



Full wwPDB NMR Structure Validation Report ⓘ

Mar 1, 2026 – 09:46 AM UTC

PDB ID : 2NCH / pdb_00002nch
BMRB ID : 26022
Title : Solution structure of translation initiation factor IF1 from wolbachia endosymbiont strain TRS of Brugia malayi
Authors : Kabra, A.; Nag, J.; Arora, A.; Bhattacharya, S.M.
Deposited on : 2016-03-31

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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

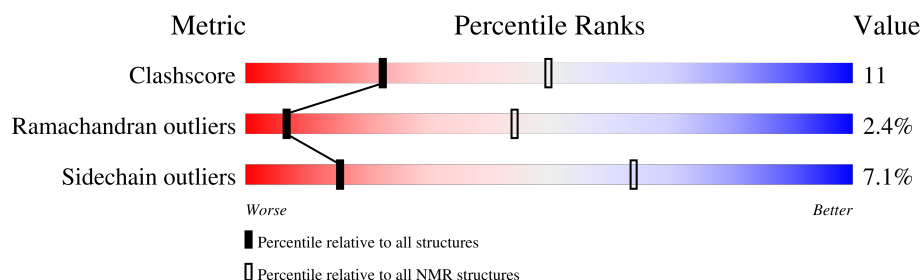
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 84%.

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	87	

2 Ensemble composition and analysis

This entry contains 10 models. Model 2 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:10-A:76 (67)	0.85	2

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

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

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

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1451 atoms, of which 755 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Translation initiation factor IF-1.

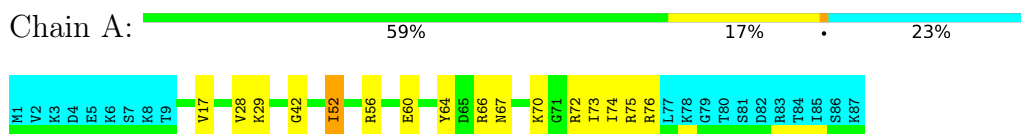
Mol	Chain	Residues	Atoms						Trace
1	A	87	Total	C	H	N	O	S	0
			1451	435	755	133	125	3	

4 Residue-property plots [i](#)

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: Translation initiation factor IF-1

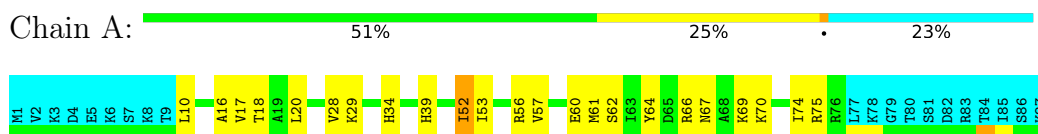


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

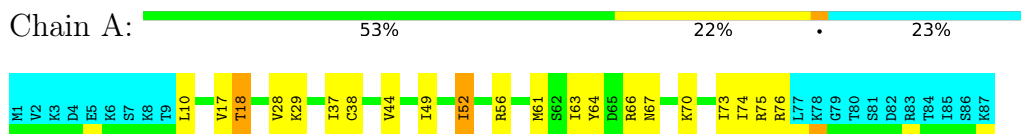
4.2.1 Score per residue for model 1

- Molecule 1: Translation initiation factor IF-1



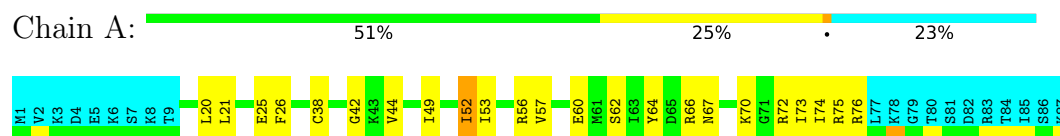
4.2.2 Score per residue for model 2 (medoid)

- Molecule 1: Translation initiation factor IF-1



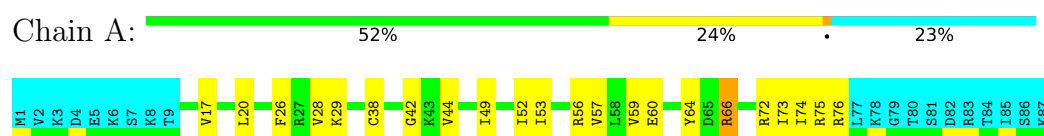
4.2.3 Score per residue for model 3

- Molecule 1: Translation initiation factor IF-1



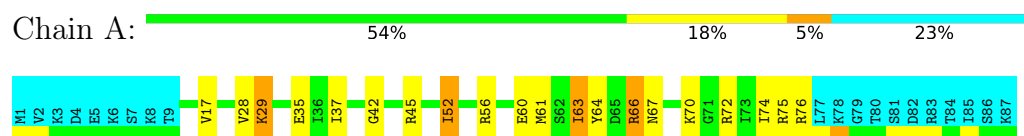
4.2.4 Score per residue for model 4

- Molecule 1: Translation initiation factor IF-1



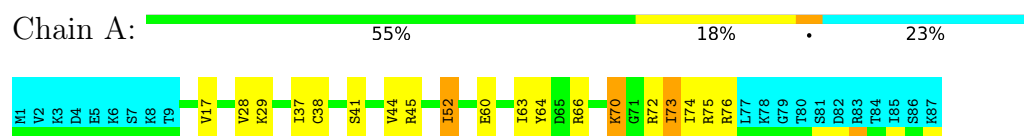
4.2.5 Score per residue for model 5

- Molecule 1: Translation initiation factor IF-1



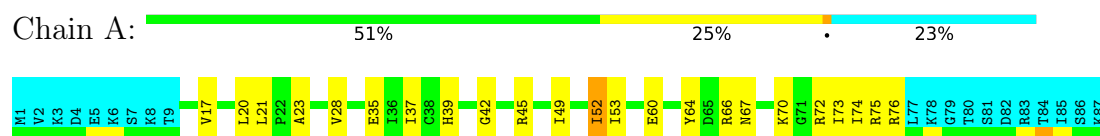
4.2.6 Score per residue for model 6

- Molecule 1: Translation initiation factor IF-1



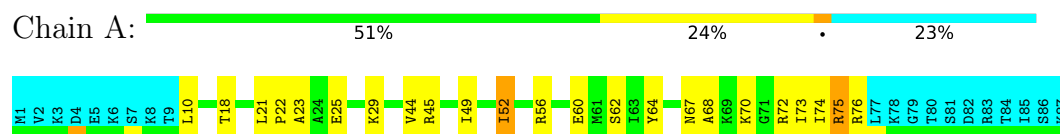
4.2.7 Score per residue for model 7

- Molecule 1: Translation initiation factor IF-1



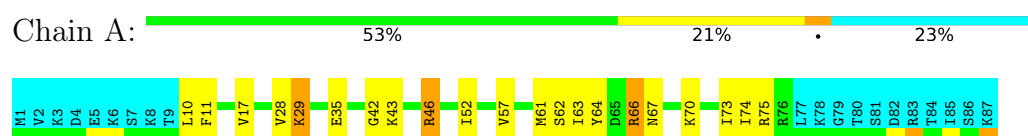
4.2.8 Score per residue for model 8

- Molecule 1: Translation initiation factor IF-1



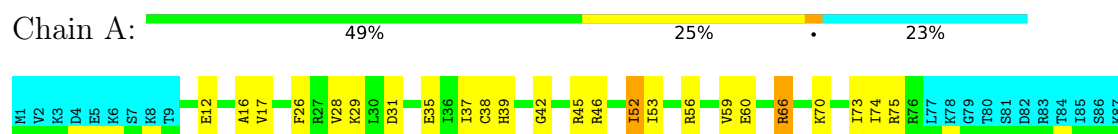
4.2.9 Score per residue for model 9

- Molecule 1: Translation initiation factor IF-1



4.2.10 Score per residue for model 10

- Molecule 1: Translation initiation factor IF-1



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 10 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
CYANA	structure solution	
CNS	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	1078
Number of shifts mapped to atoms	1078
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	84%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	540	582	580	13±2
All	All	5400	5820	5800	126

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:29:LYS:HB3	1:A:35:GLU:HG2	0.89	1.43	5	3
1:A:18:THR:HB	1:A:29:LYS:HD2	0.85	1.48	8	3
1:A:66:ARG:HD3	1:A:66:ARG:H	0.70	1.47	6	3
1:A:56:ARG:H	1:A:56:ARG:HD3	0.69	1.48	3	1
1:A:17:VAL:HA	1:A:28:VAL:HG12	0.68	1.65	5	8
1:A:66:ARG:HD2	1:A:66:ARG:H	0.66	1.49	4	3
1:A:26:PHE:HB2	1:A:38:CYS:HB3	0.66	1.67	10	1
1:A:26:PHE:HB2	1:A:38:CYS:HB2	0.65	1.67	4	2
1:A:56:ARG:O	1:A:76:ARG:HB2	0.64	1.93	3	3
1:A:52:ILE:H	1:A:52:ILE:HD13	0.63	1.54	10	8
1:A:49:ILE:HD12	1:A:74:ILE:HD11	0.61	1.71	4	1
1:A:49:ILE:HG12	1:A:74:ILE:HG13	0.60	1.73	7	1
1:A:49:ILE:HG21	1:A:74:ILE:HG13	0.60	1.74	3	1
1:A:44:VAL:HG23	1:A:49:ILE:HB	0.60	1.72	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:LEU:HD22	1:A:53:ILE:HD11	0.59	1.73	3	4
1:A:37:ILE:O	1:A:70:LYS:HA	0.59	1.98	6	5
1:A:29:LYS:HA	1:A:35:GLU:HA	0.58	1.76	5	1
1:A:63:ILE:HD12	1:A:63:ILE:H	0.58	1.58	5	2
1:A:10:LEU:HD11	1:A:60:GLU:HG2	0.57	1.75	8	1
1:A:74:ILE:HG23	1:A:75:ARG:H	0.56	1.59	9	10
1:A:62:SER:HB2	1:A:67:ASN:HB2	0.55	1.79	9	1
1:A:60:GLU:OE2	1:A:72:ARG:HD2	0.55	2.02	5	3
1:A:21:LEU:HB3	1:A:25:GLU:HB3	0.54	1.78	3	2
1:A:29:LYS:HD3	1:A:29:LYS:H	0.53	1.61	4	1
1:A:11:PHE:HB3	1:A:61:MET:SD	0.51	2.45	9	1
1:A:28:VAL:HG11	1:A:57:VAL:HG21	0.51	1.82	1	2
1:A:60:GLU:O	1:A:72:ARG:HG2	0.50	2.07	5	2
1:A:62:SER:H	1:A:67:ASN:HB2	0.50	1.67	1	1
1:A:11:PHE:HB2	1:A:63:ILE:HD11	0.50	1.82	9	1
1:A:39:HIS:O	1:A:72:ARG:HA	0.49	2.07	7	1
1:A:75:ARG:HG2	1:A:76:ARG:H	0.49	1.67	5	2
1:A:57:VAL:HG21	1:A:73:ILE:HD11	0.49	1.85	3	1
1:A:61:MET:HB2	1:A:67:ASN:O	0.49	2.08	5	2
1:A:67:ASN:HA	1:A:70:LYS:O	0.49	2.08	7	1
1:A:16:ALA:HB2	1:A:56:ARG:HD3	0.48	1.84	10	2
1:A:44:VAL:HG13	1:A:49:ILE:HB	0.47	1.85	3	1
1:A:62:SER:HB3	1:A:67:ASN:HB2	0.47	1.84	3	1
1:A:57:VAL:HB	1:A:73:ILE:HG23	0.47	1.85	4	2
1:A:66:ARG:HD3	1:A:66:ARG:N	0.47	2.20	6	2
1:A:38:CYS:HB3	1:A:73:ILE:HB	0.47	1.87	6	2
1:A:45:ARG:HD3	1:A:45:ARG:C	0.47	2.35	10	2
1:A:69:LYS:HD2	1:A:69:LYS:H	0.46	1.71	1	1
1:A:59:VAL:HB	1:A:73:ILE:HG13	0.46	1.88	4	1
1:A:67:ASN:HA	1:A:70:LYS:HE3	0.46	1.88	8	1
1:A:43:LYS:HA	1:A:46:ARG:HD3	0.45	1.88	9	1
1:A:59:VAL:HB	1:A:73:ILE:HG12	0.45	1.88	10	1
1:A:44:VAL:HG22	1:A:74:ILE:HB	0.45	1.89	4	1
1:A:75:ARG:HD3	1:A:76:ARG:N	0.45	2.25	4	1
1:A:21:LEU:C	1:A:23:ALA:H	0.45	2.18	8	2
1:A:75:ARG:HG2	1:A:76:ARG:N	0.45	2.27	7	1
1:A:44:VAL:HB	1:A:74:ILE:HB	0.45	1.87	6	1
1:A:74:ILE:O	1:A:75:ARG:HB2	0.44	2.11	9	4
1:A:12:GLU:HG2	1:A:60:GLU:HB3	0.44	1.89	10	1
1:A:10:LEU:HD21	1:A:60:GLU:HB3	0.44	1.90	1	1
1:A:60:GLU:HG3	1:A:72:ARG:HB2	0.44	1.89	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:62:SER:O	1:A:68:ALA:HA	0.44	2.13	8	1
1:A:42:GLY:HA3	1:A:72:ARG:HD3	0.43	1.89	4	1
1:A:56:ARG:O	1:A:76:ARG:HB3	0.43	2.13	5	1
1:A:70:LYS:HD2	1:A:70:LYS:C	0.43	2.37	10	1
1:A:60:GLU:CG	1:A:72:ARG:HB2	0.43	2.43	4	1
1:A:29:LYS:CB	1:A:35:GLU:HG2	0.43	2.40	10	1
1:A:29:LYS:HD3	1:A:29:LYS:N	0.42	2.30	4	1
1:A:17:VAL:HG11	1:A:52:ILE:O	0.41	2.15	9	1
1:A:17:VAL:HG11	1:A:53:ILE:HA	0.41	1.91	10	1
1:A:10:LEU:HB2	1:A:61:MET:O	0.41	2.15	9	1
1:A:60:GLU:HB2	1:A:72:ARG:HG3	0.41	1.93	3	1
1:A:10:LEU:HA	1:A:63:ILE:HG12	0.40	1.93	2	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	67/87 (77%)	58±1 (87±2%)	7±1 (10±2%)	2±0 (2±1%)	7	44
All	All	670/870 (77%)	585 (87%)	69 (10%)	16 (2%)	7	44

All 4 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	64	TYR	9
1	A	42	GLY	5
1	A	41	SER	1
1	A	22	PRO	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	58/77 (75%)	54±1 (93±2%)	4±1 (7±2%)	15 64
All	All	580/770 (75%)	539 (93%)	41 (7%)	15 64

All 16 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	52	ILE	9
1	A	66	ARG	7
1	A	70	LYS	4
1	A	29	LYS	3
1	A	45	ARG	3
1	A	73	ILE	3
1	A	39	HIS	2
1	A	46	ARG	2
1	A	34	HIS	1
1	A	61	MET	1
1	A	18	THR	1
1	A	63	ILE	1
1	A	76	ARG	1
1	A	35	GLU	1
1	A	75	ARG	1
1	A	31	ASP	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 84% for the well-defined parts and 85% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *Chemical_shifts*

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	1078
Number of shifts mapped to atoms	1078
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	87	-0.21 ± 0.12	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	82	0.26 ± 0.18	None needed (< 0.5 ppm)
$^{13}\text{C}'$	87	-0.12 ± 0.16	None needed (< 0.5 ppm)
^{15}N	83	0.78 ± 0.45	None needed (imprecise)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 84%, i.e. 836 atoms were assigned a chemical shift out of a possible 1001. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	333/337 (99%)	135/137 (99%)	134/134 (100%)	64/66 (97%)
Sidechain	490/619 (79%)	334/402 (83%)	156/183 (85%)	0/34 (0%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	13/45 (29%)	13/22 (59%)	0/19 (0%)	0/4 (0%)
Overall	836/1001 (84%)	482/561 (86%)	290/336 (86%)	64/104 (62%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 85%, i.e. 1077 atoms were assigned a chemical shift out of a possible 1273. 0 out of 14 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	431/438 (98%)	174/178 (98%)	174/174 (100%)	83/86 (97%)
Sidechain	633/790 (80%)	431/511 (84%)	202/237 (85%)	0/42 (0%)
Aromatic	13/45 (29%)	13/22 (59%)	0/19 (0%)	0/4 (0%)
Overall	1077/1273 (85%)	618/711 (87%)	376/430 (87%)	83/132 (63%)

7.1.4 Statistically unusual chemical shifts [i](#)

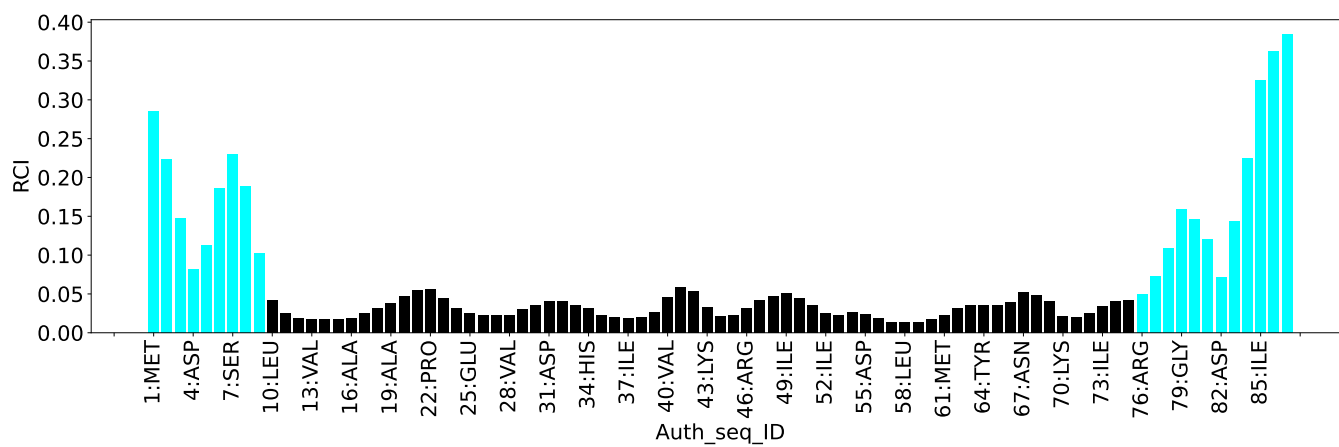
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	22	PRO	CD	42.18	45.11 – 55.58	-7.8
1	A	22	PRO	HD2	1.51	1.93 – 5.38	-6.2
1	A	22	PRO	HD3	1.51	1.76 – 5.48	-5.7

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

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	1123
Intra-residue ($ i-j =0$)	430
Sequential ($ i-j =1$)	346
Medium range ($ i-j >1$ and $ i-j <5$)	76
Long range ($ i-j \geq 5$)	216
Inter-chain	0
Hydrogen bond restraints	55
Disulfide bond restraints	0
Total dihedral-angle restraints	126
Number of unmapped restraints	0
Number of restraints per residue	14.4
Number of long range restraints per residue ¹	3.0

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)	37.1	0.2
0.2-0.5 (Medium)	45.7	0.5
>0.5 (Large)	54.1	2.64

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)	13.9	7.39
10.0-20.0 (Medium)	0.5	14.4
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

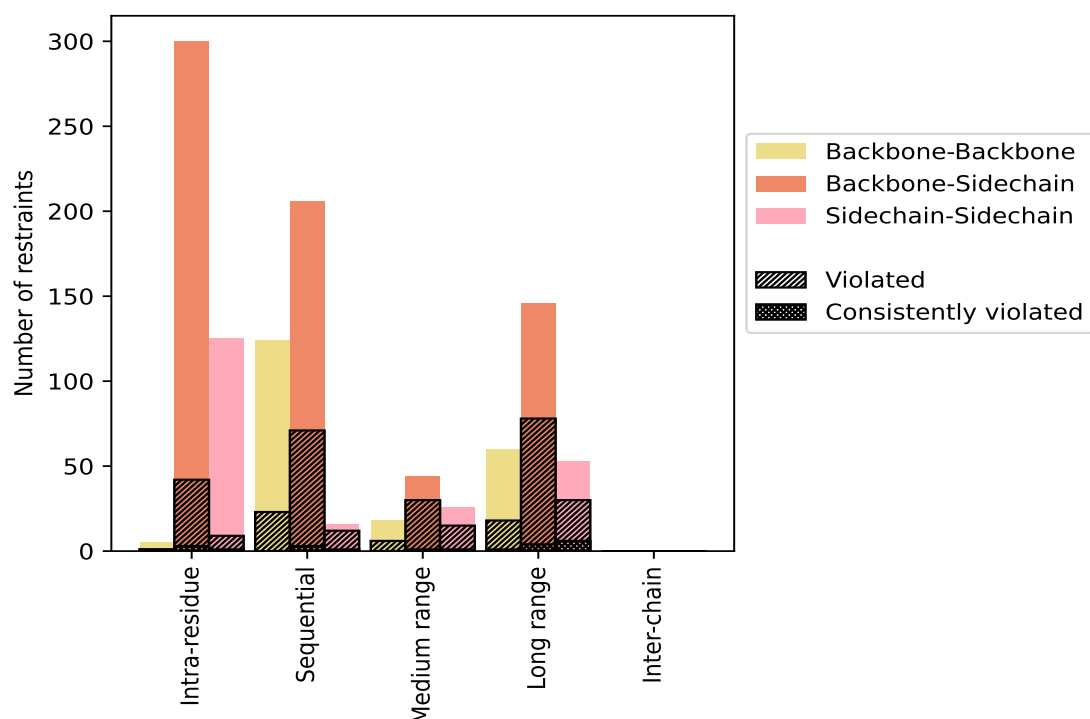
9.1 Summary of distance violations ⓘ

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 ($i-j =0$)	430	38.3	52	12.1	4.6	5	1.2	0.4
Backbone-Backbone	5	0.4	1	20.0	0.1	1	20.0	0.1
Backbone-Sidechain	300	26.7	42	14.0	3.7	3	1.0	0.3
Sidechain-Sidechain	125	11.1	9	7.2	0.8	1	0.8	0.1
Sequential ($i-j =1$)	346	30.8	106	30.6	9.4	4	1.2	0.4
Backbone-Backbone	124	11.0	23	18.5	2.0	0	0.0	0.0
Backbone-Sidechain	206	18.3	71	34.5	6.3	3	1.5	0.3
Sidechain-Sidechain	16	1.4	12	75.0	1.1	1	6.2	0.1
Medium range ($i-j >1$ & $i-j <5$)	76	6.8	43	56.6	3.8	2	2.6	0.2
Backbone-Backbone	18	1.6	6	33.3	0.5	0	0.0	0.0
Backbone-Sidechain	32	2.8	22	68.8	2.0	1	3.1	0.1
Sidechain-Sidechain	26	2.3	15	57.7	1.3	1	3.8	0.1
Long range ($i-j \geq 5$)	216	19.2	108	50.0	9.6	11	5.1	1.0
Backbone-Backbone	60	5.3	18	30.0	1.6	1	1.7	0.1
Backbone-Sidechain	103	9.2	60	58.3	5.3	4	3.9	0.4
Sidechain-Sidechain	53	4.7	30	56.6	2.7	6	11.3	0.5
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	55	4.9	26	47.3	2.3	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1123	100.0	335	29.8	29.8	22	2.0	2.0
Backbone-Backbone	207	18.4	48	23.2	4.3	2	1.0	0.2
Backbone-Sidechain	696	62.0	221	31.8	19.7	11	1.6	1.0
Sidechain-Sidechain	220	19.6	66	30.0	5.9	9	4.1	0.8

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

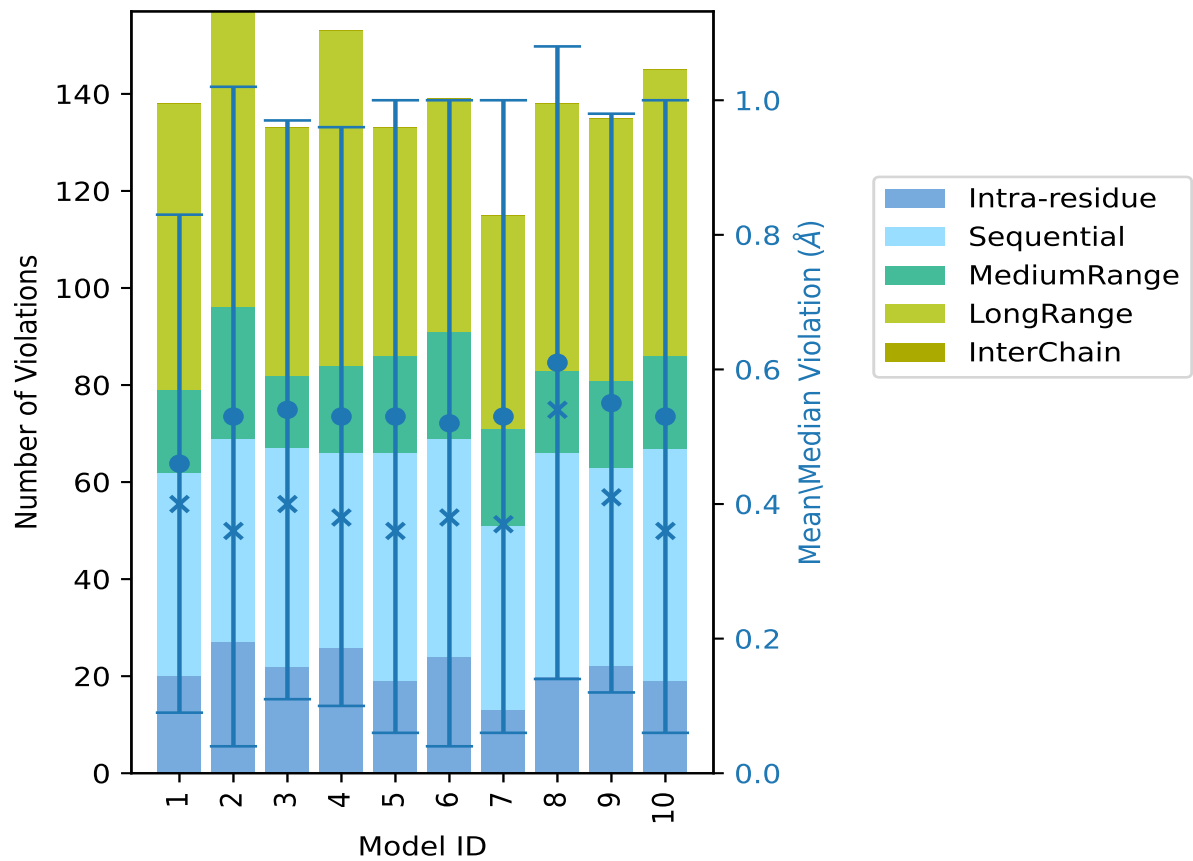
9.2 Distance violation statistics for each model [i](#)

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	20	42	17	59	0	138	0.46	2.39	0.37	0.4
2	27	42	27	61	0	157	0.53	2.39	0.49	0.36
3	22	45	15	51	0	133	0.54	2.02	0.43	0.4
4	26	40	18	69	0	153	0.53	2.25	0.43	0.38
5	19	47	20	47	0	133	0.53	2.23	0.47	0.36
6	24	45	22	48	0	139	0.52	2.64	0.48	0.38
7	13	38	20	44	0	115	0.53	2.51	0.47	0.37
8	20	46	17	55	0	138	0.61	2.45	0.47	0.54
9	22	41	18	54	0	135	0.55	1.92	0.43	0.41
10	19	48	19	59	0	145	0.53	2.27	0.47	0.36

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 ⓘ



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

9.3 Distance violation statistics for the ensemble ⓘ

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 759(IR:378, SQ:240, MR:33, LR:108, 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	%
12	27	14	20	0	73	1	10.0
12	16	7	16	0	51	2	20.0
4	14	3	18	0	39	3	30.0

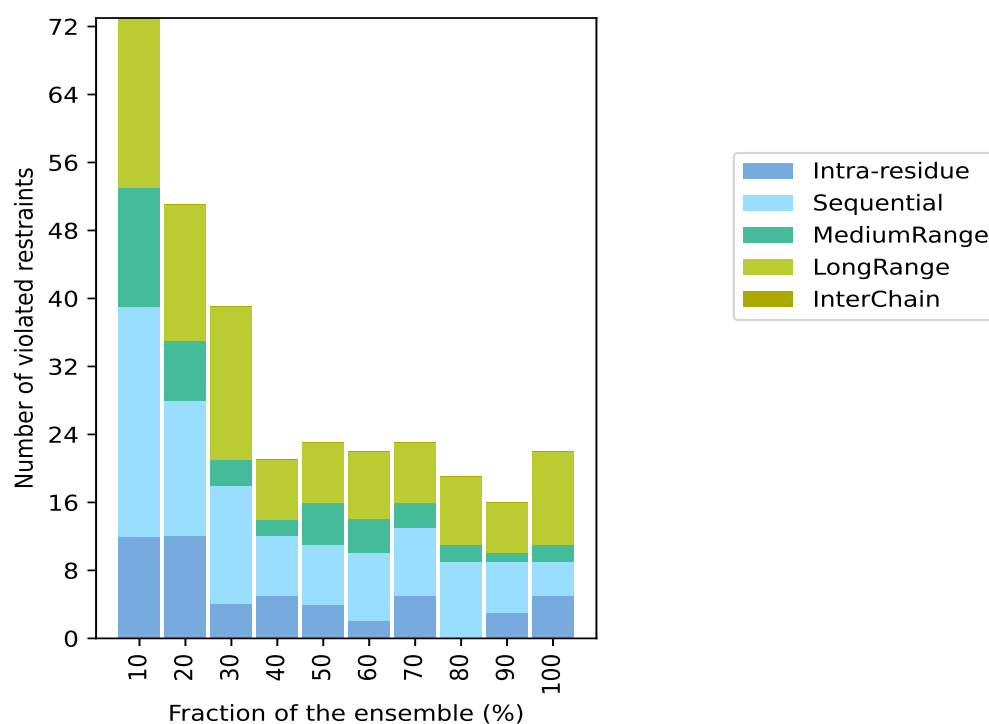
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
5	7	2	7	0	21	4	40.0
4	7	5	7	0	23	5	50.0
2	8	4	8	0	22	6	60.0
5	8	3	7	0	23	7	70.0
0	9	2	8	0	19	8	80.0
3	6	1	6	0	16	9	90.0
5	4	2	11	0	22	10	100.0

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

9.3.1 Bar graph : Distance violation statistics for the ensemble ⓘ

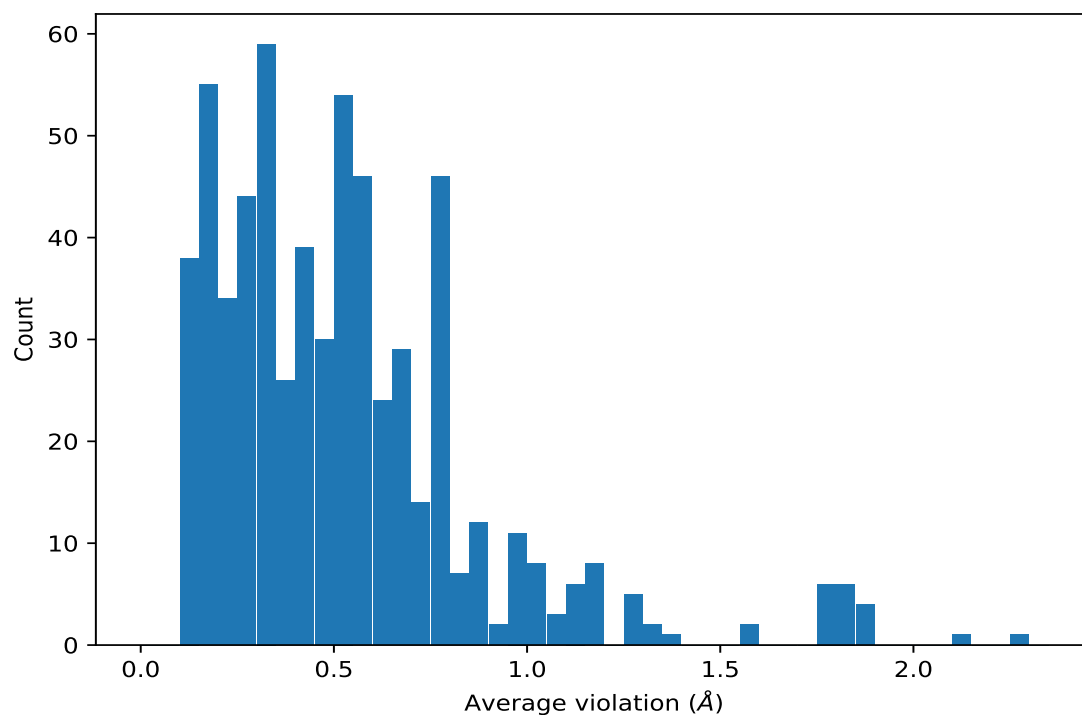


9.4 Most violated distance restraints in the ensemble ⓘ

9.4.1 Histogram : Distribution of mean distance violations ⓘ

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

in the ensemble



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,662)	1:50:A:ARG:HD2	1:75:A:ARG:HG2	10	1.87	0.1	1.92
(1,662)	1:50:A:ARG:HD2	1:75:A:ARG:HG3	10	1.87	0.1	1.92
(1,662)	1:50:A:ARG:HD3	1:75:A:ARG:HG2	10	1.87	0.1	1.92
(1,662)	1:50:A:ARG:HD3	1:75:A:ARG:HG3	10	1.87	0.1	1.92
(1,1012)	1:83:A:ARG:HD2	1:85:A:ILE:HD11	10	1.81	0.56	1.86
(1,1012)	1:83:A:ARG:HD2	1:85:A:ILE:HD12	10	1.81	0.56	1.86
(1,1012)	1:83:A:ARG:HD2	1:85:A:ILE:HD13	10	1.81	0.56	1.86
(1,1012)	1:83:A:ARG:HD3	1:85:A:ILE:HD11	10	1.81	0.56	1.86
(1,1012)	1:83:A:ARG:HD3	1:85:A:ILE:HD12	10	1.81	0.56	1.86
(1,1012)	1:83:A:ARG:HD3	1:85:A:ILE:HD13	10	1.81	0.56	1.86
(1,287)	1:18:A:THR:HG21	1:28:A:VAL:HB	10	1.28	0.65	0.94
(1,287)	1:18:A:THR:HG22	1:28:A:VAL:HB	10	1.28	0.65	0.94
(1,287)	1:18:A:THR:HG23	1:28:A:VAL:HB	10	1.28	0.65	0.94
(1,60)	1:6:A:LYS:HD3	1:7:A:SER:H	10	1.18	0.61	1.21
(1,855)	1:69:A:LYS:HD2	1:70:A:LYS:H	10	1.14	0.55	0.96

