL:HG22	7	1.5
(1,430)	1:30:A:LEU:HD22	1:72:A:VAL:HG23	7	1.5
(1,430)	1:30:A:LEU:HD23	1:72:A:VAL:HG21	7	1.5
(1,430)	1:30:A:LEU:HD23	1:72:A:VAL:HG22	7	1.5
(1,430)	1:30:A:LEU:HD23	1:72:A:VAL:HG23	7	1.5
(1,1627)	1:104:A:LEU:HB2	1:111:A:VAL:H	2	1.49
(1,1627)	1:104:A:LEU:HB2	1:111:A:VAL:H	7	1.49
(1,1627)	1:104:A:LEU:HB2	1:111:A:VAL:H	8	1.49
(1,853)	1:58:A:VAL:HG21	1:64:A:LEU:HB3	1	1.49
(1,853)	1:58:A:VAL:HG22	1:64:A:LEU:HB3	1	1.49
(1,853)	1:58:A:VAL:HG23	1:64:A:LEU:HB3	1	1.49
(1,727)	1:49:A:LEU:HB2	1:50:A:PRO:HD2	3	1.49
(1,4)	1:2:A:ALA:HB1	1:6:A:ASP:HB2	3	1.49
(1,4)	1:2:A:ALA:HB2	1:6:A:ASP:HB2	3	1.49
(1,4)	1:2:A:ALA:HB3	1:6:A:ASP:HB2	3	1.49
(1,881)	1:59:A:GLN:HB3	1:60:A:ASN:HD21	4	1.48
(1,167)	1:14:A:PHE:HB2	1:18:A:VAL:H	10	1.48
(1,1257)	1:96:A:ILE:HG13	1:107:A:LYS:HE2	6	1.47
(1,804)	1:56:A:SER:H	1:57:A:LEU:HB3	1	1.47
(1,575)	1:39:A:PHE:HA	1:124:A:HIS:HB3	3	1.47
(1,518)	1:36:A:PHE:HB2	1:72:A:VAL:HG11	7	1.47
(1,518)	1:36:A:PHE:HB2	1:72:A:VAL:HG12	7	1.47
(1,518)	1:36:A:PHE:HB2	1:72:A:VAL:HG13	7	1.47
(1,1647)	1:106:A:VAL:HG11	1:104:A:LEU:HD11	10	1.46
(1,1647)	1:106:A:VAL:HG11	1:104:A:LEU:HD12	10	1.46
(1,1647)	1:106:A:VAL:HG11	1:104:A:LEU:HD13	10	1.46
(1,1647)	1:106:A:VAL:HG12	1:104:A:LEU:HD11	10	1.46
(1,1647)	1:106:A:VAL:HG12	1:104:A:LEU:HD12	10	1.46
(1,1647)	1:106:A:VAL:HG12	1:104:A:LEU:HD13	10	1.46
(1,1647)	1:106:A:VAL:HG13	1:104:A:LEU:HD11	10	1.46
(1,1647)	1:106:A:VAL:HG13	1:104:A:LEU:HD12	10	1.46
(1,1647)	1:106:A:VAL:HG13	1:104:A:LEU:HD13	10	1.46
(1,915)	1:62:A:PRO:HB3	1:92:A:GLU:HB3	10	1.46
(1,853)	1:58:A:VAL:HG21	1:64:A:LEU:HB3	10	1.46
(1,853)	1:58:A:VAL:HG22	1:64:A:LEU:HB3	10	1.46
(1,853)	1:58:A:VAL:HG23	1:64:A:LEU:HB3	10	1.46
(1,774)	1:54:A:ILE:HG12	1:63:A:GLN:HE22	6	1.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,769)	1:54:A:ILE:HG12	1:57:A:LEU:HD21	7	1.46
(1,769)	1:54:A:ILE:HG12	1:57:A:LEU:HD22	7	1.46
(1,769)	1:54:A:ILE:HG12	1:57:A:LEU:HD23	7	1.46
(1,727)	1:49:A:LEU:HB2	1:50:A:PRO:HD2	5	1.46
(1,530)	1:36:A:PHE:HB3	1:121:A:GLY:H	10	1.46
(1,430)	1:30:A:LEU:HD21	1:72:A:VAL:HG21	6	1.46
(1,430)	1:30:A:LEU:HD21	1:72:A:VAL:HG22	6	1.46
(1,430)	1:30:A:LEU:HD21	1:72:A:VAL:HG23	6	1.46
(1,430)	1:30:A:LEU:HD22	1:72:A:VAL:HG21	6	1.46
(1,430)	1:30:A:LEU:HD22	1:72:A:VAL:HG22	6	1.46
(1,430)	1:30:A:LEU:HD22	1:72:A:VAL:HG23	6	1.46
(1,430)	1:30:A:LEU:HD23	1:72:A:VAL:HG21	6	1.46
(1,430)	1:30:A:LEU:HD23	1:72:A:VAL:HG22	6	1.46
(1,430)	1:30:A:LEU:HD23	1:72:A:VAL:HG23	6	1.46
(1,232)	1:20:A:ALA:HA	1:68:A:LEU:HD11	9	1.46
(1,232)	1:20:A:ALA:HA	1:68:A:LEU:HD12	9	1.46
(1,232)	1:20:A:ALA:HA	1:68:A:LEU:HD13	9	1.46
(1,167)	1:14:A:PHE:HB2	1:18:A:VAL:H	6	1.46
(1,4)	1:2:A:ALA:HB1	1:6:A:ASP:HB2	4	1.46
(1,4)	1:2:A:ALA:HB2	1:6:A:ASP:HB2	4	1.46
(1,4)	1:2:A:ALA:HB3	1:6:A:ASP:HB2	4	1.46
(1,1923)	1:122:A:ILE:HG13	1:121:A:GLY:HA2	5	1.45
(1,1256)	1:83:A:LYS:HD3	1:104:A:LEU:HD21	10	1.45
(1,1256)	1:83:A:LYS:HD3	1:104:A:LEU:HD22	10	1.45
(1,1256)	1:83:A:LYS:HD3	1:104:A:LEU:HD23	10	1.45
(1,1519)	1:96:A:ILE:HG13	1:107:A:LYS:HE2	9	1.44
(1,1519)	1:96:A:ILE:HG13	1:107:A:LYS:HE3	9	1.44
(1,955)	1:64:A:LEU:HD21	1:64:A:LEU:HA	2	1.44
(1,955)	1:64:A:LEU:HD22	1:64:A:LEU:HA	2	1.44
(1,955)	1:64:A:LEU:HD23	1:64:A:LEU:HA	2	1.44
(1,955)	1:64:A:LEU:HD21	1:64:A:LEU:HA	9	1.44
(1,955)	1:64:A:LEU:HD22	1:64:A:LEU:HA	9	1.44
(1,955)	1:64:A:LEU:HD23	1:64:A:LEU:HA	9	1.44
(1,853)	1:58:A:VAL:HG21	1:64:A:LEU:HB3	4	1.44
(1,853)	1:58:A:VAL:HG22	1:64:A:LEU:HB3	4	1.44
(1,853)	1:58:A:VAL:HG23	1:64:A:LEU:HB3	4	1.44
(1,167)	1:14:A:PHE:HB2	1:18:A:VAL:H	9	1.44
(1,1923)	1:122:A:ILE:HG13	1:121:A:GLY:HA2	3	1.43
(1,1774)	1:113:A:ALA:H	1:111:A:VAL:HG21	5	1.43
(1,1774)	1:113:A:ALA:H	1:111:A:VAL:HG22	5	1.43
(1,1774)	1:113:A:ALA:H	1:111:A:VAL:HG23	5	1.43
(1,1518)	1:96:A:ILE:HG13	1:107:A:LYS:HD2	8	1.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1518)	1:96:A:ILE:HG13	1:107:A:LYS:HD3	8	1.43
(1,955)	1:64:A:LEU:HD21	1:64:A:LEU:HA	8	1.43
(1,955)	1:64:A:LEU:HD22	1:64:A:LEU:HA	8	1.43
(1,955)	1:64:A:LEU:HD23	1:64:A:LEU:HA	8	1.43
(1,855)	1:59:A:GLN:HE22	1:56:A:SER:HA	5	1.43
(1,855)	1:59:A:GLN:HE22	1:56:A:SER:HA	7	1.43
(1,769)	1:54:A:ILE:HG12	1:57:A:LEU:HD21	10	1.43
(1,769)	1:54:A:ILE:HG12	1:57:A:LEU:HD22	10	1.43
(1,769)	1:54:A:ILE:HG12	1:57:A:LEU:HD23	10	1.43
(1,232)	1:20:A:ALA:HA	1:68:A:LEU:HD11	8	1.43
(1,232)	1:20:A:ALA:HA	1:68:A:LEU:HD12	8	1.43
(1,232)	1:20:A:ALA:HA	1:68:A:LEU:HD13	8	1.43
(1,4)	1:2:A:ALA:HB1	1:6:A:ASP:HB2	6	1.43
(1,4)	1:2:A:ALA:HB2	1:6:A:ASP:HB2	6	1.43
(1,4)	1:2:A:ALA:HB3	1:6:A:ASP:HB2	6	1.43
(1,955)	1:64:A:LEU:HD21	1:64:A:LEU:HA	3	1.42
(1,955)	1:64:A:LEU:HD22	1:64:A:LEU:HA	3	1.42
(1,955)	1:64:A:LEU:HD23	1:64:A:LEU:HA	3	1.42
(1,955)	1:64:A:LEU:HD21	1:64:A:LEU:HA	6	1.42
(1,955)	1:64:A:LEU:HD22	1:64:A:LEU:HA	6	1.42
(1,955)	1:64:A:LEU:HD23	1:64:A:LEU:HA	6	1.42
(1,955)	1:64:A:LEU:HD21	1:64:A:LEU:HA	10	1.42
(1,955)	1:64:A:LEU:HD22	1:64:A:LEU:HA	10	1.42
(1,955)	1:64:A:LEU:HD23	1:64:A:LEU:HA	10	1.42
(1,855)	1:59:A:GLN:HE22	1:56:A:SER:HA	2	1.42
(1,853)	1:58:A:VAL:HG21	1:64:A:LEU:HB3	6	1.42
(1,853)	1:58:A:VAL:HG22	1:64:A:LEU:HB3	6	1.42
(1,853)	1:58:A:VAL:HG23	1:64:A:LEU:HB3	6	1.42
(1,727)	1:49:A:LEU:HB2	1:50:A:PRO:HD2	7	1.42
(1,4)	1:2:A:ALA:HB1	1:6:A:ASP:HB2	5	1.42
(1,4)	1:2:A:ALA:HB2	1:6:A:ASP:HB2	5	1.42
(1,4)	1:2:A:ALA:HB3	1:6:A:ASP:HB2	5	1.42
(1,4)	1:2:A:ALA:HB1	1:6:A:ASP:HB2	8	1.42
(1,4)	1:2:A:ALA:HB2	1:6:A:ASP:HB2	8	1.42
(1,4)	1:2:A:ALA:HB3	1:6:A:ASP:HB2	8	1.42
(1,955)	1:64:A:LEU:HD21	1:64:A:LEU:HA	1	1.41
(1,955)	1:64:A:LEU:HD22	1:64:A:LEU:HA	1	1.41
(1,955)	1:64:A:LEU:HD23	1:64:A:LEU:HA	1	1.41
(1,955)	1:64:A:LEU:HD21	1:64:A:LEU:HA	5	1.41
(1,955)	1:64:A:LEU:HD22	1:64:A:LEU:HA	5	1.41
(1,955)	1:64:A:LEU:HD23	1:64:A:LEU:HA	5	1.41
(1,855)	1:59:A:GLN:HE22	1:56:A:SER:HA	4	1.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,855)	1:59:A:GLN:HE22	1:56:A:SER:HA	6	1.41
(1,955)	1:64:A:LEU:HD21	1:64:A:LEU:HA	4	1.4
(1,955)	1:64:A:LEU:HD22	1:64:A:LEU:HA	4	1.4
(1,955)	1:64:A:LEU:HD23	1:64:A:LEU:HA	4	1.4
(1,855)	1:59:A:GLN:HE22	1:56:A:SER:HA	1	1.4
(1,855)	1:59:A:GLN:HE22	1:56:A:SER:HA	8	1.4
(1,1923)	1:122:A:ILE:HG13	1:121:A:GLY:HA2	1	1.39
(1,955)	1:64:A:LEU:HD21	1:64:A:LEU:HA	7	1.39
(1,955)	1:64:A:LEU:HD22	1:64:A:LEU:HA	7	1.39
(1,955)	1:64:A:LEU:HD23	1:64:A:LEU:HA	7	1.39
(1,855)	1:59:A:GLN:HE22	1:56:A:SER:HA	10	1.39
(1,612)	1:42:A:ASN:HB3	1:125:A:VAL:HG21	8	1.38
(1,612)	1:42:A:ASN:HB3	1:125:A:VAL:HG22	8	1.38
(1,612)	1:42:A:ASN:HB3	1:125:A:VAL:HG23	8	1.38
(1,612)	1:42:A:ASN:HB3	1:125:A:VAL:HG21	10	1.38
(1,612)	1:42:A:ASN:HB3	1:125:A:VAL:HG22	10	1.38
(1,612)	1:42:A:ASN:HB3	1:125:A:VAL:HG23	10	1.38
(1,543)	1:37:A:THR:H	1:72:A:VAL:HG11	4	1.38
(1,543)	1:37:A:THR:H	1:72:A:VAL:HG12	4	1.38
(1,543)	1:37:A:THR:H	1:72:A:VAL:HG13	4	1.38
(1,232)	1:20:A:ALA:HA	1:68:A:LEU:HD11	7	1.38
(1,232)	1:20:A:ALA:HA	1:68:A:LEU:HD12	7	1.38
(1,232)	1:20:A:ALA:HA	1:68:A:LEU:HD13	7	1.38
(1,167)	1:14:A:PHE:HB2	1:18:A:VAL:H	1	1.38
(1,1627)	1:104:A:LEU:HB2	1:111:A:VAL:H	5	1.37
(1,1577)	1:101:A:ASP:H	1:103:A:PRO:HG3	3	1.37
(1,774)	1:54:A:ILE:HG12	1:63:A:GLN:HE22	5	1.37
(1,612)	1:42:A:ASN:HB3	1:125:A:VAL:HG21	3	1.37
(1,612)	1:42:A:ASN:HB3	1:125:A:VAL:HG22	3	1.37
(1,612)	1:42:A:ASN:HB3	1:125:A:VAL:HG23	3	1.37
(1,855)	1:59:A:GLN:HE22	1:56:A:SER:HA	9	1.36
(1,582)	1:40:A:ALA:H	1:124:A:HIS:HB3	5	1.36
(1,543)	1:37:A:THR:H	1:72:A:VAL:HG11	9	1.36
(1,543)	1:37:A:THR:H	1:72:A:VAL:HG12	9	1.36
(1,543)	1:37:A:THR:H	1:72:A:VAL:HG13	9	1.36
(1,1923)	1:122:A:ILE:HG13	1:121:A:GLY:HA2	2	1.35
(1,1577)	1:101:A:ASP:H	1:103:A:PRO:HG3	4	1.35
(1,611)	1:42:A:ASN:HB2	1:112:A:LEU:HD11	6	1.35
(1,611)	1:42:A:ASN:HB2	1:112:A:LEU:HD12	6	1.35
(1,611)	1:42:A:ASN:HB2	1:112:A:LEU:HD13	6	1.35
(1,1629)	1:104:A:LEU:HD11	1:114:A:ALA:HB1	9	1.34
(1,1629)	1:104:A:LEU:HD11	1:114:A:ALA:HB2	9	1.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1629)	1:104:A:LEU:HD11	1:114:A:ALA:HB3	9	1.34
(1,1629)	1:104:A:LEU:HD12	1:114:A:ALA:HB1	9	1.34
(1,1629)	1:104:A:LEU:HD12	1:114:A:ALA:HB2	9	1.34
(1,1629)	1:104:A:LEU:HD12	1:114:A:ALA:HB3	9	1.34
(1,1629)	1:104:A:LEU:HD13	1:114:A:ALA:HB1	9	1.34
(1,1629)	1:104:A:LEU:HD13	1:114:A:ALA:HB2	9	1.34
(1,1629)	1:104:A:LEU:HD13	1:114:A:ALA:HB3	9	1.34
(1,1186)	1:80:A:THR:HA	1:83:A:LYS:HB3	10	1.34
(1,726)	1:49:A:LEU:HB3	1:50:A:PRO:HD3	7	1.34
(1,543)	1:37:A:THR:H	1:72:A:VAL:HG11	6	1.34
(1,543)	1:37:A:THR:H	1:72:A:VAL:HG12	6	1.34
(1,543)	1:37:A:THR:H	1:72:A:VAL:HG13	6	1.34
(1,232)	1:20:A:ALA:HA	1:68:A:LEU:HD11	3	1.34
(1,232)	1:20:A:ALA:HA	1:68:A:LEU:HD12	3	1.34
(1,232)	1:20:A:ALA:HA	1:68:A:LEU:HD13	3	1.34
(1,1923)	1:122:A:ILE:HG13	1:121:A:GLY:HA2	4	1.33
(1,1627)	1:104:A:LEU:HB2	1:111:A:VAL:H	3	1.33
(1,611)	1:42:A:ASN:HB2	1:112:A:LEU:HD11	1	1.33
(1,611)	1:42:A:ASN:HB2	1:112:A:LEU:HD12	1	1.33
(1,611)	1:42:A:ASN:HB2	1:112:A:LEU:HD13	1	1.33
(1,232)	1:20:A:ALA:HA	1:68:A:LEU:HD11	2	1.33
(1,232)	1:20:A:ALA:HA	1:68:A:LEU:HD12	2	1.33
(1,232)	1:20:A:ALA:HA	1:68:A:LEU:HD13	2	1.33
(1,1629)	1:104:A:LEU:HD11	1:114:A:ALA:HB1	3	1.32
(1,1629)	1:104:A:LEU:HD11	1:114:A:ALA:HB2	3	1.32
(1,1629)	1:104:A:LEU:HD11	1:114:A:ALA:HB3	3	1.32
(1,1629)	1:104:A:LEU:HD12	1:114:A:ALA:HB1	3	1.32
(1,1629)	1:104:A:LEU:HD12	1:114:A:ALA:HB2	3	1.32
(1,1629)	1:104:A:LEU:HD12	1:114:A:ALA:HB3	3	1.32
(1,1629)	1:104:A:LEU:HD13	1:114:A:ALA:HB1	3	1.32
(1,1629)	1:104:A:LEU:HD13	1:114:A:ALA:HB2	3	1.32
(1,1629)	1:104:A:LEU:HD13	1:114:A:ALA:HB3	3	1.32
(1,1258)	1:83:A:LYS:HB2	1:104:A:LEU:HD21	6	1.32
(1,1258)	1:83:A:LYS:HB2	1:104:A:LEU:HD22	6	1.32
(1,1258)	1:83:A:LYS:HB2	1:104:A:LEU:HD23	6	1.32
(1,881)	1:59:A:GLN:HB3	1:60:A:ASN:HD21	1	1.32
(1,726)	1:49:A:LEU:HB3	1:50:A:PRO:HD3	3	1.32
(1,711)	1:48:A:LYS:HG2	1:128:A:THR:HG21	3	1.32
(1,711)	1:48:A:LYS:HG2	1:128:A:THR:HG22	3	1.32
(1,711)	1:48:A:LYS:HG2	1:128:A:THR:HG23	3	1.32
(1,611)	1:42:A:ASN:HB2	1:112:A:LEU:HD11	10	1.32
(1,611)	1:42:A:ASN:HB2	1:112:A:LEU:HD12	10	1.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,611)	1:42:A:ASN:HB2	1:112:A:LEU:HD13	10	1.32
(1,582)	1:40:A:ALA:H	1:124:A:HIS:HB3	2	1.32
(1,582)	1:40:A:ALA:H	1:124:A:HIS:HB3	7	1.32
(1,232)	1:20:A:ALA:HA	1:68:A:LEU:HD11	1	1.32
(1,232)	1:20:A:ALA:HA	1:68:A:LEU:HD12	1	1.32
(1,232)	1:20:A:ALA:HA	1:68:A:LEU:HD13	1	1.32
(1,1629)	1:104:A:LEU:HD11	1:114:A:ALA:HB1	10	1.31
(1,1629)	1:104:A:LEU:HD11	1:114:A:ALA:HB2	10	1.31
(1,1629)	1:104:A:LEU:HD11	1:114:A:ALA:HB3	10	1.31
(1,1629)	1:104:A:LEU:HD12	1:114:A:ALA:HB1	10	1.31
(1,1629)	1:104:A:LEU:HD12	1:114:A:ALA:HB2	10	1.31
(1,1629)	1:104:A:LEU:HD12	1:114:A:ALA:HB3	10	1.31
(1,1629)	1:104:A:LEU:HD13	1:114:A:ALA:HB1	10	1.31
(1,1629)	1:104:A:LEU:HD13	1:114:A:ALA:HB2	10	1.31
(1,1629)	1:104:A:LEU:HD13	1:114:A:ALA:HB3	10	1.31
(1,1258)	1:83:A:LYS:HB2	1:104:A:LEU:HD21	8	1.31
(1,1258)	1:83:A:LYS:HB2	1:104:A:LEU:HD22	8	1.31
(1,1258)	1:83:A:LYS:HB2	1:104:A:LEU:HD23	8	1.31
(1,1257)	1:96:A:ILE:HG13	1:107:A:LYS:HE2	4	1.31
(1,881)	1:59:A:GLN:HB3	1:60:A:ASN:HD21	10	1.31
(1,853)	1:58:A:VAL:HG21	1:64:A:LEU:HB3	2	1.31
(1,853)	1:58:A:VAL:HG22	1:64:A:LEU:HB3	2	1.31
(1,853)	1:58:A:VAL:HG23	1:64:A:LEU:HB3	2	1.31
(1,773)	1:54:A:ILE:HG12	1:58:A:VAL:H	2	1.31
(1,773)	1:54:A:ILE:HG12	1:58:A:VAL:H	3	1.31
(1,232)	1:20:A:ALA:HA	1:68:A:LEU:HD11	5	1.31
(1,232)	1:20:A:ALA:HA	1:68:A:LEU:HD12	5	1.31
(1,232)	1:20:A:ALA:HA	1:68:A:LEU:HD13	5	1.31
(1,1577)	1:101:A:ASP:H	1:103:A:PRO:HG3	10	1.3
(1,1334)	1:87:A:ILE:H	1:88:A:VAL:HG21	6	1.3
(1,1334)	1:87:A:ILE:H	1:88:A:VAL:HG22	6	1.3
(1,1334)	1:87:A:ILE:H	1:88:A:VAL:HG23	6	1.3
(1,1186)	1:80:A:THR:HA	1:83:A:LYS:HB3	2	1.3
(1,881)	1:59:A:GLN:HB3	1:60:A:ASN:HD21	5	1.3
(1,543)	1:37:A:THR:H	1:72:A:VAL:HG11	7	1.3
(1,543)	1:37:A:THR:H	1:72:A:VAL:HG12	7	1.3
(1,543)	1:37:A:THR:H	1:72:A:VAL:HG13	7	1.3
(1,1334)	1:87:A:ILE:H	1:88:A:VAL:HG21	3	1.29
(1,1334)	1:87:A:ILE:H	1:88:A:VAL:HG22	3	1.29
(1,1334)	1:87:A:ILE:H	1:88:A:VAL:HG23	3	1.29
(1,1186)	1:80:A:THR:HA	1:83:A:LYS:HB3	9	1.29
(1,769)	1:54:A:ILE:HG12	1:57:A:LEU:HD21	2	1.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,769)	1:54:A:ILE:HG12	1:57:A:LEU:HD22	2	1.29
(1,769)	1:54:A:ILE:HG12	1:57:A:LEU:HD23	2	1.29
(1,611)	1:42:A:ASN:HB2	1:112:A:LEU:HD11	2	1.29
(1,611)	1:42:A:ASN:HB2	1:112:A:LEU:HD12	2	1.29
(1,611)	1:42:A:ASN:HB2	1:112:A:LEU:HD13	2	1.29
(1,575)	1:39:A:PHE:HA	1:124:A:HIS:HB3	10	1.29
(1,518)	1:36:A:PHE:HB2	1:72:A:VAL:HG11	5	1.29
(1,518)	1:36:A:PHE:HB2	1:72:A:VAL:HG12	5	1.29
(1,518)	1:36:A:PHE:HB2	1:72:A:VAL:HG13	5	1.29
(1,1186)	1:80:A:THR:HA	1:83:A:LYS:HB3	7	1.28
(1,853)	1:58:A:VAL:HG21	1:64:A:LEU:HB3	7	1.28
(1,853)	1:58:A:VAL:HG22	1:64:A:LEU:HB3	7	1.28
(1,853)	1:58:A:VAL:HG23	1:64:A:LEU:HB3	7	1.28
(1,774)	1:54:A:ILE:HG12	1:63:A:GLN:HE22	10	1.28
(1,711)	1:48:A:LYS:HG2	1:128:A:THR:HG21	9	1.28
(1,711)	1:48:A:LYS:HG2	1:128:A:THR:HG22	9	1.28
(1,711)	1:48:A:LYS:HG2	1:128:A:THR:HG23	9	1.28
(1,711)	1:48:A:LYS:HG2	1:128:A:THR:HG21	10	1.28
(1,711)	1:48:A:LYS:HG2	1:128:A:THR:HG22	10	1.28
(1,711)	1:48:A:LYS:HG2	1:128:A:THR:HG23	10	1.28
(1,612)	1:42:A:ASN:HB3	1:125:A:VAL:HG21	9	1.28
(1,612)	1:42:A:ASN:HB3	1:125:A:VAL:HG22	9	1.28
(1,612)	1:42:A:ASN:HB3	1:125:A:VAL:HG23	9	1.28
(1,530)	1:36:A:PHE:HB3	1:121:A:GLY:H	3	1.28
(1,530)	1:36:A:PHE:HB3	1:121:A:GLY:H	8	1.28
(1,1615)	1:104:A:LEU:HA	1:105:A:GLU:HG2	1	1.27
(1,1334)	1:87:A:ILE:H	1:88:A:VAL:HG21	2	1.27
(1,1334)	1:87:A:ILE:H	1:88:A:VAL:HG22	2	1.27
(1,1334)	1:87:A:ILE:H	1:88:A:VAL:HG23	2	1.27
(1,1334)	1:87:A:ILE:H	1:88:A:VAL:HG21	5	1.27
(1,1334)	1:87:A:ILE:H	1:88:A:VAL:HG22	5	1.27
(1,1334)	1:87:A:ILE:H	1:88:A:VAL:HG23	5	1.27
(1,726)	1:49:A:LEU:HB3	1:50:A:PRO:HD3	5	1.27
(1,340)	1:25:A:ASN:HD22	1:92:A:GLU:HB3	7	1.27
(1,1938)	1:122:A:ILE:HG13	1:122:A:ILE:H	5	1.26
(1,1923)	1:122:A:ILE:HG13	1:121:A:GLY:HA2	10	1.26
(1,1774)	1:113:A:ALA:H	1:111:A:VAL:HG21	9	1.26
(1,1774)	1:113:A:ALA:H	1:111:A:VAL:HG22	9	1.26
(1,1774)	1:113:A:ALA:H	1:111:A:VAL:HG23	9	1.26
(1,1577)	1:101:A:ASP:H	1:103:A:PRO:HG3	1	1.26
(1,1577)	1:101:A:ASP:H	1:103:A:PRO:HG3	5	1.26
(1,1334)	1:87:A:ILE:H	1:88:A:VAL:HG21	10	1.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1334)	1:87:A:ILE:H	1:88:A:VAL:HG22	10	1.26
(1,1334)	1:87:A:ILE:H	1:88:A:VAL:HG23	10	1.26
(1,773)	1:54:A:ILE:HG12	1:58:A:VAL:H	5	1.26
(1,611)	1:42:A:ASN:HB2	1:112:A:LEU:HD11	9	1.26
(1,611)	1:42:A:ASN:HB2	1:112:A:LEU:HD12	9	1.26
(1,611)	1:42:A:ASN:HB2	1:112:A:LEU:HD13	9	1.26
(1,582)	1:40:A:ALA:H	1:124:A:HIS:HB3	9	1.26
(1,530)	1:36:A:PHE:HB3	1:121:A:GLY:H	1	1.26
(1,530)	1:36:A:PHE:HB3	1:121:A:GLY:H	4	1.26
(1,1615)	1:104:A:LEU:HA	1:105:A:GLU:HG2	7	1.25
(1,1516)	1:96:A:ILE:HG13	1:107:A:LYS:HB2	4	1.25
(1,1421)	1:91:A:LEU:HA	1:91:A:LEU:HD21	3	1.25
(1,1421)	1:91:A:LEU:HA	1:91:A:LEU:HD22	3	1.25
(1,1421)	1:91:A:LEU:HA	1:91:A:LEU:HD23	3	1.25
(1,1421)	1:91:A:LEU:HA	1:91:A:LEU:HD21	5	1.25
(1,1421)	1:91:A:LEU:HA	1:91:A:LEU:HD22	5	1.25
(1,1421)	1:91:A:LEU:HA	1:91:A:LEU:HD23	5	1.25
(1,769)	1:54:A:ILE:HG12	1:57:A:LEU:HD21	1	1.25
(1,769)	1:54:A:ILE:HG12	1:57:A:LEU:HD22	1	1.25
(1,769)	1:54:A:ILE:HG12	1:57:A:LEU:HD23	1	1.25
(1,611)	1:42:A:ASN:HB2	1:112:A:LEU:HD11	5	1.25
(1,611)	1:42:A:ASN:HB2	1:112:A:LEU:HD12	5	1.25
(1,611)	1:42:A:ASN:HB2	1:112:A:LEU:HD13	5	1.25
(1,1970)	1:124:A:HIS:HB2	1:113:A:ALA:H	10	1.24
(1,1923)	1:122:A:ILE:HG13	1:121:A:GLY:HA2	7	1.24
(1,1615)	1:104:A:LEU:HA	1:105:A:GLU:HG2	5	1.24
(1,1334)	1:87:A:ILE:H	1:88:A:VAL:HG21	1	1.24
(1,1334)	1:87:A:ILE:H	1:88:A:VAL:HG22	1	1.24
(1,1334)	1:87:A:ILE:H	1:88:A:VAL:HG23	1	1.24
(1,1334)	1:87:A:ILE:H	1:88:A:VAL:HG21	4	1.24
(1,1334)	1:87:A:ILE:H	1:88:A:VAL:HG22	4	1.24
(1,1334)	1:87:A:ILE:H	1:88:A:VAL:HG23	4	1.24
(1,1334)	1:87:A:ILE:H	1:88:A:VAL:HG21	8	1.24
(1,1334)	1:87:A:ILE:H	1:88:A:VAL:HG22	8	1.24
(1,1334)	1:87:A:ILE:H	1:88:A:VAL:HG23	8	1.24
(1,340)	1:25:A:ASN:HD22	1:92:A:GLU:HB3	8	1.24
(1,1923)	1:122:A:ILE:HG13	1:121:A:GLY:HA2	9	1.23
(1,1578)	1:102:A:ASN:HB3	1:101:A:ASP:H	10	1.23
(1,1528)	1:98:A:ILE:HG21	1:83:A:LYS:HB2	2	1.23
(1,1528)	1:98:A:ILE:HG22	1:83:A:LYS:HB2	2	1.23
(1,1528)	1:98:A:ILE:HG23	1:83:A:LYS:HB2	2	1.23
(1,1334)	1:87:A:ILE:H	1:88:A:VAL:HG21	7	1.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1334)	1:87:A:ILE:H	1:88:A:VAL:HG22	7	1.23
(1,1334)	1:87:A:ILE:H	1:88:A:VAL:HG23	7	1.23
(1,855)	1:59:A:GLN:HE22	1:56:A:SER:HA	3	1.23
(1,773)	1:54:A:ILE:HG12	1:58:A:VAL:H	7	1.23
(1,769)	1:54:A:ILE:HG12	1:57:A:LEU:HD21	9	1.23
(1,769)	1:54:A:ILE:HG12	1:57:A:LEU:HD22	9	1.23
(1,769)	1:54:A:ILE:HG12	1:57:A:LEU:HD23	9	1.23
(1,711)	1:48:A:LYS:HG2	1:128:A:THR:HG21	1	1.23
(1,711)	1:48:A:LYS:HG2	1:128:A:THR:HG22	1	1.23
(1,711)	1:48:A:LYS:HG2	1:128:A:THR:HG23	1	1.23
(1,4)	1:2:A:ALA:HB1	1:6:A:ASP:HB2	10	1.23
(1,4)	1:2:A:ALA:HB2	1:6:A:ASP:HB2	10	1.23
(1,4)	1:2:A:ALA:HB3	1:6:A:ASP:HB2	10	1.23
(1,1774)	1:113:A:ALA:H	1:111:A:VAL:HG21	4	1.22
(1,1774)	1:113:A:ALA:H	1:111:A:VAL:HG22	4	1.22
(1,1774)	1:113:A:ALA:H	1:111:A:VAL:HG23	4	1.22
(1,1421)	1:91:A:LEU:HA	1:91:A:LEU:HD21	10	1.22
(1,1421)	1:91:A:LEU:HA	1:91:A:LEU:HD22	10	1.22
(1,1421)	1:91:A:LEU:HA	1:91:A:LEU:HD23	10	1.22
(1,938)	1:63:A:GLN:HG2	1:67:A:ILE:HG13	10	1.22
(1,769)	1:54:A:ILE:HG12	1:57:A:LEU:HD21	3	1.22
(1,769)	1:54:A:ILE:HG12	1:57:A:LEU:HD22	3	1.22
(1,769)	1:54:A:ILE:HG12	1:57:A:LEU:HD23	3	1.22
(1,543)	1:37:A:THR:H	1:72:A:VAL:HG11	5	1.22
(1,543)	1:37:A:THR:H	1:72:A:VAL:HG12	5	1.22
(1,543)	1:37:A:THR:H	1:72:A:VAL:HG13	5	1.22
(1,340)	1:25:A:ASN:HD22	1:92:A:GLU:HB3	1	1.22
(1,4)	1:2:A:ALA:HB1	1:6:A:ASP:HB2	1	1.22
(1,4)	1:2:A:ALA:HB2	1:6:A:ASP:HB2	1	1.22
(1,4)	1:2:A:ALA:HB3	1:6:A:ASP:HB2	1	1.22
(1,1528)	1:98:A:ILE:HG21	1:83:A:LYS:HB2	10	1.21
(1,1528)	1:98:A:ILE:HG22	1:83:A:LYS:HB2	10	1.21
(1,1528)	1:98:A:ILE:HG23	1:83:A:LYS:HB2	10	1.21
(1,1334)	1:87:A:ILE:H	1:88:A:VAL:HG21	9	1.21
(1,1334)	1:87:A:ILE:H	1:88:A:VAL:HG22	9	1.21
(1,1334)	1:87:A:ILE:H	1:88:A:VAL:HG23	9	1.21
(1,775)	1:57:A:LEU:HD23	1:66:A:ARG:HD3	5	1.21
(1,4)	1:2:A:ALA:HB1	1:6:A:ASP:HB2	7	1.21
(1,4)	1:2:A:ALA:HB2	1:6:A:ASP:HB2	7	1.21
(1,4)	1:2:A:ALA:HB3	1:6:A:ASP:HB2	7	1.21
(1,1938)	1:122:A:ILE:HG13	1:122:A:ILE:H	7	1.2
(1,1577)	1:101:A:ASP:H	1:103:A:PRO:HG3	8	1.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1528)	1:98:A:ILE:HG21	1:83:A:LYS:HB2	7	1.2
(1,1528)	1:98:A:ILE:HG22	1:83:A:LYS:HB2	7	1.2
(1,1528)	1:98:A:ILE:HG23	1:83:A:LYS:HB2	7	1.2
(1,1528)	1:98:A:ILE:HG21	1:83:A:LYS:HB2	9	1.2
(1,1528)	1:98:A:ILE:HG22	1:83:A:LYS:HB2	9	1.2
(1,1528)	1:98:A:ILE:HG23	1:83:A:LYS:HB2	9	1.2
(1,1421)	1:91:A:LEU:HA	1:91:A:LEU:HD21	7	1.2
(1,1421)	1:91:A:LEU:HA	1:91:A:LEU:HD22	7	1.2
(1,1421)	1:91:A:LEU:HA	1:91:A:LEU:HD23	7	1.2
(1,936)	1:63:A:GLN:HG2	1:66:A:ARG:HD2	2	1.2
(1,881)	1:59:A:GLN:HB3	1:60:A:ASN:HD21	8	1.2
(1,807)	1:56:A:SER:HA	1:59:A:GLN:HB3	9	1.2
(1,612)	1:42:A:ASN:HB3	1:125:A:VAL:HG21	4	1.2
(1,612)	1:42:A:ASN:HB3	1:125:A:VAL:HG22	4	1.2
(1,612)	1:42:A:ASN:HB3	1:125:A:VAL:HG23	4	1.2
(1,430)	1:30:A:LEU:HD21	1:72:A:VAL:HG21	9	1.2
(1,430)	1:30:A:LEU:HD21	1:72:A:VAL:HG22	9	1.2
(1,430)	1:30:A:LEU:HD21	1:72:A:VAL:HG23	9	1.2
(1,430)	1:30:A:LEU:HD22	1:72:A:VAL:HG21	9	1.2
(1,430)	1:30:A:LEU:HD22	1:72:A:VAL:HG22	9	1.2
(1,430)	1:30:A:LEU:HD22	1:72:A:VAL:HG23	9	1.2
(1,430)	1:30:A:LEU:HD23	1:72:A:VAL:HG21	9	1.2
(1,430)	1:30:A:LEU:HD23	1:72:A:VAL:HG22	9	1.2
(1,430)	1:30:A:LEU:HD23	1:72:A:VAL:HG23	9	1.2
(1,232)	1:20:A:ALA:HA	1:68:A:LEU:HD11	10	1.2
(1,232)	1:20:A:ALA:HA	1:68:A:LEU:HD12	10	1.2
(1,232)	1:20:A:ALA:HA	1:68:A:LEU:HD13	10	1.2
(1,1938)	1:122:A:ILE:HG13	1:122:A:ILE:H	2	1.19
(1,1938)	1:122:A:ILE:HG13	1:122:A:ILE:H	4	1.19
(1,1938)	1:122:A:ILE:HG13	1:122:A:ILE:H	8	1.19
(1,1938)	1:122:A:ILE:HG13	1:122:A:ILE:H	9	1.19
(1,1938)	1:122:A:ILE:HG13	1:122:A:ILE:H	10	1.19
(1,1577)	1:101:A:ASP:H	1:103:A:PRO:HG3	2	1.19
(1,1421)	1:91:A:LEU:HA	1:91:A:LEU:HD21	1	1.19
(1,1421)	1:91:A:LEU:HA	1:91:A:LEU:HD22	1	1.19
(1,1421)	1:91:A:LEU:HA	1:91:A:LEU:HD23	1	1.19
(1,1421)	1:91:A:LEU:HA	1:91:A:LEU:HD21	2	1.19
(1,1421)	1:91:A:LEU:HA	1:91:A:LEU:HD22	2	1.19
(1,1421)	1:91:A:LEU:HA	1:91:A:LEU:HD23	2	1.19
(1,1258)	1:83:A:LYS:HB2	1:104:A:LEU:HD21	4	1.19
(1,1258)	1:83:A:LYS:HB2	1:104:A:LEU:HD22	4	1.19
(1,1258)	1:83:A:LYS:HB2	1:104:A:LEU:HD23	4	1.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1257)	1:96:A:ILE:HG13	1:107:A:LYS:HE2	7	1.19
(1,582)	1:40:A:ALA:H	1:124:A:HIS:HB3	3	1.19
(1,582)	1:40:A:ALA:H	1:124:A:HIS:HB3	8	1.19
(1,1970)	1:124:A:HIS:HB2	1:113:A:ALA:H	3	1.18
(1,1938)	1:122:A:ILE:HG13	1:122:A:ILE:H	1	1.18
(1,1647)	1:106:A:VAL:HG11	1:104:A:LEU:HD11	7	1.18
(1,1647)	1:106:A:VAL:HG11	1:104:A:LEU:HD12	7	1.18
(1,1647)	1:106:A:VAL:HG11	1:104:A:LEU:HD13	7	1.18
(1,1647)	1:106:A:VAL:HG12	1:104:A:LEU:HD11	7	1.18
(1,1647)	1:106:A:VAL:HG12	1:104:A:LEU:HD12	7	1.18
(1,1647)	1:106:A:VAL:HG12	1:104:A:LEU:HD13	7	1.18
(1,1647)	1:106:A:VAL:HG13	1:104:A:LEU:HD11	7	1.18
(1,1647)	1:106:A:VAL:HG13	1:104:A:LEU:HD12	7	1.18
(1,1647)	1:106:A:VAL:HG13	1:104:A:LEU:HD13	7	1.18
(1,1578)	1:102:A:ASN:HB3	1:101:A:ASP:H	3	1.18
(1,1577)	1:101:A:ASP:H	1:103:A:PRO:HG3	6	1.18
(1,1421)	1:91:A:LEU:HA	1:91:A:LEU:HD21	8	1.18
(1,1421)	1:91:A:LEU:HA	1:91:A:LEU:HD22	8	1.18
(1,1421)	1:91:A:LEU:HA	1:91:A:LEU:HD23	8	1.18
(1,1215)	1:104:A:LEU:HD13	1:79:A:ALA:H	10	1.18
(1,612)	1:42:A:ASN:HB3	1:125:A:VAL:HG21	2	1.18
(1,612)	1:42:A:ASN:HB3	1:125:A:VAL:HG22	2	1.18
(1,612)	1:42:A:ASN:HB3	1:125:A:VAL:HG23	2	1.18
(1,174)	1:15:A:SER:HB3	1:18:A:VAL:H	4	1.18
(1,1421)	1:91:A:LEU:HA	1:91:A:LEU:HD21	6	1.17
(1,1421)	1:91:A:LEU:HA	1:91:A:LEU:HD22	6	1.17
(1,1421)	1:91:A:LEU:HA	1:91:A:LEU:HD23	6	1.17
(1,1258)	1:83:A:LYS:HB2	1:104:A:LEU:HD21	1	1.17
(1,1258)	1:83:A:LYS:HB2	1:104:A:LEU:HD22	1	1.17
(1,1258)	1:83:A:LYS:HB2	1:104:A:LEU:HD23	1	1.17
(1,1938)	1:122:A:ILE:HG13	1:122:A:ILE:H	3	1.16
(1,1923)	1:122:A:ILE:HG13	1:121:A:GLY:HA2	6	1.16
(1,1629)	1:104:A:LEU:HD11	1:114:A:ALA:HB1	8	1.16
(1,1629)	1:104:A:LEU:HD11	1:114:A:ALA:HB2	8	1.16
(1,1629)	1:104:A:LEU:HD11	1:114:A:ALA:HB3	8	1.16
(1,1629)	1:104:A:LEU:HD12	1:114:A:ALA:HB1	8	1.16
(1,1629)	1:104:A:LEU:HD12	1:114:A:ALA:HB2	8	1.16
(1,1629)	1:104:A:LEU:HD12	1:114:A:ALA:HB3	8	1.16
(1,1629)	1:104:A:LEU:HD13	1:114:A:ALA:HB1	8	1.16
(1,1629)	1:104:A:LEU:HD13	1:114:A:ALA:HB2	8	1.16
(1,1629)	1:104:A:LEU:HD13	1:114:A:ALA:HB3	8	1.16
(1,1578)	1:102:A:ASN:HB3	1:101:A:ASP:H	1	1.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1519)	1:96:A:ILE:HG13	1:107:A:LYS:HE2	6	1.16
(1,1519)	1:96:A:ILE:HG13	1:107:A:LYS:HE3	6	1.16
(1,881)	1:59:A:GLN:HB3	1:60:A:ASN:HD21	2	1.16
(1,774)	1:54:A:ILE:HG12	1:63:A:GLN:HE22	2	1.16
(1,612)	1:42:A:ASN:HB3	1:125:A:VAL:HG21	7	1.16
(1,612)	1:42:A:ASN:HB3	1:125:A:VAL:HG22	7	1.16
(1,612)	1:42:A:ASN:HB3	1:125:A:VAL:HG23	7	1.16
(1,340)	1:25:A:ASN:HD22	1:92:A:GLU:HB3	6	1.16
(1,340)	1:25:A:ASN:HD22	1:92:A:GLU:HB3	10	1.16
(1,1774)	1:113:A:ALA:H	1:111:A:VAL:HG21	3	1.15
(1,1774)	1:113:A:ALA:H	1:111:A:VAL:HG22	3	1.15
(1,1774)	1:113:A:ALA:H	1:111:A:VAL:HG23	3	1.15
(1,1577)	1:101:A:ASP:H	1:103:A:PRO:HG3	7	1.15
(1,1258)	1:83:A:LYS:HB2	1:104:A:LEU:HD21	3	1.15
(1,1258)	1:83:A:LYS:HB2	1:104:A:LEU:HD22	3	1.15
(1,1258)	1:83:A:LYS:HB2	1:104:A:LEU:HD23	3	1.15
(1,881)	1:59:A:GLN:HB3	1:60:A:ASN:HD21	7	1.15
(1,773)	1:54:A:ILE:HG12	1:58:A:VAL:H	9	1.15
(1,174)	1:15:A:SER:HB3	1:18:A:VAL:H	5	1.15
(1,174)	1:15:A:SER:HB3	1:18:A:VAL:H	9	1.15
(1,167)	1:14:A:PHE:HB2	1:18:A:VAL:H	7	1.15
(1,1615)	1:104:A:LEU:HA	1:105:A:GLU:HG2	9	1.14
(1,1421)	1:91:A:LEU:HA	1:91:A:LEU:HD21	4	1.14
(1,1421)	1:91:A:LEU:HA	1:91:A:LEU:HD22	4	1.14
(1,1421)	1:91:A:LEU:HA	1:91:A:LEU:HD23	4	1.14
(1,1130)	1:77:A:TYR:HB3	1:81:A:ASP:HB3	6	1.14
(1,807)	1:56:A:SER:HA	1:59:A:GLN:HB3	3	1.14
(1,769)	1:54:A:ILE:HG12	1:57:A:LEU:HD21	6	1.14
(1,769)	1:54:A:ILE:HG12	1:57:A:LEU:HD22	6	1.14
(1,769)	1:54:A:ILE:HG12	1:57:A:LEU:HD23	6	1.14
(1,174)	1:15:A:SER:HB3	1:18:A:VAL:H	6	1.14
(1,167)	1:14:A:PHE:HB2	1:18:A:VAL:H	3	1.14
(1,1605)	1:104:A:LEU:HA	1:104:A:LEU:HD21	6	1.13
(1,1605)	1:104:A:LEU:HA	1:104:A:LEU:HD22	6	1.13
(1,1605)	1:104:A:LEU:HA	1:104:A:LEU:HD23	6	1.13
(1,1518)	1:96:A:ILE:HG13	1:107:A:LYS:HD2	7	1.13
(1,1518)	1:96:A:ILE:HG13	1:107:A:LYS:HD3	7	1.13
(1,898)	1:62:A:PRO:HB2	1:26:A:LEU:H	10	1.13
(1,520)	1:36:A:PHE:HA	1:72:A:VAL:HG11	2	1.13
(1,520)	1:36:A:PHE:HA	1:72:A:VAL:HG12	2	1.13
(1,520)	1:36:A:PHE:HA	1:72:A:VAL:HG13	2	1.13
(1,174)	1:15:A:SER:HB3	1:18:A:VAL:H	10	1.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1774)	1:113:A:ALA:H	1:111:A:VAL:HG21	7	1.12
(1,1774)	1:113:A:ALA:H	1:111:A:VAL:HG22	7	1.12
(1,1774)	1:113:A:ALA:H	1:111:A:VAL:HG23	7	1.12
(1,1774)	1:113:A:ALA:H	1:111:A:VAL:HG21	8	1.12
(1,1774)	1:113:A:ALA:H	1:111:A:VAL:HG22	8	1.12
(1,1774)	1:113:A:ALA:H	1:111:A:VAL:HG23	8	1.12
(1,1258)	1:83:A:LYS:HB2	1:104:A:LEU:HD21	5	1.12
(1,1258)	1:83:A:LYS:HB2	1:104:A:LEU:HD22	5	1.12
(1,1258)	1:83:A:LYS:HB2	1:104:A:LEU:HD23	5	1.12
(1,1215)	1:104:A:LEU:HD11	1:79:A:ALA:H	3	1.12
(1,936)	1:63:A:GLN:HG2	1:66:A:ARG:HD2	10	1.12
(1,914)	1:62:A:PRO:HB3	1:63:A:GLN:H	3	1.12
(1,853)	1:58:A:VAL:HG21	1:64:A:LEU:HB3	3	1.12
(1,853)	1:58:A:VAL:HG22	1:64:A:LEU:HB3	3	1.12
(1,853)	1:58:A:VAL:HG23	1:64:A:LEU:HB3	3	1.12
(1,1629)	1:104:A:LEU:HD11	1:114:A:ALA:HB1	6	1.11
(1,1629)	1:104:A:LEU:HD11	1:114:A:ALA:HB2	6	1.11
(1,1629)	1:104:A:LEU:HD11	1:114:A:ALA:HB3	6	1.11
(1,1629)	1:104:A:LEU:HD12	1:114:A:ALA:HB1	6	1.11
(1,1629)	1:104:A:LEU:HD12	1:114:A:ALA:HB2	6	1.11
(1,1629)	1:104:A:LEU:HD12	1:114:A:ALA:HB3	6	1.11
(1,1629)	1:104:A:LEU:HD13	1:114:A:ALA:HB1	6	1.11
(1,1629)	1:104:A:LEU:HD13	1:114:A:ALA:HB2	6	1.11
(1,1629)	1:104:A:LEU:HD13	1:114:A:ALA:HB3	6	1.11
(1,1605)	1:104:A:LEU:HA	1:104:A:LEU:HD21	1	1.11
(1,1605)	1:104:A:LEU:HA	1:104:A:LEU:HD22	1	1.11
(1,1605)	1:104:A:LEU:HA	1:104:A:LEU:HD23	1	1.11
(1,1605)	1:104:A:LEU:HA	1:104:A:LEU:HD21	4	1.11
(1,1605)	1:104:A:LEU:HA	1:104:A:LEU:HD22	4	1.11
(1,1605)	1:104:A:LEU:HA	1:104:A:LEU:HD23	4	1.11
(1,1257)	1:96:A:ILE:HG13	1:107:A:LYS:HE2	1	1.11
(1,853)	1:58:A:VAL:HG21	1:64:A:LEU:HB3	5	1.11
(1,853)	1:58:A:VAL:HG22	1:64:A:LEU:HB3	5	1.11
(1,853)	1:58:A:VAL:HG23	1:64:A:LEU:HB3	5	1.11
(1,773)	1:54:A:ILE:HG12	1:58:A:VAL:H	10	1.11
(1,769)	1:54:A:ILE:HG12	1:57:A:LEU:HD21	4	1.11
(1,769)	1:54:A:ILE:HG12	1:57:A:LEU:HD22	4	1.11
(1,769)	1:54:A:ILE:HG12	1:57:A:LEU:HD23	4	1.11
(1,313)	1:24:A:ALA:HB1	1:25:A:ASN:HB2	9	1.11
(1,313)	1:24:A:ALA:HB2	1:25:A:ASN:HB2	9	1.11
(1,313)	1:24:A:ALA:HB3	1:25:A:ASN:HB2	9	1.11
(1,1938)	1:122:A:ILE:HG13	1:122:A:ILE:H	6	1.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1629)	1:104:A:LEU:HD11	1:114:A:ALA:HB1	4	1.1
(1,1629)	1:104:A:LEU:HD11	1:114:A:ALA:HB2	4	1.1
(1,1629)	1:104:A:LEU:HD11	1:114:A:ALA:HB3	4	1.1
(1,1629)	1:104:A:LEU:HD12	1:114:A:ALA:HB1	4	1.1
(1,1629)	1:104:A:LEU:HD12	1:114:A:ALA:HB2	4	1.1
(1,1629)	1:104:A:LEU:HD12	1:114:A:ALA:HB3	4	1.1
(1,1629)	1:104:A:LEU:HD13	1:114:A:ALA:HB1	4	1.1
(1,1629)	1:104:A:LEU:HD13	1:114:A:ALA:HB2	4	1.1
(1,1629)	1:104:A:LEU:HD13	1:114:A:ALA:HB3	4	1.1
(1,1605)	1:104:A:LEU:HA	1:104:A:LEU:HD21	2	1.1
(1,1605)	1:104:A:LEU:HA	1:104:A:LEU:HD22	2	1.1
(1,1605)	1:104:A:LEU:HA	1:104:A:LEU:HD23	2	1.1
(1,914)	1:62:A:PRO:HB3	1:63:A:GLN:H	5	1.1
(1,313)	1:24:A:ALA:HB1	1:25:A:ASN:HB2	1	1.1
(1,313)	1:24:A:ALA:HB2	1:25:A:ASN:HB2	1	1.1
(1,313)	1:24:A:ALA:HB3	1:25:A:ASN:HB2	1	1.1
(1,313)	1:24:A:ALA:HB1	1:25:A:ASN:HB2	6	1.1
(1,313)	1:24:A:ALA:HB2	1:25:A:ASN:HB2	6	1.1
(1,313)	1:24:A:ALA:HB3	1:25:A:ASN:HB2	6	1.1
(1,313)	1:24:A:ALA:HB1	1:25:A:ASN:HB2	8	1.1
(1,313)	1:24:A:ALA:HB2	1:25:A:ASN:HB2	8	1.1
(1,313)	1:24:A:ALA:HB3	1:25:A:ASN:HB2	8	1.1
(1,1629)	1:104:A:LEU:HD11	1:114:A:ALA:HB1	7	1.09
(1,1629)	1:104:A:LEU:HD11	1:114:A:ALA:HB2	7	1.09
(1,1629)	1:104:A:LEU:HD11	1:114:A:ALA:HB3	7	1.09
(1,1629)	1:104:A:LEU:HD12	1:114:A:ALA:HB1	7	1.09
(1,1629)	1:104:A:LEU:HD12	1:114:A:ALA:HB2	7	1.09
(1,1629)	1:104:A:LEU:HD12	1:114:A:ALA:HB3	7	1.09
(1,1629)	1:104:A:LEU:HD13	1:114:A:ALA:HB1	7	1.09
(1,1629)	1:104:A:LEU:HD13	1:114:A:ALA:HB2	7	1.09
(1,1629)	1:104:A:LEU:HD13	1:114:A:ALA:HB3	7	1.09
(1,1605)	1:104:A:LEU:HA	1:104:A:LEU:HD21	7	1.09
(1,1605)	1:104:A:LEU:HA	1:104:A:LEU:HD22	7	1.09
(1,1605)	1:104:A:LEU:HA	1:104:A:LEU:HD23	7	1.09
(1,1605)	1:104:A:LEU:HA	1:104:A:LEU:HD21	9	1.09
(1,1605)	1:104:A:LEU:HA	1:104:A:LEU:HD22	9	1.09
(1,1605)	1:104:A:LEU:HA	1:104:A:LEU:HD23	9	1.09
(1,1605)	1:104:A:LEU:HA	1:104:A:LEU:HD21	10	1.09
(1,1605)	1:104:A:LEU:HA	1:104:A:LEU:HD22	10	1.09
(1,1605)	1:104:A:LEU:HA	1:104:A:LEU:HD23	10	1.09
(1,1257)	1:96:A:ILE:HG13	1:107:A:LYS:HE2	8	1.09
(1,914)	1:62:A:PRO:HB3	1:63:A:GLN:H	1	1.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,914)	1:62:A:PRO:HB3	1:63:A:GLN:H	4	1.09
(1,773)	1:54:A:ILE:HG12	1:58:A:VAL:H	8	1.09
(1,711)	1:48:A:LYS:HG2	1:128:A:THR:HG21	8	1.09
(1,711)	1:48:A:LYS:HG2	1:128:A:THR:HG22	8	1.09
(1,711)	1:48:A:LYS:HG2	1:128:A:THR:HG23	8	1.09
(1,313)	1:24:A:ALA:HB1	1:25:A:ASN:HB2	2	1.09
(1,313)	1:24:A:ALA:HB2	1:25:A:ASN:HB2	2	1.09
(1,313)	1:24:A:ALA:HB3	1:25:A:ASN:HB2	2	1.09
(1,313)	1:24:A:ALA:HB1	1:25:A:ASN:HB2	3	1.09
(1,313)	1:24:A:ALA:HB2	1:25:A:ASN:HB2	3	1.09
(1,313)	1:24:A:ALA:HB3	1:25:A:ASN:HB2	3	1.09
(1,174)	1:15:A:SER:HB3	1:18:A:VAL:H	3	1.09
(1,1629)	1:104:A:LEU:HD11	1:114:A:ALA:HB1	5	1.08
(1,1629)	1:104:A:LEU:HD11	1:114:A:ALA:HB2	5	1.08
(1,1629)	1:104:A:LEU:HD11	1:114:A:ALA:HB3	5	1.08
(1,1629)	1:104:A:LEU:HD12	1:114:A:ALA:HB1	5	1.08
(1,1629)	1:104:A:LEU:HD12	1:114:A:ALA:HB2	5	1.08
(1,1629)	1:104:A:LEU:HD12	1:114:A:ALA:HB3	5	1.08
(1,1629)	1:104:A:LEU:HD13	1:114:A:ALA:HB1	5	1.08
(1,1629)	1:104:A:LEU:HD13	1:114:A:ALA:HB2	5	1.08
(1,1629)	1:104:A:LEU:HD13	1:114:A:ALA:HB3	5	1.08
(1,1605)	1:104:A:LEU:HA	1:104:A:LEU:HD21	3	1.08
(1,1605)	1:104:A:LEU:HA	1:104:A:LEU:HD22	3	1.08
(1,1605)	1:104:A:LEU:HA	1:104:A:LEU:HD23	3	1.08
(1,1605)	1:104:A:LEU:HA	1:104:A:LEU:HD21	5	1.08
(1,1605)	1:104:A:LEU:HA	1:104:A:LEU:HD22	5	1.08
(1,1605)	1:104:A:LEU:HA	1:104:A:LEU:HD23	5	1.08
(1,1605)	1:104:A:LEU:HA	1:104:A:LEU:HD21	8	1.08
(1,1605)	1:104:A:LEU:HA	1:104:A:LEU:HD22	8	1.08
(1,1605)	1:104:A:LEU:HA	1:104:A:LEU:HD23	8	1.08
(1,1577)	1:101:A:ASP:H	1:103:A:PRO:HG3	9	1.08
(1,1441)	1:91:A:LEU:HD21	1:93:A:GLY:H	1	1.08
(1,1441)	1:91:A:LEU:HD22	1:93:A:GLY:H	1	1.08
(1,1441)	1:91:A:LEU:HD23	1:93:A:GLY:H	1	1.08
(1,1441)	1:91:A:LEU:HD21	1:93:A:GLY:H	8	1.08
(1,1441)	1:91:A:LEU:HD22	1:93:A:GLY:H	8	1.08
(1,1441)	1:91:A:LEU:HD23	1:93:A:GLY:H	8	1.08
(1,1147)	1:78:A:LYS:HA	1:78:A:LYS:HD3	1	1.08
(1,914)	1:62:A:PRO:HB3	1:63:A:GLN:H	7	1.08
(1,914)	1:62:A:PRO:HB3	1:63:A:GLN:H	8	1.08
(1,914)	1:62:A:PRO:HB3	1:63:A:GLN:H	10	1.08
(1,612)	1:42:A:ASN:HB3	1:125:A:VAL:HG21	5	1.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,612)	1:42:A:ASN:HB3	1:125:A:VAL:HG22	5	1.08
(1,612)	1:42:A:ASN:HB3	1:125:A:VAL:HG23	5	1.08
(1,340)	1:25:A:ASN:HD22	1:92:A:GLU:HB3	2	1.08
(1,313)	1:24:A:ALA:HB1	1:25:A:ASN:HB2	4	1.08
(1,313)	1:24:A:ALA:HB2	1:25:A:ASN:HB2	4	1.08
(1,313)	1:24:A:ALA:HB3	1:25:A:ASN:HB2	4	1.08
(1,313)	1:24:A:ALA:HB1	1:25:A:ASN:HB2	10	1.08
(1,313)	1:24:A:ALA:HB2	1:25:A:ASN:HB2	10	1.08
(1,313)	1:24:A:ALA:HB3	1:25:A:ASN:HB2	10	1.08
(1,174)	1:15:A:SER:HB3	1:18:A:VAL:H	7	1.08
(1,1600)	1:103:A:PRO:HG3	1:111:A:VAL:H	1	1.07
(1,1518)	1:96:A:ILE:HG13	1:107:A:LYS:HD2	4	1.07
(1,1518)	1:96:A:ILE:HG13	1:107:A:LYS:HD3	4	1.07
(1,1215)	1:104:A:LEU:HD13	1:79:A:ALA:H	2	1.07
(1,1147)	1:78:A:LYS:HA	1:78:A:LYS:HD3	7	1.07
(1,914)	1:62:A:PRO:HB3	1:63:A:GLN:H	2	1.07
(1,914)	1:62:A:PRO:HB3	1:63:A:GLN:H	9	1.07
(1,769)	1:54:A:ILE:HG12	1:57:A:LEU:HD21	5	1.07
(1,769)	1:54:A:ILE:HG12	1:57:A:LEU:HD22	5	1.07
(1,769)	1:54:A:ILE:HG12	1:57:A:LEU:HD23	5	1.07
(1,622)	1:44:A:ASP:HB2	1:42:A:ASN:HD21	1	1.07
(1,313)	1:24:A:ALA:HB1	1:25:A:ASN:HB2	5	1.07
(1,313)	1:24:A:ALA:HB2	1:25:A:ASN:HB2	5	1.07
(1,313)	1:24:A:ALA:HB3	1:25:A:ASN:HB2	5	1.07
(1,313)	1:24:A:ALA:HB1	1:25:A:ASN:HB2	7	1.07
(1,313)	1:24:A:ALA:HB2	1:25:A:ASN:HB2	7	1.07
(1,313)	1:24:A:ALA:HB3	1:25:A:ASN:HB2	7	1.07
(1,1629)	1:104:A:LEU:HD11	1:114:A:ALA:HB1	1	1.06
(1,1629)	1:104:A:LEU:HD11	1:114:A:ALA:HB2	1	1.06
(1,1629)	1:104:A:LEU:HD11	1:114:A:ALA:HB3	1	1.06
(1,1629)	1:104:A:LEU:HD12	1:114:A:ALA:HB1	1	1.06
(1,1629)	1:104:A:LEU:HD12	1:114:A:ALA:HB2	1	1.06
(1,1629)	1:104:A:LEU:HD12	1:114:A:ALA:HB3	1	1.06
(1,1629)	1:104:A:LEU:HD13	1:114:A:ALA:HB1	1	1.06
(1,1629)	1:104:A:LEU:HD13	1:114:A:ALA:HB2	1	1.06
(1,1629)	1:104:A:LEU:HD13	1:114:A:ALA:HB3	1	1.06
(1,1578)	1:102:A:ASN:HB3	1:101:A:ASP:H	2	1.06
(1,1441)	1:91:A:LEU:HD21	1:93:A:GLY:H	2	1.06
(1,1441)	1:91:A:LEU:HD22	1:93:A:GLY:H	2	1.06
(1,1441)	1:91:A:LEU:HD23	1:93:A:GLY:H	2	1.06
(1,1441)	1:91:A:LEU:HD21	1:93:A:GLY:H	6	1.06
(1,1441)	1:91:A:LEU:HD22	1:93:A:GLY:H	6	1.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1441)	1:91:A:LEU:HD23	1:93:A:GLY:H	6	1.06
(1,1147)	1:78:A:LYS:HA	1:78:A:LYS:HD3	9	1.06
(1,1029)	1:68:A:LEU:HD21	1:67:A:ILE:HG21	7	1.06
(1,1029)	1:68:A:LEU:HD21	1:67:A:ILE:HG22	7	1.06
(1,1029)	1:68:A:LEU:HD21	1:67:A:ILE:HG23	7	1.06
(1,1029)	1:68:A:LEU:HD22	1:67:A:ILE:HG21	7	1.06
(1,1029)	1:68:A:LEU:HD22	1:67:A:ILE:HG22	7	1.06
(1,1029)	1:68:A:LEU:HD22	1:67:A:ILE:HG23	7	1.06
(1,1029)	1:68:A:LEU:HD23	1:67:A:ILE:HG21	7	1.06
(1,1029)	1:68:A:LEU:HD23	1:67:A:ILE:HG22	7	1.06
(1,1029)	1:68:A:LEU:HD23	1:67:A:ILE:HG23	7	1.06
(1,914)	1:62:A:PRO:HB3	1:63:A:GLN:H	6	1.06
(1,142)	1:12:A:PRO:HB2	1:12:A:PRO:HD2	7	1.06
(1,1578)	1:102:A:ASN:HB3	1:101:A:ASP:H	8	1.05
(1,1215)	1:104:A:LEU:HD11	1:79:A:ALA:H	8	1.05
(1,1187)	1:80:A:THR:H	1:115:A:ASP:HB2	3	1.05
(1,1057)	1:70:A:TYR:HB2	1:70:A:TYR:H	10	1.05
(1,807)	1:56:A:SER:HA	1:59:A:GLN:HB3	10	1.05
(1,272)	1:22:A:LYS:HB3	1:22:A:LYS:HE2	6	1.05
(1,111)	1:9:A:VAL:H	1:9:A:VAL:HG21	9	1.05
(1,111)	1:9:A:VAL:H	1:9:A:VAL:HG22	9	1.05
(1,111)	1:9:A:VAL:H	1:9:A:VAL:HG23	9	1.05
(1,1600)	1:103:A:PRO:HG3	1:111:A:VAL:H	3	1.04
(1,1215)	1:104:A:LEU:HD12	1:79:A:ALA:H	9	1.04
(1,322)	1:24:A:ALA:HB1	1:64:A:LEU:HB2	2	1.04
(1,322)	1:24:A:ALA:HB2	1:64:A:LEU:HB2	2	1.04
(1,322)	1:24:A:ALA:HB3	1:64:A:LEU:HB2	2	1.04
(1,272)	1:22:A:LYS:HB3	1:22:A:LYS:HE2	5	1.04
(1,272)	1:22:A:LYS:HB3	1:22:A:LYS:HE2	9	1.04
(1,1377)	1:88:A:VAL:HG11	1:98:A:ILE:H	2	1.03
(1,775)	1:57:A:LEU:HD21	1:66:A:ARG:HD3	4	1.03
(1,773)	1:54:A:ILE:HG12	1:58:A:VAL:H	1	1.03
(1,174)	1:15:A:SER:HB3	1:18:A:VAL:H	2	1.03
(1,1662)	1:106:A:VAL:HG11	1:107:A:LYS:HG3	6	1.02
(1,1662)	1:106:A:VAL:HG12	1:107:A:LYS:HG3	6	1.02
(1,1662)	1:106:A:VAL:HG13	1:107:A:LYS:HG3	6	1.02
(1,1641)	1:106:A:VAL:HG21	1:39:A:PHE:HB2	6	1.02
(1,1641)	1:106:A:VAL:HG22	1:39:A:PHE:HB2	6	1.02
(1,1641)	1:106:A:VAL:HG23	1:39:A:PHE:HB2	6	1.02
(1,1629)	1:104:A:LEU:HD11	1:114:A:ALA:HB1	2	1.02
(1,1629)	1:104:A:LEU:HD11	1:114:A:ALA:HB2	2	1.02
(1,1629)	1:104:A:LEU:HD11	1:114:A:ALA:HB3	2	1.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1629)	1:104:A:LEU:HD12	1:114:A:ALA:HB1	2	1.02