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,855)	1:69:A:LYS:HD3	1:70:A:LYS:H	10	1.14	0.55	0.96
(1,318)	1:20:A:LEU:HB2	1:25:A:GLU:H	10	0.99	0.16	1.04
(1,664)	1:50:A:ARG:HG2	1:75:A:ARG:HG2	10	0.96	0.32	0.93
(1,664)	1:50:A:ARG:HG2	1:75:A:ARG:HG3	10	0.96	0.32	0.93
(1,664)	1:50:A:ARG:HG3	1:75:A:ARG:HG2	10	0.96	0.32	0.93
(1,664)	1:50:A:ARG:HG3	1:75:A:ARG:HG3	10	0.96	0.32	0.93
(1,769)	1:61:A:MET:HG2	1:70:A:LYS:HB2	10	0.96	0.15	1.02
(1,769)	1:61:A:MET:HG2	1:70:A:LYS:HB3	10	0.96	0.15	1.02
(1,769)	1:61:A:MET:HG3	1:70:A:LYS:HB2	10	0.96	0.15	1.02
(1,769)	1:61:A:MET:HG3	1:70:A:LYS:HB3	10	0.96	0.15	1.02
(1,561)	1:43:A:LYS:HG3	1:47:A:SER:HA	10	0.89	0.39	0.8
(1,323)	1:20:A:LEU:HB3	1:25:A:GLU:H	10	0.87	0.14	0.9
(1,128)	1:10:A:LEU:HD11	1:61:A:MET:HB2	10	0.76	0.39	0.78
(1,128)	1:10:A:LEU:HD11	1:61:A:MET:HB3	10	0.76	0.39	0.78
(1,128)	1:10:A:LEU:HD12	1:61:A:MET:HB2	10	0.76	0.39	0.78
(1,128)	1:10:A:LEU:HD12	1:61:A:MET:HB3	10	0.76	0.39	0.78
(1,128)	1:10:A:LEU:HD13	1:61:A:MET:HB2	10	0.76	0.39	0.78
(1,128)	1:10:A:LEU:HD13	1:61:A:MET:HB3	10	0.76	0.39	0.78
(1,128)	1:10:A:LEU:HD21	1:61:A:MET:HB2	10	0.76	0.39	0.78
(1,128)	1:10:A:LEU:HD21	1:61:A:MET:HB3	10	0.76	0.39	0.78
(1,128)	1:10:A:LEU:HD22	1:61:A:MET:HB2	10	0.76	0.39	0.78
(1,128)	1:10:A:LEU:HD22	1:61:A:MET:HB3	10	0.76	0.39	0.78
(1,128)	1:10:A:LEU:HD23	1:61:A:MET:HB2	10	0.76	0.39	0.78
(1,128)	1:10:A:LEU:HD23	1:61:A:MET:HB3	10	0.76	0.39	0.78
(1,540)	1:41:A:SER:H	1:72:A:ARG:H	10	0.62	0.21	0.74
(1,407)	1:27:A:ARG:HG2	1:38:A:CYS:HA	10	0.61	0.12	0.66
(1,257)	1:17:A:VAL:HG21	1:53:A:ILE:HB	10	0.58	0.21	0.6
(1,257)	1:17:A:VAL:HG22	1:53:A:ILE:HB	10	0.58	0.21	0.6
(1,257)	1:17:A:VAL:HG23	1:53:A:ILE:HB	10	0.58	0.21	0.6
(1,66)	1:6:A:LYS:HG3	1:7:A:SER:H	10	0.57	0.34	0.52
(1,327)	1:20:A:LEU:HG	1:21:A:LEU:HB2	10	0.57	0.44	0.43
(1,327)	1:20:A:LEU:HG	1:21:A:LEU:HB3	10	0.57	0.44	0.43
(2,5)	1:12:A:GLU:HG2	1:62:A:SER:HA	10	0.42	0.12	0.43
(2,5)	1:12:A:GLU:HG3	1:62:A:SER:HA	10	0.42	0.12	0.43
(1,307)	1:20:A:LEU:HA	1:20:A:LEU:HG	10	0.19	0.01	0.19
(1,891)	1:73:A:ILE:H	1:73:A:ILE:HA	10	0.19	0.01	0.19
(1,618)	1:48:A:LYS:HB3	1:48:A:LYS:HE2	10	0.16	0.03	0.16
(1,618)	1:48:A:LYS:HB3	1:48:A:LYS:HE3	10	0.16	0.03	0.16
(1,923)	1:75:A:ARG:HA	1:75:A:ARG:HB2	10	0.16	0.02	0.15
(1,923)	1:75:A:ARG:HA	1:75:A:ARG:HB3	10	0.16	0.02	0.15
(1,784)	1:63:A:ILE:HA	1:63:A:ILE:HB	10	0.12	0.0	0.12
(1,117)	1:10:A:LEU:HG	1:61:A:MET:HB2	9	1.08	0.38	1.17

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,117)	1:10:A:LEU:HG	1:61:A:MET:HB3	9	1.08	0.38	1.17
(1,63)	1:6:A:LYS:HG2	1:7:A:SER:H	9	1.0	0.47	1.26
(1,44)	1:5:A:GLU:HB3	1:6:A:LYS:H	9	0.88	0.51	0.81
(1,559)	1:43:A:LYS:HG2	1:47:A:SER:HA	9	0.83	0.36	0.81
(1,847)	1:69:A:LYS:HD2	1:70:A:LYS:H	9	0.75	0.65	0.34
(1,847)	1:69:A:LYS:HD3	1:70:A:LYS:H	9	0.75	0.65	0.34
(1,438)	1:29:A:LYS:HD2	1:30:A:LEU:H	9	0.64	0.18	0.59
(1,438)	1:29:A:LYS:HD3	1:30:A:LEU:H	9	0.64	0.18	0.59
(1,172)	1:12:A:GLU:HB2	1:61:A:MET:H	9	0.44	0.07	0.46
(1,172)	1:12:A:GLU:HB3	1:61:A:MET:H	9	0.44	0.07	0.46
(1,587)	1:45:A:ARG:HG2	1:46:A:ARG:H	9	0.41	0.13	0.45
(1,587)	1:45:A:ARG:HG3	1:46:A:ARG:H	9	0.41	0.13	0.45
(1,246)	1:17:A:VAL:HA	1:27:A:ARG:HB3	9	0.36	0.17	0.35
(1,337)	1:20:A:LEU:HD11	1:21:A:LEU:HB2	9	0.35	0.11	0.36
(1,337)	1:20:A:LEU:HD11	1:21:A:LEU:HB3	9	0.35	0.11	0.36
(1,337)	1:20:A:LEU:HD12	1:21:A:LEU:HB2	9	0.35	0.11	0.36
(1,337)	1:20:A:LEU:HD12	1:21:A:LEU:HB3	9	0.35	0.11	0.36
(1,337)	1:20:A:LEU:HD13	1:21:A:LEU:HB2	9	0.35	0.11	0.36
(1,337)	1:20:A:LEU:HD13	1:21:A:LEU:HB3	9	0.35	0.11	0.36
(1,337)	1:20:A:LEU:HD21	1:21:A:LEU:HB2	9	0.35	0.11	0.36
(1,337)	1:20:A:LEU:HD21	1:21:A:LEU:HB3	9	0.35	0.11	0.36
(1,337)	1:20:A:LEU:HD22	1:21:A:LEU:HB2	9	0.35	0.11	0.36
(1,337)	1:20:A:LEU:HD22	1:21:A:LEU:HB3	9	0.35	0.11	0.36
(1,337)	1:20:A:LEU:HD23	1:21:A:LEU:HB2	9	0.35	0.11	0.36
(1,337)	1:20:A:LEU:HD23	1:21:A:LEU:HB3	9	0.35	0.11	0.36
(1,338)	1:20:A:LEU:HD11	1:26:A:PHE:HB2	9	0.31	0.14	0.33
(1,338)	1:20:A:LEU:HD11	1:26:A:PHE:HB3	9	0.31	0.14	0.33
(1,338)	1:20:A:LEU:HD12	1:26:A:PHE:HB2	9	0.31	0.14	0.33
(1,338)	1:20:A:LEU:HD12	1:26:A:PHE:HB3	9	0.31	0.14	0.33
(1,338)	1:20:A:LEU:HD13	1:26:A:PHE:HB2	9	0.31	0.14	0.33
(1,338)	1:20:A:LEU:HD13	1:26:A:PHE:HB3	9	0.31	0.14	0.33
(1,338)	1:20:A:LEU:HD21	1:26:A:PHE:HB2	9	0.31	0.14	0.33
(1,338)	1:20:A:LEU:HD21	1:26:A:PHE:HB3	9	0.31	0.14	0.33
(1,338)	1:20:A:LEU:HD22	1:26:A:PHE:HB2	9	0.31	0.14	0.33
(1,338)	1:20:A:LEU:HD22	1:26:A:PHE:HB3	9	0.31	0.14	0.33
(1,338)	1:20:A:LEU:HD23	1:26:A:PHE:HB2	9	0.31	0.14	0.33
(1,338)	1:20:A:LEU:HD23	1:26:A:PHE:HB3	9	0.31	0.14	0.33
(1,191)	1:13:A:VAL:HG11	1:59:A:VAL:HB	9	0.28	0.17	0.22
(1,191)	1:13:A:VAL:HG12	1:59:A:VAL:HB	9	0.28	0.17	0.22
(1,191)	1:13:A:VAL:HG13	1:59:A:VAL:HB	9	0.28	0.17	0.22
(1,191)	1:13:A:VAL:HG21	1:59:A:VAL:HB	9	0.28	0.17	0.22
(1,191)	1:13:A:VAL:HG22	1:59:A:VAL:HB	9	0.28	0.17	0.22

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,191)	1:13:A:VAL:HG23	1:59:A:VAL:HB	9	0.28	0.17	0.22
(1,266)	1:17:A:VAL:HG11	1:53:A:ILE:HB	9	0.23	0.08	0.23
(1,266)	1:17:A:VAL:HG12	1:53:A:ILE:HB	9	0.23	0.08	0.23
(1,266)	1:17:A:VAL:HG13	1:53:A:ILE:HB	9	0.23	0.08	0.23
(1,266)	1:17:A:VAL:HG21	1:53:A:ILE:HB	9	0.23	0.08	0.23
(1,266)	1:17:A:VAL:HG22	1:53:A:ILE:HB	9	0.23	0.08	0.23
(1,266)	1:17:A:VAL:HG23	1:53:A:ILE:HB	9	0.23	0.08	0.23
(1,611)	1:48:A:LYS:HA	1:48:A:LYS:HE2	9	0.18	0.06	0.18
(1,611)	1:48:A:LYS:HA	1:48:A:LYS:HE3	9	0.18	0.06	0.18
(1,315)	1:20:A:LEU:HB2	1:20:A:LEU:HG	9	0.18	0.15	0.13
(1,627)	1:49:A:ILE:HA	1:49:A:ILE:HB	9	0.13	0.0	0.13
(1,58)	1:6:A:LYS:HD2	1:7:A:SER:H	8	1.38	0.59	1.66
(1,960)	1:77:A:LEU:HG	1:78:A:LYS:HE2	8	1.26	0.66	1.46
(1,960)	1:77:A:LEU:HG	1:78:A:LYS:HE3	8	1.26	0.66	1.46
(1,283)	1:18:A:THR:HB	1:53:A:ILE:HG21	8	1.0	0.43	0.84
(1,283)	1:18:A:THR:HB	1:53:A:ILE:HG22	8	1.0	0.43	0.84
(1,283)	1:18:A:THR:HB	1:53:A:ILE:HG23	8	1.0	0.43	0.84
(1,300)	1:19:A:ALA:HA	1:53:A:ILE:HB	8	0.91	0.43	1.0
(1,712)	1:56:A:ARG:H	1:75:A:ARG:HG2	8	0.8	0.56	0.72
(1,1022)	1:84:A:THR:HG21	1:85:A:ILE:HB	8	0.71	0.4	0.68
(1,1022)	1:84:A:THR:HG22	1:85:A:ILE:HB	8	0.71	0.4	0.68
(1,1022)	1:84:A:THR:HG23	1:85:A:ILE:HB	8	0.71	0.4	0.68
(1,586)	1:45:A:ARG:HD2	1:46:A:ARG:H	8	0.7	0.18	0.76
(1,586)	1:45:A:ARG:HD3	1:46:A:ARG:H	8	0.7	0.18	0.76
(1,422)	1:28:A:VAL:HB	1:29:A:LYS:HD2	8	0.6	0.35	0.54
(1,422)	1:28:A:VAL:HB	1:29:A:LYS:HD3	8	0.6	0.35	0.54
(3,54)	1:44:A:VAL:O	1:47:A:SER:H	8	0.58	0.34	0.54
(1,739)	1:58:A:LEU:HD11	1:60:A:GLU:HB2	8	0.53	0.35	0.44
(1,739)	1:58:A:LEU:HD11	1:60:A:GLU:HB3	8	0.53	0.35	0.44
(1,739)	1:58:A:LEU:HD12	1:60:A:GLU:HB2	8	0.53	0.35	0.44
(1,739)	1:58:A:LEU:HD12	1:60:A:GLU:HB3	8	0.53	0.35	0.44
(1,739)	1:58:A:LEU:HD13	1:60:A:GLU:HB2	8	0.53	0.35	0.44
(1,739)	1:58:A:LEU:HD13	1:60:A:GLU:HB3	8	0.53	0.35	0.44
(1,739)	1:58:A:LEU:HD21	1:60:A:GLU:HB2	8	0.53	0.35	0.44
(1,739)	1:58:A:LEU:HD21	1:60:A:GLU:HB3	8	0.53	0.35	0.44
(1,739)	1:58:A:LEU:HD22	1:60:A:GLU:HB2	8	0.53	0.35	0.44
(1,739)	1:58:A:LEU:HD22	1:60:A:GLU:HB3	8	0.53	0.35	0.44
(1,739)	1:58:A:LEU:HD23	1:60:A:GLU:HB2	8	0.53	0.35	0.44
(1,739)	1:58:A:LEU:HD23	1:60:A:GLU:HB3	8	0.53	0.35	0.44
(1,406)	1:27:A:ARG:HG2	1:28:A:VAL:H	8	0.52	0.18	0.6
(1,409)	1:27:A:ARG:HG2	1:38:A:CYS:HB2	8	0.51	0.2	0.53
(1,409)	1:27:A:ARG:HG2	1:38:A:CYS:HB3	8	0.51	0.2	0.53

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,409)	1:27:A:ARG:HG3	1:38:A:CYS:HB2	8	0.51	0.2	0.53
(1,409)	1:27:A:ARG:HG3	1:38:A:CYS:HB3	8	0.51	0.2	0.53
(1,690)	1:52:A:ILE:HG21	1:75:A:ARG:HB2	8	0.45	0.18	0.48
(1,690)	1:52:A:ILE:HG22	1:75:A:ARG:HB2	8	0.45	0.18	0.48
(1,690)	1:52:A:ILE:HG23	1:75:A:ARG:HB2	8	0.45	0.18	0.48
(1,118)	1:10:A:LEU:HG	1:61:A:MET:HG2	8	0.42	0.18	0.37
(1,118)	1:10:A:LEU:HG	1:61:A:MET:HG3	8	0.42	0.18	0.37
(1,206)	1:15:A:GLY:H	1:56:A:ARG:HA	8	0.41	0.14	0.37
(1,167)	1:12:A:GLU:HG2	1:61:A:MET:H	8	0.4	0.25	0.28
(1,17)	1:3:A:LYS:H	1:4:A:ASP:H	8	0.34	0.11	0.34
(1,530)	1:40:A:VAL:HG11	1:44:A:VAL:HA	8	0.32	0.28	0.22
(1,530)	1:40:A:VAL:HG12	1:44:A:VAL:HA	8	0.32	0.28	0.22
(1,530)	1:40:A:VAL:HG13	1:44:A:VAL:HA	8	0.32	0.28	0.22
(1,530)	1:40:A:VAL:HG21	1:44:A:VAL:HA	8	0.32	0.28	0.22
(1,530)	1:40:A:VAL:HG22	1:44:A:VAL:HA	8	0.32	0.28	0.22
(1,530)	1:40:A:VAL:HG23	1:44:A:VAL:HA	8	0.32	0.28	0.22
(1,871)	1:70:A:LYS:HG2	1:71:A:GLY:H	8	0.3	0.14	0.26
(1,763)	1:61:A:MET:H	1:62:A:SER:H	8	0.17	0.03	0.17
(1,959)	1:77:A:LEU:HG	1:78:A:LYS:HD2	7	1.31	0.55	1.39
(1,959)	1:77:A:LEU:HG	1:78:A:LYS:HD3	7	1.31	0.55	1.39
(1,993)	1:83:A:ARG:H	1:83:A:ARG:HD2	7	1.14	0.22	1.19
(1,993)	1:83:A:ARG:H	1:83:A:ARG:HD3	7	1.14	0.22	1.19
(1,347)	1:21:A:LEU:HG	1:23:A:ALA:H	7	0.81	0.36	0.61
(1,638)	1:49:A:ILE:HD11	1:75:A:ARG:HD2	7	0.73	0.39	0.69
(1,638)	1:49:A:ILE:HD12	1:75:A:ARG:HD2	7	0.73	0.39	0.69
(1,638)	1:49:A:ILE:HD13	1:75:A:ARG:HD2	7	0.73	0.39	0.69
(1,638)	1:49:A:ILE:HD11	1:75:A:ARG:HD3	7	0.73	0.39	0.69
(1,638)	1:49:A:ILE:HD12	1:75:A:ARG:HD3	7	0.73	0.39	0.69
(1,638)	1:49:A:ILE:HD13	1:75:A:ARG:HD3	7	0.73	0.39	0.69
(1,860)	1:70:A:LYS:H	1:70:A:LYS:HD2	7	0.67	0.45	0.69
(1,860)	1:70:A:LYS:H	1:70:A:LYS:HD3	7	0.67	0.45	0.69
(1,713)	1:56:A:ARG:H	1:76:A:ARG:H	7	0.59	0.3	0.53
(1,299)	1:19:A:ALA:HA	1:53:A:ILE:HA	7	0.59	0.21	0.52
(1,220)	1:15:A:GLY:HA2	1:56:A:ARG:HB2	7	0.55	0.22	0.53
(1,220)	1:15:A:GLY:HA2	1:56:A:ARG:HB3	7	0.55	0.22	0.53
(1,220)	1:15:A:GLY:HA3	1:56:A:ARG:HB2	7	0.55	0.22	0.53
(1,220)	1:15:A:GLY:HA3	1:56:A:ARG:HB3	7	0.55	0.22	0.53
(1,291)	1:18:A:THR:HG21	1:53:A:ILE:HD11	7	0.55	0.42	0.28
(1,291)	1:18:A:THR:HG21	1:53:A:ILE:HD12	7	0.55	0.42	0.28
(1,291)	1:18:A:THR:HG21	1:53:A:ILE:HD13	7	0.55	0.42	0.28
(1,291)	1:18:A:THR:HG22	1:53:A:ILE:HD11	7	0.55	0.42	0.28
(1,291)	1:18:A:THR:HG22	1:53:A:ILE:HD12	7	0.55	0.42	0.28

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,291)	1:18:A:THR:HG22	1:53:A:ILE:HD13	7	0.55	0.42	0.28
(1,291)	1:18:A:THR:HG23	1:53:A:ILE:HD11	7	0.55	0.42	0.28
(1,291)	1:18:A:THR:HG23	1:53:A:ILE:HD12	7	0.55	0.42	0.28
(1,291)	1:18:A:THR:HG23	1:53:A:ILE:HD13	7	0.55	0.42	0.28
(1,572)	1:44:A:VAL:HG11	1:51:A:ILE:HG21	7	0.54	0.3	0.54
(1,572)	1:44:A:VAL:HG11	1:51:A:ILE:HG22	7	0.54	0.3	0.54
(1,572)	1:44:A:VAL:HG11	1:51:A:ILE:HG23	7	0.54	0.3	0.54
(1,572)	1:44:A:VAL:HG12	1:51:A:ILE:HG21	7	0.54	0.3	0.54
(1,572)	1:44:A:VAL:HG12	1:51:A:ILE:HG22	7	0.54	0.3	0.54
(1,572)	1:44:A:VAL:HG12	1:51:A:ILE:HG23	7	0.54	0.3	0.54
(1,572)	1:44:A:VAL:HG13	1:51:A:ILE:HG21	7	0.54	0.3	0.54
(1,572)	1:44:A:VAL:HG13	1:51:A:ILE:HG22	7	0.54	0.3	0.54
(1,572)	1:44:A:VAL:HG13	1:51:A:ILE:HG23	7	0.54	0.3	0.54
(1,76)	1:8:A:LYS:HA	1:8:A:LYS:HE2	7	0.5	0.07	0.5
(1,76)	1:8:A:LYS:HA	1:8:A:LYS:HE3	7	0.5	0.07	0.5
(1,355)	1:22:A:PRO:HG2	1:24:A:ALA:H	7	0.48	0.23	0.63
(1,87)	1:8:A:LYS:HD3	1:9:A:THR:H	7	0.48	0.26	0.3
(1,413)	1:28:A:VAL:H	1:35:A:GLU:HB2	7	0.47	0.19	0.46
(1,413)	1:28:A:VAL:H	1:35:A:GLU:HB3	7	0.47	0.19	0.46
(1,99)	1:9:A:THR:HA	1:9:A:THR:HB	7	0.47	0.0	0.47
(1,806)	1:64:A:TYR:HB2	1:68:A:ALA:HA	7	0.39	0.13	0.38
(1,408)	1:27:A:ARG:HG3	1:28:A:VAL:H	7	0.35	0.12	0.34
(1,311)	1:20:A:LEU:HA	1:21:A:LEU:HB2	7	0.27	0.06	0.31
(1,311)	1:20:A:LEU:HA	1:21:A:LEU:HB3	7	0.27	0.06	0.31
(1,752)	1:60:A:GLU:H	1:61:A:MET:H	7	0.16	0.02	0.17
(1,149)	1:11:A:PHE:HB2	1:12:A:GLU:H	7	0.16	0.04	0.16
(1,149)	1:11:A:PHE:HB3	1:12:A:GLU:H	7	0.16	0.04	0.16
(1,693)	1:53:A:ILE:H	1:53:A:ILE:HD11	7	0.16	0.04	0.15
(1,693)	1:53:A:ILE:H	1:53:A:ILE:HD12	7	0.16	0.04	0.15
(1,693)	1:53:A:ILE:H	1:53:A:ILE:HD13	7	0.16	0.04	0.15
(1,33)	1:4:A:ASP:HA	1:5:A:GLU:H	7	0.13	0.02	0.13
(1,1013)	1:83:A:ARG:HD2	1:85:A:ILE:HG21	6	1.16	0.57	0.96
(1,1013)	1:83:A:ARG:HD2	1:85:A:ILE:HG22	6	1.16	0.57	0.96
(1,1013)	1:83:A:ARG:HD2	1:85:A:ILE:HG23	6	1.16	0.57	0.96
(1,1013)	1:83:A:ARG:HD3	1:85:A:ILE:HG21	6	1.16	0.57	0.96
(1,1013)	1:83:A:ARG:HD3	1:85:A:ILE:HG22	6	1.16	0.57	0.96
(1,1013)	1:83:A:ARG:HD3	1:85:A:ILE:HG23	6	1.16	0.57	0.96
(1,964)	1:77:A:LEU:HD11	1:78:A:LYS:HD2	6	0.76	0.36	0.55
(1,964)	1:77:A:LEU:HD11	1:78:A:LYS:HD3	6	0.76	0.36	0.55
(1,964)	1:77:A:LEU:HD12	1:78:A:LYS:HD2	6	0.76	0.36	0.55
(1,964)	1:77:A:LEU:HD12	1:78:A:LYS:HD3	6	0.76	0.36	0.55
(1,964)	1:77:A:LEU:HD13	1:78:A:LYS:HD2	6	0.76	0.36	0.55

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,964)	1:77:A:LEU:HD13	1:78:A:LYS:HD3	6	0.76	0.36	0.55
(1,964)	1:77:A:LEU:HD21	1:78:A:LYS:HD2	6	0.76	0.36	0.55
(1,964)	1:77:A:LEU:HD21	1:78:A:LYS:HD3	6	0.76	0.36	0.55
(1,964)	1:77:A:LEU:HD22	1:78:A:LYS:HD2	6	0.76	0.36	0.55
(1,964)	1:77:A:LEU:HD22	1:78:A:LYS:HD3	6	0.76	0.36	0.55
(1,964)	1:77:A:LEU:HD23	1:78:A:LYS:HD2	6	0.76	0.36	0.55
(1,964)	1:77:A:LEU:HD23	1:78:A:LYS:HD3	6	0.76	0.36	0.55
(1,116)	1:10:A:LEU:HG	1:61:A:MET:HA	6	0.74	0.31	0.81
(3,46)	1:39:A:HIS:O	1:73:A:ILE:H	6	0.72	0.41	0.78
(1,989)	1:82:A:ASP:HA	1:85:A:ILE:HG21	6	0.67	0.44	0.44
(1,989)	1:82:A:ASP:HA	1:85:A:ILE:HG22	6	0.67	0.44	0.44
(1,989)	1:82:A:ASP:HA	1:85:A:ILE:HG23	6	0.67	0.44	0.44
(1,691)	1:52:A:ILE:HG21	1:75:A:ARG:HG2	6	0.66	0.32	0.54
(1,691)	1:52:A:ILE:HG21	1:75:A:ARG:HG3	6	0.66	0.32	0.54
(1,691)	1:52:A:ILE:HG22	1:75:A:ARG:HG2	6	0.66	0.32	0.54
(1,691)	1:52:A:ILE:HG22	1:75:A:ARG:HG3	6	0.66	0.32	0.54
(1,691)	1:52:A:ILE:HG23	1:75:A:ARG:HG2	6	0.66	0.32	0.54
(1,691)	1:52:A:ILE:HG23	1:75:A:ARG:HG3	6	0.66	0.32	0.54
(3,47)	1:39:A:HIS:O	1:73:A:ILE:N	6	0.63	0.37	0.71
(1,1006)	1:83:A:ARG:HD2	1:84:A:THR:H	6	0.56	0.36	0.4
(1,1006)	1:83:A:ARG:HD3	1:84:A:THR:H	6	0.56	0.36	0.4
(1,14)	1:3:A:LYS:H	1:3:A:LYS:HD2	6	0.52	0.25	0.48
(1,14)	1:3:A:LYS:H	1:3:A:LYS:HD3	6	0.52	0.25	0.48
(1,122)	1:10:A:LEU:HB2	1:61:A:MET:HB2	6	0.49	0.46	0.34
(1,122)	1:10:A:LEU:HB2	1:61:A:MET:HB3	6	0.49	0.46	0.34
(1,122)	1:10:A:LEU:HB3	1:61:A:MET:HB2	6	0.49	0.46	0.34
(1,122)	1:10:A:LEU:HB3	1:61:A:MET:HB3	6	0.49	0.46	0.34
(1,169)	1:12:A:GLU:HG3	1:61:A:MET:H	6	0.4	0.18	0.34
(1,574)	1:44:A:VAL:HG11	1:51:A:ILE:HG21	6	0.38	0.16	0.37
(1,574)	1:44:A:VAL:HG11	1:51:A:ILE:HG22	6	0.38	0.16	0.37
(1,574)	1:44:A:VAL:HG11	1:51:A:ILE:HG23	6	0.38	0.16	0.37
(1,574)	1:44:A:VAL:HG12	1:51:A:ILE:HG21	6	0.38	0.16	0.37
(1,574)	1:44:A:VAL:HG12	1:51:A:ILE:HG22	6	0.38	0.16	0.37
(1,574)	1:44:A:VAL:HG12	1:51:A:ILE:HG23	6	0.38	0.16	0.37
(1,574)	1:44:A:VAL:HG13	1:51:A:ILE:HG21	6	0.38	0.16	0.37
(1,574)	1:44:A:VAL:HG13	1:51:A:ILE:HG22	6	0.38	0.16	0.37
(1,574)	1:44:A:VAL:HG13	1:51:A:ILE:HG23	6	0.38	0.16	0.37
(1,574)	1:44:A:VAL:HG21	1:51:A:ILE:HG21	6	0.38	0.16	0.37
(1,574)	1:44:A:VAL:HG21	1:51:A:ILE:HG22	6	0.38	0.16	0.37
(1,574)	1:44:A:VAL:HG21	1:51:A:ILE:HG23	6	0.38	0.16	0.37
(1,574)	1:44:A:VAL:HG22	1:51:A:ILE:HG21	6	0.38	0.16	0.37
(1,574)	1:44:A:VAL:HG22	1:51:A:ILE:HG22	6	0.38	0.16	0.37

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,574)	1:44:A:VAL:HG22	1:51:A:ILE:HG23	6	0.38	0.16	0.37
(1,574)	1:44:A:VAL:HG23	1:51:A:ILE:HG21	6	0.38	0.16	0.37
(1,574)	1:44:A:VAL:HG23	1:51:A:ILE:HG22	6	0.38	0.16	0.37
(1,574)	1:44:A:VAL:HG23	1:51:A:ILE:HG23	6	0.38	0.16	0.37
(1,772)	1:62:A:SER:H	1:64:A:TYR:HB2	6	0.35	0.16	0.32
(1,772)	1:62:A:SER:H	1:64:A:TYR:HB2	6	0.35	0.16	0.32
(1,772)	1:62:A:SER:H	1:64:A:TYR:HB3	6	0.35	0.16	0.32
(1,332)	1:20:A:LEU:HD11	1:27:A:ARG:H	6	0.32	0.11	0.33
(1,332)	1:20:A:LEU:HD12	1:27:A:ARG:H	6	0.32	0.11	0.33
(1,332)	1:20:A:LEU:HD13	1:27:A:ARG:H	6	0.32	0.11	0.33
(1,653)	1:50:A:ARG:HB2	1:52:A:ILE:HD11	6	0.29	0.19	0.2
(1,653)	1:50:A:ARG:HB2	1:52:A:ILE:HD12	6	0.29	0.19	0.2
(1,653)	1:50:A:ARG:HB2	1:52:A:ILE:HD13	6	0.29	0.19	0.2
(1,312)	1:20:A:LEU:HA	1:25:A:GLU:H	6	0.23	0.07	0.24
(1,419)	1:28:A:VAL:HB	1:29:A:LYS:H	6	0.21	0.07	0.2
(1,250)	1:17:A:VAL:HB	1:53:A:ILE:HA	6	0.21	0.05	0.2
(1,11)	1:2:A:VAL:HA	1:3:A:LYS:H	6	0.18	0.04	0.2
(1,162)	1:12:A:GLU:HB2	1:13:A:VAL:H	6	0.16	0.04	0.16
(1,616)	1:48:A:LYS:HB2	1:49:A:ILE:H	6	0.16	0.02	0.16
(1,706)	1:55:A:ASP:H	1:56:A:ARG:H	6	0.16	0.04	0.15
(1,668)	1:51:A:ILE:H	1:52:A:ILE:H	6	0.14	0.03	0.14
(1,75)	1:8:A:LYS:HA	1:8:A:LYS:HD2	6	0.11	0.01	0.11
(1,75)	1:8:A:LYS:HA	1:8:A:LYS:HD3	6	0.11	0.01	0.11
(1,966)	1:77:A:LEU:HD11	1:80:A:THR:HB	5	1.79	0.58	2.01
(1,966)	1:77:A:LEU:HD12	1:80:A:THR:HB	5	1.79	0.58	2.01
(1,966)	1:77:A:LEU:HD13	1:80:A:THR:HB	5	1.79	0.58	2.01
(1,966)	1:77:A:LEU:HD21	1:80:A:THR:HB	5	1.79	0.58	2.01
(1,966)	1:77:A:LEU:HD22	1:80:A:THR:HB	5	1.79	0.58	2.01
(1,966)	1:77:A:LEU:HD23	1:80:A:THR:HB	5	1.79	0.58	2.01
(1,958)	1:77:A:LEU:HG	1:78:A:LYS:HB2	5	1.55	0.53	1.24
(1,958)	1:77:A:LEU:HG	1:78:A:LYS:HB3	5	1.55	0.53	1.24
(1,589)	1:46:A:ARG:H	1:46:A:ARG:HD2	5	1.11	0.11	1.08
(1,589)	1:46:A:ARG:H	1:46:A:ARG:HD3	5	1.11	0.11	1.08
(1,957)	1:77:A:LEU:HG	1:78:A:LYS:H	5	0.9	0.39	0.81
(1,735)	1:58:A:LEU:HG	1:73:A:ILE:HA	5	0.7	0.34	0.72
(1,499)	1:38:A:CYS:HA	1:70:A:LYS:HD2	5	0.66	0.35	0.68
(1,499)	1:38:A:CYS:HA	1:70:A:LYS:HD3	5	0.66	0.35	0.68
(3,42)	1:37:A:ILE:H	1:69:A:LYS:O	5	0.66	0.3	0.54
(1,963)	1:77:A:LEU:HD11	1:78:A:LYS:HB2	5	0.61	0.37	0.76
(1,963)	1:77:A:LEU:HD11	1:78:A:LYS:HB3	5	0.61	0.37	0.76
(1,963)	1:77:A:LEU:HD12	1:78:A:LYS:HB2	5	0.61	0.37	0.76
(1,963)	1:77:A:LEU:HD12	1:78:A:LYS:HB3	5	0.61	0.37	0.76

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,963)	1:77:A:LEU:HD13	1:78:A:LYS:HB2	5	0.61	0.37	0.76
(1,963)	1:77:A:LEU:HD13	1:78:A:LYS:HB3	5	0.61	0.37	0.76
(1,963)	1:77:A:LEU:HD21	1:78:A:LYS:HB2	5	0.61	0.37	0.76
(1,963)	1:77:A:LEU:HD21	1:78:A:LYS:HB3	5	0.61	0.37	0.76
(1,963)	1:77:A:LEU:HD22	1:78:A:LYS:HB2	5	0.61	0.37	0.76
(1,963)	1:77:A:LEU:HD22	1:78:A:LYS:HB3	5	0.61	0.37	0.76
(1,963)	1:77:A:LEU:HD23	1:78:A:LYS:HB2	5	0.61	0.37	0.76
(1,963)	1:77:A:LEU:HD23	1:78:A:LYS:HB3	5	0.61	0.37	0.76
(1,852)	1:69:A:LYS:HG3	1:70:A:LYS:H	5	0.6	0.22	0.66
(1,848)	1:69:A:LYS:HE2	1:70:A:LYS:H	5	0.6	0.12	0.57
(1,848)	1:69:A:LYS:HE3	1:70:A:LYS:H	5	0.6	0.12	0.57
(1,858)	1:70:A:LYS:H	1:70:A:LYS:HD2	5	0.6	0.41	0.59
(1,858)	1:70:A:LYS:H	1:70:A:LYS:HD3	5	0.6	0.41	0.59
(1,292)	1:18:A:THR:HG21	1:53:A:ILE:HG21	5	0.47	0.18	0.44
(1,292)	1:18:A:THR:HG21	1:53:A:ILE:HG22	5	0.47	0.18	0.44
(1,292)	1:18:A:THR:HG21	1:53:A:ILE:HG23	5	0.47	0.18	0.44
(1,292)	1:18:A:THR:HG22	1:53:A:ILE:HG21	5	0.47	0.18	0.44
(1,292)	1:18:A:THR:HG22	1:53:A:ILE:HG22	5	0.47	0.18	0.44
(1,292)	1:18:A:THR:HG22	1:53:A:ILE:HG23	5	0.47	0.18	0.44
(1,292)	1:18:A:THR:HG23	1:53:A:ILE:HG21	5	0.47	0.18	0.44
(1,292)	1:18:A:THR:HG23	1:53:A:ILE:HG22	5	0.47	0.18	0.44
(1,292)	1:18:A:THR:HG23	1:53:A:ILE:HG23	5	0.47	0.18	0.44
(1,604)	1:47:A:SER:HA	1:49:A:ILE:H	5	0.45	0.12	0.49
(2,24)	1:66:A:ARG:HD2	1:68:A:ALA:HB1	5	0.44	0.01	0.44
(2,24)	1:66:A:ARG:HD2	1:68:A:ALA:HB2	5	0.44	0.01	0.44
(2,24)	1:66:A:ARG:HD2	1:68:A:ALA:HB3	5	0.44	0.01	0.44
(2,18)	1:44:A:VAL:HG21	1:51:A:ILE:HG21	5	0.43	0.01	0.42
(2,18)	1:44:A:VAL:HG21	1:51:A:ILE:HG22	5	0.43	0.01	0.42
(2,18)	1:44:A:VAL:HG21	1:51:A:ILE:HG23	5	0.43	0.01	0.42
(2,18)	1:44:A:VAL:HG22	1:51:A:ILE:HG21	5	0.43	0.01	0.42
(2,18)	1:44:A:VAL:HG22	1:51:A:ILE:HG22	5	0.43	0.01	0.42
(2,18)	1:44:A:VAL:HG22	1:51:A:ILE:HG23	5	0.43	0.01	0.42
(2,18)	1:44:A:VAL:HG23	1:51:A:ILE:HG21	5	0.43	0.01	0.42
(2,18)	1:44:A:VAL:HG23	1:51:A:ILE:HG22	5	0.43	0.01	0.42
(2,18)	1:44:A:VAL:HG23	1:51:A:ILE:HG23	5	0.43	0.01	0.42
(3,16)	1:16:A:ALA:H	1:29:A:LYS:O	5	0.42	0.23	0.38
(1,503)	1:39:A:HIS:H	1:70:A:LYS:HA	5	0.42	0.21	0.57
(1,218)	1:15:A:GLY:HA2	1:29:A:LYS:HD2	5	0.41	0.21	0.37
(1,218)	1:15:A:GLY:HA2	1:29:A:LYS:HD3	5	0.41	0.21	0.37
(1,218)	1:15:A:GLY:HA3	1:29:A:LYS:HD2	5	0.41	0.21	0.37
(1,218)	1:15:A:GLY:HA3	1:29:A:LYS:HD3	5	0.41	0.21	0.37
(1,773)	1:62:A:SER:H	1:66:A:ARG:HG2	5	0.35	0.18	0.25