(1,1629)	1:104:A:LEU:HD12	1:114:A:ALA:HB2	2	1.02
(1,1629)	1:104:A:LEU:HD12	1:114:A:ALA:HB3	2	1.02
(1,1629)	1:104:A:LEU:HD13	1:114:A:ALA:HB1	2	1.02
(1,1629)	1:104:A:LEU:HD13	1:114:A:ALA:HB2	2	1.02
(1,1629)	1:104:A:LEU:HD13	1:114:A:ALA:HB3	2	1.02
(1,1441)	1:91:A:LEU:HD21	1:93:A:GLY:H	10	1.02
(1,1441)	1:91:A:LEU:HD22	1:93:A:GLY:H	10	1.02
(1,1441)	1:91:A:LEU:HD23	1:93:A:GLY:H	10	1.02
(1,1147)	1:78:A:LYS:HA	1:78:A:LYS:HD3	6	1.02
(1,960)	1:64:A:LEU:HB3	1:67:A:ILE:HD11	10	1.02
(1,960)	1:64:A:LEU:HB3	1:67:A:ILE:HD12	10	1.02
(1,960)	1:64:A:LEU:HB3	1:67:A:ILE:HD13	10	1.02
(1,807)	1:56:A:SER:HA	1:59:A:GLN:HB3	1	1.02
(1,775)	1:57:A:LEU:HD21	1:66:A:ARG:HD3	9	1.02
(1,272)	1:22:A:LYS:HB3	1:22:A:LYS:HE2	1	1.02
(1,272)	1:22:A:LYS:HB3	1:22:A:LYS:HE2	4	1.02
(1,174)	1:15:A:SER:HB3	1:18:A:VAL:H	8	1.02
(1,111)	1:9:A:VAL:H	1:9:A:VAL:HG21	3	1.02
(1,111)	1:9:A:VAL:H	1:9:A:VAL:HG22	3	1.02
(1,111)	1:9:A:VAL:H	1:9:A:VAL:HG23	3	1.02
(1,1774)	1:113:A:ALA:H	1:111:A:VAL:HG21	2	1.01
(1,1774)	1:113:A:ALA:H	1:111:A:VAL:HG22	2	1.01
(1,1774)	1:113:A:ALA:H	1:111:A:VAL:HG23	2	1.01
(1,1600)	1:103:A:PRO:HG3	1:111:A:VAL:H	6	1.01
(1,1377)	1:88:A:VAL:HG13	1:98:A:ILE:H	9	1.01
(1,1215)	1:104:A:LEU:HD11	1:79:A:ALA:H	7	1.01
(1,1091)	1:73:A:VAL:HG11	1:74:A:ALA:H	10	1.01
(1,1091)	1:73:A:VAL:HG12	1:74:A:ALA:H	10	1.01
(1,1091)	1:73:A:VAL:HG13	1:74:A:ALA:H	10	1.01
(1,960)	1:64:A:LEU:HB3	1:67:A:ILE:HD11	2	1.01
(1,960)	1:64:A:LEU:HB3	1:67:A:ILE:HD12	2	1.01
(1,960)	1:64:A:LEU:HB3	1:67:A:ILE:HD13	2	1.01
(1,960)	1:64:A:LEU:HB3	1:67:A:ILE:HD11	6	1.01
(1,960)	1:64:A:LEU:HB3	1:67:A:ILE:HD12	6	1.01
(1,960)	1:64:A:LEU:HB3	1:67:A:ILE:HD13	6	1.01
(1,807)	1:56:A:SER:HA	1:59:A:GLN:HB3	6	1.01
(1,807)	1:56:A:SER:HA	1:59:A:GLN:HB3	7	1.01
(1,775)	1:57:A:LEU:HD22	1:66:A:ARG:HD2	1	1.01
(1,711)	1:48:A:LYS:HG2	1:128:A:THR:HG21	2	1.01
(1,711)	1:48:A:LYS:HG2	1:128:A:THR:HG22	2	1.01
(1,711)	1:48:A:LYS:HG2	1:128:A:THR:HG23	2	1.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,272)	1:22:A:LYS:HB3	1:22:A:LYS:HE2	10	1.01
(1,174)	1:15:A:SER:HB3	1:18:A:VAL:H	1	1.01
(1,1377)	1:88:A:VAL:HG11	1:98:A:ILE:H	7	1.0
(1,1253)	1:83:A:LYS:HG3	1:98:A:ILE:HG21	10	1.0
(1,1253)	1:83:A:LYS:HG3	1:98:A:ILE:HG22	10	1.0
(1,1253)	1:83:A:LYS:HG3	1:98:A:ILE:HG23	10	1.0
(1,1215)	1:104:A:LEU:HD13	1:79:A:ALA:H	4	1.0
(1,1091)	1:73:A:VAL:HG11	1:74:A:ALA:H	4	1.0
(1,1091)	1:73:A:VAL:HG12	1:74:A:ALA:H	4	1.0
(1,1091)	1:73:A:VAL:HG13	1:74:A:ALA:H	4	1.0
(1,960)	1:64:A:LEU:HB3	1:67:A:ILE:HD11	5	1.0
(1,960)	1:64:A:LEU:HB3	1:67:A:ILE:HD12	5	1.0
(1,960)	1:64:A:LEU:HB3	1:67:A:ILE:HD13	5	1.0
(1,775)	1:57:A:LEU:HD22	1:66:A:ARG:HD3	2	1.0
(1,430)	1:30:A:LEU:HD21	1:72:A:VAL:HG21	2	1.0
(1,430)	1:30:A:LEU:HD21	1:72:A:VAL:HG22	2	1.0
(1,430)	1:30:A:LEU:HD21	1:72:A:VAL:HG23	2	1.0
(1,430)	1:30:A:LEU:HD22	1:72:A:VAL:HG21	2	1.0
(1,430)	1:30:A:LEU:HD22	1:72:A:VAL:HG22	2	1.0
(1,430)	1:30:A:LEU:HD22	1:72:A:VAL:HG23	2	1.0
(1,430)	1:30:A:LEU:HD23	1:72:A:VAL:HG21	2	1.0
(1,430)	1:30:A:LEU:HD23	1:72:A:VAL:HG22	2	1.0
(1,430)	1:30:A:LEU:HD23	1:72:A:VAL:HG23	2	1.0
(1,272)	1:22:A:LYS:HB3	1:22:A:LYS:HE2	2	1.0
(1,1970)	1:124:A:HIS:HB2	1:113:A:ALA:H	8	0.99
(1,1848)	1:117:A:GLU:HB3	1:117:A:GLU:H	1	0.99
(1,1848)	1:117:A:GLU:HB3	1:117:A:GLU:H	5	0.99
(1,1774)	1:113:A:ALA:H	1:111:A:VAL:HG21	10	0.99
(1,1774)	1:113:A:ALA:H	1:111:A:VAL:HG22	10	0.99
(1,1774)	1:113:A:ALA:H	1:111:A:VAL:HG23	10	0.99
(1,1516)	1:96:A:ILE:HG13	1:107:A:LYS:HB2	1	0.99
(1,1441)	1:91:A:LEU:HD21	1:93:A:GLY:H	4	0.99
(1,1441)	1:91:A:LEU:HD22	1:93:A:GLY:H	4	0.99
(1,1441)	1:91:A:LEU:HD23	1:93:A:GLY:H	4	0.99
(1,1377)	1:88:A:VAL:HG11	1:98:A:ILE:H	10	0.99
(1,1215)	1:104:A:LEU:HD13	1:79:A:ALA:H	5	0.99
(1,1029)	1:68:A:LEU:HD21	1:67:A:ILE:HG21	3	0.99
(1,1029)	1:68:A:LEU:HD21	1:67:A:ILE:HG22	3	0.99
(1,1029)	1:68:A:LEU:HD21	1:67:A:ILE:HG23	3	0.99
(1,1029)	1:68:A:LEU:HD22	1:67:A:ILE:HG21	3	0.99
(1,1029)	1:68:A:LEU:HD22	1:67:A:ILE:HG22	3	0.99
(1,1029)	1:68:A:LEU:HD22	1:67:A:ILE:HG23	3	0.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1029)	1:68:A:LEU:HD23	1:67:A:ILE:HG21	3	0.99
(1,1029)	1:68:A:LEU:HD23	1:67:A:ILE:HG22	3	0.99
(1,1029)	1:68:A:LEU:HD23	1:67:A:ILE:HG23	3	0.99
(1,1029)	1:68:A:LEU:HD21	1:67:A:ILE:HG21	5	0.99
(1,1029)	1:68:A:LEU:HD21	1:67:A:ILE:HG22	5	0.99
(1,1029)	1:68:A:LEU:HD21	1:67:A:ILE:HG23	5	0.99
(1,1029)	1:68:A:LEU:HD22	1:67:A:ILE:HG21	5	0.99
(1,1029)	1:68:A:LEU:HD22	1:67:A:ILE:HG22	5	0.99
(1,1029)	1:68:A:LEU:HD22	1:67:A:ILE:HG23	5	0.99
(1,1029)	1:68:A:LEU:HD23	1:67:A:ILE:HG21	5	0.99
(1,1029)	1:68:A:LEU:HD23	1:67:A:ILE:HG22	5	0.99
(1,1029)	1:68:A:LEU:HD23	1:67:A:ILE:HG23	5	0.99
(1,960)	1:64:A:LEU:HB3	1:67:A:ILE:HD11	4	0.99
(1,960)	1:64:A:LEU:HB3	1:67:A:ILE:HD12	4	0.99
(1,960)	1:64:A:LEU:HB3	1:67:A:ILE:HD13	4	0.99
(1,960)	1:64:A:LEU:HB3	1:67:A:ILE:HD11	8	0.99
(1,960)	1:64:A:LEU:HB3	1:67:A:ILE:HD12	8	0.99
(1,960)	1:64:A:LEU:HB3	1:67:A:ILE:HD13	8	0.99
(1,960)	1:64:A:LEU:HB3	1:67:A:ILE:HD11	9	0.99
(1,960)	1:64:A:LEU:HB3	1:67:A:ILE:HD12	9	0.99
(1,960)	1:64:A:LEU:HB3	1:67:A:ILE:HD13	9	0.99
(1,898)	1:62:A:PRO:HB2	1:26:A:LEU:H	5	0.99
(1,898)	1:62:A:PRO:HB2	1:26:A:LEU:H	7	0.99
(1,807)	1:56:A:SER:HA	1:59:A:GLN:HB3	8	0.99
(1,612)	1:42:A:ASN:HB3	1:125:A:VAL:HG21	1	0.99
(1,612)	1:42:A:ASN:HB3	1:125:A:VAL:HG22	1	0.99
(1,612)	1:42:A:ASN:HB3	1:125:A:VAL:HG23	1	0.99
(1,1970)	1:124:A:HIS:HB2	1:113:A:ALA:H	2	0.98
(1,1970)	1:124:A:HIS:HB2	1:113:A:ALA:H	7	0.98
(1,1848)	1:117:A:GLU:HB3	1:117:A:GLU:H	3	0.98
(1,1848)	1:117:A:GLU:HB3	1:117:A:GLU:H	6	0.98
(1,1848)	1:117:A:GLU:HB3	1:117:A:GLU:H	7	0.98
(1,1848)	1:117:A:GLU:HB3	1:117:A:GLU:H	8	0.98
(1,1441)	1:91:A:LEU:HD21	1:93:A:GLY:H	7	0.98
(1,1441)	1:91:A:LEU:HD22	1:93:A:GLY:H	7	0.98
(1,1441)	1:91:A:LEU:HD23	1:93:A:GLY:H	7	0.98
(1,1253)	1:83:A:LYS:HG3	1:98:A:ILE:HG21	2	0.98
(1,1253)	1:83:A:LYS:HG3	1:98:A:ILE:HG22	2	0.98
(1,1253)	1:83:A:LYS:HG3	1:98:A:ILE:HG23	2	0.98
(1,1094)	1:73:A:VAL:HG11	1:91:A:LEU:H	9	0.98
(1,1094)	1:73:A:VAL:HG12	1:91:A:LEU:H	9	0.98
(1,1094)	1:73:A:VAL:HG13	1:91:A:LEU:H	9	0.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1091)	1:73:A:VAL:HG11	1:74:A:ALA:H	2	0.98
(1,1091)	1:73:A:VAL:HG12	1:74:A:ALA:H	2	0.98
(1,1091)	1:73:A:VAL:HG13	1:74:A:ALA:H	2	0.98
(1,1091)	1:73:A:VAL:HG11	1:74:A:ALA:H	6	0.98
(1,1091)	1:73:A:VAL:HG12	1:74:A:ALA:H	6	0.98
(1,1091)	1:73:A:VAL:HG13	1:74:A:ALA:H	6	0.98
(1,1075)	1:72:A:VAL:HG21	1:72:A:VAL:H	3	0.98
(1,1075)	1:72:A:VAL:HG22	1:72:A:VAL:H	3	0.98
(1,1075)	1:72:A:VAL:HG23	1:72:A:VAL:H	3	0.98
(1,4)	1:2:A:ALA:HB1	1:6:A:ASP:HB2	9	0.98
(1,4)	1:2:A:ALA:HB2	1:6:A:ASP:HB2	9	0.98
(1,4)	1:2:A:ALA:HB3	1:6:A:ASP:HB2	9	0.98
(1,1970)	1:124:A:HIS:HB2	1:113:A:ALA:H	9	0.97
(1,1848)	1:117:A:GLU:HB3	1:117:A:GLU:H	9	0.97
(1,1641)	1:106:A:VAL:HG21	1:39:A:PHE:HB2	4	0.97
(1,1641)	1:106:A:VAL:HG22	1:39:A:PHE:HB2	4	0.97
(1,1641)	1:106:A:VAL:HG23	1:39:A:PHE:HB2	4	0.97
(1,1615)	1:104:A:LEU:HA	1:105:A:GLU:HG2	10	0.97
(1,1600)	1:103:A:PRO:HG3	1:111:A:VAL:H	9	0.97
(1,1091)	1:73:A:VAL:HG11	1:74:A:ALA:H	1	0.97
(1,1091)	1:73:A:VAL:HG12	1:74:A:ALA:H	1	0.97
(1,1091)	1:73:A:VAL:HG13	1:74:A:ALA:H	1	0.97
(1,1029)	1:68:A:LEU:HD21	1:67:A:ILE:HG21	2	0.97
(1,1029)	1:68:A:LEU:HD21	1:67:A:ILE:HG22	2	0.97
(1,1029)	1:68:A:LEU:HD21	1:67:A:ILE:HG23	2	0.97
(1,1029)	1:68:A:LEU:HD22	1:67:A:ILE:HG21	2	0.97
(1,1029)	1:68:A:LEU:HD22	1:67:A:ILE:HG22	2	0.97
(1,1029)	1:68:A:LEU:HD22	1:67:A:ILE:HG23	2	0.97
(1,1029)	1:68:A:LEU:HD23	1:67:A:ILE:HG21	2	0.97
(1,1029)	1:68:A:LEU:HD23	1:67:A:ILE:HG22	2	0.97
(1,1029)	1:68:A:LEU:HD23	1:67:A:ILE:HG23	2	0.97
(1,960)	1:64:A:LEU:HB3	1:67:A:ILE:HD11	7	0.97
(1,960)	1:64:A:LEU:HB3	1:67:A:ILE:HD12	7	0.97
(1,960)	1:64:A:LEU:HB3	1:67:A:ILE:HD13	7	0.97
(1,807)	1:56:A:SER:HA	1:59:A:GLN:HB3	4	0.97
(1,807)	1:56:A:SER:HA	1:59:A:GLN:HB3	5	0.97
(1,582)	1:40:A:ALA:H	1:124:A:HIS:HB3	10	0.97
(1,1600)	1:103:A:PRO:HG3	1:111:A:VAL:H	10	0.96
(1,1377)	1:88:A:VAL:HG12	1:98:A:ILE:H	4	0.96
(1,1091)	1:73:A:VAL:HG11	1:74:A:ALA:H	3	0.96
(1,1091)	1:73:A:VAL:HG12	1:74:A:ALA:H	3	0.96
(1,1091)	1:73:A:VAL:HG13	1:74:A:ALA:H	3	0.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1091)	1:73:A:VAL:HG11	1:74:A:ALA:H	7	0.96
(1,1091)	1:73:A:VAL:HG12	1:74:A:ALA:H	7	0.96
(1,1091)	1:73:A:VAL:HG13	1:74:A:ALA:H	7	0.96
(1,1075)	1:72:A:VAL:HG21	1:72:A:VAL:H	1	0.96
(1,1075)	1:72:A:VAL:HG22	1:72:A:VAL:H	1	0.96
(1,1075)	1:72:A:VAL:HG23	1:72:A:VAL:H	1	0.96
(1,1075)	1:72:A:VAL:HG21	1:72:A:VAL:H	5	0.96
(1,1075)	1:72:A:VAL:HG22	1:72:A:VAL:H	5	0.96
(1,1075)	1:72:A:VAL:HG23	1:72:A:VAL:H	5	0.96
(1,1029)	1:68:A:LEU:HD21	1:67:A:ILE:HG21	8	0.96
(1,1029)	1:68:A:LEU:HD21	1:67:A:ILE:HG22	8	0.96
(1,1029)	1:68:A:LEU:HD21	1:67:A:ILE:HG23	8	0.96
(1,1029)	1:68:A:LEU:HD22	1:67:A:ILE:HG21	8	0.96
(1,1029)	1:68:A:LEU:HD22	1:67:A:ILE:HG22	8	0.96
(1,1029)	1:68:A:LEU:HD22	1:67:A:ILE:HG23	8	0.96
(1,1029)	1:68:A:LEU:HD23	1:67:A:ILE:HG21	8	0.96
(1,1029)	1:68:A:LEU:HD23	1:67:A:ILE:HG22	8	0.96
(1,1029)	1:68:A:LEU:HD23	1:67:A:ILE:HG23	8	0.96
(1,1029)	1:68:A:LEU:HD21	1:67:A:ILE:HG21	10	0.96
(1,1029)	1:68:A:LEU:HD21	1:67:A:ILE:HG22	10	0.96
(1,1029)	1:68:A:LEU:HD21	1:67:A:ILE:HG23	10	0.96
(1,1029)	1:68:A:LEU:HD22	1:67:A:ILE:HG21	10	0.96
(1,1029)	1:68:A:LEU:HD22	1:67:A:ILE:HG22	10	0.96
(1,1029)	1:68:A:LEU:HD22	1:67:A:ILE:HG23	10	0.96
(1,1029)	1:68:A:LEU:HD23	1:67:A:ILE:HG21	10	0.96
(1,1029)	1:68:A:LEU:HD23	1:67:A:ILE:HG22	10	0.96
(1,1029)	1:68:A:LEU:HD23	1:67:A:ILE:HG23	10	0.96
(1,960)	1:64:A:LEU:HB3	1:67:A:ILE:HD11	3	0.96
(1,960)	1:64:A:LEU:HB3	1:67:A:ILE:HD12	3	0.96
(1,960)	1:64:A:LEU:HB3	1:67:A:ILE:HD13	3	0.96
(1,807)	1:56:A:SER:HA	1:59:A:GLN:HB3	2	0.96
(1,775)	1:57:A:LEU:HD22	1:66:A:ARG:HD3	7	0.96
(1,769)	1:54:A:ILE:HG12	1:57:A:LEU:HD21	8	0.96
(1,769)	1:54:A:ILE:HG12	1:57:A:LEU:HD22	8	0.96
(1,769)	1:54:A:ILE:HG12	1:57:A:LEU:HD23	8	0.96
(1,711)	1:48:A:LYS:HG2	1:128:A:THR:HG21	5	0.96
(1,711)	1:48:A:LYS:HG2	1:128:A:THR:HG22	5	0.96
(1,711)	1:48:A:LYS:HG2	1:128:A:THR:HG23	5	0.96
(1,711)	1:48:A:LYS:HG2	1:128:A:THR:HG21	6	0.96
(1,711)	1:48:A:LYS:HG2	1:128:A:THR:HG22	6	0.96
(1,711)	1:48:A:LYS:HG2	1:128:A:THR:HG23	6	0.96
(1,4)	1:2:A:ALA:HB1	1:6:A:ASP:HB2	2	0.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4)	1:2:A:ALA:HB2	1:6:A:ASP:HB2	2	0.96
(1,4)	1:2:A:ALA:HB3	1:6:A:ASP:HB2	2	0.96
(1,1983)	1:125:A:VAL:HG11	1:40:A:ALA:HB1	1	0.95
(1,1983)	1:125:A:VAL:HG11	1:40:A:ALA:HB2	1	0.95
(1,1983)	1:125:A:VAL:HG11	1:40:A:ALA:HB3	1	0.95
(1,1983)	1:125:A:VAL:HG12	1:40:A:ALA:HB1	1	0.95
(1,1983)	1:125:A:VAL:HG12	1:40:A:ALA:HB2	1	0.95
(1,1983)	1:125:A:VAL:HG12	1:40:A:ALA:HB3	1	0.95
(1,1983)	1:125:A:VAL:HG13	1:40:A:ALA:HB1	1	0.95
(1,1983)	1:125:A:VAL:HG13	1:40:A:ALA:HB2	1	0.95
(1,1983)	1:125:A:VAL:HG13	1:40:A:ALA:HB3	1	0.95
(1,1377)	1:88:A:VAL:HG11	1:98:A:ILE:H	1	0.95
(1,1377)	1:88:A:VAL:HG12	1:98:A:ILE:H	3	0.95
(1,1091)	1:73:A:VAL:HG11	1:74:A:ALA:H	5	0.95
(1,1091)	1:73:A:VAL:HG12	1:74:A:ALA:H	5	0.95
(1,1091)	1:73:A:VAL:HG13	1:74:A:ALA:H	5	0.95
(1,1075)	1:72:A:VAL:HG21	1:72:A:VAL:H	4	0.95
(1,1075)	1:72:A:VAL:HG22	1:72:A:VAL:H	4	0.95
(1,1075)	1:72:A:VAL:HG23	1:72:A:VAL:H	4	0.95
(1,1029)	1:68:A:LEU:HD21	1:67:A:ILE:HG21	9	0.95
(1,1029)	1:68:A:LEU:HD21	1:67:A:ILE:HG22	9	0.95
(1,1029)	1:68:A:LEU:HD21	1:67:A:ILE:HG23	9	0.95
(1,1029)	1:68:A:LEU:HD22	1:67:A:ILE:HG21	9	0.95
(1,1029)	1:68:A:LEU:HD22	1:67:A:ILE:HG22	9	0.95
(1,1029)	1:68:A:LEU:HD22	1:67:A:ILE:HG23	9	0.95
(1,1029)	1:68:A:LEU:HD23	1:67:A:ILE:HG21	9	0.95
(1,1029)	1:68:A:LEU:HD23	1:67:A:ILE:HG22	9	0.95
(1,1029)	1:68:A:LEU:HD23	1:67:A:ILE:HG23	9	0.95
(1,612)	1:42:A:ASN:HB3	1:125:A:VAL:HG21	6	0.95
(1,612)	1:42:A:ASN:HB3	1:125:A:VAL:HG22	6	0.95
(1,612)	1:42:A:ASN:HB3	1:125:A:VAL:HG23	6	0.95
(1,527)	1:36:A:PHE:HB2	1:120:A:ASN:HD22	2	0.95
(1,527)	1:36:A:PHE:HB2	1:120:A:ASN:HD22	6	0.95
(1,1377)	1:88:A:VAL:HG13	1:98:A:ILE:H	5	0.94
(1,1377)	1:88:A:VAL:HG13	1:98:A:ILE:H	8	0.94
(1,1253)	1:83:A:LYS:HG3	1:98:A:ILE:HG21	9	0.94
(1,1253)	1:83:A:LYS:HG3	1:98:A:ILE:HG22	9	0.94
(1,1253)	1:83:A:LYS:HG3	1:98:A:ILE:HG23	9	0.94
(1,1147)	1:78:A:LYS:HA	1:78:A:LYS:HD3	10	0.94
(1,1075)	1:72:A:VAL:HG21	1:72:A:VAL:H	6	0.94
(1,1075)	1:72:A:VAL:HG22	1:72:A:VAL:H	6	0.94
(1,1075)	1:72:A:VAL:HG23	1:72:A:VAL:H	6	0.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1075)	1:72:A:VAL:HG21	1:72:A:VAL:H	9	0.94
(1,1075)	1:72:A:VAL:HG22	1:72:A:VAL:H	9	0.94
(1,1075)	1:72:A:VAL:HG23	1:72:A:VAL:H	9	0.94
(1,711)	1:48:A:LYS:HG2	1:128:A:THR:HG21	4	0.94
(1,711)	1:48:A:LYS:HG2	1:128:A:THR:HG22	4	0.94
(1,711)	1:48:A:LYS:HG2	1:128:A:THR:HG23	4	0.94
(1,342)	1:36:A:PHE:HB2	1:75:A:GLY:H	10	0.94
(1,272)	1:22:A:LYS:HB3	1:22:A:LYS:HE2	3	0.94
(1,1662)	1:106:A:VAL:HG11	1:107:A:LYS:HG3	2	0.93
(1,1662)	1:106:A:VAL:HG12	1:107:A:LYS:HG3	2	0.93
(1,1662)	1:106:A:VAL:HG13	1:107:A:LYS:HG3	2	0.93
(1,1253)	1:83:A:LYS:HG3	1:98:A:ILE:HG21	7	0.93
(1,1253)	1:83:A:LYS:HG3	1:98:A:ILE:HG22	7	0.93
(1,1253)	1:83:A:LYS:HG3	1:98:A:ILE:HG23	7	0.93
(1,1149)	1:78:A:LYS:HG3	1:78:A:LYS:HE2	5	0.93
(1,1149)	1:78:A:LYS:HG3	1:78:A:LYS:HE3	5	0.93
(1,1091)	1:73:A:VAL:HG11	1:74:A:ALA:H	8	0.93
(1,1091)	1:73:A:VAL:HG12	1:74:A:ALA:H	8	0.93
(1,1091)	1:73:A:VAL:HG13	1:74:A:ALA:H	8	0.93
(1,1075)	1:72:A:VAL:HG21	1:72:A:VAL:H	8	0.93
(1,1075)	1:72:A:VAL:HG22	1:72:A:VAL:H	8	0.93
(1,1075)	1:72:A:VAL:HG23	1:72:A:VAL:H	8	0.93
(1,898)	1:62:A:PRO:HB2	1:26:A:LEU:H	6	0.93
(1,775)	1:57:A:LEU:HD21	1:66:A:ARG:HD3	6	0.93
(1,622)	1:44:A:ASP:HB2	1:42:A:ASN:HD21	10	0.93
(1,186)	1:18:A:VAL:HG11	1:14:A:PHE:H	8	0.93
(1,186)	1:18:A:VAL:HG12	1:14:A:PHE:H	8	0.93
(1,186)	1:18:A:VAL:HG13	1:14:A:PHE:H	8	0.93
(1,186)	1:18:A:VAL:HG11	1:14:A:PHE:H	9	0.93
(1,186)	1:18:A:VAL:HG12	1:14:A:PHE:H	9	0.93
(1,186)	1:18:A:VAL:HG13	1:14:A:PHE:H	9	0.93
(1,1600)	1:103:A:PRO:HG3	1:111:A:VAL:H	7	0.92
(1,1519)	1:96:A:ILE:HG13	1:107:A:LYS:HE2	7	0.92
(1,1519)	1:96:A:ILE:HG13	1:107:A:LYS:HE3	7	0.92
(1,1391)	1:89:A:THR:HG21	1:93:A:GLY:HA3	7	0.92
(1,1391)	1:89:A:THR:HG22	1:93:A:GLY:HA3	7	0.92
(1,1391)	1:89:A:THR:HG23	1:93:A:GLY:HA3	7	0.92
(1,1147)	1:78:A:LYS:HA	1:78:A:LYS:HD3	4	0.92
(1,1075)	1:72:A:VAL:HG21	1:72:A:VAL:H	7	0.92
(1,1075)	1:72:A:VAL:HG22	1:72:A:VAL:H	7	0.92
(1,1075)	1:72:A:VAL:HG23	1:72:A:VAL:H	7	0.92
(1,1029)	1:68:A:LEU:HD21	1:67:A:ILE:HG21	4	0.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1029)	1:68:A:LEU:HD21	1:67:A:ILE:HG22	4	0.92
(1,1029)	1:68:A:LEU:HD21	1:67:A:ILE:HG23	4	0.92
(1,1029)	1:68:A:LEU:HD22	1:67:A:ILE:HG21	4	0.92
(1,1029)	1:68:A:LEU:HD22	1:67:A:ILE:HG22	4	0.92
(1,1029)	1:68:A:LEU:HD22	1:67:A:ILE:HG23	4	0.92
(1,1029)	1:68:A:LEU:HD23	1:67:A:ILE:HG21	4	0.92
(1,1029)	1:68:A:LEU:HD23	1:67:A:ILE:HG22	4	0.92
(1,1029)	1:68:A:LEU:HD23	1:67:A:ILE:HG23	4	0.92
(1,1029)	1:68:A:LEU:HD21	1:67:A:ILE:HG21	6	0.92
(1,1029)	1:68:A:LEU:HD21	1:67:A:ILE:HG22	6	0.92
(1,1029)	1:68:A:LEU:HD21	1:67:A:ILE:HG23	6	0.92
(1,1029)	1:68:A:LEU:HD22	1:67:A:ILE:HG21	6	0.92
(1,1029)	1:68:A:LEU:HD22	1:67:A:ILE:HG22	6	0.92
(1,1029)	1:68:A:LEU:HD22	1:67:A:ILE:HG23	6	0.92
(1,1029)	1:68:A:LEU:HD23	1:67:A:ILE:HG21	6	0.92
(1,1029)	1:68:A:LEU:HD23	1:67:A:ILE:HG22	6	0.92
(1,1029)	1:68:A:LEU:HD23	1:67:A:ILE:HG23	6	0.92
(1,898)	1:62:A:PRO:HB2	1:26:A:LEU:H	1	0.92
(1,708)	1:48:A:LYS:HG3	1:49:A:LEU:H	1	0.92
(1,708)	1:48:A:LYS:HG3	1:49:A:LEU:H	2	0.92
(1,527)	1:36:A:PHE:HB2	1:120:A:ASN:HD22	7	0.92
(1,186)	1:18:A:VAL:HG11	1:14:A:PHE:H	4	0.92
(1,186)	1:18:A:VAL:HG12	1:14:A:PHE:H	4	0.92
(1,186)	1:18:A:VAL:HG13	1:14:A:PHE:H	4	0.92
(1,186)	1:18:A:VAL:HG11	1:14:A:PHE:H	5	0.92
(1,186)	1:18:A:VAL:HG12	1:14:A:PHE:H	5	0.92
(1,186)	1:18:A:VAL:HG13	1:14:A:PHE:H	5	0.92
(1,186)	1:18:A:VAL:HG11	1:14:A:PHE:H	7	0.92
(1,186)	1:18:A:VAL:HG12	1:14:A:PHE:H	7	0.92
(1,186)	1:18:A:VAL:HG13	1:14:A:PHE:H	7	0.92
(1,169)	1:15:A:SER:HB3	1:15:A:SER:H	3	0.92
(1,1983)	1:125:A:VAL:HG11	1:40:A:ALA:HB1	4	0.91
(1,1983)	1:125:A:VAL:HG11	1:40:A:ALA:HB2	4	0.91
(1,1983)	1:125:A:VAL:HG11	1:40:A:ALA:HB3	4	0.91
(1,1983)	1:125:A:VAL:HG12	1:40:A:ALA:HB1	4	0.91
(1,1983)	1:125:A:VAL:HG12	1:40:A:ALA:HB2	4	0.91
(1,1983)	1:125:A:VAL:HG12	1:40:A:ALA:HB3	4	0.91
(1,1983)	1:125:A:VAL:HG13	1:40:A:ALA:HB1	4	0.91
(1,1983)	1:125:A:VAL:HG13	1:40:A:ALA:HB2	4	0.91
(1,1983)	1:125:A:VAL:HG13	1:40:A:ALA:HB3	4	0.91
(1,1600)	1:103:A:PRO:HG3	1:111:A:VAL:H	8	0.91
(1,1519)	1:96:A:ILE:HG13	1:107:A:LYS:HE2	4	0.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1519)	1:96:A:ILE:HG13	1:107:A:LYS:HE3	4	0.91
(1,1414)	1:91:A:LEU:HD22	1:74:A:ALA:HB1	10	0.91
(1,1391)	1:89:A:THR:HG21	1:93:A:GLY:HA3	5	0.91
(1,1391)	1:89:A:THR:HG22	1:93:A:GLY:HA3	5	0.91
(1,1391)	1:89:A:THR:HG23	1:93:A:GLY:HA3	5	0.91
(1,1377)	1:88:A:VAL:HG13	1:98:A:ILE:H	6	0.91
(1,1187)	1:80:A:THR:H	1:115:A:ASP:HB2	7	0.91
(1,1075)	1:72:A:VAL:HG21	1:72:A:VAL:H	10	0.91
(1,1075)	1:72:A:VAL:HG22	1:72:A:VAL:H	10	0.91
(1,1075)	1:72:A:VAL:HG23	1:72:A:VAL:H	10	0.91
(1,874)	1:59:A:GLN:HE22	1:59:A:GLN:HB2	1	0.91
(1,874)	1:59:A:GLN:HE22	1:59:A:GLN:HB2	2	0.91
(1,874)	1:59:A:GLN:HE22	1:59:A:GLN:HB2	5	0.91
(1,874)	1:59:A:GLN:HE22	1:59:A:GLN:HB2	6	0.91
(1,874)	1:59:A:GLN:HE22	1:59:A:GLN:HB2	7	0.91
(1,775)	1:57:A:LEU:HD21	1:66:A:ARG:HD3	8	0.91
(1,735)	1:52:A:GLY:HA2	1:54:A:ILE:H	8	0.91
(1,708)	1:48:A:LYS:HG3	1:49:A:LEU:H	8	0.91
(1,169)	1:15:A:SER:HB3	1:15:A:SER:H	1	0.91
(1,169)	1:15:A:SER:HB3	1:15:A:SER:H	2	0.91
(1,169)	1:15:A:SER:HB3	1:15:A:SER:H	8	0.91
(1,169)	1:15:A:SER:HB3	1:15:A:SER:H	9	0.91
(1,1600)	1:103:A:PRO:HG3	1:111:A:VAL:H	5	0.9
(1,1441)	1:91:A:LEU:HD21	1:93:A:GLY:H	3	0.9
(1,1441)	1:91:A:LEU:HD22	1:93:A:GLY:H	3	0.9
(1,1441)	1:91:A:LEU:HD23	1:93:A:GLY:H	3	0.9
(1,1391)	1:89:A:THR:HG21	1:93:A:GLY:HA3	8	0.9
(1,1391)	1:89:A:THR:HG22	1:93:A:GLY:HA3	8	0.9
(1,1391)	1:89:A:THR:HG23	1:93:A:GLY:HA3	8	0.9
(1,1215)	1:104:A:LEU:HD12	1:79:A:ALA:H	1	0.9
(1,1094)	1:73:A:VAL:HG11	1:91:A:LEU:H	4	0.9
(1,1094)	1:73:A:VAL:HG12	1:91:A:LEU:H	4	0.9
(1,1094)	1:73:A:VAL:HG13	1:91:A:LEU:H	4	0.9
(1,874)	1:59:A:GLN:HE22	1:59:A:GLN:HB2	4	0.9
(1,874)	1:59:A:GLN:HE22	1:59:A:GLN:HB2	8	0.9
(1,874)	1:59:A:GLN:HE22	1:59:A:GLN:HB2	10	0.9
(1,342)	1:36:A:PHE:HB2	1:75:A:GLY:H	4	0.9
(1,169)	1:15:A:SER:HB3	1:15:A:SER:H	4	0.9
(1,169)	1:15:A:SER:HB3	1:15:A:SER:H	5	0.9
(1,1519)	1:96:A:ILE:HG13	1:107:A:LYS:HE2	8	0.89
(1,1519)	1:96:A:ILE:HG13	1:107:A:LYS:HE3	8	0.89
(1,1391)	1:89:A:THR:HG21	1:93:A:GLY:HA3	6	0.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1391)	1:89:A:THR:HG22	1:93:A:GLY:HA3	6	0.89
(1,1391)	1:89:A:THR:HG23	1:93:A:GLY:HA3	6	0.89
(1,898)	1:62:A:PRO:HB2	1:26:A:LEU:H	3	0.89
(1,272)	1:22:A:LYS:HB3	1:22:A:LYS:HE2	8	0.89
(1,186)	1:18:A:VAL:HG11	1:14:A:PHE:H	2	0.89
(1,186)	1:18:A:VAL:HG12	1:14:A:PHE:H	2	0.89
(1,186)	1:18:A:VAL:HG13	1:14:A:PHE:H	2	0.89
(1,169)	1:15:A:SER:HB3	1:15:A:SER:H	7	0.89
(1,169)	1:15:A:SER:HB3	1:15:A:SER:H	10	0.89
(1,1720)	1:110:A:THR:HG21	1:103:A:PRO:HB3	1	0.88
(1,1720)	1:110:A:THR:HG22	1:103:A:PRO:HB3	1	0.88
(1,1720)	1:110:A:THR:HG23	1:103:A:PRO:HB3	1	0.88
(1,1391)	1:89:A:THR:HG21	1:93:A:GLY:HA3	1	0.88
(1,1391)	1:89:A:THR:HG22	1:93:A:GLY:HA3	1	0.88
(1,1391)	1:89:A:THR:HG23	1:93:A:GLY:HA3	1	0.88
(1,960)	1:64:A:LEU:HB3	1:67:A:ILE:HD11	1	0.88
(1,960)	1:64:A:LEU:HB3	1:67:A:ILE:HD12	1	0.88
(1,960)	1:64:A:LEU:HB3	1:67:A:ILE:HD13	1	0.88
(1,898)	1:62:A:PRO:HB2	1:26:A:LEU:H	4	0.88
(1,874)	1:59:A:GLN:HE22	1:59:A:GLN:HB2	3	0.88
(1,874)	1:59:A:GLN:HE22	1:59:A:GLN:HB2	9	0.88
(1,773)	1:54:A:ILE:HG12	1:58:A:VAL:H	4	0.88
(1,622)	1:44:A:ASP:HB2	1:42:A:ASN:HD21	9	0.88
(1,342)	1:36:A:PHE:HB2	1:75:A:GLY:H	8	0.88
(1,340)	1:25:A:ASN:HD22	1:92:A:GLU:HB3	5	0.88
(1,322)	1:24:A:ALA:HB1	1:64:A:LEU:HB2	8	0.88
(1,322)	1:24:A:ALA:HB2	1:64:A:LEU:HB2	8	0.88
(1,322)	1:24:A:ALA:HB3	1:64:A:LEU:HB2	8	0.88
(1,1994)	1:125:A:VAL:HG11	1:125:A:VAL:H	6	0.87
(1,1994)	1:125:A:VAL:HG12	1:125:A:VAL:H	6	0.87
(1,1994)	1:125:A:VAL:HG13	1:125:A:VAL:H	6	0.87
(1,1983)	1:125:A:VAL:HG11	1:40:A:ALA:HB1	5	0.87
(1,1983)	1:125:A:VAL:HG11	1:40:A:ALA:HB2	5	0.87
(1,1983)	1:125:A:VAL:HG11	1:40:A:ALA:HB3	5	0.87
(1,1983)	1:125:A:VAL:HG12	1:40:A:ALA:HB1	5	0.87
(1,1983)	1:125:A:VAL:HG12	1:40:A:ALA:HB2	5	0.87
(1,1983)	1:125:A:VAL:HG12	1:40:A:ALA:HB3	5	0.87
(1,1983)	1:125:A:VAL:HG13	1:40:A:ALA:HB1	5	0.87
(1,1983)	1:125:A:VAL:HG13	1:40:A:ALA:HB2	5	0.87
(1,1983)	1:125:A:VAL:HG13	1:40:A:ALA:HB3	5	0.87
(1,1970)	1:124:A:HIS:HB2	1:113:A:ALA:H	5	0.87
(1,1391)	1:89:A:THR:HG21	1:93:A:GLY:HA3	2	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1391)	1:89:A:THR:HG22	1:93:A:GLY:HA3	2	0.87
(1,1391)	1:89:A:THR:HG23	1:93:A:GLY:HA3	2	0.87
(1,1391)	1:89:A:THR:HG21	1:93:A:GLY:HA3	3	0.87
(1,1391)	1:89:A:THR:HG22	1:93:A:GLY:HA3	3	0.87
(1,1391)	1:89:A:THR:HG23	1:93:A:GLY:HA3	3	0.87
(1,1215)	1:104:A:LEU:HD13	1:79:A:ALA:H	6	0.87
(1,1075)	1:72:A:VAL:HG21	1:72:A:VAL:H	2	0.87
(1,1075)	1:72:A:VAL:HG22	1:72:A:VAL:H	2	0.87
(1,1075)	1:72:A:VAL:HG23	1:72:A:VAL:H	2	0.87
(1,708)	1:48:A:LYS:HG3	1:49:A:LEU:H	6	0.87
(1,186)	1:18:A:VAL:HG11	1:14:A:PHE:H	3	0.87
(1,186)	1:18:A:VAL:HG12	1:14:A:PHE:H	3	0.87
(1,186)	1:18:A:VAL:HG13	1:14:A:PHE:H	3	0.87
(1,169)	1:15:A:SER:HB3	1:15:A:SER:H	6	0.87
(1,1994)	1:125:A:VAL:HG11	1:125:A:VAL:H	1	0.86
(1,1994)	1:125:A:VAL:HG12	1:125:A:VAL:H	1	0.86
(1,1994)	1:125:A:VAL:HG13	1:125:A:VAL:H	1	0.86
(1,1994)	1:125:A:VAL:HG11	1:125:A:VAL:H	4	0.86
(1,1994)	1:125:A:VAL:HG12	1:125:A:VAL:H	4	0.86
(1,1994)	1:125:A:VAL:HG13	1:125:A:VAL:H	4	0.86
(1,1720)	1:110:A:THR:HG21	1:103:A:PRO:HB3	9	0.86
(1,1720)	1:110:A:THR:HG22	1:103:A:PRO:HB3	9	0.86
(1,1720)	1:110:A:THR:HG23	1:103:A:PRO:HB3	9	0.86
(1,1720)	1:110:A:THR:HG21	1:103:A:PRO:HB3	10	0.86
(1,1720)	1:110:A:THR:HG22	1:103:A:PRO:HB3	10	0.86
(1,1720)	1:110:A:THR:HG23	1:103:A:PRO:HB3	10	0.86
(1,1641)	1:106:A:VAL:HG21	1:39:A:PHE:HB2	5	0.86
(1,1641)	1:106:A:VAL:HG22	1:39:A:PHE:HB2	5	0.86
(1,1641)	1:106:A:VAL:HG23	1:39:A:PHE:HB2	5	0.86
(1,1600)	1:103:A:PRO:HG3	1:111:A:VAL:H	2	0.86
(1,1441)	1:91:A:LEU:HD21	1:93:A:GLY:H	5	0.86
(1,1441)	1:91:A:LEU:HD22	1:93:A:GLY:H	5	0.86
(1,1441)	1:91:A:LEU:HD23	1:93:A:GLY:H	5	0.86
(1,1391)	1:89:A:THR:HG21	1:93:A:GLY:HA3	9	0.86
(1,1391)	1:89:A:THR:HG22	1:93:A:GLY:HA3	9	0.86
(1,1391)	1:89:A:THR:HG23	1:93:A:GLY:HA3	9	0.86
(1,1029)	1:68:A:LEU:HD21	1:67:A:ILE:HG21	1	0.86
(1,1029)	1:68:A:LEU:HD21	1:67:A:ILE:HG22	1	0.86
(1,1029)	1:68:A:LEU:HD21	1:67:A:ILE:HG23	1	0.86
(1,1029)	1:68:A:LEU:HD22	1:67:A:ILE:HG21	1	0.86
(1,1029)	1:68:A:LEU:HD22	1:67:A:ILE:HG22	1	0.86
(1,1029)	1:68:A:LEU:HD22	1:67:A:ILE:HG23	1	0.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1029)	1:68:A:LEU:HD23	1:67:A:ILE:HG21	1	0.86
(1,1029)	1:68:A:LEU:HD23	1:67:A:ILE:HG22	1	0.86
(1,1029)	1:68:A:LEU:HD23	1:67:A:ILE:HG23	1	0.86
(1,775)	1:26:A:LEU:HD13	1:66:A:ARG:HD2	3	0.86
(1,735)	1:52:A:GLY:HA2	1:54:A:ILE:H	1	0.86
(1,708)	1:48:A:LYS:HG3	1:49:A:LEU:H	4	0.86
(1,342)	1:36:A:PHE:HB2	1:75:A:GLY:H	1	0.86
(1,1995)	1:125:A:VAL:HG21	1:126:A:ILE:H	4	0.85
(1,1995)	1:125:A:VAL:HG22	1:126:A:ILE:H	4	0.85
(1,1995)	1:125:A:VAL:HG23	1:126:A:ILE:H	4	0.85
(1,1994)	1:125:A:VAL:HG11	1:125:A:VAL:H	10	0.85
(1,1994)	1:125:A:VAL:HG12	1:125:A:VAL:H	10	0.85
(1,1994)	1:125:A:VAL:HG13	1:125:A:VAL:H	10	0.85
(1,1983)	1:125:A:VAL:HG11	1:40:A:ALA:HB1	6	0.85
(1,1983)	1:125:A:VAL:HG11	1:40:A:ALA:HB2	6	0.85
(1,1983)	1:125:A:VAL:HG11	1:40:A:ALA:HB3	6	0.85
(1,1983)	1:125:A:VAL:HG12	1:40:A:ALA:HB1	6	0.85
(1,1983)	1:125:A:VAL:HG12	1:40:A:ALA:HB2	6	0.85
(1,1983)	1:125:A:VAL:HG12	1:40:A:ALA:HB3	6	0.85
(1,1983)	1:125:A:VAL:HG13	1:40:A:ALA:HB1	6	0.85
(1,1983)	1:125:A:VAL:HG13	1:40:A:ALA:HB2	6	0.85
(1,1983)	1:125:A:VAL:HG13	1:40:A:ALA:HB3	6	0.85
(1,1616)	1:104:A:LEU:HD21	1:105:A:GLU:H	7	0.85
(1,1616)	1:104:A:LEU:HD22	1:105:A:GLU:H	7	0.85
(1,1616)	1:104:A:LEU:HD23	1:105:A:GLU:H	7	0.85
(1,1091)	1:73:A:VAL:HG11	1:74:A:ALA:H	9	0.85
(1,1091)	1:73:A:VAL:HG12	1:74:A:ALA:H	9	0.85
(1,1091)	1:73:A:VAL:HG13	1:74:A:ALA:H	9	0.85
(1,969)	1:65:A:GLY:HA2	1:26:A:LEU:HD11	8	0.85
(1,969)	1:65:A:GLY:HA2	1:26:A:LEU:HD12	8	0.85
(1,969)	1:65:A:GLY:HA2	1:26:A:LEU:HD13	8	0.85
(1,525)	1:107:A:LYS:HB3	1:107:A:LYS:HE2	9	0.85
(1,340)	1:25:A:ASN:HD22	1:92:A:GLU:HB3	9	0.85
(1,322)	1:24:A:ALA:HB1	1:64:A:LEU:HB2	9	0.85
(1,322)	1:24:A:ALA:HB2	1:64:A:LEU:HB2	9	0.85
(1,322)	1:24:A:ALA:HB3	1:64:A:LEU:HB2	9	0.85
(1,322)	1:24:A:ALA:HB1	1:64:A:LEU:HB2	10	0.85
(1,322)	1:24:A:ALA:HB2	1:64:A:LEU:HB2	10	0.85
(1,322)	1:24:A:ALA:HB3	1:64:A:LEU:HB2	10	0.85
(1,1994)	1:125:A:VAL:HG11	1:125:A:VAL:H	2	0.84
(1,1994)	1:125:A:VAL:HG12	1:125:A:VAL:H	2	0.84
(1,1994)	1:125:A:VAL:HG13	1:125:A:VAL:H	2	0.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1994)	1:125:A:VAL:HG11	1:125:A:VAL:H	8	0.84
(1,1994)	1:125:A:VAL:HG12	1:125:A:VAL:H	8	0.84
(1,1994)	1:125:A:VAL:HG13	1:125:A:VAL:H	8	0.84
(1,1994)	1:125:A:VAL:HG11	1:125:A:VAL:H	9	0.84
(1,1994)	1:125:A:VAL:HG12	1:125:A:VAL:H	9	0.84
(1,1994)	1:125:A:VAL:HG13	1:125:A:VAL:H	9	0.84
(1,1983)	1:125:A:VAL:HG11	1:40:A:ALA:HB1	7	0.84
(1,1983)	1:125:A:VAL:HG11	1:40:A:ALA:HB2	7	0.84
(1,1983)	1:125:A:VAL:HG11	1:40:A:ALA:HB3	7	0.84
(1,1983)	1:125:A:VAL:HG12	1:40:A:ALA:HB1	7	0.84
(1,1983)	1:125:A:VAL:HG12	1:40:A:ALA:HB2	7	0.84
(1,1983)	1:125:A:VAL:HG12	1:40:A:ALA:HB3	7	0.84
(1,1983)	1:125:A:VAL:HG13	1:40:A:ALA:HB1	7	0.84
(1,1983)	1:125:A:VAL:HG13	1:40:A:ALA:HB2	7	0.84
(1,1983)	1:125:A:VAL:HG13	1:40:A:ALA:HB3	7	0.84
(1,1639)	1:105:A:GLU:H	1:105:A:GLU:HG2	1	0.84
(1,1616)	1:104:A:LEU:HD21	1:105:A:GLU:H	10	0.84
(1,1616)	1:104:A:LEU:HD22	1:105:A:GLU:H	10	0.84
(1,1616)	1:104:A:LEU:HD23	1:105:A:GLU:H	10	0.84
(1,1391)	1:89:A:THR:HG21	1:93:A:GLY:HA3	10	0.84
(1,1391)	1:89:A:THR:HG22	1:93:A:GLY:HA3	10	0.84
(1,1391)	1:89:A:THR:HG23	1:93:A:GLY:HA3	10	0.84
(1,1327)	1:87:A:ILE:HG13	1:87:A:ILE:HG21	2	0.84
(1,1327)	1:87:A:ILE:HG13	1:87:A:ILE:HG22	2	0.84
(1,1327)	1:87:A:ILE:HG13	1:87:A:ILE:HG23	2	0.84
(1,1094)	1:73:A:VAL:HG11	1:91:A:LEU:H	8	0.84
(1,1094)	1:73:A:VAL:HG12	1:91:A:LEU:H	8	0.84
(1,1094)	1:73:A:VAL:HG13	1:91:A:LEU:H	8	0.84
(1,1040)	1:68:A:LEU:HD21	1:68:A:LEU:HA	4	0.84
(1,1040)	1:68:A:LEU:HD22	1:68:A:LEU:HA	4	0.84
(1,1040)	1:68:A:LEU:HD23	1:68:A:LEU:HA	4	0.84
(1,708)	1:48:A:LYS:HG3	1:49:A:LEU:H	10	0.84
(1,601)	1:42:A:ASN:HA	1:42:A:ASN:HD22	1	0.84
(1,370)	1:89:A:THR:HG22	1:92:A:GLU:H	5	0.84
(1,186)	1:18:A:VAL:HG11	1:14:A:PHE:H	1	0.84
(1,186)	1:18:A:VAL:HG12	1:14:A:PHE:H	1	0.84
(1,186)	1:18:A:VAL:HG13	1:14:A:PHE:H	1	0.84
(1,1995)	1:125:A:VAL:HG21	1:126:A:ILE:H	3	0.83
(1,1995)	1:125:A:VAL:HG22	1:126:A:ILE:H	3	0.83
(1,1995)	1:125:A:VAL:HG23	1:126:A:ILE:H	3	0.83
(1,1995)	1:125:A:VAL:HG21	1:126:A:ILE:H	8	0.83
(1,1995)	1:125:A:VAL:HG22	1:126:A:ILE:H	8	0.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1995)	1:125:A:VAL:HG23	1:126:A:ILE:H	8	0.83
(1,1995)	1:125:A:VAL:HG21	1:126:A:ILE:H	10	0.83
(1,1995)	1:125:A:VAL:HG22	1:126:A:ILE:H	10	0.83
(1,1995)	1:125:A:VAL:HG23	1:126:A:ILE:H	10	0.83
(1,1994)	1:125:A:VAL:HG11	1:125:A:VAL:H	3	0.83
(1,1994)	1:125:A:VAL:HG12	1:125:A:VAL:H	3	0.83
(1,1994)	1:125:A:VAL:HG13	1:125:A:VAL:H	3	0.83
(1,1994)	1:125:A:VAL:HG11	1:125:A:VAL:H	5	0.83
(1,1994)	1:125:A:VAL:HG12	1:125:A:VAL:H	5	0.83
(1,1994)	1:125:A:VAL:HG13	1:125:A:VAL:H	5	0.83
(1,1994)	1:125:A:VAL:HG11	1:125:A:VAL:H	7	0.83
(1,1994)	1:125:A:VAL:HG12	1:125:A:VAL:H	7	0.83
(1,1994)	1:125:A:VAL:HG13	1:125:A:VAL:H	7	0.83
(1,1600)	1:103:A:PRO:HG3	1:111:A:VAL:H	4	0.83
(1,1414)	1:91:A:LEU:HD22	1:74:A:ALA:HB1	2	0.83
(1,1327)	1:87:A:ILE:HG13	1:87:A:ILE:HG21	1	0.83
(1,1327)	1:87:A:ILE:HG13	1:87:A:ILE:HG22	1	0.83
(1,1327)	1:87:A:ILE:HG13	1:87:A:ILE:HG23	1	0.83
(1,1327)	1:87:A:ILE:HG13	1:87:A:ILE:HG21	3	0.83
(1,1327)	1:87:A:ILE:HG13	1:87:A:ILE:HG22	3	0.83
(1,1327)	1:87:A:ILE:HG13	1:87:A:ILE:HG23	3	0.83
(1,1327)	1:87:A:ILE:HG13	1:87:A:ILE:HG21	4	0.83
(1,1327)	1:87:A:ILE:HG13	1:87:A:ILE:HG22	4	0.83
(1,1327)	1:87:A:ILE:HG13	1:87:A:ILE:HG23	4	0.83
(1,1327)	1:87:A:ILE:HG13	1:87:A:ILE:HG21	6	0.83
(1,1327)	1:87:A:ILE:HG13	1:87:A:ILE:HG22	6	0.83
(1,1327)	1:87:A:ILE:HG13	1:87:A:ILE:HG23	6	0.83
(1,1327)	1:87:A:ILE:HG13	1:87:A:ILE:HG21	7	0.83
(1,1327)	1:87:A:ILE:HG13	1:87:A:ILE:HG22	7	0.83
(1,1327)	1:87:A:ILE:HG13	1:87:A:ILE:HG23	7	0.83
(1,1327)	1:87:A:ILE:HG13	1:87:A:ILE:HG21	8	0.83
(1,1327)	1:87:A:ILE:HG13	1:87:A:ILE:HG22	8	0.83
(1,1327)	1:87:A:ILE:HG13	1:87:A:ILE:HG23	8	0.83
(1,1327)	1:87:A:ILE:HG13	1:87:A:ILE:HG21	9	0.83
(1,1327)	1:87:A:ILE:HG13	1:87:A:ILE:HG22	9	0.83
(1,1327)	1:87:A:ILE:HG13	1:87:A:ILE:HG23	9	0.83
(1,1327)	1:87:A:ILE:HG13	1:87:A:ILE:HG21	10	0.83
(1,1327)	1:87:A:ILE:HG13	1:87:A:ILE:HG22	10	0.83
(1,1327)	1:87:A:ILE:HG13	1:87:A:ILE:HG23	10	0.83
(1,1040)	1:68:A:LEU:HD21	1:68:A:LEU:HA	6	0.83
(1,1040)	1:68:A:LEU:HD22	1:68:A:LEU:HA	6	0.83
(1,1040)	1:68:A:LEU:HD23	1:68:A:LEU:HA	6	0.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,898)	1:62:A:PRO:HB2	1:26:A:LEU:H	2	0.83
(1,775)	1:57:A:LEU:HD22	1:66:A:ARG:HD2	10	0.83
(1,735)	1:52:A:GLY:HA2	1:54:A:ILE:H	9	0.83
(1,553)	1:37:A:THR:HG21	1:82:A:LEU:HD11	6	0.83
(1,553)	1:37:A:THR:HG21	1:82:A:LEU:HD12	6	0.83
(1,553)	1:37:A:THR:HG21	1:82:A:LEU:HD13	6	0.83
(1,553)	1:37:A:THR:HG22	1:82:A:LEU:HD11	6	0.83
(1,553)	1:37:A:THR:HG22	1:82:A:LEU:HD12	6	0.83
(1,553)	1:37:A:THR:HG22	1:82:A:LEU:HD13	6	0.83
(1,553)	1:37:A:THR:HG23	1:82:A:LEU:HD11	6	0.83
(1,553)	1:37:A:THR:HG23	1:82:A:LEU:HD12	6	0.83
(1,553)	1:37:A:THR:HG23	1:82:A:LEU:HD13	6	0.83
(1,429)	1:30:A:LEU:HD11	1:70:A:TYR:H	7	0.83
(1,109)	1:9:A:VAL:HG11	1:9:A:VAL:HA	9	0.83
(1,109)	1:9:A:VAL:HG12	1:9:A:VAL:HA	9	0.83
(1,109)	1:9:A:VAL:HG13	1:9:A:VAL:HA	9	0.83
(1,1995)	1:125:A:VAL:HG21	1:126:A:ILE:H	2	0.82
(1,1995)	1:125:A:VAL:HG22	1:126:A:ILE:H	2	0.82
(1,1995)	1:125:A:VAL:HG23	1:126:A:ILE:H	2	0.82
(1,1983)	1:125:A:VAL:HG11	1:40:A:ALA:HB1	10	0.82
(1,1983)	1:125:A:VAL:HG11	1:40:A:ALA:HB2	10	0.82
(1,1983)	1:125:A:VAL:HG11	1:40:A:ALA:HB3	10	0.82
(1,1983)	1:125:A:VAL:HG12	1:40:A:ALA:HB1	10	0.82
(1,1983)	1:125:A:VAL:HG12	1:40:A:ALA:HB2	10	0.82
(1,1983)	1:125:A:VAL:HG12	1:40:A:ALA:HB3	10	0.82
(1,1983)	1:125:A:VAL:HG13	1:40:A:ALA:HB1	10	0.82
(1,1983)	1:125:A:VAL:HG13	1:40:A:ALA:HB2	10	0.82
(1,1983)	1:125:A:VAL:HG13	1:40:A:ALA:HB3	10	0.82
(1,1720)	1:110:A:THR:HG21	1:103:A:PRO:HB3	3	0.82
(1,1720)	1:110:A:THR:HG22	1:103:A:PRO:HB3	3	0.82
(1,1720)	1:110:A:THR:HG23	1:103:A:PRO:HB3	3	0.82
(1,1662)	1:106:A:VAL:HG11	1:107:A:LYS:HG3	3	0.82
(1,1662)	1:106:A:VAL:HG12	1:107:A:LYS:HG3	3	0.82
(1,1662)	1:106:A:VAL:HG13	1:107:A:LYS:HG3	3	0.82
(1,1639)	1:105:A:GLU:H	1:105:A:GLU:HG2	7	0.82
(1,1616)	1:104:A:LEU:HD21	1:105:A:GLU:H	2	0.82
(1,1616)	1:104:A:LEU:HD22	1:105:A:GLU:H	2	0.82
(1,1616)	1:104:A:LEU:HD23	1:105:A:GLU:H	2	0.82
(1,1616)	1:104:A:LEU:HD21	1:105:A:GLU:H	3	0.82
(1,1616)	1:104:A:LEU:HD22	1:105:A:GLU:H	3	0.82
(1,1616)	1:104:A:LEU:HD23	1:105:A:GLU:H	3	0.82
(1,1616)	1:104:A:LEU:HD21	1:105:A:GLU:H	6	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1616)	1:104:A:LEU:HD22	1:105:A:GLU:H	6	0.82
(1,1616)	1:104:A:LEU:HD23	1:105:A:GLU:H	6	0.82
(1,1616)	1:104:A:LEU:HD21	1:105:A:GLU:H	9	0.82
(1,1616)	1:104:A:LEU:HD22	1:105:A:GLU:H	9	0.82
(1,1616)	1:104:A:LEU:HD23	1:105:A:GLU:H	9	0.82
(1,1327)	1:87:A:ILE:HG13	1:87:A:ILE:HG21	5	0.82
(1,1327)	1:87:A:ILE:HG13	1:87:A:ILE:HG22	5	0.82
(1,1327)	1:87:A:ILE:HG13	1:87:A:ILE:HG23	5	0.82
(1,1094)	1:73:A:VAL:HG11	1:91:A:LEU:H	2	0.82
(1,1094)	1:73:A:VAL:HG12	1:91:A:LEU:H	2	0.82
(1,1094)	1:73:A:VAL:HG13	1:91:A:LEU:H	2	0.82
(1,1076)	1:72:A:VAL:HG11	1:73:A:VAL:H	2	0.82
(1,1076)	1:72:A:VAL:HG12	1:73:A:VAL:H	2	0.82
(1,1076)	1:72:A:VAL:HG13	1:73:A:VAL:H	2	0.82
(1,1040)	1:68:A:LEU:HD21	1:68:A:LEU:HA	8	0.82
(1,1040)	1:68:A:LEU:HD22	1:68:A:LEU:HA	8	0.82
(1,1040)	1:68:A:LEU:HD23	1:68:A:LEU:HA	8	0.82
(1,1040)	1:68:A:LEU:HD21	1:68:A:LEU:HA	9	0.82
(1,1040)	1:68:A:LEU:HD22	1:68:A:LEU:HA	9	0.82
(1,1040)	1:68:A:LEU:HD23	1:68:A:LEU:HA	9	0.82
(1,969)	1:65:A:GLY:HA2	1:26:A:LEU:HD11	9	0.82
(1,969)	1:65:A:GLY:HA2	1:26:A:LEU:HD12	9	0.82
(1,969)	1:65:A:GLY:HA2	1:26:A:LEU:HD13	9	0.82
(1,898)	1:62:A:PRO:HB2	1:26:A:LEU:H	9	0.82
(1,735)	1:52:A:GLY:HA2	1:54:A:ILE:H	10	0.82
(1,525)	1:107:A:LYS:HB3	1:107:A:LYS:HE3	6	0.82
(1,448)	1:3:A:THR:HG22	1:31:A:GLN:HE21	10	0.82
(1,109)	1:9:A:VAL:HG11	1:9:A:VAL:HA	3	0.82
(1,109)	1:9:A:VAL:HG12	1:9:A:VAL:HA	3	0.82
(1,109)	1:9:A:VAL:HG13	1:9:A:VAL:HA	3	0.82
(1,1995)	1:125:A:VAL:HG21	1:126:A:ILE:H	7	0.81
(1,1995)	1:125:A:VAL:HG22	1:126:A:ILE:H	7	0.81
(1,1995)	1:125:A:VAL:HG23	1:126:A:ILE:H	7	0.81
(1,1720)	1:110:A:THR:HG21	1:103:A:PRO:HB3	6	0.81
(1,1720)	1:110:A:THR:HG22	1:103:A:PRO:HB3	6	0.81
(1,1720)	1:110:A:THR:HG23	1:103:A:PRO:HB3	6	0.81
(1,1641)	1:106:A:VAL:HG21	1:39:A:PHE:HB2	1	0.81
(1,1641)	1:106:A:VAL:HG22	1:39:A:PHE:HB2	1	0.81
(1,1641)	1:106:A:VAL:HG23	1:39:A:PHE:HB2	1	0.81
(1,1641)	1:106:A:VAL:HG21	1:39:A:PHE:HB2	8	0.81
(1,1641)	1:106:A:VAL:HG22	1:39:A:PHE:HB2	8	0.81
(1,1641)	1:106:A:VAL:HG23	1:39:A:PHE:HB2	8	0.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1639)	1:105:A:GLU:H	1:105:A:GLU:HG2	5	0.81
(1,1616)	1:104:A:LEU:HD21	1:105:A:GLU:H	8	0.81
(1,1616)	1:104:A:LEU:HD22	1:105:A:GLU:H	8	0.81
(1,1616)	1:104:A:LEU:HD23	1:105:A:GLU:H	8	0.81
(1,1300)	1:85:A:MET:HG2	1:86:A:GLY:H	4	0.81
(1,1094)	1:73:A:VAL:HG11	1:91:A:LEU:H	6	0.81
(1,1094)	1:73:A:VAL:HG12	1:91:A:LEU:H	6	0.81
(1,1094)	1:73:A:VAL:HG13	1:91:A:LEU:H	6	0.81
(1,1040)	1:68:A:LEU:HD21	1:68:A:LEU:HA	7	0.81
(1,1040)	1:68:A:LEU:HD22	1:68:A:LEU:HA	7	0.81
(1,1040)	1:68:A:LEU:HD23	1:68:A:LEU:HA	7	0.81
(1,370)	1:89:A:THR:HG23	1:92:A:GLU:H	4	0.81
(1,186)	1:18:A:VAL:HG11	1:14:A:PHE:H	6	0.81
(1,186)	1:18:A:VAL:HG12	1:14:A:PHE:H	6	0.81
(1,186)	1:18:A:VAL:HG13	1:14:A:PHE:H	6	0.81
(1,186)	1:18:A:VAL:HG11	1:14:A:PHE:H	10	0.81
(1,186)	1:18:A:VAL:HG12	1:14:A:PHE:H	10	0.81
(1,186)	1:18:A:VAL:HG13	1:14:A:PHE:H	10	0.81
(1,1824)	1:116:A:ILE:HG21	1:116:A:ILE:HG13	1	0.8
(1,1824)	1:116:A:ILE:HG22	1:116:A:ILE:HG13	1	0.8
(1,1824)	1:116:A:ILE:HG23	1:116:A:ILE:HG13	1	0.8
(1,1824)	1:116:A:ILE:HG21	1:116:A:ILE:HG13	2	0.8
(1,1824)	1:116:A:ILE:HG22	1:116:A:ILE:HG13	2	0.8
(1,1824)	1:116:A:ILE:HG23	1:116:A:ILE:HG13	2	0.8
(1,1824)	1:116:A:ILE:HG21	1:116:A:ILE:HG13	4	0.8
(1,1824)	1:116:A:ILE:HG22	1:116:A:ILE:HG13	4	0.8
(1,1824)	1:116:A:ILE:HG23	1:116:A:ILE:HG13	4	0.8
(1,1824)	1:116:A:ILE:HG21	1:116:A:ILE:HG13	6	0.8
(1,1824)	1:116:A:ILE:HG22	1:116:A:ILE:HG13	6	0.8
(1,1824)	1:116:A:ILE:HG23	1:116:A:ILE:HG13	6	0.8
(1,1824)	1:116:A:ILE:HG21	1:116:A:ILE:HG13	9	0.8
(1,1824)	1:116:A:ILE:HG22	1:116:A:ILE:HG13	9	0.8
(1,1824)	1:116:A:ILE:HG23	1:116:A:ILE:HG13	9	0.8
(1,1824)	1:116:A:ILE:HG21	1:116:A:ILE:HG13	10	0.8
(1,1824)	1:116:A:ILE:HG22	1:116:A:ILE:HG13	10	0.8
(1,1824)	1:116:A:ILE:HG23	1:116:A:ILE:HG13	10	0.8
(1,1616)	1:104:A:LEU:HD21	1:105:A:GLU:H	1	0.8
(1,1616)	1:104:A:LEU:HD22	1:105:A:GLU:H	1	0.8
(1,1616)	1:104:A:LEU:HD23	1:105:A:GLU:H	1	0.8
(1,1094)	1:73:A:VAL:HG11	1:91:A:LEU:H	1	0.8
(1,1094)	1:73:A:VAL:HG12	1:91:A:LEU:H	1	0.8
(1,1094)	1:73:A:VAL:HG13	1:91:A:LEU:H	1	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1040)	1:68:A:LEU:HD21	1:68:A:LEU:HA	1	0.8
(1,1040)	1:68:A:LEU:HD22	1:68:A:LEU:HA	1	0.8
(1,1040)	1:68:A:LEU:HD23	1:68:A:LEU:HA	1	0.8
(1,1040)	1:68:A:LEU:HD21	1:68:A:LEU:HA	2	0.8
(1,1040)	1:68:A:LEU:HD22	1:68:A:LEU:HA	2	0.8
(1,1040)	1:68:A:LEU:HD23	1:68:A:LEU:HA	2	0.8
(1,1040)	1:68:A:LEU:HD21	1:68:A:LEU:HA	5	0.8
(1,1040)	1:68:A:LEU:HD22	1:68:A:LEU:HA	5	0.8
(1,1040)	1:68:A:LEU:HD23	1:68:A:LEU:HA	5	0.8
(1,969)	1:65:A:GLY:HA2	1:26:A:LEU:HD11	7	0.8
(1,969)	1:65:A:GLY:HA2	1:26:A:LEU:HD12	7	0.8
(1,969)	1:65:A:GLY:HA2	1:26:A:LEU:HD13	7	0.8
(1,860)	1:59:A:GLN:H	1:59:A:GLN:HB3	3	0.8
(1,1995)	1:125:A:VAL:HG21	1:126:A:ILE:H	6	0.79
(1,1995)	1:125:A:VAL:HG22	1:126:A:ILE:H	6	0.79
(1,1995)	1:125:A:VAL:HG23	1:126:A:ILE:H	6	0.79
(1,1983)	1:125:A:VAL:HG11	1:40:A:ALA:HB1	9	0.79
(1,1983)	1:125:A:VAL:HG11	1:40:A:ALA:HB2	9	0.79
(1,1983)	1:125:A:VAL:HG11	1:40:A:ALA:HB3	9	0.79
(1,1983)	1:125:A:VAL:HG12	1:40:A:ALA:HB1	9	0.79
(1,1983)	1:125:A:VAL:HG12	1:40:A:ALA:HB2	9	0.79
(1,1983)	1:125:A:VAL:HG12	1:40:A:ALA:HB3	9	0.79
(1,1983)	1:125:A:VAL:HG13	1:40:A:ALA:HB1	9	0.79
(1,1983)	1:125:A:VAL:HG13	1:40:A:ALA:HB2	9	0.79
(1,1983)	1:125:A:VAL:HG13	1:40:A:ALA:HB3	9	0.79
(1,1824)	1:116:A:ILE:HG21	1:116:A:ILE:HG13	3	0.79
(1,1824)	1:116:A:ILE:HG22	1:116:A:ILE:HG13	3	0.79
(1,1824)	1:116:A:ILE:HG23	1:116:A:ILE:HG13	3	0.79
(1,1824)	1:116:A:ILE:HG21	1:116:A:ILE:HG13	5	0.79
(1,1824)	1:116:A:ILE:HG22	1:116:A:ILE:HG13	5	0.79
(1,1824)	1:116:A:ILE:HG23	1:116:A:ILE:HG13	5	0.79
(1,1824)	1:116:A:ILE:HG21	1:116:A:ILE:HG13	7	0.79
(1,1824)	1:116:A:ILE:HG22	1:116:A:ILE:HG13	7	0.79
(1,1824)	1:116:A:ILE:HG23	1:116:A:ILE:HG13	7	0.79
(1,1824)	1:116:A:ILE:HG21	1:116:A:ILE:HG13	8	0.79
(1,1824)	1:116:A:ILE:HG22	1:116:A:ILE:HG13	8	0.79
(1,1824)	1:116:A:ILE:HG23	1:116:A:ILE:HG13	8	0.79
(1,1616)	1:104:A:LEU:HD21	1:105:A:GLU:H	4	0.79
(1,1616)	1:104:A:LEU:HD22	1:105:A:GLU:H	4	0.79
(1,1616)	1:104:A:LEU:HD23	1:105:A:GLU:H	4	0.79
(1,1601)	1:104:A:LEU:HD11	1:79:A:ALA:H	10	0.79
(1,1601)	1:104:A:LEU:HD12	1:79:A:ALA:H	10	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1601)	1:104:A:LEU:HD13	1:79:A:ALA:H	10	0.79
(1,1300)	1:85:A:MET:HG2	1:86:A:GLY:H	7	0.79
(1,1257)	1:96:A:ILE:HG13	1:107:A:LYS:HE3	10	0.79
(1,1040)	1:68:A:LEU:HD21	1:68:A:LEU:HA	3	0.79
(1,1040)	1:68:A:LEU:HD22	1:68:A:LEU:HA	3	0.79
(1,1040)	1:68:A:LEU:HD23	1:68:A:LEU:HA	3	0.79
(1,860)	1:59:A:GLN:H	1:59:A:GLN:HB3	9	0.79
(1,680)	1:47:A:ALA:HB1	1:44:A:ASP:H	9	0.79
(1,370)	1:89:A:THR:HG23	1:92:A:GLU:H	3	0.79
(1,322)	1:24:A:ALA:HB1	1:64:A:LEU:HB2	3	0.79
(1,322)	1:24:A:ALA:HB2	1:64:A:LEU:HB2	3	0.79
(1,322)	1:24:A:ALA:HB3	1:64:A:LEU:HB2	3	0.79
(1,322)	1:24:A:ALA:HB1	1:64:A:LEU:HB2	6	0.79
(1,322)	1:24:A:ALA:HB2	1:64:A:LEU:HB2	6	0.79
(1,322)	1:24:A:ALA:HB3	1:64:A:LEU:HB2	6	0.79
(1,1995)	1:125:A:VAL:HG21	1:126:A:ILE:H	1	0.78
(1,1995)	1:125:A:VAL:HG22	1:126:A:ILE:H	1	0.78
(1,1995)	1:125:A:VAL:HG23	1:126:A:ILE:H	1	0.78
(1,1995)	1:125:A:VAL:HG21	1:126:A:ILE:H	5	0.78
(1,1995)	1:125:A:VAL:HG22	1:126:A:ILE:H	5	0.78
(1,1995)	1:125:A:VAL:HG23	1:126:A:ILE:H	5	0.78
(1,1720)	1:110:A:THR:HG21	1:103:A:PRO:HB3	7	0.78
(1,1720)	1:110:A:THR:HG22	1:103:A:PRO:HB3	7	0.78
(1,1720)	1:110:A:THR:HG23	1:103:A:PRO:HB3	7	0.78
(1,1616)	1:104:A:LEU:HD21	1:105:A:GLU:H	5	0.78
(1,1616)	1:104:A:LEU:HD22	1:105:A:GLU:H	5	0.78
(1,1616)	1:104:A:LEU:HD23	1:105:A:GLU:H	5	0.78
(1,1441)	1:91:A:LEU:HD21	1:93:A:GLY:H	9	0.78
(1,1441)	1:91:A:LEU:HD22	1:93:A:GLY:H	9	0.78
(1,1441)	1:91:A:LEU:HD23	1:93:A:GLY:H	9	0.78
(1,1414)	1:91:A:LEU:HD21	1:74:A:ALA:HB2	4	0.78
(1,1300)	1:85:A:MET:HG2	1:86:A:GLY:H	2	0.78
(1,1300)	1:85:A:MET:HG2	1:86:A:GLY:H	9	0.78
(1,1300)	1:85:A:MET:HG2	1:86:A:GLY:H	10	0.78
(1,860)	1:59:A:GLN:H	1:59:A:GLN:HB3	5	0.78
(1,860)	1:59:A:GLN:H	1:59:A:GLN:HB3	8	0.78
(1,860)	1:59:A:GLN:H	1:59:A:GLN:HB3	10	0.78
(1,631)	1:44:A:ASP:HB2	1:45:A:ALA:H	4	0.78
(1,476)	1:33:A:PRO:HB3	1:34:A:GLY:H	6	0.78
(1,448)	1:3:A:THR:HG22	1:31:A:GLN:HE21	1	0.78
(1,1995)	1:125:A:VAL:HG21	1:126:A:ILE:H	9	0.77
(1,1995)	1:125:A:VAL:HG22	1:126:A:ILE:H	9	0.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1995)	1:125:A:VAL:HG23	1:126:A:ILE:H	9	0.77
(1,1566)	1:100:A:GLY:HA3	1:101:A:ASP:H	1	0.77
(1,1566)	1:100:A:GLY:HA3	1:101:A:ASP:H	10	0.77
(1,1300)	1:85:A:MET:HG2	1:86:A:GLY:H	1	0.77
(1,1300)	1:85:A:MET:HG2	1:86:A:GLY:H	3	0.77
(1,1300)	1:85:A:MET:HG2	1:86:A:GLY:H	5	0.77
(1,1300)	1:85:A:MET:HG2	1:86:A:GLY:H	8	0.77
(1,1040)	1:68:A:LEU:HD21	1:68:A:LEU:HA	10	0.77
(1,1040)	1:68:A:LEU:HD22	1:68:A:LEU:HA	10	0.77
(1,1040)	1:68:A:LEU:HD23	1:68:A:LEU:HA	10	0.77
(1,860)	1:59:A:GLN:H	1:59:A:GLN:HB3	1	0.77
(1,860)	1:59:A:GLN:H	1:59:A:GLN:HB3	2	0.77
(1,860)	1:59:A:GLN:H	1:59:A:GLN:HB3	4	0.77
(1,860)	1:59:A:GLN:H	1:59:A:GLN:HB3	6	0.77
(1,860)	1:59:A:GLN:H	1:59:A:GLN:HB3	7	0.77
(1,708)	1:48:A:LYS:HG3	1:49:A:LEU:H	9	0.77
(1,680)	1:47:A:ALA:HB2	1:44:A:ASP:H	10	0.77
(1,527)	1:36:A:PHE:HB2	1:120:A:ASN:HD22	5	0.77
(1,476)	1:33:A:PRO:HB3	1:34:A:GLY:H	4	0.77
(1,476)	1:33:A:PRO:HB3	1:34:A:GLY:H	7	0.77
(1,342)	1:36:A:PHE:HB2	1:75:A:GLY:H	3	0.77
(1,322)	1:24:A:ALA:HB1	1:64:A:LEU:HB2	1	0.77
(1,322)	1:24:A:ALA:HB2	1:64:A:LEU:HB2	1	0.77
(1,322)	1:24:A:ALA:HB3	1:64:A:LEU:HB2	1	0.77
(1,1850)	1:117:A:GLU:HB2	1:118:A:ALA:H	1	0.76
(1,1641)	1:106:A:VAL:HG21	1:39:A:PHE:HB2	2	0.76
(1,1641)	1:106:A:VAL:HG22	1:39:A:PHE:HB2	2	0.76
(1,1641)	1:106:A:VAL:HG23	1:39:A:PHE:HB2	2	0.76
(1,1641)	1:106:A:VAL:HG21	1:39:A:PHE:HB2	3	0.76
(1,1641)	1:106:A:VAL:HG22	1:39:A:PHE:HB2	3	0.76
(1,1641)	1:106:A:VAL:HG23	1:39:A:PHE:HB2	3	0.76
(1,1612)	1:104:A:LEU:HB3	1:104:A:LEU:HD11	10	0.76
(1,1612)	1:104:A:LEU:HB3	1:104:A:LEU:HD12	10	0.76
(1,1612)	1:104:A:LEU:HB3	1:104:A:LEU:HD13	10	0.76
(1,1566)	1:100:A:GLY:HA3	1:101:A:ASP:H	5	0.76
(1,1566)	1:100:A:GLY:HA3	1:101:A:ASP:H	7	0.76
(1,1391)	1:89:A:THR:HG21	1:93:A:GLY:HA3	4	0.76
(1,1391)	1:89:A:THR:HG22	1:93:A:GLY:HA3	4	0.76
(1,1391)	1:89:A:THR:HG23	1:93:A:GLY:HA3	4	0.76
(1,1211)	1:82:A:LEU:HD21	1:77:A:TYR:HD1	8	0.76
(1,1211)	1:82:A:LEU:HD21	1:77:A:TYR:HD2	8	0.76
(1,1211)	1:82:A:LEU:HD22	1:77:A:TYR:HD1	8	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1211)	1:82:A:LEU:HD22	1:77:A:TYR:HD2	8	0.76
(1,1211)	1:82:A:LEU:HD23	1:77:A:TYR:HD1	8	0.76
(1,1211)	1:82:A:LEU:HD23	1:77:A:TYR:HD2	8	0.76
(1,476)	1:33:A:PRO:HB3	1:34:A:GLY:H	3	0.76
(1,370)	1:89:A:THR:HG22	1:92:A:GLU:H	2	0.76
(1,1850)	1:117:A:GLU:HB2	1:118:A:ALA:H	6	0.75
(1,1850)	1:117:A:GLU:HB2	1:118:A:ALA:H	8	0.75
(1,1850)	1:117:A:GLU:HB2	1:118:A:ALA:H	9	0.75
(1,1720)	1:110:A:THR:HG21	1:103:A:PRO:HB3	8	0.75
(1,1720)	1:110:A:THR:HG22	1:103:A:PRO:HB3	8	0.75
(1,1720)	1:110:A:THR:HG23	1:103:A:PRO:HB3	8	0.75
(1,1662)	1:106:A:VAL:HG11	1:107:A:LYS:HG3	8	0.75
(1,1662)	1:106:A:VAL:HG12	1:107:A:LYS:HG3	8	0.75
(1,1662)	1:106:A:VAL:HG13	1:107:A:LYS:HG3	8	0.75
(1,1612)	1:104:A:LEU:HB3	1:104:A:LEU:HD11	8	0.75
(1,1612)	1:104:A:LEU:HB3	1:104:A:LEU:HD12	8	0.75
(1,1612)	1:104:A:LEU:HB3	1:104:A:LEU:HD13	8	0.75
(1,1094)	1:73:A:VAL:HG11	1:91:A:LEU:H	10	0.75
(1,1094)	1:73:A:VAL:HG12	1:91:A:LEU:H	10	0.75
(1,1094)	1:73:A:VAL:HG13	1:91:A:LEU:H	10	0.75
(1,1076)	1:72:A:VAL:HG11	1:73:A:VAL:H	3	0.75
(1,1076)	1:72:A:VAL:HG12	1:73:A:VAL:H	3	0.75
(1,1076)	1:72:A:VAL:HG13	1:73:A:VAL:H	3	0.75
(1,1076)	1:72:A:VAL:HG11	1:73:A:VAL:H	9	0.75
(1,1076)	1:72:A:VAL:HG12	1:73:A:VAL:H	9	0.75
(1,1076)	1:72:A:VAL:HG13	1:73:A:VAL:H	9	0.75
(1,429)	1:30:A:LEU:HD11	1:70:A:TYR:H	8	0.75
(1,322)	1:24:A:ALA:HB1	1:64:A:LEU:HB2	5	0.75
(1,322)	1:24:A:ALA:HB2	1:64:A:LEU:HB2	5	0.75
(1,322)	1:24:A:ALA:HB3	1:64:A:LEU:HB2	5	0.75
(1,1921)	1:122:A:ILE:HG13	1:118:A:ALA:H	8	0.74
(1,1850)	1:117:A:GLU:HB2	1:118:A:ALA:H	5	0.74
(1,1850)	1:117:A:GLU:HB2	1:118:A:ALA:H	7	0.74
(1,1662)	1:106:A:VAL:HG11	1:107:A:LYS:HG3	7	0.74
(1,1662)	1:106:A:VAL:HG12	1:107:A:LYS:HG3	7	0.74
(1,1662)	1:106:A:VAL:HG13	1:107:A:LYS:HG3	7	0.74
(1,1612)	1:104:A:LEU:HB3	1:104:A:LEU:HD11	2	0.74
(1,1612)	1:104:A:LEU:HB3	1:104:A:LEU:HD12	2	0.74
(1,1612)	1:104:A:LEU:HB3	1:104:A:LEU:HD13	2	0.74
(1,1612)	1:104:A:LEU:HB3	1:104:A:LEU:HD11	9	0.74
(1,1612)	1:104:A:LEU:HB3	1:104:A:LEU:HD12	9	0.74
(1,1612)	1:104:A:LEU:HB3	1:104:A:LEU:HD13	9	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1421)	1:91:A:LEU:HA	1:91:A:LEU:HD21	9	0.74
(1,1421)	1:91:A:LEU:HA	1:91:A:LEU:HD22	9	0.74
(1,1421)	1:91:A:LEU:HA	1:91:A:LEU:HD23	9	0.74
(1,1414)	1:91:A:LEU:HD21	1:74:A:ALA:HB3	8	0.74
(1,1240)	1:83:A:LYS:HA	1:83:A:LYS:HG3	2	0.74
(1,1240)	1:83:A:LYS:HA	1:83:A:LYS:HG3	10	0.74
(1,1076)	1:72:A:VAL:HG11	1:73:A:VAL:H	5	0.74
(1,1076)	1:72:A:VAL:HG12	1:73:A:VAL:H	5	0.74
(1,1076)	1:72:A:VAL:HG13	1:73:A:VAL:H	5	0.74
(1,1076)	1:72:A:VAL:HG11	1:73:A:VAL:H	7	0.74
(1,1076)	1:72:A:VAL:HG12	1:73:A:VAL:H	7	0.74
(1,1076)	1:72:A:VAL:HG13	1:73:A:VAL:H	7	0.74
(1,1076)	1:72:A:VAL:HG11	1:73:A:VAL:H	8	0.74
(1,1076)	1:72:A:VAL:HG12	1:73:A:VAL:H	8	0.74
(1,1076)	1:72:A:VAL:HG13	1:73:A:VAL:H	8	0.74
(1,969)	1:65:A:GLY:HA2	1:26:A:LEU:HD11	4	0.74
(1,969)	1:65:A:GLY:HA2	1:26:A:LEU:HD12	4	0.74
(1,969)	1:65:A:GLY:HA2	1:26:A:LEU:HD13	4	0.74
(1,969)	1:65:A:GLY:HA2	1:26:A:LEU:HD11	6	0.74
(1,969)	1:65:A:GLY:HA2	1:26:A:LEU:HD12	6	0.74
(1,969)	1:65:A:GLY:HA2	1:26:A:LEU:HD13	6	0.74
(1,773)	1:54:A:ILE:HG12	1:58:A:VAL:H	6	0.74
(1,680)	1:47:A:ALA:HB2	1:44:A:ASP:H	1	0.74
(1,476)	1:33:A:PRO:HB3	1:34:A:GLY:H	1	0.74
(1,448)	1:3:A:THR:HG23	1:31:A:GLN:HE21	6	0.74
(1,1983)	1:125:A:VAL:HG11	1:40:A:ALA:HB1	3	0.73
(1,1983)	1:125:A:VAL:HG11	1:40:A:ALA:HB2	3	0.73
(1,1983)	1:125:A:VAL:HG11	1:40:A:ALA:HB3	3	0.73
(1,1983)	1:125:A:VAL:HG12	1:40:A:ALA:HB1	3	0.73
(1,1983)	1:125:A:VAL:HG12	1:40:A:ALA:HB2	3	0.73
(1,1983)	1:125:A:VAL:HG12	1:40:A:ALA:HB3	3	0.73
(1,1983)	1:125:A:VAL:HG13	1:40:A:ALA:HB1	3	0.73
(1,1983)	1:125:A:VAL:HG13	1:40:A:ALA:HB2	3	0.73
(1,1983)	1:125:A:VAL:HG13	1:40:A:ALA:HB3	3	0.73
(1,1921)	1:122:A:ILE:HG13	1:118:A:ALA:H	3	0.73
(1,1612)	1:104:A:LEU:HB3	1:104:A:LEU:HD11	1	0.73
(1,1612)	1:104:A:LEU:HB3	1:104:A:LEU:HD12	1	0.73
(1,1612)	1:104:A:LEU:HB3	1:104:A:LEU:HD13	1	0.73
(1,1612)	1:104:A:LEU:HB3	1:104:A:LEU:HD11	4	0.73
(1,1612)	1:104:A:LEU:HB3	1:104:A:LEU:HD12	4	0.73
(1,1612)	1:104:A:LEU:HB3	1:104:A:LEU:HD13	4	0.73
(1,1612)	1:104:A:LEU:HB3	1:104:A:LEU:HD11	7	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1612)	1:104:A:LEU:HB3	1:104:A:LEU:HD12	7	0.73
(1,1612)	1:104:A:LEU:HB3	1:104:A:LEU:HD13	7	0.73
(1,1604)	1:104:A:LEU:H	1:103:A:PRO:HG3	10	0.73
(1,1601)	1:104:A:LEU:HD11	1:79:A:ALA:H	3	0.73
(1,1601)	1:104:A:LEU:HD12	1:79:A:ALA:H	3	0.73
(1,1601)	1:104:A:LEU:HD13	1:79:A:ALA:H	3	0.73
(1,1566)	1:100:A:GLY:HA3	1:101:A:ASP:H	4	0.73
(1,1414)	1:91:A:LEU:HD22	1:74:A:ALA:HB1	3	0.73
(1,1300)	1:85:A:MET:HG2	1:86:A:GLY:H	6	0.73
(1,1187)	1:80:A:THR:H	1:115:A:ASP:HB2	5	0.73
(1,898)	1:62:A:PRO:HB2	1:26:A:LEU:H	8	0.73
(1,631)	1:44:A:ASP:HB2	1:45:A:ALA:H	2	0.73
(1,476)	1:33:A:PRO:HB3	1:34:A:GLY:H	5	0.73
(1,1641)	1:106:A:VAL:HG21	1:39:A:PHE:HB2	7	0.72
(1,1641)	1:106:A:VAL:HG22	1:39:A:PHE:HB2	7	0.72
(1,1641)	1:106:A:VAL:HG23	1:39:A:PHE:HB2	7	0.72
(1,1612)	1:104:A:LEU:HB3	1:104:A:LEU:HD11	3	0.72
(1,1612)	1:104:A:LEU:HB3	1:104:A:LEU:HD12	3	0.72
(1,1612)	1:104:A:LEU:HB3	1:104:A:LEU:HD13	3	0.72
(1,1612)	1:104:A:LEU:HB3	1:104:A:LEU:HD11	5	0.72
(1,1612)	1:104:A:LEU:HB3	1:104:A:LEU:HD12	5	0.72
(1,1612)	1:104:A:LEU:HB3	1:104:A:LEU:HD13	5	0.72
(1,1612)	1:104:A:LEU:HB3	1:104:A:LEU:HD11	6	0.72
(1,1612)	1:104:A:LEU:HB3	1:104:A:LEU:HD12	6	0.72
(1,1612)	1:104:A:LEU:HB3	1:104:A:LEU:HD13	6	0.72
(1,1604)	1:104:A:LEU:H	1:103:A:PRO:HG3	7	0.72
(1,1519)	1:96:A:ILE:HG13	1:107:A:LYS:HE2	1	0.72
(1,1519)	1:96:A:ILE:HG13	1:107:A:LYS:HE3	1	0.72
(1,1240)	1:83:A:LYS:HA	1:83:A:LYS:HG3	9	0.72
(1,1076)	1:72:A:VAL:HG11	1:73:A:VAL:H	1	0.72
(1,1076)	1:72:A:VAL:HG12	1:73:A:VAL:H	1	0.72
(1,1076)	1:72:A:VAL:HG13	1:73:A:VAL:H	1	0.72
(1,1076)	1:72:A:VAL:HG11	1:73:A:VAL:H	6	0.72
(1,1076)	1:72:A:VAL:HG12	1:73:A:VAL:H	6	0.72
(1,1076)	1:72:A:VAL:HG13	1:73:A:VAL:H	6	0.72
(1,631)	1:44:A:ASP:HB2	1:45:A:ALA:H	3	0.72
(1,631)	1:44:A:ASP:HB2	1:45:A:ALA:H	5	0.72
(1,631)	1:44:A:ASP:HB2	1:45:A:ALA:H	7	0.72
(1,520)	1:36:A:PHE:HA	1:72:A:VAL:HG11	9	0.72
(1,520)	1:36:A:PHE:HA	1:72:A:VAL:HG12	9	0.72
(1,520)	1:36:A:PHE:HA	1:72:A:VAL:HG13	9	0.72
(1,448)	1:3:A:THR:HG23	1:31:A:GLN:HE21	7	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,448)	1:3:A:THR:HG23	1:31:A:GLN:HE21	9	0.72
(1,1983)	1:125:A:VAL:HG11	1:40:A:ALA:HB1	2	0.71
(1,1983)	1:125:A:VAL:HG11	1:40:A:ALA:HB2	2	0.71
(1,1983)	1:125:A:VAL:HG11	1:40:A:ALA:HB3	2	0.71
(1,1983)	1:125:A:VAL:HG12	1:40:A:ALA:HB1	2	0.71
(1,1983)	1:125:A:VAL:HG12	1:40:A:ALA:HB2	2	0.71
(1,1983)	1:125:A:VAL:HG12	1:40:A:ALA:HB3	2	0.71
(1,1983)	1:125:A:VAL:HG13	1:40:A:ALA:HB1	2	0.71
(1,1983)	1:125:A:VAL:HG13	1:40:A:ALA:HB2	2	0.71
(1,1983)	1:125:A:VAL:HG13	1:40:A:ALA:HB3	2	0.71
(1,1850)	1:117:A:GLU:HB2	1:118:A:ALA:H	3	0.71
(1,1604)	1:104:A:LEU:H	1:103:A:PRO:HG3	1	0.71
(1,1604)	1:104:A:LEU:H	1:103:A:PRO:HG3	5	0.71
(1,1601)	1:104:A:LEU:HD11	1:79:A:ALA:H	2	0.71
(1,1601)	1:104:A:LEU:HD12	1:79:A:ALA:H	2	0.71
(1,1601)	1:104:A:LEU:HD13	1:79:A:ALA:H	2	0.71
(1,1566)	1:100:A:GLY:HA3	1:101:A:ASP:H	6	0.71
(1,1263)	1:84:A:ARG:HD3	1:84:A:ARG:HA	9	0.71
(1,1076)	1:72:A:VAL:HG11	1:73:A:VAL:H	4	0.71
(1,1076)	1:72:A:VAL:HG12	1:73:A:VAL:H	4	0.71
(1,1076)	1:72:A:VAL:HG13	1:73:A:VAL:H	4	0.71
(1,989)	1:66:A:ARG:HA	1:66:A:ARG:HB3	1	0.71
(1,969)	1:65:A:GLY:HA2	1:26:A:LEU:HD11	1	0.71
(1,969)	1:65:A:GLY:HA2	1:26:A:LEU:HD12	1	0.71
(1,969)	1:65:A:GLY:HA2	1:26:A:LEU:HD13	1	0.71
(1,679)	1:44:A:ASP:HB3	1:47:A:ALA:H	8	0.71
(1,476)	1:33:A:PRO:HB3	1:34:A:GLY:H	2	0.71
(1,476)	1:33:A:PRO:HB3	1:34:A:GLY:H	10	0.71
(1,340)	1:25:A:ASN:HD22	1:92:A:GLU:HB3	3	0.71
(1,1639)	1:105:A:GLU:H	1:105:A:GLU:HG2	9	0.7
(1,1604)	1:104:A:LEU:H	1:103:A:PRO:HG3	2	0.7
(1,1604)	1:104:A:LEU:H	1:103:A:PRO:HG3	4	0.7
(1,1516)	1:96:A:ILE:HG13	1:107:A:LYS:HB2	2	0.7
(1,1414)	1:91:A:LEU:HD22	1:74:A:ALA:HB1	9	0.7
(1,1263)	1:84:A:ARG:HD3	1:84:A:ARG:HA	5	0.7
(1,1240)	1:83:A:LYS:HA	1:83:A:LYS:HG3	7	0.7
(1,1211)	1:82:A:LEU:HD21	1:77:A:TYR:HD1	2	0.7
(1,1211)	1:82:A:LEU:HD21	1:77:A:TYR:HD2	2	0.7
(1,1211)	1:82:A:LEU:HD22	1:77:A:TYR:HD1	2	0.7
(1,1211)	1:82:A:LEU:HD22	1:77:A:TYR:HD2	2	0.7
(1,1211)	1:82:A:LEU:HD23	1:77:A:TYR:HD1	2	0.7
(1,1211)	1:82:A:LEU:HD23	1:77:A:TYR:HD2	2	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1094)	1:73:A:VAL:HG11	1:91:A:LEU:H	7	0.7
(1,1094)	1:73:A:VAL:HG12	1:91:A:LEU:H	7	0.7
(1,1094)	1:73:A:VAL:HG13	1:91:A:LEU:H	7	0.7
(1,989)	1:66:A:ARG:HA	1:66:A:ARG:HB3	4	0.7
(1,819)	1:57:A:LEU:HD11	1:57:A:LEU:HB3	3	0.7
(1,819)	1:57:A:LEU:HD12	1:57:A:LEU:HB3	3	0.7
(1,819)	1:57:A:LEU:HD13	1:57:A:LEU:HB3	3	0.7
(1,819)	1:57:A:LEU:HD11	1:57:A:LEU:HB3	4	0.7
(1,819)	1:57:A:LEU:HD12	1:57:A:LEU:HB3	4	0.7
(1,819)	1:57:A:LEU:HD13	1:57:A:LEU:HB3	4	0.7
(1,819)	1:57:A:LEU:HD11	1:57:A:LEU:HB3	6	0.7
(1,819)	1:57:A:LEU:HD12	1:57:A:LEU:HB3	6	0.7
(1,819)	1:57:A:LEU:HD13	1:57:A:LEU:HB3	6	0.7
(1,819)	1:57:A:LEU:HD11	1:57:A:LEU:HB3	7	0.7
(1,819)	1:57:A:LEU:HD12	1:57:A:LEU:HB3	7	0.7
(1,819)	1:57:A:LEU:HD13	1:57:A:LEU:HB3	7	0.7
(1,819)	1:57:A:LEU:HD11	1:57:A:LEU:HB3	9	0.7
(1,819)	1:57:A:LEU:HD12	1:57:A:LEU:HB3	9	0.7
(1,819)	1:57:A:LEU:HD13	1:57:A:LEU:HB3	9	0.7
(1,819)	1:57:A:LEU:HD11	1:57:A:LEU:HB3	10	0.7
(1,819)	1:57:A:LEU:HD12	1:57:A:LEU:HB3	10	0.7
(1,819)	1:57:A:LEU:HD13	1:57:A:LEU:HB3	10	0.7
(1,680)	1:47:A:ALA:HB3	1:44:A:ASP:H	2	0.7
(1,680)	1:47:A:ALA:HB2	1:44:A:ASP:H	6	0.7
(1,679)	1:44:A:ASP:HB3	1:47:A:ALA:H	10	0.7
(1,631)	1:44:A:ASP:HB2	1:45:A:ALA:H	9	0.7
(1,631)	1:44:A:ASP:HB2	1:45:A:ALA:H	10	0.7
(1,622)	1:44:A:ASP:HB2	1:42:A:ASN:HD21	2	0.7
(1,563)	1:38:A:VAL:HG21	1:38:A:VAL:H	2	0.7
(1,563)	1:38:A:VAL:HG22	1:38:A:VAL:H	2	0.7
(1,563)	1:38:A:VAL:HG23	1:38:A:VAL:H	2	0.7
(1,476)	1:33:A:PRO:HB3	1:34:A:GLY:H	8	0.7
(1,448)	1:3:A:THR:HG21	1:31:A:GLN:HE21	3	0.7
(1,448)	1:3:A:THR:HG22	1:31:A:GLN:HE21	5	0.7
(1,429)	1:30:A:LEU:HD13	1:70:A:TYR:H	3	0.7
(1,370)	1:89:A:THR:HG21	1:92:A:GLU:H	8	0.7
(1,322)	1:24:A:ALA:HB1	1:64:A:LEU:HB2	7	0.7
(1,322)	1:24:A:ALA:HB2	1:64:A:LEU:HB2	7	0.7
(1,322)	1:24:A:ALA:HB3	1:64:A:LEU:HB2	7	0.7
(1,262)	1:22:A:LYS:HE2	1:19:A:THR:HG21	9	0.7
(1,262)	1:22:A:LYS:HE2	1:19:A:THR:HG22	9	0.7
(1,262)	1:22:A:LYS:HE2	1:19:A:THR:HG23	9	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1921)	1:122:A:ILE:HG13	1:118:A:ALA:H	2	0.69
(1,1921)	1:122:A:ILE:HG13	1:118:A:ALA:H	5	0.69
(1,1604)	1:104:A:LEU:H	1:103:A:PRO:HG3	6	0.69
(1,1604)	1:104:A:LEU:H	1:103:A:PRO:HG3	8	0.69
(1,1604)	1:104:A:LEU:H	1:103:A:PRO:HG3	9	0.69
(1,1263)	1:84:A:ARG:HD3	1:84:A:ARG:HA	3	0.69
(1,1263)	1:84:A:ARG:HD3	1:84:A:ARG:HA	8	0.69
(1,989)	1:66:A:ARG:HA	1:66:A:ARG:HB3	8	0.69
(1,989)	1:66:A:ARG:HA	1:66:A:ARG:HB3	10	0.69
(1,969)	1:65:A:GLY:HA2	1:26:A:LEU:HD11	10	0.69
(1,969)	1:65:A:GLY:HA2	1:26:A:LEU:HD12	10	0.69
(1,969)	1:65:A:GLY:HA2	1:26:A:LEU:HD13	10	0.69
(1,819)	1:57:A:LEU:HD11	1:57:A:LEU:HB3	1	0.69
(1,819)	1:57:A:LEU:HD12	1:57:A:LEU:HB3	1	0.69
(1,819)	1:57:A:LEU:HD13	1:57:A:LEU:HB3	1	0.69
(1,819)	1:57:A:LEU:HD11	1:57:A:LEU:HB3	2	0.69
(1,819)	1:57:A:LEU:HD12	1:57:A:LEU:HB3	2	0.69
(1,819)	1:57:A:LEU:HD13	1:57:A:LEU:HB3	2	0.69
(1,819)	1:57:A:LEU:HD11	1:57:A:LEU:HB3	5	0.69
(1,819)	1:57:A:LEU:HD12	1:57:A:LEU:HB3	5	0.69
(1,819)	1:57:A:LEU:HD13	1:57:A:LEU:HB3	5	0.69
(1,819)	1:57:A:LEU:HD11	1:57:A:LEU:HB3	8	0.69
(1,819)	1:57:A:LEU:HD12	1:57:A:LEU:HB3	8	0.69
(1,819)	1:57:A:LEU:HD13	1:57:A:LEU:HB3	8	0.69
(1,776)	1:54:A:ILE:HG13	1:67:A:ILE:HG21	9	0.69
(1,776)	1:54:A:ILE:HG13	1:67:A:ILE:HG22	9	0.69
(1,776)	1:54:A:ILE:HG13	1:67:A:ILE:HG23	9	0.69
(1,728)	1:49:A:LEU:HB2	1:50:A:PRO:HD3	5	0.69
(1,680)	1:47:A:ALA:HB3	1:44:A:ASP:H	4	0.69
(1,680)	1:47:A:ALA:HB3	1:44:A:ASP:H	8	0.69
(1,631)	1:44:A:ASP:HB2	1:45:A:ALA:H	8	0.69
(1,563)	1:38:A:VAL:HG21	1:38:A:VAL:H	10	0.69
(1,563)	1:38:A:VAL:HG22	1:38:A:VAL:H	10	0.69
(1,563)	1:38:A:VAL:HG23	1:38:A:VAL:H	10	0.69
(1,429)	1:30:A:LEU:HD13	1:70:A:TYR:H	1	0.69
(1,429)	1:30:A:LEU:HD12	1:70:A:TYR:H	5	0.69
(1,370)	1:89:A:THR:HG23	1:92:A:GLU:H	10	0.69
(1,270)	1:22:A:LYS:HG2	1:22:A:LYS:HE3	2	0.69
(1,270)	1:22:A:LYS:HG2	1:22:A:LYS:HE3	3	0.69
(1,262)	1:22:A:LYS:HE2	1:19:A:THR:HG21	10	0.69
(1,262)	1:22:A:LYS:HE2	1:19:A:THR:HG22	10	0.69
(1,262)	1:22:A:LYS:HE2	1:19:A:THR:HG23	10	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1984)	1:125:A:VAL:HG21	1:112:A:LEU:H	9	0.68
(1,1984)	1:125:A:VAL:HG22	1:112:A:LEU:H	9	0.68
(1,1984)	1:125:A:VAL:HG23	1:112:A:LEU:H	9	0.68
(1,1604)	1:104:A:LEU:H	1:103:A:PRO:HG3	3	0.68
(1,1601)	1:104:A:LEU:HD11	1:79:A:ALA:H	8	0.68
(1,1601)	1:104:A:LEU:HD12	1:79:A:ALA:H	8	0.68
(1,1601)	1:104:A:LEU:HD13	1:79:A:ALA:H	8	0.68
(1,1601)	1:104:A:LEU:HD11	1:79:A:ALA:H	9	0.68
(1,1601)	1:104:A:LEU:HD12	1:79:A:ALA:H	9	0.68
(1,1601)	1:104:A:LEU:HD13	1:79:A:ALA:H	9	0.68
(1,1519)	1:96:A:ILE:HG13	1:107:A:LYS:HE2	10	0.68
(1,1519)	1:96:A:ILE:HG13	1:107:A:LYS:HE3	10	0.68
(1,1408)	1:91:A:LEU:HD11	1:30:A:LEU:HA	2	0.68
(1,1408)	1:91:A:LEU:HD12	1:30:A:LEU:HA	2	0.68
(1,1408)	1:91:A:LEU:HD13	1:30:A:LEU:HA	2	0.68
(1,1263)	1:84:A:ARG:HD3	1:84:A:ARG:HA	1	0.68
(1,1263)	1:84:A:ARG:HD3	1:84:A:ARG:HA	6	0.68
(1,1257)	1:96:A:ILE:HG13	1:107:A:LYS:HE2	2	0.68
(1,1211)	1:82:A:LEU:HD21	1:77:A:TYR:HD1	4	0.68
(1,1211)	1:82:A:LEU:HD21	1:77:A:TYR:HD2	4	0.68
(1,1211)	1:82:A:LEU:HD22	1:77:A:TYR:HD1	4	0.68
(1,1211)	1:82:A:LEU:HD22	1:77:A:TYR:HD2	4	0.68
(1,1211)	1:82:A:LEU:HD23	1:77:A:TYR:HD1	4	0.68
(1,1211)	1:82:A:LEU:HD23	1:77:A:TYR:HD2	4	0.68
(1,728)	1:49:A:LEU:HB2	1:50:A:PRO:HD3	7	0.68
(1,708)	1:48:A:LYS:HG3	1:49:A:LEU:H	3	0.68
(1,679)	1:44:A:ASP:HB3	1:47:A:ALA:H	1	0.68
(1,679)	1:44:A:ASP:HB3	1:47:A:ALA:H	4	0.68
(1,601)	1:42:A:ASN:HA	1:42:A:ASN:HD22	7	0.68
(1,322)	1:24:A:ALA:HB1	1:64:A:LEU:HB2	4	0.68
(1,322)	1:24:A:ALA:HB2	1:64:A:LEU:HB2	4	0.68
(1,322)	1:24:A:ALA:HB3	1:64:A:LEU:HB2	4	0.68
(1,270)	1:22:A:LYS:HG2	1:22:A:LYS:HE3	1	0.68
(1,270)	1:22:A:LYS:HG2	1:22:A:LYS:HE3	5	0.68
(1,270)	1:22:A:LYS:HG2	1:22:A:LYS:HE3	7	0.68
(1,270)	1:22:A:LYS:HG2	1:22:A:LYS:HE3	10	0.68
(1,262)	1:22:A:LYS:HE2	1:19:A:THR:HG21	1	0.68
(1,262)	1:22:A:LYS:HE2	1:19:A:THR:HG22	1	0.68
(1,262)	1:22:A:LYS:HE2	1:19:A:THR:HG23	1	0.68
(1,262)	1:22:A:LYS:HE2	1:19:A:THR:HG21	3	0.68
(1,262)	1:22:A:LYS:HE2	1:19:A:THR:HG22	3	0.68
(1,262)	1:22:A:LYS:HE2	1:19:A:THR:HG23	3	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,262)	1:22:A:LYS:HE2	1:19:A:THR:HG21	5	0.68
(1,262)	1:22:A:LYS:HE2	1:19:A:THR:HG22	5	0.68
(1,262)	1:22:A:LYS:HE2	1:19:A:THR:HG23	5	0.68
(1,262)	1:22:A:LYS:HE2	1:19:A:THR:HG21	6	0.68
(1,262)	1:22:A:LYS:HE2	1:19:A:THR:HG22	6	0.68
(1,262)	1:22:A:LYS:HE2	1:19:A:THR:HG23	6	0.68
(1,262)	1:22:A:LYS:HE2	1:19:A:THR:HG21	8	0.68
(1,262)	1:22:A:LYS:HE2	1:19:A:THR:HG22	8	0.68
(1,262)	1:22:A:LYS:HE2	1:19:A:THR:HG23	8	0.68
(1,1984)	1:125:A:VAL:HG21	1:112:A:LEU:H	8	0.67
(1,1984)	1:125:A:VAL:HG22	1:112:A:LEU:H	8	0.67
(1,1984)	1:125:A:VAL:HG23	1:112:A:LEU:H	8	0.67
(1,1983)	1:125:A:VAL:HG11	1:40:A:ALA:HB1	8	0.67
(1,1983)	1:125:A:VAL:HG11	1:40:A:ALA:HB2	8	0.67
(1,1983)	1:125:A:VAL:HG11	1:40:A:ALA:HB3	8	0.67
(1,1983)	1:125:A:VAL:HG12	1:40:A:ALA:HB1	8	0.67
(1,1983)	1:125:A:VAL:HG12	1:40:A:ALA:HB2	8	0.67
(1,1983)	1:125:A:VAL:HG12	1:40:A:ALA:HB3	8	0.67
(1,1983)	1:125:A:VAL:HG13	1:40:A:ALA:HB1	8	0.67
(1,1983)	1:125:A:VAL:HG13	1:40:A:ALA:HB2	8	0.67
(1,1983)	1:125:A:VAL:HG13	1:40:A:ALA:HB3	8	0.67
(1,1737)	1:20:A:ALA:HB3	1:64:A:LEU:HD11	7	0.67
(1,1720)	1:110:A:THR:HG21	1:103:A:PRO:HB3	5	0.67
(1,1720)	1:110:A:THR:HG22	1:103:A:PRO:HB3	5	0.67
(1,1720)	1:110:A:THR:HG23	1:103:A:PRO:HB3	5	0.67
(1,1639)	1:105:A:GLU:H	1:105:A:GLU:HG2	10	0.67
(1,1601)	1:104:A:LEU:HD11	1:79:A:ALA:H	7	0.67
(1,1601)	1:104:A:LEU:HD12	1:79:A:ALA:H	7	0.67
(1,1601)	1:104:A:LEU:HD13	1:79:A:ALA:H	7	0.67
(1,1566)	1:100:A:GLY:HA3	1:101:A:ASP:H	3	0.67
(1,1566)	1:100:A:GLY:HA3	1:101:A:ASP:H	8	0.67
(1,1113)	1:76:A:ALA:HB3	1:36:A:PHE:H	7	0.67
(1,1027)	1:68:A:LEU:HD11	1:65:A:GLY:HA2	3	0.67
(1,1027)	1:68:A:LEU:HD12	1:65:A:GLY:HA2	3	0.67
(1,1027)	1:68:A:LEU:HD13	1:65:A:GLY:HA2	3	0.67
(1,680)	1:47:A:ALA:HB1	1:44:A:ASP:H	3	0.67
(1,631)	1:44:A:ASP:HB2	1:45:A:ALA:H	1	0.67
(1,622)	1:44:A:ASP:HB2	1:42:A:ASN:HD21	5	0.67
(1,476)	1:33:A:PRO:HB3	1:34:A:GLY:H	9	0.67
(1,448)	1:3:A:THR:HG21	1:31:A:GLN:HE21	4	0.67
(1,270)	1:22:A:LYS:HG2	1:22:A:LYS:HE3	4	0.67
(1,262)	1:22:A:LYS:HE2	1:19:A:THR:HG21	2	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,262)	1:22:A:LYS:HE2	1:19:A:THR:HG22	2	0.67
(1,262)	1:22:A:LYS:HE2	1:19:A:THR:HG23	2	0.67
(1,262)	1:22:A:LYS:HE2	1:19:A:THR:HG21	4	0.67
(1,262)	1:22:A:LYS:HE2	1:19:A:THR:HG22	4	0.67
(1,262)	1:22:A:LYS:HE2	1:19:A:THR:HG23	4	0.67
(1,1984)	1:125:A:VAL:HG21	1:112:A:LEU:H	5	0.66
(1,1984)	1:125:A:VAL:HG22	1:112:A:LEU:H	5	0.66
(1,1984)	1:125:A:VAL:HG23	1:112:A:LEU:H	5	0.66
(1,1984)	1:125:A:VAL:HG21	1:112:A:LEU:H	10	0.66
(1,1984)	1:125:A:VAL:HG22	1:112:A:LEU:H	10	0.66
(1,1984)	1:125:A:VAL:HG23	1:112:A:LEU:H	10	0.66
(1,1981)	1:124:A:HIS:HB2	1:125:A:VAL:H	10	0.66
(1,1684)	1:107:A:LYS:HG2	1:107:A:LYS:HE2	1	0.66
(1,1684)	1:107:A:LYS:HG2	1:107:A:LYS:HE3	1	0.66
(1,1684)	1:107:A:LYS:HG2	1:107:A:LYS:HE2	4	0.66
(1,1684)	1:107:A:LYS:HG2	1:107:A:LYS:HE3	4	0.66
(1,1684)	1:107:A:LYS:HG2	1:107:A:LYS:HE2	8	0.66
(1,1684)	1:107:A:LYS:HG2	1:107:A:LYS:HE3	8	0.66
(1,1566)	1:100:A:GLY:HA3	1:101:A:ASP:H	9	0.66
(1,1263)	1:84:A:ARG:HD3	1:84:A:ARG:HA	4	0.66
(1,1263)	1:84:A:ARG:HD3	1:84:A:ARG:HA	10	0.66
(1,1027)	1:68:A:LEU:HD11	1:65:A:GLY:HA2	6	0.66
(1,1027)	1:68:A:LEU:HD12	1:65:A:GLY:HA2	6	0.66
(1,1027)	1:68:A:LEU:HD13	1:65:A:GLY:HA2	6	0.66
(1,1027)	1:68:A:LEU:HD11	1:65:A:GLY:HA2	9	0.66
(1,1027)	1:68:A:LEU:HD12	1:65:A:GLY:HA2	9	0.66
(1,1027)	1:68:A:LEU:HD13	1:65:A:GLY:HA2	9	0.66
(1,680)	1:47:A:ALA:HB2	1:44:A:ASP:H	7	0.66
(1,601)	1:42:A:ASN:HA	1:42:A:ASN:HD22	10	0.66
(1,563)	1:38:A:VAL:HG21	1:38:A:VAL:H	5	0.66
(1,563)	1:38:A:VAL:HG22	1:38:A:VAL:H	5	0.66
(1,563)	1:38:A:VAL:HG23	1:38:A:VAL:H	5	0.66
(1,448)	1:3:A:THR:HG23	1:31:A:GLN:HE21	8	0.66
(1,150)	1:12:A:PRO:HA	1:12:A:PRO:HG3	7	0.66
(1,1984)	1:125:A:VAL:HG21	1:112:A:LEU:H	3	0.65
(1,1984)	1:125:A:VAL:HG22	1:112:A:LEU:H	3	0.65
(1,1984)	1:125:A:VAL:HG23	1:112:A:LEU:H	3	0.65
(1,1921)	1:122:A:ILE:HG13	1:118:A:ALA:H	1	0.65
(1,1894)	1:120:A:ASN:HB3	1:121:A:GLY:H	1	0.65
(1,1737)	1:20:A:ALA:HB2	1:64:A:LEU:HD13	4	0.65
(1,1641)	1:106:A:VAL:HG21	1:39:A:PHE:HB2	9	0.65
(1,1641)	1:106:A:VAL:HG22	1:39:A:PHE:HB2	9	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1641)	1:106:A:VAL:HG23	1:39:A:PHE:HB2	9	0.65
(1,1641)	1:106:A:VAL:HG21	1:39:A:PHE:HB2	10	0.65
(1,1641)	1:106:A:VAL:HG22	1:39:A:PHE:HB2	10	0.65
(1,1641)	1:106:A:VAL:HG23	1:39:A:PHE:HB2	10	0.65
(1,1423)	1:91:A:LEU:HB3	1:91:A:LEU:HD11	3	0.65
(1,1423)	1:91:A:LEU:HB3	1:91:A:LEU:HD12	3	0.65
(1,1423)	1:91:A:LEU:HB3	1:91:A:LEU:HD13	3	0.65
(1,1423)	1:91:A:LEU:HB3	1:91:A:LEU:HD11	10	0.65
(1,1423)	1:91:A:LEU:HB3	1:91:A:LEU:HD12	10	0.65
(1,1423)	1:91:A:LEU:HB3	1:91:A:LEU:HD13	10	0.65
(1,1414)	1:91:A:LEU:HD23	1:74:A:ALA:HB1	6	0.65
(1,1211)	1:82:A:LEU:HD21	1:77:A:TYR:HD1	5	0.65
(1,1211)	1:82:A:LEU:HD21	1:77:A:TYR:HD2	5	0.65
(1,1211)	1:82:A:LEU:HD22	1:77:A:TYR:HD1	5	0.65
(1,1211)	1:82:A:LEU:HD22	1:77:A:TYR:HD2	5	0.65
(1,1211)	1:82:A:LEU:HD23	1:77:A:TYR:HD1	5	0.65
(1,1211)	1:82:A:LEU:HD23	1:77:A:TYR:HD2	5	0.65
(1,1094)	1:73:A:VAL:HG11	1:91:A:LEU:H	5	0.65
(1,1094)	1:73:A:VAL:HG12	1:91:A:LEU:H	5	0.65
(1,1094)	1:73:A:VAL:HG13	1:91:A:LEU:H	5	0.65
(1,700)	1:48:A:LYS:HG3	1:48:A:LYS:HA	9	0.65
(1,631)	1:44:A:ASP:HB2	1:45:A:ALA:H	6	0.65
(1,601)	1:42:A:ASN:HA	1:42:A:ASN:HD22	5	0.65
(1,563)	1:38:A:VAL:HG21	1:38:A:VAL:H	6	0.65
(1,563)	1:38:A:VAL:HG22	1:38:A:VAL:H	6	0.65
(1,563)	1:38:A:VAL:HG23	1:38:A:VAL:H	6	0.65
(1,270)	1:22:A:LYS:HG2	1:22:A:LYS:HE3	6	0.65
(1,1921)	1:122:A:ILE:HG13	1:118:A:ALA:H	7	0.64
(1,1921)	1:122:A:ILE:HG13	1:118:A:ALA:H	9	0.64
(1,1894)	1:120:A:ASN:HB3	1:121:A:GLY:H	4	0.64
(1,1601)	1:104:A:LEU:HD11	1:79:A:ALA:H	5	0.64
(1,1601)	1:104:A:LEU:HD12	1:79:A:ALA:H	5	0.64
(1,1601)	1:104:A:LEU:HD13	1:79:A:ALA:H	5	0.64
(1,1516)	1:96:A:ILE:HG13	1:107:A:LYS:HB2	5	0.64
(1,1423)	1:91:A:LEU:HB3	1:91:A:LEU:HD11	1	0.64
(1,1423)	1:91:A:LEU:HB3	1:91:A:LEU:HD12	1	0.64
(1,1423)	1:91:A:LEU:HB3	1:91:A:LEU:HD13	1	0.64
(1,1423)	1:91:A:LEU:HB3	1:91:A:LEU:HD11	2	0.64
(1,1423)	1:91:A:LEU:HB3	1:91:A:LEU:HD12	2	0.64
(1,1423)	1:91:A:LEU:HB3	1:91:A:LEU:HD13	2	0.64
(1,1423)	1:91:A:LEU:HB3	1:91:A:LEU:HD11	5	0.64
(1,1423)	1:91:A:LEU:HB3	1:91:A:LEU:HD12	5	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1423)	1:91:A:LEU:HB3	1:91:A:LEU:HD13	5	0.64
(1,1423)	1:91:A:LEU:HB3	1:91:A:LEU:HD11	7	0.64
(1,1423)	1:91:A:LEU:HB3	1:91:A:LEU:HD12	7	0.64
(1,1423)	1:91:A:LEU:HB3	1:91:A:LEU:HD13	7	0.64
(1,1168)	1:78:A:LYS:HG3	1:122:A:ILE:HD11	2	0.64
(1,1168)	1:78:A:LYS:HG3	1:122:A:ILE:HD12	2	0.64
(1,1168)	1:78:A:LYS:HG3	1:122:A:ILE:HD13	2	0.64
(1,1148)	1:78:A:LYS:H	1:78:A:LYS:HD3	6	0.64
(1,1113)	1:76:A:ALA:HB1	1:77:A:TYR:H	4	0.64
(1,989)	1:66:A:ARG:HA	1:66:A:ARG:HB3	7	0.64
(1,679)	1:44:A:ASP:HB3	1:47:A:ALA:H	2	0.64
(1,622)	1:44:A:ASP:HB2	1:42:A:ASN:HD21	4	0.64
(1,601)	1:42:A:ASN:HA	1:42:A:ASN:HD22	6	0.64
(1,601)	1:42:A:ASN:HA	1:42:A:ASN:HD22	9	0.64
(1,448)	1:3:A:THR:HG22	1:31:A:GLN:HE21	2	0.64
(1,429)	1:30:A:LEU:HD12	1:70:A:TYR:H	4	0.64
(1,370)	1:89:A:THR:HG21	1:92:A:GLU:H	7	0.64
(1,270)	1:22:A:LYS:HG2	1:22:A:LYS:HE3	9	0.64
(1,1984)	1:125:A:VAL:HG21	1:112:A:LEU:H	2	0.63
(1,1984)	1:125:A:VAL:HG22	1:112:A:LEU:H	2	0.63
(1,1984)	1:125:A:VAL:HG23	1:112:A:LEU:H	2	0.63
(1,1894)	1:120:A:ASN:HB3	1:121:A:GLY:H	5	0.63
(1,1864)	1:118:A:ALA:HB3	1:121:A:GLY:HA2	6	0.63
(1,1601)	1:104:A:LEU:HD11	1:79:A:ALA:H	4	0.63
(1,1601)	1:104:A:LEU:HD12	1:79:A:ALA:H	4	0.63
(1,1601)	1:104:A:LEU:HD13	1:79:A:ALA:H	4	0.63
(1,1423)	1:91:A:LEU:HB3	1:91:A:LEU:HD11	4	0.63
(1,1423)	1:91:A:LEU:HB3	1:91:A:LEU:HD12	4	0.63
(1,1423)	1:91:A:LEU:HB3	1:91:A:LEU:HD13	4	0.63
(1,1423)	1:91:A:LEU:HB3	1:91:A:LEU:HD11	6	0.63
(1,1423)	1:91:A:LEU:HB3	1:91:A:LEU:HD12	6	0.63
(1,1423)	1:91:A:LEU:HB3	1:91:A:LEU:HD13	6	0.63
(1,1423)	1:91:A:LEU:HB3	1:91:A:LEU:HD11	8	0.63
(1,1423)	1:91:A:LEU:HB3	1:91:A:LEU:HD12	8	0.63
(1,1423)	1:91:A:LEU:HB3	1:91:A:LEU:HD13	8	0.63
(1,1211)	1:82:A:LEU:HD21	1:77:A:TYR:HD1	1	0.63
(1,1211)	1:82:A:LEU:HD21	1:77:A:TYR:HD2	1	0.63
(1,1211)	1:82:A:LEU:HD22	1:77:A:TYR:HD1	1	0.63
(1,1211)	1:82:A:LEU:HD22	1:77:A:TYR:HD2	1	0.63
(1,1211)	1:82:A:LEU:HD23	1:77:A:TYR:HD1	1	0.63
(1,1211)	1:82:A:LEU:HD23	1:77:A:TYR:HD2	1	0.63
(1,1176)	1:79:A:ALA:HA	1:104:A:LEU:HD11	10	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1176)	1:79:A:ALA:HA	1:104:A:LEU:HD12	10	0.63
(1,1176)	1:79:A:ALA:HA	1:104:A:LEU:HD13	10	0.63
(1,1168)	1:78:A:LYS:HG3	1:122:A:ILE:HD11	3	0.63
(1,1168)	1:78:A:LYS:HG3	1:122:A:ILE:HD12	3	0.63
(1,1168)	1:78:A:LYS:HG3	1:122:A:ILE:HD13	3	0.63
(1,1148)	1:78:A:LYS:H	1:78:A:LYS:HD3	4	0.63
(1,1113)	1:76:A:ALA:HB3	1:36:A:PHE:H	2	0.63
(1,989)	1:66:A:ARG:HA	1:66:A:ARG:HB3	2	0.63
(1,920)	1:54:A:ILE:HD13	1:63:A:GLN:HE21	1	0.63
(1,728)	1:49:A:LEU:HB2	1:50:A:PRO:HD3	3	0.63
(1,680)	1:47:A:ALA:HB3	1:44:A:ASP:H	5	0.63
(1,525)	1:107:A:LYS:HB3	1:107:A:LYS:HE2	2	0.63
(1,1684)	1:107:A:LYS:HG2	1:107:A:LYS:HE2	7	0.62
(1,1684)	1:107:A:LYS:HG2	1:107:A:LYS:HE3	7	0.62
(1,1566)	1:100:A:GLY:HA3	1:101:A:ASP:H	2	0.62
(1,1518)	1:96:A:ILE:HG13	1:107:A:LYS:HD2	1	0.62
(1,1518)	1:96:A:ILE:HG13	1:107:A:LYS:HD3	1	0.62
(1,1516)	1:96:A:ILE:HG13	1:107:A:LYS:HB2	6	0.62
(1,1408)	1:91:A:LEU:HD11	1:30:A:LEU:HA	4	0.62
(1,1408)	1:91:A:LEU:HD12	1:30:A:LEU:HA	4	0.62
(1,1408)	1:91:A:LEU:HD13	1:30:A:LEU:HA	4	0.62
(1,1408)	1:91:A:LEU:HD11	1:30:A:LEU:HA	6	0.62
(1,1408)	1:91:A:LEU:HD12	1:30:A:LEU:HA	6	0.62
(1,1408)	1:91:A:LEU:HD13	1:30:A:LEU:HA	6	0.62
(1,1259)	1:84:A:ARG:H	1:83:A:LYS:HB3	2	0.62
(1,1168)	1:78:A:LYS:HG3	1:122:A:ILE:HD11	8	0.62
(1,1168)	1:78:A:LYS:HG3	1:122:A:ILE:HD12	8	0.62
(1,1168)	1:78:A:LYS:HG3	1:122:A:ILE:HD13	8	0.62
(1,1113)	1:76:A:ALA:HB2	1:36:A:PHE:H	10	0.62
(1,974)	1:65:A:GLY:H	1:64:A:LEU:HB2	9	0.62
(1,708)	1:48:A:LYS:HG3	1:49:A:LEU:H	7	0.62
(1,700)	1:48:A:LYS:HG3	1:48:A:LYS:HA	10	0.62
(1,601)	1:42:A:ASN:HA	1:42:A:ASN:HD22	2	0.62
(1,2029)	1:126:A:ILE:HA	1:127:A:ASP:HB3	6	0.61
(1,1984)	1:125:A:VAL:HG21	1:112:A:LEU:H	7	0.61
(1,1984)	1:125:A:VAL:HG22	1:112:A:LEU:H	7	0.61
(1,1984)	1:125:A:VAL:HG23	1:112:A:LEU:H	7	0.61
(1,1684)	1:107:A:LYS:HG2	1:107:A:LYS:HE2	2	0.61
(1,1684)	1:107:A:LYS:HG2	1:107:A:LYS:HE3	2	0.61
(1,1505)	1:96:A:ILE:HG13	1:96:A:ILE:HG21	10	0.61
(1,1505)	1:96:A:ILE:HG13	1:96:A:ILE:HG22	10	0.61
(1,1505)	1:96:A:ILE:HG13	1:96:A:ILE:HG23	10	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1113)	1:76:A:ALA:HB2	1:77:A:TYR:H	8	0.61
(1,1094)	1:73:A:VAL:HG11	1:91:A:LEU:H	3	0.61
(1,1094)	1:73:A:VAL:HG12	1:91:A:LEU:H	3	0.61
(1,1094)	1:73:A:VAL:HG13	1:91:A:LEU:H	3	0.61
(1,969)	1:65:A:GLY:HA2	1:26:A:LEU:HD11	2	0.61
(1,969)	1:65:A:GLY:HA2	1:26:A:LEU:HD12	2	0.61
(1,969)	1:65:A:GLY:HA2	1:26:A:LEU:HD13	2	0.61
(1,700)	1:48:A:LYS:HG3	1:48:A:LYS:HA	4	0.61
(1,679)	1:44:A:ASP:HB3	1:47:A:ALA:H	6	0.61
(1,679)	1:44:A:ASP:HB3	1:47:A:ALA:H	9	0.61
(1,433)	1:31:A:GLN:HE21	1:6:A:ASP:HB3	8	0.61
(1,344)	1:60:A:ASN:HB3	1:60:A:ASN:HD22	1	0.61
(1,344)	1:60:A:ASN:HB3	1:60:A:ASN:HD22	2	0.61
(1,344)	1:60:A:ASN:HB3	1:60:A:ASN:HD22	5	0.61
(1,344)	1:60:A:ASN:HB3	1:60:A:ASN:HD22	8	0.61
(1,1981)	1:124:A:HIS:HB2	1:125:A:VAL:H	3	0.6
(1,1737)	1:20:A:ALA:HB1	1:64:A:LEU:HD13	1	0.6
(1,1720)	1:110:A:THR:HG21	1:103:A:PRO:HB3	2	0.6
(1,1720)	1:110:A:THR:HG22	1:103:A:PRO:HB3	2	0.6
(1,1720)	1:110:A:THR:HG23	1:103:A:PRO:HB3	2	0.6
(1,1662)	1:106:A:VAL:HG11	1:107:A:LYS:HG3	4	0.6
(1,1662)	1:106:A:VAL:HG12	1:107:A:LYS:HG3	4	0.6
(1,1662)	1:106:A:VAL:HG13	1:107:A:LYS:HG3	4	0.6
(1,1505)	1:96:A:ILE:HG13	1:96:A:ILE:HG21	3	0.6
(1,1505)	1:96:A:ILE:HG13	1:96:A:ILE:HG22	3	0.6
(1,1505)	1:96:A:ILE:HG13	1:96:A:ILE:HG23	3	0.6
(1,1259)	1:84:A:ARG:H	1:83:A:LYS:HB3	7	0.6
(1,990)	1:66:A:ARG:H	1:66:A:ARG:HB2	3	0.6
(1,989)	1:66:A:ARG:HA	1:66:A:ARG:HB3	5	0.6
(1,989)	1:66:A:ARG:HA	1:66:A:ARG:HB3	6	0.6
(1,974)	1:65:A:GLY:H	1:64:A:LEU:HB2	2	0.6
(1,974)	1:65:A:GLY:H	1:64:A:LEU:HB2	3	0.6
(1,974)	1:65:A:GLY:H	1:64:A:LEU:HB2	5	0.6
(1,974)	1:65:A:GLY:H	1:64:A:LEU:HB2	6	0.6
(1,974)	1:65:A:GLY:H	1:64:A:LEU:HB2	10	0.6
(1,856)	1:59:A:GLN:HA	1:59:A:GLN:HB2	1	0.6
(1,856)	1:59:A:GLN:HA	1:59:A:GLN:HB2	2	0.6
(1,856)	1:59:A:GLN:HA	1:59:A:GLN:HB2	4	0.6
(1,856)	1:59:A:GLN:HA	1:59:A:GLN:HB2	6	0.6
(1,856)	1:59:A:GLN:HA	1:59:A:GLN:HB2	7	0.6
(1,856)	1:59:A:GLN:HA	1:59:A:GLN:HB2	8	0.6
(1,856)	1:59:A:GLN:HA	1:59:A:GLN:HB2	10	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,774)	1:54:A:ILE:HG12	1:63:A:GLN:HE22	7	0.6
(1,772)	1:55:A:THR:HG21	1:58:A:VAL:H	1	0.6
(1,772)	1:55:A:THR:HG22	1:58:A:VAL:H	5	0.6
(1,723)	1:49:A:LEU:HB3	1:49:A:LEU:H	3	0.6
(1,723)	1:49:A:LEU:HB3	1:49:A:LEU:H	7	0.6
(1,700)	1:48:A:LYS:HG3	1:48:A:LYS:HA	1	0.6
(1,520)	1:36:A:PHE:HA	1:72:A:VAL:HG11	6	0.6
(1,520)	1:36:A:PHE:HA	1:72:A:VAL:HG12	6	0.6
(1,520)	1:36:A:PHE:HA	1:72:A:VAL:HG13	6	0.6
(1,344)	1:60:A:ASN:HB3	1:60:A:ASN:HD22	6	0.6
(1,344)	1:60:A:ASN:HB3	1:60:A:ASN:HD22	7	0.6
(1,344)	1:60:A:ASN:HB3	1:60:A:ASN:HD22	10	0.6
(1,1720)	1:110:A:THR:HG21	1:103:A:PRO:HB3	4	0.59
(1,1720)	1:110:A:THR:HG22	1:103:A:PRO:HB3	4	0.59
(1,1720)	1:110:A:THR:HG23	1:103:A:PRO:HB3	4	0.59
(1,1518)	1:96:A:ILE:HG13	1:107:A:LYS:HD2	10	0.59
(1,1518)	1:96:A:ILE:HG13	1:107:A:LYS:HD3	10	0.59
(1,1211)	1:82:A:LEU:HD21	1:77:A:TYR:HD1	10	0.59
(1,1211)	1:82:A:LEU:HD21	1:77:A:TYR:HD2	10	0.59
(1,1211)	1:82:A:LEU:HD22	1:77:A:TYR:HD1	10	0.59
(1,1211)	1:82:A:LEU:HD22	1:77:A:TYR:HD2	10	0.59
(1,1211)	1:82:A:LEU:HD23	1:77:A:TYR:HD1	10	0.59
(1,1211)	1:82:A:LEU:HD23	1:77:A:TYR:HD2	10	0.59
(1,1027)	1:68:A:LEU:HD11	1:65:A:GLY:HA2	7	0.59
(1,1027)	1:68:A:LEU:HD12	1:65:A:GLY:HA2	7	0.59
(1,1027)	1:68:A:LEU:HD13	1:65:A:GLY:HA2	7	0.59
(1,981)	1:65:A:GLY:HA3	1:68:A:LEU:H	2	0.59
(1,856)	1:59:A:GLN:HA	1:59:A:GLN:HB2	3	0.59
(1,856)	1:59:A:GLN:HA	1:59:A:GLN:HB2	5	0.59
(1,772)	1:55:A:THR:HG22	1:58:A:VAL:H	2	0.59
(1,723)	1:49:A:LEU:HB3	1:49:A:LEU:H	5	0.59
(1,700)	1:48:A:LYS:HG3	1:48:A:LYS:HA	8	0.59
(1,679)	1:44:A:ASP:HB3	1:47:A:ALA:H	7	0.59