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,12)	1:17:A:VAL:H	1:55:A:ASP:O	5	0.35	0.21	0.24
(3,52)	1:43:A:LYS:O	1:46:A:ARG:H	5	0.28	0.2	0.16
(3,36)	1:30:A:LEU:O	1:34:A:HIS:H	5	0.28	0.14	0.28
(1,485)	1:37:A:ILE:H	1:70:A:LYS:H	5	0.28	0.09	0.29
(1,30)	1:3:A:LYS:HG3	1:4:A:ASP:H	5	0.23	0.03	0.22
(1,814)	1:64:A:TYR:HB2	1:66:A:ARG:H	5	0.15	0.04	0.16
(1,814)	1:64:A:TYR:HB3	1:66:A:ARG:H	5	0.15	0.04	0.16
(1,657)	1:50:A:ARG:HD2	1:51:A:ILE:H	5	0.15	0.03	0.16
(1,657)	1:50:A:ARG:HD3	1:51:A:ILE:H	5	0.15	0.03	0.16
(1,953)	1:77:A:LEU:HB2	1:77:A:LEU:HG	5	0.14	0.01	0.14
(1,921)	1:75:A:ARG:HA	1:75:A:ARG:HD2	5	0.13	0.02	0.12
(1,921)	1:75:A:ARG:HA	1:75:A:ARG:HD3	5	0.13	0.02	0.12
(1,942)	1:76:A:ARG:HD2	1:77:A:LEU:HG	4	1.17	0.26	1.27
(1,68)	1:7:A:SER:H	1:8:A:LYS:H	4	1.08	0.46	1.3
(1,824)	1:66:A:ARG:HD3	1:68:A:ALA:HB1	4	1.0	0.15	1.06
(1,824)	1:66:A:ARG:HD3	1:68:A:ALA:HB2	4	1.0	0.15	1.06
(1,824)	1:66:A:ARG:HD3	1:68:A:ALA:HB3	4	1.0	0.15	1.06
(1,875)	1:70:A:LYS:HD2	1:71:A:GLY:H	4	0.96	0.5	1.1
(1,875)	1:70:A:LYS:HD3	1:71:A:GLY:H	4	0.96	0.5	1.1
(1,42)	1:5:A:GLU:HB2	1:6:A:LYS:H	4	0.87	0.11	0.84
(1,112)	1:10:A:LEU:HB2	1:61:A:MET:HA	4	0.79	0.34	0.86
(1,50)	1:6:A:LYS:HA	1:6:A:LYS:HD2	4	0.56	0.02	0.56
(1,50)	1:6:A:LYS:HA	1:6:A:LYS:HD3	4	0.56	0.02	0.56
(1,839)	1:69:A:LYS:HA	1:69:A:LYS:HE2	4	0.54	0.05	0.52
(1,839)	1:69:A:LYS:HA	1:69:A:LYS:HE3	4	0.54	0.05	0.52
(1,518)	1:40:A:VAL:HA	1:72:A:ARG:HB2	4	0.48	0.05	0.47
(1,504)	1:39:A:HIS:H	1:71:A:GLY:HA2	4	0.44	0.26	0.38
(1,504)	1:39:A:HIS:H	1:71:A:GLY:HA3	4	0.44	0.26	0.38
(1,226)	1:16:A:ALA:H	1:30:A:LEU:HA	4	0.44	0.16	0.4
(1,1019)	1:84:A:THR:HB	1:85:A:ILE:H	4	0.4	0.2	0.3
(3,22)	1:21:A:LEU:O	1:25:A:GLU:H	4	0.39	0.11	0.37
(2,12)	1:26:A:PHE:HE2	1:51:A:ILE:H	4	0.39	0.16	0.45
(3,55)	1:44:A:VAL:O	1:47:A:SER:N	4	0.38	0.15	0.39
(1,405)	1:27:A:ARG:HB2	1:38:A:CYS:H	4	0.34	0.11	0.34
(1,405)	1:27:A:ARG:HB3	1:38:A:CYS:H	4	0.34	0.11	0.34
(1,376)	1:25:A:GLU:HG2	1:39:A:HIS:HA	4	0.33	0.27	0.2
(1,850)	1:69:A:LYS:HG2	1:70:A:LYS:H	4	0.3	0.09	0.3
(3,17)	1:16:A:ALA:N	1:29:A:LYS:O	4	0.26	0.05	0.27
(1,354)	1:22:A:PRO:HG2	1:23:A:ALA:H	4	0.26	0.12	0.22
(1,617)	1:48:A:LYS:HB3	1:48:A:LYS:HD2	4	0.16	0.04	0.17
(1,617)	1:48:A:LYS:HB3	1:48:A:LYS:HD3	4	0.16	0.04	0.17
(1,447)	1:30:A:LEU:HG	1:33:A:GLU:H	4	0.16	0.03	0.17

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,430)	1:29:A:LYS:HA	1:29:A:LYS:HD2	4	0.16	0.03	0.16
(1,430)	1:29:A:LYS:HA	1:29:A:LYS:HD3	4	0.16	0.03	0.16
(1,950)	1:77:A:LEU:HA	1:77:A:LEU:HG	4	0.14	0.01	0.14
(1,521)	1:40:A:VAL:HB	1:45:A:ARG:HA	3	1.01	0.47	0.92
(1,534)	1:40:A:VAL:HG11	1:45:A:ARG:HA	3	0.87	0.39	0.67
(1,534)	1:40:A:VAL:HG12	1:45:A:ARG:HA	3	0.87	0.39	0.67
(1,534)	1:40:A:VAL:HG13	1:45:A:ARG:HA	3	0.87	0.39	0.67
(1,534)	1:40:A:VAL:HG21	1:45:A:ARG:HA	3	0.87	0.39	0.67
(1,534)	1:40:A:VAL:HG22	1:45:A:ARG:HA	3	0.87	0.39	0.67
(1,534)	1:40:A:VAL:HG23	1:45:A:ARG:HA	3	0.87	0.39	0.67
(1,288)	1:18:A:THR:HG21	1:29:A:LYS:H	3	0.82	0.13	0.87
(1,288)	1:18:A:THR:HG22	1:29:A:LYS:H	3	0.82	0.13	0.87
(1,288)	1:18:A:THR:HG23	1:29:A:LYS:H	3	0.82	0.13	0.87
(1,74)	1:8:A:LYS:H	1:9:A:THR:H	3	0.81	0.35	0.95
(1,525)	1:40:A:VAL:HG11	1:45:A:ARG:HA	3	0.77	0.5	0.6
(1,525)	1:40:A:VAL:HG12	1:45:A:ARG:HA	3	0.77	0.5	0.6
(1,525)	1:40:A:VAL:HG13	1:45:A:ARG:HA	3	0.77	0.5	0.6
(1,965)	1:77:A:LEU:HD11	1:78:A:LYS:HE2	3	0.77	0.39	0.96
(1,965)	1:77:A:LEU:HD11	1:78:A:LYS:HE3	3	0.77	0.39	0.96
(1,965)	1:77:A:LEU:HD12	1:78:A:LYS:HE2	3	0.77	0.39	0.96
(1,965)	1:77:A:LEU:HD12	1:78:A:LYS:HE3	3	0.77	0.39	0.96
(1,965)	1:77:A:LEU:HD13	1:78:A:LYS:HE2	3	0.77	0.39	0.96
(1,965)	1:77:A:LEU:HD13	1:78:A:LYS:HE3	3	0.77	0.39	0.96
(1,965)	1:77:A:LEU:HD21	1:78:A:LYS:HE2	3	0.77	0.39	0.96
(1,965)	1:77:A:LEU:HD21	1:78:A:LYS:HE3	3	0.77	0.39	0.96
(1,965)	1:77:A:LEU:HD22	1:78:A:LYS:HE2	3	0.77	0.39	0.96
(1,965)	1:77:A:LEU:HD22	1:78:A:LYS:HE3	3	0.77	0.39	0.96
(1,965)	1:77:A:LEU:HD23	1:78:A:LYS:HE2	3	0.77	0.39	0.96
(1,965)	1:77:A:LEU:HD23	1:78:A:LYS:HE3	3	0.77	0.39	0.96
(1,216)	1:15:A:GLY:HA3	1:30:A:LEU:HA	3	0.68	0.31	0.78
(1,26)	1:3:A:LYS:HD2	1:4:A:ASP:H	3	0.67	0.48	0.41
(1,26)	1:3:A:LYS:HD3	1:4:A:ASP:H	3	0.67	0.48	0.41
(1,544)	1:41:A:SER:HB2	1:72:A:ARG:HD2	3	0.67	0.61	0.28
(1,544)	1:41:A:SER:HB2	1:72:A:ARG:HD3	3	0.67	0.61	0.28
(1,544)	1:41:A:SER:HB3	1:72:A:ARG:HD2	3	0.67	0.61	0.28
(1,544)	1:41:A:SER:HB3	1:72:A:ARG:HD3	3	0.67	0.61	0.28
(1,528)	1:40:A:VAL:HG21	1:45:A:ARG:HA	3	0.67	0.38	0.4
(1,528)	1:40:A:VAL:HG22	1:45:A:ARG:HA	3	0.67	0.38	0.4
(1,528)	1:40:A:VAL:HG23	1:45:A:ARG:HA	3	0.67	0.38	0.4
(1,8)	1:2:A:VAL:H	1:3:A:LYS:H	3	0.66	0.41	0.71
(1,393)	1:26:A:PHE:HE1	1:51:A:ILE:H	3	0.64	0.17	0.67
(1,746)	1:59:A:VAL:HA	1:72:A:ARG:HG3	3	0.6	0.07	0.64

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,456)	1:33:A:GLU:H	1:33:A:GLU:HG2	3	0.6	0.1	0.56
(1,456)	1:33:A:GLU:H	1:33:A:GLU:HG3	3	0.6	0.1	0.56
(1,990)	1:82:A:ASP:HB2	1:85:A:ILE:HD11	3	0.59	0.25	0.54
(1,990)	1:82:A:ASP:HB2	1:85:A:ILE:HD12	3	0.59	0.25	0.54
(1,990)	1:82:A:ASP:HB2	1:85:A:ILE:HD13	3	0.59	0.25	0.54
(1,990)	1:82:A:ASP:HB3	1:85:A:ILE:HD11	3	0.59	0.25	0.54
(1,990)	1:82:A:ASP:HB3	1:85:A:ILE:HD12	3	0.59	0.25	0.54
(1,990)	1:82:A:ASP:HB3	1:85:A:ILE:HD13	3	0.59	0.25	0.54
(3,43)	1:37:A:ILE:N	1:69:A:LYS:O	3	0.55	0.23	0.47
(1,34)	1:4:A:ASP:HB2	1:5:A:GLU:H	3	0.54	0.52	0.23
(1,34)	1:4:A:ASP:HB3	1:5:A:GLU:H	3	0.54	0.52	0.23
(1,285)	1:18:A:THR:HG21	1:27:A:ARG:H	3	0.54	0.3	0.7
(1,285)	1:18:A:THR:HG22	1:27:A:ARG:H	3	0.54	0.3	0.7
(1,285)	1:18:A:THR:HG23	1:27:A:ARG:H	3	0.54	0.3	0.7
(1,130)	1:10:A:LEU:HD11	1:62:A:SER:HB2	3	0.51	0.11	0.44
(1,130)	1:10:A:LEU:HD11	1:62:A:SER:HB3	3	0.51	0.11	0.44
(1,130)	1:10:A:LEU:HD12	1:62:A:SER:HB2	3	0.51	0.11	0.44
(1,130)	1:10:A:LEU:HD12	1:62:A:SER:HB3	3	0.51	0.11	0.44
(1,130)	1:10:A:LEU:HD13	1:62:A:SER:HB2	3	0.51	0.11	0.44
(1,130)	1:10:A:LEU:HD13	1:62:A:SER:HB3	3	0.51	0.11	0.44
(1,130)	1:10:A:LEU:HD21	1:62:A:SER:HB2	3	0.51	0.11	0.44
(1,130)	1:10:A:LEU:HD21	1:62:A:SER:HB3	3	0.51	0.11	0.44
(1,130)	1:10:A:LEU:HD22	1:62:A:SER:HB2	3	0.51	0.11	0.44
(1,130)	1:10:A:LEU:HD22	1:62:A:SER:HB3	3	0.51	0.11	0.44
(1,130)	1:10:A:LEU:HD23	1:62:A:SER:HB2	3	0.51	0.11	0.44
(1,130)	1:10:A:LEU:HD23	1:62:A:SER:HB3	3	0.51	0.11	0.44
(1,280)	1:18:A:THR:HA	1:53:A:ILE:HG21	3	0.48	0.21	0.54
(1,280)	1:18:A:THR:HA	1:53:A:ILE:HG22	3	0.48	0.21	0.54
(1,280)	1:18:A:THR:HA	1:53:A:ILE:HG23	3	0.48	0.21	0.54
(2,25)	1:76:A:ARG:HD3	1:77:A:LEU:HG	3	0.47	0.06	0.43
(1,378)	1:25:A:GLU:HG3	1:39:A:HIS:HA	3	0.44	0.18	0.5
(3,13)	1:17:A:VAL:N	1:55:A:ASP:O	3	0.42	0.15	0.52
(2,9)	1:17:A:VAL:H	1:56:A:ARG:HB3	3	0.31	0.08	0.36
(1,356)	1:22:A:PRO:HG3	1:23:A:ALA:H	3	0.3	0.14	0.2
(1,85)	1:8:A:LYS:HD2	1:9:A:THR:H	3	0.28	0.12	0.36
(1,1021)	1:84:A:THR:HG21	1:85:A:ILE:HA	3	0.28	0.11	0.27
(1,1021)	1:84:A:THR:HG22	1:85:A:ILE:HA	3	0.28	0.11	0.27
(1,1021)	1:84:A:THR:HG23	1:85:A:ILE:HA	3	0.28	0.11	0.27
(1,336)	1:20:A:LEU:HD21	1:27:A:ARG:H	3	0.28	0.04	0.25
(1,336)	1:20:A:LEU:HD22	1:27:A:ARG:H	3	0.28	0.04	0.25
(1,336)	1:20:A:LEU:HD23	1:27:A:ARG:H	3	0.28	0.04	0.25
(1,566)	1:44:A:VAL:H	1:47:A:SER:H	3	0.28	0.12	0.3

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,179)	1:13:A:VAL:H	1:60:A:GLU:HB2	3	0.27	0.1	0.3
(1,179)	1:13:A:VAL:H	1:60:A:GLU:HB3	3	0.27	0.1	0.3
(1,35)	1:5:A:GLU:H	1:5:A:GLU:HB2	3	0.26	0.1	0.33
(1,35)	1:5:A:GLU:H	1:5:A:GLU:HB3	3	0.26	0.1	0.33
(3,37)	1:30:A:LEU:O	1:34:A:HIS:N	3	0.21	0.08	0.2
(3,23)	1:21:A:LEU:O	1:25:A:GLU:N	3	0.21	0.03	0.21
(1,277)	1:18:A:THR:HA	1:18:A:THR:HB	3	0.19	0.01	0.18
(1,517)	1:40:A:VAL:HA	1:72:A:ARG:HA	3	0.19	0.07	0.14
(1,659)	1:50:A:ARG:HB2	1:52:A:ILE:HG12	3	0.18	0.09	0.12
(1,659)	1:50:A:ARG:HB2	1:52:A:ILE:HG13	3	0.18	0.09	0.12
(1,659)	1:50:A:ARG:HB3	1:52:A:ILE:HG12	3	0.18	0.09	0.12
(1,659)	1:50:A:ARG:HB3	1:52:A:ILE:HG13	3	0.18	0.09	0.12
(1,136)	1:11:A:PHE:H	1:61:A:MET:HB2	3	0.17	0.06	0.14
(1,827)	1:67:A:ASN:HA	1:68:A:ALA:HB1	3	0.17	0.06	0.13
(1,827)	1:67:A:ASN:HA	1:68:A:ALA:HB2	3	0.17	0.06	0.13
(1,827)	1:67:A:ASN:HA	1:68:A:ALA:HB3	3	0.17	0.06	0.13
(1,185)	1:13:A:VAL:HB	1:14:A:GLU:H	3	0.17	0.06	0.14
(1,760)	1:60:A:GLU:HG2	1:61:A:MET:H	3	0.16	0.08	0.12
(1,760)	1:60:A:GLU:HG3	1:61:A:MET:H	3	0.16	0.08	0.12
(1,760)	1:60:A:GLU:HG2	1:61:A:MET:H	3	0.16	0.08	0.12
(1,760)	1:60:A:GLU:HG3	1:61:A:MET:H	3	0.16	0.08	0.12
(1,119)	1:10:A:LEU:HB2	1:10:A:LEU:HG	3	0.15	0.03	0.15
(1,119)	1:10:A:LEU:HB3	1:10:A:LEU:HG	3	0.15	0.03	0.15
(1,330)	1:20:A:LEU:HD11	1:21:A:LEU:HA	3	0.15	0.03	0.15
(1,330)	1:20:A:LEU:HD12	1:21:A:LEU:HA	3	0.15	0.03	0.15
(1,330)	1:20:A:LEU:HD13	1:21:A:LEU:HA	3	0.15	0.03	0.15
(1,175)	1:13:A:VAL:H	1:14:A:GLU:H	3	0.11	0.0	0.11
(1,392)	1:26:A:PHE:HD2	1:40:A:VAL:H	2	2.29	0.35	2.29
(1,394)	1:26:A:PHE:HE2	1:40:A:VAL:H	2	2.11	0.45	2.11
(1,672)	1:51:A:ILE:HA	1:75:A:ARG:HG2	2	0.86	0.08	0.86
(1,672)	1:51:A:ILE:HA	1:75:A:ARG:HG3	2	0.86	0.08	0.86
(1,15)	1:3:A:LYS:H	1:3:A:LYS:HE2	2	0.79	0.07	0.79
(1,15)	1:3:A:LYS:H	1:3:A:LYS:HE3	2	0.79	0.07	0.79
(1,522)	1:40:A:VAL:HB	1:45:A:ARG:HB2	2	0.77	0.23	0.77
(1,522)	1:40:A:VAL:HB	1:45:A:ARG:HB3	2	0.77	0.23	0.77
(1,988)	1:82:A:ASP:HA	1:85:A:ILE:HD11	2	0.73	0.0	0.73
(1,988)	1:82:A:ASP:HA	1:85:A:ILE:HD12	2	0.73	0.0	0.73
(1,988)	1:82:A:ASP:HA	1:85:A:ILE:HD13	2	0.73	0.0	0.73
(3,44)	1:37:A:ILE:O	1:71:A:GLY:H	2	0.66	0.43	0.66
(1,991)	1:82:A:ASP:HB2	1:85:A:ILE:HG21	2	0.62	0.42	0.62
(1,991)	1:82:A:ASP:HB2	1:85:A:ILE:HG22	2	0.62	0.42	0.62
(1,991)	1:82:A:ASP:HB2	1:85:A:ILE:HG23	2	0.62	0.42	0.62

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,991)	1:82:A:ASP:HB3	1:85:A:ILE:HG21	2	0.62	0.42	0.62
(1,991)	1:82:A:ASP:HB3	1:85:A:ILE:HG22	2	0.62	0.42	0.62
(1,991)	1:82:A:ASP:HB3	1:85:A:ILE:HG23	2	0.62	0.42	0.62
(1,121)	1:10:A:LEU:HB2	1:61:A:MET:HA	2	0.57	0.19	0.57
(1,121)	1:10:A:LEU:HB3	1:61:A:MET:HA	2	0.57	0.19	0.57
(1,475)	1:36:A:ILE:HB	1:37:A:ILE:H	2	0.55	0.02	0.55
(1,776)	1:62:A:SER:HA	1:63:A:ILE:HD11	2	0.5	0.31	0.5
(1,776)	1:62:A:SER:HA	1:63:A:ILE:HD12	2	0.5	0.31	0.5
(1,776)	1:62:A:SER:HA	1:63:A:ILE:HD13	2	0.5	0.31	0.5
(1,360)	1:23:A:ALA:HA	1:25:A:GLU:HB2	2	0.5	0.16	0.5
(1,360)	1:23:A:ALA:HA	1:25:A:GLU:HB3	2	0.5	0.16	0.5
(1,972)	1:78:A:LYS:HA	1:78:A:LYS:HD2	2	0.49	0.19	0.49
(1,972)	1:78:A:LYS:HA	1:78:A:LYS:HD3	2	0.49	0.19	0.49
(1,542)	1:41:A:SER:H	1:73:A:ILE:H	2	0.46	0.06	0.46
(1,231)	1:16:A:ALA:HA	1:56:A:ARG:HD2	2	0.43	0.24	0.43
(1,231)	1:16:A:ALA:HA	1:56:A:ARG:HD3	2	0.43	0.24	0.43
(3,34)	1:28:A:VAL:H	1:36:A:ILE:O	2	0.42	0.08	0.42
(1,201)	1:14:A:GLU:HG2	1:59:A:VAL:H	2	0.4	0.15	0.4
(1,505)	1:39:A:HIS:H	1:72:A:ARG:H	2	0.39	0.17	0.39
(1,985)	1:80:A:THR:HA	1:80:A:THR:HB	2	0.38	0.23	0.38
(3,40)	1:39:A:HIS:H	1:71:A:GLY:O	2	0.36	0.18	0.36
(1,477)	1:36:A:ILE:HD11	1:37:A:ILE:H	2	0.35	0.02	0.35
(1,477)	1:36:A:ILE:HD12	1:37:A:ILE:H	2	0.35	0.02	0.35
(1,477)	1:36:A:ILE:HD13	1:37:A:ILE:H	2	0.35	0.02	0.35
(1,637)	1:49:A:ILE:HD11	1:74:A:ILE:HG12	2	0.35	0.06	0.35
(1,637)	1:49:A:ILE:HD12	1:74:A:ILE:HG12	2	0.35	0.06	0.35
(1,637)	1:49:A:ILE:HD13	1:74:A:ILE:HG12	2	0.35	0.06	0.35
(1,637)	1:49:A:ILE:HD11	1:74:A:ILE:HG13	2	0.35	0.06	0.35
(1,637)	1:49:A:ILE:HD12	1:74:A:ILE:HG13	2	0.35	0.06	0.35
(1,637)	1:49:A:ILE:HD13	1:74:A:ILE:HG13	2	0.35	0.06	0.35
(1,1002)	1:83:A:ARG:HB2	1:84:A:THR:H	2	0.34	0.13	0.34
(1,937)	1:76:A:ARG:HA	1:76:A:ARG:HD2	2	0.32	0.06	0.32
(1,937)	1:76:A:ARG:HA	1:76:A:ARG:HD3	2	0.32	0.06	0.32
(1,19)	1:3:A:LYS:HA	1:3:A:LYS:HE2	2	0.32	0.2	0.32
(1,19)	1:3:A:LYS:HA	1:3:A:LYS:HE3	2	0.32	0.2	0.32
(3,41)	1:39:A:HIS:N	1:71:A:GLY:O	2	0.32	0.2	0.32
(1,1038)	1:87:A:LYS:H	1:87:A:LYS:HE2	2	0.3	0.08	0.3
(1,1038)	1:87:A:LYS:H	1:87:A:LYS:HE3	2	0.3	0.08	0.3
(1,188)	1:13:A:VAL:HG11	1:30:A:LEU:HA	2	0.3	0.01	0.3
(1,188)	1:13:A:VAL:HG12	1:30:A:LEU:HA	2	0.3	0.01	0.3
(1,188)	1:13:A:VAL:HG13	1:30:A:LEU:HA	2	0.3	0.01	0.3
(1,188)	1:13:A:VAL:HG21	1:30:A:LEU:HA	2	0.3	0.01	0.3

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,188)	1:13:A:VAL:HG22	1:30:A:LEU:HA	2	0.3	0.01	0.3
(1,188)	1:13:A:VAL:HG23	1:30:A:LEU:HA	2	0.3	0.01	0.3
(1,286)	1:18:A:THR:HG21	1:28:A:VAL:HA	2	0.29	0.06	0.29
(1,286)	1:18:A:THR:HG22	1:28:A:VAL:HA	2	0.29	0.06	0.29
(1,286)	1:18:A:THR:HG23	1:28:A:VAL:HA	2	0.29	0.06	0.29
(1,95)	1:9:A:THR:H	1:10:A:LEU:H	2	0.26	0.12	0.26
(1,282)	1:18:A:THR:HB	1:29:A:LYS:H	2	0.26	0.12	0.26
(1,607)	1:48:A:LYS:H	1:48:A:LYS:HE2	2	0.24	0.03	0.24
(1,607)	1:48:A:LYS:H	1:48:A:LYS:HE3	2	0.24	0.03	0.24
(1,335)	1:20:A:LEU:HD21	1:26:A:PHE:HA	2	0.24	0.04	0.24
(1,335)	1:20:A:LEU:HD22	1:26:A:PHE:HA	2	0.24	0.04	0.24
(1,335)	1:20:A:LEU:HD23	1:26:A:PHE:HA	2	0.24	0.04	0.24
(1,531)	1:40:A:VAL:HG11	1:44:A:VAL:HB	2	0.22	0.02	0.22
(1,531)	1:40:A:VAL:HG12	1:44:A:VAL:HB	2	0.22	0.02	0.22
(1,531)	1:40:A:VAL:HG13	1:44:A:VAL:HB	2	0.22	0.02	0.22
(1,531)	1:40:A:VAL:HG21	1:44:A:VAL:HB	2	0.22	0.02	0.22
(1,531)	1:40:A:VAL:HG22	1:44:A:VAL:HB	2	0.22	0.02	0.22
(1,531)	1:40:A:VAL:HG23	1:44:A:VAL:HB	2	0.22	0.02	0.22
(1,973)	1:78:A:LYS:HA	1:78:A:LYS:HE2	2	0.22	0.04	0.22
(1,973)	1:78:A:LYS:HA	1:78:A:LYS:HE3	2	0.22	0.04	0.22
(1,1005)	1:83:A:ARG:HB3	1:84:A:THR:H	2	0.22	0.08	0.22
(1,926)	1:75:A:ARG:HB2	1:76:A:ARG:H	2	0.2	0.09	0.2
(2,1)	1:8:A:LYS:HB2	1:10:A:LEU:H	2	0.2	0.06	0.2
(1,259)	1:17:A:VAL:HG11	1:19:A:ALA:HA	2	0.2	0.02	0.2
(1,259)	1:17:A:VAL:HG12	1:19:A:ALA:HA	2	0.2	0.02	0.2
(1,259)	1:17:A:VAL:HG13	1:19:A:ALA:HA	2	0.2	0.02	0.2
(1,259)	1:17:A:VAL:HG21	1:19:A:ALA:HA	2	0.2	0.02	0.2
(1,259)	1:17:A:VAL:HG22	1:19:A:ALA:HA	2	0.2	0.02	0.2
(1,259)	1:17:A:VAL:HG23	1:19:A:ALA:HA	2	0.2	0.02	0.2
(1,583)	1:45:A:ARG:HB2	1:46:A:ARG:H	2	0.19	0.08	0.19
(3,50)	1:60:A:GLU:H	1:72:A:ARG:O	2	0.18	0.02	0.18
(1,147)	1:11:A:PHE:HB3	1:12:A:GLU:H	2	0.18	0.06	0.18
(1,180)	1:13:A:VAL:H	1:60:A:GLU:HG2	2	0.18	0.0	0.18
(1,180)	1:13:A:VAL:H	1:60:A:GLU:HG3	2	0.18	0.0	0.18
(1,596)	1:46:A:ARG:HB2	1:47:A:SER:H	2	0.18	0.06	0.18
(1,736)	1:58:A:LEU:HD11	1:60:A:GLU:HA	2	0.17	0.0	0.17
(1,736)	1:58:A:LEU:HD12	1:60:A:GLU:HA	2	0.17	0.0	0.17
(1,736)	1:58:A:LEU:HD13	1:60:A:GLU:HA	2	0.17	0.0	0.17
(1,72)	1:8:A:LYS:H	1:8:A:LYS:HE2	2	0.16	0.01	0.16
(1,72)	1:8:A:LYS:H	1:8:A:LYS:HE3	2	0.16	0.01	0.16
(1,12)	1:2:A:VAL:HB	1:3:A:LYS:H	2	0.16	0.02	0.16
(1,593)	1:46:A:ARG:HA	1:46:A:ARG:HD2	2	0.16	0.04	0.16

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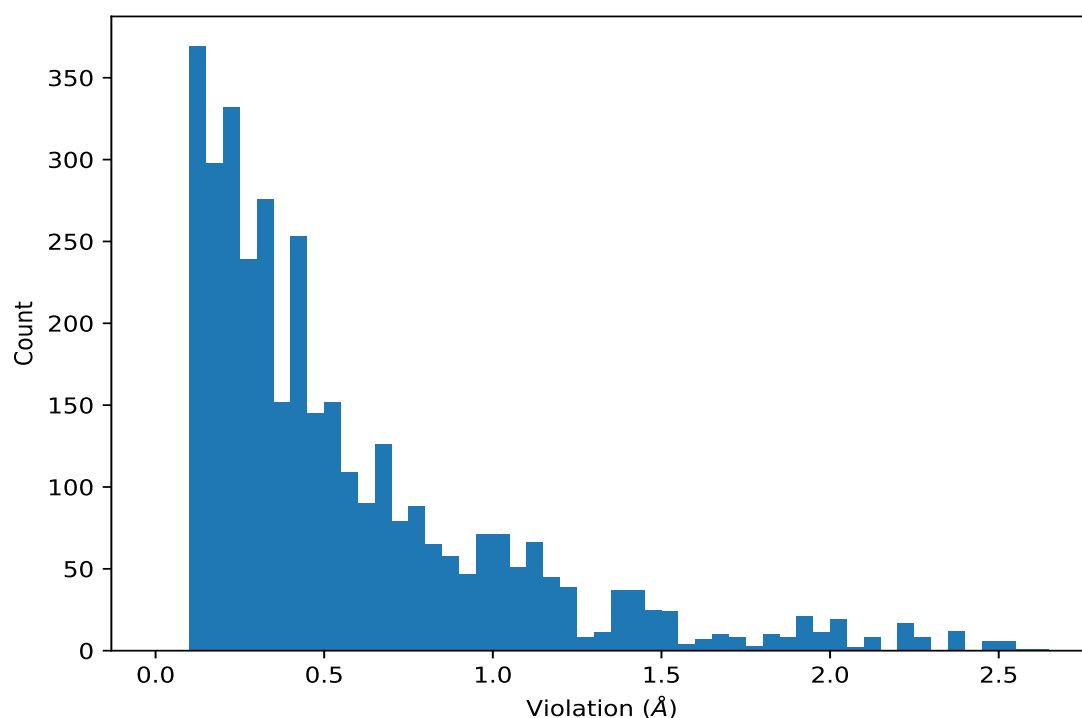
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,593)	1:46:A:ARG:HA	1:46:A:ARG:HD3	2	0.16	0.04	0.16
(1,619)	1:48:A:LYS:HB3	1:49:A:ILE:H	2	0.16	0.02	0.16
(1,1011)	1:83:A:ARG:HB2	1:84:A:THR:H	2	0.15	0.01	0.15
(1,1011)	1:83:A:ARG:HB3	1:84:A:THR:H	2	0.15	0.01	0.15
(1,961)	1:77:A:LEU:HB2	1:78:A:LYS:H	2	0.15	0.04	0.15
(1,961)	1:77:A:LEU:HB3	1:78:A:LYS:H	2	0.15	0.04	0.15
(3,51)	1:60:A:GLU:N	1:72:A:ARG:O	2	0.15	0.0	0.15
(1,279)	1:18:A:THR:HA	1:28:A:VAL:HG11	2	0.15	0.03	0.15
(1,279)	1:18:A:THR:HA	1:28:A:VAL:HG12	2	0.15	0.03	0.15
(1,279)	1:18:A:THR:HA	1:28:A:VAL:HG13	2	0.15	0.03	0.15
(1,279)	1:18:A:THR:HA	1:28:A:VAL:HG21	2	0.15	0.03	0.15
(1,279)	1:18:A:THR:HA	1:28:A:VAL:HG22	2	0.15	0.03	0.15
(1,279)	1:18:A:THR:HA	1:28:A:VAL:HG23	2	0.15	0.03	0.15
(1,51)	1:6:A:LYS:HA	1:6:A:LYS:HE2	2	0.14	0.02	0.14
(1,51)	1:6:A:LYS:HA	1:6:A:LYS:HE3	2	0.14	0.02	0.14
(1,476)	1:36:A:ILE:HG12	1:37:A:ILE:H	2	0.14	0.01	0.14
(1,476)	1:36:A:ILE:HG13	1:37:A:ILE:H	2	0.14	0.01	0.14
(1,995)	1:83:A:ARG:H	1:83:A:ARG:HB2	2	0.12	0.0	0.12
(1,995)	1:83:A:ARG:H	1:83:A:ARG:HB3	2	0.12	0.0	0.12
(1,695)	1:53:A:ILE:H	1:54:A:GLY:H	2	0.11	0.0	0.11