(1,370)	1:89:A:THR:HG23	1:92:A:GLU:H	6	0.59
(1,344)	1:60:A:ASN:HB3	1:60:A:ASN:HD22	9	0.59
(1,1984)	1:125:A:VAL:HG21	1:112:A:LEU:H	4	0.58
(1,1984)	1:125:A:VAL:HG22	1:112:A:LEU:H	4	0.58
(1,1984)	1:125:A:VAL:HG23	1:112:A:LEU:H	4	0.58
(1,1894)	1:120:A:ASN:HB3	1:121:A:GLY:H	9	0.58
(1,1864)	1:118:A:ALA:HB2	1:121:A:GLY:HA2	10	0.58
(1,1737)	1:20:A:ALA:HB3	1:64:A:LEU:HD12	6	0.58
(1,1289)	1:85:A:MET:HB3	1:85:A:MET:H	6	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1289)	1:85:A:MET:HB3	1:85:A:MET:H	7	0.58
(1,1259)	1:84:A:ARG:H	1:83:A:LYS:HB3	9	0.58
(1,989)	1:66:A:ARG:HA	1:66:A:ARG:HB3	9	0.58
(1,974)	1:65:A:GLY:H	1:64:A:LEU:HB2	8	0.58
(1,856)	1:59:A:GLN:HA	1:59:A:GLN:HB2	9	0.58
(1,700)	1:48:A:LYS:HG3	1:48:A:LYS:HA	6	0.58
(1,527)	1:36:A:PHE:HB2	1:120:A:ASN:HD22	9	0.58
(1,370)	1:89:A:THR:HG23	1:92:A:GLU:H	1	0.58
(1,195)	1:18:A:VAL:HG21	1:18:A:VAL:HA	8	0.58
(1,195)	1:18:A:VAL:HG22	1:18:A:VAL:HA	8	0.58
(1,195)	1:18:A:VAL:HG23	1:18:A:VAL:HA	8	0.58
(1,1921)	1:122:A:ILE:HG13	1:118:A:ALA:H	10	0.57
(1,1894)	1:120:A:ASN:HB3	1:121:A:GLY:H	7	0.57
(1,1516)	1:96:A:ILE:HG13	1:107:A:LYS:HB2	9	0.57
(1,1464)	1:93:A:GLY:H	1:92:A:GLU:HG3	5	0.57
(1,1414)	1:91:A:LEU:HD23	1:74:A:ALA:HB2	7	0.57
(1,1289)	1:85:A:MET:HB3	1:85:A:MET:H	2	0.57
(1,1289)	1:85:A:MET:HB3	1:85:A:MET:H	5	0.57
(1,1289)	1:85:A:MET:HB3	1:85:A:MET:H	8	0.57
(1,1289)	1:85:A:MET:HB3	1:85:A:MET:H	9	0.57
(1,1211)	1:82:A:LEU:HD21	1:77:A:TYR:HD1	9	0.57
(1,1211)	1:82:A:LEU:HD21	1:77:A:TYR:HD2	9	0.57
(1,1211)	1:82:A:LEU:HD22	1:77:A:TYR:HD1	9	0.57
(1,1211)	1:82:A:LEU:HD22	1:77:A:TYR:HD2	9	0.57
(1,1211)	1:82:A:LEU:HD23	1:77:A:TYR:HD1	9	0.57
(1,1211)	1:82:A:LEU:HD23	1:77:A:TYR:HD2	9	0.57
(1,1113)	1:76:A:ALA:HB3	1:36:A:PHE:H	9	0.57
(1,1027)	1:68:A:LEU:HD11	1:65:A:GLY:HA2	2	0.57
(1,1027)	1:68:A:LEU:HD12	1:65:A:GLY:HA2	2	0.57
(1,1027)	1:68:A:LEU:HD13	1:65:A:GLY:HA2	2	0.57
(1,1027)	1:68:A:LEU:HD11	1:65:A:GLY:HA2	5	0.57
(1,1027)	1:68:A:LEU:HD12	1:65:A:GLY:HA2	5	0.57
(1,1027)	1:68:A:LEU:HD13	1:65:A:GLY:HA2	5	0.57
(1,983)	1:66:A:ARG:HB2	1:66:A:ARG:HD2	5	0.57
(1,974)	1:65:A:GLY:H	1:64:A:LEU:HB2	1	0.57
(1,974)	1:65:A:GLY:H	1:64:A:LEU:HB2	4	0.57
(1,974)	1:65:A:GLY:H	1:64:A:LEU:HB2	7	0.57
(1,920)	1:54:A:ILE:HD12	1:63:A:GLN:HE21	6	0.57
(1,776)	1:54:A:ILE:HG13	1:67:A:ILE:HG21	3	0.57
(1,776)	1:54:A:ILE:HG13	1:67:A:ILE:HG22	3	0.57
(1,776)	1:54:A:ILE:HG13	1:67:A:ILE:HG23	3	0.57
(1,772)	1:55:A:THR:HG23	1:58:A:VAL:H	4	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,679)	1:44:A:ASP:HB3	1:47:A:ALA:H	5	0.57
(1,520)	1:36:A:PHE:HA	1:72:A:VAL:HG11	7	0.57
(1,520)	1:36:A:PHE:HA	1:72:A:VAL:HG12	7	0.57
(1,520)	1:36:A:PHE:HA	1:72:A:VAL:HG13	7	0.57
(1,517)	1:36:A:PHE:HB2	1:37:A:THR:H	4	0.57
(1,370)	1:89:A:THR:HG23	1:92:A:GLU:H	9	0.57
(1,195)	1:18:A:VAL:HG21	1:18:A:VAL:HA	5	0.57
(1,195)	1:18:A:VAL:HG22	1:18:A:VAL:HA	5	0.57
(1,195)	1:18:A:VAL:HG23	1:18:A:VAL:HA	5	0.57
(1,195)	1:18:A:VAL:HG21	1:18:A:VAL:HA	6	0.57
(1,195)	1:18:A:VAL:HG22	1:18:A:VAL:HA	6	0.57
(1,195)	1:18:A:VAL:HG23	1:18:A:VAL:HA	6	0.57
(1,33)	1:5:A:VAL:HG11	1:6:A:ASP:HB3	4	0.57
(1,33)	1:5:A:VAL:HG12	1:6:A:ASP:HB3	4	0.57
(1,33)	1:5:A:VAL:HG13	1:6:A:ASP:HB3	4	0.57
(1,1968)	1:124:A:HIS:HB3	1:39:A:PHE:HD1	5	0.56
(1,1968)	1:124:A:HIS:HB3	1:39:A:PHE:HD2	5	0.56
(1,1921)	1:122:A:ILE:HG13	1:118:A:ALA:H	6	0.56
(1,1516)	1:96:A:ILE:HG13	1:107:A:LYS:HB2	10	0.56
(1,1505)	1:96:A:ILE:HG13	1:96:A:ILE:HG21	4	0.56
(1,1505)	1:96:A:ILE:HG13	1:96:A:ILE:HG22	4	0.56
(1,1505)	1:96:A:ILE:HG13	1:96:A:ILE:HG23	4	0.56
(1,1447)	1:92:A:GLU:HA	1:92:A:GLU:HG3	3	0.56
(1,1447)	1:92:A:GLU:HA	1:92:A:GLU:HG3	5	0.56
(1,1408)	1:91:A:LEU:HD11	1:30:A:LEU:HA	8	0.56
(1,1408)	1:91:A:LEU:HD12	1:30:A:LEU:HA	8	0.56
(1,1408)	1:91:A:LEU:HD13	1:30:A:LEU:HA	8	0.56
(1,1289)	1:85:A:MET:HB3	1:85:A:MET:H	1	0.56
(1,1289)	1:85:A:MET:HB3	1:85:A:MET:H	3	0.56
(1,1289)	1:85:A:MET:HB3	1:85:A:MET:H	4	0.56
(1,1289)	1:85:A:MET:HB3	1:85:A:MET:H	10	0.56
(1,1259)	1:84:A:ARG:H	1:83:A:LYS:HB3	10	0.56
(1,690)	1:48:A:LYS:HG2	1:48:A:LYS:HB3	1	0.56
(1,679)	1:44:A:ASP:HB3	1:47:A:ALA:H	3	0.56
(1,622)	1:44:A:ASP:HB2	1:42:A:ASN:HD21	6	0.56
(1,601)	1:42:A:ASN:HA	1:42:A:ASN:HD22	4	0.56
(1,601)	1:42:A:ASN:HA	1:42:A:ASN:HD22	8	0.56
(1,517)	1:36:A:PHE:HB2	1:37:A:THR:H	1	0.56
(1,195)	1:18:A:VAL:HG21	1:18:A:VAL:HA	1	0.56
(1,195)	1:18:A:VAL:HG22	1:18:A:VAL:HA	1	0.56
(1,195)	1:18:A:VAL:HG23	1:18:A:VAL:HA	1	0.56
(1,195)	1:18:A:VAL:HG21	1:18:A:VAL:HA	2	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,195)	1:18:A:VAL:HG22	1:18:A:VAL:HA	2	0.56
(1,195)	1:18:A:VAL:HG23	1:18:A:VAL:HA	2	0.56
(1,195)	1:18:A:VAL:HG21	1:18:A:VAL:HA	3	0.56
(1,195)	1:18:A:VAL:HG22	1:18:A:VAL:HA	3	0.56
(1,195)	1:18:A:VAL:HG23	1:18:A:VAL:HA	3	0.56
(1,195)	1:18:A:VAL:HG21	1:18:A:VAL:HA	4	0.56
(1,195)	1:18:A:VAL:HG22	1:18:A:VAL:HA	4	0.56
(1,195)	1:18:A:VAL:HG23	1:18:A:VAL:HA	4	0.56
(1,195)	1:18:A:VAL:HG21	1:18:A:VAL:HA	7	0.56
(1,195)	1:18:A:VAL:HG22	1:18:A:VAL:HA	7	0.56
(1,195)	1:18:A:VAL:HG23	1:18:A:VAL:HA	7	0.56
(1,195)	1:18:A:VAL:HG21	1:18:A:VAL:HA	9	0.56
(1,195)	1:18:A:VAL:HG22	1:18:A:VAL:HA	9	0.56
(1,195)	1:18:A:VAL:HG23	1:18:A:VAL:HA	9	0.56
(1,195)	1:18:A:VAL:HG21	1:18:A:VAL:HA	10	0.56
(1,195)	1:18:A:VAL:HG22	1:18:A:VAL:HA	10	0.56
(1,195)	1:18:A:VAL:HG23	1:18:A:VAL:HA	10	0.56
(1,33)	1:5:A:VAL:HG11	1:6:A:ASP:HB3	8	0.56
(1,33)	1:5:A:VAL:HG12	1:6:A:ASP:HB3	8	0.56
(1,33)	1:5:A:VAL:HG13	1:6:A:ASP:HB3	8	0.56
(1,1894)	1:120:A:ASN:HB3	1:121:A:GLY:H	8	0.55
(1,1894)	1:120:A:ASN:HB3	1:121:A:GLY:H	10	0.55
(1,1662)	1:106:A:VAL:HG11	1:107:A:LYS:HG3	1	0.55
(1,1662)	1:106:A:VAL:HG12	1:107:A:LYS:HG3	1	0.55
(1,1662)	1:106:A:VAL:HG13	1:107:A:LYS:HG3	1	0.55
(1,1601)	1:104:A:LEU:HD11	1:79:A:ALA:H	1	0.55
(1,1601)	1:104:A:LEU:HD12	1:79:A:ALA:H	1	0.55
(1,1601)	1:104:A:LEU:HD13	1:79:A:ALA:H	1	0.55
(1,1519)	1:96:A:ILE:HG13	1:107:A:LYS:HE2	2	0.55
(1,1519)	1:96:A:ILE:HG13	1:107:A:LYS:HE3	2	0.55
(1,1505)	1:96:A:ILE:HG13	1:96:A:ILE:HG21	7	0.55
(1,1505)	1:96:A:ILE:HG13	1:96:A:ILE:HG22	7	0.55
(1,1505)	1:96:A:ILE:HG13	1:96:A:ILE:HG23	7	0.55
(1,1414)	1:91:A:LEU:HD23	1:74:A:ALA:HB1	1	0.55
(1,1176)	1:79:A:ALA:HA	1:104:A:LEU:HD11	3	0.55
(1,1176)	1:79:A:ALA:HA	1:104:A:LEU:HD12	3	0.55
(1,1176)	1:79:A:ALA:HA	1:104:A:LEU:HD13	3	0.55
(1,1116)	1:76:A:ALA:H	1:75:A:GLY:HA3	6	0.55
(1,1027)	1:68:A:LEU:HD11	1:65:A:GLY:HA2	8	0.55
(1,1027)	1:68:A:LEU:HD12	1:65:A:GLY:HA2	8	0.55
(1,1027)	1:68:A:LEU:HD13	1:65:A:GLY:HA2	8	0.55
(1,772)	1:55:A:THR:HG21	1:58:A:VAL:H	6	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,772)	1:55:A:THR:HG23	1:58:A:VAL:H	8	0.55
(1,772)	1:55:A:THR:HG21	1:58:A:VAL:H	10	0.55
(1,723)	1:49:A:LEU:HB3	1:49:A:LEU:H	4	0.55
(1,723)	1:49:A:LEU:HB3	1:49:A:LEU:H	9	0.55
(1,690)	1:48:A:LYS:HG2	1:48:A:LYS:HB3	4	0.55
(1,690)	1:48:A:LYS:HG2	1:48:A:LYS:HB3	6	0.55
(1,690)	1:48:A:LYS:HG2	1:48:A:LYS:HB3	8	0.55
(1,690)	1:48:A:LYS:HG2	1:48:A:LYS:HB3	9	0.55
(1,690)	1:48:A:LYS:HG2	1:48:A:LYS:HB3	10	0.55
(1,622)	1:44:A:ASP:HB2	1:42:A:ASN:HD21	3	0.55
(1,622)	1:44:A:ASP:HB2	1:42:A:ASN:HD21	8	0.55
(1,517)	1:36:A:PHE:HB2	1:37:A:THR:H	8	0.55
(1,433)	1:31:A:GLN:HE21	1:6:A:ASP:HB3	7	0.55
(1,393)	1:28:A:GLU:H	1:28:A:GLU:HB2	1	0.55
(1,393)	1:28:A:GLU:H	1:28:A:GLU:HB2	7	0.55
(1,393)	1:28:A:GLU:H	1:28:A:GLU:HB2	8	0.55
(1,33)	1:5:A:VAL:HG11	1:6:A:ASP:HB3	3	0.55
(1,33)	1:5:A:VAL:HG12	1:6:A:ASP:HB3	3	0.55
(1,33)	1:5:A:VAL:HG13	1:6:A:ASP:HB3	3	0.55
(1,33)	1:5:A:VAL:HG11	1:6:A:ASP:HB3	5	0.55
(1,33)	1:5:A:VAL:HG12	1:6:A:ASP:HB3	5	0.55
(1,33)	1:5:A:VAL:HG13	1:6:A:ASP:HB3	5	0.55
(1,2029)	1:126:A:ILE:HA	1:127:A:ASP:HB3	10	0.54
(1,1981)	1:124:A:HIS:HB2	1:125:A:VAL:H	8	0.54
(1,1921)	1:122:A:ILE:HG13	1:118:A:ALA:H	4	0.54
(1,1505)	1:96:A:ILE:HG13	1:96:A:ILE:HG21	1	0.54
(1,1505)	1:96:A:ILE:HG13	1:96:A:ILE:HG22	1	0.54
(1,1505)	1:96:A:ILE:HG13	1:96:A:ILE:HG23	1	0.54
(1,1505)	1:96:A:ILE:HG13	1:96:A:ILE:HG21	2	0.54
(1,1505)	1:96:A:ILE:HG13	1:96:A:ILE:HG22	2	0.54
(1,1505)	1:96:A:ILE:HG13	1:96:A:ILE:HG23	2	0.54
(1,1505)	1:96:A:ILE:HG13	1:96:A:ILE:HG21	6	0.54
(1,1505)	1:96:A:ILE:HG13	1:96:A:ILE:HG22	6	0.54
(1,1505)	1:96:A:ILE:HG13	1:96:A:ILE:HG23	6	0.54
(1,1238)	1:82:A:LEU:HB3	1:104:A:LEU:HD21	7	0.54
(1,1238)	1:82:A:LEU:HB3	1:104:A:LEU:HD22	7	0.54
(1,1238)	1:82:A:LEU:HB3	1:104:A:LEU:HD23	7	0.54
(1,1125)	1:77:A:TYR:HB2	1:37:A:THR:HG21	6	0.54
(1,1125)	1:77:A:TYR:HB2	1:37:A:THR:HG22	6	0.54
(1,1125)	1:77:A:TYR:HB2	1:37:A:THR:HG23	6	0.54
(1,920)	1:54:A:ILE:HD12	1:63:A:GLN:HE21	4	0.54
(1,772)	1:55:A:THR:HG21	1:58:A:VAL:H	7	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,723)	1:49:A:LEU:HB3	1:49:A:LEU:H	2	0.54
(1,723)	1:49:A:LEU:HB3	1:49:A:LEU:H	6	0.54
(1,700)	1:48:A:LYS:HG3	1:48:A:LYS:HA	2	0.54
(1,690)	1:48:A:LYS:HG2	1:48:A:LYS:HB3	2	0.54
(1,517)	1:36:A:PHE:HB2	1:37:A:THR:H	3	0.54
(1,393)	1:28:A:GLU:H	1:28:A:GLU:HB2	6	0.54
(1,393)	1:28:A:GLU:H	1:28:A:GLU:HB2	9	0.54
(1,343)	1:25:A:ASN:HD22	1:92:A:GLU:HB3	9	0.54
(1,342)	1:36:A:PHE:HB2	1:75:A:GLY:H	6	0.54
(1,227)	1:20:A:ALA:HB1	1:64:A:LEU:HD11	7	0.54
(1,227)	1:20:A:ALA:HB1	1:64:A:LEU:HD12	7	0.54
(1,227)	1:20:A:ALA:HB1	1:64:A:LEU:HD13	7	0.54
(1,227)	1:20:A:ALA:HB2	1:64:A:LEU:HD11	7	0.54
(1,227)	1:20:A:ALA:HB2	1:64:A:LEU:HD12	7	0.54
(1,227)	1:20:A:ALA:HB2	1:64:A:LEU:HD13	7	0.54
(1,227)	1:20:A:ALA:HB3	1:64:A:LEU:HD11	7	0.54
(1,227)	1:20:A:ALA:HB3	1:64:A:LEU:HD12	7	0.54
(1,227)	1:20:A:ALA:HB3	1:64:A:LEU:HD13	7	0.54
(1,33)	1:5:A:VAL:HG11	1:6:A:ASP:HB3	1	0.54
(1,33)	1:5:A:VAL:HG12	1:6:A:ASP:HB3	1	0.54
(1,33)	1:5:A:VAL:HG13	1:6:A:ASP:HB3	1	0.54
(1,1984)	1:125:A:VAL:HG21	1:112:A:LEU:H	1	0.53
(1,1984)	1:125:A:VAL:HG22	1:112:A:LEU:H	1	0.53
(1,1984)	1:125:A:VAL:HG23	1:112:A:LEU:H	1	0.53
(1,1984)	1:125:A:VAL:HG21	1:112:A:LEU:H	6	0.53
(1,1984)	1:125:A:VAL:HG22	1:112:A:LEU:H	6	0.53
(1,1984)	1:125:A:VAL:HG23	1:112:A:LEU:H	6	0.53
(1,1894)	1:120:A:ASN:HB3	1:121:A:GLY:H	6	0.53
(1,1737)	1:20:A:ALA:HB1	1:64:A:LEU:HD11	5	0.53
(1,1603)	1:104:A:LEU:H	1:103:A:PRO:HG3	10	0.53
(1,1505)	1:96:A:ILE:HG13	1:96:A:ILE:HG21	9	0.53
(1,1505)	1:96:A:ILE:HG13	1:96:A:ILE:HG22	9	0.53
(1,1505)	1:96:A:ILE:HG13	1:96:A:ILE:HG23	9	0.53
(1,1435)	1:91:A:LEU:HD21	1:91:A:LEU:H	5	0.53
(1,1435)	1:91:A:LEU:HD22	1:91:A:LEU:H	5	0.53
(1,1435)	1:91:A:LEU:HD23	1:91:A:LEU:H	5	0.53
(1,1176)	1:79:A:ALA:HA	1:104:A:LEU:HD11	2	0.53
(1,1176)	1:79:A:ALA:HA	1:104:A:LEU:HD12	2	0.53
(1,1176)	1:79:A:ALA:HA	1:104:A:LEU:HD13	2	0.53
(1,1113)	1:76:A:ALA:HB3	1:36:A:PHE:H	5	0.53
(1,981)	1:65:A:GLY:HA3	1:68:A:LEU:H	6	0.53
(1,981)	1:65:A:GLY:HA3	1:68:A:LEU:H	9	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,920)	1:54:A:ILE:HD13	1:63:A:GLN:HE21	9	0.53
(1,723)	1:49:A:LEU:HB3	1:49:A:LEU:H	1	0.53
(1,723)	1:49:A:LEU:HB3	1:49:A:LEU:H	8	0.53
(1,700)	1:48:A:LYS:HG3	1:48:A:LYS:HA	5	0.53
(1,601)	1:42:A:ASN:HA	1:42:A:ASN:HD22	3	0.53
(1,553)	1:37:A:THR:HG21	1:82:A:LEU:HD11	3	0.53
(1,553)	1:37:A:THR:HG21	1:82:A:LEU:HD12	3	0.53
(1,553)	1:37:A:THR:HG21	1:82:A:LEU:HD13	3	0.53
(1,553)	1:37:A:THR:HG22	1:82:A:LEU:HD11	3	0.53
(1,553)	1:37:A:THR:HG22	1:82:A:LEU:HD12	3	0.53
(1,553)	1:37:A:THR:HG22	1:82:A:LEU:HD13	3	0.53
(1,553)	1:37:A:THR:HG23	1:82:A:LEU:HD11	3	0.53
(1,553)	1:37:A:THR:HG23	1:82:A:LEU:HD12	3	0.53
(1,553)	1:37:A:THR:HG23	1:82:A:LEU:HD13	3	0.53
(1,520)	1:36:A:PHE:HA	1:72:A:VAL:HG11	1	0.53
(1,520)	1:36:A:PHE:HA	1:72:A:VAL:HG12	1	0.53
(1,520)	1:36:A:PHE:HA	1:72:A:VAL:HG13	1	0.53
(1,520)	1:36:A:PHE:HA	1:72:A:VAL:HG11	8	0.53
(1,520)	1:36:A:PHE:HA	1:72:A:VAL:HG12	8	0.53
(1,520)	1:36:A:PHE:HA	1:72:A:VAL:HG13	8	0.53
(1,393)	1:28:A:GLU:H	1:28:A:GLU:HB2	2	0.53
(1,393)	1:28:A:GLU:H	1:28:A:GLU:HB2	3	0.53
(1,393)	1:28:A:GLU:H	1:28:A:GLU:HB2	5	0.53
(1,393)	1:28:A:GLU:H	1:28:A:GLU:HB2	10	0.53
(1,33)	1:5:A:VAL:HG11	1:6:A:ASP:HB3	6	0.53
(1,33)	1:5:A:VAL:HG12	1:6:A:ASP:HB3	6	0.53
(1,33)	1:5:A:VAL:HG13	1:6:A:ASP:HB3	6	0.53
(1,33)	1:5:A:VAL:HG11	1:6:A:ASP:HB3	9	0.53
(1,33)	1:5:A:VAL:HG12	1:6:A:ASP:HB3	9	0.53
(1,33)	1:5:A:VAL:HG13	1:6:A:ASP:HB3	9	0.53
(1,2029)	1:126:A:ILE:HA	1:127:A:ASP:HB3	3	0.52
(1,1981)	1:124:A:HIS:HB2	1:125:A:VAL:H	9	0.52
(1,1603)	1:104:A:LEU:H	1:103:A:PRO:HG3	7	0.52
(1,1601)	1:104:A:LEU:HD11	1:79:A:ALA:H	6	0.52
(1,1601)	1:104:A:LEU:HD12	1:79:A:ALA:H	6	0.52
(1,1601)	1:104:A:LEU:HD13	1:79:A:ALA:H	6	0.52
(1,1464)	1:93:A:GLY:H	1:92:A:GLU:HG3	3	0.52
(1,1358)	1:88:A:VAL:HA	1:88:A:VAL:HG21	1	0.52
(1,1358)	1:88:A:VAL:HA	1:88:A:VAL:HG22	1	0.52
(1,1358)	1:88:A:VAL:HA	1:88:A:VAL:HG23	1	0.52
(1,1358)	1:88:A:VAL:HA	1:88:A:VAL:HG21	2	0.52
(1,1358)	1:88:A:VAL:HA	1:88:A:VAL:HG22	2	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1358)	1:88:A:VAL:HA	1:88:A:VAL:HG23	2	0.52
(1,1358)	1:88:A:VAL:HA	1:88:A:VAL:HG21	3	0.52
(1,1358)	1:88:A:VAL:HA	1:88:A:VAL:HG22	3	0.52
(1,1358)	1:88:A:VAL:HA	1:88:A:VAL:HG23	3	0.52
(1,1358)	1:88:A:VAL:HA	1:88:A:VAL:HG21	4	0.52
(1,1358)	1:88:A:VAL:HA	1:88:A:VAL:HG22	4	0.52
(1,1358)	1:88:A:VAL:HA	1:88:A:VAL:HG23	4	0.52
(1,1358)	1:88:A:VAL:HA	1:88:A:VAL:HG21	5	0.52
(1,1358)	1:88:A:VAL:HA	1:88:A:VAL:HG22	5	0.52
(1,1358)	1:88:A:VAL:HA	1:88:A:VAL:HG23	5	0.52
(1,1358)	1:88:A:VAL:HA	1:88:A:VAL:HG21	6	0.52
(1,1358)	1:88:A:VAL:HA	1:88:A:VAL:HG22	6	0.52
(1,1358)	1:88:A:VAL:HA	1:88:A:VAL:HG23	6	0.52
(1,1358)	1:88:A:VAL:HA	1:88:A:VAL:HG21	7	0.52
(1,1358)	1:88:A:VAL:HA	1:88:A:VAL:HG22	7	0.52
(1,1358)	1:88:A:VAL:HA	1:88:A:VAL:HG23	7	0.52
(1,1358)	1:88:A:VAL:HA	1:88:A:VAL:HG21	8	0.52
(1,1358)	1:88:A:VAL:HA	1:88:A:VAL:HG22	8	0.52
(1,1358)	1:88:A:VAL:HA	1:88:A:VAL:HG23	8	0.52
(1,1358)	1:88:A:VAL:HA	1:88:A:VAL:HG21	9	0.52
(1,1358)	1:88:A:VAL:HA	1:88:A:VAL:HG22	9	0.52
(1,1358)	1:88:A:VAL:HA	1:88:A:VAL:HG23	9	0.52
(1,1358)	1:88:A:VAL:HA	1:88:A:VAL:HG21	10	0.52
(1,1358)	1:88:A:VAL:HA	1:88:A:VAL:HG22	10	0.52
(1,1358)	1:88:A:VAL:HA	1:88:A:VAL:HG23	10	0.52
(1,1201)	1:81:A:ASP:HB3	1:81:A:ASP:H	4	0.52
(1,1148)	1:78:A:LYS:H	1:78:A:LYS:HD3	10	0.52
(1,1076)	1:72:A:VAL:HG11	1:73:A:VAL:H	10	0.52
(1,1076)	1:72:A:VAL:HG12	1:73:A:VAL:H	10	0.52
(1,1076)	1:72:A:VAL:HG13	1:73:A:VAL:H	10	0.52
(1,992)	1:66:A:ARG:HG3	1:67:A:ILE:H	8	0.52
(1,723)	1:49:A:LEU:HB3	1:49:A:LEU:H	10	0.52
(1,393)	1:28:A:GLU:H	1:28:A:GLU:HB2	4	0.52
(1,227)	1:20:A:ALA:HB1	1:64:A:LEU:HD11	4	0.52
(1,227)	1:20:A:ALA:HB1	1:64:A:LEU:HD12	4	0.52
(1,227)	1:20:A:ALA:HB1	1:64:A:LEU:HD13	4	0.52
(1,227)	1:20:A:ALA:HB2	1:64:A:LEU:HD11	4	0.52
(1,227)	1:20:A:ALA:HB2	1:64:A:LEU:HD12	4	0.52
(1,227)	1:20:A:ALA:HB2	1:64:A:LEU:HD13	4	0.52
(1,227)	1:20:A:ALA:HB3	1:64:A:LEU:HD11	4	0.52
(1,227)	1:20:A:ALA:HB3	1:64:A:LEU:HD12	4	0.52
(1,227)	1:20:A:ALA:HB3	1:64:A:LEU:HD13	4	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,200)	1:18:A:VAL:HG11	1:19:A:THR:H	2	0.52
(1,200)	1:18:A:VAL:HG12	1:19:A:THR:H	2	0.52
(1,200)	1:18:A:VAL:HG13	1:19:A:THR:H	2	0.52
(1,200)	1:18:A:VAL:HG11	1:19:A:THR:H	4	0.52
(1,200)	1:18:A:VAL:HG12	1:19:A:THR:H	4	0.52
(1,200)	1:18:A:VAL:HG13	1:19:A:THR:H	4	0.52
(1,200)	1:18:A:VAL:HG11	1:19:A:THR:H	6	0.52
(1,200)	1:18:A:VAL:HG12	1:19:A:THR:H	6	0.52
(1,200)	1:18:A:VAL:HG13	1:19:A:THR:H	6	0.52
(1,33)	1:5:A:VAL:HG11	1:6:A:ASP:HB3	7	0.52
(1,33)	1:5:A:VAL:HG12	1:6:A:ASP:HB3	7	0.52
(1,33)	1:5:A:VAL:HG13	1:6:A:ASP:HB3	7	0.52
(1,33)	1:5:A:VAL:HG11	1:6:A:ASP:HB3	10	0.52
(1,33)	1:5:A:VAL:HG12	1:6:A:ASP:HB3	10	0.52
(1,33)	1:5:A:VAL:HG13	1:6:A:ASP:HB3	10	0.52
(1,1603)	1:104:A:LEU:H	1:103:A:PRO:HG3	1	0.51
(1,1603)	1:104:A:LEU:H	1:103:A:PRO:HG3	5	0.51
(1,1596)	1:103:A:PRO:HB3	1:104:A:LEU:H	2	0.51
(1,1596)	1:103:A:PRO:HB3	1:104:A:LEU:H	5	0.51
(1,1596)	1:103:A:PRO:HB3	1:104:A:LEU:H	6	0.51
(1,1596)	1:103:A:PRO:HB3	1:104:A:LEU:H	8	0.51
(1,1596)	1:103:A:PRO:HB3	1:104:A:LEU:H	9	0.51
(1,1505)	1:96:A:ILE:HG13	1:96:A:ILE:HG21	8	0.51
(1,1505)	1:96:A:ILE:HG13	1:96:A:ILE:HG22	8	0.51
(1,1505)	1:96:A:ILE:HG13	1:96:A:ILE:HG23	8	0.51
(1,1493)	1:96:A:ILE:HD13	1:90:A:SER:H	7	0.51
(1,1414)	1:91:A:LEU:HD23	1:74:A:ALA:HB1	5	0.51
(1,1211)	1:82:A:LEU:HD21	1:77:A:TYR:HD1	3	0.51
(1,1211)	1:82:A:LEU:HD21	1:77:A:TYR:HD2	3	0.51
(1,1211)	1:82:A:LEU:HD22	1:77:A:TYR:HD1	3	0.51
(1,1211)	1:82:A:LEU:HD22	1:77:A:TYR:HD2	3	0.51
(1,1211)	1:82:A:LEU:HD23	1:77:A:TYR:HD1	3	0.51
(1,1211)	1:82:A:LEU:HD23	1:77:A:TYR:HD2	3	0.51
(1,1116)	1:76:A:ALA:H	1:75:A:GLY:HA3	10	0.51
(1,1113)	1:76:A:ALA:HB2	1:36:A:PHE:H	6	0.51
(1,690)	1:48:A:LYS:HG2	1:48:A:LYS:HB3	3	0.51
(1,690)	1:48:A:LYS:HG2	1:48:A:LYS:HB3	7	0.51
(1,200)	1:18:A:VAL:HG11	1:19:A:THR:H	1	0.51
(1,200)	1:18:A:VAL:HG12	1:19:A:THR:H	1	0.51
(1,200)	1:18:A:VAL:HG13	1:19:A:THR:H	1	0.51
(1,200)	1:18:A:VAL:HG11	1:19:A:THR:H	3	0.51
(1,200)	1:18:A:VAL:HG12	1:19:A:THR:H	3	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,200)	1:18:A:VAL:HG13	1:19:A:THR:H	3	0.51
(1,200)	1:18:A:VAL:HG11	1:19:A:THR:H	5	0.51
(1,200)	1:18:A:VAL:HG12	1:19:A:THR:H	5	0.51
(1,200)	1:18:A:VAL:HG13	1:19:A:THR:H	5	0.51
(1,200)	1:18:A:VAL:HG11	1:19:A:THR:H	10	0.51
(1,200)	1:18:A:VAL:HG12	1:19:A:THR:H	10	0.51
(1,200)	1:18:A:VAL:HG13	1:19:A:THR:H	10	0.51
(1,1737)	1:20:A:ALA:HB2	1:64:A:LEU:HD11	8	0.5
(1,1603)	1:104:A:LEU:H	1:103:A:PRO:HG3	9	0.5
(1,1596)	1:103:A:PRO:HB3	1:104:A:LEU:H	10	0.5
(1,1435)	1:91:A:LEU:HD21	1:91:A:LEU:H	3	0.5
(1,1435)	1:91:A:LEU:HD22	1:91:A:LEU:H	3	0.5
(1,1435)	1:91:A:LEU:HD23	1:91:A:LEU:H	3	0.5
(1,1408)	1:91:A:LEU:HD11	1:30:A:LEU:HA	1	0.5
(1,1408)	1:91:A:LEU:HD12	1:30:A:LEU:HA	1	0.5
(1,1408)	1:91:A:LEU:HD13	1:30:A:LEU:HA	1	0.5
(1,1408)	1:91:A:LEU:HD11	1:30:A:LEU:HA	3	0.5
(1,1408)	1:91:A:LEU:HD12	1:30:A:LEU:HA	3	0.5
(1,1408)	1:91:A:LEU:HD13	1:30:A:LEU:HA	3	0.5
(1,1408)	1:91:A:LEU:HD11	1:30:A:LEU:HA	5	0.5
(1,1408)	1:91:A:LEU:HD12	1:30:A:LEU:HA	5	0.5
(1,1408)	1:91:A:LEU:HD13	1:30:A:LEU:HA	5	0.5
(1,1408)	1:91:A:LEU:HD11	1:30:A:LEU:HA	9	0.5
(1,1408)	1:91:A:LEU:HD12	1:30:A:LEU:HA	9	0.5
(1,1408)	1:91:A:LEU:HD13	1:30:A:LEU:HA	9	0.5
(1,1211)	1:82:A:LEU:HD21	1:77:A:TYR:HD1	7	0.5
(1,1211)	1:82:A:LEU:HD21	1:77:A:TYR:HD2	7	0.5
(1,1211)	1:82:A:LEU:HD22	1:77:A:TYR:HD1	7	0.5
(1,1211)	1:82:A:LEU:HD22	1:77:A:TYR:HD2	7	0.5
(1,1211)	1:82:A:LEU:HD23	1:77:A:TYR:HD1	7	0.5
(1,1211)	1:82:A:LEU:HD23	1:77:A:TYR:HD2	7	0.5
(1,1149)	1:78:A:LYS:HG3	1:78:A:LYS:HE2	3	0.5
(1,1149)	1:78:A:LYS:HG3	1:78:A:LYS:HE3	3	0.5
(1,1116)	1:76:A:ALA:H	1:75:A:GLY:HA3	1	0.5
(1,1116)	1:76:A:ALA:H	1:75:A:GLY:HA3	5	0.5
(1,983)	1:66:A:ARG:HB2	1:66:A:ARG:HD2	2	0.5
(1,981)	1:65:A:GLY:HA3	1:68:A:LEU:H	3	0.5
(1,981)	1:65:A:GLY:HA3	1:68:A:LEU:H	7	0.5
(1,700)	1:48:A:LYS:HG3	1:48:A:LYS:HA	3	0.5
(1,700)	1:48:A:LYS:HG3	1:48:A:LYS:HA	7	0.5
(1,1981)	1:124:A:HIS:HB2	1:125:A:VAL:H	7	0.49
(1,1864)	1:118:A:ALA:HB3	1:121:A:GLY:HA2	5	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1596)	1:103:A:PRO:HB3	1:104:A:LEU:H	1	0.49
(1,1176)	1:79:A:ALA:HA	1:104:A:LEU:HD11	7	0.49
(1,1176)	1:79:A:ALA:HA	1:104:A:LEU:HD12	7	0.49
(1,1176)	1:79:A:ALA:HA	1:104:A:LEU:HD13	7	0.49
(1,1176)	1:79:A:ALA:HA	1:104:A:LEU:HD11	9	0.49
(1,1176)	1:79:A:ALA:HA	1:104:A:LEU:HD12	9	0.49
(1,1176)	1:79:A:ALA:HA	1:104:A:LEU:HD13	9	0.49
(1,1116)	1:76:A:ALA:H	1:75:A:GLY:HA3	2	0.49
(1,1116)	1:76:A:ALA:H	1:75:A:GLY:HA3	3	0.49
(1,1116)	1:76:A:ALA:H	1:75:A:GLY:HA3	4	0.49
(1,1116)	1:76:A:ALA:H	1:75:A:GLY:HA3	9	0.49
(1,342)	1:36:A:PHE:HB2	1:75:A:GLY:H	2	0.49
(1,200)	1:18:A:VAL:HG11	1:19:A:THR:H	7	0.49
(1,200)	1:18:A:VAL:HG12	1:19:A:THR:H	7	0.49
(1,200)	1:18:A:VAL:HG13	1:19:A:THR:H	7	0.49
(1,200)	1:18:A:VAL:HG11	1:19:A:THR:H	9	0.49
(1,200)	1:18:A:VAL:HG12	1:19:A:THR:H	9	0.49
(1,200)	1:18:A:VAL:HG13	1:19:A:THR:H	9	0.49
(1,2029)	1:126:A:ILE:HA	1:127:A:ASP:HB3	9	0.48
(1,1684)	1:107:A:LYS:HG2	1:107:A:LYS:HE2	3	0.48
(1,1684)	1:107:A:LYS:HG2	1:107:A:LYS:HE3	3	0.48
(1,1596)	1:103:A:PRO:HB3	1:104:A:LEU:H	4	0.48
(1,1596)	1:103:A:PRO:HB3	1:104:A:LEU:H	7	0.48
(1,1454)	1:92:A:GLU:HB3	1:93:A:GLY:H	4	0.48
(1,1116)	1:76:A:ALA:H	1:75:A:GLY:HA3	7	0.48
(1,1024)	1:68:A:LEU:HD21	1:64:A:LEU:HD21	9	0.48
(1,1024)	1:68:A:LEU:HD21	1:64:A:LEU:HD22	9	0.48
(1,1024)	1:68:A:LEU:HD21	1:64:A:LEU:HD23	9	0.48
(1,1024)	1:68:A:LEU:HD22	1:64:A:LEU:HD21	9	0.48
(1,1024)	1:68:A:LEU:HD22	1:64:A:LEU:HD22	9	0.48
(1,1024)	1:68:A:LEU:HD22	1:64:A:LEU:HD23	9	0.48
(1,1024)	1:68:A:LEU:HD23	1:64:A:LEU:HD21	9	0.48
(1,1024)	1:68:A:LEU:HD23	1:64:A:LEU:HD22	9	0.48
(1,1024)	1:68:A:LEU:HD23	1:64:A:LEU:HD23	9	0.48
(1,989)	1:66:A:ARG:HA	1:66:A:ARG:HB3	3	0.48
(1,920)	1:54:A:ILE:HD11	1:63:A:GLN:HE21	7	0.48
(1,920)	1:54:A:ILE:HD11	1:63:A:GLN:HE21	8	0.48
(1,652)	1:45:A:ALA:HB1	1:48:A:LYS:HG2	5	0.48
(1,652)	1:45:A:ALA:HB2	1:48:A:LYS:HG2	5	0.48
(1,652)	1:45:A:ALA:HB3	1:48:A:LYS:HG2	5	0.48
(1,517)	1:36:A:PHE:HB2	1:37:A:THR:H	10	0.48
(1,227)	1:20:A:ALA:HB1	1:64:A:LEU:HD11	1	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,227)	1:20:A:ALA:HB1	1:64:A:LEU:HD12	1	0.48
(1,227)	1:20:A:ALA:HB1	1:64:A:LEU:HD13	1	0.48
(1,227)	1:20:A:ALA:HB2	1:64:A:LEU:HD11	1	0.48
(1,227)	1:20:A:ALA:HB2	1:64:A:LEU:HD12	1	0.48
(1,227)	1:20:A:ALA:HB2	1:64:A:LEU:HD13	1	0.48
(1,227)	1:20:A:ALA:HB3	1:64:A:LEU:HD11	1	0.48
(1,227)	1:20:A:ALA:HB3	1:64:A:LEU:HD12	1	0.48
(1,227)	1:20:A:ALA:HB3	1:64:A:LEU:HD13	1	0.48
(1,113)	1:10:A:ASN:HB2	1:7:A:ILE:HG21	1	0.48
(1,113)	1:10:A:ASN:HB2	1:7:A:ILE:HG22	1	0.48
(1,113)	1:10:A:ASN:HB2	1:7:A:ILE:HG23	1	0.48
(1,1981)	1:124:A:HIS:HB2	1:125:A:VAL:H	2	0.47
(1,1894)	1:120:A:ASN:HB3	1:121:A:GLY:H	3	0.47
(1,1684)	1:107:A:LYS:HG2	1:107:A:LYS:HE2	10	0.47
(1,1684)	1:107:A:LYS:HG2	1:107:A:LYS:HE3	10	0.47
(1,1345)	1:87:A:ILE:HG13	1:95:A:THR:HB	3	0.47
(1,1238)	1:82:A:LEU:HB3	1:104:A:LEU:HD21	6	0.47
(1,1238)	1:82:A:LEU:HB3	1:104:A:LEU:HD22	6	0.47
(1,1238)	1:82:A:LEU:HB3	1:104:A:LEU:HD23	6	0.47
(1,1147)	1:78:A:LYS:HA	1:78:A:LYS:HD3	5	0.47
(1,1116)	1:76:A:ALA:H	1:75:A:GLY:HA3	8	0.47
(1,1113)	1:76:A:ALA:HB3	1:36:A:PHE:H	3	0.47
(1,1024)	1:68:A:LEU:HD21	1:64:A:LEU:HD21	2	0.47
(1,1024)	1:68:A:LEU:HD21	1:64:A:LEU:HD22	2	0.47
(1,1024)	1:68:A:LEU:HD21	1:64:A:LEU:HD23	2	0.47
(1,1024)	1:68:A:LEU:HD22	1:64:A:LEU:HD21	2	0.47
(1,1024)	1:68:A:LEU:HD22	1:64:A:LEU:HD22	2	0.47
(1,1024)	1:68:A:LEU:HD22	1:64:A:LEU:HD23	2	0.47
(1,1024)	1:68:A:LEU:HD23	1:64:A:LEU:HD21	2	0.47
(1,1024)	1:68:A:LEU:HD23	1:64:A:LEU:HD22	2	0.47
(1,1024)	1:68:A:LEU:HD23	1:64:A:LEU:HD23	2	0.47
(1,992)	1:66:A:ARG:HG3	1:67:A:ILE:H	2	0.47
(1,1979)	1:124:A:HIS:HB3	1:124:A:HIS:H	2	0.46
(1,1979)	1:124:A:HIS:HB3	1:124:A:HIS:H	5	0.46
(1,1740)	1:111:A:VAL:HG11	1:111:A:VAL:HA	3	0.46
(1,1740)	1:111:A:VAL:HG12	1:111:A:VAL:HA	3	0.46
(1,1740)	1:111:A:VAL:HG13	1:111:A:VAL:HA	3	0.46
(1,1740)	1:111:A:VAL:HG11	1:111:A:VAL:HA	10	0.46
(1,1740)	1:111:A:VAL:HG12	1:111:A:VAL:HA	10	0.46
(1,1740)	1:111:A:VAL:HG13	1:111:A:VAL:HA	10	0.46
(1,1493)	1:98:A:ILE:HD12	1:106:A:VAL:H	10	0.46
(1,1435)	1:91:A:LEU:HD21	1:91:A:LEU:H	10	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1435)	1:91:A:LEU:HD22	1:91:A:LEU:H	10	0.46
(1,1435)	1:91:A:LEU:HD23	1:91:A:LEU:H	10	0.46
(1,1410)	1:58:A:VAL:HG13	1:59:A:GLN:HA	2	0.46
(1,1070)	1:72:A:VAL:HG11	1:72:A:VAL:HA	1	0.46
(1,1070)	1:72:A:VAL:HG12	1:72:A:VAL:HA	1	0.46
(1,1070)	1:72:A:VAL:HG13	1:72:A:VAL:HA	1	0.46
(1,1070)	1:72:A:VAL:HG11	1:72:A:VAL:HA	3	0.46
(1,1070)	1:72:A:VAL:HG12	1:72:A:VAL:HA	3	0.46
(1,1070)	1:72:A:VAL:HG13	1:72:A:VAL:HA	3	0.46
(1,1070)	1:72:A:VAL:HG11	1:72:A:VAL:HA	4	0.46
(1,1070)	1:72:A:VAL:HG12	1:72:A:VAL:HA	4	0.46
(1,1070)	1:72:A:VAL:HG13	1:72:A:VAL:HA	4	0.46
(1,1070)	1:72:A:VAL:HG11	1:72:A:VAL:HA	5	0.46
(1,1070)	1:72:A:VAL:HG12	1:72:A:VAL:HA	5	0.46
(1,1070)	1:72:A:VAL:HG13	1:72:A:VAL:HA	5	0.46
(1,1070)	1:72:A:VAL:HG11	1:72:A:VAL:HA	6	0.46
(1,1070)	1:72:A:VAL:HG12	1:72:A:VAL:HA	6	0.46
(1,1070)	1:72:A:VAL:HG13	1:72:A:VAL:HA	6	0.46
(1,1070)	1:72:A:VAL:HG11	1:72:A:VAL:HA	7	0.46
(1,1070)	1:72:A:VAL:HG12	1:72:A:VAL:HA	7	0.46
(1,1070)	1:72:A:VAL:HG13	1:72:A:VAL:HA	7	0.46
(1,1070)	1:72:A:VAL:HG11	1:72:A:VAL:HA	8	0.46
(1,1070)	1:72:A:VAL:HG12	1:72:A:VAL:HA	8	0.46
(1,1070)	1:72:A:VAL:HG13	1:72:A:VAL:HA	8	0.46
(1,1070)	1:72:A:VAL:HG11	1:72:A:VAL:HA	9	0.46
(1,1070)	1:72:A:VAL:HG12	1:72:A:VAL:HA	9	0.46
(1,1070)	1:72:A:VAL:HG13	1:72:A:VAL:HA	9	0.46
(1,690)	1:48:A:LYS:HG2	1:48:A:LYS:HB3	5	0.46
(1,544)	1:37:A:THR:HB	1:73:A:VAL:HG21	6	0.46
(1,544)	1:37:A:THR:HB	1:73:A:VAL:HG22	6	0.46
(1,544)	1:37:A:THR:HB	1:73:A:VAL:HG23	6	0.46
(1,544)	1:37:A:THR:HB	1:73:A:VAL:HG21	9	0.46
(1,544)	1:37:A:THR:HB	1:73:A:VAL:HG22	9	0.46
(1,544)	1:37:A:THR:HB	1:73:A:VAL:HG23	9	0.46
(1,520)	1:36:A:PHE:HA	1:72:A:VAL:HG11	3	0.46
(1,520)	1:36:A:PHE:HA	1:72:A:VAL:HG12	3	0.46
(1,520)	1:36:A:PHE:HA	1:72:A:VAL:HG13	3	0.46
(1,429)	1:30:A:LEU:HD11	1:70:A:TYR:H	2	0.46
(1,332)	1:25:A:ASN:HB3	1:25:A:ASN:HD22	3	0.46
(1,332)	1:25:A:ASN:HB3	1:25:A:ASN:HD22	4	0.46
(1,332)	1:25:A:ASN:HB3	1:25:A:ASN:HD22	5	0.46
(1,332)	1:25:A:ASN:HB3	1:25:A:ASN:HD22	10	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,227)	1:20:A:ALA:HB1	1:64:A:LEU:HD11	6	0.46
(1,227)	1:20:A:ALA:HB1	1:64:A:LEU:HD12	6	0.46
(1,227)	1:20:A:ALA:HB1	1:64:A:LEU:HD13	6	0.46
(1,227)	1:20:A:ALA:HB2	1:64:A:LEU:HD11	6	0.46
(1,227)	1:20:A:ALA:HB2	1:64:A:LEU:HD12	6	0.46
(1,227)	1:20:A:ALA:HB2	1:64:A:LEU:HD13	6	0.46
(1,227)	1:20:A:ALA:HB3	1:64:A:LEU:HD11	6	0.46
(1,227)	1:20:A:ALA:HB3	1:64:A:LEU:HD12	6	0.46
(1,227)	1:20:A:ALA:HB3	1:64:A:LEU:HD13	6	0.46
(1,200)	1:18:A:VAL:HG11	1:19:A:THR:H	8	0.46
(1,200)	1:18:A:VAL:HG12	1:19:A:THR:H	8	0.46
(1,200)	1:18:A:VAL:HG13	1:19:A:THR:H	8	0.46
(1,1979)	1:124:A:HIS:HB3	1:124:A:HIS:H	9	0.45
(1,1740)	1:111:A:VAL:HG11	1:111:A:VAL:HA	2	0.45
(1,1740)	1:111:A:VAL:HG12	1:111:A:VAL:HA	2	0.45
(1,1740)	1:111:A:VAL:HG13	1:111:A:VAL:HA	2	0.45
(1,1410)	1:58:A:VAL:HG13	1:59:A:GLN:HA	5	0.45
(1,1345)	1:87:A:ILE:HG13	1:95:A:THR:HB	7	0.45
(1,1070)	1:72:A:VAL:HG11	1:72:A:VAL:HA	2	0.45
(1,1070)	1:72:A:VAL:HG12	1:72:A:VAL:HA	2	0.45
(1,1070)	1:72:A:VAL:HG13	1:72:A:VAL:HA	2	0.45
(1,983)	1:66:A:ARG:HB2	1:66:A:ARG:HD2	4	0.45
(1,772)	1:55:A:THR:HG22	1:58:A:VAL:H	3	0.45
(1,433)	1:31:A:GLN:HE21	1:6:A:ASP:HB3	3	0.45
(1,433)	1:31:A:GLN:HE21	1:6:A:ASP:HB3	4	0.45
(1,433)	1:31:A:GLN:HE21	1:6:A:ASP:HB3	9	0.45
(1,371)	1:91:A:LEU:HB2	1:93:A:GLY:H	1	0.45
(1,371)	1:91:A:LEU:HB2	1:93:A:GLY:H	2	0.45
(1,371)	1:91:A:LEU:HB2	1:93:A:GLY:H	8	0.45
(1,332)	1:25:A:ASN:HB3	1:25:A:ASN:HD22	1	0.45
(1,332)	1:25:A:ASN:HB3	1:25:A:ASN:HD22	2	0.45
(1,332)	1:25:A:ASN:HB3	1:25:A:ASN:HD22	6	0.45
(1,332)	1:25:A:ASN:HB3	1:25:A:ASN:HD22	7	0.45
(1,332)	1:25:A:ASN:HB3	1:25:A:ASN:HD22	8	0.45
(1,332)	1:25:A:ASN:HB3	1:25:A:ASN:HD22	9	0.45
(1,183)	1:18:A:VAL:HG11	1:11:A:THR:H	8	0.45
(1,183)	1:18:A:VAL:HG12	1:11:A:THR:H	8	0.45
(1,183)	1:18:A:VAL:HG13	1:11:A:THR:H	8	0.45
(1,180)	1:18:A:VAL:HG11	1:11:A:THR:HB	2	0.45
(1,180)	1:18:A:VAL:HG12	1:11:A:THR:HB	2	0.45
(1,180)	1:18:A:VAL:HG13	1:11:A:THR:HB	2	0.45
(1,1979)	1:124:A:HIS:HB3	1:124:A:HIS:H	3	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1979)	1:124:A:HIS:HB3	1:124:A:HIS:H	8	0.44
(1,1979)	1:124:A:HIS:HB3	1:124:A:HIS:H	10	0.44
(1,1864)	1:118:A:ALA:HB3	1:121:A:GLY:HA2	2	0.44
(1,1410)	1:58:A:VAL:HG12	1:59:A:GLN:HA	7	0.44
(1,990)	1:66:A:ARG:H	1:66:A:ARG:HB2	5	0.44
(1,983)	1:66:A:ARG:HB2	1:66:A:ARG:HD2	1	0.44
(1,726)	1:49:A:LEU:HB3	1:50:A:PRO:HD3	10	0.44
(1,544)	1:37:A:THR:HB	1:73:A:VAL:HG21	1	0.44
(1,544)	1:37:A:THR:HB	1:73:A:VAL:HG22	1	0.44
(1,544)	1:37:A:THR:HB	1:73:A:VAL:HG23	1	0.44
(1,371)	1:91:A:LEU:HB2	1:93:A:GLY:H	6	0.44
(1,157)	1:13:A:GLY:HA3	1:13:A:GLY:H	5	0.44
(1,1737)	1:20:A:ALA:HB2	1:64:A:LEU:HD12	3	0.43
(1,1596)	1:103:A:PRO:HB3	1:104:A:LEU:H	3	0.43
(1,1493)	1:96:A:ILE:HD12	1:90:A:SER:H	9	0.43
(1,1435)	1:91:A:LEU:HD21	1:91:A:LEU:H	1	0.43
(1,1435)	1:91:A:LEU:HD22	1:91:A:LEU:H	1	0.43
(1,1435)	1:91:A:LEU:HD23	1:91:A:LEU:H	1	0.43
(1,1435)	1:91:A:LEU:HD21	1:91:A:LEU:H	2	0.43
(1,1435)	1:91:A:LEU:HD22	1:91:A:LEU:H	2	0.43
(1,1435)	1:91:A:LEU:HD23	1:91:A:LEU:H	2	0.43
(1,1435)	1:91:A:LEU:HD21	1:91:A:LEU:H	6	0.43
(1,1435)	1:91:A:LEU:HD22	1:91:A:LEU:H	6	0.43
(1,1435)	1:91:A:LEU:HD23	1:91:A:LEU:H	6	0.43
(1,1410)	1:58:A:VAL:HG13	1:59:A:GLN:HA	4	0.43
(1,1410)	1:58:A:VAL:HG13	1:59:A:GLN:HA	8	0.43
(1,1408)	1:91:A:LEU:HD11	1:30:A:LEU:HA	10	0.43
(1,1408)	1:91:A:LEU:HD12	1:30:A:LEU:HA	10	0.43
(1,1408)	1:91:A:LEU:HD13	1:30:A:LEU:HA	10	0.43
(1,1070)	1:72:A:VAL:HG11	1:72:A:VAL:HA	10	0.43
(1,1070)	1:72:A:VAL:HG12	1:72:A:VAL:HA	10	0.43
(1,1070)	1:72:A:VAL:HG13	1:72:A:VAL:HA	10	0.43
(1,830)	1:57:A:LEU:HB3	1:58:A:VAL:H	9	0.43
(1,726)	1:49:A:LEU:HB3	1:50:A:PRO:HD3	1	0.43
(1,553)	1:37:A:THR:HG21	1:82:A:LEU:HD11	7	0.43
(1,553)	1:37:A:THR:HG21	1:82:A:LEU:HD12	7	0.43
(1,553)	1:37:A:THR:HG21	1:82:A:LEU:HD13	7	0.43
(1,553)	1:37:A:THR:HG22	1:82:A:LEU:HD11	7	0.43
(1,553)	1:37:A:THR:HG22	1:82:A:LEU:HD12	7	0.43
(1,553)	1:37:A:THR:HG22	1:82:A:LEU:HD13	7	0.43
(1,553)	1:37:A:THR:HG23	1:82:A:LEU:HD11	7	0.43
(1,553)	1:37:A:THR:HG23	1:82:A:LEU:HD12	7	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,553)	1:37:A:THR:HG23	1:82:A:LEU:HD13	7	0.43
(1,553)	1:37:A:THR:HG21	1:82:A:LEU:HD11	10	0.43
(1,553)	1:37:A:THR:HG21	1:82:A:LEU:HD12	10	0.43
(1,553)	1:37:A:THR:HG21	1:82:A:LEU:HD13	10	0.43
(1,553)	1:37:A:THR:HG22	1:82:A:LEU:HD11	10	0.43
(1,553)	1:37:A:THR:HG22	1:82:A:LEU:HD12	10	0.43
(1,553)	1:37:A:THR:HG22	1:82:A:LEU:HD13	10	0.43
(1,553)	1:37:A:THR:HG23	1:82:A:LEU:HD11	10	0.43
(1,553)	1:37:A:THR:HG23	1:82:A:LEU:HD12	10	0.43
(1,553)	1:37:A:THR:HG23	1:82:A:LEU:HD13	10	0.43
(1,544)	1:37:A:THR:HB	1:73:A:VAL:HG21	3	0.43
(1,544)	1:37:A:THR:HB	1:73:A:VAL:HG22	3	0.43
(1,544)	1:37:A:THR:HB	1:73:A:VAL:HG23	3	0.43
(1,544)	1:37:A:THR:HB	1:73:A:VAL:HG21	4	0.43
(1,544)	1:37:A:THR:HB	1:73:A:VAL:HG22	4	0.43
(1,544)	1:37:A:THR:HB	1:73:A:VAL:HG23	4	0.43
(1,544)	1:37:A:THR:HB	1:73:A:VAL:HG21	7	0.43
(1,544)	1:37:A:THR:HB	1:73:A:VAL:HG22	7	0.43
(1,544)	1:37:A:THR:HB	1:73:A:VAL:HG23	7	0.43
(1,433)	1:31:A:GLN:HE21	1:6:A:ASP:HB3	1	0.43
(1,331)	1:25:A:ASN:H	1:25:A:ASN:HB2	5	0.43
(1,331)	1:25:A:ASN:H	1:25:A:ASN:HB2	10	0.43
(1,157)	1:13:A:GLY:HA3	1:13:A:GLY:H	7	0.43
(1,33)	1:5:A:VAL:HG11	1:6:A:ASP:HB3	2	0.43
(1,33)	1:5:A:VAL:HG12	1:6:A:ASP:HB3	2	0.43
(1,33)	1:5:A:VAL:HG13	1:6:A:ASP:HB3	2	0.43
(1,1981)	1:124:A:HIS:HB2	1:125:A:VAL:H	5	0.42
(1,1979)	1:124:A:HIS:HB3	1:124:A:HIS:H	7	0.42
(1,1894)	1:120:A:ASN:HB3	1:121:A:GLY:H	2	0.42
(1,1740)	1:111:A:VAL:HG11	1:111:A:VAL:HA	7	0.42
(1,1740)	1:111:A:VAL:HG12	1:111:A:VAL:HA	7	0.42
(1,1740)	1:111:A:VAL:HG13	1:111:A:VAL:HA	7	0.42
(1,1567)	1:100:A:GLY:HA2	1:105:A:GLU:H	9	0.42
(1,1451)	1:92:A:GLU:H	1:92:A:GLU:HG3	5	0.42
(1,1435)	1:91:A:LEU:HD21	1:91:A:LEU:H	7	0.42
(1,1435)	1:91:A:LEU:HD22	1:91:A:LEU:H	7	0.42
(1,1435)	1:91:A:LEU:HD23	1:91:A:LEU:H	7	0.42
(1,1435)	1:91:A:LEU:HD21	1:91:A:LEU:H	8	0.42
(1,1435)	1:91:A:LEU:HD22	1:91:A:LEU:H	8	0.42
(1,1435)	1:91:A:LEU:HD23	1:91:A:LEU:H	8	0.42
(1,1410)	1:58:A:VAL:HG12	1:59:A:GLN:HA	1	0.42
(1,1410)	1:58:A:VAL:HG13	1:59:A:GLN:HA	6	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1410)	1:58:A:VAL:HG11	1:59:A:GLN:HA	10	0.42
(1,1345)	1:87:A:ILE:HG13	1:95:A:THR:HB	9	0.42
(1,1176)	1:79:A:ALA:HA	1:104:A:LEU:HD11	8	0.42
(1,1176)	1:79:A:ALA:HA	1:104:A:LEU:HD12	8	0.42
(1,1176)	1:79:A:ALA:HA	1:104:A:LEU:HD13	8	0.42
(1,1027)	1:68:A:LEU:HD11	1:65:A:GLY:HA2	1	0.42
(1,1027)	1:68:A:LEU:HD12	1:65:A:GLY:HA2	1	0.42
(1,1027)	1:68:A:LEU:HD13	1:65:A:GLY:HA2	1	0.42
(1,990)	1:66:A:ARG:H	1:66:A:ARG:HB2	2	0.42
(1,981)	1:65:A:GLY:HA3	1:68:A:LEU:H	8	0.42
(1,920)	1:54:A:ILE:HD13	1:63:A:GLN:HE21	5	0.42
(1,830)	1:57:A:LEU:HB3	1:58:A:VAL:H	3	0.42
(1,544)	1:37:A:THR:HB	1:73:A:VAL:HG21	8	0.42
(1,544)	1:37:A:THR:HB	1:73:A:VAL:HG22	8	0.42
(1,544)	1:37:A:THR:HB	1:73:A:VAL:HG23	8	0.42
(1,433)	1:31:A:GLN:HE21	1:6:A:ASP:HB3	6	0.42
(1,371)	1:91:A:LEU:HB2	1:93:A:GLY:H	10	0.42
(1,331)	1:25:A:ASN:H	1:25:A:ASN:HB2	3	0.42
(1,331)	1:25:A:ASN:H	1:25:A:ASN:HB2	4	0.42
(1,331)	1:25:A:ASN:H	1:25:A:ASN:HB2	7	0.42
(1,227)	1:20:A:ALA:HB1	1:64:A:LEU:HD11	5	0.42
(1,227)	1:20:A:ALA:HB1	1:64:A:LEU:HD12	5	0.42
(1,227)	1:20:A:ALA:HB1	1:64:A:LEU:HD13	5	0.42
(1,227)	1:20:A:ALA:HB2	1:64:A:LEU:HD11	5	0.42
(1,227)	1:20:A:ALA:HB2	1:64:A:LEU:HD12	5	0.42
(1,227)	1:20:A:ALA:HB2	1:64:A:LEU:HD13	5	0.42
(1,227)	1:20:A:ALA:HB3	1:64:A:LEU:HD11	5	0.42
(1,227)	1:20:A:ALA:HB3	1:64:A:LEU:HD12	5	0.42
(1,227)	1:20:A:ALA:HB3	1:64:A:LEU:HD13	5	0.42
(1,180)	1:18:A:VAL:HG11	1:11:A:THR:HB	5	0.42
(1,180)	1:18:A:VAL:HG12	1:11:A:THR:HB	5	0.42
(1,180)	1:18:A:VAL:HG13	1:11:A:THR:HB	5	0.42
(1,180)	1:18:A:VAL:HG11	1:11:A:THR:HB	8	0.42
(1,180)	1:18:A:VAL:HG12	1:11:A:THR:HB	8	0.42
(1,180)	1:18:A:VAL:HG13	1:11:A:THR:HB	8	0.42
(1,157)	1:13:A:GLY:HA3	1:13:A:GLY:H	2	0.42
(1,157)	1:13:A:GLY:HA3	1:13:A:GLY:H	3	0.42
(1,157)	1:13:A:GLY:HA3	1:13:A:GLY:H	4	0.42
(1,2029)	1:126:A:ILE:HA	1:127:A:ASP:HB3	5	0.41
(1,1827)	1:116:A:ILE:H	1:116:A:ILE:HG12	8	0.41
(1,1176)	1:79:A:ALA:HA	1:104:A:LEU:HD11	5	0.41
(1,1176)	1:79:A:ALA:HA	1:104:A:LEU:HD12	5	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1176)	1:79:A:ALA:HA	1:104:A:LEU:HD13	5	0.41
(1,1024)	1:68:A:LEU:HD21	1:64:A:LEU:HD21	10	0.41
(1,1024)	1:68:A:LEU:HD21	1:64:A:LEU:HD22	10	0.41
(1,1024)	1:68:A:LEU:HD21	1:64:A:LEU:HD23	10	0.41
(1,1024)	1:68:A:LEU:HD22	1:64:A:LEU:HD21	10	0.41
(1,1024)	1:68:A:LEU:HD22	1:64:A:LEU:HD22	10	0.41
(1,1024)	1:68:A:LEU:HD22	1:64:A:LEU:HD23	10	0.41
(1,1024)	1:68:A:LEU:HD23	1:64:A:LEU:HD21	10	0.41
(1,1024)	1:68:A:LEU:HD23	1:64:A:LEU:HD22	10	0.41
(1,1024)	1:68:A:LEU:HD23	1:64:A:LEU:HD23	10	0.41
(1,624)	1:44:A:ASP:HB3	1:44:A:ASP:HA	2	0.41
(1,544)	1:37:A:THR:HB	1:73:A:VAL:HG21	2	0.41
(1,544)	1:37:A:THR:HB	1:73:A:VAL:HG22	2	0.41
(1,544)	1:37:A:THR:HB	1:73:A:VAL:HG23	2	0.41
(1,544)	1:37:A:THR:HB	1:73:A:VAL:HG21	5	0.41
(1,544)	1:37:A:THR:HB	1:73:A:VAL:HG22	5	0.41
(1,544)	1:37:A:THR:HB	1:73:A:VAL:HG23	5	0.41
(1,520)	1:36:A:PHE:HA	1:72:A:VAL:HG11	5	0.41
(1,520)	1:36:A:PHE:HA	1:72:A:VAL:HG12	5	0.41
(1,520)	1:36:A:PHE:HA	1:72:A:VAL:HG13	5	0.41
(1,342)	1:36:A:PHE:HB2	1:75:A:GLY:H	5	0.41
(1,331)	1:25:A:ASN:H	1:25:A:ASN:HB2	1	0.41
(1,331)	1:25:A:ASN:H	1:25:A:ASN:HB2	2	0.41
(1,331)	1:25:A:ASN:H	1:25:A:ASN:HB2	6	0.41
(1,331)	1:25:A:ASN:H	1:25:A:ASN:HB2	9	0.41
(1,183)	1:18:A:VAL:HG11	1:11:A:THR:H	2	0.41
(1,183)	1:18:A:VAL:HG12	1:11:A:THR:H	2	0.41
(1,183)	1:18:A:VAL:HG13	1:11:A:THR:H	2	0.41
(1,180)	1:18:A:VAL:HG11	1:11:A:THR:HB	4	0.41
(1,180)	1:18:A:VAL:HG12	1:11:A:THR:HB	4	0.41
(1,180)	1:18:A:VAL:HG13	1:11:A:THR:HB	4	0.41
(1,180)	1:18:A:VAL:HG11	1:11:A:THR:HB	9	0.41
(1,180)	1:18:A:VAL:HG12	1:11:A:THR:HB	9	0.41
(1,180)	1:18:A:VAL:HG13	1:11:A:THR:HB	9	0.41
(1,157)	1:13:A:GLY:HA3	1:13:A:GLY:H	1	0.41
(1,157)	1:13:A:GLY:HA3	1:13:A:GLY:H	6	0.41
(1,157)	1:13:A:GLY:HA3	1:13:A:GLY:H	8	0.41
(1,1968)	1:124:A:HIS:HB3	1:39:A:PHE:HD1	7	0.4
(1,1968)	1:124:A:HIS:HB3	1:39:A:PHE:HD2	7	0.4
(1,1827)	1:116:A:ILE:H	1:116:A:ILE:HG12	2	0.4
(1,1827)	1:116:A:ILE:H	1:116:A:ILE:HG12	3	0.4
(1,1827)	1:116:A:ILE:H	1:116:A:ILE:HG12	5	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1827)	1:116:A:ILE:H	1:116:A:ILE:HG12	7	0.4
(1,1827)	1:116:A:ILE:H	1:116:A:ILE:HG12	9	0.4
(1,1827)	1:116:A:ILE:H	1:116:A:ILE:HG12	10	0.4
(1,1740)	1:111:A:VAL:HG11	1:111:A:VAL:HA	8	0.4
(1,1740)	1:111:A:VAL:HG12	1:111:A:VAL:HA	8	0.4
(1,1740)	1:111:A:VAL:HG13	1:111:A:VAL:HA	8	0.4
(1,1740)	1:111:A:VAL:HG11	1:111:A:VAL:HA	9	0.4
(1,1740)	1:111:A:VAL:HG12	1:111:A:VAL:HA	9	0.4
(1,1740)	1:111:A:VAL:HG13	1:111:A:VAL:HA	9	0.4
(1,1424)	1:91:A:LEU:HB2	1:91:A:LEU:HD11	9	0.4
(1,1424)	1:91:A:LEU:HB2	1:91:A:LEU:HD12	9	0.4
(1,1424)	1:91:A:LEU:HB2	1:91:A:LEU:HD13	9	0.4
(1,1345)	1:87:A:ILE:HG13	1:95:A:THR:HB	5	0.4
(1,1176)	1:79:A:ALA:HA	1:104:A:LEU:HD11	4	0.4
(1,1176)	1:79:A:ALA:HA	1:104:A:LEU:HD12	4	0.4
(1,1176)	1:79:A:ALA:HA	1:104:A:LEU:HD13	4	0.4
(1,981)	1:65:A:GLY:HA3	1:68:A:LEU:H	5	0.4
(1,969)	1:65:A:GLY:HA2	1:26:A:LEU:HD11	3	0.4
(1,969)	1:65:A:GLY:HA2	1:26:A:LEU:HD12	3	0.4
(1,969)	1:65:A:GLY:HA2	1:26:A:LEU:HD13	3	0.4
(1,920)	1:54:A:ILE:HD13	1:63:A:GLN:HE21	3	0.4
(1,901)	1:62:A:PRO:HB2	1:62:A:PRO:HA	4	0.4
(1,901)	1:62:A:PRO:HB2	1:62:A:PRO:HA	6	0.4
(1,901)	1:62:A:PRO:HB2	1:62:A:PRO:HA	7	0.4
(1,901)	1:62:A:PRO:HB2	1:62:A:PRO:HA	8	0.4
(1,878)	1:59:A:GLN:HB3	1:60:A:ASN:H	1	0.4
(1,726)	1:49:A:LEU:HB3	1:50:A:PRO:HD3	6	0.4
(1,708)	1:48:A:LYS:HG3	1:49:A:LEU:H	5	0.4
(1,624)	1:44:A:ASP:HB3	1:44:A:ASP:HA	1	0.4
(1,624)	1:44:A:ASP:HB3	1:44:A:ASP:HA	3	0.4
(1,624)	1:44:A:ASP:HB3	1:44:A:ASP:HA	4	0.4
(1,624)	1:44:A:ASP:HB3	1:44:A:ASP:HA	5	0.4
(1,624)	1:44:A:ASP:HB3	1:44:A:ASP:HA	6	0.4
(1,624)	1:44:A:ASP:HB3	1:44:A:ASP:HA	7	0.4
(1,624)	1:44:A:ASP:HB3	1:44:A:ASP:HA	8	0.4
(1,624)	1:44:A:ASP:HB3	1:44:A:ASP:HA	9	0.4
(1,624)	1:44:A:ASP:HB3	1:44:A:ASP:HA	10	0.4
(1,520)	1:36:A:PHE:HA	1:72:A:VAL:HG11	10	0.4
(1,520)	1:36:A:PHE:HA	1:72:A:VAL:HG12	10	0.4
(1,520)	1:36:A:PHE:HA	1:72:A:VAL:HG13	10	0.4
(1,343)	1:25:A:ASN:HD22	1:92:A:GLU:HB3	3	0.4
(1,331)	1:25:A:ASN:H	1:25:A:ASN:HB2	8	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,157)	1:13:A:GLY:HA3	1:13:A:GLY:H	9	0.4
(1,2029)	1:126:A:ILE:HA	1:127:A:ASP:HB3	8	0.39
(1,1968)	1:124:A:HIS:HB3	1:39:A:PHE:HD1	2	0.39
(1,1968)	1:124:A:HIS:HB3	1:39:A:PHE:HD2	2	0.39
(1,1493)	1:96:A:ILE:HD13	1:90:A:SER:H	3	0.39
(1,1454)	1:92:A:GLU:HB3	1:93:A:GLY:H	3	0.39
(1,1303)	1:85:A:MET:HB3	1:86:A:GLY:H	2	0.39
(1,1273)	1:84:A:ARG:HB3	1:84:A:ARG:HD2	1	0.39
(1,1238)	1:82:A:LEU:HB3	1:104:A:LEU:HD21	10	0.39
(1,1238)	1:82:A:LEU:HB3	1:104:A:LEU:HD22	10	0.39
(1,1238)	1:82:A:LEU:HB3	1:104:A:LEU:HD23	10	0.39
(1,1191)	1:81:A:ASP:H	1:78:A:LYS:HB3	1	0.39
(1,1149)	1:78:A:LYS:HG3	1:78:A:LYS:HE2	2	0.39
(1,1149)	1:78:A:LYS:HG3	1:78:A:LYS:HE3	2	0.39
(1,1024)	1:68:A:LEU:HD21	1:64:A:LEU:HD21	3	0.39
(1,1024)	1:68:A:LEU:HD21	1:64:A:LEU:HD22	3	0.39
(1,1024)	1:68:A:LEU:HD21	1:64:A:LEU:HD23	3	0.39
(1,1024)	1:68:A:LEU:HD22	1:64:A:LEU:HD21	3	0.39
(1,1024)	1:68:A:LEU:HD22	1:64:A:LEU:HD22	3	0.39
(1,1024)	1:68:A:LEU:HD22	1:64:A:LEU:HD23	3	0.39
(1,1024)	1:68:A:LEU:HD23	1:64:A:LEU:HD21	3	0.39
(1,1024)	1:68:A:LEU:HD23	1:64:A:LEU:HD22	3	0.39
(1,1024)	1:68:A:LEU:HD23	1:64:A:LEU:HD23	3	0.39
(1,1024)	1:68:A:LEU:HD21	1:64:A:LEU:HD21	4	0.39
(1,1024)	1:68:A:LEU:HD21	1:64:A:LEU:HD22	4	0.39
(1,1024)	1:68:A:LEU:HD21	1:64:A:LEU:HD23	4	0.39
(1,1024)	1:68:A:LEU:HD22	1:64:A:LEU:HD21	4	0.39
(1,1024)	1:68:A:LEU:HD22	1:64:A:LEU:HD22	4	0.39
(1,1024)	1:68:A:LEU:HD22	1:64:A:LEU:HD23	4	0.39
(1,1024)	1:68:A:LEU:HD23	1:64:A:LEU:HD21	4	0.39
(1,1024)	1:68:A:LEU:HD23	1:64:A:LEU:HD22	4	0.39
(1,1024)	1:68:A:LEU:HD23	1:64:A:LEU:HD23	4	0.39
(1,1024)	1:68:A:LEU:HD21	1:64:A:LEU:HD21	6	0.39
(1,1024)	1:68:A:LEU:HD21	1:64:A:LEU:HD22	6	0.39
(1,1024)	1:68:A:LEU:HD21	1:64:A:LEU:HD23	6	0.39
(1,1024)	1:68:A:LEU:HD22	1:64:A:LEU:HD21	6	0.39
(1,1024)	1:68:A:LEU:HD22	1:64:A:LEU:HD22	6	0.39
(1,1024)	1:68:A:LEU:HD22	1:64:A:LEU:HD23	6	0.39
(1,1024)	1:68:A:LEU:HD23	1:64:A:LEU:HD21	6	0.39
(1,1024)	1:68:A:LEU:HD23	1:64:A:LEU:HD22	6	0.39
(1,1024)	1:68:A:LEU:HD23	1:64:A:LEU:HD23	6	0.39
(1,1024)	1:68:A:LEU:HD21	1:64:A:LEU:HD21	7	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1024)	1:68:A:LEU:HD21	1:64:A:LEU:HD22	7	0.39
(1,1024)	1:68:A:LEU:HD21	1:64:A:LEU:HD23	7	0.39
(1,1024)	1:68:A:LEU:HD22	1:64:A:LEU:HD21	7	0.39
(1,1024)	1:68:A:LEU:HD22	1:64:A:LEU:HD22	7	0.39
(1,1024)	1:68:A:LEU:HD22	1:64:A:LEU:HD23	7	0.39
(1,1024)	1:68:A:LEU:HD23	1:64:A:LEU:HD21	7	0.39
(1,1024)	1:68:A:LEU:HD23	1:64:A:LEU:HD22	7	0.39
(1,1024)	1:68:A:LEU:HD23	1:64:A:LEU:HD23	7	0.39
(1,1024)	1:68:A:LEU:HD21	1:64:A:LEU:HD21	8	0.39
(1,1024)	1:68:A:LEU:HD21	1:64:A:LEU:HD22	8	0.39
(1,1024)	1:68:A:LEU:HD21	1:64:A:LEU:HD23	8	0.39
(1,1024)	1:68:A:LEU:HD22	1:64:A:LEU:HD21	8	0.39
(1,1024)	1:68:A:LEU:HD22	1:64:A:LEU:HD22	8	0.39
(1,1024)	1:68:A:LEU:HD22	1:64:A:LEU:HD23	8	0.39
(1,1024)	1:68:A:LEU:HD23	1:64:A:LEU:HD21	8	0.39
(1,1024)	1:68:A:LEU:HD23	1:64:A:LEU:HD22	8	0.39
(1,1024)	1:68:A:LEU:HD23	1:64:A:LEU:HD23	8	0.39
(1,990)	1:66:A:ARG:H	1:66:A:ARG:HB2	9	0.39
(1,983)	1:66:A:ARG:HB2	1:66:A:ARG:HD2	3	0.39
(1,901)	1:62:A:PRO:HB2	1:62:A:PRO:HA	1	0.39
(1,901)	1:62:A:PRO:HB2	1:62:A:PRO:HA	2	0.39
(1,901)	1:62:A:PRO:HB2	1:62:A:PRO:HA	5	0.39
(1,901)	1:62:A:PRO:HB2	1:62:A:PRO:HA	10	0.39
(1,726)	1:49:A:LEU:HB3	1:50:A:PRO:HD3	4	0.39
(1,544)	1:37:A:THR:HB	1:73:A:VAL:HG21	10	0.39
(1,544)	1:37:A:THR:HB	1:73:A:VAL:HG22	10	0.39
(1,544)	1:37:A:THR:HB	1:73:A:VAL:HG23	10	0.39
(1,433)	1:31:A:GLN:HE21	1:6:A:ASP:HB3	5	0.39
(1,344)	1:25:A:ASN:HD22	1:92:A:GLU:HB3	4	0.39
(1,276)	1:22:A:LYS:HG2	1:22:A:LYS:HE2	9	0.39
(1,227)	1:20:A:ALA:HB1	1:64:A:LEU:HD11	8	0.39
(1,227)	1:20:A:ALA:HB1	1:64:A:LEU:HD12	8	0.39
(1,227)	1:20:A:ALA:HB1	1:64:A:LEU:HD13	8	0.39
(1,227)	1:20:A:ALA:HB2	1:64:A:LEU:HD11	8	0.39
(1,227)	1:20:A:ALA:HB2	1:64:A:LEU:HD12	8	0.39
(1,227)	1:20:A:ALA:HB2	1:64:A:LEU:HD13	8	0.39
(1,227)	1:20:A:ALA:HB3	1:64:A:LEU:HD11	8	0.39
(1,227)	1:20:A:ALA:HB3	1:64:A:LEU:HD12	8	0.39
(1,227)	1:20:A:ALA:HB3	1:64:A:LEU:HD13	8	0.39
(1,183)	1:18:A:VAL:HG11	1:11:A:THR:H	10	0.39
(1,183)	1:18:A:VAL:HG12	1:11:A:THR:H	10	0.39
(1,183)	1:18:A:VAL:HG13	1:11:A:THR:H	10	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,157)	1:13:A:GLY:HA3	1:13:A:GLY:H	10	0.39
(1,1827)	1:116:A:ILE:H	1:116:A:ILE:HG12	4	0.38
(1,1827)	1:116:A:ILE:H	1:116:A:ILE:HG12	6	0.38
(1,1771)	1:112:A:LEU:HD11	1:127:A:ASP:HB3	8	0.38
(1,1771)	1:112:A:LEU:HD12	1:127:A:ASP:HB3	8	0.38
(1,1771)	1:112:A:LEU:HD13	1:127:A:ASP:HB3	8	0.38
(1,1493)	1:96:A:ILE:HD13	1:90:A:SER:H	2	0.38
(1,1454)	1:92:A:GLU:HB3	1:93:A:GLY:H	5	0.38
(1,1435)	1:91:A:LEU:HD21	1:91:A:LEU:H	4	0.38
(1,1435)	1:91:A:LEU:HD22	1:91:A:LEU:H	4	0.38
(1,1435)	1:91:A:LEU:HD23	1:91:A:LEU:H	4	0.38
(1,1379)	1:89:A:THR:H	1:77:A:TYR:HD2	6	0.38
(1,1345)	1:87:A:ILE:HG13	1:95:A:THR:HB	1	0.38
(1,1238)	1:82:A:LEU:HB3	1:104:A:LEU:HD21	2	0.38
(1,1238)	1:82:A:LEU:HB3	1:104:A:LEU:HD22	2	0.38
(1,1238)	1:82:A:LEU:HB3	1:104:A:LEU:HD23	2	0.38
(1,1024)	1:68:A:LEU:HD21	1:64:A:LEU:HD21	1	0.38
(1,1024)	1:68:A:LEU:HD21	1:64:A:LEU:HD22	1	0.38
(1,1024)	1:68:A:LEU:HD21	1:64:A:LEU:HD23	1	0.38
(1,1024)	1:68:A:LEU:HD22	1:64:A:LEU:HD21	1	0.38
(1,1024)	1:68:A:LEU:HD22	1:64:A:LEU:HD22	1	0.38
(1,1024)	1:68:A:LEU:HD22	1:64:A:LEU:HD23	1	0.38
(1,1024)	1:68:A:LEU:HD23	1:64:A:LEU:HD21	1	0.38
(1,1024)	1:68:A:LEU:HD23	1:64:A:LEU:HD22	1	0.38
(1,1024)	1:68:A:LEU:HD23	1:64:A:LEU:HD23	1	0.38
(1,1024)	1:68:A:LEU:HD21	1:64:A:LEU:HD21	5	0.38
(1,1024)	1:68:A:LEU:HD21	1:64:A:LEU:HD22	5	0.38
(1,1024)	1:68:A:LEU:HD21	1:64:A:LEU:HD23	5	0.38
(1,1024)	1:68:A:LEU:HD22	1:64:A:LEU:HD21	5	0.38
(1,1024)	1:68:A:LEU:HD22	1:64:A:LEU:HD22	5	0.38
(1,1024)	1:68:A:LEU:HD22	1:64:A:LEU:HD23	5	0.38
(1,1024)	1:68:A:LEU:HD23	1:64:A:LEU:HD21	5	0.38
(1,1024)	1:68:A:LEU:HD23	1:64:A:LEU:HD22	5	0.38
(1,1024)	1:68:A:LEU:HD23	1:64:A:LEU:HD23	5	0.38
(1,878)	1:59:A:GLN:HB3	1:60:A:ASN:H	2	0.38
(1,878)	1:59:A:GLN:HB3	1:60:A:ASN:H	4	0.38
(1,878)	1:59:A:GLN:HB3	1:60:A:ASN:H	6	0.38
(1,878)	1:59:A:GLN:HB3	1:60:A:ASN:H	7	0.38
(1,878)	1:59:A:GLN:HB3	1:60:A:ASN:H	8	0.38
(1,878)	1:59:A:GLN:HB3	1:60:A:ASN:H	10	0.38
(1,652)	1:45:A:ALA:HB1	1:48:A:LYS:HG2	7	0.38
(1,652)	1:45:A:ALA:HB2	1:48:A:LYS:HG2	7	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,652)	1:45:A:ALA:HB3	1:48:A:LYS:HG2	7	0.38
(1,276)	1:22:A:LYS:HG2	1:22:A:LYS:HE2	6	0.38
(1,180)	1:18:A:VAL:HG11	1:11:A:THR:HB	10	0.38
(1,180)	1:18:A:VAL:HG12	1:11:A:THR:HB	10	0.38
(1,180)	1:18:A:VAL:HG13	1:11:A:THR:HB	10	0.38
(1,117)	1:10:A:ASN:HB3	1:10:A:ASN:H	9	0.38
(1,1864)	1:118:A:ALA:HB2	1:121:A:GLY:HA2	3	0.37
(1,1864)	1:118:A:ALA:HB1	1:121:A:GLY:HA2	8	0.37
(1,1345)	1:87:A:ILE:HG13	1:95:A:THR:HB	4	0.37
(1,1337)	1:87:A:ILE:HA	1:88:A:VAL:HG11	2	0.37
(1,1337)	1:87:A:ILE:HA	1:88:A:VAL:HG12	2	0.37
(1,1337)	1:87:A:ILE:HA	1:88:A:VAL:HG13	2	0.37
(1,1337)	1:87:A:ILE:HA	1:88:A:VAL:HG11	9	0.37
(1,1337)	1:87:A:ILE:HA	1:88:A:VAL:HG12	9	0.37
(1,1337)	1:87:A:ILE:HA	1:88:A:VAL:HG13	9	0.37
(1,1303)	1:85:A:MET:HB3	1:86:A:GLY:H	1	0.37
(1,1303)	1:85:A:MET:HB3	1:86:A:GLY:H	3	0.37
(1,1303)	1:85:A:MET:HB3	1:86:A:GLY:H	7	0.37
(1,1303)	1:85:A:MET:HB3	1:86:A:GLY:H	10	0.37
(1,901)	1:62:A:PRO:HB2	1:62:A:PRO:HA	9	0.37
(1,774)	1:54:A:ILE:HG12	1:63:A:GLN:HE22	3	0.37
(1,571)	1:39:A:PHE:HB3	1:39:A:PHE:H	10	0.37
(1,368)	1:26:A:LEU:HD21	1:66:A:ARG:HB3	1	0.37
(1,368)	1:26:A:LEU:HD22	1:66:A:ARG:HB3	1	0.37
(1,368)	1:26:A:LEU:HD23	1:66:A:ARG:HB3	1	0.37
(1,257)	1:21:A:VAL:HG21	1:65:A:GLY:HA2	2	0.37
(1,257)	1:21:A:VAL:HG22	1:65:A:GLY:HA2	2	0.37
(1,257)	1:21:A:VAL:HG23	1:65:A:GLY:HA2	2	0.37
(1,183)	1:18:A:VAL:HG11	1:11:A:THR:H	5	0.37
(1,183)	1:18:A:VAL:HG12	1:11:A:THR:H	5	0.37
(1,183)	1:18:A:VAL:HG13	1:11:A:THR:H	5	0.37
(1,113)	1:10:A:ASN:HB2	1:7:A:ILE:HG21	8	0.37
(1,113)	1:10:A:ASN:HB2	1:7:A:ILE:HG22	8	0.37
(1,113)	1:10:A:ASN:HB2	1:7:A:ILE:HG23	8	0.37
(1,2029)	1:126:A:ILE:HA	1:127:A:ASP:HB3	4	0.36
(1,1827)	1:116:A:ILE:H	1:116:A:ILE:HG12	1	0.36
(1,1771)	1:112:A:LEU:HD11	1:127:A:ASP:HB3	4	0.36
(1,1771)	1:112:A:LEU:HD12	1:127:A:ASP:HB3	4	0.36
(1,1771)	1:112:A:LEU:HD13	1:127:A:ASP:HB3	4	0.36
(1,1740)	1:111:A:VAL:HG11	1:111:A:VAL:HA	5	0.36
(1,1740)	1:111:A:VAL:HG12	1:111:A:VAL:HA	5	0.36
(1,1740)	1:111:A:VAL:HG13	1:111:A:VAL:HA	5	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1737)	1:20:A:ALA:HB1	1:64:A:LEU:HD13	10	0.36
(1,1451)	1:92:A:GLU:H	1:92:A:GLU:HG3	3	0.36
(1,1337)	1:87:A:ILE:HA	1:88:A:VAL:HG11	1	0.36
(1,1337)	1:87:A:ILE:HA	1:88:A:VAL:HG12	1	0.36
(1,1337)	1:87:A:ILE:HA	1:88:A:VAL:HG13	1	0.36
(1,1337)	1:87:A:ILE:HA	1:88:A:VAL:HG11	4	0.36
(1,1337)	1:87:A:ILE:HA	1:88:A:VAL:HG12	4	0.36
(1,1337)	1:87:A:ILE:HA	1:88:A:VAL:HG13	4	0.36
(1,1337)	1:87:A:ILE:HA	1:88:A:VAL:HG11	7	0.36
(1,1337)	1:87:A:ILE:HA	1:88:A:VAL:HG12	7	0.36
(1,1337)	1:87:A:ILE:HA	1:88:A:VAL:HG13	7	0.36
(1,1337)	1:87:A:ILE:HA	1:88:A:VAL:HG11	8	0.36
(1,1337)	1:87:A:ILE:HA	1:88:A:VAL:HG12	8	0.36
(1,1337)	1:87:A:ILE:HA	1:88:A:VAL:HG13	8	0.36
(1,1337)	1:87:A:ILE:HA	1:88:A:VAL:HG11	10	0.36
(1,1337)	1:87:A:ILE:HA	1:88:A:VAL:HG12	10	0.36
(1,1337)	1:87:A:ILE:HA	1:88:A:VAL:HG13	10	0.36
(1,1303)	1:85:A:MET:HB3	1:86:A:GLY:H	4	0.36
(1,1303)	1:85:A:MET:HB3	1:86:A:GLY:H	8	0.36
(1,1273)	1:84:A:ARG:HB3	1:84:A:ARG:HD2	6	0.36
(1,1149)	1:78:A:LYS:HG3	1:78:A:LYS:HE2	8	0.36
(1,1149)	1:78:A:LYS:HG3	1:78:A:LYS:HE3	8	0.36
(1,1113)	1:76:A:ALA:HB2	1:36:A:PHE:H	1	0.36
(1,901)	1:62:A:PRO:HB2	1:62:A:PRO:HA	3	0.36
(1,726)	1:49:A:LEU:HB3	1:50:A:PRO:HD3	8	0.36
(1,652)	1:45:A:ALA:HB1	1:48:A:LYS:HG2	3	0.36
(1,652)	1:45:A:ALA:HB2	1:48:A:LYS:HG2	3	0.36
(1,652)	1:45:A:ALA:HB3	1:48:A:LYS:HG2	3	0.36
(1,571)	1:39:A:PHE:HB3	1:39:A:PHE:H	2	0.36
(1,571)	1:39:A:PHE:HB3	1:39:A:PHE:H	3	0.36
(1,571)	1:39:A:PHE:HB3	1:39:A:PHE:H	5	0.36
(1,371)	1:91:A:LEU:HB2	1:93:A:GLY:H	7	0.36
(1,183)	1:18:A:VAL:HG11	1:11:A:THR:H	4	0.36
(1,183)	1:18:A:VAL:HG12	1:11:A:THR:H	4	0.36
(1,183)	1:18:A:VAL:HG13	1:11:A:THR:H	4	0.36
(1,183)	1:18:A:VAL:HG11	1:11:A:THR:H	9	0.36
(1,183)	1:18:A:VAL:HG12	1:11:A:THR:H	9	0.36
(1,183)	1:18:A:VAL:HG13	1:11:A:THR:H	9	0.36
(1,1603)	1:104:A:LEU:H	1:105:A:GLU:HG2	3	0.35
(1,1516)	1:96:A:ILE:HG13	1:107:A:LYS:HB2	7	0.35
(1,1453)	1:92:A:GLU:H	1:93:A:GLY:HA3	3	0.35
(1,1453)	1:92:A:GLU:H	1:93:A:GLY:HA3	5	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1303)	1:85:A:MET:HB3	1:86:A:GLY:H	5	0.35
(1,1303)	1:85:A:MET:HB3	1:86:A:GLY:H	6	0.35
(1,1303)	1:85:A:MET:HB3	1:86:A:GLY:H	9	0.35
(1,869)	1:59:A:GLN:HE22	1:59:A:GLN:HG3	3	0.35
(1,869)	1:59:A:GLN:HE22	1:59:A:GLN:HG3	9	0.35
(1,762)	1:54:A:ILE:HG12	1:54:A:ILE:H	4	0.35
(1,762)	1:54:A:ILE:HG12	1:54:A:ILE:H	6	0.35
(1,726)	1:49:A:LEU:HB3	1:50:A:PRO:HD3	2	0.35
(1,483)	1:35:A:PRO:HD2	1:35:A:PRO:HB2	3	0.35
(1,368)	1:26:A:LEU:HD21	1:66:A:ARG:HB3	10	0.35
(1,368)	1:26:A:LEU:HD22	1:66:A:ARG:HB3	10	0.35
(1,368)	1:26:A:LEU:HD23	1:66:A:ARG:HB3	10	0.35
(1,257)	1:21:A:VAL:HG21	1:65:A:GLY:HA2	4	0.35
(1,257)	1:21:A:VAL:HG22	1:65:A:GLY:HA2	4	0.35
(1,257)	1:21:A:VAL:HG23	1:65:A:GLY:HA2	4	0.35
(1,148)	1:12:A:PRO:HD3	1:12:A:PRO:HG2	7	0.35
(1,1737)	1:20:A:ALA:HB2	1:64:A:LEU:HD11	2	0.34
(1,1558)	1:99:A:HIS:HB2	1:100:A:GLY:H	2	0.34
(1,1451)	1:92:A:GLU:H	1:92:A:GLU:HG3	7	0.34
(1,1345)	1:87:A:ILE:HG13	1:95:A:THR:HB	10	0.34
(1,1337)	1:87:A:ILE:HA	1:88:A:VAL:HG11	3	0.34
(1,1337)	1:87:A:ILE:HA	1:88:A:VAL:HG12	3	0.34
(1,1337)	1:87:A:ILE:HA	1:88:A:VAL:HG13	3	0.34
(1,1337)	1:87:A:ILE:HA	1:88:A:VAL:HG11	5	0.34
(1,1337)	1:87:A:ILE:HA	1:88:A:VAL:HG12	5	0.34
(1,1337)	1:87:A:ILE:HA	1:88:A:VAL:HG13	5	0.34
(1,1337)	1:87:A:ILE:HA	1:88:A:VAL:HG11	6	0.34
(1,1337)	1:87:A:ILE:HA	1:88:A:VAL:HG12	6	0.34
(1,1337)	1:87:A:ILE:HA	1:88:A:VAL:HG13	6	0.34
(1,1277)	1:84:A:ARG:HD2	1:84:A:ARG:HG2	2	0.34
(1,1257)	1:96:A:ILE:HG13	1:107:A:LYS:HE3	3	0.34
(1,1244)	1:83:A:LYS:HB3	1:83:A:LYS:H	9	0.34
(1,1231)	1:82:A:LEU:HD11	1:83:A:LYS:H	7	0.34
(1,1231)	1:82:A:LEU:HD12	1:83:A:LYS:H	7	0.34
(1,1231)	1:82:A:LEU:HD13	1:83:A:LYS:H	7	0.34
(1,1231)	1:82:A:LEU:HD11	1:83:A:LYS:H	9	0.34
(1,1231)	1:82:A:LEU:HD12	1:83:A:LYS:H	9	0.34
(1,1231)	1:82:A:LEU:HD13	1:83:A:LYS:H	9	0.34
(1,990)	1:66:A:ARG:H	1:66:A:ARG:HB2	6	0.34
(1,878)	1:59:A:GLN:HB3	1:60:A:ASN:H	5	0.34
(1,825)	1:57:A:LEU:HB3	1:57:A:LEU:H	9	0.34
(1,762)	1:54:A:ILE:HG12	1:54:A:ILE:H	9	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,758)	1:54:A:ILE:HG12	1:54:A:ILE:HA	2	0.34
(1,758)	1:54:A:ILE:HG12	1:54:A:ILE:HA	5	0.34
(1,758)	1:54:A:ILE:HG12	1:54:A:ILE:HA	7	0.34
(1,709)	1:48:A:LYS:HD2	1:50:A:PRO:HD3	7	0.34
(1,709)	1:48:A:LYS:HD3	1:50:A:PRO:HD3	7	0.34
(1,571)	1:39:A:PHE:HB3	1:39:A:PHE:H	9	0.34
(1,553)	1:37:A:THR:HG21	1:82:A:LEU:HD11	5	0.34
(1,553)	1:37:A:THR:HG21	1:82:A:LEU:HD12	5	0.34
(1,553)	1:37:A:THR:HG21	1:82:A:LEU:HD13	5	0.34
(1,553)	1:37:A:THR:HG22	1:82:A:LEU:HD11	5	0.34
(1,553)	1:37:A:THR:HG22	1:82:A:LEU:HD12	5	0.34
(1,553)	1:37:A:THR:HG22	1:82:A:LEU:HD13	5	0.34
(1,553)	1:37:A:THR:HG23	1:82:A:LEU:HD11	5	0.34
(1,553)	1:37:A:THR:HG23	1:82:A:LEU:HD12	5	0.34
(1,553)	1:37:A:THR:HG23	1:82:A:LEU:HD13	5	0.34
(1,391)	1:28:A:GLU:HA	1:28:A:GLU:HB2	2	0.34
(1,391)	1:28:A:GLU:HA	1:28:A:GLU:HB2	4	0.34
(1,391)	1:28:A:GLU:HA	1:28:A:GLU:HB2	10	0.34
(1,380)	1:26:A:LEU:HD23	1:66:A:ARG:HA	8	0.34
(1,371)	1:91:A:LEU:HB2	1:93:A:GLY:H	4	0.34
(1,1583)	1:103:A:PRO:HD2	1:103:A:PRO:HB2	4	0.33
(1,1558)	1:99:A:HIS:HB2	1:100:A:GLY:H	4	0.33
(1,1493)	1:96:A:ILE:HD13	1:90:A:SER:H	4	0.33
(1,1453)	1:92:A:GLU:H	1:93:A:GLY:HA3	8	0.33
(1,1410)	1:58:A:VAL:HG12	1:59:A:GLN:HA	9	0.33
(1,1345)	1:87:A:ILE:HG13	1:95:A:THR:HB	2	0.33
(1,1277)	1:84:A:ARG:HD2	1:84:A:ARG:HG2	1	0.33
(1,1277)	1:84:A:ARG:HD2	1:84:A:ARG:HG2	3	0.33
(1,1277)	1:84:A:ARG:HD2	1:84:A:ARG:HG2	5	0.33
(1,1277)	1:84:A:ARG:HD2	1:84:A:ARG:HG2	6	0.33
(1,1277)	1:84:A:ARG:HD2	1:84:A:ARG:HG2	8	0.33
(1,1277)	1:84:A:ARG:HD2	1:84:A:ARG:HG2	9	0.33
(1,1273)	1:84:A:ARG:HB3	1:84:A:ARG:HD2	4	0.33
(1,1273)	1:84:A:ARG:HB3	1:84:A:ARG:HD2	9	0.33
(1,1027)	1:68:A:LEU:HD11	1:65:A:GLY:HA2	10	0.33
(1,1027)	1:68:A:LEU:HD12	1:65:A:GLY:HA2	10	0.33
(1,1027)	1:68:A:LEU:HD13	1:65:A:GLY:HA2	10	0.33
(1,957)	1:64:A:LEU:HD11	1:65:A:GLY:H	7	0.33
(1,957)	1:64:A:LEU:HD12	1:65:A:GLY:H	7	0.33
(1,957)	1:64:A:LEU:HD13	1:65:A:GLY:H	7	0.33
(1,929)	1:63:A:GLN:HG2	1:63:A:GLN:HE22	9	0.33
(1,929)	1:63:A:GLN:HG3	1:63:A:GLN:HE22	9	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,869)	1:59:A:GLN:HE22	1:59:A:GLN:HG3	6	0.33
(1,869)	1:59:A:GLN:HE22	1:59:A:GLN:HG3	10	0.33
(1,825)	1:57:A:LEU:HB3	1:57:A:LEU:H	3	0.33
(1,758)	1:54:A:ILE:HG12	1:54:A:ILE:HA	3	0.33
(1,571)	1:39:A:PHE:HB3	1:39:A:PHE:H	1	0.33
(1,571)	1:39:A:PHE:HB3	1:39:A:PHE:H	7	0.33
(1,553)	1:37:A:THR:HG21	1:82:A:LEU:HD11	2	0.33
(1,553)	1:37:A:THR:HG21	1:82:A:LEU:HD12	2	0.33
(1,553)	1:37:A:THR:HG21	1:82:A:LEU:HD13	2	0.33
(1,553)	1:37:A:THR:HG22	1:82:A:LEU:HD11	2	0.33
(1,553)	1:37:A:THR:HG22	1:82:A:LEU:HD12	2	0.33
(1,553)	1:37:A:THR:HG22	1:82:A:LEU:HD13	2	0.33
(1,553)	1:37:A:THR:HG23	1:82:A:LEU:HD11	2	0.33
(1,553)	1:37:A:THR:HG23	1:82:A:LEU:HD12	2	0.33
(1,553)	1:37:A:THR:HG23	1:82:A:LEU:HD13	2	0.33
(1,483)	1:35:A:PRO:HD2	1:35:A:PRO:HB2	10	0.33
(1,435)	1:31:A:GLN:HE22	1:27:A:VAL:HG23	2	0.33
(1,429)	1:30:A:LEU:HD11	1:70:A:TYR:H	6	0.33
(1,391)	1:28:A:GLU:HA	1:28:A:GLU:HB2	3	0.33
(1,391)	1:28:A:GLU:HA	1:28:A:GLU:HB2	5	0.33
(1,342)	1:36:A:PHE:HB2	1:75:A:GLY:H	7	0.33
(1,342)	1:36:A:PHE:HB2	1:75:A:GLY:H	9	0.33
(1,276)	1:22:A:LYS:HG2	1:22:A:LYS:HE2	1	0.33
(1,276)	1:22:A:LYS:HG2	1:22:A:LYS:HE2	4	0.33
(1,276)	1:22:A:LYS:HG2	1:22:A:LYS:HE2	10	0.33
(1,227)	1:20:A:ALA:HB1	1:64:A:LEU:HD11	3	0.33
(1,227)	1:20:A:ALA:HB1	1:64:A:LEU:HD12	3	0.33
(1,227)	1:20:A:ALA:HB1	1:64:A:LEU:HD13	3	0.33
(1,227)	1:20:A:ALA:HB2	1:64:A:LEU:HD11	3	0.33
(1,227)	1:20:A:ALA:HB2	1:64:A:LEU:HD12	3	0.33
(1,227)	1:20:A:ALA:HB2	1:64:A:LEU:HD13	3	0.33
(1,227)	1:20:A:ALA:HB3	1:64:A:LEU:HD11	3	0.33
(1,227)	1:20:A:ALA:HB3	1:64:A:LEU:HD12	3	0.33
(1,227)	1:20:A:ALA:HB3	1:64:A:LEU:HD13	3	0.33
(1,1842)	1:117:A:GLU:HB2	1:117:A:GLU:HA	1	0.32
(1,1842)	1:117:A:GLU:HB2	1:117:A:GLU:HA	3	0.32
(1,1842)	1:117:A:GLU:HB2	1:117:A:GLU:HA	5	0.32
(1,1842)	1:117:A:GLU:HB2	1:117:A:GLU:HA	6	0.32
(1,1842)	1:117:A:GLU:HB2	1:117:A:GLU:HA	7	0.32
(1,1842)	1:117:A:GLU:HB2	1:117:A:GLU:HA	8	0.32
(1,1842)	1:117:A:GLU:HB2	1:117:A:GLU:HA	9	0.32
(1,1740)	1:111:A:VAL:HG11	1:111:A:VAL:HA	4	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1740)	1:111:A:VAL:HG12	1:111:A:VAL:HA	4	0.32
(1,1740)	1:111:A:VAL:HG13	1:111:A:VAL:HA	4	0.32
(1,1593)	1:103:A:PRO:HD3	1:103:A:PRO:HG2	9	0.32
(1,1453)	1:92:A:GLU:H	1:93:A:GLY:HA3	10	0.32
(1,1361)	1:88:A:VAL:H	1:88:A:VAL:HG11	9	0.32
(1,1361)	1:88:A:VAL:H	1:88:A:VAL:HG12	9	0.32
(1,1361)	1:88:A:VAL:H	1:88:A:VAL:HG13	9	0.32
(1,1345)	1:87:A:ILE:HG13	1:95:A:THR:HB	8	0.32
(1,1277)	1:84:A:ARG:HD2	1:84:A:ARG:HG2	4	0.32
(1,1277)	1:84:A:ARG:HD2	1:84:A:ARG:HG2	10	0.32
(1,1273)	1:84:A:ARG:HB3	1:84:A:ARG:HD2	3	0.32
(1,1273)	1:84:A:ARG:HB3	1:84:A:ARG:HD2	8	0.32
(1,1252)	1:83:A:LYS:HG2	1:86:A:GLY:H	10	0.32
(1,1252)	1:83:A:LYS:HG3	1:86:A:GLY:H	10	0.32
(1,1244)	1:83:A:LYS:HB3	1:83:A:LYS:H	7	0.32
(1,1244)	1:83:A:LYS:HB3	1:83:A:LYS:H	10	0.32
(1,1027)	1:68:A:LEU:HD11	1:65:A:GLY:HA2	4	0.32
(1,1027)	1:68:A:LEU:HD12	1:65:A:GLY:HA2	4	0.32
(1,1027)	1:68:A:LEU:HD13	1:65:A:GLY:HA2	4	0.32
(1,992)	1:66:A:ARG:HG3	1:67:A:ILE:H	5	0.32
(1,992)	1:66:A:ARG:HG3	1:67:A:ILE:H	7	0.32
(1,983)	1:66:A:ARG:HB2	1:66:A:ARG:HD2	10	0.32
(1,929)	1:63:A:GLN:HG2	1:63:A:GLN:HE22	6	0.32
(1,929)	1:63:A:GLN:HG3	1:63:A:GLN:HE22	6	0.32
(1,869)	1:59:A:GLN:HE22	1:59:A:GLN:HG3	1	0.32
(1,869)	1:59:A:GLN:HE22	1:59:A:GLN:HG3	2	0.32
(1,869)	1:59:A:GLN:HE22	1:59:A:GLN:HG3	4	0.32
(1,869)	1:59:A:GLN:HE22	1:59:A:GLN:HG3	5	0.32
(1,869)	1:59:A:GLN:HE22	1:59:A:GLN:HG3	8	0.32
(1,825)	1:57:A:LEU:HB3	1:57:A:LEU:H	8	0.32
(1,772)	1:55:A:THR:HG22	1:58:A:VAL:H	9	0.32
(1,571)	1:39:A:PHE:HB3	1:39:A:PHE:H	6	0.32
(1,553)	1:37:A:THR:HG21	1:82:A:LEU:HD11	9	0.32
(1,553)	1:37:A:THR:HG21	1:82:A:LEU:HD12	9	0.32
(1,553)	1:37:A:THR:HG21	1:82:A:LEU:HD13	9	0.32
(1,553)	1:37:A:THR:HG22	1:82:A:LEU:HD11	9	0.32
(1,553)	1:37:A:THR:HG22	1:82:A:LEU:HD12	9	0.32
(1,553)	1:37:A:THR:HG22	1:82:A:LEU:HD13	9	0.32
(1,553)	1:37:A:THR:HG23	1:82:A:LEU:HD11	9	0.32
(1,553)	1:37:A:THR:HG23	1:82:A:LEU:HD12	9	0.32
(1,553)	1:37:A:THR:HG23	1:82:A:LEU:HD13	9	0.32
(1,433)	1:31:A:GLN:HE21	1:6:A:ASP:HB3	2	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,429)	1:30:A:LEU:HD11	1:70:A:TYR:H	10	0.32
(1,391)	1:28:A:GLU:HA	1:28:A:GLU:HB2	1	0.32
(1,276)	1:22:A:LYS:HG2	1:22:A:LYS:HE2	2	0.32
(1,276)	1:22:A:LYS:HG2	1:22:A:LYS:HE2	5	0.32
(1,1593)	1:103:A:PRO:HD3	1:103:A:PRO:HG2	1	0.31
(1,1593)	1:103:A:PRO:HD3	1:103:A:PRO:HG2	3	0.31
(1,1593)	1:103:A:PRO:HD3	1:103:A:PRO:HG2	4	0.31
(1,1593)	1:103:A:PRO:HD3	1:103:A:PRO:HG2	6	0.31
(1,1593)	1:103:A:PRO:HD3	1:103:A:PRO:HG2	7	0.31
(1,1593)	1:103:A:PRO:HD3	1:103:A:PRO:HG2	10	0.31
(1,1453)	1:92:A:GLU:H	1:93:A:GLY:HA3	2	0.31
(1,1252)	1:83:A:LYS:HG2	1:86:A:GLY:H	7	0.31
(1,1252)	1:83:A:LYS:HG3	1:86:A:GLY:H	7	0.31
(1,1177)	1:79:A:ALA:HB1	1:104:A:LEU:HD21	1	0.31
(1,1177)	1:79:A:ALA:HB1	1:104:A:LEU:HD22	1	0.31
(1,1177)	1:79:A:ALA:HB1	1:104:A:LEU:HD23	1	0.31
(1,1177)	1:79:A:ALA:HB2	1:104:A:LEU:HD21	1	0.31
(1,1177)	1:79:A:ALA:HB2	1:104:A:LEU:HD22	1	0.31
(1,1177)	1:79:A:ALA:HB2	1:104:A:LEU:HD23	1	0.31
(1,1177)	1:79:A:ALA:HB3	1:104:A:LEU:HD21	1	0.31
(1,1177)	1:79:A:ALA:HB3	1:104:A:LEU:HD22	1	0.31
(1,1177)	1:79:A:ALA:HB3	1:104:A:LEU:HD23	1	0.31
(1,957)	1:64:A:LEU:HD11	1:65:A:GLY:H	5	0.31
(1,957)	1:64:A:LEU:HD12	1:65:A:GLY:H	5	0.31
(1,957)	1:64:A:LEU:HD13	1:65:A:GLY:H	5	0.31
(1,957)	1:64:A:LEU:HD11	1:65:A:GLY:H	6	0.31
(1,957)	1:64:A:LEU:HD12	1:65:A:GLY:H	6	0.31
(1,957)	1:64:A:LEU:HD13	1:65:A:GLY:H	6	0.31
(1,920)	1:54:A:ILE:HD11	1:63:A:GLN:HE21	10	0.31
(1,869)	1:59:A:GLN:HE22	1:59:A:GLN:HG3	7	0.31
(1,825)	1:57:A:LEU:HB3	1:57:A:LEU:H	4	0.31
(1,825)	1:57:A:LEU:HB3	1:57:A:LEU:H	6	0.31
(1,758)	1:54:A:ILE:HG12	1:54:A:ILE:HA	10	0.31
(1,435)	1:31:A:GLN:HE22	1:27:A:VAL:HG22	5	0.31
(1,435)	1:31:A:GLN:HE22	1:27:A:VAL:HG21	10	0.31
(1,429)	1:30:A:LEU:HD13	1:70:A:TYR:H	9	0.31
(1,391)	1:28:A:GLU:HA	1:28:A:GLU:HB2	7	0.31
(1,391)	1:28:A:GLU:HA	1:28:A:GLU:HB2	8	0.31
(1,368)	1:26:A:LEU:HD21	1:66:A:ARG:HB3	4	0.31
(1,368)	1:26:A:LEU:HD22	1:66:A:ARG:HB3	4	0.31
(1,368)	1:26:A:LEU:HD23	1:66:A:ARG:HB3	4	0.31
(1,180)	1:18:A:VAL:HG11	1:11:A:THR:HB	1	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,180)	1:18:A:VAL:HG12	1:11:A:THR:HB	1	0.31
(1,180)	1:18:A:VAL:HG13	1:11:A:THR:HB	1	0.31
(1,107)	1:8:A:ALA:HA	1:18:A:VAL:HG21	9	0.31
(1,107)	1:8:A:ALA:HA	1:18:A:VAL:HG22	9	0.31
(1,107)	1:8:A:ALA:HA	1:18:A:VAL:HG23	9	0.31
(1,1771)	1:112:A:LEU:HD11	1:127:A:ASP:HB3	3	0.3
(1,1771)	1:112:A:LEU:HD12	1:127:A:ASP:HB3	3	0.3
(1,1771)	1:112:A:LEU:HD13	1:127:A:ASP:HB3	3	0.3
(1,1593)	1:103:A:PRO:HD3	1:103:A:PRO:HG2	2	0.3
(1,1593)	1:103:A:PRO:HD3	1:103:A:PRO:HG2	5	0.3
(1,1593)	1:103:A:PRO:HD3	1:103:A:PRO:HG2	8	0.3
(1,1516)	1:96:A:ILE:HG13	1:107:A:LYS:HB2	8	0.3
(1,1252)	1:83:A:LYS:HG2	1:86:A:GLY:H	9	0.3
(1,1252)	1:83:A:LYS:HG3	1:86:A:GLY:H	9	0.3
(1,1244)	1:83:A:LYS:HB3	1:83:A:LYS:H	2	0.3
(1,1052)	1:69:A:LYS:HB2	1:70:A:TYR:H	8	0.3
(1,957)	1:64:A:LEU:HD11	1:65:A:GLY:H	1	0.3
(1,957)	1:64:A:LEU:HD12	1:65:A:GLY:H	1	0.3
(1,957)	1:64:A:LEU:HD13	1:65:A:GLY:H	1	0.3
(1,929)	1:63:A:GLN:HG2	1:63:A:GLN:HE22	1	0.3
(1,929)	1:63:A:GLN:HG3	1:63:A:GLN:HE22	1	0.3
(1,825)	1:57:A:LEU:HB3	1:57:A:LEU:H	5	0.3
(1,762)	1:54:A:ILE:HG12	1:54:A:ILE:H	10	0.3
(1,758)	1:54:A:ILE:HG12	1:54:A:ILE:HA	8	0.3
(1,726)	1:49:A:LEU:HB3	1:50:A:PRO:HD3	9	0.3
(1,709)	1:48:A:LYS:HD2	1:50:A:PRO:HD3	3	0.3
(1,709)	1:48:A:LYS:HD3	1:50:A:PRO:HD3	3	0.3
(1,571)	1:39:A:PHE:HB3	1:39:A:PHE:H	4	0.3
(1,435)	1:31:A:GLN:HE22	1:27:A:VAL:HG22	1	0.3
(1,435)	1:31:A:GLN:HE22	1:27:A:VAL:HG21	3	0.3
(1,435)	1:31:A:GLN:HE22	1:27:A:VAL:HG23	4	0.3
(1,435)	1:31:A:GLN:HE22	1:27:A:VAL:HG21	9	0.3
(1,391)	1:28:A:GLU:HA	1:28:A:GLU:HB2	6	0.3
(1,391)	1:28:A:GLU:HA	1:28:A:GLU:HB2	9	0.3
(1,371)	1:91:A:LEU:HB2	1:93:A:GLY:H	3	0.3
(1,321)	1:24:A:ALA:HB1	1:62:A:PRO:HB2	7	0.3
(1,321)	1:24:A:ALA:HB2	1:62:A:PRO:HB2	7	0.3
(1,321)	1:24:A:ALA:HB3	1:62:A:PRO:HB2	7	0.3
(1,276)	1:22:A:LYS:HG2	1:22:A:LYS:HE2	3	0.3
(1,275)	1:22:A:LYS:HG3	1:22:A:LYS:HE2	8	0.3
(1,257)	1:21:A:VAL:HG21	1:65:A:GLY:HA2	1	0.3
(1,257)	1:21:A:VAL:HG22	1:65:A:GLY:HA2	1	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,257)	1:21:A:VAL:HG23	1:65:A:GLY:HA2	1	0.3
(1,1968)	1:124:A:HIS:HB3	1:39:A:PHE:HD1	8	0.29
(1,1968)	1:124:A:HIS:HB3	1:39:A:PHE:HD2	8	0.29
(1,1771)	1:112:A:LEU:HD11	1:127:A:ASP:HB3	6	0.29
(1,1771)	1:112:A:LEU:HD12	1:127:A:ASP:HB3	6	0.29
(1,1771)	1:112:A:LEU:HD13	1:127:A:ASP:HB3	6	0.29
(1,1453)	1:92:A:GLU:H	1:93:A:GLY:HA3	9	0.29
(1,1410)	1:58:A:VAL:HG13	1:59:A:GLN:HA	3	0.29
(1,1361)	1:88:A:VAL:H	1:88:A:VAL:HG11	7	0.29
(1,1361)	1:88:A:VAL:H	1:88:A:VAL:HG12	7	0.29
(1,1361)	1:88:A:VAL:H	1:88:A:VAL:HG13	7	0.29
(1,1273)	1:84:A:ARG:HB3	1:84:A:ARG:HD2	5	0.29
(1,1271)	1:84:A:ARG:HD3	1:84:A:ARG:HG3	1	0.29
(1,1271)	1:84:A:ARG:HD3	1:84:A:ARG:HG3	2	0.29
(1,1271)	1:84:A:ARG:HD3	1:84:A:ARG:HG3	3	0.29
(1,1271)	1:84:A:ARG:HD3	1:84:A:ARG:HG3	5	0.29
(1,1271)	1:84:A:ARG:HD3	1:84:A:ARG:HG3	6	0.29
(1,1271)	1:84:A:ARG:HD3	1:84:A:ARG:HG3	8	0.29
(1,1271)	1:84:A:ARG:HD3	1:84:A:ARG:HG3	9	0.29
(1,1252)	1:83:A:LYS:HG2	1:86:A:GLY:H	2	0.29
(1,1252)	1:83:A:LYS:HG3	1:86:A:GLY:H	2	0.29
(1,1231)	1:82:A:LEU:HD11	1:83:A:LYS:H	2	0.29
(1,1231)	1:82:A:LEU:HD12	1:83:A:LYS:H	2	0.29
(1,1231)	1:82:A:LEU:HD13	1:83:A:LYS:H	2	0.29
(1,1231)	1:82:A:LEU:HD11	1:83:A:LYS:H	4	0.29
(1,1231)	1:82:A:LEU:HD12	1:83:A:LYS:H	4	0.29
(1,1231)	1:82:A:LEU:HD13	1:83:A:LYS:H	4	0.29
(1,1214)	1:78:A:LYS:HG2	1:79:A:ALA:H	2	0.29
(1,1214)	1:78:A:LYS:HG2	1:79:A:ALA:H	8	0.29
(1,981)	1:65:A:GLY:HA3	1:68:A:LEU:H	1	0.29
(1,957)	1:64:A:LEU:HD11	1:65:A:GLY:H	8	0.29
(1,957)	1:64:A:LEU:HD12	1:65:A:GLY:H	8	0.29
(1,957)	1:64:A:LEU:HD13	1:65:A:GLY:H	8	0.29
(1,825)	1:57:A:LEU:HB3	1:57:A:LEU:H	2	0.29
(1,435)	1:31:A:GLN:HE22	1:27:A:VAL:HG22	6	0.29
(1,433)	1:31:A:GLN:HE21	1:6:A:ASP:HB3	10	0.29
(1,1864)	1:118:A:ALA:HB3	1:121:A:GLY:HA2	4	0.28
(1,1816)	1:116:A:ILE:HA	1:116:A:ILE:HG13	4	0.28
(1,1579)	1:102:A:ASN:HB2	1:102:A:ASN:HA	8	0.28
(1,1415)	1:91:A:LEU:HD21	1:74:A:ALA:HB1	10	0.28
(1,1415)	1:91:A:LEU:HD21	1:74:A:ALA:HB2	10	0.28
(1,1415)	1:91:A:LEU:HD21	1:74:A:ALA:HB3	10	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1415)	1:91:A:LEU:HD22	1:74:A:ALA:HB1	10	0.28
(1,1415)	1:91:A:LEU:HD22	1:74:A:ALA:HB2	10	0.28
(1,1415)	1:91:A:LEU:HD22	1:74:A:ALA:HB3	10	0.28
(1,1415)	1:91:A:LEU:HD23	1:74:A:ALA:HB1	10	0.28
(1,1415)	1:91:A:LEU:HD23	1:74:A:ALA:HB2	10	0.28
(1,1415)	1:91:A:LEU:HD23	1:74:A:ALA:HB3	10	0.28
(1,1277)	1:84:A:ARG:HD2	1:84:A:ARG:HG2	7	0.28
(1,1273)	1:84:A:ARG:HB3	1:84:A:ARG:HD2	10	0.28
(1,1271)	1:84:A:ARG:HD3	1:84:A:ARG:HG3	4	0.28
(1,1271)	1:84:A:ARG:HD3	1:84:A:ARG:HG3	10	0.28
(1,1231)	1:82:A:LEU:HD11	1:83:A:LYS:H	10	0.28
(1,1231)	1:82:A:LEU:HD12	1:83:A:LYS:H	10	0.28
(1,1231)	1:82:A:LEU:HD13	1:83:A:LYS:H	10	0.28
(1,1214)	1:78:A:LYS:HG2	1:79:A:ALA:H	3	0.28
(1,1177)	1:79:A:ALA:HB1	1:104:A:LEU:HD21	8	0.28
(1,1177)	1:79:A:ALA:HB1	1:104:A:LEU:HD22	8	0.28
(1,1177)	1:79:A:ALA:HB1	1:104:A:LEU:HD23	8	0.28
(1,1177)	1:79:A:ALA:HB2	1:104:A:LEU:HD21	8	0.28
(1,1177)	1:79:A:ALA:HB2	1:104:A:LEU:HD22	8	0.28
(1,1177)	1:79:A:ALA:HB2	1:104:A:LEU:HD23	8	0.28
(1,1177)	1:79:A:ALA:HB3	1:104:A:LEU:HD21	8	0.28
(1,1177)	1:79:A:ALA:HB3	1:104:A:LEU:HD22	8	0.28
(1,1177)	1:79:A:ALA:HB3	1:104:A:LEU:HD23	8	0.28
(1,1176)	1:79:A:ALA:HA	1:104:A:LEU:HD11	1	0.28
(1,1176)	1:79:A:ALA:HA	1:104:A:LEU:HD12	1	0.28
(1,1176)	1:79:A:ALA:HA	1:104:A:LEU:HD13	1	0.28
(1,923)	1:63:A:GLN:HE21	1:63:A:GLN:HB2	2	0.28
(1,923)	1:63:A:GLN:HE21	1:63:A:GLN:HB3	2	0.28
(1,830)	1:57:A:LEU:HB3	1:58:A:VAL:H	6	0.28
(1,825)	1:57:A:LEU:HB3	1:57:A:LEU:H	7	0.28
(1,825)	1:57:A:LEU:HB3	1:57:A:LEU:H	10	0.28
(1,571)	1:39:A:PHE:HB3	1:39:A:PHE:H	8	0.28
(1,520)	1:36:A:PHE:HA	1:72:A:VAL:HG11	4	0.28
(1,520)	1:36:A:PHE:HA	1:72:A:VAL:HG12	4	0.28
(1,520)	1:36:A:PHE:HA	1:72:A:VAL:HG13	4	0.28
(1,483)	1:35:A:PRO:HD2	1:35:A:PRO:HB2	1	0.28
(1,435)	1:31:A:GLN:HE22	1:27:A:VAL:HG21	7	0.28
(1,1999)	1:126:A:ILE:HG21	1:39:A:PHE:HD1	4	0.27
(1,1999)	1:126:A:ILE:HG21	1:39:A:PHE:HD2	4	0.27
(1,1999)	1:126:A:ILE:HG22	1:39:A:PHE:HD1	4	0.27
(1,1999)	1:126:A:ILE:HG22	1:39:A:PHE:HD2	4	0.27
(1,1999)	1:126:A:ILE:HG23	1:39:A:PHE:HD1	4	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1999)	1:126:A:ILE:HG23	1:39:A:PHE:HD2	4	0.27
(1,1816)	1:116:A:ILE:HA	1:116:A:ILE:HG13	2	0.27
(1,1621)	1:104:A:LEU:HB2	1:105:A:GLU:H	5	0.27
(1,1583)	1:103:A:PRO:HD2	1:103:A:PRO:HB2	3	0.27
(1,1583)	1:103:A:PRO:HD2	1:103:A:PRO:HB2	7	0.27
(1,1583)	1:103:A:PRO:HD2	1:103:A:PRO:HB2	8	0.27
(1,1579)	1:102:A:ASN:HB2	1:102:A:ASN:HA	2	0.27
(1,1493)	1:96:A:ILE:HD13	1:90:A:SER:H	8	0.27
(1,1423)	1:91:A:LEU:HB3	1:91:A:LEU:HD11	9	0.27
(1,1423)	1:91:A:LEU:HB3	1:91:A:LEU:HD12	9	0.27
(1,1423)	1:91:A:LEU:HB3	1:91:A:LEU:HD13	9	0.27
(1,1361)	1:88:A:VAL:H	1:88:A:VAL:HG11	1	0.27
(1,1361)	1:88:A:VAL:H	1:88:A:VAL:HG12	1	0.27
(1,1361)	1:88:A:VAL:H	1:88:A:VAL:HG13	1	0.27
(1,1361)	1:88:A:VAL:H	1:88:A:VAL:HG11	2	0.27
(1,1361)	1:88:A:VAL:H	1:88:A:VAL:HG12	2	0.27
(1,1361)	1:88:A:VAL:H	1:88:A:VAL:HG13	2	0.27
(1,1361)	1:88:A:VAL:H	1:88:A:VAL:HG11	4	0.27
(1,1361)	1:88:A:VAL:H	1:88:A:VAL:HG12	4	0.27
(1,1361)	1:88:A:VAL:H	1:88:A:VAL:HG13	4	0.27
(1,1361)	1:88:A:VAL:H	1:88:A:VAL:HG11	8	0.27
(1,1361)	1:88:A:VAL:H	1:88:A:VAL:HG12	8	0.27
(1,1361)	1:88:A:VAL:H	1:88:A:VAL:HG13	8	0.27
(1,1145)	1:78:A:LYS:HG2	1:78:A:LYS:HD2	3	0.27
(1,1145)	1:78:A:LYS:HG2	1:78:A:LYS:HD2	8	0.27
(1,1126)	1:77:A:TYR:HB3	1:77:A:TYR:H	4	0.27
(1,1126)	1:77:A:TYR:HB3	1:77:A:TYR:H	5	0.27
(1,762)	1:54:A:ILE:HG12	1:54:A:ILE:H	1	0.27
(1,758)	1:54:A:ILE:HG12	1:54:A:ILE:HA	4	0.27
(1,472)	1:33:A:PRO:HB2	1:33:A:PRO:HG3	6	0.27
(1,371)	1:91:A:LEU:HB2	1:93:A:GLY:H	5	0.27
(1,371)	1:91:A:LEU:HB2	1:93:A:GLY:H	9	0.27
(1,227)	1:20:A:ALA:HB1	1:64:A:LEU:HD11	10	0.27
(1,227)	1:20:A:ALA:HB1	1:64:A:LEU:HD12	10	0.27
(1,227)	1:20:A:ALA:HB1	1:64:A:LEU:HD13	10	0.27
(1,227)	1:20:A:ALA:HB2	1:64:A:LEU:HD11	10	0.27
(1,227)	1:20:A:ALA:HB2	1:64:A:LEU:HD12	10	0.27
(1,227)	1:20:A:ALA:HB2	1:64:A:LEU:HD13	10	0.27
(1,227)	1:20:A:ALA:HB3	1:64:A:LEU:HD11	10	0.27
(1,227)	1:20:A:ALA:HB3	1:64:A:LEU:HD12	10	0.27
(1,227)	1:20:A:ALA:HB3	1:64:A:LEU:HD13	10	0.27
(1,183)	1:18:A:VAL:HG11	1:11:A:THR:H	1	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,183)	1:18:A:VAL:HG12	1:11:A:THR:H	1	0.27
(1,183)	1:18:A:VAL:HG13	1:11:A:THR:H	1	0.27
(1,1848)	1:117:A:GLU:HB3	1:117:A:GLU:H	4	0.26
(1,1816)	1:116:A:ILE:HA	1:116:A:ILE:HG13	1	0.26
(1,1816)	1:116:A:ILE:HA	1:116:A:ILE:HG13	8	0.26
(1,1771)	1:112:A:LEU:HD11	1:127:A:ASP:HB3	9	0.26
(1,1771)	1:112:A:LEU:HD12	1:127:A:ASP:HB3	9	0.26
(1,1771)	1:112:A:LEU:HD13	1:127:A:ASP:HB3	9	0.26
(1,1598)	1:110:A:THR:H	1:111:A:VAL:HB	1	0.26
(1,1583)	1:103:A:PRO:HD2	1:103:A:PRO:HB2	2	0.26
(1,1583)	1:103:A:PRO:HD2	1:103:A:PRO:HB2	6	0.26
(1,1583)	1:103:A:PRO:HD2	1:103:A:PRO:HB2	9	0.26
(1,1583)	1:103:A:PRO:HD2	1:103:A:PRO:HB2	10	0.26
(1,1579)	1:102:A:ASN:HB2	1:102:A:ASN:HA	3	0.26
(1,1519)	1:96:A:ILE:HG13	1:107:A:LYS:HE2	3	0.26
(1,1519)	1:96:A:ILE:HG13	1:107:A:LYS:HE3	3	0.26
(1,1453)	1:92:A:GLU:H	1:93:A:GLY:HA3	6	0.26
(1,1453)	1:92:A:GLU:H	1:93:A:GLY:HA3	7	0.26
(1,1231)	1:82:A:LEU:HD11	1:83:A:LYS:H	1	0.26
(1,1231)	1:82:A:LEU:HD12	1:83:A:LYS:H	1	0.26
(1,1231)	1:82:A:LEU:HD13	1:83:A:LYS:H	1	0.26
(1,1155)	1:78:A:LYS:HA	1:78:A:LYS:HE2	2	0.26
(1,1155)	1:78:A:LYS:HA	1:78:A:LYS:HE3	2	0.26
(1,1145)	1:78:A:LYS:HG2	1:78:A:LYS:HD2	2	0.26
(1,1126)	1:77:A:TYR:HB3	1:77:A:TYR:H	7	0.26
(1,1126)	1:77:A:TYR:HB3	1:77:A:TYR:H	8	0.26
(1,1052)	1:69:A:LYS:HB2	1:70:A:TYR:H	4	0.26
(1,990)	1:66:A:ARG:H	1:66:A:ARG:HB2	7	0.26
(1,981)	1:65:A:GLY:HA3	1:68:A:LEU:H	10	0.26
(1,969)	1:65:A:GLY:HA2	1:26:A:LEU:HD11	5	0.26
(1,969)	1:65:A:GLY:HA2	1:26:A:LEU:HD12	5	0.26
(1,969)	1:65:A:GLY:HA2	1:26:A:LEU:HD13	5	0.26
(1,957)	1:64:A:LEU:HD11	1:65:A:GLY:H	3	0.26
(1,957)	1:64:A:LEU:HD12	1:65:A:GLY:H	3	0.26
(1,957)	1:64:A:LEU:HD13	1:65:A:GLY:H	3	0.26
(1,830)	1:57:A:LEU:HB3	1:58:A:VAL:H	4	0.26
(1,830)	1:57:A:LEU:HB3	1:58:A:VAL:H	8	0.26
(1,553)	1:37:A:THR:HG21	1:82:A:LEU:HD11	8	0.26
(1,553)	1:37:A:THR:HG21	1:82:A:LEU:HD12	8	0.26
(1,553)	1:37:A:THR:HG21	1:82:A:LEU:HD13	8	0.26
(1,553)	1:37:A:THR:HG22	1:82:A:LEU:HD11	8	0.26
(1,553)	1:37:A:THR:HG22	1:82:A:LEU:HD12	8	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,553)	1:37:A:THR:HG22	1:82:A:LEU:HD13	8	0.26
(1,553)	1:37:A:THR:HG23	1:82:A:LEU:HD11	8	0.26
(1,553)	1:37:A:THR:HG23	1:82:A:LEU:HD12	8	0.26
(1,553)	1:37:A:THR:HG23	1:82:A:LEU:HD13	8	0.26
(1,483)	1:35:A:PRO:HD2	1:35:A:PRO:HB2	2	0.26
(1,483)	1:35:A:PRO:HD2	1:35:A:PRO:HB2	5	0.26
(1,483)	1:35:A:PRO:HD2	1:35:A:PRO:HB2	9	0.26
(1,380)	1:26:A:LEU:HD23	1:66:A:ARG:HA	1	0.26
(1,270)	1:22:A:LYS:HG2	1:22:A:LYS:HE3	8	0.26
(1,267)	1:22:A:LYS:HB3	1:22:A:LYS:HD2	8	0.26
(1,267)	1:22:A:LYS:HB3	1:22:A:LYS:HD3	8	0.26
(1,227)	1:20:A:ALA:HB1	1:64:A:LEU:HD11	2	0.26
(1,227)	1:20:A:ALA:HB1	1:64:A:LEU:HD12	2	0.26
(1,227)	1:20:A:ALA:HB1	1:64:A:LEU:HD13	2	0.26
(1,227)	1:20:A:ALA:HB2	1:64:A:LEU:HD11	2	0.26
(1,227)	1:20:A:ALA:HB2	1:64:A:LEU:HD12	2	0.26
(1,227)	1:20:A:ALA:HB2	1:64:A:LEU:HD13	2	0.26
(1,227)	1:20:A:ALA:HB3	1:64:A:LEU:HD11	2	0.26
(1,227)	1:20:A:ALA:HB3	1:64:A:LEU:HD12	2	0.26
(1,227)	1:20:A:ALA:HB3	1:64:A:LEU:HD13	2	0.26
(1,180)	1:18:A:VAL:HG11	1:11:A:THR:HB	6	0.26
(1,180)	1:18:A:VAL:HG12	1:11:A:THR:HB	6	0.26
(1,180)	1:18:A:VAL:HG13	1:11:A:THR:HB	6	0.26
(1,1848)	1:117:A:GLU:HB3	1:117:A:GLU:H	2	0.25
(1,1848)	1:117:A:GLU:HB3	1:117:A:GLU:H	10	0.25
(1,1816)	1:116:A:ILE:HA	1:116:A:ILE:HG13	3	0.25
(1,1816)	1:116:A:ILE:HA	1:116:A:ILE:HG13	5	0.25
(1,1816)	1:116:A:ILE:HA	1:116:A:ILE:HG13	6	0.25
(1,1816)	1:116:A:ILE:HA	1:116:A:ILE:HG13	10	0.25
(1,1583)	1:103:A:PRO:HD2	1:103:A:PRO:HB2	1	0.25
(1,1583)	1:103:A:PRO:HD2	1:103:A:PRO:HB2	5	0.25
(1,1493)	1:96:A:ILE:HD13	1:90:A:SER:H	6	0.25
(1,1453)	1:92:A:GLU:H	1:93:A:GLY:HA3	1	0.25
(1,1361)	1:88:A:VAL:H	1:88:A:VAL:HG11	5	0.25
(1,1361)	1:88:A:VAL:H	1:88:A:VAL:HG12	5	0.25
(1,1361)	1:88:A:VAL:H	1:88:A:VAL:HG13	5	0.25
(1,1361)	1:88:A:VAL:H	1:88:A:VAL:HG11	10	0.25
(1,1361)	1:88:A:VAL:H	1:88:A:VAL:HG12	10	0.25
(1,1361)	1:88:A:VAL:H	1:88:A:VAL:HG13	10	0.25
(1,1275)	1:84:A:ARG:HB3	1:84:A:ARG:HG3	4	0.25
(1,1275)	1:84:A:ARG:HB3	1:84:A:ARG:HG3	10	0.25