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



9.5.2 Table : All distance violations [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)
(1,392)	1:26:A:PHE:HD2	1:40:A:VAL:H	6	2.64
(1,394)	1:26:A:PHE:HE2	1:40:A:VAL:H	6	2.57
(1,1012)	1:83:A:ARG:HD2	1:85:A:ILE:HD11	7	2.51
(1,1012)	1:83:A:ARG:HD2	1:85:A:ILE:HD12	7	2.51
(1,1012)	1:83:A:ARG:HD2	1:85:A:ILE:HD13	7	2.51
(1,1012)	1:83:A:ARG:HD3	1:85:A:ILE:HD11	7	2.51
(1,1012)	1:83:A:ARG:HD3	1:85:A:ILE:HD12	7	2.51
(1,1012)	1:83:A:ARG:HD3	1:85:A:ILE:HD13	7	2.51
(1,1012)	1:83:A:ARG:HD2	1:85:A:ILE:HD11	8	2.45
(1,1012)	1:83:A:ARG:HD2	1:85:A:ILE:HD12	8	2.45
(1,1012)	1:83:A:ARG:HD2	1:85:A:ILE:HD13	8	2.45
(1,1012)	1:83:A:ARG:HD3	1:85:A:ILE:HD11	8	2.45
(1,1012)	1:83:A:ARG:HD3	1:85:A:ILE:HD12	8	2.45
(1,1012)	1:83:A:ARG:HD3	1:85:A:ILE:HD13	8	2.45
(1,1013)	1:83:A:ARG:HD2	1:85:A:ILE:HG21	2	2.39
(1,1013)	1:83:A:ARG:HD2	1:85:A:ILE:HG22	2	2.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1013)	1:83:A:ARG:HD2	1:85:A:ILE:HG23	2	2.39
(1,1013)	1:83:A:ARG:HD3	1:85:A:ILE:HG21	2	2.39
(1,1013)	1:83:A:ARG:HD3	1:85:A:ILE:HG22	2	2.39
(1,1013)	1:83:A:ARG:HD3	1:85:A:ILE:HG23	2	2.39
(1,1012)	1:83:A:ARG:HD2	1:85:A:ILE:HD11	1	2.39
(1,1012)	1:83:A:ARG:HD2	1:85:A:ILE:HD12	1	2.39
(1,1012)	1:83:A:ARG:HD2	1:85:A:ILE:HD13	1	2.39
(1,1012)	1:83:A:ARG:HD3	1:85:A:ILE:HD11	1	2.39
(1,1012)	1:83:A:ARG:HD3	1:85:A:ILE:HD12	1	2.39
(1,1012)	1:83:A:ARG:HD3	1:85:A:ILE:HD13	1	2.39
(1,287)	1:18:A:THR:HG21	1:28:A:VAL:HB	10	2.27
(1,287)	1:18:A:THR:HG22	1:28:A:VAL:HB	10	2.27
(1,287)	1:18:A:THR:HG23	1:28:A:VAL:HB	10	2.27
(1,855)	1:69:A:LYS:HD2	1:70:A:LYS:H	2	2.25
(1,855)	1:69:A:LYS:HD3	1:70:A:LYS:H	2	2.25
(1,287)	1:18:A:THR:HG21	1:28:A:VAL:HB	4	2.25
(1,287)	1:18:A:THR:HG22	1:28:A:VAL:HB	4	2.25
(1,287)	1:18:A:THR:HG23	1:28:A:VAL:HB	4	2.25
(1,966)	1:77:A:LEU:HD11	1:80:A:THR:HB	1	2.24
(1,966)	1:77:A:LEU:HD12	1:80:A:THR:HB	1	2.24
(1,966)	1:77:A:LEU:HD13	1:80:A:THR:HB	1	2.24
(1,966)	1:77:A:LEU:HD21	1:80:A:THR:HB	1	2.24
(1,966)	1:77:A:LEU:HD22	1:80:A:THR:HB	1	2.24
(1,966)	1:77:A:LEU:HD23	1:80:A:THR:HB	1	2.24
(1,966)	1:77:A:LEU:HD11	1:80:A:THR:HB	5	2.23
(1,966)	1:77:A:LEU:HD12	1:80:A:THR:HB	5	2.23
(1,966)	1:77:A:LEU:HD13	1:80:A:THR:HB	5	2.23
(1,966)	1:77:A:LEU:HD21	1:80:A:THR:HB	5	2.23
(1,966)	1:77:A:LEU:HD22	1:80:A:THR:HB	5	2.23
(1,966)	1:77:A:LEU:HD23	1:80:A:THR:HB	5	2.23
(1,958)	1:77:A:LEU:HG	1:78:A:LYS:HB2	7	2.23
(1,958)	1:77:A:LEU:HG	1:78:A:LYS:HB3	7	2.23
(1,287)	1:18:A:THR:HG21	1:28:A:VAL:HB	5	2.22
(1,287)	1:18:A:THR:HG22	1:28:A:VAL:HB	5	2.22
(1,287)	1:18:A:THR:HG23	1:28:A:VAL:HB	5	2.22
(1,958)	1:77:A:LEU:HG	1:78:A:LYS:HB2	10	2.14
(1,958)	1:77:A:LEU:HG	1:78:A:LYS:HB3	10	2.14
(1,1012)	1:83:A:ARG:HD2	1:85:A:ILE:HD11	2	2.13
(1,1012)	1:83:A:ARG:HD2	1:85:A:ILE:HD12	2	2.13
(1,1012)	1:83:A:ARG:HD2	1:85:A:ILE:HD13	2	2.13
(1,1012)	1:83:A:ARG:HD3	1:85:A:ILE:HD11	2	2.13
(1,1012)	1:83:A:ARG:HD3	1:85:A:ILE:HD12	2	2.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1012)	1:83:A:ARG:HD3	1:85:A:ILE:HD13	2	2.13
(1,847)	1:69:A:LYS:HD2	1:70:A:LYS:H	2	2.07
(1,847)	1:69:A:LYS:HD3	1:70:A:LYS:H	2	2.07
(1,60)	1:6:A:LYS:HD3	1:7:A:SER:H	8	2.04
(1,1012)	1:83:A:ARG:HD2	1:85:A:ILE:HD11	10	2.02
(1,1012)	1:83:A:ARG:HD2	1:85:A:ILE:HD12	10	2.02
(1,1012)	1:83:A:ARG:HD2	1:85:A:ILE:HD13	10	2.02
(1,1012)	1:83:A:ARG:HD3	1:85:A:ILE:HD11	10	2.02
(1,1012)	1:83:A:ARG:HD3	1:85:A:ILE:HD12	10	2.02
(1,1012)	1:83:A:ARG:HD3	1:85:A:ILE:HD13	10	2.02
(1,959)	1:77:A:LEU:HG	1:78:A:LYS:HD2	3	2.02
(1,959)	1:77:A:LEU:HG	1:78:A:LYS:HD3	3	2.02
(1,58)	1:6:A:LYS:HD2	1:7:A:SER:H	3	2.02
(1,58)	1:6:A:LYS:HD2	1:7:A:SER:H	8	2.02
(1,966)	1:77:A:LEU:HD11	1:80:A:THR:HB	2	2.01
(1,966)	1:77:A:LEU:HD12	1:80:A:THR:HB	2	2.01
(1,966)	1:77:A:LEU:HD13	1:80:A:THR:HB	2	2.01
(1,966)	1:77:A:LEU:HD21	1:80:A:THR:HB	2	2.01
(1,966)	1:77:A:LEU:HD22	1:80:A:THR:HB	2	2.01
(1,966)	1:77:A:LEU:HD23	1:80:A:THR:HB	2	2.01
(1,855)	1:69:A:LYS:HD2	1:70:A:LYS:H	4	2.0
(1,855)	1:69:A:LYS:HD3	1:70:A:LYS:H	4	2.0
(1,662)	1:50:A:ARG:HD2	1:75:A:ARG:HG2	6	1.98
(1,662)	1:50:A:ARG:HD2	1:75:A:ARG:HG3	6	1.98
(1,662)	1:50:A:ARG:HD3	1:75:A:ARG:HG2	6	1.98
(1,662)	1:50:A:ARG:HD3	1:75:A:ARG:HG3	6	1.98
(1,960)	1:77:A:LEU:HG	1:78:A:LYS:HE2	8	1.97
(1,960)	1:77:A:LEU:HG	1:78:A:LYS:HE3	8	1.97
(1,960)	1:77:A:LEU:HG	1:78:A:LYS:HE2	10	1.97
(1,960)	1:77:A:LEU:HG	1:78:A:LYS:HE3	10	1.97
(1,959)	1:77:A:LEU:HG	1:78:A:LYS:HD2	6	1.97
(1,959)	1:77:A:LEU:HG	1:78:A:LYS:HD3	6	1.97
(1,60)	1:6:A:LYS:HD3	1:7:A:SER:H	6	1.96
(1,662)	1:50:A:ARG:HD2	1:75:A:ARG:HG2	7	1.94
(1,662)	1:50:A:ARG:HD2	1:75:A:ARG:HG3	7	1.94
(1,662)	1:50:A:ARG:HD3	1:75:A:ARG:HG2	7	1.94
(1,662)	1:50:A:ARG:HD3	1:75:A:ARG:HG3	7	1.94
(1,392)	1:26:A:PHE:HD2	1:40:A:VAL:H	5	1.94
(1,662)	1:50:A:ARG:HD2	1:75:A:ARG:HG2	3	1.93
(1,662)	1:50:A:ARG:HD2	1:75:A:ARG:HG3	3	1.93
(1,662)	1:50:A:ARG:HD3	1:75:A:ARG:HG2	3	1.93
(1,662)	1:50:A:ARG:HD3	1:75:A:ARG:HG3	3	1.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,662)	1:50:A:ARG:HD2	1:75:A:ARG:HG2	5	1.92
(1,662)	1:50:A:ARG:HD2	1:75:A:ARG:HG3	5	1.92
(1,662)	1:50:A:ARG:HD3	1:75:A:ARG:HG2	5	1.92
(1,662)	1:50:A:ARG:HD3	1:75:A:ARG:HG3	5	1.92
(1,662)	1:50:A:ARG:HD2	1:75:A:ARG:HG2	9	1.92
(1,662)	1:50:A:ARG:HD2	1:75:A:ARG:HG3	9	1.92
(1,662)	1:50:A:ARG:HD3	1:75:A:ARG:HG2	9	1.92
(1,662)	1:50:A:ARG:HD3	1:75:A:ARG:HG3	9	1.92
(1,662)	1:50:A:ARG:HD2	1:75:A:ARG:HG2	10	1.92
(1,662)	1:50:A:ARG:HD2	1:75:A:ARG:HG3	10	1.92
(1,662)	1:50:A:ARG:HD3	1:75:A:ARG:HG2	10	1.92
(1,662)	1:50:A:ARG:HD3	1:75:A:ARG:HG3	10	1.92
(1,662)	1:50:A:ARG:HD2	1:75:A:ARG:HG2	4	1.89
(1,662)	1:50:A:ARG:HD2	1:75:A:ARG:HG3	4	1.89
(1,662)	1:50:A:ARG:HD3	1:75:A:ARG:HG2	4	1.89
(1,662)	1:50:A:ARG:HD3	1:75:A:ARG:HG3	4	1.89
(1,662)	1:50:A:ARG:HD2	1:75:A:ARG:HG2	2	1.87
(1,662)	1:50:A:ARG:HD2	1:75:A:ARG:HG3	2	1.87
(1,662)	1:50:A:ARG:HD3	1:75:A:ARG:HG2	2	1.87
(1,662)	1:50:A:ARG:HD3	1:75:A:ARG:HG3	2	1.87
(1,327)	1:20:A:LEU:HG	1:21:A:LEU:HB2	9	1.82
(1,327)	1:20:A:LEU:HG	1:21:A:LEU:HB3	9	1.82
(1,960)	1:77:A:LEU:HG	1:78:A:LYS:HE2	4	1.81
(1,960)	1:77:A:LEU:HG	1:78:A:LYS:HE3	4	1.81
(1,966)	1:77:A:LEU:HD11	1:80:A:THR:HB	7	1.8
(1,966)	1:77:A:LEU:HD12	1:80:A:THR:HB	7	1.8
(1,966)	1:77:A:LEU:HD13	1:80:A:THR:HB	7	1.8
(1,966)	1:77:A:LEU:HD21	1:80:A:THR:HB	7	1.8
(1,966)	1:77:A:LEU:HD22	1:80:A:THR:HB	7	1.8
(1,966)	1:77:A:LEU:HD23	1:80:A:THR:HB	7	1.8
(1,960)	1:77:A:LEU:HG	1:78:A:LYS:HE2	9	1.78
(1,960)	1:77:A:LEU:HG	1:78:A:LYS:HE3	9	1.78
(1,44)	1:5:A:GLU:HB3	1:6:A:LYS:H	2	1.77
(1,58)	1:6:A:LYS:HD2	1:7:A:SER:H	6	1.73
(1,58)	1:6:A:LYS:HD2	1:7:A:SER:H	5	1.72
(1,1012)	1:83:A:ARG:HD2	1:85:A:ILE:HD11	5	1.7
(1,1012)	1:83:A:ARG:HD2	1:85:A:ILE:HD12	5	1.7
(1,1012)	1:83:A:ARG:HD2	1:85:A:ILE:HD13	5	1.7
(1,1012)	1:83:A:ARG:HD3	1:85:A:ILE:HD11	5	1.7
(1,1012)	1:83:A:ARG:HD3	1:85:A:ILE:HD12	5	1.7
(1,1012)	1:83:A:ARG:HD3	1:85:A:ILE:HD13	5	1.7
(1,662)	1:50:A:ARG:HD2	1:75:A:ARG:HG2	1	1.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,662)	1:50:A:ARG:HD2	1:75:A:ARG:HG3	1	1.68
(1,662)	1:50:A:ARG:HD3	1:75:A:ARG:HG2	1	1.68
(1,662)	1:50:A:ARG:HD3	1:75:A:ARG:HG3	1	1.68
(1,662)	1:50:A:ARG:HD2	1:75:A:ARG:HG2	8	1.67
(1,662)	1:50:A:ARG:HD2	1:75:A:ARG:HG3	8	1.67
(1,662)	1:50:A:ARG:HD3	1:75:A:ARG:HG2	8	1.67
(1,662)	1:50:A:ARG:HD3	1:75:A:ARG:HG3	8	1.67
(1,394)	1:26:A:PHE:HE2	1:40:A:VAL:H	5	1.66
(1,561)	1:43:A:LYS:HG3	1:47:A:SER:HA	10	1.65
(1,521)	1:40:A:VAL:HB	1:45:A:ARG:HA	4	1.63
(1,60)	1:6:A:LYS:HD3	1:7:A:SER:H	3	1.63
(1,283)	1:18:A:THR:HB	1:53:A:ILE:HG21	8	1.62
(1,283)	1:18:A:THR:HB	1:53:A:ILE:HG22	8	1.62
(1,283)	1:18:A:THR:HB	1:53:A:ILE:HG23	8	1.62
(1,959)	1:77:A:LEU:HG	1:78:A:LYS:HD2	10	1.6
(1,959)	1:77:A:LEU:HG	1:78:A:LYS:HD3	10	1.6
(1,58)	1:6:A:LYS:HD2	1:7:A:SER:H	7	1.59
(1,283)	1:18:A:THR:HB	1:53:A:ILE:HG21	10	1.55
(1,283)	1:18:A:THR:HB	1:53:A:ILE:HG22	10	1.55
(1,283)	1:18:A:THR:HB	1:53:A:ILE:HG23	10	1.55
(1,347)	1:21:A:LEU:HG	1:23:A:ALA:H	9	1.54
(1,1012)	1:83:A:ARG:HD2	1:85:A:ILE:HD11	6	1.53
(1,1012)	1:83:A:ARG:HD2	1:85:A:ILE:HD12	6	1.53
(1,1012)	1:83:A:ARG:HD2	1:85:A:ILE:HD13	6	1.53
(1,1012)	1:83:A:ARG:HD3	1:85:A:ILE:HD11	6	1.53
(1,1012)	1:83:A:ARG:HD3	1:85:A:ILE:HD12	6	1.53
(1,1012)	1:83:A:ARG:HD3	1:85:A:ILE:HD13	6	1.53
(1,712)	1:56:A:ARG:H	1:75:A:ARG:HG2	3	1.53
(1,559)	1:43:A:LYS:HG2	1:47:A:SER:HA	10	1.53
(1,544)	1:41:A:SER:HB2	1:72:A:ARG:HD2	8	1.53
(1,544)	1:41:A:SER:HB2	1:72:A:ARG:HD3	8	1.53
(1,544)	1:41:A:SER:HB3	1:72:A:ARG:HD2	8	1.53
(1,544)	1:41:A:SER:HB3	1:72:A:ARG:HD3	8	1.53
(1,117)	1:10:A:LEU:HG	1:61:A:MET:HB2	3	1.52
(1,117)	1:10:A:LEU:HG	1:61:A:MET:HB3	3	1.52
(1,63)	1:6:A:LYS:HG2	1:7:A:SER:H	5	1.51
(1,60)	1:6:A:LYS:HD3	1:7:A:SER:H	9	1.51
(1,1012)	1:83:A:ARG:HD2	1:85:A:ILE:HD11	3	1.5
(1,1012)	1:83:A:ARG:HD2	1:85:A:ILE:HD12	3	1.5
(1,1012)	1:83:A:ARG:HD2	1:85:A:ILE:HD13	3	1.5
(1,1012)	1:83:A:ARG:HD3	1:85:A:ILE:HD11	3	1.5
(1,1012)	1:83:A:ARG:HD3	1:85:A:ILE:HD12	3	1.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1012)	1:83:A:ARG:HD3	1:85:A:ILE:HD13	3	1.5
(1,63)	1:6:A:LYS:HG2	1:7:A:SER:H	10	1.5
(1,875)	1:70:A:LYS:HD2	1:71:A:GLY:H	2	1.49
(1,875)	1:70:A:LYS:HD3	1:71:A:GLY:H	2	1.49
(1,545)	1:41:A:SER:HB2	1:72:A:ARG:HG2	8	1.49
(1,545)	1:41:A:SER:HB2	1:72:A:ARG:HG3	8	1.49
(1,545)	1:41:A:SER:HB3	1:72:A:ARG:HG2	8	1.49
(1,545)	1:41:A:SER:HB3	1:72:A:ARG:HG3	8	1.49
(1,122)	1:10:A:LEU:HB2	1:61:A:MET:HB2	1	1.49
(1,122)	1:10:A:LEU:HB2	1:61:A:MET:HB3	1	1.49
(1,122)	1:10:A:LEU:HB3	1:61:A:MET:HB2	1	1.49
(1,122)	1:10:A:LEU:HB3	1:61:A:MET:HB3	1	1.49
(1,860)	1:70:A:LYS:H	1:70:A:LYS:HD2	9	1.48
(1,860)	1:70:A:LYS:H	1:70:A:LYS:HD3	9	1.48
(1,847)	1:69:A:LYS:HD2	1:70:A:LYS:H	4	1.48
(1,847)	1:69:A:LYS:HD3	1:70:A:LYS:H	4	1.48
(1,117)	1:10:A:LEU:HG	1:61:A:MET:HB2	9	1.48
(1,117)	1:10:A:LEU:HG	1:61:A:MET:HB3	9	1.48
(1,712)	1:56:A:ARG:H	1:75:A:ARG:HG2	2	1.47
(1,957)	1:77:A:LEU:HG	1:78:A:LYS:H	10	1.46
(1,664)	1:50:A:ARG:HG2	1:75:A:ARG:HG2	9	1.45
(1,664)	1:50:A:ARG:HG2	1:75:A:ARG:HG3	9	1.45
(1,664)	1:50:A:ARG:HG3	1:75:A:ARG:HG2	9	1.45
(1,664)	1:50:A:ARG:HG3	1:75:A:ARG:HG3	9	1.45
(1,525)	1:40:A:VAL:HG11	1:45:A:ARG:HA	4	1.45
(1,525)	1:40:A:VAL:HG12	1:45:A:ARG:HA	4	1.45
(1,525)	1:40:A:VAL:HG13	1:45:A:ARG:HA	4	1.45
(1,964)	1:77:A:LEU:HD11	1:78:A:LYS:HD2	3	1.44
(1,964)	1:77:A:LEU:HD11	1:78:A:LYS:HD3	3	1.44
(1,964)	1:77:A:LEU:HD12	1:78:A:LYS:HD2	3	1.44
(1,964)	1:77:A:LEU:HD12	1:78:A:LYS:HD3	3	1.44
(1,964)	1:77:A:LEU:HD13	1:78:A:LYS:HD2	3	1.44
(1,964)	1:77:A:LEU:HD13	1:78:A:LYS:HD3	3	1.44
(1,964)	1:77:A:LEU:HD21	1:78:A:LYS:HD2	3	1.44
(1,964)	1:77:A:LEU:HD21	1:78:A:LYS:HD3	3	1.44
(1,964)	1:77:A:LEU:HD22	1:78:A:LYS:HD2	3	1.44
(1,964)	1:77:A:LEU:HD22	1:78:A:LYS:HD3	3	1.44
(1,964)	1:77:A:LEU:HD23	1:78:A:LYS:HD2	3	1.44
(1,964)	1:77:A:LEU:HD23	1:78:A:LYS:HD3	3	1.44
(1,638)	1:49:A:ILE:HD11	1:75:A:ARG:HD2	10	1.43
(1,638)	1:49:A:ILE:HD12	1:75:A:ARG:HD2	10	1.43
(1,638)	1:49:A:ILE:HD13	1:75:A:ARG:HD2	10	1.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,638)	1:49:A:ILE:HD11	1:75:A:ARG:HD3	10	1.43
(1,638)	1:49:A:ILE:HD12	1:75:A:ARG:HD3	10	1.43
(1,638)	1:49:A:ILE:HD13	1:75:A:ARG:HD3	10	1.43
(1,300)	1:19:A:ALA:HA	1:53:A:ILE:HB	8	1.43
(1,989)	1:82:A:ASP:HA	1:85:A:ILE:HG21	8	1.42
(1,989)	1:82:A:ASP:HA	1:85:A:ILE:HG22	8	1.42
(1,989)	1:82:A:ASP:HA	1:85:A:ILE:HG23	8	1.42
(1,855)	1:69:A:LYS:HD2	1:70:A:LYS:H	7	1.42
(1,855)	1:69:A:LYS:HD3	1:70:A:LYS:H	7	1.42
(1,66)	1:6:A:LYS:HG3	1:7:A:SER:H	7	1.42
(1,63)	1:6:A:LYS:HG2	1:7:A:SER:H	2	1.42
(1,561)	1:43:A:LYS:HG3	1:47:A:SER:HA	4	1.41
(1,534)	1:40:A:VAL:HG11	1:45:A:ARG:HA	4	1.41
(1,534)	1:40:A:VAL:HG12	1:45:A:ARG:HA	4	1.41
(1,534)	1:40:A:VAL:HG13	1:45:A:ARG:HA	4	1.41
(1,534)	1:40:A:VAL:HG21	1:45:A:ARG:HA	4	1.41
(1,534)	1:40:A:VAL:HG22	1:45:A:ARG:HA	4	1.41
(1,534)	1:40:A:VAL:HG23	1:45:A:ARG:HA	4	1.41
(1,68)	1:7:A:SER:H	1:8:A:LYS:H	2	1.41
(1,942)	1:76:A:ARG:HD2	1:77:A:LEU:HG	5	1.4
(1,117)	1:10:A:LEU:HG	1:61:A:MET:HB2	7	1.4
(1,117)	1:10:A:LEU:HG	1:61:A:MET:HB3	7	1.4
(1,959)	1:77:A:LEU:HG	1:78:A:LYS:HD2	7	1.39
(1,959)	1:77:A:LEU:HG	1:78:A:LYS:HD3	7	1.39
(1,300)	1:19:A:ALA:HA	1:53:A:ILE:HB	10	1.39
(1,117)	1:10:A:LEU:HG	1:61:A:MET:HB2	2	1.39
(1,117)	1:10:A:LEU:HG	1:61:A:MET:HB3	2	1.39
(1,68)	1:7:A:SER:H	1:8:A:LYS:H	9	1.38
(1,60)	1:6:A:LYS:HD3	1:7:A:SER:H	4	1.38
(1,993)	1:83:A:ARG:H	1:83:A:ARG:HD2	8	1.37
(1,993)	1:83:A:ARG:H	1:83:A:ARG:HD3	8	1.37
(1,664)	1:50:A:ARG:HG2	1:75:A:ARG:HG2	10	1.37
(1,664)	1:50:A:ARG:HG2	1:75:A:ARG:HG3	10	1.37
(1,664)	1:50:A:ARG:HG3	1:75:A:ARG:HG2	10	1.37
(1,664)	1:50:A:ARG:HG3	1:75:A:ARG:HG3	10	1.37
(1,283)	1:18:A:THR:HB	1:53:A:ILE:HG21	2	1.37
(1,283)	1:18:A:THR:HB	1:53:A:ILE:HG22	2	1.37
(1,283)	1:18:A:THR:HB	1:53:A:ILE:HG23	2	1.37
(1,44)	1:5:A:GLU:HB3	1:6:A:LYS:H	6	1.37
(1,1022)	1:84:A:THR:HG21	1:85:A:ILE:HB	5	1.36
(1,1022)	1:84:A:THR:HG22	1:85:A:ILE:HB	5	1.36
(1,1022)	1:84:A:THR:HG23	1:85:A:ILE:HB	5	1.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,128)	1:10:A:LEU:HD11	1:61:A:MET:HB2	3	1.36
(1,128)	1:10:A:LEU:HD11	1:61:A:MET:HB3	3	1.36
(1,128)	1:10:A:LEU:HD12	1:61:A:MET:HB2	3	1.36
(1,128)	1:10:A:LEU:HD12	1:61:A:MET:HB3	3	1.36
(1,128)	1:10:A:LEU:HD13	1:61:A:MET:HB2	3	1.36
(1,128)	1:10:A:LEU:HD13	1:61:A:MET:HB3	3	1.36
(1,128)	1:10:A:LEU:HD21	1:61:A:MET:HB2	3	1.36
(1,128)	1:10:A:LEU:HD21	1:61:A:MET:HB3	3	1.36
(1,128)	1:10:A:LEU:HD22	1:61:A:MET:HB2	3	1.36
(1,128)	1:10:A:LEU:HD22	1:61:A:MET:HB3	3	1.36
(1,128)	1:10:A:LEU:HD23	1:61:A:MET:HB2	3	1.36
(1,128)	1:10:A:LEU:HD23	1:61:A:MET:HB3	3	1.36
(1,1006)	1:83:A:ARG:HD2	1:84:A:THR:H	6	1.35
(1,1006)	1:83:A:ARG:HD3	1:84:A:THR:H	6	1.35
(1,712)	1:56:A:ARG:H	1:75:A:ARG:HG2	8	1.35
(1,26)	1:3:A:LYS:HD2	1:4:A:ASP:H	5	1.35
(1,26)	1:3:A:LYS:HD3	1:4:A:ASP:H	5	1.35
(1,664)	1:50:A:ARG:HG2	1:75:A:ARG:HG2	6	1.32
(1,664)	1:50:A:ARG:HG2	1:75:A:ARG:HG3	6	1.32
(1,664)	1:50:A:ARG:HG3	1:75:A:ARG:HG2	6	1.32
(1,664)	1:50:A:ARG:HG3	1:75:A:ARG:HG3	6	1.32
(1,589)	1:46:A:ARG:H	1:46:A:ARG:HD2	6	1.32
(1,589)	1:46:A:ARG:H	1:46:A:ARG:HD3	6	1.32
(1,44)	1:5:A:GLU:HB3	1:6:A:LYS:H	5	1.32
(1,942)	1:76:A:ARG:HD2	1:77:A:LEU:HG	8	1.31
(1,993)	1:83:A:ARG:H	1:83:A:ARG:HD2	2	1.3
(1,993)	1:83:A:ARG:H	1:83:A:ARG:HD3	2	1.3
(1,63)	1:6:A:LYS:HG2	1:7:A:SER:H	4	1.3
(1,858)	1:70:A:LYS:H	1:70:A:LYS:HD2	9	1.29
(1,858)	1:70:A:LYS:H	1:70:A:LYS:HD3	9	1.29
(1,34)	1:4:A:ASP:HB2	1:5:A:GLU:H	8	1.27
(1,34)	1:4:A:ASP:HB3	1:5:A:GLU:H	8	1.27
(1,993)	1:83:A:ARG:H	1:83:A:ARG:HD2	10	1.26
(1,993)	1:83:A:ARG:H	1:83:A:ARG:HD3	10	1.26
(1,63)	1:6:A:LYS:HG2	1:7:A:SER:H	9	1.26
(1,326)	1:20:A:LEU:HG	1:21:A:LEU:HA	9	1.25
(1,958)	1:77:A:LEU:HG	1:78:A:LYS:HB2	3	1.24
(1,958)	1:77:A:LEU:HG	1:78:A:LYS:HB3	3	1.24
(1,847)	1:69:A:LYS:HD2	1:70:A:LYS:H	7	1.24
(1,847)	1:69:A:LYS:HD3	1:70:A:LYS:H	7	1.24
(1,499)	1:38:A:CYS:HA	1:70:A:LYS:HD2	2	1.24
(1,499)	1:38:A:CYS:HA	1:70:A:LYS:HD3	2	1.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1035)	1:86:A:SER:H	1:87:A:LYS:H	3	1.23
(1,942)	1:76:A:ARG:HD2	1:77:A:LEU:HG	4	1.23
(1,561)	1:43:A:LYS:HG3	1:47:A:SER:HA	3	1.23
(1,300)	1:19:A:ALA:HA	1:53:A:ILE:HB	2	1.23
(1,68)	1:7:A:SER:H	1:8:A:LYS:H	4	1.23
(1,958)	1:77:A:LEU:HG	1:78:A:LYS:HB2	8	1.22
(1,958)	1:77:A:LEU:HG	1:78:A:LYS:HB3	8	1.22
(1,957)	1:77:A:LEU:HG	1:78:A:LYS:H	7	1.22
(1,287)	1:18:A:THR:HG21	1:28:A:VAL:HB	2	1.22
(1,287)	1:18:A:THR:HG22	1:28:A:VAL:HB	2	1.22
(1,287)	1:18:A:THR:HG23	1:28:A:VAL:HB	2	1.22
(1,691)	1:52:A:ILE:HG21	1:75:A:ARG:HG2	9	1.21
(1,691)	1:52:A:ILE:HG21	1:75:A:ARG:HG3	9	1.21
(1,691)	1:52:A:ILE:HG22	1:75:A:ARG:HG2	9	1.21
(1,691)	1:52:A:ILE:HG22	1:75:A:ARG:HG3	9	1.21
(1,691)	1:52:A:ILE:HG23	1:75:A:ARG:HG2	9	1.21
(1,691)	1:52:A:ILE:HG23	1:75:A:ARG:HG3	9	1.21
(3,42)	1:37:A:ILE:H	1:69:A:LYS:O	8	1.2
(1,528)	1:40:A:VAL:HG21	1:45:A:ARG:HA	4	1.2
(1,528)	1:40:A:VAL:HG22	1:45:A:ARG:HA	4	1.2
(1,528)	1:40:A:VAL:HG23	1:45:A:ARG:HA	4	1.2
(1,128)	1:10:A:LEU:HD11	1:61:A:MET:HB2	9	1.2
(1,128)	1:10:A:LEU:HD11	1:61:A:MET:HB3	9	1.2
(1,128)	1:10:A:LEU:HD12	1:61:A:MET:HB2	9	1.2
(1,128)	1:10:A:LEU:HD12	1:61:A:MET:HB3	9	1.2
(1,128)	1:10:A:LEU:HD13	1:61:A:MET:HB2	9	1.2
(1,128)	1:10:A:LEU:HD13	1:61:A:MET:HB3	9	1.2
(1,128)	1:10:A:LEU:HD21	1:61:A:MET:HB2	9	1.2
(1,128)	1:10:A:LEU:HD21	1:61:A:MET:HB3	9	1.2
(1,128)	1:10:A:LEU:HD22	1:61:A:MET:HB2	9	1.2
(1,128)	1:10:A:LEU:HD22	1:61:A:MET:HB3	9	1.2
(1,128)	1:10:A:LEU:HD23	1:61:A:MET:HB2	9	1.2
(1,128)	1:10:A:LEU:HD23	1:61:A:MET:HB3	9	1.2
(1,993)	1:83:A:ARG:H	1:83:A:ARG:HD2	4	1.19
(1,993)	1:83:A:ARG:H	1:83:A:ARG:HD3	4	1.19
(1,559)	1:43:A:LYS:HG2	1:47:A:SER:HA	4	1.19
(1,318)	1:20:A:LEU:HB2	1:25:A:GLU:H	6	1.19
(1,739)	1:58:A:LEU:HD11	1:60:A:GLU:HB2	6	1.18
(1,739)	1:58:A:LEU:HD11	1:60:A:GLU:HB3	6	1.18
(1,739)	1:58:A:LEU:HD12	1:60:A:GLU:HB2	6	1.18
(1,739)	1:58:A:LEU:HD12	1:60:A:GLU:HB3	6	1.18
(1,739)	1:58:A:LEU:HD13	1:60:A:GLU:HB2	6	1.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,739)	1:58:A:LEU:HD13	1:60:A:GLU:HB3	6	1.18
(1,739)	1:58:A:LEU:HD21	1:60:A:GLU:HB2	6	1.18
(1,739)	1:58:A:LEU:HD21	1:60:A:GLU:HB3	6	1.18
(1,739)	1:58:A:LEU:HD22	1:60:A:GLU:HB2	6	1.18
(1,739)	1:58:A:LEU:HD22	1:60:A:GLU:HB3	6	1.18
(1,739)	1:58:A:LEU:HD23	1:60:A:GLU:HB2	6	1.18
(1,739)	1:58:A:LEU:HD23	1:60:A:GLU:HB3	6	1.18
(1,422)	1:28:A:VAL:HB	1:29:A:LYS:HD2	9	1.18
(1,422)	1:28:A:VAL:HB	1:29:A:LYS:HD3	9	1.18
(1,300)	1:19:A:ALA:HA	1:53:A:ILE:HB	3	1.18
(1,291)	1:18:A:THR:HG21	1:53:A:ILE:HD11	10	1.18
(1,291)	1:18:A:THR:HG21	1:53:A:ILE:HD12	10	1.18
(1,291)	1:18:A:THR:HG21	1:53:A:ILE:HD13	10	1.18
(1,291)	1:18:A:THR:HG22	1:53:A:ILE:HD11	10	1.18
(1,291)	1:18:A:THR:HG22	1:53:A:ILE:HD12	10	1.18
(1,291)	1:18:A:THR:HG22	1:53:A:ILE:HD13	10	1.18
(1,291)	1:18:A:THR:HG23	1:53:A:ILE:HD11	10	1.18
(1,291)	1:18:A:THR:HG23	1:53:A:ILE:HD12	10	1.18
(1,291)	1:18:A:THR:HG23	1:53:A:ILE:HD13	10	1.18
(3,46)	1:39:A:HIS:O	1:73:A:ILE:H	10	1.17
(1,993)	1:83:A:ARG:H	1:83:A:ARG:HD2	3	1.17
(1,993)	1:83:A:ARG:H	1:83:A:ARG:HD3	3	1.17
(1,291)	1:18:A:THR:HG21	1:53:A:ILE:HD11	2	1.17
(1,291)	1:18:A:THR:HG21	1:53:A:ILE:HD12	2	1.17
(1,291)	1:18:A:THR:HG21	1:53:A:ILE:HD13	2	1.17
(1,291)	1:18:A:THR:HG22	1:53:A:ILE:HD11	2	1.17
(1,291)	1:18:A:THR:HG22	1:53:A:ILE:HD12	2	1.17
(1,291)	1:18:A:THR:HG22	1:53:A:ILE:HD13	2	1.17
(1,291)	1:18:A:THR:HG23	1:53:A:ILE:HD11	2	1.17
(1,291)	1:18:A:THR:HG23	1:53:A:ILE:HD12	2	1.17
(1,291)	1:18:A:THR:HG23	1:53:A:ILE:HD13	2	1.17
(1,117)	1:10:A:LEU:HG	1:61:A:MET:HB2	4	1.17
(1,117)	1:10:A:LEU:HG	1:61:A:MET:HB3	4	1.17
(1,112)	1:10:A:LEU:HB2	1:61:A:MET:HA	1	1.16
(3,46)	1:39:A:HIS:O	1:73:A:ILE:H	9	1.15
(1,74)	1:8:A:LYS:H	1:9:A:THR:H	3	1.15
(1,1013)	1:83:A:ARG:HD2	1:85:A:ILE:HG21	8	1.14
(1,1013)	1:83:A:ARG:HD2	1:85:A:ILE:HG22	8	1.14
(1,1013)	1:83:A:ARG:HD2	1:85:A:ILE:HG23	8	1.14
(1,1013)	1:83:A:ARG:HD3	1:85:A:ILE:HG21	8	1.14
(1,1013)	1:83:A:ARG:HD3	1:85:A:ILE:HG22	8	1.14
(1,1013)	1:83:A:ARG:HD3	1:85:A:ILE:HG23	8	1.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,960)	1:77:A:LEU:HG	1:78:A:LYS:HE2	6	1.14
(1,960)	1:77:A:LEU:HG	1:78:A:LYS:HE3	6	1.14
(1,824)	1:66:A:ARG:HD3	1:68:A:ALA:HB1	9	1.14
(1,824)	1:66:A:ARG:HD3	1:68:A:ALA:HB2	9	1.14
(1,824)	1:66:A:ARG:HD3	1:68:A:ALA:HB3	9	1.14
(1,318)	1:20:A:LEU:HB2	1:25:A:GLU:H	9	1.13
(1,128)	1:10:A:LEU:HD11	1:61:A:MET:HB2	7	1.13
(1,128)	1:10:A:LEU:HD11	1:61:A:MET:HB3	7	1.13