(1,1208)	1:81:A:ASP:HA	1:84:A:ARG:HB3	3	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1155)	1:78:A:LYS:HA	1:78:A:LYS:HE2	8	0.25
(1,1155)	1:78:A:LYS:HA	1:78:A:LYS:HE3	8	0.25
(1,1145)	1:78:A:LYS:HG2	1:78:A:LYS:HD2	4	0.25
(1,1126)	1:77:A:TYR:HB3	1:77:A:TYR:H	9	0.25
(1,957)	1:64:A:LEU:HD11	1:65:A:GLY:H	4	0.25
(1,957)	1:64:A:LEU:HD12	1:65:A:GLY:H	4	0.25
(1,957)	1:64:A:LEU:HD13	1:65:A:GLY:H	4	0.25
(1,923)	1:63:A:GLN:HE21	1:63:A:GLN:HB2	10	0.25
(1,923)	1:63:A:GLN:HE21	1:63:A:GLN:HB3	10	0.25
(1,909)	1:62:A:PRO:HB2	1:62:A:PRO:HG3	1	0.25
(1,909)	1:62:A:PRO:HB2	1:62:A:PRO:HG3	2	0.25
(1,909)	1:62:A:PRO:HB2	1:62:A:PRO:HG3	4	0.25
(1,909)	1:62:A:PRO:HB2	1:62:A:PRO:HG3	8	0.25
(1,909)	1:62:A:PRO:HB2	1:62:A:PRO:HG3	9	0.25
(1,758)	1:54:A:ILE:HG12	1:54:A:ILE:HA	6	0.25
(1,709)	1:48:A:LYS:HD2	1:50:A:PRO:HD3	5	0.25
(1,709)	1:48:A:LYS:HD3	1:50:A:PRO:HD3	5	0.25
(1,652)	1:45:A:ALA:HB1	1:48:A:LYS:HG2	2	0.25
(1,652)	1:45:A:ALA:HB2	1:48:A:LYS:HG2	2	0.25
(1,652)	1:45:A:ALA:HB3	1:48:A:LYS:HG2	2	0.25
(1,483)	1:35:A:PRO:HD2	1:35:A:PRO:HB2	7	0.25
(1,257)	1:21:A:VAL:HG21	1:65:A:GLY:HA2	10	0.25
(1,257)	1:21:A:VAL:HG22	1:65:A:GLY:HA2	10	0.25
(1,257)	1:21:A:VAL:HG23	1:65:A:GLY:HA2	10	0.25
(1,1968)	1:124:A:HIS:HB3	1:39:A:PHE:HD1	6	0.24
(1,1968)	1:124:A:HIS:HB3	1:39:A:PHE:HD2	6	0.24
(1,1859)	1:118:A:ALA:HB1	1:119:A:GLU:HG3	3	0.24
(1,1859)	1:118:A:ALA:HB2	1:119:A:GLU:HG3	3	0.24
(1,1859)	1:118:A:ALA:HB3	1:119:A:GLU:HG3	3	0.24
(1,1845)	1:117:A:GLU:HA	1:117:A:GLU:HG3	10	0.24
(1,1816)	1:116:A:ILE:HA	1:116:A:ILE:HG13	7	0.24
(1,1816)	1:116:A:ILE:HA	1:116:A:ILE:HG13	9	0.24
(1,1662)	1:106:A:VAL:HG11	1:107:A:LYS:HG3	10	0.24
(1,1662)	1:106:A:VAL:HG12	1:107:A:LYS:HG3	10	0.24
(1,1662)	1:106:A:VAL:HG13	1:107:A:LYS:HG3	10	0.24
(1,1621)	1:104:A:LEU:HB2	1:105:A:GLU:H	1	0.24
(1,1453)	1:92:A:GLU:H	1:93:A:GLY:HA3	4	0.24
(1,1361)	1:88:A:VAL:H	1:88:A:VAL:HG11	3	0.24
(1,1361)	1:88:A:VAL:H	1:88:A:VAL:HG12	3	0.24
(1,1361)	1:88:A:VAL:H	1:88:A:VAL:HG13	3	0.24
(1,1361)	1:88:A:VAL:H	1:88:A:VAL:HG11	6	0.24
(1,1361)	1:88:A:VAL:H	1:88:A:VAL:HG12	6	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1361)	1:88:A:VAL:H	1:88:A:VAL:HG13	6	0.24
(1,1275)	1:84:A:ARG:HB3	1:84:A:ARG:HG3	3	0.24
(1,1275)	1:84:A:ARG:HB3	1:84:A:ARG:HG3	5	0.24
(1,1275)	1:84:A:ARG:HB3	1:84:A:ARG:HG3	8	0.24
(1,1271)	1:84:A:ARG:HD3	1:84:A:ARG:HG3	7	0.24
(1,1261)	1:84:A:ARG:HB3	1:84:A:ARG:H	5	0.24
(1,1231)	1:82:A:LEU:HD11	1:83:A:LYS:H	3	0.24
(1,1231)	1:82:A:LEU:HD12	1:83:A:LYS:H	3	0.24
(1,1231)	1:82:A:LEU:HD13	1:83:A:LYS:H	3	0.24
(1,1176)	1:79:A:ALA:HA	1:104:A:LEU:HD11	6	0.24
(1,1176)	1:79:A:ALA:HA	1:104:A:LEU:HD12	6	0.24
(1,1176)	1:79:A:ALA:HA	1:104:A:LEU:HD13	6	0.24
(1,1168)	1:78:A:LYS:HG3	1:122:A:ILE:HD11	5	0.24
(1,1168)	1:78:A:LYS:HG3	1:122:A:ILE:HD12	5	0.24
(1,1168)	1:78:A:LYS:HG3	1:122:A:ILE:HD13	5	0.24
(1,1155)	1:78:A:LYS:HA	1:78:A:LYS:HE2	3	0.24
(1,1155)	1:78:A:LYS:HA	1:78:A:LYS:HE3	3	0.24
(1,1145)	1:78:A:LYS:HG2	1:78:A:LYS:HD2	10	0.24
(1,1126)	1:77:A:TYR:HB3	1:77:A:TYR:H	10	0.24
(1,909)	1:62:A:PRO:HB2	1:62:A:PRO:HG3	3	0.24
(1,909)	1:62:A:PRO:HB2	1:62:A:PRO:HG3	5	0.24
(1,909)	1:62:A:PRO:HB2	1:62:A:PRO:HG3	6	0.24
(1,909)	1:62:A:PRO:HB2	1:62:A:PRO:HG3	7	0.24
(1,758)	1:54:A:ILE:HG12	1:54:A:ILE:HA	1	0.24
(1,758)	1:54:A:ILE:HG12	1:54:A:ILE:HA	9	0.24
(1,380)	1:26:A:LEU:HD22	1:66:A:ARG:HA	10	0.24
(1,368)	1:26:A:LEU:HD21	1:66:A:ARG:HB3	8	0.24
(1,368)	1:26:A:LEU:HD22	1:66:A:ARG:HB3	8	0.24
(1,368)	1:26:A:LEU:HD23	1:66:A:ARG:HB3	8	0.24
(1,257)	1:21:A:VAL:HG21	1:65:A:GLY:HA2	3	0.24
(1,257)	1:21:A:VAL:HG22	1:65:A:GLY:HA2	3	0.24
(1,257)	1:21:A:VAL:HG23	1:65:A:GLY:HA2	3	0.24
(1,1999)	1:126:A:ILE:HG21	1:39:A:PHE:HD1	1	0.23
(1,1999)	1:126:A:ILE:HG21	1:39:A:PHE:HD2	1	0.23
(1,1999)	1:126:A:ILE:HG22	1:39:A:PHE:HD1	1	0.23
(1,1999)	1:126:A:ILE:HG22	1:39:A:PHE:HD2	1	0.23
(1,1999)	1:126:A:ILE:HG23	1:39:A:PHE:HD1	1	0.23
(1,1999)	1:126:A:ILE:HG23	1:39:A:PHE:HD2	1	0.23
(1,1864)	1:118:A:ALA:HB3	1:121:A:GLY:HA2	1	0.23
(1,1859)	1:118:A:ALA:HB1	1:119:A:GLU:HG3	8	0.23
(1,1859)	1:118:A:ALA:HB2	1:119:A:GLU:HG3	8	0.23
(1,1859)	1:118:A:ALA:HB3	1:119:A:GLU:HG3	8	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1771)	1:112:A:LEU:HD11	1:127:A:ASP:HB3	5	0.23
(1,1771)	1:112:A:LEU:HD12	1:127:A:ASP:HB3	5	0.23
(1,1771)	1:112:A:LEU:HD13	1:127:A:ASP:HB3	5	0.23
(1,1621)	1:104:A:LEU:HB2	1:105:A:GLU:H	8	0.23
(1,1579)	1:102:A:ASN:HB2	1:102:A:ASN:HA	10	0.23
(1,1408)	1:91:A:LEU:HD11	1:30:A:LEU:HA	7	0.23
(1,1408)	1:91:A:LEU:HD12	1:30:A:LEU:HA	7	0.23
(1,1408)	1:91:A:LEU:HD13	1:30:A:LEU:HA	7	0.23
(1,1275)	1:84:A:ARG:HB3	1:84:A:ARG:HG3	1	0.23
(1,1275)	1:84:A:ARG:HB3	1:84:A:ARG:HG3	6	0.23
(1,1275)	1:84:A:ARG:HB3	1:84:A:ARG:HG3	9	0.23
(1,1261)	1:84:A:ARG:HB3	1:84:A:ARG:H	1	0.23
(1,1261)	1:84:A:ARG:HB3	1:84:A:ARG:H	6	0.23
(1,1261)	1:84:A:ARG:HB3	1:84:A:ARG:H	9	0.23
(1,1208)	1:81:A:ASP:HA	1:84:A:ARG:HB3	1	0.23
(1,1130)	1:77:A:TYR:HB3	1:81:A:ASP:HB3	4	0.23
(1,1126)	1:77:A:TYR:HB3	1:77:A:TYR:H	1	0.23
(1,957)	1:64:A:LEU:HD11	1:65:A:GLY:H	10	0.23
(1,957)	1:64:A:LEU:HD12	1:65:A:GLY:H	10	0.23
(1,957)	1:64:A:LEU:HD13	1:65:A:GLY:H	10	0.23
(1,909)	1:62:A:PRO:HB2	1:62:A:PRO:HG3	10	0.23
(1,886)	1:60:A:ASN:HB2	1:60:A:ASN:H	3	0.23
(1,879)	1:59:A:GLN:HA	1:60:A:ASN:H	9	0.23
(1,825)	1:57:A:LEU:HB3	1:57:A:LEU:H	1	0.23
(1,710)	1:48:A:LYS:HE2	1:128:A:THR:HG21	5	0.23
(1,710)	1:48:A:LYS:HE2	1:128:A:THR:HG22	5	0.23
(1,710)	1:48:A:LYS:HE2	1:128:A:THR:HG23	5	0.23
(1,710)	1:48:A:LYS:HE3	1:128:A:THR:HG21	5	0.23
(1,710)	1:48:A:LYS:HE3	1:128:A:THR:HG22	5	0.23
(1,710)	1:48:A:LYS:HE3	1:128:A:THR:HG23	5	0.23
(1,380)	1:26:A:LEU:HD22	1:66:A:ARG:HA	4	0.23
(1,321)	1:24:A:ALA:HB1	1:62:A:PRO:HB2	5	0.23
(1,321)	1:24:A:ALA:HB2	1:62:A:PRO:HB2	5	0.23
(1,321)	1:24:A:ALA:HB3	1:62:A:PRO:HB2	5	0.23
(1,280)	1:22:A:LYS:HG2	1:22:A:LYS:H	7	0.23
(1,180)	1:18:A:VAL:HG11	1:11:A:THR:HB	7	0.23
(1,180)	1:18:A:VAL:HG12	1:11:A:THR:HB	7	0.23
(1,180)	1:18:A:VAL:HG13	1:11:A:THR:HB	7	0.23
(1,120)	1:10:A:ASN:HB3	1:10:A:ASN:HD22	9	0.23
(1,48)	1:5:A:VAL:HB	1:31:A:GLN:HE21	5	0.23
(1,48)	1:5:A:VAL:HB	1:31:A:GLN:HE21	9	0.23
(1,1859)	1:118:A:ALA:HB1	1:119:A:GLU:HG3	2	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1859)	1:118:A:ALA:HB2	1:119:A:GLU:HG3	2	0.22
(1,1859)	1:118:A:ALA:HB3	1:119:A:GLU:HG3	2	0.22
(1,1845)	1:117:A:GLU:HA	1:117:A:GLU:HG3	2	0.22
(1,1809)	1:115:A:ASP:HB3	1:115:A:ASP:H	5	0.22
(1,1771)	1:112:A:LEU:HD11	1:127:A:ASP:HB3	10	0.22
(1,1771)	1:112:A:LEU:HD12	1:127:A:ASP:HB3	10	0.22
(1,1771)	1:112:A:LEU:HD13	1:127:A:ASP:HB3	10	0.22
(1,1740)	1:111:A:VAL:HG11	1:111:A:VAL:HA	6	0.22
(1,1740)	1:111:A:VAL:HG12	1:111:A:VAL:HA	6	0.22
(1,1740)	1:111:A:VAL:HG13	1:111:A:VAL:HA	6	0.22
(1,1701)	1:108:A:ASN:HB3	1:108:A:ASN:HD22	10	0.22
(1,1621)	1:104:A:LEU:HB2	1:105:A:GLU:H	4	0.22
(1,1621)	1:104:A:LEU:HB2	1:105:A:GLU:H	7	0.22
(1,1598)	1:110:A:THR:H	1:111:A:VAL:HB	6	0.22
(1,1579)	1:102:A:ASN:HB2	1:102:A:ASN:HA	1	0.22
(1,1403)	1:90:A:SER:HB2	1:92:A:GLU:H	9	0.22
(1,1261)	1:84:A:ARG:HB3	1:84:A:ARG:H	3	0.22
(1,1261)	1:84:A:ARG:HB3	1:84:A:ARG:H	8	0.22
(1,1208)	1:81:A:ASP:HA	1:84:A:ARG:HB3	6	0.22
(1,1177)	1:79:A:ALA:HB1	1:104:A:LEU:HD21	2	0.22
(1,1177)	1:79:A:ALA:HB1	1:104:A:LEU:HD22	2	0.22
(1,1177)	1:79:A:ALA:HB1	1:104:A:LEU:HD23	2	0.22
(1,1177)	1:79:A:ALA:HB2	1:104:A:LEU:HD21	2	0.22
(1,1177)	1:79:A:ALA:HB2	1:104:A:LEU:HD22	2	0.22
(1,1177)	1:79:A:ALA:HB2	1:104:A:LEU:HD23	2	0.22
(1,1177)	1:79:A:ALA:HB3	1:104:A:LEU:HD21	2	0.22
(1,1177)	1:79:A:ALA:HB3	1:104:A:LEU:HD22	2	0.22
(1,1177)	1:79:A:ALA:HB3	1:104:A:LEU:HD23	2	0.22
(1,1148)	1:78:A:LYS:H	1:78:A:LYS:HD3	5	0.22
(1,1126)	1:77:A:TYR:HB3	1:77:A:TYR:H	2	0.22
(1,1126)	1:77:A:TYR:HB3	1:77:A:TYR:H	3	0.22
(1,1052)	1:69:A:LYS:HB2	1:70:A:TYR:H	5	0.22
(1,957)	1:64:A:LEU:HD11	1:65:A:GLY:H	2	0.22
(1,957)	1:64:A:LEU:HD12	1:65:A:GLY:H	2	0.22
(1,957)	1:64:A:LEU:HD13	1:65:A:GLY:H	2	0.22
(1,830)	1:57:A:LEU:HB3	1:58:A:VAL:H	2	0.22
(1,652)	1:45:A:ALA:HB1	1:48:A:LYS:HG2	6	0.22
(1,652)	1:45:A:ALA:HB2	1:48:A:LYS:HG2	6	0.22
(1,652)	1:45:A:ALA:HB3	1:48:A:LYS:HG2	6	0.22
(1,582)	1:40:A:ALA:H	1:124:A:HIS:HB3	1	0.22
(1,180)	1:18:A:VAL:HG11	1:11:A:THR:HB	3	0.22
(1,180)	1:18:A:VAL:HG12	1:11:A:THR:HB	3	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,180)	1:18:A:VAL:HG13	1:11:A:THR:HB	3	0.22
(1,146)	1:12:A:PRO:HB3	1:12:A:PRO:HG2	7	0.22
(1,64)	1:6:A:ASP:HA	1:9:A:VAL:HB	9	0.22
(1,48)	1:5:A:VAL:HB	1:31:A:GLN:HE21	1	0.22
(1,48)	1:5:A:VAL:HB	1:31:A:GLN:HE21	2	0.22
(1,48)	1:5:A:VAL:HB	1:31:A:GLN:HE21	4	0.22
(1,48)	1:5:A:VAL:HB	1:31:A:GLN:HE21	10	0.22
(1,1970)	1:124:A:HIS:HB2	1:113:A:ALA:H	4	0.21
(1,1859)	1:118:A:ALA:HB1	1:119:A:GLU:HG3	1	0.21
(1,1859)	1:118:A:ALA:HB2	1:119:A:GLU:HG3	1	0.21
(1,1859)	1:118:A:ALA:HB3	1:119:A:GLU:HG3	1	0.21
(1,1859)	1:118:A:ALA:HB1	1:119:A:GLU:HG3	4	0.21
(1,1859)	1:118:A:ALA:HB2	1:119:A:GLU:HG3	4	0.21
(1,1859)	1:118:A:ALA:HB3	1:119:A:GLU:HG3	4	0.21
(1,1809)	1:115:A:ASP:HB3	1:115:A:ASP:H	3	0.21
(1,1621)	1:104:A:LEU:HB2	1:105:A:GLU:H	3	0.21
(1,1621)	1:104:A:LEU:HB2	1:105:A:GLU:H	10	0.21
(1,1415)	1:91:A:LEU:HD21	1:74:A:ALA:HB1	2	0.21
(1,1415)	1:91:A:LEU:HD21	1:74:A:ALA:HB2	2	0.21
(1,1415)	1:91:A:LEU:HD21	1:74:A:ALA:HB3	2	0.21
(1,1415)	1:91:A:LEU:HD22	1:74:A:ALA:HB1	2	0.21
(1,1415)	1:91:A:LEU:HD22	1:74:A:ALA:HB2	2	0.21
(1,1415)	1:91:A:LEU:HD22	1:74:A:ALA:HB3	2	0.21
(1,1415)	1:91:A:LEU:HD23	1:74:A:ALA:HB1	2	0.21
(1,1415)	1:91:A:LEU:HD23	1:74:A:ALA:HB2	2	0.21
(1,1415)	1:91:A:LEU:HD23	1:74:A:ALA:HB3	2	0.21
(1,1351)	1:87:A:ILE:H	1:97:A:PRO:HA	3	0.21
(1,1351)	1:87:A:ILE:H	1:97:A:PRO:HA	4	0.21
(1,1351)	1:87:A:ILE:H	1:97:A:PRO:HA	5	0.21
(1,1351)	1:87:A:ILE:H	1:97:A:PRO:HA	7	0.21
(1,1276)	1:84:A:ARG:HB3	1:84:A:ARG:HG2	7	0.21
(1,1248)	1:83:A:LYS:HG2	1:83:A:LYS:H	2	0.21
(1,1248)	1:83:A:LYS:HG3	1:83:A:LYS:H	2	0.21
(1,1238)	1:82:A:LEU:HB3	1:104:A:LEU:HD21	9	0.21
(1,1238)	1:82:A:LEU:HB3	1:104:A:LEU:HD22	9	0.21
(1,1238)	1:82:A:LEU:HB3	1:104:A:LEU:HD23	9	0.21
(1,1234)	1:86:A:GLY:H	1:98:A:ILE:HG12	2	0.21
(1,1231)	1:82:A:LEU:HD11	1:83:A:LYS:H	5	0.21
(1,1231)	1:82:A:LEU:HD12	1:83:A:LYS:H	5	0.21
(1,1231)	1:82:A:LEU:HD13	1:83:A:LYS:H	5	0.21
(1,1208)	1:81:A:ASP:HA	1:84:A:ARG:HB3	10	0.21
(1,762)	1:54:A:ILE:HG12	1:54:A:ILE:H	7	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,730)	1:40:A:ALA:H	1:126:A:ILE:HG21	1	0.21
(1,553)	1:37:A:THR:HG21	1:82:A:LEU:HD11	1	0.21
(1,553)	1:37:A:THR:HG21	1:82:A:LEU:HD12	1	0.21
(1,553)	1:37:A:THR:HG21	1:82:A:LEU:HD13	1	0.21
(1,553)	1:37:A:THR:HG22	1:82:A:LEU:HD11	1	0.21
(1,553)	1:37:A:THR:HG22	1:82:A:LEU:HD12	1	0.21
(1,553)	1:37:A:THR:HG22	1:82:A:LEU:HD13	1	0.21
(1,553)	1:37:A:THR:HG23	1:82:A:LEU:HD11	1	0.21
(1,553)	1:37:A:THR:HG23	1:82:A:LEU:HD12	1	0.21
(1,553)	1:37:A:THR:HG23	1:82:A:LEU:HD13	1	0.21
(1,321)	1:24:A:ALA:HB1	1:62:A:PRO:HB2	6	0.21
(1,321)	1:24:A:ALA:HB2	1:62:A:PRO:HB2	6	0.21
(1,321)	1:24:A:ALA:HB3	1:62:A:PRO:HB2	6	0.21
(1,321)	1:24:A:ALA:HB1	1:62:A:PRO:HB2	10	0.21
(1,321)	1:24:A:ALA:HB2	1:62:A:PRO:HB2	10	0.21
(1,321)	1:24:A:ALA:HB3	1:62:A:PRO:HB2	10	0.21
(1,280)	1:22:A:LYS:HG2	1:22:A:LYS:H	9	0.21
(1,257)	1:21:A:VAL:HG21	1:65:A:GLY:HA2	7	0.21
(1,257)	1:21:A:VAL:HG22	1:65:A:GLY:HA2	7	0.21
(1,257)	1:21:A:VAL:HG23	1:65:A:GLY:HA2	7	0.21
(1,120)	1:10:A:ASN:HB3	1:10:A:ASN:HD22	6	0.21
(1,107)	1:8:A:ALA:HA	1:18:A:VAL:HG21	8	0.21
(1,107)	1:8:A:ALA:HA	1:18:A:VAL:HG22	8	0.21
(1,107)	1:8:A:ALA:HA	1:18:A:VAL:HG23	8	0.21
(1,64)	1:6:A:ASP:HA	1:9:A:VAL:HB	3	0.21
(1,48)	1:5:A:VAL:HB	1:31:A:GLN:HE21	3	0.21
(1,48)	1:5:A:VAL:HB	1:31:A:GLN:HE21	6	0.21
(1,1970)	1:124:A:HIS:HB2	1:113:A:ALA:H	6	0.2
(1,1859)	1:118:A:ALA:HB1	1:119:A:GLU:HG3	6	0.2
(1,1859)	1:118:A:ALA:HB2	1:119:A:GLU:HG3	6	0.2
(1,1859)	1:118:A:ALA:HB3	1:119:A:GLU:HG3	6	0.2
(1,1859)	1:118:A:ALA:HB1	1:119:A:GLU:HG3	7	0.2
(1,1859)	1:118:A:ALA:HB2	1:119:A:GLU:HG3	7	0.2
(1,1859)	1:118:A:ALA:HB3	1:119:A:GLU:HG3	7	0.2
(1,1859)	1:118:A:ALA:HB1	1:119:A:GLU:HG3	10	0.2
(1,1859)	1:118:A:ALA:HB2	1:119:A:GLU:HG3	10	0.2
(1,1859)	1:118:A:ALA:HB3	1:119:A:GLU:HG3	10	0.2
(1,1845)	1:117:A:GLU:HA	1:117:A:GLU:HG3	4	0.2
(1,1740)	1:111:A:VAL:HG11	1:111:A:VAL:HA	1	0.2
(1,1740)	1:111:A:VAL:HG12	1:111:A:VAL:HA	1	0.2
(1,1740)	1:111:A:VAL:HG13	1:111:A:VAL:HA	1	0.2
(1,1621)	1:104:A:LEU:HB2	1:105:A:GLU:H	2	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1621)	1:104:A:LEU:HB2	1:105:A:GLU:H	6	0.2
(1,1493)	1:96:A:ILE:HD12	1:90:A:SER:H	1	0.2
(1,1403)	1:90:A:SER:HB2	1:92:A:GLU:H	1	0.2
(1,1403)	1:90:A:SER:HB2	1:92:A:GLU:H	6	0.2
(1,1351)	1:87:A:ILE:H	1:97:A:PRO:HA	1	0.2
(1,1351)	1:87:A:ILE:H	1:97:A:PRO:HA	2	0.2
(1,1351)	1:87:A:ILE:H	1:97:A:PRO:HA	6	0.2
(1,1284)	1:85:A:MET:HA	1:85:A:MET:HG3	9	0.2
(1,1261)	1:84:A:ARG:HB3	1:84:A:ARG:H	4	0.2
(1,1261)	1:84:A:ARG:HB3	1:84:A:ARG:H	10	0.2
(1,1248)	1:83:A:LYS:HG2	1:83:A:LYS:H	7	0.2
(1,1248)	1:83:A:LYS:HG3	1:83:A:LYS:H	7	0.2
(1,1234)	1:86:A:GLY:H	1:98:A:ILE:HG12	6	0.2
(1,1231)	1:82:A:LEU:HD11	1:83:A:LYS:H	6	0.2
(1,1231)	1:82:A:LEU:HD12	1:83:A:LYS:H	6	0.2
(1,1231)	1:82:A:LEU:HD13	1:83:A:LYS:H	6	0.2
(1,1219)	1:82:A:LEU:HD11	1:82:A:LEU:HB2	7	0.2
(1,1219)	1:82:A:LEU:HD12	1:82:A:LEU:HB2	7	0.2
(1,1219)	1:82:A:LEU:HD13	1:82:A:LEU:HB2	7	0.2
(1,1219)	1:82:A:LEU:HD11	1:82:A:LEU:HB2	9	0.2
(1,1219)	1:82:A:LEU:HD12	1:82:A:LEU:HB2	9	0.2
(1,1219)	1:82:A:LEU:HD13	1:82:A:LEU:HB2	9	0.2
(1,1214)	1:78:A:LYS:HG2	1:79:A:ALA:H	1	0.2
(1,1205)	1:81:A:ASP:H	1:82:A:LEU:HD11	9	0.2
(1,1205)	1:81:A:ASP:H	1:82:A:LEU:HD12	9	0.2
(1,1205)	1:81:A:ASP:H	1:82:A:LEU:HD13	9	0.2
(1,1177)	1:79:A:ALA:HB1	1:104:A:LEU:HD21	6	0.2
(1,1177)	1:79:A:ALA:HB1	1:104:A:LEU:HD22	6	0.2
(1,1177)	1:79:A:ALA:HB1	1:104:A:LEU:HD23	6	0.2
(1,1177)	1:79:A:ALA:HB2	1:104:A:LEU:HD21	6	0.2
(1,1177)	1:79:A:ALA:HB2	1:104:A:LEU:HD22	6	0.2
(1,1177)	1:79:A:ALA:HB2	1:104:A:LEU:HD23	6	0.2
(1,1177)	1:79:A:ALA:HB3	1:104:A:LEU:HD21	6	0.2
(1,1177)	1:79:A:ALA:HB3	1:104:A:LEU:HD22	6	0.2
(1,1177)	1:79:A:ALA:HB3	1:104:A:LEU:HD23	6	0.2
(1,1148)	1:78:A:LYS:H	1:78:A:LYS:HD3	2	0.2
(1,1148)	1:78:A:LYS:H	1:78:A:LYS:HD3	8	0.2
(1,1145)	1:78:A:LYS:HG2	1:78:A:LYS:HD2	6	0.2
(1,998)	1:67:A:ILE:HG23	1:68:A:LEU:HA	9	0.2
(1,990)	1:66:A:ARG:H	1:66:A:ARG:HB2	8	0.2
(1,929)	1:63:A:GLN:HG2	1:63:A:GLN:HE22	4	0.2
(1,929)	1:63:A:GLN:HG3	1:63:A:GLN:HE22	4	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,879)	1:59:A:GLN:HA	1:60:A:ASN:H	3	0.2
(1,830)	1:57:A:LEU:HB3	1:58:A:VAL:H	7	0.2
(1,582)	1:40:A:ALA:H	1:124:A:HIS:HB3	4	0.2
(1,290)	1:22:A:LYS:HG3	1:27:A:VAL:HG21	2	0.2
(1,290)	1:22:A:LYS:HG3	1:27:A:VAL:HG22	2	0.2
(1,290)	1:22:A:LYS:HG3	1:27:A:VAL:HG23	2	0.2
(1,280)	1:22:A:LYS:HG2	1:22:A:LYS:H	6	0.2
(1,183)	1:18:A:VAL:HG11	1:11:A:THR:H	3	0.2
(1,183)	1:18:A:VAL:HG12	1:11:A:THR:H	3	0.2
(1,183)	1:18:A:VAL:HG13	1:11:A:THR:H	3	0.2
(1,48)	1:5:A:VAL:HB	1:31:A:GLN:HE21	8	0.2
(1,1809)	1:115:A:ASP:HB3	1:115:A:ASP:H	7	0.19
(1,1701)	1:108:A:ASN:HB3	1:108:A:ASN:HD22	2	0.19
(1,1701)	1:108:A:ASN:HB3	1:108:A:ASN:HD22	3	0.19
(1,1621)	1:104:A:LEU:HB2	1:105:A:GLU:H	9	0.19
(1,1598)	1:110:A:THR:H	1:111:A:VAL:HB	4	0.19
(1,1351)	1:87:A:ILE:H	1:97:A:PRO:HA	8	0.19
(1,1351)	1:87:A:ILE:H	1:97:A:PRO:HA	9	0.19
(1,1351)	1:87:A:ILE:H	1:97:A:PRO:HA	10	0.19
(1,1296)	1:85:A:MET:H	1:85:A:MET:HG2	2	0.19
(1,1284)	1:85:A:MET:HA	1:85:A:MET:HG3	2	0.19
(1,1284)	1:85:A:MET:HA	1:85:A:MET:HG3	6	0.19
(1,1284)	1:85:A:MET:HA	1:85:A:MET:HG3	7	0.19
(1,1284)	1:85:A:MET:HA	1:85:A:MET:HG3	10	0.19
(1,1275)	1:84:A:ARG:HB3	1:84:A:ARG:HG3	2	0.19
(1,1262)	1:84:A:ARG:HG3	1:84:A:ARG:HA	7	0.19
(1,1248)	1:83:A:LYS:HG2	1:83:A:LYS:H	10	0.19
(1,1248)	1:83:A:LYS:HG3	1:83:A:LYS:H	10	0.19
(1,1231)	1:82:A:LEU:HD11	1:83:A:LYS:H	8	0.19
(1,1231)	1:82:A:LEU:HD12	1:83:A:LYS:H	8	0.19
(1,1231)	1:82:A:LEU:HD13	1:83:A:LYS:H	8	0.19
(1,1219)	1:82:A:LEU:HD11	1:82:A:LEU:HB2	2	0.19
(1,1219)	1:82:A:LEU:HD12	1:82:A:LEU:HB2	2	0.19
(1,1219)	1:82:A:LEU:HD13	1:82:A:LEU:HB2	2	0.19
(1,1163)	1:78:A:LYS:H	1:80:A:THR:H	2	0.19
(1,1145)	1:78:A:LYS:HG2	1:78:A:LYS:HD2	9	0.19
(1,967)	1:65:A:GLY:HA2	1:26:A:LEU:HD21	3	0.19
(1,967)	1:65:A:GLY:HA2	1:26:A:LEU:HD22	3	0.19
(1,967)	1:65:A:GLY:HA2	1:26:A:LEU:HD23	3	0.19
(1,967)	1:65:A:GLY:HA2	1:26:A:LEU:HD21	9	0.19
(1,967)	1:65:A:GLY:HA2	1:26:A:LEU:HD22	9	0.19
(1,967)	1:65:A:GLY:HA2	1:26:A:LEU:HD23	9	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,929)	1:63:A:GLN:HG2	1:63:A:GLN:HE22	8	0.19
(1,929)	1:63:A:GLN:HG3	1:63:A:GLN:HE22	8	0.19
(1,882)	1:60:A:ASN:HA	1:59:A:GLN:H	9	0.19
(1,762)	1:54:A:ILE:HG12	1:54:A:ILE:H	2	0.19
(1,527)	1:36:A:PHE:HB2	1:120:A:ASN:HD22	10	0.19
(1,504)	1:35:A:PRO:HG3	1:76:A:ALA:HB1	8	0.19
(1,504)	1:35:A:PRO:HG3	1:76:A:ALA:HB2	8	0.19
(1,504)	1:35:A:PRO:HG3	1:76:A:ALA:HB3	8	0.19
(1,290)	1:22:A:LYS:HG3	1:27:A:VAL:HG21	9	0.19
(1,290)	1:22:A:LYS:HG3	1:27:A:VAL:HG22	9	0.19
(1,290)	1:22:A:LYS:HG3	1:27:A:VAL:HG23	9	0.19
(1,272)	1:22:A:LYS:HB3	1:22:A:LYS:HE2	7	0.19
(1,257)	1:21:A:VAL:HG21	1:65:A:GLY:HA2	8	0.19
(1,257)	1:21:A:VAL:HG22	1:65:A:GLY:HA2	8	0.19
(1,257)	1:21:A:VAL:HG23	1:65:A:GLY:HA2	8	0.19
(1,230)	1:20:A:ALA:HB1	1:68:A:LEU:HD11	4	0.19
(1,230)	1:20:A:ALA:HB1	1:68:A:LEU:HD12	4	0.19
(1,230)	1:20:A:ALA:HB1	1:68:A:LEU:HD13	4	0.19
(1,230)	1:20:A:ALA:HB2	1:68:A:LEU:HD11	4	0.19
(1,230)	1:20:A:ALA:HB2	1:68:A:LEU:HD12	4	0.19
(1,230)	1:20:A:ALA:HB2	1:68:A:LEU:HD13	4	0.19
(1,230)	1:20:A:ALA:HB3	1:68:A:LEU:HD11	4	0.19
(1,230)	1:20:A:ALA:HB3	1:68:A:LEU:HD12	4	0.19
(1,230)	1:20:A:ALA:HB3	1:68:A:LEU:HD13	4	0.19
(1,230)	1:20:A:ALA:HB1	1:68:A:LEU:HD11	6	0.19
(1,230)	1:20:A:ALA:HB1	1:68:A:LEU:HD12	6	0.19
(1,230)	1:20:A:ALA:HB1	1:68:A:LEU:HD13	6	0.19
(1,230)	1:20:A:ALA:HB2	1:68:A:LEU:HD11	6	0.19
(1,230)	1:20:A:ALA:HB2	1:68:A:LEU:HD12	6	0.19
(1,230)	1:20:A:ALA:HB2	1:68:A:LEU:HD13	6	0.19
(1,230)	1:20:A:ALA:HB3	1:68:A:LEU:HD11	6	0.19
(1,230)	1:20:A:ALA:HB3	1:68:A:LEU:HD12	6	0.19
(1,230)	1:20:A:ALA:HB3	1:68:A:LEU:HD13	6	0.19
(1,115)	1:10:A:ASN:HB2	1:10:A:ASN:HA	9	0.19
(1,32)	1:5:A:VAL:HG11	1:6:A:ASP:HA	5	0.19
(1,32)	1:5:A:VAL:HG12	1:6:A:ASP:HA	5	0.19
(1,32)	1:5:A:VAL:HG13	1:6:A:ASP:HA	5	0.19
(1,1981)	1:124:A:HIS:HB2	1:125:A:VAL:H	6	0.18
(1,1571)	1:101:A:ASP:HB3	1:101:A:ASP:HA	3	0.18
(1,1454)	1:92:A:GLU:HB3	1:93:A:GLY:H	10	0.18
(1,1296)	1:85:A:MET:H	1:85:A:MET:HG2	1	0.18
(1,1284)	1:85:A:MET:HA	1:85:A:MET:HG3	3	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1272)	1:84:A:ARG:HB3	1:84:A:ARG:HD3	9	0.18
(1,1261)	1:84:A:ARG:HB3	1:84:A:ARG:H	2	0.18
(1,1219)	1:82:A:LEU:HD11	1:82:A:LEU:HB2	1	0.18
(1,1219)	1:82:A:LEU:HD12	1:82:A:LEU:HB2	1	0.18
(1,1219)	1:82:A:LEU:HD13	1:82:A:LEU:HB2	1	0.18
(1,1191)	1:81:A:ASP:H	1:78:A:LYS:HB3	9	0.18
(1,1148)	1:78:A:LYS:H	1:78:A:LYS:HD3	3	0.18
(1,1145)	1:78:A:LYS:HG2	1:78:A:LYS:HD2	1	0.18
(1,967)	1:65:A:GLY:HA2	1:26:A:LEU:HD21	6	0.18
(1,967)	1:65:A:GLY:HA2	1:26:A:LEU:HD22	6	0.18
(1,967)	1:65:A:GLY:HA2	1:26:A:LEU:HD23	6	0.18
(1,967)	1:65:A:GLY:HA2	1:26:A:LEU:HD21	7	0.18
(1,967)	1:65:A:GLY:HA2	1:26:A:LEU:HD22	7	0.18
(1,967)	1:65:A:GLY:HA2	1:26:A:LEU:HD23	7	0.18
(1,957)	1:64:A:LEU:HD11	1:65:A:GLY:H	9	0.18
(1,957)	1:64:A:LEU:HD12	1:65:A:GLY:H	9	0.18
(1,957)	1:64:A:LEU:HD13	1:65:A:GLY:H	9	0.18
(1,887)	1:60:A:ASN:HB3	1:60:A:ASN:H	9	0.18
(1,834)	1:57:A:LEU:HD11	1:108:A:ASN:HD22	9	0.18
(1,834)	1:57:A:LEU:HD12	1:108:A:ASN:HD22	9	0.18
(1,834)	1:57:A:LEU:HD13	1:108:A:ASN:HD22	9	0.18
(1,834)	1:57:A:LEU:HD21	1:108:A:ASN:HD22	9	0.18
(1,834)	1:57:A:LEU:HD22	1:108:A:ASN:HD22	9	0.18
(1,834)	1:57:A:LEU:HD23	1:108:A:ASN:HD22	9	0.18
(1,794)	1:55:A:THR:HG21	1:59:A:GLN:HE22	1	0.18
(1,794)	1:55:A:THR:HG22	1:59:A:GLN:HE22	1	0.18
(1,794)	1:55:A:THR:HG23	1:59:A:GLN:HE22	1	0.18
(1,776)	1:54:A:ILE:HG13	1:67:A:ILE:HG21	2	0.18
(1,776)	1:54:A:ILE:HG13	1:67:A:ILE:HG22	2	0.18
(1,776)	1:54:A:ILE:HG13	1:67:A:ILE:HG23	2	0.18
(1,730)	1:40:A:ALA:H	1:126:A:ILE:HG21	4	0.18
(1,730)	1:40:A:ALA:H	1:126:A:ILE:HG21	6	0.18
(1,547)	1:37:A:THR:H	1:73:A:VAL:HG21	7	0.18
(1,547)	1:37:A:THR:H	1:73:A:VAL:HG22	7	0.18
(1,547)	1:37:A:THR:H	1:73:A:VAL:HG23	7	0.18
(1,280)	1:22:A:LYS:HG2	1:22:A:LYS:H	3	0.18
(1,179)	1:18:A:VAL:HG21	1:8:A:ALA:HB1	9	0.18
(1,179)	1:18:A:VAL:HG21	1:8:A:ALA:HB2	9	0.18
(1,179)	1:18:A:VAL:HG21	1:8:A:ALA:HB3	9	0.18
(1,179)	1:18:A:VAL:HG22	1:8:A:ALA:HB1	9	0.18
(1,179)	1:18:A:VAL:HG22	1:8:A:ALA:HB2	9	0.18
(1,179)	1:18:A:VAL:HG22	1:8:A:ALA:HB3	9	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,179)	1:18:A:VAL:HG23	1:8:A:ALA:HB1	9	0.18
(1,179)	1:18:A:VAL:HG23	1:8:A:ALA:HB2	9	0.18
(1,179)	1:18:A:VAL:HG23	1:8:A:ALA:HB3	9	0.18
(1,135)	1:11:A:THR:HG21	1:12:A:PRO:HD3	7	0.18
(1,135)	1:11:A:THR:HG22	1:12:A:PRO:HD3	7	0.18
(1,135)	1:11:A:THR:HG23	1:12:A:PRO:HD3	7	0.18
(1,48)	1:5:A:VAL:HB	1:31:A:GLN:HE21	7	0.18
(1,1970)	1:124:A:HIS:HB2	1:113:A:ALA:H	1	0.17
(1,1915)	1:122:A:ILE:HD11	1:117:A:GLU:HG2	2	0.17
(1,1915)	1:122:A:ILE:HD12	1:117:A:GLU:HG2	2	0.17
(1,1915)	1:122:A:ILE:HD13	1:117:A:GLU:HG2	2	0.17
(1,1859)	1:118:A:ALA:HB1	1:119:A:GLU:HG3	9	0.17
(1,1859)	1:118:A:ALA:HB2	1:119:A:GLU:HG3	9	0.17
(1,1859)	1:118:A:ALA:HB3	1:119:A:GLU:HG3	9	0.17
(1,1737)	1:20:A:ALA:HB1	1:64:A:LEU:HD11	9	0.17
(1,1719)	1:110:A:THR:HG21	1:103:A:PRO:HG3	9	0.17
(1,1719)	1:110:A:THR:HG22	1:103:A:PRO:HG3	9	0.17
(1,1719)	1:110:A:THR:HG23	1:103:A:PRO:HG3	9	0.17
(1,1598)	1:110:A:THR:H	1:111:A:VAL:HB	7	0.17
(1,1571)	1:101:A:ASP:HB3	1:101:A:ASP:HA	1	0.17
(1,1571)	1:101:A:ASP:HB3	1:101:A:ASP:HA	2	0.17
(1,1571)	1:101:A:ASP:HB3	1:101:A:ASP:HA	4	0.17
(1,1571)	1:101:A:ASP:HB3	1:101:A:ASP:HA	6	0.17
(1,1571)	1:101:A:ASP:HB3	1:101:A:ASP:HA	7	0.17
(1,1571)	1:101:A:ASP:HB3	1:101:A:ASP:HA	9	0.17
(1,1518)	1:96:A:ILE:HG13	1:107:A:LYS:HD2	3	0.17
(1,1518)	1:96:A:ILE:HG13	1:107:A:LYS:HD3	3	0.17
(1,1403)	1:90:A:SER:HB2	1:92:A:GLU:H	7	0.17
(1,1296)	1:85:A:MET:H	1:85:A:MET:HG2	7	0.17
(1,1284)	1:85:A:MET:HA	1:85:A:MET:HG3	5	0.17
(1,1284)	1:85:A:MET:HA	1:85:A:MET:HG3	8	0.17
(1,1248)	1:83:A:LYS:HG2	1:83:A:LYS:H	9	0.17
(1,1248)	1:83:A:LYS:HG3	1:83:A:LYS:H	9	0.17
(1,1205)	1:81:A:ASP:H	1:82:A:LEU:HD11	7	0.17
(1,1205)	1:81:A:ASP:H	1:82:A:LEU:HD12	7	0.17
(1,1205)	1:81:A:ASP:H	1:82:A:LEU:HD13	7	0.17
(1,1177)	1:79:A:ALA:HB1	1:104:A:LEU:HD21	9	0.17
(1,1177)	1:79:A:ALA:HB1	1:104:A:LEU:HD22	9	0.17
(1,1177)	1:79:A:ALA:HB1	1:104:A:LEU:HD23	9	0.17
(1,1177)	1:79:A:ALA:HB2	1:104:A:LEU:HD21	9	0.17
(1,1177)	1:79:A:ALA:HB2	1:104:A:LEU:HD22	9	0.17
(1,1177)	1:79:A:ALA:HB2	1:104:A:LEU:HD23	9	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1177)	1:79:A:ALA:HB3	1:104:A:LEU:HD21	9	0.17
(1,1177)	1:79:A:ALA:HB3	1:104:A:LEU:HD22	9	0.17
(1,1177)	1:79:A:ALA:HB3	1:104:A:LEU:HD23	9	0.17
(1,1177)	1:79:A:ALA:HB1	1:104:A:LEU:HD21	10	0.17
(1,1177)	1:79:A:ALA:HB1	1:104:A:LEU:HD22	10	0.17
(1,1177)	1:79:A:ALA:HB1	1:104:A:LEU:HD23	10	0.17
(1,1177)	1:79:A:ALA:HB2	1:104:A:LEU:HD21	10	0.17
(1,1177)	1:79:A:ALA:HB2	1:104:A:LEU:HD22	10	0.17
(1,1177)	1:79:A:ALA:HB2	1:104:A:LEU:HD23	10	0.17
(1,1177)	1:79:A:ALA:HB3	1:104:A:LEU:HD21	10	0.17
(1,1177)	1:79:A:ALA:HB3	1:104:A:LEU:HD22	10	0.17
(1,1177)	1:79:A:ALA:HB3	1:104:A:LEU:HD23	10	0.17
(1,1163)	1:78:A:LYS:H	1:80:A:THR:H	3	0.17
(1,1155)	1:78:A:LYS:HA	1:78:A:LYS:HE2	4	0.17
(1,1155)	1:78:A:LYS:HA	1:78:A:LYS:HE3	4	0.17
(1,1145)	1:78:A:LYS:HG2	1:78:A:LYS:HD2	7	0.17
(1,998)	1:67:A:ILE:HG23	1:68:A:LEU:HA	6	0.17
(1,992)	1:66:A:ARG:HG3	1:67:A:ILE:H	10	0.17
(1,967)	1:65:A:GLY:HA2	1:26:A:LEU:HD21	5	0.17
(1,967)	1:65:A:GLY:HA2	1:26:A:LEU:HD22	5	0.17
(1,967)	1:65:A:GLY:HA2	1:26:A:LEU:HD23	5	0.17
(1,927)	1:63:A:GLN:HE22	1:57:A:LEU:HB3	2	0.17
(1,830)	1:57:A:LEU:HB3	1:58:A:VAL:H	10	0.17
(1,794)	1:55:A:THR:HG21	1:59:A:GLN:HE22	5	0.17
(1,794)	1:55:A:THR:HG22	1:59:A:GLN:HE22	5	0.17
(1,794)	1:55:A:THR:HG23	1:59:A:GLN:HE22	5	0.17
(1,794)	1:55:A:THR:HG21	1:59:A:GLN:HE22	7	0.17
(1,794)	1:55:A:THR:HG22	1:59:A:GLN:HE22	7	0.17
(1,794)	1:55:A:THR:HG23	1:59:A:GLN:HE22	7	0.17
(1,762)	1:54:A:ILE:HG12	1:54:A:ILE:H	3	0.17
(1,623)	1:44:A:ASP:H	1:43:A:ASP:HB2	7	0.17
(1,280)	1:22:A:LYS:HG2	1:22:A:LYS:H	1	0.17
(1,280)	1:22:A:LYS:HG2	1:22:A:LYS:H	4	0.17
(1,2084)	1:129:A:VAL:HG11	1:129:A:VAL:H	1	0.16
(1,2084)	1:129:A:VAL:HG12	1:129:A:VAL:H	1	0.16
(1,2084)	1:129:A:VAL:HG13	1:129:A:VAL:H	1	0.16
(1,2084)	1:129:A:VAL:HG11	1:129:A:VAL:H	2	0.16
(1,2084)	1:129:A:VAL:HG12	1:129:A:VAL:H	2	0.16
(1,2084)	1:129:A:VAL:HG13	1:129:A:VAL:H	2	0.16
(1,2084)	1:129:A:VAL:HG11	1:129:A:VAL:H	8	0.16
(1,2084)	1:129:A:VAL:HG12	1:129:A:VAL:H	8	0.16
(1,2084)	1:129:A:VAL:HG13	1:129:A:VAL:H	8	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2084)	1:129:A:VAL:HG11	1:129:A:VAL:H	10	0.16
(1,2084)	1:129:A:VAL:HG12	1:129:A:VAL:H	10	0.16
(1,2084)	1:129:A:VAL:HG13	1:129:A:VAL:H	10	0.16
(1,1942)	1:122:A:ILE:HD11	1:123:A:ILE:H	2	0.16
(1,1942)	1:122:A:ILE:HD12	1:123:A:ILE:H	2	0.16
(1,1942)	1:122:A:ILE:HD13	1:123:A:ILE:H	2	0.16
(1,1942)	1:122:A:ILE:HD11	1:123:A:ILE:H	3	0.16
(1,1942)	1:122:A:ILE:HD12	1:123:A:ILE:H	3	0.16
(1,1942)	1:122:A:ILE:HD13	1:123:A:ILE:H	3	0.16
(1,1942)	1:122:A:ILE:HD11	1:123:A:ILE:H	8	0.16
(1,1942)	1:122:A:ILE:HD12	1:123:A:ILE:H	8	0.16
(1,1942)	1:122:A:ILE:HD13	1:123:A:ILE:H	8	0.16
(1,1671)	1:106:A:VAL:HG11	1:111:A:VAL:HB	6	0.16
(1,1671)	1:106:A:VAL:HG12	1:111:A:VAL:HB	6	0.16
(1,1671)	1:106:A:VAL:HG13	1:111:A:VAL:HB	6	0.16
(1,1571)	1:101:A:ASP:HB3	1:101:A:ASP:HA	5	0.16
(1,1571)	1:101:A:ASP:HB3	1:101:A:ASP:HA	8	0.16
(1,1571)	1:101:A:ASP:HB3	1:101:A:ASP:HA	10	0.16
(1,1475)	1:94:A:SER:HB3	1:94:A:SER:H	7	0.16
(1,1454)	1:92:A:GLU:HB3	1:93:A:GLY:H	9	0.16
(1,1420)	1:91:A:LEU:HA	1:91:A:LEU:HB2	9	0.16
(1,1364)	1:87:A:ILE:HG22	1:88:A:VAL:H	1	0.16
(1,1364)	1:87:A:ILE:HG23	1:88:A:VAL:H	4	0.16
(1,1364)	1:87:A:ILE:HG22	1:88:A:VAL:H	5	0.16
(1,1364)	1:87:A:ILE:HG23	1:88:A:VAL:H	6	0.16
(1,1364)	1:87:A:ILE:HG21	1:88:A:VAL:H	10	0.16
(1,1345)	1:87:A:ILE:HG13	1:95:A:THR:HB	6	0.16
(1,1272)	1:84:A:ARG:HB3	1:84:A:ARG:HD3	1	0.16
(1,1234)	1:86:A:GLY:H	1:98:A:ILE:HG12	10	0.16
(1,1219)	1:82:A:LEU:HD11	1:82:A:LEU:HB2	4	0.16
(1,1219)	1:82:A:LEU:HD12	1:82:A:LEU:HB2	4	0.16
(1,1219)	1:82:A:LEU:HD13	1:82:A:LEU:HB2	4	0.16
(1,1219)	1:82:A:LEU:HD11	1:82:A:LEU:HB2	6	0.16
(1,1219)	1:82:A:LEU:HD12	1:82:A:LEU:HB2	6	0.16
(1,1219)	1:82:A:LEU:HD13	1:82:A:LEU:HB2	6	0.16
(1,1219)	1:82:A:LEU:HD11	1:82:A:LEU:HB2	10	0.16
(1,1219)	1:82:A:LEU:HD12	1:82:A:LEU:HB2	10	0.16
(1,1219)	1:82:A:LEU:HD13	1:82:A:LEU:HB2	10	0.16
(1,1205)	1:81:A:ASP:H	1:82:A:LEU:HD11	4	0.16
(1,1205)	1:81:A:ASP:H	1:82:A:LEU:HD12	4	0.16
(1,1205)	1:81:A:ASP:H	1:82:A:LEU:HD13	4	0.16
(1,1148)	1:78:A:LYS:H	1:78:A:LYS:HD3	7	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1136)	1:77:A:TYR:H	1:121:A:GLY:HA3	6	0.16
(1,998)	1:67:A:ILE:HG22	1:68:A:LEU:HA	5	0.16
(1,967)	1:65:A:GLY:HA2	1:26:A:LEU:HD21	1	0.16
(1,967)	1:65:A:GLY:HA2	1:26:A:LEU:HD22	1	0.16
(1,967)	1:65:A:GLY:HA2	1:26:A:LEU:HD23	1	0.16
(1,967)	1:65:A:GLY:HA2	1:26:A:LEU:HD21	2	0.16
(1,967)	1:65:A:GLY:HA2	1:26:A:LEU:HD22	2	0.16
(1,967)	1:65:A:GLY:HA2	1:26:A:LEU:HD23	2	0.16
(1,967)	1:65:A:GLY:HA2	1:26:A:LEU:HD21	8	0.16
(1,967)	1:65:A:GLY:HA2	1:26:A:LEU:HD22	8	0.16
(1,967)	1:65:A:GLY:HA2	1:26:A:LEU:HD23	8	0.16
(1,929)	1:63:A:GLN:HG2	1:63:A:GLN:HE22	3	0.16
(1,929)	1:63:A:GLN:HG3	1:63:A:GLN:HE22	3	0.16
(1,882)	1:60:A:ASN:HA	1:59:A:GLN:H	3	0.16
(1,794)	1:55:A:THR:HG21	1:59:A:GLN:HE22	4	0.16
(1,794)	1:55:A:THR:HG22	1:59:A:GLN:HE22	4	0.16
(1,794)	1:55:A:THR:HG23	1:59:A:GLN:HE22	4	0.16
(1,794)	1:55:A:THR:HG21	1:59:A:GLN:HE22	8	0.16
(1,794)	1:55:A:THR:HG22	1:59:A:GLN:HE22	8	0.16
(1,794)	1:55:A:THR:HG23	1:59:A:GLN:HE22	8	0.16
(1,748)	1:54:A:ILE:HG13	1:54:A:ILE:HB	2	0.16
(1,652)	1:45:A:ALA:HB1	1:48:A:LYS:HG2	4	0.16
(1,652)	1:45:A:ALA:HB2	1:48:A:LYS:HG2	4	0.16
(1,652)	1:45:A:ALA:HB3	1:48:A:LYS:HG2	4	0.16
(1,642)	1:45:A:ALA:HB1	1:44:A:ASP:H	7	0.16
(1,642)	1:45:A:ALA:HB2	1:44:A:ASP:H	7	0.16
(1,642)	1:45:A:ALA:HB3	1:44:A:ASP:H	7	0.16
(1,582)	1:40:A:ALA:H	1:124:A:HIS:HB3	6	0.16
(1,547)	1:37:A:THR:H	1:73:A:VAL:HG21	2	0.16
(1,547)	1:37:A:THR:H	1:73:A:VAL:HG22	2	0.16
(1,547)	1:37:A:THR:H	1:73:A:VAL:HG23	2	0.16
(1,538)	1:37:A:THR:HG21	1:37:A:THR:H	6	0.16
(1,538)	1:37:A:THR:HG22	1:37:A:THR:H	6	0.16
(1,538)	1:37:A:THR:HG23	1:37:A:THR:H	6	0.16
(1,64)	1:6:A:ASP:HA	1:9:A:VAL:HB	7	0.16
(1,32)	1:5:A:VAL:HG11	1:6:A:ASP:HA	2	0.16
(1,32)	1:5:A:VAL:HG12	1:6:A:ASP:HA	2	0.16
(1,32)	1:5:A:VAL:HG13	1:6:A:ASP:HA	2	0.16
(1,32)	1:5:A:VAL:HG11	1:6:A:ASP:HA	4	0.16
(1,32)	1:5:A:VAL:HG12	1:6:A:ASP:HA	4	0.16
(1,32)	1:5:A:VAL:HG13	1:6:A:ASP:HA	4	0.16
(1,2084)	1:129:A:VAL:HG11	1:129:A:VAL:H	3	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2084)	1:129:A:VAL:HG12	1:129:A:VAL:H	3	0.15
(1,2084)	1:129:A:VAL:HG13	1:129:A:VAL:H	3	0.15
(1,2084)	1:129:A:VAL:HG11	1:129:A:VAL:H	4	0.15
(1,2084)	1:129:A:VAL:HG12	1:129:A:VAL:H	4	0.15
(1,2084)	1:129:A:VAL:HG13	1:129:A:VAL:H	4	0.15
(1,2084)	1:129:A:VAL:HG11	1:129:A:VAL:H	6	0.15
(1,2084)	1:129:A:VAL:HG12	1:129:A:VAL:H	6	0.15
(1,2084)	1:129:A:VAL:HG13	1:129:A:VAL:H	6	0.15
(1,1981)	1:124:A:HIS:HB2	1:125:A:VAL:H	1	0.15
(1,1981)	1:124:A:HIS:HB2	1:125:A:VAL:H	4	0.15
(1,1971)	1:124:A:HIS:HB3	1:114:A:ALA:HB1	6	0.15
(1,1971)	1:124:A:HIS:HB3	1:114:A:ALA:HB2	6	0.15
(1,1971)	1:124:A:HIS:HB3	1:114:A:ALA:HB3	6	0.15
(1,1947)	1:123:A:ILE:HG12	1:38:A:VAL:HB	6	0.15
(1,1840)	1:117:A:GLU:H	1:116:A:ILE:H	5	0.15
(1,1840)	1:117:A:GLU:H	1:116:A:ILE:H	7	0.15
(1,1598)	1:110:A:THR:H	1:111:A:VAL:HB	8	0.15
(1,1567)	1:100:A:GLY:HA2	1:105:A:GLU:H	2	0.15
(1,1475)	1:94:A:SER:HB3	1:94:A:SER:H	3	0.15
(1,1475)	1:94:A:SER:HB3	1:94:A:SER:H	5	0.15
(1,1415)	1:91:A:LEU:HD21	1:74:A:ALA:HB1	4	0.15
(1,1415)	1:91:A:LEU:HD21	1:74:A:ALA:HB2	4	0.15
(1,1415)	1:91:A:LEU:HD21	1:74:A:ALA:HB3	4	0.15
(1,1415)	1:91:A:LEU:HD22	1:74:A:ALA:HB1	4	0.15
(1,1415)	1:91:A:LEU:HD22	1:74:A:ALA:HB2	4	0.15
(1,1415)	1:91:A:LEU:HD22	1:74:A:ALA:HB3	4	0.15
(1,1415)	1:91:A:LEU:HD23	1:74:A:ALA:HB1	4	0.15
(1,1415)	1:91:A:LEU:HD23	1:74:A:ALA:HB2	4	0.15
(1,1415)	1:91:A:LEU:HD23	1:74:A:ALA:HB3	4	0.15
(1,1415)	1:91:A:LEU:HD21	1:74:A:ALA:HB1	9	0.15
(1,1415)	1:91:A:LEU:HD21	1:74:A:ALA:HB2	9	0.15
(1,1415)	1:91:A:LEU:HD21	1:74:A:ALA:HB3	9	0.15
(1,1415)	1:91:A:LEU:HD22	1:74:A:ALA:HB1	9	0.15
(1,1415)	1:91:A:LEU:HD22	1:74:A:ALA:HB2	9	0.15
(1,1415)	1:91:A:LEU:HD22	1:74:A:ALA:HB3	9	0.15
(1,1415)	1:91:A:LEU:HD23	1:74:A:ALA:HB1	9	0.15
(1,1415)	1:91:A:LEU:HD23	1:74:A:ALA:HB2	9	0.15
(1,1415)	1:91:A:LEU:HD23	1:74:A:ALA:HB3	9	0.15
(1,1364)	1:87:A:ILE:HG21	1:88:A:VAL:H	2	0.15
(1,1364)	1:87:A:ILE:HG23	1:88:A:VAL:H	7	0.15
(1,1364)	1:87:A:ILE:HG22	1:88:A:VAL:H	8	0.15
(1,1296)	1:85:A:MET:H	1:85:A:MET:HG2	8	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1224)	1:82:A:LEU:H	1:82:A:LEU:HG	3	0.15
(1,1219)	1:82:A:LEU:HD11	1:82:A:LEU:HB2	8	0.15
(1,1219)	1:82:A:LEU:HD12	1:82:A:LEU:HB2	8	0.15
(1,1219)	1:82:A:LEU:HD13	1:82:A:LEU:HB2	8	0.15
(1,1191)	1:81:A:ASP:H	1:78:A:LYS:HB3	7	0.15
(1,1122)	1:76:A:ALA:H	1:77:A:TYR:H	8	0.15
(1,992)	1:66:A:ARG:HG3	1:67:A:ILE:H	1	0.15
(1,967)	1:65:A:GLY:HA2	1:26:A:LEU:HD21	4	0.15
(1,967)	1:65:A:GLY:HA2	1:26:A:LEU:HD22	4	0.15
(1,967)	1:65:A:GLY:HA2	1:26:A:LEU:HD23	4	0.15
(1,929)	1:63:A:GLN:HG2	1:63:A:GLN:HE22	7	0.15
(1,929)	1:63:A:GLN:HG3	1:63:A:GLN:HE22	7	0.15
(1,852)	1:58:A:VAL:H	1:60:A:ASN:H	3	0.15
(1,845)	1:58:A:VAL:HG11	1:59:A:GLN:HA	2	0.15
(1,845)	1:58:A:VAL:HG12	1:59:A:GLN:HA	2	0.15
(1,845)	1:58:A:VAL:HG13	1:59:A:GLN:HA	2	0.15
(1,794)	1:55:A:THR:HG21	1:59:A:GLN:HE22	2	0.15
(1,794)	1:55:A:THR:HG22	1:59:A:GLN:HE22	2	0.15
(1,794)	1:55:A:THR:HG23	1:59:A:GLN:HE22	2	0.15
(1,794)	1:55:A:THR:HG21	1:59:A:GLN:HE22	10	0.15
(1,794)	1:55:A:THR:HG22	1:59:A:GLN:HE22	10	0.15
(1,794)	1:55:A:THR:HG23	1:59:A:GLN:HE22	10	0.15
(1,748)	1:54:A:ILE:HG13	1:54:A:ILE:HB	5	0.15
(1,748)	1:54:A:ILE:HG13	1:54:A:ILE:HB	7	0.15
(1,748)	1:54:A:ILE:HG13	1:54:A:ILE:HB	8	0.15
(1,748)	1:54:A:ILE:HG13	1:54:A:ILE:HB	10	0.15
(1,730)	1:40:A:ALA:H	1:126:A:ILE:HG21	8	0.15
(1,730)	1:40:A:ALA:H	1:126:A:ILE:HG21	10	0.15
(1,622)	1:44:A:ASP:HB2	1:42:A:ASN:HD21	7	0.15
(1,547)	1:37:A:THR:H	1:73:A:VAL:HG21	5	0.15
(1,547)	1:37:A:THR:H	1:73:A:VAL:HG22	5	0.15
(1,547)	1:37:A:THR:H	1:73:A:VAL:HG23	5	0.15
(1,427)	1:30:A:LEU:HD11	1:31:A:GLN:H	7	0.15
(1,427)	1:30:A:LEU:HD12	1:31:A:GLN:H	7	0.15
(1,427)	1:30:A:LEU:HD13	1:31:A:GLN:H	7	0.15
(1,380)	1:26:A:LEU:HD21	1:66:A:ARG:HA	2	0.15
(1,280)	1:22:A:LYS:HG2	1:22:A:LYS:H	10	0.15
(1,276)	1:22:A:LYS:HG2	1:22:A:LYS:HE2	7	0.15
(1,257)	1:21:A:VAL:HG21	1:65:A:GLY:HA2	5	0.15
(1,257)	1:21:A:VAL:HG22	1:65:A:GLY:HA2	5	0.15
(1,257)	1:21:A:VAL:HG23	1:65:A:GLY:HA2	5	0.15
(1,183)	1:18:A:VAL:HG11	1:11:A:THR:H	7	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,183)	1:18:A:VAL:HG12	1:11:A:THR:H	7	0.15
(1,183)	1:18:A:VAL:HG13	1:11:A:THR:H	7	0.15
(1,64)	1:6:A:ASP:HA	1:9:A:VAL:HB	4	0.15
(1,64)	1:6:A:ASP:HA	1:9:A:VAL:HB	5	0.15
(1,2084)	1:129:A:VAL:HG11	1:129:A:VAL:H	7	0.14
(1,2084)	1:129:A:VAL:HG12	1:129:A:VAL:H	7	0.14
(1,2084)	1:129:A:VAL:HG13	1:129:A:VAL:H	7	0.14
(1,2084)	1:129:A:VAL:HG11	1:129:A:VAL:H	9	0.14
(1,2084)	1:129:A:VAL:HG12	1:129:A:VAL:H	9	0.14
(1,2084)	1:129:A:VAL:HG13	1:129:A:VAL:H	9	0.14
(1,2031)	1:126:A:ILE:H	1:127:A:ASP:HA	4	0.14
(1,2006)	1:126:A:ILE:HD11	1:109:A:ALA:HB1	1	0.14
(1,2006)	1:126:A:ILE:HD11	1:109:A:ALA:HB2	1	0.14
(1,2006)	1:126:A:ILE:HD11	1:109:A:ALA:HB3	1	0.14
(1,2006)	1:126:A:ILE:HD12	1:109:A:ALA:HB1	1	0.14
(1,2006)	1:126:A:ILE:HD12	1:109:A:ALA:HB2	1	0.14
(1,2006)	1:126:A:ILE:HD12	1:109:A:ALA:HB3	1	0.14
(1,2006)	1:126:A:ILE:HD13	1:109:A:ALA:HB1	1	0.14
(1,2006)	1:126:A:ILE:HD13	1:109:A:ALA:HB2	1	0.14
(1,2006)	1:126:A:ILE:HD13	1:109:A:ALA:HB3	1	0.14
(1,1999)	1:126:A:ILE:HG21	1:39:A:PHE:HD1	6	0.14
(1,1999)	1:126:A:ILE:HG21	1:39:A:PHE:HD2	6	0.14
(1,1999)	1:126:A:ILE:HG22	1:39:A:PHE:HD1	6	0.14
(1,1999)	1:126:A:ILE:HG22	1:39:A:PHE:HD2	6	0.14
(1,1999)	1:126:A:ILE:HG23	1:39:A:PHE:HD1	6	0.14
(1,1999)	1:126:A:ILE:HG23	1:39:A:PHE:HD2	6	0.14
(1,1968)	1:124:A:HIS:HB3	1:39:A:PHE:HD1	4	0.14
(1,1968)	1:124:A:HIS:HB3	1:39:A:PHE:HD2	4	0.14
(1,1968)	1:124:A:HIS:HB3	1:39:A:PHE:HD1	9	0.14
(1,1968)	1:124:A:HIS:HB3	1:39:A:PHE:HD2	9	0.14
(1,1603)	1:104:A:LEU:H	1:105:A:GLU:HG2	6	0.14
(1,1493)	1:96:A:ILE:HD11	1:90:A:SER:H	5	0.14
(1,1454)	1:92:A:GLU:HB3	1:93:A:GLY:H	2	0.14
(1,1415)	1:91:A:LEU:HD21	1:74:A:ALA:HB1	8	0.14
(1,1415)	1:91:A:LEU:HD21	1:74:A:ALA:HB2	8	0.14
(1,1415)	1:91:A:LEU:HD21	1:74:A:ALA:HB3	8	0.14
(1,1415)	1:91:A:LEU:HD22	1:74:A:ALA:HB1	8	0.14
(1,1415)	1:91:A:LEU:HD22	1:74:A:ALA:HB2	8	0.14
(1,1415)	1:91:A:LEU:HD22	1:74:A:ALA:HB3	8	0.14
(1,1415)	1:91:A:LEU:HD23	1:74:A:ALA:HB1	8	0.14
(1,1415)	1:91:A:LEU:HD23	1:74:A:ALA:HB2	8	0.14
(1,1415)	1:91:A:LEU:HD23	1:74:A:ALA:HB3	8	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1364)	1:87:A:ILE:HG21	1:88:A:VAL:H	3	0.14