(1,128)	1:10:A:LEU:HD12	1:61:A:MET:HB2	7	1.13
(1,128)	1:10:A:LEU:HD12	1:61:A:MET:HB3	7	1.13
(1,128)	1:10:A:LEU:HD13	1:61:A:MET:HB2	7	1.13
(1,128)	1:10:A:LEU:HD13	1:61:A:MET:HB3	7	1.13
(1,128)	1:10:A:LEU:HD21	1:61:A:MET:HB2	7	1.13
(1,128)	1:10:A:LEU:HD21	1:61:A:MET:HB3	7	1.13
(1,128)	1:10:A:LEU:HD22	1:61:A:MET:HB2	7	1.13
(1,128)	1:10:A:LEU:HD22	1:61:A:MET:HB3	7	1.13
(1,128)	1:10:A:LEU:HD23	1:61:A:MET:HB2	7	1.13
(1,128)	1:10:A:LEU:HD23	1:61:A:MET:HB3	7	1.13
(1,8)	1:2:A:VAL:H	1:3:A:LYS:H	8	1.13
(1,989)	1:82:A:ASP:HA	1:85:A:ILE:HG21	2	1.12
(1,989)	1:82:A:ASP:HA	1:85:A:ILE:HG22	2	1.12
(1,989)	1:82:A:ASP:HA	1:85:A:ILE:HG23	2	1.12
(1,965)	1:77:A:LEU:HD11	1:78:A:LYS:HE2	8	1.12
(1,965)	1:77:A:LEU:HD11	1:78:A:LYS:HE3	8	1.12
(1,965)	1:77:A:LEU:HD12	1:78:A:LYS:HE2	8	1.12
(1,965)	1:77:A:LEU:HD12	1:78:A:LYS:HE3	8	1.12
(1,965)	1:77:A:LEU:HD13	1:78:A:LYS:HE2	8	1.12
(1,965)	1:77:A:LEU:HD13	1:78:A:LYS:HE3	8	1.12
(1,965)	1:77:A:LEU:HD21	1:78:A:LYS:HE2	8	1.12
(1,965)	1:77:A:LEU:HD21	1:78:A:LYS:HE3	8	1.12
(1,965)	1:77:A:LEU:HD22	1:78:A:LYS:HE2	8	1.12
(1,965)	1:77:A:LEU:HD22	1:78:A:LYS:HE3	8	1.12
(1,965)	1:77:A:LEU:HD23	1:78:A:LYS:HE2	8	1.12
(1,965)	1:77:A:LEU:HD23	1:78:A:LYS:HE3	8	1.12
(1,769)	1:61:A:MET:HG2	1:70:A:LYS:HB2	2	1.12
(1,769)	1:61:A:MET:HG2	1:70:A:LYS:HB3	2	1.12
(1,769)	1:61:A:MET:HG3	1:70:A:LYS:HB2	2	1.12
(1,769)	1:61:A:MET:HG3	1:70:A:LYS:HB3	2	1.12
(1,875)	1:70:A:LYS:HD2	1:71:A:GLY:H	5	1.11
(1,875)	1:70:A:LYS:HD3	1:71:A:GLY:H	5	1.11
(1,664)	1:50:A:ARG:HG2	1:75:A:ARG:HG2	7	1.11
(1,664)	1:50:A:ARG:HG2	1:75:A:ARG:HG3	7	1.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,664)	1:50:A:ARG:HG3	1:75:A:ARG:HG2	7	1.11
(1,664)	1:50:A:ARG:HG3	1:75:A:ARG:HG3	7	1.11
(1,318)	1:20:A:LEU:HB2	1:25:A:GLU:H	8	1.11
(1,875)	1:70:A:LYS:HD2	1:71:A:GLY:H	7	1.1
(1,875)	1:70:A:LYS:HD3	1:71:A:GLY:H	7	1.1
(1,769)	1:61:A:MET:HG2	1:70:A:LYS:HB2	4	1.1
(1,769)	1:61:A:MET:HG2	1:70:A:LYS:HB3	4	1.1
(1,769)	1:61:A:MET:HG3	1:70:A:LYS:HB2	4	1.1
(1,769)	1:61:A:MET:HG3	1:70:A:LYS:HB3	4	1.1
(1,638)	1:49:A:ILE:HD11	1:75:A:ARG:HD2	9	1.1
(1,638)	1:49:A:ILE:HD12	1:75:A:ARG:HD2	9	1.1
(1,638)	1:49:A:ILE:HD13	1:75:A:ARG:HD2	9	1.1
(1,638)	1:49:A:ILE:HD11	1:75:A:ARG:HD3	9	1.1
(1,638)	1:49:A:ILE:HD12	1:75:A:ARG:HD3	9	1.1
(1,638)	1:49:A:ILE:HD13	1:75:A:ARG:HD3	9	1.1
(1,589)	1:46:A:ARG:H	1:46:A:ARG:HD2	4	1.1
(1,589)	1:46:A:ARG:H	1:46:A:ARG:HD3	4	1.1
(1,347)	1:21:A:LEU:HG	1:23:A:ALA:H	2	1.1
(3,44)	1:37:A:ILE:O	1:71:A:GLY:H	4	1.09
(1,1012)	1:83:A:ARG:HD2	1:85:A:ILE:HD11	4	1.09
(1,1012)	1:83:A:ARG:HD2	1:85:A:ILE:HD12	4	1.09
(1,1012)	1:83:A:ARG:HD2	1:85:A:ILE:HD13	4	1.09
(1,1012)	1:83:A:ARG:HD3	1:85:A:ILE:HD11	4	1.09
(1,1012)	1:83:A:ARG:HD3	1:85:A:ILE:HD12	4	1.09
(1,1012)	1:83:A:ARG:HD3	1:85:A:ILE:HD13	4	1.09
(1,735)	1:58:A:LEU:HG	1:73:A:ILE:HA	8	1.09
(3,54)	1:44:A:VAL:O	1:47:A:SER:H	1	1.08
(1,589)	1:46:A:ARG:H	1:46:A:ARG:HD2	5	1.08
(1,589)	1:46:A:ARG:H	1:46:A:ARG:HD3	5	1.08
(1,318)	1:20:A:LEU:HB2	1:25:A:GLU:H	7	1.08
(1,116)	1:10:A:LEU:HG	1:61:A:MET:HA	9	1.08
(1,1022)	1:84:A:THR:HG21	1:85:A:ILE:HB	4	1.07
(1,1022)	1:84:A:THR:HG22	1:85:A:ILE:HB	4	1.07
(1,1022)	1:84:A:THR:HG23	1:85:A:ILE:HB	4	1.07
(1,964)	1:77:A:LEU:HD11	1:78:A:LYS:HD2	6	1.07
(1,964)	1:77:A:LEU:HD11	1:78:A:LYS:HD3	6	1.07
(1,964)	1:77:A:LEU:HD12	1:78:A:LYS:HD2	6	1.07
(1,964)	1:77:A:LEU:HD12	1:78:A:LYS:HD3	6	1.07
(1,964)	1:77:A:LEU:HD13	1:78:A:LYS:HD2	6	1.07
(1,964)	1:77:A:LEU:HD13	1:78:A:LYS:HD3	6	1.07
(1,964)	1:77:A:LEU:HD21	1:78:A:LYS:HD2	6	1.07
(1,964)	1:77:A:LEU:HD21	1:78:A:LYS:HD3	6	1.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,964)	1:77:A:LEU:HD22	1:78:A:LYS:HD2	6	1.07
(1,964)	1:77:A:LEU:HD22	1:78:A:LYS:HD3	6	1.07
(1,964)	1:77:A:LEU:HD23	1:78:A:LYS:HD2	6	1.07
(1,964)	1:77:A:LEU:HD23	1:78:A:LYS:HD3	6	1.07
(1,855)	1:69:A:LYS:HD2	1:70:A:LYS:H	3	1.07
(1,855)	1:69:A:LYS:HD3	1:70:A:LYS:H	3	1.07
(1,735)	1:58:A:LEU:HG	1:73:A:ILE:HA	2	1.07
(1,44)	1:5:A:GLU:HB3	1:6:A:LYS:H	9	1.07
(3,47)	1:39:A:HIS:O	1:73:A:ILE:N	10	1.06
(1,1013)	1:83:A:ARG:HD2	1:85:A:ILE:HG21	7	1.06
(1,1013)	1:83:A:ARG:HD2	1:85:A:ILE:HG22	7	1.06
(1,1013)	1:83:A:ARG:HD2	1:85:A:ILE:HG23	7	1.06
(1,1013)	1:83:A:ARG:HD3	1:85:A:ILE:HG21	7	1.06
(1,1013)	1:83:A:ARG:HD3	1:85:A:ILE:HG22	7	1.06
(1,1013)	1:83:A:ARG:HD3	1:85:A:ILE:HG23	7	1.06
(1,824)	1:66:A:ARG:HD3	1:68:A:ALA:HB1	3	1.06
(1,824)	1:66:A:ARG:HD3	1:68:A:ALA:HB2	3	1.06
(1,824)	1:66:A:ARG:HD3	1:68:A:ALA:HB3	3	1.06
(1,824)	1:66:A:ARG:HD3	1:68:A:ALA:HB1	5	1.06
(1,824)	1:66:A:ARG:HD3	1:68:A:ALA:HB2	5	1.06
(1,824)	1:66:A:ARG:HD3	1:68:A:ALA:HB3	5	1.06
(1,769)	1:61:A:MET:HG2	1:70:A:LYS:HB2	3	1.06
(1,769)	1:61:A:MET:HG2	1:70:A:LYS:HB3	3	1.06
(1,769)	1:61:A:MET:HG3	1:70:A:LYS:HB2	3	1.06
(1,769)	1:61:A:MET:HG3	1:70:A:LYS:HB3	3	1.06
(1,318)	1:20:A:LEU:HB2	1:25:A:GLU:H	2	1.06
(1,60)	1:6:A:LYS:HD3	1:7:A:SER:H	10	1.05
(1,769)	1:61:A:MET:HG2	1:70:A:LYS:HB2	9	1.04
(1,769)	1:61:A:MET:HG2	1:70:A:LYS:HB3	9	1.04
(1,769)	1:61:A:MET:HG3	1:70:A:LYS:HB2	9	1.04
(1,769)	1:61:A:MET:HG3	1:70:A:LYS:HB3	9	1.04
(1,713)	1:56:A:ARG:H	1:76:A:ARG:H	10	1.04
(1,589)	1:46:A:ARG:H	1:46:A:ARG:HD2	8	1.04
(1,589)	1:46:A:ARG:H	1:46:A:ARG:HD3	8	1.04
(1,323)	1:20:A:LEU:HB3	1:25:A:GLU:H	6	1.04
(1,323)	1:20:A:LEU:HB3	1:25:A:GLU:H	8	1.04
(1,1022)	1:84:A:THR:HG21	1:85:A:ILE:HB	8	1.03
(1,1022)	1:84:A:THR:HG22	1:85:A:ILE:HB	8	1.03
(1,1022)	1:84:A:THR:HG23	1:85:A:ILE:HB	8	1.03
(1,991)	1:82:A:ASP:HB2	1:85:A:ILE:HG21	1	1.03
(1,991)	1:82:A:ASP:HB2	1:85:A:ILE:HG22	1	1.03
(1,991)	1:82:A:ASP:HB2	1:85:A:ILE:HG23	1	1.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,991)	1:82:A:ASP:HB3	1:85:A:ILE:HG21	1	1.03
(1,991)	1:82:A:ASP:HB3	1:85:A:ILE:HG22	1	1.03
(1,991)	1:82:A:ASP:HB3	1:85:A:ILE:HG23	1	1.03
(1,769)	1:61:A:MET:HG2	1:70:A:LYS:HB2	5	1.03
(1,769)	1:61:A:MET:HG2	1:70:A:LYS:HB3	5	1.03
(1,769)	1:61:A:MET:HG3	1:70:A:LYS:HB2	5	1.03
(1,769)	1:61:A:MET:HG3	1:70:A:LYS:HB3	5	1.03
(1,589)	1:46:A:ARG:H	1:46:A:ARG:HD2	1	1.03
(1,589)	1:46:A:ARG:H	1:46:A:ARG:HD3	1	1.03
(1,559)	1:43:A:LYS:HG2	1:47:A:SER:HA	3	1.03
(1,530)	1:40:A:VAL:HG11	1:44:A:VAL:HA	3	1.03
(1,530)	1:40:A:VAL:HG12	1:44:A:VAL:HA	3	1.03
(1,530)	1:40:A:VAL:HG13	1:44:A:VAL:HA	3	1.03
(1,530)	1:40:A:VAL:HG21	1:44:A:VAL:HA	3	1.03
(1,530)	1:40:A:VAL:HG22	1:44:A:VAL:HA	3	1.03
(1,530)	1:40:A:VAL:HG23	1:44:A:VAL:HA	3	1.03
(1,318)	1:20:A:LEU:HB2	1:25:A:GLU:H	5	1.03
(1,112)	1:10:A:LEU:HB2	1:61:A:MET:HA	5	1.03
(1,42)	1:5:A:GLU:HB2	1:6:A:LYS:H	4	1.03
(3,54)	1:44:A:VAL:O	1:47:A:SER:H	6	1.02
(1,860)	1:70:A:LYS:H	1:70:A:LYS:HD2	2	1.02
(1,860)	1:70:A:LYS:H	1:70:A:LYS:HD3	2	1.02
(1,769)	1:61:A:MET:HG2	1:70:A:LYS:HB2	10	1.02
(1,769)	1:61:A:MET:HG2	1:70:A:LYS:HB3	10	1.02
(1,769)	1:61:A:MET:HG3	1:70:A:LYS:HB2	10	1.02
(1,769)	1:61:A:MET:HG3	1:70:A:LYS:HB3	10	1.02
(1,116)	1:10:A:LEU:HG	1:61:A:MET:HA	2	1.02
(1,60)	1:6:A:LYS:HD3	1:7:A:SER:H	2	1.02
(1,993)	1:83:A:ARG:H	1:83:A:ARG:HD2	7	1.01
(1,993)	1:83:A:ARG:H	1:83:A:ARG:HD3	7	1.01
(1,664)	1:50:A:ARG:HG2	1:75:A:ARG:HG2	5	1.01
(1,664)	1:50:A:ARG:HG2	1:75:A:ARG:HG3	5	1.01
(1,664)	1:50:A:ARG:HG3	1:75:A:ARG:HG2	5	1.01
(1,664)	1:50:A:ARG:HG3	1:75:A:ARG:HG3	5	1.01
(1,323)	1:20:A:LEU:HB3	1:25:A:GLU:H	2	1.01
(1,216)	1:15:A:GLY:HA3	1:30:A:LEU:HA	2	1.01
(1,14)	1:3:A:LYS:H	1:3:A:LYS:HD2	5	1.01
(1,14)	1:3:A:LYS:H	1:3:A:LYS:HD3	5	1.01
(3,46)	1:39:A:HIS:O	1:73:A:ILE:H	4	1.0
(1,963)	1:77:A:LEU:HD11	1:78:A:LYS:HB2	3	1.0
(1,963)	1:77:A:LEU:HD11	1:78:A:LYS:HB3	3	1.0
(1,963)	1:77:A:LEU:HD12	1:78:A:LYS:HB2	3	1.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,963)	1:77:A:LEU:HD12	1:78:A:LYS:HB3	3	1.0
(1,963)	1:77:A:LEU:HD13	1:78:A:LYS:HB2	3	1.0
(1,963)	1:77:A:LEU:HD13	1:78:A:LYS:HB3	3	1.0
(1,963)	1:77:A:LEU:HD21	1:78:A:LYS:HB2	3	1.0
(1,963)	1:77:A:LEU:HD21	1:78:A:LYS:HB3	3	1.0
(1,963)	1:77:A:LEU:HD22	1:78:A:LYS:HB2	3	1.0
(1,963)	1:77:A:LEU:HD22	1:78:A:LYS:HB3	3	1.0
(1,963)	1:77:A:LEU:HD23	1:78:A:LYS:HB2	3	1.0
(1,963)	1:77:A:LEU:HD23	1:78:A:LYS:HB3	3	1.0
(1,522)	1:40:A:VAL:HB	1:45:A:ARG:HB2	4	1.0
(1,522)	1:40:A:VAL:HB	1:45:A:ARG:HB3	4	1.0
(1,287)	1:18:A:THR:HG21	1:28:A:VAL:HB	3	1.0
(1,287)	1:18:A:THR:HG22	1:28:A:VAL:HB	3	1.0
(1,287)	1:18:A:THR:HG23	1:28:A:VAL:HB	3	1.0
(1,855)	1:69:A:LYS:HD2	1:70:A:LYS:H	8	0.99
(1,855)	1:69:A:LYS:HD3	1:70:A:LYS:H	8	0.99
(1,712)	1:56:A:ARG:H	1:75:A:ARG:HG2	10	0.99
(1,438)	1:29:A:LYS:HD2	1:30:A:LEU:H	9	0.98
(1,438)	1:29:A:LYS:HD3	1:30:A:LEU:H	9	0.98
(1,769)	1:61:A:MET:HG2	1:70:A:LYS:HB2	6	0.97
(1,769)	1:61:A:MET:HG2	1:70:A:LYS:HB3	6	0.97
(1,769)	1:61:A:MET:HG3	1:70:A:LYS:HB2	6	0.97
(1,769)	1:61:A:MET:HG3	1:70:A:LYS:HB3	6	0.97
(1,323)	1:20:A:LEU:HB3	1:25:A:GLU:H	7	0.97
(1,318)	1:20:A:LEU:HB2	1:25:A:GLU:H	4	0.97
(1,58)	1:6:A:LYS:HD2	1:7:A:SER:H	1	0.97
(1,965)	1:77:A:LEU:HD11	1:78:A:LYS:HE2	9	0.96
(1,965)	1:77:A:LEU:HD11	1:78:A:LYS:HE3	9	0.96
(1,965)	1:77:A:LEU:HD12	1:78:A:LYS:HE2	9	0.96
(1,965)	1:77:A:LEU:HD12	1:78:A:LYS:HE3	9	0.96
(1,965)	1:77:A:LEU:HD13	1:78:A:LYS:HE2	9	0.96
(1,965)	1:77:A:LEU:HD13	1:78:A:LYS:HE3	9	0.96
(1,965)	1:77:A:LEU:HD21	1:78:A:LYS:HE2	9	0.96
(1,965)	1:77:A:LEU:HD21	1:78:A:LYS:HE3	9	0.96
(1,965)	1:77:A:LEU:HD22	1:78:A:LYS:HE2	9	0.96
(1,965)	1:77:A:LEU:HD22	1:78:A:LYS:HE3	9	0.96
(1,965)	1:77:A:LEU:HD23	1:78:A:LYS:HE2	9	0.96
(1,965)	1:77:A:LEU:HD23	1:78:A:LYS:HE3	9	0.96
(1,963)	1:77:A:LEU:HD11	1:78:A:LYS:HB2	8	0.96
(1,963)	1:77:A:LEU:HD11	1:78:A:LYS:HB3	8	0.96
(1,963)	1:77:A:LEU:HD12	1:78:A:LYS:HB2	8	0.96
(1,963)	1:77:A:LEU:HD12	1:78:A:LYS:HB3	8	0.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,963)	1:77:A:LEU:HD13	1:78:A:LYS:HB2	8	0.96
(1,963)	1:77:A:LEU:HD13	1:78:A:LYS:HB3	8	0.96
(1,963)	1:77:A:LEU:HD21	1:78:A:LYS:HB2	8	0.96
(1,963)	1:77:A:LEU:HD21	1:78:A:LYS:HB3	8	0.96
(1,963)	1:77:A:LEU:HD22	1:78:A:LYS:HB2	8	0.96
(1,963)	1:77:A:LEU:HD22	1:78:A:LYS:HB3	8	0.96
(1,963)	1:77:A:LEU:HD23	1:78:A:LYS:HB2	8	0.96
(1,963)	1:77:A:LEU:HD23	1:78:A:LYS:HB3	8	0.96
(1,691)	1:52:A:ILE:HG21	1:75:A:ARG:HG2	7	0.96
(1,691)	1:52:A:ILE:HG21	1:75:A:ARG:HG3	7	0.96
(1,691)	1:52:A:ILE:HG22	1:75:A:ARG:HG2	7	0.96
(1,691)	1:52:A:ILE:HG22	1:75:A:ARG:HG3	7	0.96
(1,691)	1:52:A:ILE:HG23	1:75:A:ARG:HG2	7	0.96
(1,691)	1:52:A:ILE:HG23	1:75:A:ARG:HG3	7	0.96
(1,128)	1:10:A:LEU:HD11	1:61:A:MET:HB2	4	0.96
(1,128)	1:10:A:LEU:HD11	1:61:A:MET:HB3	4	0.96
(1,128)	1:10:A:LEU:HD12	1:61:A:MET:HB2	4	0.96
(1,128)	1:10:A:LEU:HD12	1:61:A:MET:HB3	4	0.96
(1,128)	1:10:A:LEU:HD13	1:61:A:MET:HB2	4	0.96
(1,128)	1:10:A:LEU:HD13	1:61:A:MET:HB3	4	0.96
(1,128)	1:10:A:LEU:HD21	1:61:A:MET:HB2	4	0.96
(1,128)	1:10:A:LEU:HD21	1:61:A:MET:HB3	4	0.96
(1,128)	1:10:A:LEU:HD22	1:61:A:MET:HB2	4	0.96
(1,128)	1:10:A:LEU:HD22	1:61:A:MET:HB3	4	0.96
(1,128)	1:10:A:LEU:HD23	1:61:A:MET:HB2	4	0.96
(1,128)	1:10:A:LEU:HD23	1:61:A:MET:HB3	4	0.96
(1,288)	1:18:A:THR:HG21	1:29:A:LYS:H	4	0.95
(1,288)	1:18:A:THR:HG22	1:29:A:LYS:H	4	0.95
(1,288)	1:18:A:THR:HG23	1:29:A:LYS:H	4	0.95
(1,128)	1:10:A:LEU:HD11	1:61:A:MET:HB2	2	0.95
(1,128)	1:10:A:LEU:HD11	1:61:A:MET:HB3	2	0.95
(1,128)	1:10:A:LEU:HD12	1:61:A:MET:HB2	2	0.95
(1,128)	1:10:A:LEU:HD12	1:61:A:MET:HB3	2	0.95
(1,128)	1:10:A:LEU:HD13	1:61:A:MET:HB2	2	0.95
(1,128)	1:10:A:LEU:HD13	1:61:A:MET:HB3	2	0.95
(1,128)	1:10:A:LEU:HD21	1:61:A:MET:HB2	2	0.95
(1,128)	1:10:A:LEU:HD21	1:61:A:MET:HB3	2	0.95
(1,128)	1:10:A:LEU:HD22	1:61:A:MET:HB2	2	0.95
(1,128)	1:10:A:LEU:HD22	1:61:A:MET:HB3	2	0.95
(1,128)	1:10:A:LEU:HD23	1:61:A:MET:HB2	2	0.95
(1,128)	1:10:A:LEU:HD23	1:61:A:MET:HB3	2	0.95
(1,116)	1:10:A:LEU:HG	1:61:A:MET:HA	3	0.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,74)	1:8:A:LYS:H	1:9:A:THR:H	5	0.95
(3,47)	1:39:A:HIS:O	1:73:A:ILE:N	9	0.94
(1,958)	1:77:A:LEU:HG	1:78:A:LYS:HB2	9	0.94
(1,958)	1:77:A:LEU:HG	1:78:A:LYS:HB3	9	0.94
(1,855)	1:69:A:LYS:HD2	1:70:A:LYS:H	5	0.94
(1,855)	1:69:A:LYS:HD3	1:70:A:LYS:H	5	0.94
(1,739)	1:58:A:LEU:HD11	1:60:A:GLU:HB2	9	0.94
(1,739)	1:58:A:LEU:HD11	1:60:A:GLU:HB3	9	0.94
(1,739)	1:58:A:LEU:HD12	1:60:A:GLU:HB2	9	0.94
(1,739)	1:58:A:LEU:HD12	1:60:A:GLU:HB3	9	0.94
(1,739)	1:58:A:LEU:HD13	1:60:A:GLU:HB2	9	0.94
(1,739)	1:58:A:LEU:HD13	1:60:A:GLU:HB3	9	0.94
(1,739)	1:58:A:LEU:HD21	1:60:A:GLU:HB2	9	0.94
(1,739)	1:58:A:LEU:HD21	1:60:A:GLU:HB3	9	0.94
(1,739)	1:58:A:LEU:HD22	1:60:A:GLU:HB2	9	0.94
(1,739)	1:58:A:LEU:HD22	1:60:A:GLU:HB3	9	0.94
(1,739)	1:58:A:LEU:HD23	1:60:A:GLU:HB2	9	0.94
(1,739)	1:58:A:LEU:HD23	1:60:A:GLU:HB3	9	0.94
(1,672)	1:51:A:ILE:HA	1:75:A:ARG:HG2	9	0.94
(1,672)	1:51:A:ILE:HA	1:75:A:ARG:HG3	9	0.94
(1,586)	1:45:A:ARG:HD2	1:46:A:ARG:H	9	0.94
(1,586)	1:45:A:ARG:HD3	1:46:A:ARG:H	9	0.94
(1,299)	1:19:A:ALA:HA	1:53:A:ILE:HA	3	0.94
(3,47)	1:39:A:HIS:O	1:73:A:ILE:N	4	0.93
(1,422)	1:28:A:VAL:HB	1:29:A:LYS:HD2	6	0.93
(1,422)	1:28:A:VAL:HB	1:29:A:LYS:HD3	6	0.93
(1,521)	1:40:A:VAL:HB	1:45:A:ARG:HA	1	0.92
(1,117)	1:10:A:LEU:HG	1:61:A:MET:HB2	6	0.92
(1,117)	1:10:A:LEU:HG	1:61:A:MET:HB3	6	0.92
(1,42)	1:5:A:GLU:HB2	1:6:A:LYS:H	8	0.92
(1,990)	1:82:A:ASP:HB2	1:85:A:ILE:HD11	1	0.91
(1,990)	1:82:A:ASP:HB2	1:85:A:ILE:HD12	1	0.91
(1,990)	1:82:A:ASP:HB2	1:85:A:ILE:HD13	1	0.91
(1,990)	1:82:A:ASP:HB3	1:85:A:ILE:HD11	1	0.91
(1,990)	1:82:A:ASP:HB3	1:85:A:ILE:HD12	1	0.91
(1,990)	1:82:A:ASP:HB3	1:85:A:ILE:HD13	1	0.91
(1,559)	1:43:A:LYS:HG2	1:47:A:SER:HA	9	0.91
(1,323)	1:20:A:LEU:HB3	1:25:A:GLU:H	5	0.91
(1,257)	1:17:A:VAL:HG21	1:53:A:ILE:HB	8	0.91
(1,257)	1:17:A:VAL:HG22	1:53:A:ILE:HB	8	0.91
(1,257)	1:17:A:VAL:HG23	1:53:A:ILE:HB	8	0.91
(1,283)	1:18:A:THR:HB	1:53:A:ILE:HG21	1	0.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,283)	1:18:A:THR:HB	1:53:A:ILE:HG22	1	0.9
(1,283)	1:18:A:THR:HB	1:53:A:ILE:HG23	1	0.9
(1,220)	1:15:A:GLY:HA2	1:56:A:ARG:HB2	9	0.9
(1,220)	1:15:A:GLY:HA2	1:56:A:ARG:HB3	9	0.9
(1,220)	1:15:A:GLY:HA3	1:56:A:ARG:HB2	9	0.9
(1,220)	1:15:A:GLY:HA3	1:56:A:ARG:HB3	9	0.9
(1,323)	1:20:A:LEU:HB3	1:25:A:GLU:H	4	0.89
(1,287)	1:18:A:THR:HG21	1:28:A:VAL:HB	9	0.89
(1,287)	1:18:A:THR:HG22	1:28:A:VAL:HB	9	0.89
(1,287)	1:18:A:THR:HG23	1:28:A:VAL:HB	9	0.89
(1,87)	1:8:A:LYS:HD3	1:9:A:THR:H	8	0.89
(1,572)	1:44:A:VAL:HG11	1:51:A:ILE:HG21	2	0.88
(1,572)	1:44:A:VAL:HG11	1:51:A:ILE:HG22	2	0.88
(1,572)	1:44:A:VAL:HG11	1:51:A:ILE:HG23	2	0.88
(1,572)	1:44:A:VAL:HG12	1:51:A:ILE:HG21	2	0.88
(1,572)	1:44:A:VAL:HG12	1:51:A:ILE:HG22	2	0.88
(1,572)	1:44:A:VAL:HG12	1:51:A:ILE:HG23	2	0.88
(1,572)	1:44:A:VAL:HG13	1:51:A:ILE:HG21	2	0.88
(1,572)	1:44:A:VAL:HG13	1:51:A:ILE:HG22	2	0.88
(1,572)	1:44:A:VAL:HG13	1:51:A:ILE:HG23	2	0.88
(1,572)	1:44:A:VAL:HG11	1:51:A:ILE:HG21	6	0.88
(1,572)	1:44:A:VAL:HG11	1:51:A:ILE:HG22	6	0.88
(1,572)	1:44:A:VAL:HG11	1:51:A:ILE:HG23	6	0.88
(1,572)	1:44:A:VAL:HG12	1:51:A:ILE:HG21	6	0.88
(1,572)	1:44:A:VAL:HG12	1:51:A:ILE:HG22	6	0.88
(1,572)	1:44:A:VAL:HG12	1:51:A:ILE:HG23	6	0.88
(1,572)	1:44:A:VAL:HG13	1:51:A:ILE:HG21	6	0.88
(1,572)	1:44:A:VAL:HG13	1:51:A:ILE:HG22	6	0.88
(1,572)	1:44:A:VAL:HG13	1:51:A:ILE:HG23	6	0.88
(1,561)	1:43:A:LYS:HG3	1:47:A:SER:HA	2	0.88
(1,422)	1:28:A:VAL:HB	1:29:A:LYS:HD2	7	0.88
(1,422)	1:28:A:VAL:HB	1:29:A:LYS:HD3	7	0.88
(1,102)	1:10:A:LEU:H	1:10:A:LEU:HG	1	0.88
(1,438)	1:29:A:LYS:HD2	1:30:A:LEU:H	5	0.87
(1,438)	1:29:A:LYS:HD3	1:30:A:LEU:H	5	0.87
(1,288)	1:18:A:THR:HG21	1:29:A:LYS:H	5	0.87
(1,288)	1:18:A:THR:HG22	1:29:A:LYS:H	5	0.87
(1,288)	1:18:A:THR:HG23	1:29:A:LYS:H	5	0.87
(1,167)	1:12:A:GLU:HG2	1:61:A:MET:H	2	0.87
(3,43)	1:37:A:ILE:N	1:69:A:LYS:O	8	0.86
(1,713)	1:56:A:ARG:H	1:76:A:ARG:H	3	0.86
(1,15)	1:3:A:LYS:H	1:3:A:LYS:HE2	8	0.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,15)	1:3:A:LYS:H	1:3:A:LYS:HE3	8	0.86
(1,1013)	1:83:A:ARG:HD2	1:85:A:ILE:HG21	1	0.85
(1,1013)	1:83:A:ARG:HD2	1:85:A:ILE:HG22	1	0.85
(1,1013)	1:83:A:ARG:HD2	1:85:A:ILE:HG23	1	0.85
(1,1013)	1:83:A:ARG:HD3	1:85:A:ILE:HG21	1	0.85
(1,1013)	1:83:A:ARG:HD3	1:85:A:ILE:HG22	1	0.85
(1,1013)	1:83:A:ARG:HD3	1:85:A:ILE:HG23	1	0.85
(1,664)	1:50:A:ARG:HG2	1:75:A:ARG:HG2	3	0.85
(1,664)	1:50:A:ARG:HG2	1:75:A:ARG:HG3	3	0.85
(1,664)	1:50:A:ARG:HG3	1:75:A:ARG:HG2	3	0.85
(1,664)	1:50:A:ARG:HG3	1:75:A:ARG:HG3	3	0.85
(1,540)	1:41:A:SER:H	1:72:A:ARG:H	7	0.85
(1,504)	1:39:A:HIS:H	1:71:A:GLY:HA2	4	0.85
(1,504)	1:39:A:HIS:H	1:71:A:GLY:HA3	4	0.85
(1,409)	1:27:A:ARG:HG2	1:38:A:CYS:HB2	5	0.85
(1,409)	1:27:A:ARG:HG2	1:38:A:CYS:HB3	5	0.85
(1,409)	1:27:A:ARG:HG3	1:38:A:CYS:HB2	5	0.85
(1,409)	1:27:A:ARG:HG3	1:38:A:CYS:HB3	5	0.85
(1,257)	1:17:A:VAL:HG21	1:53:A:ILE:HB	10	0.85
(1,257)	1:17:A:VAL:HG22	1:53:A:ILE:HB	10	0.85
(1,257)	1:17:A:VAL:HG23	1:53:A:ILE:HB	10	0.85
(1,87)	1:8:A:LYS:HD3	1:9:A:THR:H	2	0.85
(1,713)	1:56:A:ARG:H	1:76:A:ARG:H	8	0.84
(1,413)	1:28:A:VAL:H	1:35:A:GLU:HB2	6	0.84
(1,413)	1:28:A:VAL:H	1:35:A:GLU:HB3	6	0.84
(1,299)	1:19:A:ALA:HA	1:53:A:ILE:HA	8	0.84
(1,638)	1:49:A:ILE:HD11	1:75:A:ARG:HD2	8	0.83
(1,638)	1:49:A:ILE:HD12	1:75:A:ARG:HD2	8	0.83
(1,638)	1:49:A:ILE:HD13	1:75:A:ARG:HD2	8	0.83
(1,638)	1:49:A:ILE:HD11	1:75:A:ARG:HD3	8	0.83
(1,638)	1:49:A:ILE:HD12	1:75:A:ARG:HD3	8	0.83
(1,638)	1:49:A:ILE:HD13	1:75:A:ARG:HD3	8	0.83
(1,586)	1:45:A:ARG:HD2	1:46:A:ARG:H	2	0.83
(1,586)	1:45:A:ARG:HD3	1:46:A:ARG:H	2	0.83
(1,393)	1:26:A:PHE:HE1	1:51:A:ILE:H	5	0.83
(1,347)	1:21:A:LEU:HG	1:23:A:ALA:H	10	0.83
(3,45)	1:37:A:ILE:O	1:71:A:GLY:N	4	0.82
(1,959)	1:77:A:LEU:HG	1:78:A:LYS:HD2	8	0.82
(1,959)	1:77:A:LEU:HG	1:78:A:LYS:HD3	8	0.82
(1,959)	1:77:A:LEU:HG	1:78:A:LYS:HD2	9	0.82
(1,959)	1:77:A:LEU:HG	1:78:A:LYS:HD3	9	0.82
(1,855)	1:69:A:LYS:HD2	1:70:A:LYS:H	10	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,855)	1:69:A:LYS:HD3	1:70:A:LYS:H	10	0.82
(1,572)	1:44:A:VAL:HG11	1:51:A:ILE:HG21	8	0.82
(1,572)	1:44:A:VAL:HG11	1:51:A:ILE:HG22	8	0.82
(1,572)	1:44:A:VAL:HG11	1:51:A:ILE:HG23	8	0.82
(1,572)	1:44:A:VAL:HG12	1:51:A:ILE:HG21	8	0.82
(1,572)	1:44:A:VAL:HG12	1:51:A:ILE:HG22	8	0.82
(1,572)	1:44:A:VAL:HG12	1:51:A:ILE:HG23	8	0.82
(1,572)	1:44:A:VAL:HG13	1:51:A:ILE:HG21	8	0.82
(1,572)	1:44:A:VAL:HG13	1:51:A:ILE:HG22	8	0.82
(1,572)	1:44:A:VAL:HG13	1:51:A:ILE:HG23	8	0.82
(1,540)	1:41:A:SER:H	1:72:A:ARG:H	3	0.82
(1,540)	1:41:A:SER:H	1:72:A:ARG:H	5	0.82
(1,300)	1:19:A:ALA:HA	1:53:A:ILE:HB	6	0.82
(1,60)	1:6:A:LYS:HD3	1:7:A:SER:H	7	0.82
(1,1012)	1:83:A:ARG:HD2	1:85:A:ILE:HD11	9	0.81
(1,1012)	1:83:A:ARG:HD2	1:85:A:ILE:HD12	9	0.81
(1,1012)	1:83:A:ARG:HD2	1:85:A:ILE:HD13	9	0.81
(1,1012)	1:83:A:ARG:HD3	1:85:A:ILE:HD11	9	0.81
(1,1012)	1:83:A:ARG:HD3	1:85:A:ILE:HD12	9	0.81
(1,1012)	1:83:A:ARG:HD3	1:85:A:ILE:HD13	9	0.81
(1,957)	1:77:A:LEU:HG	1:78:A:LYS:H	3	0.81
(1,860)	1:70:A:LYS:H	1:70:A:LYS:HD2	8	0.81
(1,860)	1:70:A:LYS:H	1:70:A:LYS:HD3	8	0.81
(1,776)	1:62:A:SER:HA	1:63:A:ILE:HD11	10	0.81
(1,776)	1:62:A:SER:HA	1:63:A:ILE:HD12	10	0.81
(1,776)	1:62:A:SER:HA	1:63:A:ILE:HD13	10	0.81
(1,559)	1:43:A:LYS:HG2	1:47:A:SER:HA	5	0.81
(1,318)	1:20:A:LEU:HB2	1:25:A:GLU:H	3	0.81
(1,287)	1:18:A:THR:HG21	1:28:A:VAL:HB	1	0.81
(1,287)	1:18:A:THR:HG22	1:28:A:VAL:HB	1	0.81
(1,287)	1:18:A:THR:HG23	1:28:A:VAL:HB	1	0.81
(1,44)	1:5:A:GLU:HB3	1:6:A:LYS:H	7	0.81
(1,1013)	1:83:A:ARG:HD2	1:85:A:ILE:HG21	4	0.8
(1,1013)	1:83:A:ARG:HD2	1:85:A:ILE:HG22	4	0.8
(1,1013)	1:83:A:ARG:HD2	1:85:A:ILE:HG23	4	0.8