(1,1364)	1:87:A:ILE:HG22	1:88:A:VAL:H	9	0.14
(1,1296)	1:85:A:MET:H	1:85:A:MET:HG2	4	0.14
(1,1296)	1:85:A:MET:H	1:85:A:MET:HG2	5	0.14
(1,1272)	1:84:A:ARG:HB3	1:84:A:ARG:HD3	5	0.14
(1,1272)	1:84:A:ARG:HB3	1:84:A:ARG:HD3	6	0.14
(1,1272)	1:84:A:ARG:HB3	1:84:A:ARG:HD3	7	0.14
(1,1251)	1:83:A:LYS:HB3	1:86:A:GLY:H	3	0.14
(1,1234)	1:86:A:GLY:H	1:98:A:ILE:HG12	3	0.14
(1,1224)	1:82:A:LEU:H	1:82:A:LEU:HG	2	0.14
(1,1224)	1:82:A:LEU:H	1:82:A:LEU:HG	4	0.14
(1,1219)	1:82:A:LEU:HD11	1:82:A:LEU:HB2	3	0.14
(1,1219)	1:82:A:LEU:HD12	1:82:A:LEU:HB2	3	0.14
(1,1219)	1:82:A:LEU:HD13	1:82:A:LEU:HB2	3	0.14
(1,1216)	1:82:A:LEU:HB2	1:80:A:THR:H	6	0.14
(1,1214)	1:78:A:LYS:HG2	1:79:A:ALA:H	7	0.14
(1,1208)	1:81:A:ASP:HA	1:84:A:ARG:HB3	8	0.14
(1,1205)	1:81:A:ASP:H	1:82:A:LEU:HD11	1	0.14
(1,1205)	1:81:A:ASP:H	1:82:A:LEU:HD12	1	0.14
(1,1205)	1:81:A:ASP:H	1:82:A:LEU:HD13	1	0.14
(1,1177)	1:79:A:ALA:HB1	1:104:A:LEU:HD21	5	0.14
(1,1177)	1:79:A:ALA:HB1	1:104:A:LEU:HD22	5	0.14
(1,1177)	1:79:A:ALA:HB1	1:104:A:LEU:HD23	5	0.14
(1,1177)	1:79:A:ALA:HB2	1:104:A:LEU:HD21	5	0.14
(1,1177)	1:79:A:ALA:HB2	1:104:A:LEU:HD22	5	0.14
(1,1177)	1:79:A:ALA:HB2	1:104:A:LEU:HD23	5	0.14
(1,1177)	1:79:A:ALA:HB3	1:104:A:LEU:HD21	5	0.14
(1,1177)	1:79:A:ALA:HB3	1:104:A:LEU:HD22	5	0.14
(1,1177)	1:79:A:ALA:HB3	1:104:A:LEU:HD23	5	0.14
(1,1169)	1:78:A:LYS:HG2	1:122:A:ILE:HD11	10	0.14
(1,1169)	1:78:A:LYS:HG2	1:122:A:ILE:HD12	10	0.14
(1,1169)	1:78:A:LYS:HG2	1:122:A:ILE:HD13	10	0.14
(1,1163)	1:78:A:LYS:H	1:80:A:THR:H	7	0.14
(1,1163)	1:78:A:LYS:H	1:80:A:THR:H	10	0.14
(1,1138)	1:78:A:LYS:H	1:77:A:TYR:H	6	0.14
(1,1122)	1:76:A:ALA:H	1:77:A:TYR:H	4	0.14
(1,1115)	1:76:A:ALA:H	1:74:A:ALA:HA	1	0.14
(1,1115)	1:76:A:ALA:H	1:74:A:ALA:HA	3	0.14
(1,1115)	1:76:A:ALA:H	1:74:A:ALA:HA	7	0.14
(1,1115)	1:76:A:ALA:H	1:74:A:ALA:HA	9	0.14
(1,998)	1:67:A:ILE:HG22	1:68:A:LEU:HA	3	0.14
(1,992)	1:66:A:ARG:HG3	1:67:A:ILE:H	4	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,990)	1:66:A:ARG:H	1:66:A:ARG:HB2	10	0.14
(1,967)	1:65:A:GLY:HA2	1:26:A:LEU:HD21	10	0.14
(1,967)	1:65:A:GLY:HA2	1:26:A:LEU:HD22	10	0.14
(1,967)	1:65:A:GLY:HA2	1:26:A:LEU:HD23	10	0.14
(1,939)	1:63:A:GLN:HG2	1:67:A:ILE:HD11	2	0.14
(1,939)	1:63:A:GLN:HG2	1:67:A:ILE:HD12	2	0.14
(1,939)	1:63:A:GLN:HG2	1:67:A:ILE:HD13	2	0.14
(1,845)	1:58:A:VAL:HG11	1:59:A:GLN:HA	5	0.14
(1,845)	1:58:A:VAL:HG12	1:59:A:GLN:HA	5	0.14
(1,845)	1:58:A:VAL:HG13	1:59:A:GLN:HA	5	0.14
(1,776)	1:54:A:ILE:HG13	1:67:A:ILE:HG21	10	0.14
(1,776)	1:54:A:ILE:HG13	1:67:A:ILE:HG22	10	0.14
(1,776)	1:54:A:ILE:HG13	1:67:A:ILE:HG23	10	0.14
(1,762)	1:54:A:ILE:HG12	1:54:A:ILE:H	5	0.14
(1,748)	1:54:A:ILE:HG13	1:54:A:ILE:HB	1	0.14
(1,748)	1:54:A:ILE:HG13	1:54:A:ILE:HB	3	0.14
(1,748)	1:54:A:ILE:HG13	1:54:A:ILE:HB	4	0.14
(1,748)	1:54:A:ILE:HG13	1:54:A:ILE:HB	9	0.14
(1,730)	1:40:A:ALA:H	1:126:A:ILE:HG22	2	0.14
(1,730)	1:40:A:ALA:H	1:126:A:ILE:HG23	5	0.14
(1,692)	1:48:A:LYS:HA	1:48:A:LYS:HB3	7	0.14
(1,652)	1:45:A:ALA:HB1	1:48:A:LYS:HG2	8	0.14
(1,652)	1:45:A:ALA:HB2	1:48:A:LYS:HG2	8	0.14
(1,652)	1:45:A:ALA:HB3	1:48:A:LYS:HG2	8	0.14
(1,290)	1:22:A:LYS:HG3	1:27:A:VAL:HG21	6	0.14
(1,290)	1:22:A:LYS:HG3	1:27:A:VAL:HG22	6	0.14
(1,290)	1:22:A:LYS:HG3	1:27:A:VAL:HG23	6	0.14
(1,280)	1:22:A:LYS:HG2	1:22:A:LYS:H	8	0.14
(1,32)	1:5:A:VAL:HG11	1:6:A:ASP:HA	1	0.14
(1,32)	1:5:A:VAL:HG12	1:6:A:ASP:HA	1	0.14
(1,32)	1:5:A:VAL:HG13	1:6:A:ASP:HA	1	0.14
(1,32)	1:5:A:VAL:HG11	1:6:A:ASP:HA	6	0.14
(1,32)	1:5:A:VAL:HG12	1:6:A:ASP:HA	6	0.14
(1,32)	1:5:A:VAL:HG13	1:6:A:ASP:HA	6	0.14
(1,32)	1:5:A:VAL:HG11	1:6:A:ASP:HA	8	0.14
(1,32)	1:5:A:VAL:HG12	1:6:A:ASP:HA	8	0.14
(1,32)	1:5:A:VAL:HG13	1:6:A:ASP:HA	8	0.14
(1,32)	1:5:A:VAL:HG11	1:6:A:ASP:HA	9	0.14
(1,32)	1:5:A:VAL:HG12	1:6:A:ASP:HA	9	0.14
(1,32)	1:5:A:VAL:HG13	1:6:A:ASP:HA	9	0.14
(1,32)	1:5:A:VAL:HG11	1:6:A:ASP:HA	10	0.14
(1,32)	1:5:A:VAL:HG12	1:6:A:ASP:HA	10	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,32)	1:5:A:VAL:HG13	1:6:A:ASP:HA	10	0.14
(1,2084)	1:129:A:VAL:HG11	1:129:A:VAL:H	5	0.13
(1,2084)	1:129:A:VAL:HG12	1:129:A:VAL:H	5	0.13
(1,2084)	1:129:A:VAL:HG13	1:129:A:VAL:H	5	0.13
(1,2078)	1:129:A:VAL:HB	1:53:A:THR:H	8	0.13
(1,2054)	1:128:A:THR:HG21	1:109:A:ALA:HB1	5	0.13
(1,2054)	1:128:A:THR:HG21	1:109:A:ALA:HB2	5	0.13
(1,2054)	1:128:A:THR:HG21	1:109:A:ALA:HB3	5	0.13
(1,2054)	1:128:A:THR:HG22	1:109:A:ALA:HB1	5	0.13
(1,2054)	1:128:A:THR:HG22	1:109:A:ALA:HB2	5	0.13
(1,2054)	1:128:A:THR:HG22	1:109:A:ALA:HB3	5	0.13
(1,2054)	1:128:A:THR:HG23	1:109:A:ALA:HB1	5	0.13
(1,2054)	1:128:A:THR:HG23	1:109:A:ALA:HB2	5	0.13
(1,2054)	1:128:A:THR:HG23	1:109:A:ALA:HB3	5	0.13
(1,2046)	1:127:A:ASP:H	1:127:A:ASP:HB2	1	0.13
(1,2046)	1:127:A:ASP:H	1:127:A:ASP:HB2	2	0.13
(1,2046)	1:127:A:ASP:H	1:127:A:ASP:HB2	7	0.13
(1,1968)	1:124:A:HIS:HB3	1:39:A:PHE:HD1	1	0.13
(1,1968)	1:124:A:HIS:HB3	1:39:A:PHE:HD2	1	0.13
(1,1926)	1:122:A:ILE:H	1:121:A:GLY:HA2	3	0.13
(1,1919)	1:122:A:ILE:HB	1:118:A:ALA:H	3	0.13
(1,1919)	1:122:A:ILE:HB	1:118:A:ALA:H	5	0.13
(1,1868)	1:118:A:ALA:HA	1:121:A:GLY:H	6	0.13
(1,1840)	1:117:A:GLU:H	1:116:A:ILE:H	3	0.13
(1,1840)	1:117:A:GLU:H	1:116:A:ILE:H	8	0.13
(1,1788)	1:113:A:ALA:H	1:125:A:VAL:HG11	6	0.13
(1,1788)	1:113:A:ALA:H	1:125:A:VAL:HG12	6	0.13
(1,1788)	1:113:A:ALA:H	1:125:A:VAL:HG13	6	0.13
(1,1719)	1:110:A:THR:HG21	1:103:A:PRO:HG3	1	0.13
(1,1719)	1:110:A:THR:HG22	1:103:A:PRO:HG3	1	0.13
(1,1719)	1:110:A:THR:HG23	1:103:A:PRO:HG3	1	0.13
(1,1695)	1:107:A:LYS:HB3	1:108:A:ASN:H	3	0.13
(1,1518)	1:96:A:ILE:HG13	1:107:A:LYS:HD2	9	0.13
(1,1518)	1:96:A:ILE:HG13	1:107:A:LYS:HD3	9	0.13
(1,1454)	1:92:A:GLU:HB3	1:93:A:GLY:H	1	0.13
(1,1415)	1:91:A:LEU:HD21	1:74:A:ALA:HB1	3	0.13
(1,1415)	1:91:A:LEU:HD21	1:74:A:ALA:HB2	3	0.13
(1,1415)	1:91:A:LEU:HD21	1:74:A:ALA:HB3	3	0.13
(1,1415)	1:91:A:LEU:HD22	1:74:A:ALA:HB1	3	0.13
(1,1415)	1:91:A:LEU:HD22	1:74:A:ALA:HB2	3	0.13
(1,1415)	1:91:A:LEU:HD22	1:74:A:ALA:HB3	3	0.13
(1,1415)	1:91:A:LEU:HD23	1:74:A:ALA:HB1	3	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1415)	1:91:A:LEU:HD23	1:74:A:ALA:HB2	3	0.13
(1,1415)	1:91:A:LEU:HD23	1:74:A:ALA:HB3	3	0.13
(1,1409)	1:91:A:LEU:HB3	1:30:A:LEU:H	6	0.13
(1,1407)	1:91:A:LEU:HD11	1:29:A:ALA:HB1	10	0.13
(1,1407)	1:91:A:LEU:HD11	1:29:A:ALA:HB2	10	0.13
(1,1407)	1:91:A:LEU:HD11	1:29:A:ALA:HB3	10	0.13
(1,1407)	1:91:A:LEU:HD12	1:29:A:ALA:HB1	10	0.13
(1,1407)	1:91:A:LEU:HD12	1:29:A:ALA:HB2	10	0.13
(1,1407)	1:91:A:LEU:HD12	1:29:A:ALA:HB3	10	0.13
(1,1407)	1:91:A:LEU:HD13	1:29:A:ALA:HB1	10	0.13
(1,1407)	1:91:A:LEU:HD13	1:29:A:ALA:HB2	10	0.13
(1,1407)	1:91:A:LEU:HD13	1:29:A:ALA:HB3	10	0.13
(1,1284)	1:85:A:MET:HA	1:85:A:MET:HG3	1	0.13
(1,1261)	1:84:A:ARG:HB3	1:84:A:ARG:H	7	0.13
(1,1251)	1:83:A:LYS:HB3	1:86:A:GLY:H	4	0.13
(1,1251)	1:83:A:LYS:HB3	1:86:A:GLY:H	5	0.13
(1,1251)	1:83:A:LYS:HB3	1:86:A:GLY:H	8	0.13
(1,1224)	1:82:A:LEU:H	1:82:A:LEU:HG	5	0.13
(1,1224)	1:82:A:LEU:H	1:82:A:LEU:HG	9	0.13
(1,1219)	1:82:A:LEU:HD11	1:82:A:LEU:HB2	5	0.13
(1,1219)	1:82:A:LEU:HD12	1:82:A:LEU:HB2	5	0.13
(1,1219)	1:82:A:LEU:HD13	1:82:A:LEU:HB2	5	0.13
(1,1214)	1:78:A:LYS:HG2	1:79:A:ALA:H	6	0.13
(1,1205)	1:81:A:ASP:H	1:82:A:LEU:HD11	2	0.13
(1,1205)	1:81:A:ASP:H	1:82:A:LEU:HD12	2	0.13
(1,1205)	1:81:A:ASP:H	1:82:A:LEU:HD13	2	0.13
(1,1163)	1:78:A:LYS:H	1:80:A:THR:H	9	0.13
(1,1155)	1:78:A:LYS:HA	1:78:A:LYS:HE2	10	0.13
(1,1155)	1:78:A:LYS:HA	1:78:A:LYS:HE3	10	0.13
(1,1148)	1:78:A:LYS:H	1:78:A:LYS:HD3	1	0.13
(1,1148)	1:78:A:LYS:H	1:78:A:LYS:HD3	9	0.13
(1,1146)	1:78:A:LYS:HB3	1:78:A:LYS:HD2	1	0.13
(1,1146)	1:78:A:LYS:HB3	1:78:A:LYS:HD3	1	0.13
(1,1136)	1:77:A:TYR:H	1:121:A:GLY:HA3	1	0.13
(1,1122)	1:76:A:ALA:H	1:77:A:TYR:H	10	0.13
(1,1115)	1:76:A:ALA:H	1:74:A:ALA:HA	5	0.13
(1,1115)	1:76:A:ALA:H	1:74:A:ALA:HA	8	0.13
(1,1095)	1:74:A:ALA:HA	1:36:A:PHE:H	9	0.13
(1,998)	1:67:A:ILE:HG21	1:68:A:LEU:HA	2	0.13
(1,998)	1:67:A:ILE:HG23	1:68:A:LEU:HA	7	0.13
(1,998)	1:67:A:ILE:HG21	1:68:A:LEU:HA	8	0.13
(1,990)	1:66:A:ARG:H	1:66:A:ARG:HB2	4	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,981)	1:65:A:GLY:HA3	1:68:A:LEU:H	4	0.13
(1,929)	1:63:A:GLN:HG2	1:63:A:GLN:HE22	5	0.13
(1,929)	1:63:A:GLN:HG3	1:63:A:GLN:HE22	5	0.13
(1,929)	1:63:A:GLN:HG2	1:63:A:GLN:HE22	10	0.13
(1,929)	1:63:A:GLN:HG3	1:63:A:GLN:HE22	10	0.13
(1,887)	1:60:A:ASN:HB3	1:60:A:ASN:H	7	0.13
(1,887)	1:60:A:ASN:HB3	1:60:A:ASN:H	8	0.13
(1,845)	1:58:A:VAL:HG11	1:59:A:GLN:HA	4	0.13
(1,845)	1:58:A:VAL:HG12	1:59:A:GLN:HA	4	0.13
(1,845)	1:58:A:VAL:HG13	1:59:A:GLN:HA	4	0.13
(1,845)	1:58:A:VAL:HG11	1:59:A:GLN:HA	7	0.13
(1,845)	1:58:A:VAL:HG12	1:59:A:GLN:HA	7	0.13
(1,845)	1:58:A:VAL:HG13	1:59:A:GLN:HA	7	0.13
(1,845)	1:58:A:VAL:HG11	1:59:A:GLN:HA	8	0.13
(1,845)	1:58:A:VAL:HG12	1:59:A:GLN:HA	8	0.13
(1,845)	1:58:A:VAL:HG13	1:59:A:GLN:HA	8	0.13
(1,830)	1:57:A:LEU:HB3	1:58:A:VAL:H	1	0.13
(1,809)	1:56:A:SER:H	1:59:A:GLN:H	3	0.13
(1,762)	1:54:A:ILE:HG12	1:54:A:ILE:H	8	0.13
(1,730)	1:40:A:ALA:H	1:126:A:ILE:HG22	3	0.13
(1,692)	1:48:A:LYS:HA	1:48:A:LYS:HB3	3	0.13
(1,662)	1:46:A:PHE:HB2	1:43:A:ASP:HA	7	0.13
(1,639)	1:45:A:ALA:HB1	1:42:A:ASN:HD21	1	0.13
(1,639)	1:45:A:ALA:HB2	1:42:A:ASN:HD21	1	0.13
(1,639)	1:45:A:ALA:HB3	1:42:A:ASN:HD21	1	0.13
(1,620)	1:44:A:ASP:H	1:42:A:ASN:HD21	1	0.13
(1,596)	1:42:A:ASN:HB2	1:42:A:ASN:HD22	3	0.13
(1,575)	1:39:A:PHE:HA	1:124:A:HIS:HB3	6	0.13
(1,553)	1:37:A:THR:HG21	1:82:A:LEU:HD11	4	0.13
(1,553)	1:37:A:THR:HG21	1:82:A:LEU:HD12	4	0.13
(1,553)	1:37:A:THR:HG21	1:82:A:LEU:HD13	4	0.13
(1,553)	1:37:A:THR:HG22	1:82:A:LEU:HD11	4	0.13
(1,553)	1:37:A:THR:HG22	1:82:A:LEU:HD12	4	0.13
(1,553)	1:37:A:THR:HG22	1:82:A:LEU:HD13	4	0.13
(1,553)	1:37:A:THR:HG23	1:82:A:LEU:HD11	4	0.13
(1,553)	1:37:A:THR:HG23	1:82:A:LEU:HD12	4	0.13
(1,553)	1:37:A:THR:HG23	1:82:A:LEU:HD13	4	0.13
(1,497)	1:35:A:PRO:HG3	1:75:A:GLY:H	8	0.13
(1,290)	1:22:A:LYS:HG3	1:27:A:VAL:HG21	5	0.13
(1,290)	1:22:A:LYS:HG3	1:27:A:VAL:HG22	5	0.13
(1,290)	1:22:A:LYS:HG3	1:27:A:VAL:HG23	5	0.13
(1,163)	1:14:A:PHE:HB3	1:14:A:PHE:H	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,154)	1:12:A:PRO:HA	1:14:A:PHE:H	6	0.13
(1,2078)	1:129:A:VAL:HB	1:53:A:THR:H	7	0.12
(1,2075)	1:129:A:VAL:HG11	1:49:A:LEU:HA	5	0.12
(1,2075)	1:129:A:VAL:HG12	1:49:A:LEU:HA	5	0.12
(1,2075)	1:129:A:VAL:HG13	1:49:A:LEU:HA	5	0.12
(1,2014)	1:126:A:ILE:HD11	1:125:A:VAL:H	1	0.12
(1,2014)	1:126:A:ILE:HD12	1:125:A:VAL:H	1	0.12
(1,2014)	1:126:A:ILE:HD13	1:125:A:VAL:H	1	0.12
(1,1967)	1:123:A:ILE:HG21	1:125:A:VAL:H	6	0.12
(1,1967)	1:123:A:ILE:HG22	1:125:A:VAL:H	6	0.12
(1,1967)	1:123:A:ILE:HG23	1:125:A:VAL:H	6	0.12
(1,1926)	1:122:A:ILE:H	1:121:A:GLY:HA2	1	0.12
(1,1926)	1:122:A:ILE:H	1:121:A:GLY:HA2	4	0.12
(1,1926)	1:122:A:ILE:H	1:121:A:GLY:HA2	5	0.12
(1,1926)	1:122:A:ILE:H	1:121:A:GLY:HA2	6	0.12
(1,1926)	1:122:A:ILE:H	1:121:A:GLY:HA2	8	0.12
(1,1919)	1:122:A:ILE:HB	1:118:A:ALA:H	7	0.12
(1,1919)	1:122:A:ILE:HB	1:118:A:ALA:H	8	0.12
(1,1840)	1:117:A:GLU:H	1:116:A:ILE:H	6	0.12
(1,1823)	1:116:A:ILE:HG12	1:116:A:ILE:HB	1	0.12
(1,1823)	1:116:A:ILE:HG12	1:116:A:ILE:HB	3	0.12
(1,1823)	1:116:A:ILE:HG12	1:116:A:ILE:HB	4	0.12
(1,1823)	1:116:A:ILE:HG12	1:116:A:ILE:HB	6	0.12
(1,1798)	1:114:A:ALA:H	1:115:A:ASP:HB3	10	0.12
(1,1731)	1:110:A:THR:H	1:111:A:VAL:H	1	0.12
(1,1731)	1:110:A:THR:H	1:111:A:VAL:H	4	0.12
(1,1731)	1:110:A:THR:H	1:111:A:VAL:H	8	0.12
(1,1679)	1:107:A:LYS:H	1:97:A:PRO:HG2	8	0.12
(1,1679)	1:107:A:LYS:H	1:97:A:PRO:HG3	8	0.12
(1,1438)	1:91:A:LEU:HB2	1:92:A:GLU:H	1	0.12
(1,1416)	1:91:A:LEU:HA	1:74:A:ALA:HB1	7	0.12
(1,1416)	1:91:A:LEU:HA	1:74:A:ALA:HB2	7	0.12
(1,1416)	1:91:A:LEU:HA	1:74:A:ALA:HB3	7	0.12
(1,1409)	1:91:A:LEU:HB3	1:30:A:LEU:H	1	0.12
(1,1409)	1:91:A:LEU:HB3	1:30:A:LEU:H	2	0.12
(1,1409)	1:91:A:LEU:HB3	1:30:A:LEU:H	4	0.12
(1,1409)	1:91:A:LEU:HB3	1:30:A:LEU:H	5	0.12
(1,1409)	1:91:A:LEU:HB3	1:30:A:LEU:H	8	0.12
(1,1409)	1:91:A:LEU:HB3	1:30:A:LEU:H	10	0.12
(1,1378)	1:88:A:VAL:H	1:98:A:ILE:HD11	1	0.12
(1,1378)	1:88:A:VAL:H	1:98:A:ILE:HD12	1	0.12
(1,1378)	1:88:A:VAL:H	1:98:A:ILE:HD13	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1378)	1:88:A:VAL:H	1:98:A:ILE:HD11	2	0.12
(1,1378)	1:88:A:VAL:H	1:98:A:ILE:HD12	2	0.12
(1,1378)	1:88:A:VAL:H	1:98:A:ILE:HD13	2	0.12
(1,1378)	1:88:A:VAL:H	1:98:A:ILE:HD11	4	0.12
(1,1378)	1:88:A:VAL:H	1:98:A:ILE:HD12	4	0.12
(1,1378)	1:88:A:VAL:H	1:98:A:ILE:HD13	4	0.12
(1,1378)	1:88:A:VAL:H	1:98:A:ILE:HD11	5	0.12
(1,1378)	1:88:A:VAL:H	1:98:A:ILE:HD12	5	0.12
(1,1378)	1:88:A:VAL:H	1:98:A:ILE:HD13	5	0.12
(1,1378)	1:88:A:VAL:H	1:98:A:ILE:HD11	8	0.12
(1,1378)	1:88:A:VAL:H	1:98:A:ILE:HD12	8	0.12
(1,1378)	1:88:A:VAL:H	1:98:A:ILE:HD13	8	0.12
(1,1378)	1:88:A:VAL:H	1:98:A:ILE:HD11	10	0.12
(1,1378)	1:88:A:VAL:H	1:98:A:ILE:HD12	10	0.12
(1,1378)	1:88:A:VAL:H	1:98:A:ILE:HD13	10	0.12
(1,1238)	1:82:A:LEU:HB3	1:104:A:LEU:HD21	1	0.12
(1,1238)	1:82:A:LEU:HB3	1:104:A:LEU:HD22	1	0.12
(1,1238)	1:82:A:LEU:HB3	1:104:A:LEU:HD23	1	0.12
(1,1224)	1:82:A:LEU:H	1:82:A:LEU:HG	7	0.12
(1,1224)	1:82:A:LEU:H	1:82:A:LEU:HG	8	0.12
(1,1190)	1:81:A:ASP:H	1:78:A:LYS:H	8	0.12
(1,1167)	1:78:A:LYS:HE2	1:122:A:ILE:HG21	4	0.12
(1,1167)	1:78:A:LYS:HE2	1:122:A:ILE:HG22	4	0.12
(1,1167)	1:78:A:LYS:HE2	1:122:A:ILE:HG23	4	0.12
(1,1167)	1:78:A:LYS:HE3	1:122:A:ILE:HG21	4	0.12
(1,1167)	1:78:A:LYS:HE3	1:122:A:ILE:HG22	4	0.12
(1,1167)	1:78:A:LYS:HE3	1:122:A:ILE:HG23	4	0.12
(1,1167)	1:78:A:LYS:HE2	1:122:A:ILE:HG21	10	0.12
(1,1167)	1:78:A:LYS:HE2	1:122:A:ILE:HG22	10	0.12
(1,1167)	1:78:A:LYS:HE2	1:122:A:ILE:HG23	10	0.12
(1,1167)	1:78:A:LYS:HE3	1:122:A:ILE:HG21	10	0.12
(1,1167)	1:78:A:LYS:HE3	1:122:A:ILE:HG22	10	0.12
(1,1167)	1:78:A:LYS:HE3	1:122:A:ILE:HG23	10	0.12
(1,1163)	1:78:A:LYS:H	1:80:A:THR:H	8	0.12
(1,1162)	1:78:A:LYS:HA	1:80:A:THR:H	9	0.12
(1,1155)	1:78:A:LYS:HA	1:78:A:LYS:HE2	5	0.12
(1,1155)	1:78:A:LYS:HA	1:78:A:LYS:HE3	5	0.12
(1,1136)	1:77:A:TYR:H	1:121:A:GLY:HA3	5	0.12
(1,1122)	1:76:A:ALA:H	1:77:A:TYR:H	2	0.12
(1,1115)	1:76:A:ALA:H	1:74:A:ALA:HA	2	0.12
(1,1115)	1:76:A:ALA:H	1:74:A:ALA:HA	4	0.12
(1,1095)	1:74:A:ALA:HA	1:36:A:PHE:H	2	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,990)	1:66:A:ARG:H	1:66:A:ARG:HB2	1	0.12
(1,929)	1:63:A:GLN:HG2	1:63:A:GLN:HE22	2	0.12
(1,929)	1:63:A:GLN:HG3	1:63:A:GLN:HE22	2	0.12
(1,911)	1:62:A:PRO:HB3	1:62:A:PRO:HG2	10	0.12
(1,904)	1:62:A:PRO:HA	1:62:A:PRO:HG2	3	0.12
(1,887)	1:60:A:ASN:HB3	1:60:A:ASN:H	1	0.12
(1,887)	1:60:A:ASN:HB3	1:60:A:ASN:H	2	0.12
(1,887)	1:60:A:ASN:HB3	1:60:A:ASN:H	6	0.12
(1,887)	1:60:A:ASN:HB3	1:60:A:ASN:H	10	0.12
(1,852)	1:58:A:VAL:H	1:60:A:ASN:H	9	0.12
(1,845)	1:58:A:VAL:HG11	1:59:A:GLN:HA	1	0.12
(1,845)	1:58:A:VAL:HG12	1:59:A:GLN:HA	1	0.12
(1,845)	1:58:A:VAL:HG13	1:59:A:GLN:HA	1	0.12
(1,845)	1:58:A:VAL:HG11	1:59:A:GLN:HA	6	0.12
(1,845)	1:58:A:VAL:HG12	1:59:A:GLN:HA	6	0.12
(1,845)	1:58:A:VAL:HG13	1:59:A:GLN:HA	6	0.12
(1,845)	1:58:A:VAL:HG11	1:59:A:GLN:HA	10	0.12
(1,845)	1:58:A:VAL:HG12	1:59:A:GLN:HA	10	0.12
(1,845)	1:58:A:VAL:HG13	1:59:A:GLN:HA	10	0.12
(1,835)	1:58:A:VAL:HG11	1:55:A:THR:H	2	0.12
(1,835)	1:58:A:VAL:HG12	1:55:A:THR:H	2	0.12
(1,835)	1:58:A:VAL:HG13	1:55:A:THR:H	2	0.12
(1,809)	1:56:A:SER:H	1:59:A:GLN:H	9	0.12
(1,793)	1:55:A:THR:HG21	1:59:A:GLN:H	3	0.12
(1,793)	1:55:A:THR:HG22	1:59:A:GLN:H	3	0.12
(1,793)	1:55:A:THR:HG23	1:59:A:GLN:H	3	0.12
(1,793)	1:55:A:THR:HG21	1:59:A:GLN:H	9	0.12
(1,793)	1:55:A:THR:HG22	1:59:A:GLN:H	9	0.12
(1,793)	1:55:A:THR:HG23	1:59:A:GLN:H	9	0.12
(1,748)	1:54:A:ILE:HG13	1:54:A:ILE:HB	6	0.12
(1,742)	1:53:A:THR:HB	1:55:A:THR:H	2	0.12
(1,742)	1:53:A:THR:HB	1:55:A:THR:H	5	0.12
(1,742)	1:53:A:THR:HB	1:55:A:THR:H	8	0.12
(1,730)	1:40:A:ALA:H	1:126:A:ILE:HG21	7	0.12
(1,730)	1:40:A:ALA:H	1:126:A:ILE:HG21	9	0.12
(1,692)	1:48:A:LYS:HA	1:48:A:LYS:HB3	5	0.12
(1,686)	1:47:A:ALA:H	1:49:A:LEU:H	5	0.12
(1,686)	1:47:A:ALA:H	1:49:A:LEU:H	7	0.12
(1,652)	1:45:A:ALA:HB1	1:48:A:LYS:HG2	1	0.12
(1,652)	1:45:A:ALA:HB2	1:48:A:LYS:HG2	1	0.12
(1,652)	1:45:A:ALA:HB3	1:48:A:LYS:HG2	1	0.12
(1,596)	1:42:A:ASN:HB2	1:42:A:ASN:HD22	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,524)	1:36:A:PHE:HA	1:75:A:GLY:H	6	0.12
(1,290)	1:22:A:LYS:HG3	1:27:A:VAL:HG21	7	0.12
(1,290)	1:22:A:LYS:HG3	1:27:A:VAL:HG22	7	0.12
(1,290)	1:22:A:LYS:HG3	1:27:A:VAL:HG23	7	0.12
(1,284)	1:22:A:LYS:H	1:23:A:VAL:HG11	8	0.12
(1,284)	1:22:A:LYS:H	1:23:A:VAL:HG12	8	0.12
(1,284)	1:22:A:LYS:H	1:23:A:VAL:HG13	8	0.12
(1,280)	1:22:A:LYS:HG2	1:22:A:LYS:H	2	0.12
(1,257)	1:21:A:VAL:HG21	1:65:A:GLY:HA2	6	0.12
(1,257)	1:21:A:VAL:HG22	1:65:A:GLY:HA2	6	0.12
(1,257)	1:21:A:VAL:HG23	1:65:A:GLY:HA2	6	0.12
(1,252)	1:21:A:VAL:HG21	1:26:A:LEU:HA	9	0.12
(1,252)	1:21:A:VAL:HG22	1:26:A:LEU:HA	9	0.12
(1,252)	1:21:A:VAL:HG23	1:26:A:LEU:HA	9	0.12
(1,246)	1:21:A:VAL:HG21	1:23:A:VAL:H	3	0.12
(1,246)	1:21:A:VAL:HG22	1:23:A:VAL:H	3	0.12
(1,246)	1:21:A:VAL:HG23	1:23:A:VAL:H	3	0.12
(1,183)	1:18:A:VAL:HG11	1:11:A:THR:H	6	0.12
(1,183)	1:18:A:VAL:HG12	1:11:A:THR:H	6	0.12
(1,183)	1:18:A:VAL:HG13	1:11:A:THR:H	6	0.12
(1,154)	1:12:A:PRO:HA	1:14:A:PHE:H	5	0.12
(1,66)	1:7:A:ILE:HD11	1:5:A:VAL:H	6	0.12
(1,66)	1:7:A:ILE:HD12	1:5:A:VAL:H	6	0.12
(1,66)	1:7:A:ILE:HD13	1:5:A:VAL:H	6	0.12
(1,66)	1:7:A:ILE:HD11	1:5:A:VAL:H	8	0.12
(1,66)	1:7:A:ILE:HD12	1:5:A:VAL:H	8	0.12
(1,66)	1:7:A:ILE:HD13	1:5:A:VAL:H	8	0.12
(1,32)	1:5:A:VAL:HG11	1:6:A:ASP:HA	3	0.12
(1,32)	1:5:A:VAL:HG12	1:6:A:ASP:HA	3	0.12
(1,32)	1:5:A:VAL:HG13	1:6:A:ASP:HA	3	0.12
(1,2078)	1:129:A:VAL:HB	1:53:A:THR:H	5	0.11
(1,2037)	1:127:A:ASP:HA	1:44:A:ASP:H	1	0.11
(1,2033)	1:126:A:ILE:HG12	1:127:A:ASP:H	4	0.11
(1,2031)	1:126:A:ILE:H	1:127:A:ASP:HA	3	0.11
(1,2031)	1:126:A:ILE:H	1:127:A:ASP:HA	8	0.11
(1,1966)	1:123:A:ILE:HG12	1:124:A:HIS:H	2	0.11
(1,1966)	1:123:A:ILE:HG12	1:124:A:HIS:H	5	0.11
(1,1942)	1:122:A:ILE:HD11	1:123:A:ILE:H	5	0.11
(1,1942)	1:122:A:ILE:HD12	1:123:A:ILE:H	5	0.11
(1,1942)	1:122:A:ILE:HD13	1:123:A:ILE:H	5	0.11
(1,1926)	1:122:A:ILE:H	1:121:A:GLY:HA2	10	0.11
(1,1840)	1:117:A:GLU:H	1:116:A:ILE:H	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1840)	1:117:A:GLU:H	1:116:A:ILE:H	9	0.11
(1,1829)	1:116:A:ILE:HG21	1:118:A:ALA:H	1	0.11
(1,1829)	1:116:A:ILE:HG22	1:118:A:ALA:H	1	0.11
(1,1829)	1:116:A:ILE:HG23	1:118:A:ALA:H	1	0.11
(1,1829)	1:116:A:ILE:HG21	1:118:A:ALA:H	6	0.11
(1,1829)	1:116:A:ILE:HG22	1:118:A:ALA:H	6	0.11
(1,1829)	1:116:A:ILE:HG23	1:118:A:ALA:H	6	0.11
(1,1823)	1:116:A:ILE:HG12	1:116:A:ILE:HB	2	0.11
(1,1823)	1:116:A:ILE:HG12	1:116:A:ILE:HB	5	0.11
(1,1823)	1:116:A:ILE:HG12	1:116:A:ILE:HB	7	0.11
(1,1823)	1:116:A:ILE:HG12	1:116:A:ILE:HB	8	0.11
(1,1823)	1:116:A:ILE:HG12	1:116:A:ILE:HB	9	0.11
(1,1823)	1:116:A:ILE:HG12	1:116:A:ILE:HB	10	0.11
(1,1798)	1:114:A:ALA:H	1:115:A:ASP:HB3	8	0.11
(1,1793)	1:114:A:ALA:HB1	1:114:A:ALA:H	10	0.11
(1,1793)	1:114:A:ALA:HB2	1:114:A:ALA:H	10	0.11
(1,1793)	1:114:A:ALA:HB3	1:114:A:ALA:H	10	0.11
(1,1762)	1:112:A:LEU:HD11	1:112:A:LEU:HA	4	0.11
(1,1762)	1:112:A:LEU:HD12	1:112:A:LEU:HA	4	0.11
(1,1762)	1:112:A:LEU:HD13	1:112:A:LEU:HA	4	0.11
(1,1731)	1:110:A:THR:H	1:111:A:VAL:H	2	0.11
(1,1731)	1:110:A:THR:H	1:111:A:VAL:H	7	0.11
(1,1731)	1:110:A:THR:H	1:111:A:VAL:H	9	0.11
(1,1731)	1:110:A:THR:H	1:111:A:VAL:H	10	0.11
(1,1673)	1:106:A:VAL:H	1:111:A:VAL:H	6	0.11
(1,1671)	1:106:A:VAL:HG11	1:111:A:VAL:HB	1	0.11
(1,1671)	1:106:A:VAL:HG12	1:111:A:VAL:HB	1	0.11
(1,1671)	1:106:A:VAL:HG13	1:111:A:VAL:HB	1	0.11
(1,1615)	1:104:A:LEU:HA	1:105:A:GLU:HG2	6	0.11
(1,1598)	1:110:A:THR:H	1:111:A:VAL:HB	2	0.11
(1,1454)	1:92:A:GLU:HB3	1:93:A:GLY:H	8	0.11
(1,1447)	1:92:A:GLU:HA	1:92:A:GLU:HG3	7	0.11
(1,1429)	1:91:A:LEU:HD21	1:91:A:LEU:HD11	9	0.11
(1,1429)	1:91:A:LEU:HD21	1:91:A:LEU:HD12	9	0.11
(1,1429)	1:91:A:LEU:HD21	1:91:A:LEU:HD13	9	0.11
(1,1429)	1:91:A:LEU:HD22	1:91:A:LEU:HD11	9	0.11
(1,1429)	1:91:A:LEU:HD22	1:91:A:LEU:HD12	9	0.11
(1,1429)	1:91:A:LEU:HD22	1:91:A:LEU:HD13	9	0.11
(1,1429)	1:91:A:LEU:HD23	1:91:A:LEU:HD11	9	0.11
(1,1429)	1:91:A:LEU:HD23	1:91:A:LEU:HD12	9	0.11
(1,1429)	1:91:A:LEU:HD23	1:91:A:LEU:HD13	9	0.11
(1,1416)	1:91:A:LEU:HA	1:74:A:ALA:HB1	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1416)	1:91:A:LEU:HA	1:74:A:ALA:HB2	1	0.11
(1,1416)	1:91:A:LEU:HA	1:74:A:ALA:HB3	1	0.11
(1,1416)	1:91:A:LEU:HA	1:74:A:ALA:HB1	2	0.11
(1,1416)	1:91:A:LEU:HA	1:74:A:ALA:HB2	2	0.11
(1,1416)	1:91:A:LEU:HA	1:74:A:ALA:HB3	2	0.11
(1,1416)	1:91:A:LEU:HA	1:74:A:ALA:HB1	5	0.11
(1,1416)	1:91:A:LEU:HA	1:74:A:ALA:HB2	5	0.11
(1,1416)	1:91:A:LEU:HA	1:74:A:ALA:HB3	5	0.11
(1,1416)	1:91:A:LEU:HA	1:74:A:ALA:HB1	10	0.11
(1,1416)	1:91:A:LEU:HA	1:74:A:ALA:HB2	10	0.11
(1,1416)	1:91:A:LEU:HA	1:74:A:ALA:HB3	10	0.11
(1,1409)	1:91:A:LEU:HB3	1:30:A:LEU:H	3	0.11
(1,1394)	1:89:A:THR:HG21	1:95:A:THR:H	3	0.11
(1,1394)	1:89:A:THR:HG22	1:95:A:THR:H	3	0.11
(1,1394)	1:89:A:THR:HG23	1:95:A:THR:H	3	0.11
(1,1394)	1:89:A:THR:HG21	1:95:A:THR:H	4	0.11
(1,1394)	1:89:A:THR:HG22	1:95:A:THR:H	4	0.11
(1,1394)	1:89:A:THR:HG23	1:95:A:THR:H	4	0.11
(1,1378)	1:88:A:VAL:H	1:98:A:ILE:HD11	3	0.11
(1,1378)	1:88:A:VAL:H	1:98:A:ILE:HD12	3	0.11
(1,1378)	1:88:A:VAL:H	1:98:A:ILE:HD13	3	0.11
(1,1378)	1:88:A:VAL:H	1:98:A:ILE:HD11	6	0.11
(1,1378)	1:88:A:VAL:H	1:98:A:ILE:HD12	6	0.11
(1,1378)	1:88:A:VAL:H	1:98:A:ILE:HD13	6	0.11
(1,1378)	1:88:A:VAL:H	1:98:A:ILE:HD11	7	0.11
(1,1378)	1:88:A:VAL:H	1:98:A:ILE:HD12	7	0.11
(1,1378)	1:88:A:VAL:H	1:98:A:ILE:HD13	7	0.11
(1,1272)	1:84:A:ARG:HB3	1:84:A:ARG:HD3	3	0.11
(1,1251)	1:83:A:LYS:HB3	1:86:A:GLY:H	1	0.11
(1,1251)	1:83:A:LYS:HB3	1:86:A:GLY:H	6	0.11
(1,1224)	1:82:A:LEU:H	1:82:A:LEU:HG	10	0.11
(1,1214)	1:78:A:LYS:HG2	1:79:A:ALA:H	9	0.11
(1,1190)	1:81:A:ASP:H	1:78:A:LYS:H	2	0.11
(1,1167)	1:78:A:LYS:HE2	1:122:A:ILE:HG21	7	0.11
(1,1167)	1:78:A:LYS:HE2	1:122:A:ILE:HG22	7	0.11
(1,1167)	1:78:A:LYS:HE2	1:122:A:ILE:HG23	7	0.11
(1,1167)	1:78:A:LYS:HE3	1:122:A:ILE:HG21	7	0.11
(1,1167)	1:78:A:LYS:HE3	1:122:A:ILE:HG22	7	0.11
(1,1167)	1:78:A:LYS:HE3	1:122:A:ILE:HG23	7	0.11
(1,1167)	1:78:A:LYS:HE2	1:122:A:ILE:HG21	9	0.11
(1,1167)	1:78:A:LYS:HE2	1:122:A:ILE:HG22	9	0.11
(1,1167)	1:78:A:LYS:HE2	1:122:A:ILE:HG23	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1167)	1:78:A:LYS:HE3	1:122:A:ILE:HG21	9	0.11
(1,1167)	1:78:A:LYS:HE3	1:122:A:ILE:HG22	9	0.11
(1,1167)	1:78:A:LYS:HE3	1:122:A:ILE:HG23	9	0.11
(1,1162)	1:78:A:LYS:HA	1:80:A:THR:H	1	0.11
(1,1162)	1:78:A:LYS:HA	1:80:A:THR:H	10	0.11
(1,1146)	1:78:A:LYS:HB3	1:78:A:LYS:HD2	7	0.11
(1,1146)	1:78:A:LYS:HB3	1:78:A:LYS:HD3	7	0.11
(1,1146)	1:78:A:LYS:HB3	1:78:A:LYS:HD2	9	0.11
(1,1146)	1:78:A:LYS:HB3	1:78:A:LYS:HD3	9	0.11
(1,1136)	1:77:A:TYR:H	1:121:A:GLY:HA3	10	0.11
(1,1122)	1:76:A:ALA:H	1:77:A:TYR:H	9	0.11
(1,1115)	1:76:A:ALA:H	1:74:A:ALA:HA	10	0.11
(1,992)	1:66:A:ARG:HG3	1:67:A:ILE:H	3	0.11
(1,911)	1:62:A:PRO:HB3	1:62:A:PRO:HG2	3	0.11
(1,911)	1:62:A:PRO:HB3	1:62:A:PRO:HG2	6	0.11
(1,887)	1:60:A:ASN:HB3	1:60:A:ASN:H	4	0.11
(1,865)	1:59:A:GLN:HG3	1:59:A:GLN:H	5	0.11
(1,865)	1:59:A:GLN:HG3	1:59:A:GLN:H	9	0.11
(1,835)	1:58:A:VAL:HG11	1:55:A:THR:H	5	0.11
(1,835)	1:58:A:VAL:HG12	1:55:A:THR:H	5	0.11
(1,835)	1:58:A:VAL:HG13	1:55:A:THR:H	5	0.11
(1,803)	1:56:A:SER:HA	1:57:A:LEU:H	1	0.11
(1,803)	1:56:A:SER:HA	1:57:A:LEU:H	9	0.11
(1,779)	1:55:A:THR:HB	1:53:A:THR:H	5	0.11
(1,742)	1:53:A:THR:HB	1:55:A:THR:H	3	0.11
(1,742)	1:53:A:THR:HB	1:55:A:THR:H	4	0.11
(1,686)	1:47:A:ALA:H	1:49:A:LEU:H	3	0.11
(1,686)	1:47:A:ALA:H	1:49:A:LEU:H	8	0.11
(1,647)	1:45:A:ALA:H	1:46:A:PHE:HB3	7	0.11
(1,642)	1:45:A:ALA:HB1	1:44:A:ASP:H	3	0.11
(1,642)	1:45:A:ALA:HB2	1:44:A:ASP:H	3	0.11
(1,642)	1:45:A:ALA:HB3	1:44:A:ASP:H	3	0.11
(1,642)	1:45:A:ALA:HB1	1:44:A:ASP:H	4	0.11
(1,642)	1:45:A:ALA:HB2	1:44:A:ASP:H	4	0.11
(1,642)	1:45:A:ALA:HB3	1:44:A:ASP:H	4	0.11
(1,642)	1:45:A:ALA:HB1	1:44:A:ASP:H	8	0.11
(1,642)	1:45:A:ALA:HB2	1:44:A:ASP:H	8	0.11
(1,642)	1:45:A:ALA:HB3	1:44:A:ASP:H	8	0.11
(1,611)	1:42:A:ASN:HB2	1:112:A:LEU:HD11	3	0.11
(1,611)	1:42:A:ASN:HB2	1:112:A:LEU:HD12	3	0.11
(1,611)	1:42:A:ASN:HB2	1:112:A:LEU:HD13	3	0.11
(1,611)	1:42:A:ASN:HB2	1:112:A:LEU:HD11	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,611)	1:42:A:ASN:HB2	1:112:A:LEU:HD12	4	0.11
(1,611)	1:42:A:ASN:HB2	1:112:A:LEU:HD13	4	0.11
(1,596)	1:42:A:ASN:HB2	1:42:A:ASN:HD22	4	0.11
(1,575)	1:39:A:PHE:HA	1:124:A:HIS:HB3	4	0.11
(1,547)	1:37:A:THR:H	1:73:A:VAL:HG21	6	0.11
(1,547)	1:37:A:THR:H	1:73:A:VAL:HG22	6	0.11
(1,547)	1:37:A:THR:H	1:73:A:VAL:HG23	6	0.11
(1,547)	1:37:A:THR:H	1:73:A:VAL:HG21	9	0.11
(1,547)	1:37:A:THR:H	1:73:A:VAL:HG22	9	0.11
(1,547)	1:37:A:THR:H	1:73:A:VAL:HG23	9	0.11
(1,532)	1:36:A:PHE:H	1:122:A:ILE:H	10	0.11
(1,380)	1:26:A:LEU:HD22	1:66:A:ARG:HA	7	0.11
(1,290)	1:22:A:LYS:HG3	1:27:A:VAL:HG21	10	0.11
(1,290)	1:22:A:LYS:HG3	1:27:A:VAL:HG22	10	0.11
(1,290)	1:22:A:LYS:HG3	1:27:A:VAL:HG23	10	0.11
(1,252)	1:21:A:VAL:HG21	1:26:A:LEU:HA	3	0.11
(1,252)	1:21:A:VAL:HG22	1:26:A:LEU:HA	3	0.11
(1,252)	1:21:A:VAL:HG23	1:26:A:LEU:HA	3	0.11
(1,252)	1:21:A:VAL:HG21	1:26:A:LEU:HA	4	0.11
(1,252)	1:21:A:VAL:HG22	1:26:A:LEU:HA	4	0.11
(1,252)	1:21:A:VAL:HG23	1:26:A:LEU:HA	4	0.11
(1,252)	1:21:A:VAL:HG21	1:26:A:LEU:HA	6	0.11
(1,252)	1:21:A:VAL:HG22	1:26:A:LEU:HA	6	0.11
(1,252)	1:21:A:VAL:HG23	1:26:A:LEU:HA	6	0.11
(1,252)	1:21:A:VAL:HG21	1:26:A:LEU:HA	7	0.11
(1,252)	1:21:A:VAL:HG22	1:26:A:LEU:HA	7	0.11
(1,252)	1:21:A:VAL:HG23	1:26:A:LEU:HA	7	0.11
(1,246)	1:21:A:VAL:HG21	1:23:A:VAL:H	4	0.11
(1,246)	1:21:A:VAL:HG22	1:23:A:VAL:H	4	0.11
(1,246)	1:21:A:VAL:HG23	1:23:A:VAL:H	4	0.11
(1,246)	1:21:A:VAL:HG21	1:23:A:VAL:H	5	0.11
(1,246)	1:21:A:VAL:HG22	1:23:A:VAL:H	5	0.11
(1,246)	1:21:A:VAL:HG23	1:23:A:VAL:H	5	0.11
(1,246)	1:21:A:VAL:HG21	1:23:A:VAL:H	6	0.11
(1,246)	1:21:A:VAL:HG22	1:23:A:VAL:H	6	0.11
(1,246)	1:21:A:VAL:HG23	1:23:A:VAL:H	6	0.11
(1,246)	1:21:A:VAL:HG21	1:23:A:VAL:H	9	0.11
(1,246)	1:21:A:VAL:HG22	1:23:A:VAL:H	9	0.11
(1,246)	1:21:A:VAL:HG23	1:23:A:VAL:H	9	0.11
(1,230)	1:20:A:ALA:HB1	1:68:A:LEU:HD11	9	0.11
(1,230)	1:20:A:ALA:HB1	1:68:A:LEU:HD12	9	0.11
(1,230)	1:20:A:ALA:HB1	1:68:A:LEU:HD13	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,230)	1:20:A:ALA:HB2	1:68:A:LEU:HD11	9	0.11
(1,230)	1:20:A:ALA:HB2	1:68:A:LEU:HD12	9	0.11
(1,230)	1:20:A:ALA:HB2	1:68:A:LEU:HD13	9	0.11
(1,230)	1:20:A:ALA:HB3	1:68:A:LEU:HD11	9	0.11
(1,230)	1:20:A:ALA:HB3	1:68:A:LEU:HD12	9	0.11
(1,230)	1:20:A:ALA:HB3	1:68:A:LEU:HD13	9	0.11
(1,189)	1:18:A:VAL:H	1:16:A:THR:HA	3	0.11
(1,179)	1:18:A:VAL:HG21	1:8:A:ALA:HB1	6	0.11
(1,179)	1:18:A:VAL:HG21	1:8:A:ALA:HB2	6	0.11
(1,179)	1:18:A:VAL:HG21	1:8:A:ALA:HB3	6	0.11
(1,179)	1:18:A:VAL:HG22	1:8:A:ALA:HB1	6	0.11
(1,179)	1:18:A:VAL:HG22	1:8:A:ALA:HB2	6	0.11
(1,179)	1:18:A:VAL:HG22	1:8:A:ALA:HB3	6	0.11
(1,179)	1:18:A:VAL:HG23	1:8:A:ALA:HB1	6	0.11
(1,179)	1:18:A:VAL:HG23	1:8:A:ALA:HB2	6	0.11
(1,179)	1:18:A:VAL:HG23	1:8:A:ALA:HB3	6	0.11
(1,163)	1:14:A:PHE:HB3	1:14:A:PHE:H	3	0.11
(1,154)	1:12:A:PRO:HA	1:14:A:PHE:H	1	0.11
(1,154)	1:12:A:PRO:HA	1:14:A:PHE:H	2	0.11
(1,154)	1:12:A:PRO:HA	1:14:A:PHE:H	3	0.11
(1,154)	1:12:A:PRO:HA	1:14:A:PHE:H	4	0.11
(1,154)	1:12:A:PRO:HA	1:14:A:PHE:H	8	0.11
(1,154)	1:12:A:PRO:HA	1:14:A:PHE:H	9	0.11
(1,107)	1:8:A:ALA:HA	1:18:A:VAL:HG21	5	0.11
(1,107)	1:8:A:ALA:HA	1:18:A:VAL:HG22	5	0.11
(1,107)	1:8:A:ALA:HA	1:18:A:VAL:HG23	5	0.11
(1,107)	1:8:A:ALA:HA	1:18:A:VAL:HG21	10	0.11
(1,107)	1:8:A:ALA:HA	1:18:A:VAL:HG22	10	0.11
(1,107)	1:8:A:ALA:HA	1:18:A:VAL:HG23	10	0.11
(1,66)	1:7:A:ILE:HD11	1:5:A:VAL:H	10	0.11
(1,66)	1:7:A:ILE:HD12	1:5:A:VAL:H	10	0.11
(1,66)	1:7:A:ILE:HD13	1:5:A:VAL:H	10	0.11
(1,64)	1:6:A:ASP:HA	1:9:A:VAL:HB	2	0.11
(1,2075)	1:129:A:VAL:HG11	1:49:A:LEU:HA	7	0.1
(1,2075)	1:129:A:VAL:HG12	1:49:A:LEU:HA	7	0.1
(1,2075)	1:129:A:VAL:HG13	1:49:A:LEU:HA	7	0.1
(1,2033)	1:126:A:ILE:HG12	1:127:A:ASP:H	1	0.1
(1,1971)	1:124:A:HIS:HB3	1:114:A:ALA:HB1	1	0.1
(1,1971)	1:124:A:HIS:HB3	1:114:A:ALA:HB2	1	0.1
(1,1971)	1:124:A:HIS:HB3	1:114:A:ALA:HB3	1	0.1
(1,1942)	1:122:A:ILE:HD11	1:123:A:ILE:H	7	0.1
(1,1942)	1:122:A:ILE:HD12	1:123:A:ILE:H	7	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1942)	1:122:A:ILE:HD13	1:123:A:ILE:H	7	0.1
(1,1939)	1:122:A:ILE:H	1:122:A:ILE:HG21	2	0.1
(1,1939)	1:122:A:ILE:H	1:122:A:ILE:HG22	2	0.1
(1,1939)	1:122:A:ILE:H	1:122:A:ILE:HG23	2	0.1
(1,1939)	1:122:A:ILE:H	1:122:A:ILE:HG21	10	0.1
(1,1939)	1:122:A:ILE:H	1:122:A:ILE:HG22	10	0.1
(1,1939)	1:122:A:ILE:H	1:122:A:ILE:HG23	10	0.1
(1,1926)	1:122:A:ILE:H	1:121:A:GLY:HA2	2	0.1
(1,1903)	1:122:A:ILE:HB	1:38:A:VAL:H	7	0.1
(1,1868)	1:118:A:ALA:HA	1:121:A:GLY:H	9	0.1
(1,1840)	1:117:A:GLU:H	1:116:A:ILE:H	10	0.1
(1,1793)	1:114:A:ALA:HB1	1:114:A:ALA:H	4	0.1
(1,1793)	1:114:A:ALA:HB2	1:114:A:ALA:H	4	0.1
(1,1793)	1:114:A:ALA:HB3	1:114:A:ALA:H	4	0.1
(1,1793)	1:114:A:ALA:HB1	1:114:A:ALA:H	8	0.1
(1,1793)	1:114:A:ALA:HB2	1:114:A:ALA:H	8	0.1
(1,1793)	1:114:A:ALA:HB3	1:114:A:ALA:H	8	0.1
(1,1762)	1:112:A:LEU:HD11	1:112:A:LEU:HA	8	0.1
(1,1762)	1:112:A:LEU:HD12	1:112:A:LEU:HA	8	0.1
(1,1762)	1:112:A:LEU:HD13	1:112:A:LEU:HA	8	0.1
(1,1697)	1:107:A:LYS:HG2	1:109:A:ALA:H	5	0.1
(1,1599)	1:103:A:PRO:HB3	1:111:A:VAL:H	1	0.1
(1,1546)	1:98:A:ILE:HG21	1:98:A:ILE:H	4	0.1
(1,1546)	1:98:A:ILE:HG22	1:98:A:ILE:H	4	0.1
(1,1546)	1:98:A:ILE:HG23	1:98:A:ILE:H	4	0.1
(1,1438)	1:91:A:LEU:HB2	1:92:A:GLU:H	6	0.1
(1,1438)	1:91:A:LEU:HB2	1:92:A:GLU:H	7	0.1
(1,1418)	1:91:A:LEU:HG	1:74:A:ALA:H	10	0.1
(1,1416)	1:91:A:LEU:HA	1:74:A:ALA:HB1	3	0.1
(1,1416)	1:91:A:LEU:HA	1:74:A:ALA:HB2	3	0.1
(1,1416)	1:91:A:LEU:HA	1:74:A:ALA:HB3	3	0.1
(1,1407)	1:91:A:LEU:HD11	1:29:A:ALA:HB1	1	0.1
(1,1407)	1:91:A:LEU:HD11	1:29:A:ALA:HB2	1	0.1
(1,1407)	1:91:A:LEU:HD11	1:29:A:ALA:HB3	1	0.1
(1,1407)	1:91:A:LEU:HD12	1:29:A:ALA:HB1	1	0.1
(1,1407)	1:91:A:LEU:HD12	1:29:A:ALA:HB2	1	0.1
(1,1407)	1:91:A:LEU:HD12	1:29:A:ALA:HB3	1	0.1
(1,1407)	1:91:A:LEU:HD13	1:29:A:ALA:HB1	1	0.1
(1,1407)	1:91:A:LEU:HD13	1:29:A:ALA:HB2	1	0.1
(1,1407)	1:91:A:LEU:HD13	1:29:A:ALA:HB3	1	0.1
(1,1394)	1:89:A:THR:HG21	1:95:A:THR:H	5	0.1
(1,1394)	1:89:A:THR:HG22	1:95:A:THR:H	5	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1394)	1:89:A:THR:HG23	1:95:A:THR:H	5	0.1
(1,1378)	1:88:A:VAL:H	1:98:A:ILE:HD11	9	0.1
(1,1378)	1:88:A:VAL:H	1:98:A:ILE:HD12	9	0.1
(1,1378)	1:88:A:VAL:H	1:98:A:ILE:HD13	9	0.1
(1,1341)	1:87:A:ILE:HG21	1:88:A:VAL:H	1	0.1
(1,1341)	1:87:A:ILE:HG22	1:88:A:VAL:H	1	0.1
(1,1341)	1:87:A:ILE:HG23	1:88:A:VAL:H	1	0.1
(1,1341)	1:87:A:ILE:HG21	1:88:A:VAL:H	5	0.1
(1,1341)	1:87:A:ILE:HG22	1:88:A:VAL:H	5	0.1
(1,1341)	1:87:A:ILE:HG23	1:88:A:VAL:H	5	0.1
(1,1341)	1:87:A:ILE:HG21	1:88:A:VAL:H	10	0.1
(1,1341)	1:87:A:ILE:HG22	1:88:A:VAL:H	10	0.1
(1,1341)	1:87:A:ILE:HG23	1:88:A:VAL:H	10	0.1
(1,1296)	1:85:A:MET:H	1:85:A:MET:HG2	3	0.1
(1,1283)	1:84:A:ARG:HB2	1:85:A:MET:H	7	0.1
(1,1283)	1:84:A:ARG:HB2	1:85:A:MET:H	10	0.1
(1,1224)	1:82:A:LEU:H	1:82:A:LEU:HG	1	0.1
(1,1169)	1:78:A:LYS:HG2	1:122:A:ILE:HD11	4	0.1
(1,1169)	1:78:A:LYS:HG2	1:122:A:ILE:HD12	4	0.1
(1,1169)	1:78:A:LYS:HG2	1:122:A:ILE:HD13	4	0.1
(1,1169)	1:78:A:LYS:HG2	1:122:A:ILE:HD11	6	0.1
(1,1169)	1:78:A:LYS:HG2	1:122:A:ILE:HD12	6	0.1
(1,1169)	1:78:A:LYS:HG2	1:122:A:ILE:HD13	6	0.1
(1,1163)	1:78:A:LYS:H	1:80:A:THR:H	5	0.1
(1,1136)	1:77:A:TYR:H	1:121:A:GLY:HA3	4	0.1
(1,1133)	1:77:A:TYR:HB2	1:82:A:LEU:HG	4	0.1
(1,1122)	1:76:A:ALA:H	1:77:A:TYR:H	1	0.1
(1,1122)	1:76:A:ALA:H	1:77:A:TYR:H	3	0.1
(1,1122)	1:76:A:ALA:H	1:77:A:TYR:H	5	0.1
(1,1095)	1:74:A:ALA:HA	1:36:A:PHE:H	7	0.1
(1,1063)	1:71:A:HIS:HB2	1:71:A:HIS:H	2	0.1
(1,1063)	1:71:A:HIS:HB3	1:71:A:HIS:H	2	0.1
(1,953)	1:64:A:LEU:HD12	1:64:A:LEU:HG	4	0.1
(1,911)	1:62:A:PRO:HB3	1:62:A:PRO:HG2	7	0.1
(1,865)	1:59:A:GLN:HG3	1:59:A:GLN:H	2	0.1
(1,830)	1:57:A:LEU:HB3	1:58:A:VAL:H	5	0.1
(1,803)	1:56:A:SER:HA	1:57:A:LEU:H	6	0.1
(1,803)	1:56:A:SER:HA	1:57:A:LEU:H	7	0.1
(1,803)	1:56:A:SER:HA	1:57:A:LEU:H	10	0.1
(1,794)	1:55:A:THR:HG21	1:59:A:GLN:HE22	6	0.1
(1,794)	1:55:A:THR:HG22	1:59:A:GLN:HE22	6	0.1
(1,794)	1:55:A:THR:HG23	1:59:A:GLN:HE22	6	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,791)	1:55:A:THR:HG21	1:58:A:VAL:H	8	0.1
(1,791)	1:55:A:THR:HG22	1:58:A:VAL:H	8	0.1
(1,791)	1:55:A:THR:HG23	1:58:A:VAL:H	8	0.1
(1,779)	1:55:A:THR:HB	1:53:A:THR:H	1	0.1
(1,742)	1:53:A:THR:HB	1:55:A:THR:H	1	0.1
(1,686)	1:47:A:ALA:H	1:49:A:LEU:H	1	0.1
(1,686)	1:47:A:ALA:H	1:49:A:LEU:H	2	0.1
(1,611)	1:42:A:ASN:HB2	1:112:A:LEU:HD11	7	0.1
(1,611)	1:42:A:ASN:HB2	1:112:A:LEU:HD12	7	0.1
(1,611)	1:42:A:ASN:HB2	1:112:A:LEU:HD13	7	0.1
(1,538)	1:37:A:THR:HG21	1:37:A:THR:H	2	0.1
(1,538)	1:37:A:THR:HG22	1:37:A:THR:H	2	0.1
(1,538)	1:37:A:THR:HG23	1:37:A:THR:H	2	0.1
(1,479)	1:33:A:PRO:HG3	1:34:A:GLY:H	6	0.1
(1,427)	1:30:A:LEU:HD11	1:31:A:GLN:H	1	0.1
(1,427)	1:30:A:LEU:HD12	1:31:A:GLN:H	1	0.1
(1,427)	1:30:A:LEU:HD13	1:31:A:GLN:H	1	0.1
(1,321)	1:24:A:ALA:HB1	1:62:A:PRO:HB2	4	0.1
(1,321)	1:24:A:ALA:HB2	1:62:A:PRO:HB2	4	0.1
(1,321)	1:24:A:ALA:HB3	1:62:A:PRO:HB2	4	0.1
(1,304)	1:23:A:VAL:HG11	1:24:A:ALA:HB1	5	0.1
(1,304)	1:23:A:VAL:HG11	1:24:A:ALA:HB2	5	0.1
(1,304)	1:23:A:VAL:HG11	1:24:A:ALA:HB3	5	0.1
(1,304)	1:23:A:VAL:HG12	1:24:A:ALA:HB1	5	0.1
(1,304)	1:23:A:VAL:HG12	1:24:A:ALA:HB2	5	0.1
(1,304)	1:23:A:VAL:HG12	1:24:A:ALA:HB3	5	0.1
(1,304)	1:23:A:VAL:HG13	1:24:A:ALA:HB1	5	0.1
(1,304)	1:23:A:VAL:HG13	1:24:A:ALA:HB2	5	0.1
(1,304)	1:23:A:VAL:HG13	1:24:A:ALA:HB3	5	0.1
(1,280)	1:22:A:LYS:HG2	1:22:A:LYS:H	5	0.1
(1,252)	1:21:A:VAL:HG21	1:26:A:LEU:HA	10	0.1
(1,252)	1:21:A:VAL:HG22	1:26:A:LEU:HA	10	0.1
(1,252)	1:21:A:VAL:HG23	1:26:A:LEU:HA	10	0.1
(1,246)	1:21:A:VAL:HG21	1:23:A:VAL:H	10	0.1
(1,246)	1:21:A:VAL:HG22	1:23:A:VAL:H	10	0.1
(1,246)	1:21:A:VAL:HG23	1:23:A:VAL:H	10	0.1
(1,230)	1:20:A:ALA:HB1	1:68:A:LEU:HD11	8	0.1
(1,230)	1:20:A:ALA:HB1	1:68:A:LEU:HD12	8	0.1
(1,230)	1:20:A:ALA:HB1	1:68:A:LEU:HD13	8	0.1
(1,230)	1:20:A:ALA:HB2	1:68:A:LEU:HD11	8	0.1
(1,230)	1:20:A:ALA:HB2	1:68:A:LEU:HD12	8	0.1
(1,230)	1:20:A:ALA:HB2	1:68:A:LEU:HD13	8	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,230)	1:20:A:ALA:HB3	1:68:A:LEU:HD11	8	0.1
(1,230)	1:20:A:ALA:HB3	1:68:A:LEU:HD12	8	0.1
(1,230)	1:20:A:ALA:HB3	1:68:A:LEU:HD13	8	0.1
(1,227)	1:20:A:ALA:HB1	1:64:A:LEU:HD11	9	0.1
(1,227)	1:20:A:ALA:HB1	1:64:A:LEU:HD12	9	0.1
(1,227)	1:20:A:ALA:HB1	1:64:A:LEU:HD13	9	0.1
(1,227)	1:20:A:ALA:HB2	1:64:A:LEU:HD11	9	0.1
(1,227)	1:20:A:ALA:HB2	1:64:A:LEU:HD12	9	0.1
(1,227)	1:20:A:ALA:HB2	1:64:A:LEU:HD13	9	0.1
(1,227)	1:20:A:ALA:HB3	1:64:A:LEU:HD11	9	0.1
(1,227)	1:20:A:ALA:HB3	1:64:A:LEU:HD12	9	0.1
(1,227)	1:20:A:ALA:HB3	1:64:A:LEU:HD13	9	0.1
(1,203)	1:18:A:VAL:HA	1:21:A:VAL:HG11	3	0.1
(1,203)	1:18:A:VAL:HA	1:21:A:VAL:HG12	3	0.1
(1,203)	1:18:A:VAL:HA	1:21:A:VAL:HG13	3	0.1
(1,189)	1:18:A:VAL:H	1:16:A:THR:HA	10	0.1