(1,1013)	1:83:A:ARG:HD3	1:85:A:ILE:HG21	4	0.8
(1,1013)	1:83:A:ARG:HD3	1:85:A:ILE:HG22	4	0.8
(1,1013)	1:83:A:ARG:HD3	1:85:A:ILE:HG23	4	0.8
(1,586)	1:45:A:ARG:HD2	1:46:A:ARG:H	7	0.8
(1,586)	1:45:A:ARG:HD3	1:46:A:ARG:H	7	0.8
(1,561)	1:43:A:LYS:HG3	1:47:A:SER:HA	1	0.8
(1,561)	1:43:A:LYS:HG3	1:47:A:SER:HA	5	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,287)	1:18:A:THR:HG21	1:28:A:VAL:HB	7	0.8
(1,287)	1:18:A:THR:HG22	1:28:A:VAL:HB	7	0.8
(1,287)	1:18:A:THR:HG23	1:28:A:VAL:HB	7	0.8
(1,499)	1:38:A:CYS:HA	1:70:A:LYS:HD2	3	0.79
(1,499)	1:38:A:CYS:HA	1:70:A:LYS:HD3	3	0.79
(1,323)	1:20:A:LEU:HB3	1:25:A:GLU:H	9	0.79
(1,285)	1:18:A:THR:HG21	1:27:A:ARG:H	10	0.79
(1,285)	1:18:A:THR:HG22	1:27:A:ARG:H	10	0.79
(1,285)	1:18:A:THR:HG23	1:27:A:ARG:H	10	0.79
(1,769)	1:61:A:MET:HG2	1:70:A:LYS:HB2	1	0.78
(1,769)	1:61:A:MET:HG2	1:70:A:LYS:HB3	1	0.78
(1,769)	1:61:A:MET:HG3	1:70:A:LYS:HB2	1	0.78
(1,769)	1:61:A:MET:HG3	1:70:A:LYS:HB3	1	0.78
(1,769)	1:61:A:MET:HG2	1:70:A:LYS:HB2	7	0.78
(1,769)	1:61:A:MET:HG2	1:70:A:LYS:HB3	7	0.78
(1,769)	1:61:A:MET:HG3	1:70:A:LYS:HB2	7	0.78
(1,769)	1:61:A:MET:HG3	1:70:A:LYS:HB3	7	0.78
(1,376)	1:25:A:GLU:HG2	1:39:A:HIS:HA	5	0.78
(1,216)	1:15:A:GLY:HA3	1:30:A:LEU:HA	6	0.78
(1,852)	1:69:A:LYS:HG3	1:70:A:LYS:H	3	0.77
(1,672)	1:51:A:ILE:HA	1:75:A:ARG:HG2	10	0.77
(1,672)	1:51:A:ILE:HA	1:75:A:ARG:HG3	10	0.77
(1,540)	1:41:A:SER:H	1:72:A:ARG:H	10	0.77
(1,318)	1:20:A:LEU:HB2	1:25:A:GLU:H	1	0.77
(1,283)	1:18:A:THR:HB	1:53:A:ILE:HG21	5	0.77
(1,283)	1:18:A:THR:HB	1:53:A:ILE:HG22	5	0.77
(1,283)	1:18:A:THR:HB	1:53:A:ILE:HG23	5	0.77
(1,191)	1:13:A:VAL:HG11	1:59:A:VAL:HB	8	0.77
(1,191)	1:13:A:VAL:HG12	1:59:A:VAL:HB	8	0.77
(1,191)	1:13:A:VAL:HG13	1:59:A:VAL:HB	8	0.77
(1,191)	1:13:A:VAL:HG21	1:59:A:VAL:HB	8	0.77
(1,191)	1:13:A:VAL:HG22	1:59:A:VAL:HB	8	0.77
(1,191)	1:13:A:VAL:HG23	1:59:A:VAL:HB	8	0.77
(1,63)	1:6:A:LYS:HG2	1:7:A:SER:H	6	0.77
(1,42)	1:5:A:GLU:HB2	1:6:A:LYS:H	3	0.77
(1,963)	1:77:A:LEU:HD11	1:78:A:LYS:HB2	9	0.76
(1,963)	1:77:A:LEU:HD11	1:78:A:LYS:HB3	9	0.76
(1,963)	1:77:A:LEU:HD12	1:78:A:LYS:HB2	9	0.76
(1,963)	1:77:A:LEU:HD12	1:78:A:LYS:HB3	9	0.76
(1,963)	1:77:A:LEU:HD13	1:78:A:LYS:HB2	9	0.76
(1,963)	1:77:A:LEU:HD13	1:78:A:LYS:HB3	9	0.76
(1,963)	1:77:A:LEU:HD21	1:78:A:LYS:HB2	9	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,963)	1:77:A:LEU:HD21	1:78:A:LYS:HB3	9	0.76
(1,963)	1:77:A:LEU:HD22	1:78:A:LYS:HB2	9	0.76
(1,963)	1:77:A:LEU:HD22	1:78:A:LYS:HB3	9	0.76
(1,963)	1:77:A:LEU:HD23	1:78:A:LYS:HB2	9	0.76
(1,963)	1:77:A:LEU:HD23	1:78:A:LYS:HB3	9	0.76
(1,586)	1:45:A:ARG:HD2	1:46:A:ARG:H	1	0.76
(1,586)	1:45:A:ARG:HD3	1:46:A:ARG:H	1	0.76
(1,323)	1:20:A:LEU:HB3	1:25:A:GLU:H	3	0.76
(1,292)	1:18:A:THR:HG21	1:53:A:ILE:HG21	8	0.76
(1,292)	1:18:A:THR:HG21	1:53:A:ILE:HG22	8	0.76
(1,292)	1:18:A:THR:HG21	1:53:A:ILE:HG23	8	0.76
(1,292)	1:18:A:THR:HG22	1:53:A:ILE:HG21	8	0.76
(1,292)	1:18:A:THR:HG22	1:53:A:ILE:HG22	8	0.76
(1,292)	1:18:A:THR:HG22	1:53:A:ILE:HG23	8	0.76
(1,292)	1:18:A:THR:HG23	1:53:A:ILE:HG21	8	0.76
(1,292)	1:18:A:THR:HG23	1:53:A:ILE:HG22	8	0.76
(1,292)	1:18:A:THR:HG23	1:53:A:ILE:HG23	8	0.76
(1,283)	1:18:A:THR:HB	1:53:A:ILE:HG21	3	0.76
(1,283)	1:18:A:THR:HB	1:53:A:ILE:HG22	3	0.76
(1,283)	1:18:A:THR:HB	1:53:A:ILE:HG23	3	0.76
(1,257)	1:17:A:VAL:HG21	1:53:A:ILE:HB	1	0.76
(1,257)	1:17:A:VAL:HG22	1:53:A:ILE:HB	1	0.76
(1,257)	1:17:A:VAL:HG23	1:53:A:ILE:HB	1	0.76
(1,121)	1:10:A:LEU:HB2	1:61:A:MET:HA	1	0.76
(1,121)	1:10:A:LEU:HB3	1:61:A:MET:HA	1	0.76
(1,94)	1:8:A:LYS:HD2	1:10:A:LEU:HD11	1	0.76
(1,94)	1:8:A:LYS:HD2	1:10:A:LEU:HD12	1	0.76
(1,94)	1:8:A:LYS:HD2	1:10:A:LEU:HD13	1	0.76
(1,94)	1:8:A:LYS:HD2	1:10:A:LEU:HD21	1	0.76
(1,94)	1:8:A:LYS:HD2	1:10:A:LEU:HD22	1	0.76
(1,94)	1:8:A:LYS:HD2	1:10:A:LEU:HD23	1	0.76
(1,94)	1:8:A:LYS:HD3	1:10:A:LEU:HD11	1	0.76
(1,94)	1:8:A:LYS:HD3	1:10:A:LEU:HD12	1	0.76
(1,94)	1:8:A:LYS:HD3	1:10:A:LEU:HD13	1	0.76
(1,94)	1:8:A:LYS:HD3	1:10:A:LEU:HD21	1	0.76
(1,94)	1:8:A:LYS:HD3	1:10:A:LEU:HD22	1	0.76
(1,94)	1:8:A:LYS:HD3	1:10:A:LEU:HD23	1	0.76
(1,66)	1:6:A:LYS:HG3	1:7:A:SER:H	10	0.76
(3,54)	1:44:A:VAL:O	1:47:A:SER:H	8	0.75
(1,1019)	1:84:A:THR:HB	1:85:A:ILE:H	8	0.75
(1,852)	1:69:A:LYS:HG3	1:70:A:LYS:H	5	0.75
(1,824)	1:66:A:ARG:HD3	1:68:A:ALA:HB1	4	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,824)	1:66:A:ARG:HD3	1:68:A:ALA:HB2	4	0.75
(1,824)	1:66:A:ARG:HD3	1:68:A:ALA:HB3	4	0.75
(1,586)	1:45:A:ARG:HD2	1:46:A:ARG:H	4	0.75
(1,586)	1:45:A:ARG:HD3	1:46:A:ARG:H	4	0.75
(1,540)	1:41:A:SER:H	1:72:A:ARG:H	9	0.75
(1,167)	1:12:A:GLU:HG2	1:61:A:MET:H	3	0.75
(1,42)	1:5:A:GLU:HB2	1:6:A:LYS:H	1	0.75
(3,16)	1:16:A:ALA:H	1:29:A:LYS:O	8	0.74
(1,848)	1:69:A:LYS:HE2	1:70:A:LYS:H	3	0.74
(1,848)	1:69:A:LYS:HE3	1:70:A:LYS:H	3	0.74
(1,771)	1:62:A:SER:H	1:63:A:ILE:HD11	10	0.74
(1,771)	1:62:A:SER:H	1:63:A:ILE:HD12	10	0.74
(1,771)	1:62:A:SER:H	1:63:A:ILE:HD13	10	0.74
(1,218)	1:15:A:GLY:HA2	1:29:A:LYS:HD2	9	0.74
(1,218)	1:15:A:GLY:HA2	1:29:A:LYS:HD3	9	0.74
(1,218)	1:15:A:GLY:HA3	1:29:A:LYS:HD2	9	0.74
(1,218)	1:15:A:GLY:HA3	1:29:A:LYS:HD3	9	0.74
(1,988)	1:82:A:ASP:HA	1:85:A:ILE:HD11	6	0.73
(1,988)	1:82:A:ASP:HA	1:85:A:ILE:HD12	6	0.73
(1,988)	1:82:A:ASP:HA	1:85:A:ILE:HD13	6	0.73
(1,988)	1:82:A:ASP:HA	1:85:A:ILE:HD11	8	0.73
(1,988)	1:82:A:ASP:HA	1:85:A:ILE:HD12	8	0.73
(1,988)	1:82:A:ASP:HA	1:85:A:ILE:HD13	8	0.73
(1,942)	1:76:A:ARG:HD2	1:77:A:LEU:HG	2	0.73
(1,855)	1:69:A:LYS:HD2	1:70:A:LYS:H	1	0.73
(1,855)	1:69:A:LYS:HD3	1:70:A:LYS:H	1	0.73
(1,664)	1:50:A:ARG:HG2	1:75:A:ARG:HG2	1	0.73
(1,664)	1:50:A:ARG:HG2	1:75:A:ARG:HG3	1	0.73
(1,664)	1:50:A:ARG:HG3	1:75:A:ARG:HG2	1	0.73
(1,664)	1:50:A:ARG:HG3	1:75:A:ARG:HG3	1	0.73
(1,634)	1:49:A:ILE:HB	1:74:A:ILE:HG12	10	0.73
(1,634)	1:49:A:ILE:HB	1:74:A:ILE:HG13	10	0.73
(1,456)	1:33:A:GLU:H	1:33:A:GLU:HG2	3	0.73
(1,456)	1:33:A:GLU:H	1:33:A:GLU:HG3	3	0.73
(1,406)	1:27:A:ARG:HG2	1:28:A:VAL:H	8	0.73
(1,287)	1:18:A:THR:HG21	1:28:A:VAL:HB	6	0.73
(1,287)	1:18:A:THR:HG22	1:28:A:VAL:HB	6	0.73
(1,287)	1:18:A:THR:HG23	1:28:A:VAL:HB	6	0.73
(1,220)	1:15:A:GLY:HA2	1:56:A:ARG:HB2	6	0.73
(1,220)	1:15:A:GLY:HA2	1:56:A:ARG:HB3	6	0.73
(1,220)	1:15:A:GLY:HA3	1:56:A:ARG:HB2	6	0.73
(1,220)	1:15:A:GLY:HA3	1:56:A:ARG:HB3	6	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,42)	1:37:A:ILE:H	1:69:A:LYS:O	4	0.72
(1,1013)	1:83:A:ARG:HD2	1:85:A:ILE:HG21	5	0.72
(1,1013)	1:83:A:ARG:HD2	1:85:A:ILE:HG22	5	0.72
(1,1013)	1:83:A:ARG:HD2	1:85:A:ILE:HG23	5	0.72
(1,1013)	1:83:A:ARG:HD3	1:85:A:ILE:HG21	5	0.72
(1,1013)	1:83:A:ARG:HD3	1:85:A:ILE:HG22	5	0.72
(1,1013)	1:83:A:ARG:HD3	1:85:A:ILE:HG23	5	0.72
(1,864)	1:70:A:LYS:HA	1:70:A:LYS:HD2	2	0.72
(1,864)	1:70:A:LYS:HA	1:70:A:LYS:HD3	2	0.72
(1,735)	1:58:A:LEU:HG	1:73:A:ILE:HA	6	0.72
(1,540)	1:41:A:SER:H	1:72:A:ARG:H	6	0.72
(1,407)	1:27:A:ARG:HG2	1:38:A:CYS:HA	5	0.72
(1,318)	1:20:A:LEU:HB2	1:25:A:GLU:H	10	0.72
(1,206)	1:15:A:GLY:H	1:56:A:ARG:HA	1	0.72
(1,117)	1:10:A:LEU:HG	1:61:A:MET:HB2	5	0.72
(1,117)	1:10:A:LEU:HG	1:61:A:MET:HB3	5	0.72
(1,117)	1:10:A:LEU:HG	1:61:A:MET:HB2	8	0.72
(1,117)	1:10:A:LEU:HG	1:61:A:MET:HB3	8	0.72
(1,15)	1:3:A:LYS:H	1:3:A:LYS:HE2	3	0.72
(1,15)	1:3:A:LYS:H	1:3:A:LYS:HE3	3	0.72
(1,858)	1:70:A:LYS:H	1:70:A:LYS:HD2	8	0.71
(1,858)	1:70:A:LYS:H	1:70:A:LYS:HD3	8	0.71
(1,848)	1:69:A:LYS:HE2	1:70:A:LYS:H	5	0.71
(1,848)	1:69:A:LYS:HE3	1:70:A:LYS:H	5	0.71
(1,847)	1:69:A:LYS:HD2	1:70:A:LYS:H	8	0.71
(1,847)	1:69:A:LYS:HD3	1:70:A:LYS:H	8	0.71
(1,407)	1:27:A:ARG:HG2	1:38:A:CYS:HA	10	0.71
(1,8)	1:2:A:VAL:H	1:3:A:LYS:H	2	0.71
(1,664)	1:50:A:ARG:HG2	1:75:A:ARG:HG2	4	0.7
(1,664)	1:50:A:ARG:HG2	1:75:A:ARG:HG3	4	0.7
(1,664)	1:50:A:ARG:HG3	1:75:A:ARG:HG2	4	0.7
(1,664)	1:50:A:ARG:HG3	1:75:A:ARG:HG3	4	0.7
(1,438)	1:29:A:LYS:HD2	1:30:A:LEU:H	1	0.7
(1,438)	1:29:A:LYS:HD3	1:30:A:LEU:H	1	0.7
(1,407)	1:27:A:ARG:HG2	1:38:A:CYS:HA	7	0.7
(1,285)	1:18:A:THR:HG21	1:27:A:ARG:H	4	0.7
(1,285)	1:18:A:THR:HG22	1:27:A:ARG:H	4	0.7
(1,285)	1:18:A:THR:HG23	1:27:A:ARG:H	4	0.7
(1,280)	1:18:A:THR:HA	1:53:A:ILE:HG21	10	0.7
(1,280)	1:18:A:THR:HA	1:53:A:ILE:HG22	10	0.7
(1,280)	1:18:A:THR:HA	1:53:A:ILE:HG23	10	0.7
(1,169)	1:12:A:GLU:HG3	1:61:A:MET:H	8	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,118)	1:10:A:LEU:HG	1:61:A:MET:HG2	5	0.7
(1,118)	1:10:A:LEU:HG	1:61:A:MET:HG3	5	0.7
(1,1022)	1:84:A:THR:HG21	1:85:A:ILE:HB	3	0.69
(1,1022)	1:84:A:THR:HG22	1:85:A:ILE:HB	3	0.69
(1,1022)	1:84:A:THR:HG23	1:85:A:ILE:HB	3	0.69
(1,966)	1:77:A:LEU:HD11	1:80:A:THR:HB	6	0.69
(1,966)	1:77:A:LEU:HD12	1:80:A:THR:HB	6	0.69
(1,966)	1:77:A:LEU:HD13	1:80:A:THR:HB	6	0.69
(1,966)	1:77:A:LEU:HD21	1:80:A:THR:HB	6	0.69
(1,966)	1:77:A:LEU:HD22	1:80:A:THR:HB	6	0.69
(1,966)	1:77:A:LEU:HD23	1:80:A:THR:HB	6	0.69
(1,929)	1:75:A:ARG:HG2	1:76:A:ARG:H	2	0.69
(1,929)	1:75:A:ARG:HG3	1:76:A:ARG:H	2	0.69
(1,860)	1:70:A:LYS:H	1:70:A:LYS:HD2	6	0.69
(1,860)	1:70:A:LYS:H	1:70:A:LYS:HD3	6	0.69
(1,690)	1:52:A:ILE:HG21	1:75:A:ARG:HB2	2	0.69
(1,690)	1:52:A:ILE:HG22	1:75:A:ARG:HB2	2	0.69
(1,690)	1:52:A:ILE:HG23	1:75:A:ARG:HB2	2	0.69
(1,638)	1:49:A:ILE:HD11	1:75:A:ARG:HD2	5	0.69
(1,638)	1:49:A:ILE:HD12	1:75:A:ARG:HD2	5	0.69
(1,638)	1:49:A:ILE:HD13	1:75:A:ARG:HD2	5	0.69
(1,638)	1:49:A:ILE:HD11	1:75:A:ARG:HD3	5	0.69
(1,638)	1:49:A:ILE:HD12	1:75:A:ARG:HD3	5	0.69
(1,638)	1:49:A:ILE:HD13	1:75:A:ARG:HD3	5	0.69
(1,409)	1:27:A:ARG:HG2	1:38:A:CYS:HB2	6	0.69
(1,409)	1:27:A:ARG:HG2	1:38:A:CYS:HB3	6	0.69
(1,409)	1:27:A:ARG:HG3	1:38:A:CYS:HB2	6	0.69
(1,409)	1:27:A:ARG:HG3	1:38:A:CYS:HB3	6	0.69
(1,407)	1:27:A:ARG:HG2	1:38:A:CYS:HA	6	0.69
(1,355)	1:22:A:PRO:HG2	1:24:A:ALA:H	10	0.69
(1,226)	1:16:A:ALA:H	1:30:A:LEU:HA	8	0.69
(1,112)	1:10:A:LEU:HB2	1:61:A:MET:HA	2	0.69
(1,972)	1:78:A:LYS:HA	1:78:A:LYS:HD2	6	0.68
(1,972)	1:78:A:LYS:HA	1:78:A:LYS:HD3	6	0.68
(1,773)	1:62:A:SER:H	1:66:A:ARG:HG2	8	0.68
(1,653)	1:50:A:ARG:HB2	1:52:A:ILE:HD11	9	0.68
(1,653)	1:50:A:ARG:HB2	1:52:A:ILE:HD12	9	0.68
(1,653)	1:50:A:ARG:HB2	1:52:A:ILE:HD13	9	0.68
(1,499)	1:38:A:CYS:HA	1:70:A:LYS:HD2	4	0.68
(1,499)	1:38:A:CYS:HA	1:70:A:LYS:HD3	4	0.68
(1,406)	1:27:A:ARG:HG2	1:28:A:VAL:H	1	0.68
(1,327)	1:20:A:LEU:HG	1:21:A:LEU:HB2	6	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,327)	1:20:A:LEU:HG	1:21:A:LEU:HB3	6	0.68
(1,283)	1:18:A:THR:HB	1:53:A:ILE:HG21	9	0.68
(1,283)	1:18:A:THR:HB	1:53:A:ILE:HG22	9	0.68
(1,283)	1:18:A:THR:HB	1:53:A:ILE:HG23	9	0.68
(3,54)	1:44:A:VAL:O	1:47:A:SER:H	4	0.67
(1,1022)	1:84:A:THR:HG21	1:85:A:ILE:HB	9	0.67
(1,1022)	1:84:A:THR:HG22	1:85:A:ILE:HB	9	0.67
(1,1022)	1:84:A:THR:HG23	1:85:A:ILE:HB	9	0.67
(1,534)	1:40:A:VAL:HG11	1:45:A:ARG:HA	1	0.67
(1,534)	1:40:A:VAL:HG12	1:45:A:ARG:HA	1	0.67
(1,534)	1:40:A:VAL:HG13	1:45:A:ARG:HA	1	0.67
(1,534)	1:40:A:VAL:HG21	1:45:A:ARG:HA	1	0.67
(1,534)	1:40:A:VAL:HG22	1:45:A:ARG:HA	1	0.67
(1,534)	1:40:A:VAL:HG23	1:45:A:ARG:HA	1	0.67
(1,407)	1:27:A:ARG:HG2	1:38:A:CYS:HA	3	0.67
(1,406)	1:27:A:ARG:HG2	1:28:A:VAL:H	3	0.67
(1,406)	1:27:A:ARG:HG2	1:28:A:VAL:H	10	0.67
(1,393)	1:26:A:PHE:HE1	1:51:A:ILE:H	7	0.67
(1,334)	1:20:A:LEU:HD21	1:21:A:LEU:HA	9	0.67
(1,334)	1:20:A:LEU:HD22	1:21:A:LEU:HA	9	0.67
(1,334)	1:20:A:LEU:HD23	1:21:A:LEU:HA	9	0.67
(1,323)	1:20:A:LEU:HB3	1:25:A:GLU:H	1	0.67
(1,231)	1:16:A:ALA:HA	1:56:A:ARG:HD2	8	0.67
(1,231)	1:16:A:ALA:HA	1:56:A:ARG:HD3	8	0.67
(1,130)	1:10:A:LEU:HD11	1:62:A:SER:HB2	9	0.67
(1,130)	1:10:A:LEU:HD11	1:62:A:SER:HB3	9	0.67
(1,130)	1:10:A:LEU:HD12	1:62:A:SER:HB2	9	0.67
(1,130)	1:10:A:LEU:HD12	1:62:A:SER:HB3	9	0.67
(1,130)	1:10:A:LEU:HD13	1:62:A:SER:HB2	9	0.67
(1,130)	1:10:A:LEU:HD13	1:62:A:SER:HB3	9	0.67
(1,130)	1:10:A:LEU:HD21	1:62:A:SER:HB2	9	0.67
(1,130)	1:10:A:LEU:HD21	1:62:A:SER:HB3	9	0.67
(1,130)	1:10:A:LEU:HD22	1:62:A:SER:HB2	9	0.67
(1,130)	1:10:A:LEU:HD22	1:62:A:SER:HB3	9	0.67
(1,130)	1:10:A:LEU:HD23	1:62:A:SER:HB2	9	0.67
(1,130)	1:10:A:LEU:HD23	1:62:A:SER:HB3	9	0.67
(1,116)	1:10:A:LEU:HG	1:61:A:MET:HA	7	0.67
(1,852)	1:69:A:LYS:HG3	1:70:A:LYS:H	1	0.66
(1,769)	1:61:A:MET:HG2	1:70:A:LYS:HB2	8	0.66
(1,769)	1:61:A:MET:HG2	1:70:A:LYS:HB3	8	0.66
(1,769)	1:61:A:MET:HG3	1:70:A:LYS:HB2	8	0.66
(1,769)	1:61:A:MET:HG3	1:70:A:LYS:HB3	8	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,746)	1:59:A:VAL:HA	1:72:A:ARG:HG3	2	0.66
(1,656)	1:50:A:ARG:HB3	1:52:A:ILE:HD11	9	0.66
(1,656)	1:50:A:ARG:HB3	1:52:A:ILE:HD12	9	0.66
(1,656)	1:50:A:ARG:HB3	1:52:A:ILE:HD13	9	0.66
(1,360)	1:23:A:ALA:HA	1:25:A:GLU:HB2	7	0.66
(1,360)	1:23:A:ALA:HA	1:25:A:GLU:HB3	7	0.66
(1,355)	1:22:A:PRO:HG2	1:24:A:ALA:H	8	0.66
(1,220)	1:15:A:GLY:HA2	1:56:A:ARG:HB2	5	0.66
(1,220)	1:15:A:GLY:HA2	1:56:A:ARG:HB3	5	0.66
(1,220)	1:15:A:GLY:HA3	1:56:A:ARG:HB2	5	0.66
(1,220)	1:15:A:GLY:HA3	1:56:A:ARG:HB3	5	0.66
(1,118)	1:10:A:LEU:HG	1:61:A:MET:HG2	7	0.66
(1,118)	1:10:A:LEU:HG	1:61:A:MET:HG3	7	0.66
(1,66)	1:6:A:LYS:HG3	1:7:A:SER:H	3	0.66
(3,52)	1:43:A:LYS:O	1:46:A:ARG:H	10	0.65
(1,993)	1:83:A:ARG:H	1:83:A:ARG:HD2	6	0.65
(1,993)	1:83:A:ARG:H	1:83:A:ARG:HD3	6	0.65
(1,772)	1:62:A:SER:H	1:64:A:TYR:HB2	1	0.65
(1,772)	1:62:A:SER:H	1:64:A:TYR:HB2	1	0.65
(1,772)	1:62:A:SER:H	1:64:A:TYR:HB3	1	0.65
(1,574)	1:44:A:VAL:HG11	1:51:A:ILE:HG21	10	0.65
(1,574)	1:44:A:VAL:HG11	1:51:A:ILE:HG22	10	0.65
(1,574)	1:44:A:VAL:HG11	1:51:A:ILE:HG23	10	0.65
(1,574)	1:44:A:VAL:HG12	1:51:A:ILE:HG21	10	0.65
(1,574)	1:44:A:VAL:HG12	1:51:A:ILE:HG22	10	0.65
(1,574)	1:44:A:VAL:HG12	1:51:A:ILE:HG23	10	0.65
(1,574)	1:44:A:VAL:HG13	1:51:A:ILE:HG21	10	0.65
(1,574)	1:44:A:VAL:HG13	1:51:A:ILE:HG22	10	0.65
(1,574)	1:44:A:VAL:HG13	1:51:A:ILE:HG23	10	0.65
(1,574)	1:44:A:VAL:HG21	1:51:A:ILE:HG21	10	0.65
(1,574)	1:44:A:VAL:HG21	1:51:A:ILE:HG22	10	0.65
(1,574)	1:44:A:VAL:HG21	1:51:A:ILE:HG23	10	0.65
(1,574)	1:44:A:VAL:HG22	1:51:A:ILE:HG21	10	0.65
(1,574)	1:44:A:VAL:HG22	1:51:A:ILE:HG22	10	0.65
(1,574)	1:44:A:VAL:HG22	1:51:A:ILE:HG23	10	0.65
(1,574)	1:44:A:VAL:HG23	1:51:A:ILE:HG21	10	0.65
(1,574)	1:44:A:VAL:HG23	1:51:A:ILE:HG22	10	0.65
(1,574)	1:44:A:VAL:HG23	1:51:A:ILE:HG23	10	0.65
(1,288)	1:18:A:THR:HG21	1:29:A:LYS:H	10	0.65
(1,288)	1:18:A:THR:HG22	1:29:A:LYS:H	10	0.65
(1,288)	1:18:A:THR:HG23	1:29:A:LYS:H	10	0.65
(1,257)	1:17:A:VAL:HG21	1:53:A:ILE:HB	5	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,257)	1:17:A:VAL:HG22	1:53:A:ILE:HB	5	0.65
(1,257)	1:17:A:VAL:HG23	1:53:A:ILE:HB	5	0.65
(3,12)	1:17:A:VAL:H	1:55:A:ASP:O	1	0.64
(1,960)	1:77:A:LEU:HG	1:78:A:LYS:HE2	7	0.64
(1,960)	1:77:A:LEU:HG	1:78:A:LYS:HE3	7	0.64
(1,855)	1:69:A:LYS:HD2	1:70:A:LYS:H	6	0.64
(1,855)	1:69:A:LYS:HD3	1:70:A:LYS:H	6	0.64
(1,852)	1:69:A:LYS:HG3	1:70:A:LYS:H	10	0.64
(1,746)	1:59:A:VAL:HA	1:72:A:ARG:HG3	1	0.64
(1,664)	1:50:A:ARG:HG2	1:75:A:ARG:HG2	8	0.64
(1,664)	1:50:A:ARG:HG2	1:75:A:ARG:HG3	8	0.64
(1,664)	1:50:A:ARG:HG3	1:75:A:ARG:HG2	8	0.64
(1,664)	1:50:A:ARG:HG3	1:75:A:ARG:HG3	8	0.64
(1,561)	1:43:A:LYS:HG3	1:47:A:SER:HA	9	0.64
(1,559)	1:43:A:LYS:HG2	1:47:A:SER:HA	8	0.64
(1,407)	1:27:A:ARG:HG2	1:38:A:CYS:HA	4	0.64
(1,323)	1:20:A:LEU:HB3	1:25:A:GLU:H	10	0.64
(1,246)	1:17:A:VAL:HA	1:27:A:ARG:HB3	2	0.64
(1,66)	1:6:A:LYS:HG3	1:7:A:SER:H	2	0.64
(1,957)	1:77:A:LEU:HG	1:78:A:LYS:H	8	0.63
(1,690)	1:52:A:ILE:HG21	1:75:A:ARG:HB2	9	0.63
(1,690)	1:52:A:ILE:HG22	1:75:A:ARG:HB2	9	0.63
(1,690)	1:52:A:ILE:HG23	1:75:A:ARG:HB2	9	0.63
(1,355)	1:22:A:PRO:HG2	1:24:A:ALA:H	1	0.63
(1,355)	1:22:A:PRO:HG2	1:24:A:ALA:H	4	0.63
(1,230)	1:16:A:ALA:HA	1:56:A:ARG:HB2	9	0.63
(1,230)	1:16:A:ALA:HA	1:56:A:ARG:HB3	9	0.63
(3,16)	1:16:A:ALA:H	1:29:A:LYS:O	3	0.62
(1,1015)	1:84:A:THR:H	1:85:A:ILE:H	8	0.62
(1,839)	1:69:A:LYS:HA	1:69:A:LYS:HE2	4	0.62
(1,839)	1:69:A:LYS:HA	1:69:A:LYS:HE3	4	0.62
(1,739)	1:58:A:LEU:HD11	1:60:A:GLU:HB2	1	0.62
(1,739)	1:58:A:LEU:HD11	1:60:A:GLU:HB3	1	0.62
(1,739)	1:58:A:LEU:HD12	1:60:A:GLU:HB2	1	0.62
(1,739)	1:58:A:LEU:HD12	1:60:A:GLU:HB3	1	0.62
(1,739)	1:58:A:LEU:HD13	1:60:A:GLU:HB2	1	0.62
(1,739)	1:58:A:LEU:HD13	1:60:A:GLU:HB3	1	0.62
(1,739)	1:58:A:LEU:HD21	1:60:A:GLU:HB2	1	0.62
(1,739)	1:58:A:LEU:HD21	1:60:A:GLU:HB3	1	0.62
(1,739)	1:58:A:LEU:HD22	1:60:A:GLU:HB2	1	0.62
(1,739)	1:58:A:LEU:HD22	1:60:A:GLU:HB3	1	0.62
(1,739)	1:58:A:LEU:HD23	1:60:A:GLU:HB2	1	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,739)	1:58:A:LEU:HD23	1:60:A:GLU:HB3	1	0.62
(1,690)	1:52:A:ILE:HG21	1:75:A:ARG:HB2	1	0.62
(1,690)	1:52:A:ILE:HG22	1:75:A:ARG:HB2	1	0.62
(1,690)	1:52:A:ILE:HG23	1:75:A:ARG:HB2	1	0.62
(1,561)	1:43:A:LYS:HG3	1:47:A:SER:HA	8	0.62
(1,438)	1:29:A:LYS:HD2	1:30:A:LEU:H	3	0.62
(1,438)	1:29:A:LYS:HD3	1:30:A:LEU:H	3	0.62
(1,409)	1:27:A:ARG:HG2	1:38:A:CYS:HB2	8	0.62
(1,409)	1:27:A:ARG:HG2	1:38:A:CYS:HB3	8	0.62
(1,409)	1:27:A:ARG:HG3	1:38:A:CYS:HB2	8	0.62
(1,409)	1:27:A:ARG:HG3	1:38:A:CYS:HB3	8	0.62
(1,378)	1:25:A:GLU:HG3	1:39:A:HIS:HA	7	0.62
(1,327)	1:20:A:LEU:HG	1:21:A:LEU:HB2	7	0.62
(1,327)	1:20:A:LEU:HG	1:21:A:LEU:HB3	7	0.62
(1,287)	1:18:A:THR:HG21	1:28:A:VAL:HB	8	0.62
(1,287)	1:18:A:THR:HG22	1:28:A:VAL:HB	8	0.62
(1,287)	1:18:A:THR:HG23	1:28:A:VAL:HB	8	0.62
(1,257)	1:17:A:VAL:HG21	1:53:A:ILE:HB	2	0.62
(1,257)	1:17:A:VAL:HG22	1:53:A:ILE:HB	2	0.62
(1,257)	1:17:A:VAL:HG23	1:53:A:ILE:HB	2	0.62
(1,128)	1:10:A:LEU:HD11	1:61:A:MET:HB2	6	0.62
(1,128)	1:10:A:LEU:HD11	1:61:A:MET:HB3	6	0.62
(1,128)	1:10:A:LEU:HD12	1:61:A:MET:HB2	6	0.62
(1,128)	1:10:A:LEU:HD12	1:61:A:MET:HB3	6	0.62
(1,128)	1:10:A:LEU:HD13	1:61:A:MET:HB2	6	0.62
(1,128)	1:10:A:LEU:HD13	1:61:A:MET:HB3	6	0.62
(1,128)	1:10:A:LEU:HD21	1:61:A:MET:HB2	6	0.62
(1,128)	1:10:A:LEU:HD21	1:61:A:MET:HB3	6	0.62
(1,128)	1:10:A:LEU:HD22	1:61:A:MET:HB2	6	0.62
(1,128)	1:10:A:LEU:HD22	1:61:A:MET:HB3	6	0.62
(1,128)	1:10:A:LEU:HD23	1:61:A:MET:HB2	6	0.62
(1,128)	1:10:A:LEU:HD23	1:61:A:MET:HB3	6	0.62
(1,63)	1:6:A:LYS:HG2	1:7:A:SER:H	8	0.62
(1,44)	1:5:A:GLU:HB3	1:6:A:LYS:H	4	0.62
(1,985)	1:80:A:THR:HA	1:80:A:THR:HB	3	0.61
(1,559)	1:43:A:LYS:HG2	1:47:A:SER:HA	6	0.61
(1,503)	1:39:A:HIS:H	1:70:A:LYS:HA	9	0.61
(1,407)	1:27:A:ARG:HG2	1:38:A:CYS:HA	9	0.61
(1,347)	1:21:A:LEU:HG	1:23:A:ALA:H	7	0.61
(1,525)	1:40:A:VAL:HG11	1:45:A:ARG:HA	1	0.6
(1,525)	1:40:A:VAL:HG12	1:45:A:ARG:HA	1	0.6
(1,525)	1:40:A:VAL:HG13	1:45:A:ARG:HA	1	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,413)	1:28:A:VAL:H	1:35:A:GLU:HB2	8	0.6
(1,413)	1:28:A:VAL:H	1:35:A:GLU:HB3	8	0.6
(1,327)	1:20:A:LEU:HG	1:21:A:LEU:HB2	10	0.6
(1,327)	1:20:A:LEU:HG	1:21:A:LEU:HB3	10	0.6
(1,315)	1:20:A:LEU:HB2	1:20:A:LEU:HG	9	0.6
(1,299)	1:19:A:ALA:HA	1:53:A:ILE:HA	1	0.6
(1,76)	1:8:A:LYS:HA	1:8:A:LYS:HE2	9	0.6
(1,76)	1:8:A:LYS:HA	1:8:A:LYS:HE3	9	0.6
(1,858)	1:70:A:LYS:H	1:70:A:LYS:HD2	6	0.59
(1,858)	1:70:A:LYS:H	1:70:A:LYS:HD3	6	0.59
(1,806)	1:64:A:TYR:HB2	1:68:A:ALA:HA	7	0.59
(1,604)	1:47:A:SER:HA	1:49:A:ILE:H	9	0.59
(1,438)	1:29:A:LYS:HD2	1:30:A:LEU:H	8	0.59
(1,438)	1:29:A:LYS:HD3	1:30:A:LEU:H	8	0.59
(1,409)	1:27:A:ARG:HG2	1:38:A:CYS:HB2	7	0.59
(1,409)	1:27:A:ARG:HG2	1:38:A:CYS:HB3	7	0.59
(1,409)	1:27:A:ARG:HG3	1:38:A:CYS:HB2	7	0.59
(1,409)	1:27:A:ARG:HG3	1:38:A:CYS:HB3	7	0.59
(1,407)	1:27:A:ARG:HG2	1:38:A:CYS:HA	8	0.59
(1,257)	1:17:A:VAL:HG21	1:53:A:ILE:HB	3	0.59
(1,257)	1:17:A:VAL:HG22	1:53:A:ILE:HB	3	0.59
(1,257)	1:17:A:VAL:HG23	1:53:A:ILE:HB	3	0.59
(1,169)	1:12:A:GLU:HG3	1:61:A:MET:H	7	0.59