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

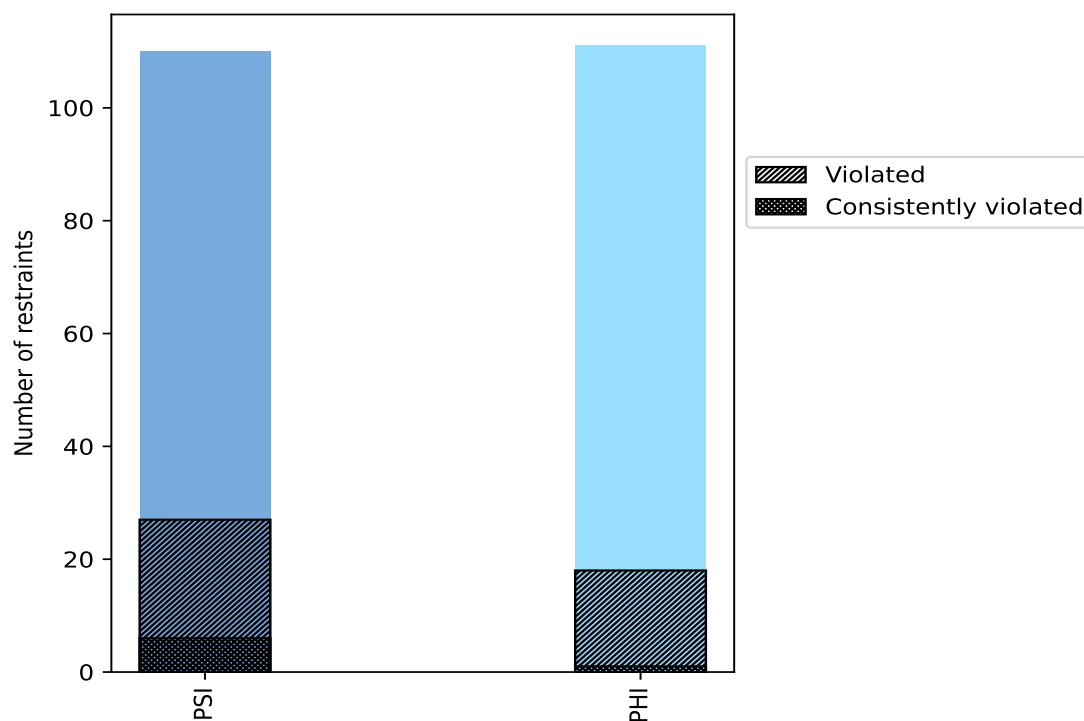
10.1 Summary of dihedral-angle violations [i](#)

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

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PSI	110	49.8	27	24.5	12.2	6	5.5	2.7
PHI	111	50.2	18	16.2	8.1	1	0.9	0.5
Total	221	100.0	45	20.4	20.4	7	3.2	3.2

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

10.1.1 Bar chart : Distribution of dihedral-angles and violations [i](#)



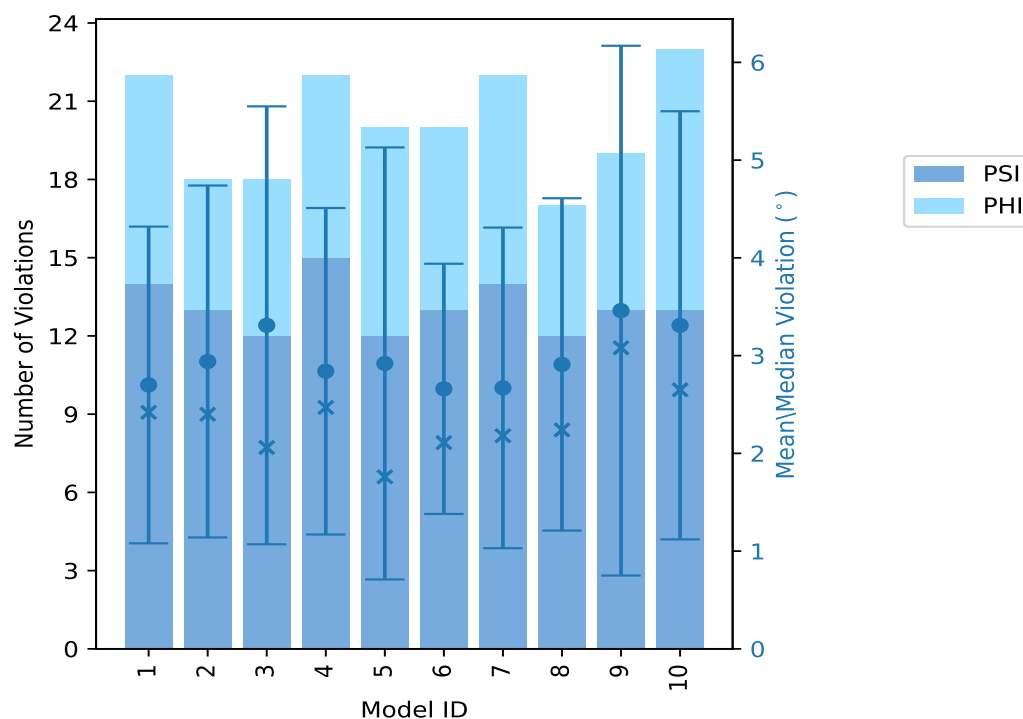
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	PHI	Total				
1	14	8	22	2.7	8.24	1.62	2.42
2	13	5	18	2.94	8.99	1.8	2.4
3	12	6	18	3.31	8.67	2.24	2.06
4	15	7	22	2.84	7.37	1.67	2.47
5	12	8	20	2.92	9.2	2.21	1.76
6	13	7	20	2.66	6.29	1.28	2.11
7	14	8	22	2.67	7.97	1.64	2.18
8	12	5	17	2.91	7.67	1.7	2.24
9	13	6	19	3.46	12.71	2.71	3.08
10	13	10	23	3.31	11.1	2.19	2.65

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



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

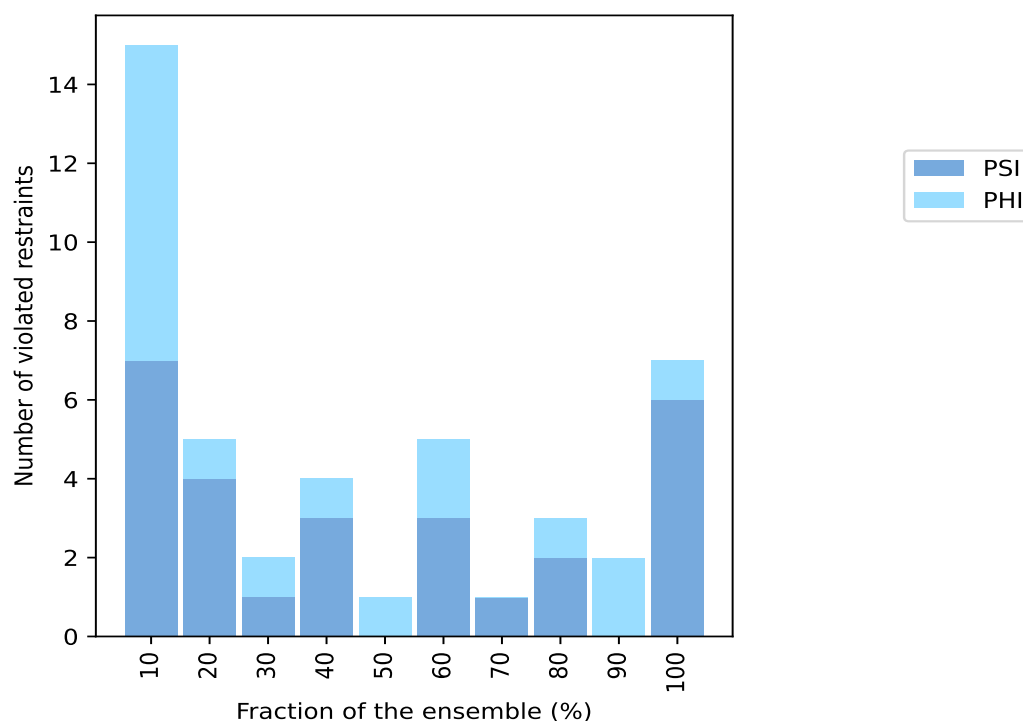
10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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

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

¹ Number of models with violations

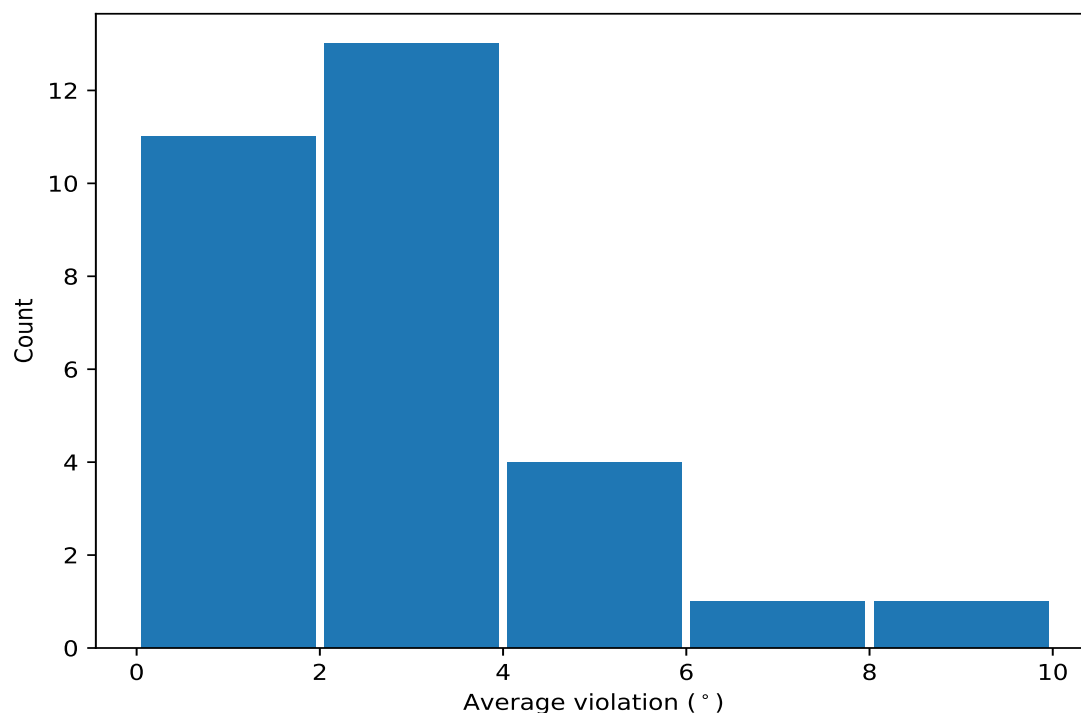
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,98)	1:60:A:ASN:N	1:60:A:ASN:CA	1:60:A:ASN:C	1:61:A:PRO:N	10	8.28	1.82	8.1
(1,116)	1:69:A:LYS:N	1:69:A:LYS:CA	1:69:A:LYS:C	1:70:A:TYR:N	10	5.23	2.28	4.94
(1,172)	1:99:A:HIS:N	1:99:A:HIS:CA	1:99:A:HIS:C	1:100:A:GLY:N	10	4.48	1.41	5.0
(1,162)	1:94:A:SER:N	1:94:A:SER:CA	1:94:A:SER:C	1:95:A:THR:N	10	4.1	0.97	4.03
(1,149)	1:86:A:GLY:C	1:87:A:ILE:N	1:87:A:ILE:CA	1:87:A:ILE:C	10	3.49	0.5	3.34
(1,196)	1:114:A:ALA:N	1:114:A:ALA:CA	1:114:A:ALA:C	1:115:A:ASP:N	10	2.98	0.71	3.06
(1,176)	1:103:A:PRO:N	1:103:A:PRO:CA	1:103:A:PRO:C	1:104:A:LEU:N	10	2.11	0.44	2.26
(1,117)	1:69:A:LYS:C	1:70:A:TYR:N	1:70:A:TYR:CA	1:70:A:TYR:C	9	4.24	1.46	4.19
(1,99)	1:60:A:ASN:C	1:61:A:PRO:N	1:61:A:PRO:CA	1:61:A:PRO:C	9	3.0	0.95	3.14
(1,102)	1:62:A:PRO:N	1:62:A:PRO:CA	1:62:A:PRO:C	1:63:A:GLN:N	8	2.57	0.88	2.6
(1,100)	1:61:A:PRO:N	1:61:A:PRO:CA	1:61:A:PRO:C	1:62:A:PRO:N	8	2.3	0.78	1.84
(1,25)	1:17:A:LEU:C	1:18:A:VAL:N	1:18:A:VAL:CA	1:18:A:VAL:C	8	2.0	0.99	1.88
(1,22)	1:16:A:THR:N	1:16:A:THR:CA	1:16:A:THR:C	1:17:A:LEU:N	7	1.71	0.38	1.73

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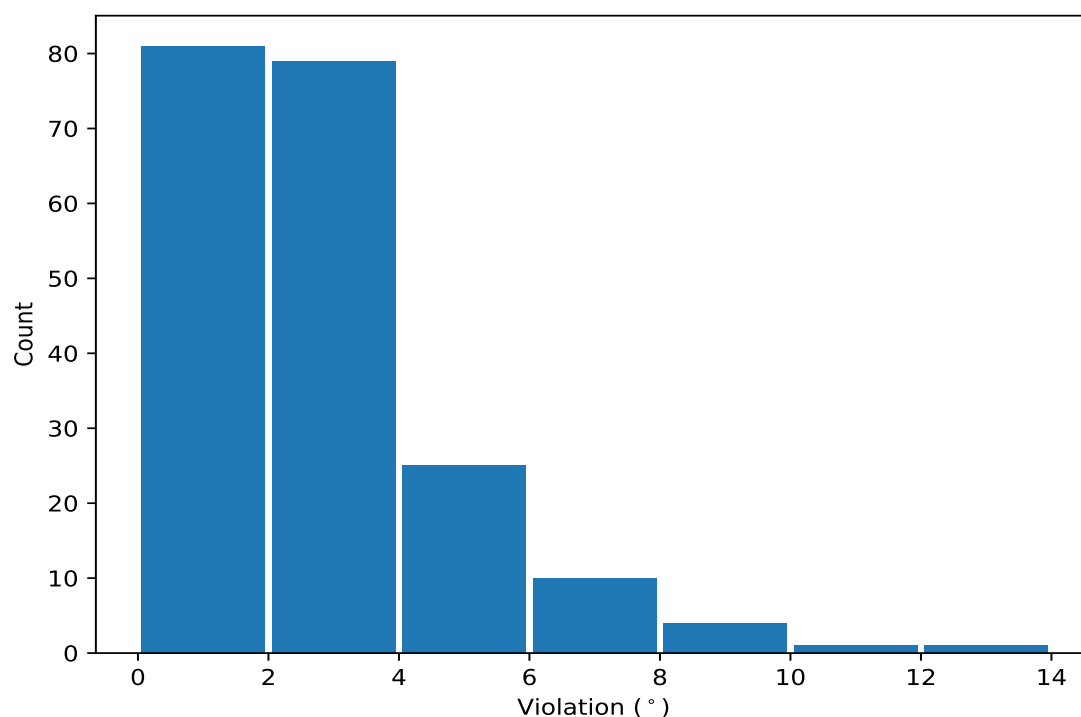
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,200)	1:116:A:ILE:N	1:116:A:ILE:CA	1:116:A:ILE:C	1:117:A:GLU:N	6	3.1	1.61	2.82
(1,198)	1:115:A:ASP:N	1:115:A:ASP:CA	1:115:A:ASP:C	1:116:A:ILE:N	6	2.23	0.6	2.13
(1,207)	1:119:A:GLU:C	1:120:A:ASN:N	1:120:A:ASN:CA	1:120:A:ASN:C	6	2.03	0.68	1.92
(1,55)	1:32:A:SER:C	1:33:A:PRO:N	1:33:A:PRO:CA	1:33:A:PRO:C	6	1.42	0.29	1.46
(1,16)	1:10:A:ASN:N	1:10:A:ASN:CA	1:10:A:ASN:C	1:11:A:THR:N	6	1.26	0.09	1.28
(1,103)	1:62:A:PRO:C	1:63:A:GLN:N	1:63:A:GLN:CA	1:63:A:GLN:C	5	2.21	0.38	2.1
(1,114)	1:68:A:LEU:N	1:68:A:LEU:CA	1:68:A:LEU:C	1:69:A:LYS:N	4	2.53	1.05	2.45
(1,115)	1:68:A:LEU:C	1:69:A:LYS:N	1:69:A:LYS:CA	1:69:A:LYS:C	4	2.27	0.49	2.38
(1,86)	1:54:A:ILE:N	1:54:A:ILE:CA	1:54:A:ILE:C	1:55:A:THR:N	4	1.53	0.38	1.54
(1,78)	1:46:A:PHE:N	1:46:A:PHE:CA	1:46:A:PHE:C	1:47:A:ALA:N	4	1.41	0.27	1.33
(1,201)	1:116:A:ILE:C	1:117:A:GLU:N	1:117:A:GLU:CA	1:117:A:GLU:C	3	1.7	0.47	1.88
(1,60)	1:36:A:PHE:N	1:36:A:PHE:CA	1:36:A:PHE:C	1:37:A:THR:N	3	1.34	0.26	1.33
(1,92)	1:57:A:LEU:N	1:57:A:LEU:CA	1:57:A:LEU:C	1:58:A:VAL:N	2	6.21	0.5	6.21
(1,2)	1:3:A:THR:N	1:3:A:THR:CA	1:3:A:THR:C	1:4:A:ILE:N	2	1.64	0.29	1.64
(1,5)	1:4:A:ILE:C	1:5:A:VAL:N	1:5:A:VAL:CA	1:5:A:VAL:C	2	1.44	0.36	1.44
(1,18)	1:13:A:GLY:N	1:13:A:GLY:CA	1:13:A:GLY:C	1:14:A:PHE:N	2	1.17	0.04	1.17
(1,10)	1:7:A:ILE:N	1:7:A:ILE:CA	1:7:A:ILE:C	1:8:A:ALA:N	2	1.1	0.04	1.1

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

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

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

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



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,98)	1:60:A:ASN:N	1:60:A:ASN:CA	1:60:A:ASN:C	1:61:A:PRO:N	9	12.71
(1,116)	1:69:A:LYS:N	1:69:A:LYS:CA	1:69:A:LYS:C	1:70:A:TYR:N	10	11.1
(1,98)	1:60:A:ASN:N	1:60:A:ASN:CA	1:60:A:ASN:C	1:61:A:PRO:N	5	9.2
(1,98)	1:60:A:ASN:N	1:60:A:ASN:CA	1:60:A:ASN:C	1:61:A:PRO:N	2	8.99
(1,98)	1:60:A:ASN:N	1:60:A:ASN:CA	1:60:A:ASN:C	1:61:A:PRO:N	3	8.67
(1,98)	1:60:A:ASN:N	1:60:A:ASN:CA	1:60:A:ASN:C	1:61:A:PRO:N	1	8.24
(1,98)	1:60:A:ASN:N	1:60:A:ASN:CA	1:60:A:ASN:C	1:61:A:PRO:N	7	7.97
(1,98)	1:60:A:ASN:N	1:60:A:ASN:CA	1:60:A:ASN:C	1:61:A:PRO:N	8	7.67
(1,98)	1:60:A:ASN:N	1:60:A:ASN:CA	1:60:A:ASN:C	1:61:A:PRO:N	4	7.37
(1,92)	1:57:A:LEU:N	1:57:A:LEU:CA	1:57:A:LEU:C	1:58:A:VAL:N	9	6.71
(1,116)	1:69:A:LYS:N	1:69:A:LYS:CA	1:69:A:LYS:C	1:70:A:TYR:N	5	6.36
(1,98)	1:60:A:ASN:N	1:60:A:ASN:CA	1:60:A:ASN:C	1:61:A:PRO:N	6	6.29
(1,200)	1:116:A:ILE:N	1:116:A:ILE:CA	1:116:A:ILE:C	1:117:A:GLU:N	4	6.28
(1,117)	1:69:A:LYS:C	1:70:A:TYR:N	1:70:A:TYR:CA	1:70:A:TYR:C	10	6.26
(1,172)	1:99:A:HIS:N	1:99:A:HIS:CA	1:99:A:HIS:C	1:100:A:GLY:N	7	6.09
(1,162)	1:94:A:SER:N	1:94:A:SER:CA	1:94:A:SER:C	1:95:A:THR:N	3	6.05
(1,172)	1:99:A:HIS:N	1:99:A:HIS:CA	1:99:A:HIS:C	1:100:A:GLY:N	9	5.98
(1,116)	1:69:A:LYS:N	1:69:A:LYS:CA	1:69:A:LYS:C	1:70:A:TYR:N	3	5.9
(1,117)	1:69:A:LYS:C	1:70:A:TYR:N	1:70:A:TYR:CA	1:70:A:TYR:C	5	5.78
(1,92)	1:57:A:LEU:N	1:57:A:LEU:CA	1:57:A:LEU:C	1:58:A:VAL:N	3	5.71
(1,117)	1:69:A:LYS:C	1:70:A:TYR:N	1:70:A:TYR:CA	1:70:A:TYR:C	3	5.69
(1,98)	1:60:A:ASN:N	1:60:A:ASN:CA	1:60:A:ASN:C	1:61:A:PRO:N	10	5.68
(1,172)	1:99:A:HIS:N	1:99:A:HIS:CA	1:99:A:HIS:C	1:100:A:GLY:N	1	5.66
(1,172)	1:99:A:HIS:N	1:99:A:HIS:CA	1:99:A:HIS:C	1:100:A:GLY:N	5	5.63
(1,172)	1:99:A:HIS:N	1:99:A:HIS:CA	1:99:A:HIS:C	1:100:A:GLY:N	3	5.13
(1,162)	1:94:A:SER:N	1:94:A:SER:CA	1:94:A:SER:C	1:95:A:THR:N	10	5.09
(1,116)	1:69:A:LYS:N	1:69:A:LYS:CA	1:69:A:LYS:C	1:70:A:TYR:N	8	4.99
(1,116)	1:69:A:LYS:N	1:69:A:LYS:CA	1:69:A:LYS:C	1:70:A:TYR:N	4	4.96
(1,116)	1:69:A:LYS:N	1:69:A:LYS:CA	1:69:A:LYS:C	1:70:A:TYR:N	9	4.91
(1,172)	1:99:A:HIS:N	1:99:A:HIS:CA	1:99:A:HIS:C	1:100:A:GLY:N	10	4.88
(1,117)	1:69:A:LYS:C	1:70:A:TYR:N	1:70:A:TYR:CA	1:70:A:TYR:C	8	4.77
(1,149)	1:86:A:GLY:C	1:87:A:ILE:N	1:87:A:ILE:CA	1:87:A:ILE:C	2	4.59
(1,162)	1:94:A:SER:N	1:94:A:SER:CA	1:94:A:SER:C	1:95:A:THR:N	5	4.54
(1,25)	1:17:A:LEU:C	1:18:A:VAL:N	1:18:A:VAL:CA	1:18:A:VAL:C	7	4.36
(1,116)	1:69:A:LYS:N	1:69:A:LYS:CA	1:69:A:LYS:C	1:70:A:TYR:N	6	4.35
(1,99)	1:60:A:ASN:C	1:61:A:PRO:N	1:61:A:PRO:CA	1:61:A:PRO:C	2	4.24
(1,117)	1:69:A:LYS:C	1:70:A:TYR:N	1:70:A:TYR:CA	1:70:A:TYR:C	4	4.19
(1,117)	1:69:A:LYS:C	1:70:A:TYR:N	1:70:A:TYR:CA	1:70:A:TYR:C	9	4.11
(1,162)	1:94:A:SER:N	1:94:A:SER:CA	1:94:A:SER:C	1:95:A:THR:N	8	4.07
(1,162)	1:94:A:SER:N	1:94:A:SER:CA	1:94:A:SER:C	1:95:A:THR:N	6	4.06
(1,149)	1:86:A:GLY:C	1:87:A:ILE:N	1:87:A:ILE:CA	1:87:A:ILE:C	6	4.03
(1,162)	1:94:A:SER:N	1:94:A:SER:CA	1:94:A:SER:C	1:95:A:THR:N	9	3.99
(1,114)	1:68:A:LEU:N	1:68:A:LEU:CA	1:68:A:LEU:C	1:69:A:LYS:N	10	3.99
(1,99)	1:60:A:ASN:C	1:61:A:PRO:N	1:61:A:PRO:CA	1:61:A:PRO:C	5	3.99
(1,100)	1:61:A:PRO:N	1:61:A:PRO:CA	1:61:A:PRO:C	1:62:A:PRO:N	2	3.97
(1,116)	1:69:A:LYS:N	1:69:A:LYS:CA	1:69:A:LYS:C	1:70:A:TYR:N	1	3.96
(1,162)	1:94:A:SER:N	1:94:A:SER:CA	1:94:A:SER:C	1:95:A:THR:N	4	3.94

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,102)	1:62:A:PRO:N	1:62:A:PRO:CA	1:62:A:PRO:C	1:63:A:GLN:N	4	3.89
(1,149)	1:86:A:GLY:C	1:87:A:ILE:N	1:87:A:ILE:CA	1:87:A:ILE:C	10	3.86
(1,196)	1:114:A:ALA:N	1:114:A:ALA:CA	1:114:A:ALA:C	1:115:A:ASP:N	10	3.85
(1,99)	1:60:A:ASN:C	1:61:A:PRO:N	1:61:A:PRO:CA	1:61:A:PRO:C	8	3.85
(1,116)	1:69:A:LYS:N	1:69:A:LYS:CA	1:69:A:LYS:C	1:70:A:TYR:N	7	3.84
(1,162)	1:94:A:SER:N	1:94:A:SER:CA	1:94:A:SER:C	1:95:A:THR:N	2	3.81
(1,196)	1:114:A:ALA:N	1:114:A:ALA:CA	1:114:A:ALA:C	1:115:A:ASP:N	3	3.71
(1,172)	1:99:A:HIS:N	1:99:A:HIS:CA	1:99:A:HIS:C	1:100:A:GLY:N	6	3.7
(1,196)	1:114:A:ALA:N	1:114:A:ALA:CA	1:114:A:ALA:C	1:115:A:ASP:N	2	3.52
(1,149)	1:86:A:GLY:C	1:87:A:ILE:N	1:87:A:ILE:CA	1:87:A:ILE:C	4	3.47
(1,102)	1:62:A:PRO:N	1:62:A:PRO:CA	1:62:A:PRO:C	1:63:A:GLN:N	10	3.45
(1,200)	1:116:A:ILE:N	1:116:A:ILE:CA	1:116:A:ILE:C	1:117:A:GLU:N	1	3.43
(1,196)	1:114:A:ALA:N	1:114:A:ALA:CA	1:114:A:ALA:C	1:115:A:ASP:N	9	3.43
(1,149)	1:86:A:GLY:C	1:87:A:ILE:N	1:87:A:ILE:CA	1:87:A:ILE:C	7	3.42
(1,149)	1:86:A:GLY:C	1:87:A:ILE:N	1:87:A:ILE:CA	1:87:A:ILE:C	3	3.27
(1,196)	1:114:A:ALA:N	1:114:A:ALA:CA	1:114:A:ALA:C	1:115:A:ASP:N	8	3.22
(1,162)	1:94:A:SER:N	1:94:A:SER:CA	1:94:A:SER:C	1:95:A:THR:N	1	3.2
(1,117)	1:69:A:LYS:C	1:70:A:TYR:N	1:70:A:TYR:CA	1:70:A:TYR:C	6	3.19
(1,149)	1:86:A:GLY:C	1:87:A:ILE:N	1:87:A:ILE:CA	1:87:A:ILE:C	9	3.17
(1,99)	1:60:A:ASN:C	1:61:A:PRO:N	1:61:A:PRO:CA	1:61:A:PRO:C	9	3.16
(1,149)	1:86:A:GLY:C	1:87:A:ILE:N	1:87:A:ILE:CA	1:87:A:ILE:C	8	3.15
(1,102)	1:62:A:PRO:N	1:62:A:PRO:CA	1:62:A:PRO:C	1:63:A:GLN:N	1	3.14
(1,99)	1:60:A:ASN:C	1:61:A:PRO:N	1:61:A:PRO:CA	1:61:A:PRO:C	1	3.14
(1,149)	1:86:A:GLY:C	1:87:A:ILE:N	1:87:A:ILE:CA	1:87:A:ILE:C	1	3.12
(1,200)	1:116:A:ILE:N	1:116:A:ILE:CA	1:116:A:ILE:C	1:117:A:GLU:N	6	3.11
(1,207)	1:119:A:GLU:C	1:120:A:ASN:N	1:120:A:ASN:CA	1:120:A:ASN:C	9	3.08
(1,198)	1:115:A:ASP:N	1:115:A:ASP:CA	1:115:A:ASP:C	1:116:A:ILE:N	6	3.05
(1,172)	1:99:A:HIS:N	1:99:A:HIS:CA	1:99:A:HIS:C	1:100:A:GLY:N	8	3.04
(1,99)	1:60:A:ASN:C	1:61:A:PRO:N	1:61:A:PRO:CA	1:61:A:PRO:C	7	3.0
(1,114)	1:68:A:LEU:N	1:68:A:LEU:CA	1:68:A:LEU:C	1:69:A:LYS:N	1	2.99
(1,102)	1:62:A:PRO:N	1:62:A:PRO:CA	1:62:A:PRO:C	1:63:A:GLN:N	2	2.96
(1,198)	1:115:A:ASP:N	1:115:A:ASP:CA	1:115:A:ASP:C	1:116:A:ILE:N	4	2.9
(1,196)	1:114:A:ALA:N	1:114:A:ALA:CA	1:114:A:ALA:C	1:115:A:ASP:N	4	2.89
(1,196)	1:114:A:ALA:N	1:114:A:ALA:CA	1:114:A:ALA:C	1:115:A:ASP:N	7	2.87
(1,100)	1:61:A:PRO:N	1:61:A:PRO:CA	1:61:A:PRO:C	1:62:A:PRO:N	1	2.87
(1,149)	1:86:A:GLY:C	1:87:A:ILE:N	1:87:A:ILE:CA	1:87:A:ILE:C	5	2.84
(1,115)	1:68:A:LEU:C	1:69:A:LYS:N	1:69:A:LYS:CA	1:69:A:LYS:C	10	2.84
(1,100)	1:61:A:PRO:N	1:61:A:PRO:CA	1:61:A:PRO:C	1:62:A:PRO:N	10	2.82
(1,103)	1:62:A:PRO:C	1:63:A:GLN:N	1:63:A:GLN:CA	1:63:A:GLN:C	10	2.65
(1,103)	1:62:A:PRO:C	1:63:A:GLN:N	1:63:A:GLN:CA	1:63:A:GLN:C	2	2.63
(1,207)	1:119:A:GLU:C	1:120:A:ASN:N	1:120:A:ASN:CA	1:120:A:ASN:C	7	2.62
(1,176)	1:103:A:PRO:N	1:103:A:PRO:CA	1:103:A:PRO:C	1:104:A:LEU:N	4	2.59
(1,196)	1:114:A:ALA:N	1:114:A:ALA:CA	1:114:A:ALA:C	1:115:A:ASP:N	1	2.56
(1,200)	1:116:A:ILE:N	1:116:A:ILE:CA	1:116:A:ILE:C	1:117:A:GLU:N	10	2.54
(1,176)	1:103:A:PRO:N	1:103:A:PRO:CA	1:103:A:PRO:C	1:104:A:LEU:N	5	2.53
(1,172)	1:99:A:HIS:N	1:99:A:HIS:CA	1:99:A:HIS:C	1:100:A:GLY:N	4	2.52
(1,176)	1:103:A:PRO:N	1:103:A:PRO:CA	1:103:A:PRO:C	1:104:A:LEU:N	9	2.46
(1,176)	1:103:A:PRO:N	1:103:A:PRO:CA	1:103:A:PRO:C	1:104:A:LEU:N	7	2.44
(1,131)	1:77:A:TYR:C	1:78:A:LYS:N	1:78:A:LYS:CA	1:78:A:LYS:C	6	2.43
(1,198)	1:115:A:ASP:N	1:115:A:ASP:CA	1:115:A:ASP:C	1:116:A:ILE:N	10	2.42
(1,99)	1:60:A:ASN:C	1:61:A:PRO:N	1:61:A:PRO:CA	1:61:A:PRO:C	4	2.42

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,176)	1:103:A:PRO:N	1:103:A:PRO:CA	1:103:A:PRO:C	1:104:A:LEU:N	2	2.41
(1,196)	1:114:A:ALA:N	1:114:A:ALA:CA	1:114:A:ALA:C	1:115:A:ASP:N	5	2.4
(1,115)	1:68:A:LEU:C	1:69:A:LYS:N	1:69:A:LYS:CA	1:69:A:LYS:C	2	2.39
(1,115)	1:68:A:LEU:C	1:69:A:LYS:N	1:69:A:LYS:CA	1:69:A:LYS:C	7	2.36
(1,96)	1:59:A:GLN:N	1:59:A:GLN:CA	1:59:A:GLN:C	1:60:A:ASN:N	9	2.35
(1,25)	1:17:A:LEU:C	1:18:A:VAL:N	1:18:A:VAL:CA	1:18:A:VAL:C	9	2.3
(1,117)	1:69:A:LYS:C	1:70:A:TYR:N	1:70:A:TYR:CA	1:70:A:TYR:C	1	2.28
(1,102)	1:62:A:PRO:N	1:62:A:PRO:CA	1:62:A:PRO:C	1:63:A:GLN:N	8	2.24
(1,162)	1:94:A:SER:N	1:94:A:SER:CA	1:94:A:SER:C	1:95:A:THR:N	7	2.21
(1,172)	1:99:A:HIS:N	1:99:A:HIS:CA	1:99:A:HIS:C	1:100:A:GLY:N	2	2.2
(1,95)	1:58:A:VAL:C	1:59:A:GLN:N	1:59:A:GLN:CA	1:59:A:GLN:C	3	2.18
(1,207)	1:119:A:GLU:C	1:120:A:ASN:N	1:120:A:ASN:CA	1:120:A:ASN:C	10	2.16
(1,201)	1:116:A:ILE:C	1:117:A:GLU:N	1:117:A:GLU:CA	1:117:A:GLU:C	7	2.16
(1,200)	1:116:A:ILE:N	1:116:A:ILE:CA	1:116:A:ILE:C	1:117:A:GLU:N	2	2.15
(1,22)	1:16:A:THR:N	1:16:A:THR:CA	1:16:A:THR:C	1:17:A:LEU:N	4	2.15
(1,176)	1:103:A:PRO:N	1:103:A:PRO:CA	1:103:A:PRO:C	1:104:A:LEU:N	6	2.11
(1,22)	1:16:A:THR:N	1:16:A:THR:CA	1:16:A:THR:C	1:17:A:LEU:N	6	2.11
(1,103)	1:62:A:PRO:C	1:63:A:GLN:N	1:63:A:GLN:CA	1:63:A:GLN:C	4	2.1
(1,99)	1:60:A:ASN:C	1:61:A:PRO:N	1:61:A:PRO:CA	1:61:A:PRO:C	6	2.09
(1,102)	1:62:A:PRO:N	1:62:A:PRO:CA	1:62:A:PRO:C	1:63:A:GLN:N	6	2.04
(1,25)	1:17:A:LEU:C	1:18:A:VAL:N	1:18:A:VAL:CA	1:18:A:VAL:C	6	2.02
(1,176)	1:103:A:PRO:N	1:103:A:PRO:CA	1:103:A:PRO:C	1:104:A:LEU:N	8	2.01
(1,86)	1:54:A:ILE:N	1:54:A:ILE:CA	1:54:A:ILE:C	1:55:A:THR:N	8	1.98
(1,103)	1:62:A:PRO:C	1:63:A:GLN:N	1:63:A:GLN:CA	1:63:A:GLN:C	6	1.96
(1,25)	1:17:A:LEU:C	1:18:A:VAL:N	1:18:A:VAL:CA	1:18:A:VAL:C	3	1.95
(1,2)	1:3:A:THR:N	1:3:A:THR:CA	1:3:A:THR:C	1:4:A:ILE:N	1	1.94
(1,117)	1:69:A:LYS:C	1:70:A:TYR:N	1:70:A:TYR:CA	1:70:A:TYR:C	7	1.93
(1,22)	1:16:A:THR:N	1:16:A:THR:CA	1:16:A:THR:C	1:17:A:LEU:N	8	1.93
(1,116)	1:69:A:LYS:N	1:69:A:LYS:CA	1:69:A:LYS:C	1:70:A:TYR:N	2	1.91
(1,114)	1:68:A:LEU:N	1:68:A:LEU:CA	1:68:A:LEU:C	1:69:A:LYS:N	2	1.9
(1,100)	1:61:A:PRO:N	1:61:A:PRO:CA	1:61:A:PRO:C	1:62:A:PRO:N	7	1.89
(1,201)	1:116:A:ILE:C	1:117:A:GLU:N	1:117:A:GLU:CA	1:117:A:GLU:C	10	1.88
(1,198)	1:115:A:ASP:N	1:115:A:ASP:CA	1:115:A:ASP:C	1:116:A:ILE:N	1	1.84
(1,78)	1:46:A:PHE:N	1:46:A:PHE:CA	1:46:A:PHE:C	1:47:A:ALA:N	10	1.83
(1,86)	1:54:A:ILE:N	1:54:A:ILE:CA	1:54:A:ILE:C	1:55:A:THR:N	3	1.82
(1,25)	1:17:A:LEU:C	1:18:A:VAL:N	1:18:A:VAL:CA	1:18:A:VAL:C	10	1.8
(1,5)	1:4:A:ILE:C	1:5:A:VAL:N	1:5:A:VAL:CA	1:5:A:VAL:C	7	1.79
(1,102)	1:62:A:PRO:N	1:62:A:PRO:CA	1:62:A:PRO:C	1:63:A:GLN:N	7	1.78
(1,100)	1:61:A:PRO:N	1:61:A:PRO:CA	1:61:A:PRO:C	1:62:A:PRO:N	4	1.78
(1,55)	1:32:A:SER:C	1:33:A:PRO:N	1:33:A:PRO:CA	1:33:A:PRO:C	5	1.78
(1,100)	1:61:A:PRO:N	1:61:A:PRO:CA	1:61:A:PRO:C	1:62:A:PRO:N	5	1.74
(1,22)	1:16:A:THR:N	1:16:A:THR:CA	1:16:A:THR:C	1:17:A:LEU:N	3	1.73
(1,22)	1:16:A:THR:N	1:16:A:THR:CA	1:16:A:THR:C	1:17:A:LEU:N	7	1.72
(1,81)	1:47:A:ALA:C	1:48:A:LYS:N	1:48:A:LYS:CA	1:48:A:LYS:C	5	1.71
(1,100)	1:61:A:PRO:N	1:61:A:PRO:CA	1:61:A:PRO:C	1:62:A:PRO:N	6	1.7
(1,103)	1:62:A:PRO:C	1:63:A:GLN:N	1:63:A:GLN:CA	1:63:A:GLN:C	1	1.69
(1,176)	1:103:A:PRO:N	1:103:A:PRO:CA	1:103:A:PRO:C	1:104:A:LEU:N	10	1.68
(1,55)	1:32:A:SER:C	1:33:A:PRO:N	1:33:A:PRO:CA	1:33:A:PRO:C	10	1.68
(1,207)	1:119:A:GLU:C	1:120:A:ASN:N	1:120:A:ASN:CA	1:120:A:ASN:C	4	1.67
(1,60)	1:36:A:PHE:N	1:36:A:PHE:CA	1:36:A:PHE:C	1:37:A:THR:N	4	1.67
(1,134)	1:79:A:ALA:N	1:79:A:ALA:CA	1:79:A:ALA:C	1:80:A:THR:N	3	1.66

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,176)	1:103:A:PRO:N	1:103:A:PRO:CA	1:103:A:PRO:C	1:104:A:LEU:N	1	1.65
(1,100)	1:61:A:PRO:N	1:61:A:PRO:CA	1:61:A:PRO:C	1:62:A:PRO:N	8	1.65
(1,55)	1:32:A:SER:C	1:33:A:PRO:N	1:33:A:PRO:CA	1:33:A:PRO:C	2	1.63
(1,198)	1:115:A:ASP:N	1:115:A:ASP:CA	1:115:A:ASP:C	1:116:A:ILE:N	5	1.61
(1,46)	1:28:A:GLU:N	1:28:A:GLU:CA	1:28:A:GLU:C	1:29:A:ALA:N	9	1.59
(1,207)	1:119:A:GLU:C	1:120:A:ASN:N	1:120:A:ASN:CA	1:120:A:ASN:C	5	1.58
(1,198)	1:115:A:ASP:N	1:115:A:ASP:CA	1:115:A:ASP:C	1:116:A:ILE:N	7	1.55
(1,101)	1:61:A:PRO:C	1:62:A:PRO:N	1:62:A:PRO:CA	1:62:A:PRO:C	10	1.55
(1,40)	1:25:A:ASN:N	1:25:A:ASN:CA	1:25:A:ASN:C	1:26:A:LEU:N	3	1.54
(1,115)	1:68:A:LEU:C	1:69:A:LYS:N	1:69:A:LYS:CA	1:69:A:LYS:C	1	1.49
(1,78)	1:46:A:PHE:N	1:46:A:PHE:CA	1:46:A:PHE:C	1:47:A:ALA:N	8	1.46
(1,25)	1:17:A:LEU:C	1:18:A:VAL:N	1:18:A:VAL:CA	1:18:A:VAL:C	1	1.4
(1,16)	1:10:A:ASN:N	1:10:A:ASN:CA	1:10:A:ASN:C	1:11:A:THR:N	8	1.35
(1,2)	1:3:A:THR:N	1:3:A:THR:CA	1:3:A:THR:C	1:4:A:ILE:N	9	1.35
(1,16)	1:10:A:ASN:N	1:10:A:ASN:CA	1:10:A:ASN:C	1:11:A:THR:N	2	1.34
(1,196)	1:114:A:ALA:N	1:114:A:ALA:CA	1:114:A:ALA:C	1:115:A:ASP:N	6	1.33
(1,60)	1:36:A:PHE:N	1:36:A:PHE:CA	1:36:A:PHE:C	1:37:A:THR:N	7	1.33
(1,16)	1:10:A:ASN:N	1:10:A:ASN:CA	1:10:A:ASN:C	1:11:A:THR:N	4	1.33
(1,55)	1:32:A:SER:C	1:33:A:PRO:N	1:33:A:PRO:CA	1:33:A:PRO:C	6	1.28
(1,86)	1:54:A:ILE:N	1:54:A:ILE:CA	1:54:A:ILE:C	1:55:A:THR:N	5	1.27
(1,114)	1:68:A:LEU:N	1:68:A:LEU:CA	1:68:A:LEU:C	1:69:A:LYS:N	7	1.25
(1,122)	1:72:A:VAL:N	1:72:A:VAL:CA	1:72:A:VAL:C	1:73:A:VAL:N	6	1.24
(1,73)	1:43:A:ASP:C	1:44:A:ASP:N	1:44:A:ASP:CA	1:44:A:ASP:C	1	1.24
(1,63)	1:38:A:VAL:C	1:39:A:PHE:N	1:39:A:PHE:CA	1:39:A:PHE:C	1	1.24
(1,22)	1:16:A:THR:N	1:16:A:THR:CA	1:16:A:THR:C	1:17:A:LEU:N	5	1.24
(1,16)	1:10:A:ASN:N	1:10:A:ASN:CA	1:10:A:ASN:C	1:11:A:THR:N	1	1.23
(1,18)	1:13:A:GLY:N	1:13:A:GLY:CA	1:13:A:GLY:C	1:14:A:PHE:N	9	1.21
(1,176)	1:103:A:PRO:N	1:103:A:PRO:CA	1:103:A:PRO:C	1:104:A:LEU:N	3	1.2
(1,78)	1:46:A:PHE:N	1:46:A:PHE:CA	1:46:A:PHE:C	1:47:A:ALA:N	1	1.2
(1,16)	1:10:A:ASN:N	1:10:A:ASN:CA	1:10:A:ASN:C	1:11:A:THR:N	7	1.17
(1,74)	1:44:A:ASP:N	1:44:A:ASP:CA	1:44:A:ASP:C	1:45:A:ALA:N	3	1.15
(1,78)	1:46:A:PHE:N	1:46:A:PHE:CA	1:46:A:PHE:C	1:47:A:ALA:N	4	1.14
(1,18)	1:13:A:GLY:N	1:13:A:GLY:CA	1:13:A:GLY:C	1:14:A:PHE:N	2	1.14
(1,10)	1:7:A:ILE:N	1:7:A:ILE:CA	1:7:A:ILE:C	1:8:A:ALA:N	5	1.14
(1,55)	1:32:A:SER:C	1:33:A:PRO:N	1:33:A:PRO:CA	1:33:A:PRO:C	3	1.13
(1,25)	1:17:A:LEU:C	1:18:A:VAL:N	1:18:A:VAL:CA	1:18:A:VAL:C	4	1.12
(1,16)	1:10:A:ASN:N	1:10:A:ASN:CA	1:10:A:ASN:C	1:11:A:THR:N	6	1.12
(1,102)	1:62:A:PRO:N	1:62:A:PRO:CA	1:62:A:PRO:C	1:63:A:GLN:N	5	1.09
(1,99)	1:60:A:ASN:C	1:61:A:PRO:N	1:61:A:PRO:CA	1:61:A:PRO:C	3	1.08
(1,5)	1:4:A:ILE:C	1:5:A:VAL:N	1:5:A:VAL:CA	1:5:A:VAL:C	9	1.08
(1,200)	1:116:A:ILE:N	1:116:A:ILE:CA	1:116:A:ILE:C	1:117:A:GLU:N	9	1.07
(1,180)	1:105:A:GLU:N	1:105:A:GLU:CA	1:105:A:GLU:C	1:106:A:VAL:N	7	1.07
(1,22)	1:16:A:THR:N	1:16:A:THR:CA	1:16:A:THR:C	1:17:A:LEU:N	2	1.07
(1,86)	1:54:A:ILE:N	1:54:A:ILE:CA	1:54:A:ILE:C	1:55:A:THR:N	9	1.06
(1,207)	1:119:A:GLU:C	1:120:A:ASN:N	1:120:A:ASN:CA	1:120:A:ASN:C	8	1.05
(1,201)	1:116:A:ILE:C	1:117:A:GLU:N	1:117:A:GLU:CA	1:117:A:GLU:C	5	1.05
(1,10)	1:7:A:ILE:N	1:7:A:ILE:CA	1:7:A:ILE:C	1:8:A:ALA:N	4	1.05
(1,75)	1:44:A:ASP:C	1:45:A:ALA:N	1:45:A:ALA:CA	1:45:A:ALA:C	10	1.03
(1,60)	1:36:A:PHE:N	1:36:A:PHE:CA	1:36:A:PHE:C	1:37:A:THR:N	10	1.03
(1,25)	1:17:A:LEU:C	1:18:A:VAL:N	1:18:A:VAL:CA	1:18:A:VAL:C	8	1.03
(1,55)	1:32:A:SER:C	1:33:A:PRO:N	1:33:A:PRO:CA	1:33:A:PRO:C	4	1.02

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,45)	1:27:A:VAL:C	1:28:A:GLU:N	1:28:A:GLU:CA	1:28:A:GLU:C	5	1.01