(1,50)	1:6:A:LYS:HA	1:6:A:LYS:HD2	3	0.59
(1,50)	1:6:A:LYS:HA	1:6:A:LYS:HD3	3	0.59
(2,5)	1:12:A:GLU:HG2	1:62:A:SER:HA	1	0.58
(2,5)	1:12:A:GLU:HG3	1:62:A:SER:HA	1	0.58
(1,587)	1:45:A:ARG:HG2	1:46:A:ARG:H	7	0.58
(1,587)	1:45:A:ARG:HG3	1:46:A:ARG:H	7	0.58
(1,586)	1:45:A:ARG:HD2	1:46:A:ARG:H	3	0.58
(1,586)	1:45:A:ARG:HD3	1:46:A:ARG:H	3	0.58
(1,503)	1:39:A:HIS:H	1:70:A:LYS:HA	8	0.58
(1,408)	1:27:A:ARG:HG3	1:28:A:VAL:H	10	0.58
(1,347)	1:21:A:LEU:HG	1:23:A:ALA:H	5	0.58
(1,338)	1:20:A:LEU:HD11	1:26:A:PHE:HB2	1	0.58
(1,338)	1:20:A:LEU:HD11	1:26:A:PHE:HB3	1	0.58
(1,338)	1:20:A:LEU:HD12	1:26:A:PHE:HB2	1	0.58
(1,338)	1:20:A:LEU:HD12	1:26:A:PHE:HB3	1	0.58
(1,338)	1:20:A:LEU:HD13	1:26:A:PHE:HB2	1	0.58
(1,338)	1:20:A:LEU:HD13	1:26:A:PHE:HB3	1	0.58
(1,338)	1:20:A:LEU:HD21	1:26:A:PHE:HB2	1	0.58
(1,338)	1:20:A:LEU:HD21	1:26:A:PHE:HB3	1	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,338)	1:20:A:LEU:HD22	1:26:A:PHE:HB2	1	0.58
(1,338)	1:20:A:LEU:HD22	1:26:A:PHE:HB3	1	0.58
(1,338)	1:20:A:LEU:HD23	1:26:A:PHE:HB2	1	0.58
(1,338)	1:20:A:LEU:HD23	1:26:A:PHE:HB3	1	0.58
(1,292)	1:18:A:THR:HG21	1:53:A:ILE:HG21	10	0.58
(1,292)	1:18:A:THR:HG21	1:53:A:ILE:HG22	10	0.58
(1,292)	1:18:A:THR:HG21	1:53:A:ILE:HG23	10	0.58
(1,292)	1:18:A:THR:HG22	1:53:A:ILE:HG21	10	0.58
(1,292)	1:18:A:THR:HG22	1:53:A:ILE:HG22	10	0.58
(1,292)	1:18:A:THR:HG22	1:53:A:ILE:HG23	10	0.58
(1,292)	1:18:A:THR:HG23	1:53:A:ILE:HG21	10	0.58
(1,292)	1:18:A:THR:HG23	1:53:A:ILE:HG22	10	0.58
(1,292)	1:18:A:THR:HG23	1:53:A:ILE:HG23	10	0.58
(1,14)	1:3:A:LYS:H	1:3:A:LYS:HD2	8	0.58
(1,14)	1:3:A:LYS:H	1:3:A:LYS:HD3	8	0.58
(3,55)	1:44:A:VAL:O	1:47:A:SER:N	6	0.57
(1,848)	1:69:A:LYS:HE2	1:70:A:LYS:H	10	0.57
(1,848)	1:69:A:LYS:HE3	1:70:A:LYS:H	10	0.57
(1,503)	1:39:A:HIS:H	1:70:A:LYS:HA	4	0.57
(1,475)	1:36:A:ILE:HB	1:37:A:ILE:H	3	0.57
(1,438)	1:29:A:LYS:HD2	1:30:A:LEU:H	4	0.57
(1,438)	1:29:A:LYS:HD3	1:30:A:LEU:H	4	0.57
(1,422)	1:28:A:VAL:HB	1:29:A:LYS:HD2	5	0.57
(1,422)	1:28:A:VAL:HB	1:29:A:LYS:HD3	5	0.57
(1,291)	1:18:A:THR:HG21	1:53:A:ILE:HD11	3	0.57
(1,291)	1:18:A:THR:HG21	1:53:A:ILE:HD12	3	0.57
(1,291)	1:18:A:THR:HG21	1:53:A:ILE:HD13	3	0.57
(1,291)	1:18:A:THR:HG22	1:53:A:ILE:HD11	3	0.57
(1,291)	1:18:A:THR:HG22	1:53:A:ILE:HD12	3	0.57
(1,291)	1:18:A:THR:HG22	1:53:A:ILE:HD13	3	0.57
(1,291)	1:18:A:THR:HG23	1:53:A:ILE:HD11	3	0.57
(1,291)	1:18:A:THR:HG23	1:53:A:ILE:HD12	3	0.57
(1,291)	1:18:A:THR:HG23	1:53:A:ILE:HD13	3	0.57
(1,50)	1:6:A:LYS:HA	1:6:A:LYS:HD2	6	0.57
(1,50)	1:6:A:LYS:HA	1:6:A:LYS:HD3	6	0.57
(3,46)	1:39:A:HIS:O	1:73:A:ILE:H	6	0.56
(3,22)	1:21:A:LEU:O	1:25:A:GLU:H	6	0.56
(3,12)	1:17:A:VAL:H	1:55:A:ASP:O	10	0.56
(1,964)	1:77:A:LEU:HD11	1:78:A:LYS:HD2	9	0.56
(1,964)	1:77:A:LEU:HD11	1:78:A:LYS:HD3	9	0.56
(1,964)	1:77:A:LEU:HD12	1:78:A:LYS:HD2	9	0.56
(1,964)	1:77:A:LEU:HD12	1:78:A:LYS:HD3	9	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,964)	1:77:A:LEU:HD13	1:78:A:LYS:HD2	9	0.56
(1,964)	1:77:A:LEU:HD13	1:78:A:LYS:HD3	9	0.56
(1,964)	1:77:A:LEU:HD21	1:78:A:LYS:HD2	9	0.56
(1,964)	1:77:A:LEU:HD21	1:78:A:LYS:HD3	9	0.56
(1,964)	1:77:A:LEU:HD22	1:78:A:LYS:HD2	9	0.56
(1,964)	1:77:A:LEU:HD22	1:78:A:LYS:HD3	9	0.56
(1,964)	1:77:A:LEU:HD23	1:78:A:LYS:HD2	9	0.56
(1,964)	1:77:A:LEU:HD23	1:78:A:LYS:HD3	9	0.56
(1,848)	1:69:A:LYS:HE2	1:70:A:LYS:H	1	0.56
(1,848)	1:69:A:LYS:HE3	1:70:A:LYS:H	1	0.56
(1,518)	1:40:A:VAL:HA	1:72:A:ARG:HB2	6	0.56
(1,505)	1:39:A:HIS:H	1:72:A:ARG:H	4	0.56
(1,456)	1:33:A:GLU:H	1:33:A:GLU:HG2	8	0.56
(1,456)	1:33:A:GLU:H	1:33:A:GLU:HG3	8	0.56
(1,50)	1:6:A:LYS:HA	1:6:A:LYS:HD2	8	0.56
(1,50)	1:6:A:LYS:HA	1:6:A:LYS:HD3	8	0.56
(2,25)	1:76:A:ARG:HD3	1:77:A:LEU:HG	4	0.55
(1,959)	1:77:A:LEU:HG	1:78:A:LYS:HD2	1	0.55
(1,959)	1:77:A:LEU:HG	1:78:A:LYS:HD3	1	0.55
(1,691)	1:52:A:ILE:HG21	1:75:A:ARG:HG2	1	0.55
(1,691)	1:52:A:ILE:HG21	1:75:A:ARG:HG3	1	0.55
(1,691)	1:52:A:ILE:HG22	1:75:A:ARG:HG2	1	0.55
(1,691)	1:52:A:ILE:HG22	1:75:A:ARG:HG3	1	0.55
(1,691)	1:52:A:ILE:HG23	1:75:A:ARG:HG2	1	0.55
(1,691)	1:52:A:ILE:HG23	1:75:A:ARG:HG3	1	0.55
(1,604)	1:47:A:SER:HA	1:49:A:ILE:H	1	0.55
(1,586)	1:45:A:ARG:HD2	1:46:A:ARG:H	5	0.55
(1,586)	1:45:A:ARG:HD3	1:46:A:ARG:H	5	0.55
(1,172)	1:12:A:GLU:HB2	1:61:A:MET:H	3	0.55
(1,172)	1:12:A:GLU:HB3	1:61:A:MET:H	3	0.55
(1,76)	1:8:A:LYS:HA	1:8:A:LYS:HE2	6	0.55
(1,76)	1:8:A:LYS:HA	1:8:A:LYS:HE3	6	0.55
(1,44)	1:5:A:GLU:HB3	1:6:A:LYS:H	10	0.55
(3,42)	1:37:A:ILE:H	1:69:A:LYS:O	1	0.54
(3,40)	1:39:A:HIS:H	1:71:A:GLY:O	4	0.54
(1,990)	1:82:A:ASP:HB2	1:85:A:ILE:HD11	2	0.54
(1,990)	1:82:A:ASP:HB2	1:85:A:ILE:HD12	2	0.54
(1,990)	1:82:A:ASP:HB2	1:85:A:ILE:HD13	2	0.54
(1,990)	1:82:A:ASP:HB3	1:85:A:ILE:HD11	2	0.54
(1,990)	1:82:A:ASP:HB3	1:85:A:ILE:HD12	2	0.54
(1,990)	1:82:A:ASP:HB3	1:85:A:ILE:HD13	2	0.54
(1,964)	1:77:A:LEU:HD11	1:78:A:LYS:HD2	8	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,964)	1:77:A:LEU:HD11	1:78:A:LYS:HD3	8	0.54
(1,964)	1:77:A:LEU:HD12	1:78:A:LYS:HD2	8	0.54
(1,964)	1:77:A:LEU:HD12	1:78:A:LYS:HD3	8	0.54
(1,964)	1:77:A:LEU:HD13	1:78:A:LYS:HD2	8	0.54
(1,964)	1:77:A:LEU:HD13	1:78:A:LYS:HD3	8	0.54
(1,964)	1:77:A:LEU:HD21	1:78:A:LYS:HD2	8	0.54
(1,964)	1:77:A:LEU:HD21	1:78:A:LYS:HD3	8	0.54
(1,964)	1:77:A:LEU:HD22	1:78:A:LYS:HD2	8	0.54
(1,964)	1:77:A:LEU:HD22	1:78:A:LYS:HD3	8	0.54
(1,964)	1:77:A:LEU:HD23	1:78:A:LYS:HD2	8	0.54
(1,964)	1:77:A:LEU:HD23	1:78:A:LYS:HD3	8	0.54
(1,739)	1:58:A:LEU:HD11	1:60:A:GLU:HB2	2	0.54
(1,739)	1:58:A:LEU:HD11	1:60:A:GLU:HB3	2	0.54
(1,739)	1:58:A:LEU:HD12	1:60:A:GLU:HB2	2	0.54
(1,739)	1:58:A:LEU:HD12	1:60:A:GLU:HB3	2	0.54
(1,739)	1:58:A:LEU:HD13	1:60:A:GLU:HB2	2	0.54
(1,739)	1:58:A:LEU:HD13	1:60:A:GLU:HB3	2	0.54
(1,739)	1:58:A:LEU:HD21	1:60:A:GLU:HB2	2	0.54
(1,739)	1:58:A:LEU:HD21	1:60:A:GLU:HB3	2	0.54
(1,739)	1:58:A:LEU:HD22	1:60:A:GLU:HB2	2	0.54
(1,739)	1:58:A:LEU:HD22	1:60:A:GLU:HB3	2	0.54
(1,739)	1:58:A:LEU:HD23	1:60:A:GLU:HB2	2	0.54
(1,739)	1:58:A:LEU:HD23	1:60:A:GLU:HB3	2	0.54
(1,587)	1:45:A:ARG:HG2	1:46:A:ARG:H	2	0.54
(1,587)	1:45:A:ARG:HG3	1:46:A:ARG:H	2	0.54
(1,572)	1:44:A:VAL:HG11	1:51:A:ILE:HG21	10	0.54
(1,572)	1:44:A:VAL:HG11	1:51:A:ILE:HG22	10	0.54
(1,572)	1:44:A:VAL:HG11	1:51:A:ILE:HG23	10	0.54
(1,572)	1:44:A:VAL:HG12	1:51:A:ILE:HG21	10	0.54
(1,572)	1:44:A:VAL:HG12	1:51:A:ILE:HG22	10	0.54
(1,572)	1:44:A:VAL:HG12	1:51:A:ILE:HG23	10	0.54
(1,572)	1:44:A:VAL:HG13	1:51:A:ILE:HG21	10	0.54
(1,572)	1:44:A:VAL:HG13	1:51:A:ILE:HG22	10	0.54
(1,572)	1:44:A:VAL:HG13	1:51:A:ILE:HG23	10	0.54
(1,522)	1:40:A:VAL:HB	1:45:A:ARG:HB2	1	0.54
(1,522)	1:40:A:VAL:HB	1:45:A:ARG:HB3	1	0.54
(1,280)	1:18:A:THR:HA	1:53:A:ILE:HG21	8	0.54
(1,280)	1:18:A:THR:HA	1:53:A:ILE:HG22	8	0.54
(1,280)	1:18:A:THR:HA	1:53:A:ILE:HG23	8	0.54
(1,201)	1:14:A:GLU:HG2	1:59:A:VAL:H	2	0.54
(1,118)	1:10:A:LEU:HG	1:61:A:MET:HG2	3	0.54
(1,118)	1:10:A:LEU:HG	1:61:A:MET:HG3	3	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,50)	1:6:A:LYS:HA	1:6:A:LYS:HD2	1	0.54
(1,50)	1:6:A:LYS:HA	1:6:A:LYS:HD3	1	0.54
(1,1022)	1:84:A:THR:HG21	1:85:A:ILE:HB	2	0.53
(1,1022)	1:84:A:THR:HG22	1:85:A:ILE:HB	2	0.53
(1,1022)	1:84:A:THR:HG23	1:85:A:ILE:HB	2	0.53
(1,713)	1:56:A:ARG:H	1:76:A:ARG:H	2	0.53
(1,691)	1:52:A:ILE:HG21	1:75:A:ARG:HG2	6	0.53
(1,691)	1:52:A:ILE:HG21	1:75:A:ARG:HG3	6	0.53
(1,691)	1:52:A:ILE:HG22	1:75:A:ARG:HG2	6	0.53
(1,691)	1:52:A:ILE:HG22	1:75:A:ARG:HG3	6	0.53
(1,691)	1:52:A:ILE:HG23	1:75:A:ARG:HG2	6	0.53
(1,691)	1:52:A:ILE:HG23	1:75:A:ARG:HG3	6	0.53
(1,534)	1:40:A:VAL:HG11	1:45:A:ARG:HA	6	0.53
(1,534)	1:40:A:VAL:HG12	1:45:A:ARG:HA	6	0.53
(1,534)	1:40:A:VAL:HG13	1:45:A:ARG:HA	6	0.53
(1,534)	1:40:A:VAL:HG21	1:45:A:ARG:HA	6	0.53
(1,534)	1:40:A:VAL:HG22	1:45:A:ARG:HA	6	0.53
(1,534)	1:40:A:VAL:HG23	1:45:A:ARG:HA	6	0.53
(1,475)	1:36:A:ILE:HB	1:37:A:ILE:H	8	0.53
(1,438)	1:29:A:LYS:HD2	1:30:A:LEU:H	10	0.53
(1,438)	1:29:A:LYS:HD3	1:30:A:LEU:H	10	0.53
(1,406)	1:27:A:ARG:HG2	1:28:A:VAL:H	2	0.53
(1,220)	1:15:A:GLY:HA2	1:56:A:ARG:HB2	7	0.53
(1,220)	1:15:A:GLY:HA2	1:56:A:ARG:HB3	7	0.53
(1,220)	1:15:A:GLY:HA3	1:56:A:ARG:HB2	7	0.53
(1,220)	1:15:A:GLY:HA3	1:56:A:ARG:HB3	7	0.53
(1,76)	1:8:A:LYS:HA	1:8:A:LYS:HE2	8	0.53
(1,76)	1:8:A:LYS:HA	1:8:A:LYS:HE3	8	0.53
(1,58)	1:6:A:LYS:HD2	1:7:A:SER:H	9	0.53
(3,13)	1:17:A:VAL:N	1:55:A:ASP:O	1	0.52
(3,13)	1:17:A:VAL:N	1:55:A:ASP:O	10	0.52
(2,12)	1:26:A:PHE:HE2	1:51:A:ILE:H	7	0.52
(1,855)	1:69:A:LYS:HD2	1:70:A:LYS:H	9	0.52
(1,855)	1:69:A:LYS:HD3	1:70:A:LYS:H	9	0.52
(1,839)	1:69:A:LYS:HA	1:69:A:LYS:HE2	6	0.52
(1,839)	1:69:A:LYS:HA	1:69:A:LYS:HE3	6	0.52
(1,839)	1:69:A:LYS:HA	1:69:A:LYS:HE2	8	0.52
(1,839)	1:69:A:LYS:HA	1:69:A:LYS:HE3	8	0.52
(1,542)	1:41:A:SER:H	1:73:A:ILE:H	9	0.52
(1,299)	1:19:A:ALA:HA	1:53:A:ILE:HA	10	0.52
(1,246)	1:17:A:VAL:HA	1:27:A:ARG:HB3	1	0.52
(1,246)	1:17:A:VAL:HA	1:27:A:ARG:HB3	5	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,218)	1:15:A:GLY:HA2	1:29:A:LYS:HD2	5	0.52
(1,218)	1:15:A:GLY:HA2	1:29:A:LYS:HD3	5	0.52
(1,218)	1:15:A:GLY:HA3	1:29:A:LYS:HD2	5	0.52
(1,218)	1:15:A:GLY:HA3	1:29:A:LYS:HD3	5	0.52
(1,172)	1:12:A:GLU:HB2	1:61:A:MET:H	8	0.52
(1,172)	1:12:A:GLU:HB3	1:61:A:MET:H	8	0.52
(1,66)	1:6:A:LYS:HG3	1:7:A:SER:H	5	0.52
(1,66)	1:6:A:LYS:HG3	1:7:A:SER:H	8	0.52
(1,19)	1:3:A:LYS:HA	1:3:A:LYS:HE2	10	0.52
(1,19)	1:3:A:LYS:HA	1:3:A:LYS:HE3	10	0.52
(3,41)	1:39:A:HIS:N	1:71:A:GLY:O	4	0.51
(2,5)	1:12:A:GLU:HG2	1:62:A:SER:HA	5	0.51
(2,5)	1:12:A:GLU:HG3	1:62:A:SER:HA	5	0.51
(2,5)	1:12:A:GLU:HG2	1:62:A:SER:HA	8	0.51
(2,5)	1:12:A:GLU:HG3	1:62:A:SER:HA	8	0.51
(1,871)	1:70:A:LYS:HG2	1:71:A:GLY:H	4	0.51
(1,806)	1:64:A:TYR:HB2	1:68:A:ALA:HA	5	0.51
(1,746)	1:59:A:VAL:HA	1:72:A:ARG:HG3	4	0.51
(1,561)	1:43:A:LYS:HG3	1:47:A:SER:HA	6	0.51
(1,438)	1:29:A:LYS:HD2	1:30:A:LEU:H	2	0.51
(1,438)	1:29:A:LYS:HD3	1:30:A:LEU:H	2	0.51
(1,422)	1:28:A:VAL:HB	1:29:A:LYS:HD2	2	0.51
(1,422)	1:28:A:VAL:HB	1:29:A:LYS:HD3	2	0.51
(1,347)	1:21:A:LEU:HG	1:23:A:ALA:H	6	0.51
(1,206)	1:15:A:GLY:H	1:56:A:ARG:HA	8	0.51
(1,172)	1:12:A:GLU:HB2	1:61:A:MET:H	9	0.51
(1,172)	1:12:A:GLU:HB3	1:61:A:MET:H	9	0.51
(3,36)	1:30:A:LEU:O	1:34:A:HIS:H	10	0.5
(3,34)	1:28:A:VAL:H	1:36:A:ILE:O	4	0.5
(2,12)	1:26:A:PHE:HE2	1:51:A:ILE:H	4	0.5
(1,1006)	1:83:A:ARG:HD2	1:84:A:THR:H	10	0.5
(1,1006)	1:83:A:ARG:HD3	1:84:A:THR:H	10	0.5
(1,518)	1:40:A:VAL:HA	1:72:A:ARG:HB2	1	0.5
(1,456)	1:33:A:GLU:H	1:33:A:GLU:HG2	1	0.5
(1,456)	1:33:A:GLU:H	1:33:A:GLU:HG3	1	0.5
(1,378)	1:25:A:GLU:HG3	1:39:A:HIS:HA	8	0.5
(1,356)	1:22:A:PRO:HG3	1:23:A:ALA:H	9	0.5
(1,347)	1:21:A:LEU:HG	1:23:A:ALA:H	1	0.5
(1,337)	1:20:A:LEU:HD11	1:21:A:LEU:HB2	6	0.5
(1,337)	1:20:A:LEU:HD11	1:21:A:LEU:HB3	6	0.5
(1,337)	1:20:A:LEU:HD12	1:21:A:LEU:HB2	6	0.5
(1,337)	1:20:A:LEU:HD12	1:21:A:LEU:HB3	6	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,337)	1:20:A:LEU:HD13	1:21:A:LEU:HB2	6	0.5
(1,337)	1:20:A:LEU:HD13	1:21:A:LEU:HB3	6	0.5
(1,337)	1:20:A:LEU:HD21	1:21:A:LEU:HB2	6	0.5
(1,337)	1:20:A:LEU:HD21	1:21:A:LEU:HB3	6	0.5
(1,337)	1:20:A:LEU:HD22	1:21:A:LEU:HB2	6	0.5
(1,337)	1:20:A:LEU:HD22	1:21:A:LEU:HB3	6	0.5
(1,337)	1:20:A:LEU:HD23	1:21:A:LEU:HB2	6	0.5
(1,337)	1:20:A:LEU:HD23	1:21:A:LEU:HB3	6	0.5
(1,325)	1:20:A:LEU:HG	1:21:A:LEU:H	9	0.5
(1,300)	1:19:A:ALA:HA	1:53:A:ILE:HB	7	0.5
(1,76)	1:8:A:LYS:HA	1:8:A:LYS:HE2	2	0.5
(1,76)	1:8:A:LYS:HA	1:8:A:LYS:HE3	2	0.5
(1,76)	1:8:A:LYS:HA	1:8:A:LYS:HE2	10	0.5
(1,76)	1:8:A:LYS:HA	1:8:A:LYS:HE3	10	0.5
(1,58)	1:6:A:LYS:HD2	1:7:A:SER:H	4	0.5
(1,14)	1:3:A:LYS:H	1:3:A:LYS:HD2	3	0.5
(1,14)	1:3:A:LYS:H	1:3:A:LYS:HD3	3	0.5
(3,47)	1:39:A:HIS:O	1:73:A:ILE:N	6	0.49
(1,964)	1:77:A:LEU:HD11	1:78:A:LYS:HD2	1	0.49
(1,964)	1:77:A:LEU:HD11	1:78:A:LYS:HD3	1	0.49
(1,964)	1:77:A:LEU:HD12	1:78:A:LYS:HD2	1	0.49
(1,964)	1:77:A:LEU:HD12	1:78:A:LYS:HD3	1	0.49
(1,964)	1:77:A:LEU:HD13	1:78:A:LYS:HD2	1	0.49
(1,964)	1:77:A:LEU:HD13	1:78:A:LYS:HD3	1	0.49
(1,964)	1:77:A:LEU:HD21	1:78:A:LYS:HD2	1	0.49
(1,964)	1:77:A:LEU:HD21	1:78:A:LYS:HD3	1	0.49
(1,964)	1:77:A:LEU:HD22	1:78:A:LYS:HD2	1	0.49
(1,964)	1:77:A:LEU:HD22	1:78:A:LYS:HD3	1	0.49
(1,964)	1:77:A:LEU:HD23	1:78:A:LYS:HD2	1	0.49
(1,964)	1:77:A:LEU:HD23	1:78:A:LYS:HD3	1	0.49
(1,690)	1:52:A:ILE:HG21	1:75:A:ARG:HB2	7	0.49
(1,690)	1:52:A:ILE:HG22	1:75:A:ARG:HB2	7	0.49
(1,690)	1:52:A:ILE:HG23	1:75:A:ARG:HB2	7	0.49
(1,604)	1:47:A:SER:HA	1:49:A:ILE:H	8	0.49
(1,587)	1:45:A:ARG:HG2	1:46:A:ARG:H	1	0.49
(1,587)	1:45:A:ARG:HG3	1:46:A:ARG:H	1	0.49
(1,337)	1:20:A:LEU:HD11	1:21:A:LEU:HB2	7	0.49
(1,337)	1:20:A:LEU:HD11	1:21:A:LEU:HB3	7	0.49
(1,337)	1:20:A:LEU:HD12	1:21:A:LEU:HB2	7	0.49
(1,337)	1:20:A:LEU:HD12	1:21:A:LEU:HB3	7	0.49
(1,337)	1:20:A:LEU:HD13	1:21:A:LEU:HB2	7	0.49
(1,337)	1:20:A:LEU:HD13	1:21:A:LEU:HB3	7	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,337)	1:20:A:LEU:HD21	1:21:A:LEU:HB2	7	0.49
(1,337)	1:20:A:LEU:HD21	1:21:A:LEU:HB3	7	0.49
(1,337)	1:20:A:LEU:HD22	1:21:A:LEU:HB2	7	0.49
(1,337)	1:20:A:LEU:HD22	1:21:A:LEU:HB3	7	0.49
(1,337)	1:20:A:LEU:HD23	1:21:A:LEU:HB2	7	0.49
(1,337)	1:20:A:LEU:HD23	1:21:A:LEU:HB3	7	0.49
(1,332)	1:20:A:LEU:HD11	1:27:A:ARG:H	1	0.49
(1,332)	1:20:A:LEU:HD12	1:27:A:ARG:H	1	0.49
(1,332)	1:20:A:LEU:HD13	1:27:A:ARG:H	1	0.49
(1,300)	1:19:A:ALA:HA	1:53:A:ILE:HB	1	0.49
(1,219)	1:15:A:GLY:HA2	1:30:A:LEU:HA	2	0.49
(1,219)	1:15:A:GLY:HA3	1:30:A:LEU:HA	2	0.49
(1,172)	1:12:A:GLU:HB2	1:61:A:MET:H	7	0.49
(1,172)	1:12:A:GLU:HB3	1:61:A:MET:H	7	0.49
(1,167)	1:12:A:GLU:HG2	1:61:A:MET:H	5	0.49
(1,116)	1:10:A:LEU:HG	1:61:A:MET:HA	4	0.49
(1,87)	1:8:A:LYS:HD3	1:9:A:THR:H	9	0.49
(1,66)	1:6:A:LYS:HG3	1:7:A:SER:H	4	0.49
(1,964)	1:77:A:LEU:HD11	1:78:A:LYS:HD2	10	0.48
(1,964)	1:77:A:LEU:HD11	1:78:A:LYS:HD3	10	0.48
(1,964)	1:77:A:LEU:HD12	1:78:A:LYS:HD2	10	0.48
(1,964)	1:77:A:LEU:HD12	1:78:A:LYS:HD3	10	0.48
(1,964)	1:77:A:LEU:HD13	1:78:A:LYS:HD2	10	0.48
(1,964)	1:77:A:LEU:HD13	1:78:A:LYS:HD3	10	0.48
(1,964)	1:77:A:LEU:HD21	1:78:A:LYS:HD2	10	0.48
(1,964)	1:77:A:LEU:HD21	1:78:A:LYS:HD3	10	0.48
(1,964)	1:77:A:LEU:HD22	1:78:A:LYS:HD2	10	0.48
(1,964)	1:77:A:LEU:HD22	1:78:A:LYS:HD3	10	0.48
(1,964)	1:77:A:LEU:HD23	1:78:A:LYS:HD2	10	0.48
(1,964)	1:77:A:LEU:HD23	1:78:A:LYS:HD3	10	0.48
(1,839)	1:69:A:LYS:HA	1:69:A:LYS:HE2	9	0.48
(1,839)	1:69:A:LYS:HA	1:69:A:LYS:HE3	9	0.48
(1,587)	1:45:A:ARG:HG2	1:46:A:ARG:H	4	0.48
(1,587)	1:45:A:ARG:HG3	1:46:A:ARG:H	4	0.48
(1,521)	1:40:A:VAL:HB	1:45:A:ARG:HA	6	0.48
(1,413)	1:28:A:VAL:H	1:35:A:GLU:HB2	9	0.48
(1,413)	1:28:A:VAL:H	1:35:A:GLU:HB3	9	0.48
(1,405)	1:27:A:ARG:HB2	1:38:A:CYS:H	10	0.48
(1,405)	1:27:A:ARG:HB3	1:38:A:CYS:H	10	0.48
(1,76)	1:8:A:LYS:HA	1:8:A:LYS:HE2	1	0.48
(1,76)	1:8:A:LYS:HA	1:8:A:LYS:HE3	1	0.48
(3,43)	1:37:A:ILE:N	1:69:A:LYS:O	4	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1002)	1:83:A:ARG:HB2	1:84:A:THR:H	9	0.47
(1,409)	1:27:A:ARG:HG2	1:38:A:CYS:HB2	1	0.47
(1,409)	1:27:A:ARG:HG2	1:38:A:CYS:HB3	1	0.47
(1,409)	1:27:A:ARG:HG3	1:38:A:CYS:HB2	1	0.47
(1,409)	1:27:A:ARG:HG3	1:38:A:CYS:HB3	1	0.47
(1,226)	1:16:A:ALA:H	1:30:A:LEU:HA	3	0.47
(1,99)	1:9:A:THR:HA	1:9:A:THR:HB	4	0.47
(1,99)	1:9:A:THR:HA	1:9:A:THR:HB	6	0.47
(1,99)	1:9:A:THR:HA	1:9:A:THR:HB	7	0.47
(1,99)	1:9:A:THR:HA	1:9:A:THR:HB	10	0.47
(1,17)	1:3:A:LYS:H	1:4:A:ASP:H	6	0.47
(1,690)	1:52:A:ILE:HG21	1:75:A:ARG:HB2	6	0.46
(1,690)	1:52:A:ILE:HG22	1:75:A:ARG:HB2	6	0.46
(1,690)	1:52:A:ILE:HG23	1:75:A:ARG:HB2	6	0.46
(1,664)	1:50:A:ARG:HG2	1:75:A:ARG:HG2	2	0.46
(1,664)	1:50:A:ARG:HG2	1:75:A:ARG:HG3	2	0.46
(1,664)	1:50:A:ARG:HG3	1:75:A:ARG:HG2	2	0.46
(1,664)	1:50:A:ARG:HG3	1:75:A:ARG:HG3	2	0.46
(1,413)	1:28:A:VAL:H	1:35:A:GLU:HB2	1	0.46
(1,413)	1:28:A:VAL:H	1:35:A:GLU:HB3	1	0.46
(1,354)	1:22:A:PRO:HG2	1:23:A:ALA:H	8	0.46
(1,299)	1:19:A:ALA:HA	1:53:A:ILE:HA	6	0.46
(1,172)	1:12:A:GLU:HB2	1:61:A:MET:H	5	0.46
(1,172)	1:12:A:GLU:HB3	1:61:A:MET:H	5	0.46
(1,99)	1:9:A:THR:HA	1:9:A:THR:HB	2	0.46
(1,99)	1:9:A:THR:HA	1:9:A:THR:HB	3	0.46
(1,99)	1:9:A:THR:HA	1:9:A:THR:HB	5	0.46
(1,63)	1:6:A:LYS:HG2	1:7:A:SER:H	7	0.46
(3,55)	1:44:A:VAL:O	1:47:A:SER:N	1	0.45
(2,24)	1:66:A:ARG:HD2	1:68:A:ALA:HB1	6	0.45
(2,24)	1:66:A:ARG:HD2	1:68:A:ALA:HB2	6	0.45
(2,24)	1:66:A:ARG:HD2	1:68:A:ALA:HB3	6	0.45
(2,24)	1:66:A:ARG:HD2	1:68:A:ALA:HB1	10	0.45
(2,24)	1:66:A:ARG:HD2	1:68:A:ALA:HB2	10	0.45
(2,24)	1:66:A:ARG:HD2	1:68:A:ALA:HB3	10	0.45
(2,18)	1:44:A:VAL:HG21	1:51:A:ILE:HG21	10	0.45
(2,18)	1:44:A:VAL:HG21	1:51:A:ILE:HG22	10	0.45
(2,18)	1:44:A:VAL:HG21	1:51:A:ILE:HG23	10	0.45
(2,18)	1:44:A:VAL:HG22	1:51:A:ILE:HG21	10	0.45
(2,18)	1:44:A:VAL:HG22	1:51:A:ILE:HG22	10	0.45
(2,18)	1:44:A:VAL:HG22	1:51:A:ILE:HG23	10	0.45
(2,18)	1:44:A:VAL:HG23	1:51:A:ILE:HG21	10	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,18)	1:44:A:VAL:HG23	1:51:A:ILE:HG22	10	0.45
(2,18)	1:44:A:VAL:HG23	1:51:A:ILE:HG23	10	0.45
(1,871)	1:70:A:LYS:HG2	1:71:A:GLY:H	3	0.45
(1,712)	1:56:A:ARG:H	1:75:A:ARG:HG2	5	0.45
(1,587)	1:45:A:ARG:HG2	1:46:A:ARG:H	9	0.45
(1,587)	1:45:A:ARG:HG3	1:46:A:ARG:H	9	0.45
(1,540)	1:41:A:SER:H	1:72:A:ARG:H	8	0.45
(1,529)	1:40:A:VAL:HG11	1:44:A:VAL:H	3	0.45
(1,529)	1:40:A:VAL:HG12	1:44:A:VAL:H	3	0.45
(1,529)	1:40:A:VAL:HG13	1:44:A:VAL:H	3	0.45
(1,529)	1:40:A:VAL:HG21	1:44:A:VAL:H	3	0.45
(1,529)	1:40:A:VAL:HG22	1:44:A:VAL:H	3	0.45
(1,529)	1:40:A:VAL:HG23	1:44:A:VAL:H	3	0.45
(1,407)	1:27:A:ARG:HG2	1:38:A:CYS:HA	1	0.45
(1,355)	1:22:A:PRO:HG2	1:24:A:ALA:H	9	0.45
(1,327)	1:20:A:LEU:HG	1:21:A:LEU:HB2	5	0.45
(1,327)	1:20:A:LEU:HG	1:21:A:LEU:HB3	5	0.45
(1,299)	1:19:A:ALA:HA	1:53:A:ILE:HA	2	0.45
(1,128)	1:10:A:LEU:HD11	1:61:A:MET:HB2	1	0.45
(1,128)	1:10:A:LEU:HD11	1:61:A:MET:HB3	1	0.45
(1,128)	1:10:A:LEU:HD12	1:61:A:MET:HB2	1	0.45
(1,128)	1:10:A:LEU:HD12	1:61:A:MET:HB3	1	0.45
(1,128)	1:10:A:LEU:HD13	1:61:A:MET:HB2	1	0.45
(1,128)	1:10:A:LEU:HD13	1:61:A:MET:HB3	1	0.45
(1,128)	1:10:A:LEU:HD21	1:61:A:MET:HB2	1	0.45
(1,128)	1:10:A:LEU:HD21	1:61:A:MET:HB3	1	0.45
(1,128)	1:10:A:LEU:HD22	1:61:A:MET:HB2	1	0.45
(1,128)	1:10:A:LEU:HD22	1:61:A:MET:HB3	1	0.45
(1,128)	1:10:A:LEU:HD23	1:61:A:MET:HB2	1	0.45
(1,128)	1:10:A:LEU:HD23	1:61:A:MET:HB3	1	0.45
(1,47)	1:6:A:LYS:H	1:6:A:LYS:HE2	4	0.45
(1,47)	1:6:A:LYS:H	1:6:A:LYS:HE3	4	0.45
(1,17)	1:3:A:LYS:H	1:4:A:ASP:H	2	0.45
(1,17)	1:3:A:LYS:H	1:4:A:ASP:H	5	0.45
(1,14)	1:3:A:LYS:H	1:3:A:LYS:HD2	2	0.45
(1,14)	1:3:A:LYS:H	1:3:A:LYS:HD3	2	0.45
(3,1)	1:11:A:PHE:O	1:61:A:MET:N	2	0.44
(2,24)	1:66:A:ARG:HD2	1:68:A:ALA:HB1	7	0.44
(2,24)	1:66:A:ARG:HD2	1:68:A:ALA:HB2	7	0.44
(2,24)	1:66:A:ARG:HD2	1:68:A:ALA:HB3	7	0.44
(2,24)	1:66:A:ARG:HD2	1:68:A:ALA:HB1	8	0.44
(2,24)	1:66:A:ARG:HD2	1:68:A:ALA:HB2	8	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,24)	1:66:A:ARG:HD2	1:68:A:ALA:HB3	8	0.44
(2,18)	1:44:A:VAL:HG21	1:51:A:ILE:HG21	5	0.44
(2,18)	1:44:A:VAL:HG21	1:51:A:ILE:HG22	5	0.44
(2,18)	1:44:A:VAL:HG21	1:51:A:ILE:HG23	5	0.44
(2,18)	1:44:A:VAL:HG22	1:51:A:ILE:HG21	5	0.44
(2,18)	1:44:A:VAL:HG22	1:51:A:ILE:HG22	5	0.44
(2,18)	1:44:A:VAL:HG22	1:51:A:ILE:HG23	5	0.44
(2,18)	1:44:A:VAL:HG23	1:51:A:ILE:HG21	5	0.44
(2,18)	1:44:A:VAL:HG23	1:51:A:ILE:HG22	5	0.44
(2,18)	1:44:A:VAL:HG23	1:51:A:ILE:HG23	5	0.44
(1,1006)	1:83:A:ARG:HD2	1:84:A:THR:H	5	0.44
(1,1006)	1:83:A:ARG:HD3	1:84:A:THR:H	5	0.44
(1,989)	1:82:A:ASP:HA	1:85:A:ILE:HG21	9	0.44
(1,989)	1:82:A:ASP:HA	1:85:A:ILE:HG22	9	0.44
(1,989)	1:82:A:ASP:HA	1:85:A:ILE:HG23	9	0.44
(1,960)	1:77:A:LEU:HG	1:78:A:LYS:HE2	1	0.44
(1,960)	1:77:A:LEU:HG	1:78:A:LYS:HE3	1	0.44
(1,871)	1:70:A:LYS:HG2	1:71:A:GLY:H	6	0.44
(1,806)	1:64:A:TYR:HB2	1:68:A:ALA:HA	4	0.44
(1,559)	1:43:A:LYS:HG2	1:47:A:SER:HA	7	0.44
(1,518)	1:40:A:VAL:HA	1:72:A:ARG:HB2	2	0.44
(1,292)	1:18:A:THR:HG21	1:53:A:ILE:HG21	2	0.44
(1,292)	1:18:A:THR:HG21	1:53:A:ILE:HG22	2	0.44
(1,292)	1:18:A:THR:HG21	1:53:A:ILE:HG23	2	0.44
(1,292)	1:18:A:THR:HG22	1:53:A:ILE:HG21	2	0.44
(1,292)	1:18:A:THR:HG22	1:53:A:ILE:HG22	2	0.44
(1,292)	1:18:A:THR:HG22	1:53:A:ILE:HG23	2	0.44
(1,292)	1:18:A:THR:HG23	1:53:A:ILE:HG21	2	0.44
(1,292)	1:18:A:THR:HG23	1:53:A:ILE:HG22	2	0.44
(1,292)	1:18:A:THR:HG23	1:53:A:ILE:HG23	2	0.44
(1,257)	1:17:A:VAL:HG21	1:53:A:ILE:HB	7	0.44
(1,257)	1:17:A:VAL:HG22	1:53:A:ILE:HB	7	0.44
(1,257)	1:17:A:VAL:HG23	1:53:A:ILE:HB	7	0.44
(1,130)	1:10:A:LEU:HD11	1:62:A:SER:HB2	7	0.44
(1,130)	1:10:A:LEU:HD11	1:62:A:SER:HB3	7	0.44
(1,130)	1:10:A:LEU:HD12	1:62:A:SER:HB2	7	0.44
(1,130)	1:10:A:LEU:HD12	1:62:A:SER:HB3	7	0.44
(1,130)	1:10:A:LEU:HD13	1:62:A:SER:HB2	7	0.44
(1,130)	1:10:A:LEU:HD13	1:62:A:SER:HB3	7	0.44
(1,130)	1:10:A:LEU:HD21	1:62:A:SER:HB2	7	0.44
(1,130)	1:10:A:LEU:HD21	1:62:A:SER:HB3	7	0.44
(1,130)	1:10:A:LEU:HD22	1:62:A:SER:HB2	7	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,130)	1:10:A:LEU:HD22	1:62:A:SER:HB3	7	0.44
(1,130)	1:10:A:LEU:HD23	1:62:A:SER:HB2	7	0.44
(1,130)	1:10:A:LEU:HD23	1:62:A:SER:HB3	7	0.44
(3,42)	1:37:A:ILE:H	1:69:A:LYS:O	3	0.43
(2,25)	1:76:A:ARG:HD3	1:77:A:LEU:HG	5	0.43
(2,5)	1:12:A:GLU:HG2	1:62:A:SER:HA	3	0.43
(2,5)	1:12:A:GLU:HG3	1:62:A:SER:HA	3	0.43
(2,5)	1:12:A:GLU:HG2	1:62:A:SER:HA	4	0.43
(2,5)	1:12:A:GLU:HG3	1:62:A:SER:HA	4	0.43
(2,5)	1:12:A:GLU:HG2	1:62:A:SER:HA	7	0.43
(2,5)	1:12:A:GLU:HG3	1:62:A:SER:HA	7	0.43
(1,989)	1:82:A:ASP:HA	1:85:A:ILE:HG21	1	0.43
(1,989)	1:82:A:ASP:HA	1:85:A:ILE:HG22	1	0.43
(1,989)	1:82:A:ASP:HA	1:85:A:ILE:HG23	1	0.43
(1,638)	1:49:A:ILE:HD11	1:75:A:ARG:HD2	1	0.43
(1,638)	1:49:A:ILE:HD12	1:75:A:ARG:HD2	1	0.43
(1,638)	1:49:A:ILE:HD13	1:75:A:ARG:HD2	1	0.43
(1,638)	1:49:A:ILE:HD11	1:75:A:ARG:HD3	1	0.43
(1,638)	1:49:A:ILE:HD12	1:75:A:ARG:HD3	1	0.43
(1,638)	1:49:A:ILE:HD13	1:75:A:ARG:HD3	1	0.43
(1,574)	1:44:A:VAL:HG11	1:51:A:ILE:HG21	3	0.43
(1,574)	1:44:A:VAL:HG11	1:51:A:ILE:HG22	3	0.43
(1,574)	1:44:A:VAL:HG11	1:51:A:ILE:HG23	3	0.43
(1,574)	1:44:A:VAL:HG12	1:51:A:ILE:HG21	3	0.43
(1,574)	1:44:A:VAL:HG12	1:51:A:ILE:HG22	3	0.43
(1,574)	1:44:A:VAL:HG12	1:51:A:ILE:HG23	3	0.43
(1,574)	1:44:A:VAL:HG13	1:51:A:ILE:HG21	3	0.43
(1,574)	1:44:A:VAL:HG13	1:51:A:ILE:HG22	3	0.43
(1,574)	1:44:A:VAL:HG13	1:51:A:ILE:HG23	3	0.43
(1,574)	1:44:A:VAL:HG21	1:51:A:ILE:HG21	3	0.43
(1,574)	1:44:A:VAL:HG21	1:51:A:ILE:HG22	3	0.43
(1,574)	1:44:A:VAL:HG21	1:51:A:ILE:HG23	3	0.43
(1,574)	1:44:A:VAL:HG22	1:51:A:ILE:HG21	3	0.43
(1,574)	1:44:A:VAL:HG22	1:51:A:ILE:HG22	3	0.43
(1,574)	1:44:A:VAL:HG22	1:51:A:ILE:HG23	3	0.43
(1,574)	1:44:A:VAL:HG23	1:51:A:ILE:HG21	3	0.43
(1,574)	1:44:A:VAL:HG23	1:51:A:ILE:HG22	3	0.43
(1,574)	1:44:A:VAL:HG23	1:51:A:ILE:HG23	3	0.43
(1,574)	1:44:A:VAL:HG11	1:51:A:ILE:HG21	9	0.43
(1,574)	1:44:A:VAL:HG11	1:51:A:ILE:HG22	9	0.43
(1,574)	1:44:A:VAL:HG11	1:51:A:ILE:HG23	9	0.43
(1,574)	1:44:A:VAL:HG12	1:51:A:ILE:HG21	9	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,574)	1:44:A:VAL:HG12	1:51:A:ILE:HG22	9	0.43
(1,574)	1:44:A:VAL:HG12	1:51:A:ILE:HG23	9	0.43
(1,574)	1:44:A:VAL:HG13	1:51:A:ILE:HG21	9	0.43
(1,574)	1:44:A:VAL:HG13	1:51:A:ILE:HG22	9	0.43
(1,574)	1:44:A:VAL:HG13	1:51:A:ILE:HG23	9	0.43
(1,574)	1:44:A:VAL:HG21	1:51:A:ILE:HG21	9	0.43
(1,574)	1:44:A:VAL:HG21	1:51:A:ILE:HG22	9	0.43
(1,574)	1:44:A:VAL:HG21	1:51:A:ILE:HG23	9	0.43
(1,574)	1:44:A:VAL:HG22	1:51:A:ILE:HG21	9	0.43
(1,574)	1:44:A:VAL:HG22	1:51:A:ILE:HG22	9	0.43
(1,574)	1:44:A:VAL:HG22	1:51:A:ILE:HG23	9	0.43
(1,574)	1:44:A:VAL:HG23	1:51:A:ILE:HG21	9	0.43
(1,574)	1:44:A:VAL:HG23	1:51:A:ILE:HG22	9	0.43
(1,574)	1:44:A:VAL:HG23	1:51:A:ILE:HG23	9	0.43
(1,518)	1:40:A:VAL:HA	1:72:A:ARG:HB2	4	0.43
(1,408)	1:27:A:ARG:HG3	1:28:A:VAL:H	3	0.43
(1,338)	1:20:A:LEU:HD11	1:26:A:PHE:HB2	4	0.43
(1,338)	1:20:A:LEU:HD11	1:26:A:PHE:HB3	4	0.43
(1,338)	1:20:A:LEU:HD12	1:26:A:PHE:HB2	4	0.43
(1,338)	1:20:A:LEU:HD12	1:26:A:PHE:HB3	4	0.43
(1,338)	1:20:A:LEU:HD13	1:26:A:PHE:HB2	4	0.43
(1,338)	1:20:A:LEU:HD13	1:26:A:PHE:HB3	4	0.43
(1,338)	1:20:A:LEU:HD21	1:26:A:PHE:HB2	4	0.43
(1,338)	1:20:A:LEU:HD21	1:26:A:PHE:HB3	4	0.43
(1,338)	1:20:A:LEU:HD22	1:26:A:PHE:HB2	4	0.43
(1,338)	1:20:A:LEU:HD22	1:26:A:PHE:HB3	4	0.43
(1,338)	1:20:A:LEU:HD23	1:26:A:PHE:HB2	4	0.43
(1,338)	1:20:A:LEU:HD23	1:26:A:PHE:HB3	4	0.43
(1,130)	1:10:A:LEU:HD11	1:62:A:SER:HB2	4	0.43
(1,130)	1:10:A:LEU:HD11	1:62:A:SER:HB3	4	0.43
(1,130)	1:10:A:LEU:HD12	1:62:A:SER:HB2	4	0.43
(1,130)	1:10:A:LEU:HD12	1:62:A:SER:HB3	4	0.43
(1,130)	1:10:A:LEU:HD13	1:62:A:SER:HB2	4	0.43
(1,130)	1:10:A:LEU:HD13	1:62:A:SER:HB3	4	0.43
(1,130)	1:10:A:LEU:HD21	1:62:A:SER:HB2	4	0.43
(1,130)	1:10:A:LEU:HD21	1:62:A:SER:HB3	4	0.43
(1,130)	1:10:A:LEU:HD22	1:62:A:SER:HB2	4	0.43
(1,130)	1:10:A:LEU:HD22	1:62:A:SER:HB3	4	0.43
(1,130)	1:10:A:LEU:HD23	1:62:A:SER:HB2	4	0.43
(1,130)	1:10:A:LEU:HD23	1:62:A:SER:HB3	4	0.43
(1,118)	1:10:A:LEU:HG	1:61:A:MET:HG2	2	0.43
(1,118)	1:10:A:LEU:HG	1:61:A:MET:HG3	2	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,117)	1:10:A:LEU:HG	1:61:A:MET:HB2	10	0.43
(1,117)	1:10:A:LEU:HG	1:61:A:MET:HB3	10	0.43
(2,25)	1:76:A:ARG:HD3	1:77:A:LEU:HG	6	0.42
(2,18)	1:44:A:VAL:HG21	1:51:A:ILE:HG21	3	0.42
(2,18)	1:44:A:VAL:HG21	1:51:A:ILE:HG22	3	0.42
(2,18)	1:44:A:VAL:HG21	1:51:A:ILE:HG23	3	0.42
(2,18)	1:44:A:VAL:HG22	1:51:A:ILE:HG21	3	0.42
(2,18)	1:44:A:VAL:HG22	1:51:A:ILE:HG22	3	0.42
(2,18)	1:44:A:VAL:HG22	1:51:A:ILE:HG23	3	0.42
(2,18)	1:44:A:VAL:HG23	1:51:A:ILE:HG21	3	0.42
(2,18)	1:44:A:VAL:HG23	1:51:A:ILE:HG22	3	0.42
(2,18)	1:44:A:VAL:HG23	1:51:A:ILE:HG23	3	0.42
(2,18)	1:44:A:VAL:HG21	1:51:A:ILE:HG21	7	0.42
(2,18)	1:44:A:VAL:HG21	1:51:A:ILE:HG22	7	0.42
(2,18)	1:44:A:VAL:HG21	1:51:A:ILE:HG23	7	0.42
(2,18)	1:44:A:VAL:HG22	1:51:A:ILE:HG21	7	0.42
(2,18)	1:44:A:VAL:HG22	1:51:A:ILE:HG22	7	0.42
(2,18)	1:44:A:VAL:HG22	1:51:A:ILE:HG23	7	0.42
(2,18)	1:44:A:VAL:HG23	1:51:A:ILE:HG21	7	0.42
(2,18)	1:44:A:VAL:HG23	1:51:A:ILE:HG22	7	0.42
(2,18)	1:44:A:VAL:HG23	1:51:A:ILE:HG23	7	0.42
(1,1021)	1:84:A:THR:HG21	1:85:A:ILE:HA	3	0.42
(1,1021)	1:84:A:THR:HG22	1:85:A:ILE:HA	3	0.42
(1,1021)	1:84:A:THR:HG23	1:85:A:ILE:HA	3	0.42
(1,772)	1:62:A:SER:H	1:64:A:TYR:HB2	10	0.42
(1,772)	1:62:A:SER:H	1:64:A:TYR:HB2	10	0.42
(1,772)	1:62:A:SER:H	1:64:A:TYR:HB3	10	0.42
(1,504)	1:39:A:HIS:H	1:71:A:GLY:HA2	3	0.42
(1,504)	1:39:A:HIS:H	1:71:A:GLY:HA3	3	0.42
(1,485)	1:37:A:ILE:H	1:70:A:LYS:H	4	0.42
(1,422)	1:28:A:VAL:HB	1:29:A:LYS:HD2	3	0.42
(1,422)	1:28:A:VAL:HB	1:29:A:LYS:HD3	3	0.42
(1,393)	1:26:A:PHE:HE1	1:51:A:ILE:H	6	0.42
(3,54)	1:44:A:VAL:O	1:47:A:SER:H	3	0.41
(2,24)	1:66:A:ARG:HD2	1:68:A:ALA:HB1	2	0.41
(2,24)	1:66:A:ARG:HD2	1:68:A:ALA:HB2	2	0.41
(2,24)	1:66:A:ARG:HD2	1:68:A:ALA:HB3	2	0.41
(2,18)	1:44:A:VAL:HG21	1:51:A:ILE:HG21	9	0.41
(2,18)	1:44:A:VAL:HG21	1:51:A:ILE:HG22	9	0.41
(2,18)	1:44:A:VAL:HG21	1:51:A:ILE:HG23	9	0.41
(2,18)	1:44:A:VAL:HG22	1:51:A:ILE:HG21	9	0.41
(2,18)	1:44:A:VAL:HG22	1:51:A:ILE:HG22	9	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,18)	1:44:A:VAL:HG22	1:51:A:ILE:HG23	9	0.41
(2,18)	1:44:A:VAL:HG23	1:51:A:ILE:HG21	9	0.41
(2,18)	1:44:A:VAL:HG23	1:51:A:ILE:HG22	9	0.41
(2,18)	1:44:A:VAL:HG23	1:51:A:ILE:HG23	9	0.41
(2,5)	1:12:A:GLU:HG2	1:62:A:SER:HA	2	0.41
(2,5)	1:12:A:GLU:HG3	1:62:A:SER:HA	2	0.41
(2,5)	1:12:A:GLU:HG2	1:62:A:SER:HA	6	0.41
(2,5)	1:12:A:GLU:HG3	1:62:A:SER:HA	6	0.41
(2,5)	1:12:A:GLU:HG2	1:62:A:SER:HA	10	0.41
(2,5)	1:12:A:GLU:HG3	1:62:A:SER:HA	10	0.41
(1,848)	1:69:A:LYS:HE2	1:70:A:LYS:H	7	0.41
(1,848)	1:69:A:LYS:HE3	1:70:A:LYS:H	7	0.41
(1,637)	1:49:A:ILE:HD11	1:74:A:ILE:HG12	8	0.41
(1,637)	1:49:A:ILE:HD12	1:74:A:ILE:HG12	8	0.41
(1,637)	1:49:A:ILE:HD13	1:74:A:ILE:HG12	8	0.41
(1,637)	1:49:A:ILE:HD11	1:74:A:ILE:HG13	8	0.41
(1,637)	1:49:A:ILE:HD12	1:74:A:ILE:HG13	8	0.41
(1,637)	1:49:A:ILE:HD13	1:74:A:ILE:HG13	8	0.41
(1,566)	1:44:A:VAL:H	1:47:A:SER:H	10	0.41
(1,542)	1:41:A:SER:H	1:73:A:ILE:H	10	0.41
(1,540)	1:41:A:SER:H	1:72:A:ARG:H	1	0.41
(1,337)	1:20:A:LEU:HD11	1:21:A:LEU:HB2	10	0.41
(1,337)	1:20:A:LEU:HD11	1:21:A:LEU:HB3	10	0.41
(1,337)	1:20:A:LEU:HD12	1:21:A:LEU:HB2	10	0.41
(1,337)	1:20:A:LEU:HD12	1:21:A:LEU:HB3	10	0.41
(1,337)	1:20:A:LEU:HD13	1:21:A:LEU:HB2	10	0.41
(1,337)	1:20:A:LEU:HD13	1:21:A:LEU:HB3	10	0.41
(1,337)	1:20:A:LEU:HD21	1:21:A:LEU:HB2	10	0.41
(1,337)	1:20:A:LEU:HD21	1:21:A:LEU:HB3	10	0.41
(1,337)	1:20:A:LEU:HD22	1:21:A:LEU:HB2	10	0.41
(1,337)	1:20:A:LEU:HD22	1:21:A:LEU:HB3	10	0.41
(1,337)	1:20:A:LEU:HD23	1:21:A:LEU:HB2	10	0.41
(1,337)	1:20:A:LEU:HD23	1:21:A:LEU:HB3	10	0.41
(1,327)	1:20:A:LEU:HG	1:21:A:LEU:HB2	1	0.41
(1,327)	1:20:A:LEU:HG	1:21:A:LEU:HB3	1	0.41
(1,220)	1:15:A:GLY:HA2	1:56:A:ARG:HB2	2	0.41
(1,220)	1:15:A:GLY:HA2	1:56:A:ARG:HB3	2	0.41
(1,220)	1:15:A:GLY:HA3	1:56:A:ARG:HB2	2	0.41
(1,220)	1:15:A:GLY:HA3	1:56:A:ARG:HB3	2	0.41
(1,206)	1:15:A:GLY:H	1:56:A:ARG:HA	10	0.41
(1,128)	1:10:A:LEU:HD11	1:61:A:MET:HB2	5	0.41
(1,128)	1:10:A:LEU:HD11	1:61:A:MET:HB3	5	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,128)	1:10:A:LEU:HD12	1:61:A:MET:HB2	5	0.41
(1,128)	1:10:A:LEU:HD12	1:61:A:MET:HB3	5	0.41
(1,128)	1:10:A:LEU:HD13	1:61:A:MET:HB2	5	0.41
(1,128)	1:10:A:LEU:HD13	1:61:A:MET:HB3	5	0.41
(1,128)	1:10:A:LEU:HD21	1:61:A:MET:HB2	5	0.41
(1,128)	1:10:A:LEU:HD21	1:61:A:MET:HB3	5	0.41
(1,128)	1:10:A:LEU:HD22	1:61:A:MET:HB2	5	0.41
(1,128)	1:10:A:LEU:HD22	1:61:A:MET:HB3	5	0.41
(1,128)	1:10:A:LEU:HD23	1:61:A:MET:HB2	5	0.41
(1,128)	1:10:A:LEU:HD23	1:61:A:MET:HB3	5	0.41
(1,26)	1:3:A:LYS:HD2	1:4:A:ASP:H	10	0.41
(1,26)	1:3:A:LYS:HD3	1:4:A:ASP:H	10	0.41
(1,14)	1:3:A:LYS:H	1:3:A:LYS:HD2	9	0.41
(1,14)	1:3:A:LYS:H	1:3:A:LYS:HD3	9	0.41
(3,35)	1:28:A:VAL:N	1:36:A:ILE:O	4	0.4
(2,12)	1:26:A:PHE:HE2	1:51:A:ILE:H	2	0.4
(1,957)	1:77:A:LEU:HG	1:78:A:LYS:H	9	0.4
(1,850)	1:69:A:LYS:HG2	1:70:A:LYS:H	9	0.4
(1,773)	1:62:A:SER:H	1:66:A:ARG:HG2	3	0.4
(1,587)	1:45:A:ARG:HG2	1:46:A:ARG:H	5	0.4
(1,587)	1:45:A:ARG:HG3	1:46:A:ARG:H	5	0.4
(1,528)	1:40:A:VAL:HG21	1:45:A:ARG:HA	1	0.4
(1,528)	1:40:A:VAL:HG22	1:45:A:ARG:HA	1	0.4
(1,528)	1:40:A:VAL:HG23	1:45:A:ARG:HA	1	0.4
(1,528)	1:40:A:VAL:HG21	1:45:A:ARG:HA	6	0.4
(1,528)	1:40:A:VAL:HG22	1:45:A:ARG:HA	6	0.4
(1,528)	1:40:A:VAL:HG23	1:45:A:ARG:HA	6	0.4
(1,413)	1:28:A:VAL:H	1:35:A:GLU:HB2	4	0.4
(1,413)	1:28:A:VAL:H	1:35:A:GLU:HB3	4	0.4
(1,257)	1:17:A:VAL:HG21	1:53:A:ILE:HB	4	0.4
(1,257)	1:17:A:VAL:HG22	1:53:A:ILE:HB	4	0.4
(1,257)	1:17:A:VAL:HG23	1:53:A:ILE:HB	4	0.4
(1,257)	1:17:A:VAL:HG21	1:53:A:ILE:HB	6	0.4
(1,257)	1:17:A:VAL:HG22	1:53:A:ILE:HB	6	0.4
(1,257)	1:17:A:VAL:HG23	1:53:A:ILE:HB	6	0.4
(1,56)	1:6:A:LYS:HB3	1:6:A:LYS:HE2	4	0.4
(1,56)	1:6:A:LYS:HB3	1:6:A:LYS:HE3	4	0.4
(3,42)	1:37:A:ILE:H	1:69:A:LYS:O	5	0.39
(1,937)	1:76:A:ARG:HA	1:76:A:ARG:HD2	5	0.39
(1,937)	1:76:A:ARG:HA	1:76:A:ARG:HD3	5	0.39
(1,772)	1:62:A:SER:H	1:64:A:TYR:HB2	4	0.39
(1,772)	1:62:A:SER:H	1:64:A:TYR:HB2	4	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,772)	1:62:A:SER:H	1:64:A:TYR:HB3	4	0.39
(1,220)	1:15:A:GLY:HA2	1:56:A:ARG:HB2	4	0.39
(1,220)	1:15:A:GLY:HA2	1:56:A:ARG:HB3	4	0.39
(1,220)	1:15:A:GLY:HA3	1:56:A:ARG:HB2	4	0.39
(1,220)	1:15:A:GLY:HA3	1:56:A:ARG:HB3	4	0.39
(3,22)	1:21:A:LEU:O	1:25:A:GLU:H	5	0.38
(3,16)	1:16:A:ALA:H	1:29:A:LYS:O	2	0.38
(1,1038)	1:87:A:LYS:H	1:87:A:LYS:HE2	2	0.38
(1,1038)	1:87:A:LYS:H	1:87:A:LYS:HE3	2	0.38
(1,1016)	1:84:A:THR:H	1:85:A:ILE:HG12	6	0.38
(1,1016)	1:84:A:THR:H	1:85:A:ILE:HG13	6	0.38
(1,841)	1:69:A:LYS:HB2	1:69:A:LYS:HD2	2	0.38
(1,841)	1:69:A:LYS:HB2	1:69:A:LYS:HD3	2	0.38
(1,806)	1:64:A:TYR:HB2	1:68:A:ALA:HA	1	0.38
(1,691)	1:52:A:ILE:HG21	1:75:A:ARG:HG2	4	0.38
(1,691)	1:52:A:ILE:HG21	1:75:A:ARG:HG3	4	0.38
(1,691)	1:52:A:ILE:HG22	1:75:A:ARG:HG2	4	0.38
(1,691)	1:52:A:ILE:HG22	1:75:A:ARG:HG3	4	0.38
(1,691)	1:52:A:ILE:HG23	1:75:A:ARG:HG2	4	0.38
(1,691)	1:52:A:ILE:HG23	1:75:A:ARG:HG3	4	0.38
(1,438)	1:29:A:LYS:HD2	1:30:A:LEU:H	7	0.38
(1,438)	1:29:A:LYS:HD3	1:30:A:LEU:H	7	0.38
(1,406)	1:27:A:ARG:HG2	1:28:A:VAL:H	5	0.38
(1,405)	1:27:A:ARG:HB2	1:38:A:CYS:H	6	0.38
(1,405)	1:27:A:ARG:HB3	1:38:A:CYS:H	6	0.38
(1,337)	1:20:A:LEU:HD11	1:21:A:LEU:HB2	1	0.38
(1,337)	1:20:A:LEU:HD11	1:21:A:LEU:HB3	1	0.38
(1,337)	1:20:A:LEU:HD12	1:21:A:LEU:HB2	1	0.38
(1,337)	1:20:A:LEU:HD12	1:21:A:LEU:HB3	1	0.38
(1,337)	1:20:A:LEU:HD13	1:21:A:LEU:HB2	1	0.38
(1,337)	1:20:A:LEU:HD13	1:21:A:LEU:HB3	1	0.38
(1,337)	1:20:A:LEU:HD21	1:21:A:LEU:HB2	1	0.38
(1,337)	1:20:A:LEU:HD21	1:21:A:LEU:HB3	1	0.38
(1,337)	1:20:A:LEU:HD22	1:21:A:LEU:HB2	1	0.38
(1,337)	1:20:A:LEU:HD22	1:21:A:LEU:HB3	1	0.38
(1,337)	1:20:A:LEU:HD23	1:21:A:LEU:HB2	1	0.38
(1,337)	1:20:A:LEU:HD23	1:21:A:LEU:HB3	1	0.38
(1,332)	1:20:A:LEU:HD11	1:27:A:ARG:H	4	0.38
(1,332)	1:20:A:LEU:HD12	1:27:A:ARG:H	4	0.38
(1,332)	1:20:A:LEU:HD13	1:27:A:ARG:H	4	0.38
(1,282)	1:18:A:THR:HB	1:29:A:LYS:H	4	0.38
(1,246)	1:17:A:VAL:HA	1:27:A:ARG:HB3	4	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,206)	1:15:A:GLY:H	1:56:A:ARG:HA	7	0.38
(1,179)	1:13:A:VAL:H	1:60:A:GLU:HB2	9	0.38
(1,179)	1:13:A:VAL:H	1:60:A:GLU:HB3	9	0.38
(1,172)	1:12:A:GLU:HB2	1:61:A:MET:H	1	0.38
(1,172)	1:12:A:GLU:HB3	1:61:A:MET:H	1	0.38
(1,172)	1:12:A:GLU:HB2	1:61:A:MET:H	6	0.38
(1,172)	1:12:A:GLU:HB3	1:61:A:MET:H	6	0.38
(1,169)	1:12:A:GLU:HG3	1:61:A:MET:H	3	0.38
(1,121)	1:10:A:LEU:HB2	1:61:A:MET:HA	2	0.38
(1,121)	1:10:A:LEU:HB3	1:61:A:MET:HA	2	0.38
(1,85)	1:8:A:LYS:HD2	1:9:A:THR:H	2	0.38
(2,9)	1:17:A:VAL:H	1:56:A:ARG:HB3	10	0.37
(1,1006)	1:83:A:ARG:HD2	1:84:A:THR:H	1	0.37
(1,1006)	1:83:A:ARG:HD3	1:84:A:THR:H	1	0.37
(1,960)	1:77:A:LEU:HG	1:78:A:LYS:HE2	3	0.37
(1,960)	1:77:A:LEU:HG	1:78:A:LYS:HE3	3	0.37
(1,806)	1:64:A:TYR:HB2	1:68:A:ALA:HA	10	0.37
(1,561)	1:43:A:LYS:HG3	1:47:A:SER:HA	7	0.37
(1,540)	1:41:A:SER:H	1:72:A:ARG:H	4	0.37
(1,499)	1:38:A:CYS:HA	1:70:A:LYS:HD2	7	0.37
(1,499)	1:38:A:CYS:HA	1:70:A:LYS:HD3	7	0.37
(1,477)	1:36:A:ILE:HD11	1:37:A:ILE:H	3	0.37
(1,477)	1:36:A:ILE:HD12	1:37:A:ILE:H	3	0.37
(1,477)	1:36:A:ILE:HD13	1:37:A:ILE:H	3	0.37
(1,218)	1:15:A:GLY:HA2	1:29:A:LYS:HD2	7	0.37
(1,218)	1:15:A:GLY:HA2	1:29:A:LYS:HD3	7	0.37
(1,218)	1:15:A:GLY:HA3	1:29:A:LYS:HD2	7	0.37
(1,218)	1:15:A:GLY:HA3	1:29:A:LYS:HD3	7	0.37
(1,122)	1:10:A:LEU:HB2	1:61:A:MET:HB2	2	0.37
(1,122)	1:10:A:LEU:HB2	1:61:A:MET:HB3	2	0.37
(1,122)	1:10:A:LEU:HB3	1:61:A:MET:HB2	2	0.37
(1,122)	1:10:A:LEU:HB3	1:61:A:MET:HB3	2	0.37
(1,95)	1:9:A:THR:H	1:10:A:LEU:H	5	0.37
(1,76)	1:8:A:LYS:HA	1:8:A:LYS:HE2	4	0.37
(1,76)	1:8:A:LYS:HA	1:8:A:LYS:HE3	4	0.37
(1,17)	1:3:A:LYS:H	1:4:A:ASP:H	3	0.37
(3,54)	1:44:A:VAL:O	1:47:A:SER:H	2	0.36
(3,22)	1:21:A:LEU:O	1:25:A:GLU:H	2	0.36
(2,9)	1:17:A:VAL:H	1:56:A:ARG:HB3	9	0.36
(1,850)	1:69:A:LYS:HG2	1:70:A:LYS:H	8	0.36
(1,653)	1:50:A:ARG:HB2	1:52:A:ILE:HD11	3	0.36
(1,653)	1:50:A:ARG:HB2	1:52:A:ILE:HD12	3	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,653)	1:50:A:ARG:HB2	1:52:A:ILE:HD13	3	0.36
(1,604)	1:47:A:SER:HA	1:49:A:ILE:H	10	0.36
(1,408)	1:27:A:ARG:HG3	1:28:A:VAL:H	2	0.36
(1,337)	1:20:A:LEU:HD11	1:21:A:LEU:HB2	5	0.36
(1,337)	1:20:A:LEU:HD11	1:21:A:LEU:HB3	5	0.36
(1,337)	1:20:A:LEU:HD12	1:21:A:LEU:HB2	5	0.36
(1,337)	1:20:A:LEU:HD12	1:21:A:LEU:HB3	5	0.36
(1,337)	1:20:A:LEU:HD13	1:21:A:LEU:HB2	5	0.36
(1,337)	1:20:A:LEU:HD13	1:21:A:LEU:HB3	5	0.36
(1,337)	1:20:A:LEU:HD21	1:21:A:LEU:HB2	5	0.36
(1,337)	1:20:A:LEU:HD21	1:21:A:LEU:HB3	5	0.36
(1,337)	1:20:A:LEU:HD22	1:21:A:LEU:HB2	5	0.36
(1,337)	1:20:A:LEU:HD22	1:21:A:LEU:HB3	5	0.36
(1,337)	1:20:A:LEU:HD23	1:21:A:LEU:HB2	5	0.36
(1,337)	1:20:A:LEU:HD23	1:21:A:LEU:HB3	5	0.36
(1,266)	1:17:A:VAL:HG11	1:53:A:ILE:HB	2	0.36
(1,266)	1:17:A:VAL:HG12	1:53:A:ILE:HB	2	0.36
(1,266)	1:17:A:VAL:HG13	1:53:A:ILE:HB	2	0.36
(1,266)	1:17:A:VAL:HG21	1:53:A:ILE:HB	2	0.36
(1,266)	1:17:A:VAL:HG22	1:53:A:ILE:HB	2	0.36
(1,266)	1:17:A:VAL:HG23	1:53:A:ILE:HB	2	0.36
(1,206)	1:15:A:GLY:H	1:56:A:ARG:HA	2	0.36
(1,206)	1:15:A:GLY:H	1:56:A:ARG:HA	5	0.36
(1,172)	1:12:A:GLU:HB2	1:61:A:MET:H	4	0.36
(1,172)	1:12:A:GLU:HB3	1:61:A:MET:H	4	0.36
(1,122)	1:10:A:LEU:HB2	1:61:A:MET:HB2	10	0.36
(1,122)	1:10:A:LEU:HB2	1:61:A:MET:HB3	10	0.36
(1,122)	1:10:A:LEU:HB3	1:61:A:MET:HB2	10	0.36
(1,122)	1:10:A:LEU:HB3	1:61:A:MET:HB3	10	0.36
(1,85)	1:8:A:LYS:HD2	1:9:A:THR:H	8	0.36
(1,66)	1:6:A:LYS:HG3	1:7:A:SER:H	6	0.36
(3,34)	1:28:A:VAL:H	1:36:A:ILE:O	2	0.35
(1,1006)	1:83:A:ARG:HD2	1:84:A:THR:H	8	0.35
(1,1006)	1:83:A:ARG:HD3	1:84:A:THR:H	8	0.35
(1,989)	1:82:A:ASP:HA	1:85:A:ILE:HG21	4	0.35
(1,989)	1:82:A:ASP:HA	1:85:A:ILE:HG22	4	0.35
(1,989)	1:82:A:ASP:HA	1:85:A:ILE:HG23	4	0.35
(1,586)	1:45:A:ARG:HD2	1:46:A:ARG:H	10	0.35
(1,586)	1:45:A:ARG:HD3	1:46:A:ARG:H	10	0.35
(1,527)	1:40:A:VAL:HG21	1:45:A:ARG:H	4	0.35
(1,527)	1:40:A:VAL:HG22	1:45:A:ARG:H	4	0.35
(1,527)	1:40:A:VAL:HG23	1:45:A:ARG:H	4	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,504)	1:39:A:HIS:H	1:71:A:GLY:HA2	10	0.35
(1,504)	1:39:A:HIS:H	1:71:A:GLY:HA3	10	0.35
(1,413)	1:28:A:VAL:H	1:35:A:GLU:HB2	3	0.35
(1,413)	1:28:A:VAL:H	1:35:A:GLU:HB3	3	0.35
(1,407)	1:27:A:ARG:HG2	1:38:A:CYS:HA	2	0.35
(1,406)	1:27:A:ARG:HG2	1:28:A:VAL:H	4	0.35
(1,338)	1:20:A:LEU:HD11	1:26:A:PHE:HB2	5	0.35
(1,338)	1:20:A:LEU:HD11	1:26:A:PHE:HB3	5	0.35
(1,338)	1:20:A:LEU:HD12	1:26:A:PHE:HB2	5	0.35
(1,338)	1:20:A:LEU:HD12	1:26:A:PHE:HB3	5	0.35
(1,338)	1:20:A:LEU:HD13	1:26:A:PHE:HB2	5	0.35
(1,338)	1:20:A:LEU:HD13	1:26:A:PHE:HB3	5	0.35
(1,338)	1:20:A:LEU:HD21	1:26:A:PHE:HB2	5	0.35
(1,338)	1:20:A:LEU:HD21	1:26:A:PHE:HB3	5	0.35
(1,338)	1:20:A:LEU:HD22	1:26:A:PHE:HB2	5	0.35
(1,338)	1:20:A:LEU:HD22	1:26:A:PHE:HB3	5	0.35
(1,338)	1:20:A:LEU:HD23	1:26:A:PHE:HB2	5	0.35
(1,338)	1:20:A:LEU:HD23	1:26:A:PHE:HB3	5	0.35
(1,246)	1:17:A:VAL:HA	1:27:A:ARG:HB3	8	0.35
(1,172)	1:12:A:GLU:HB2	1:61:A:MET:H	10	0.35
(1,172)	1:12:A:GLU:HB3	1:61:A:MET:H	10	0.35
(1,847)	1:69:A:LYS:HD2	1:70:A:LYS:H	6	0.34
(1,847)	1:69:A:LYS:HD3	1:70:A:LYS:H	6	0.34
(1,739)	1:58:A:LEU:HD11	1:60:A:GLU:HB2	4	0.34
(1,739)	1:58:A:LEU:HD11	1:60:A:GLU:HB3	4	0.34
(1,739)	1:58:A:LEU:HD12	1:60:A:GLU:HB2	4	0.34
(1,739)	1:58:A:LEU:HD12	1:60:A:GLU:HB3	4	0.34
(1,739)	1:58:A:LEU:HD13	1:60:A:GLU:HB2	4	0.34
(1,739)	1:58:A:LEU:HD13	1:60:A:GLU:HB3	4	0.34
(1,739)	1:58:A:LEU:HD21	1:60:A:GLU:HB2	4	0.34
(1,739)	1:58:A:LEU:HD21	1:60:A:GLU:HB3	4	0.34
(1,739)	1:58:A:LEU:HD22	1:60:A:GLU:HB2	4	0.34
(1,739)	1:58:A:LEU:HD22	1:60:A:GLU:HB3	4	0.34
(1,739)	1:58:A:LEU:HD23	1:60:A:GLU:HB2	4	0.34
(1,739)	1:58:A:LEU:HD23	1:60:A:GLU:HB3	4	0.34
(1,587)	1:45:A:ARG:HG2	1:46:A:ARG:H	3	0.34
(1,587)	1:45:A:ARG:HG3	1:46:A:ARG:H	3	0.34
(1,559)	1:43:A:LYS:HG2	1:47:A:SER:HA	2	0.34
(1,533)	1:40:A:VAL:HG11	1:45:A:ARG:H	4	0.34
(1,533)	1:40:A:VAL:HG12	1:45:A:ARG:H	4	0.34
(1,533)	1:40:A:VAL:HG13	1:45:A:ARG:H	4	0.34
(1,533)	1:40:A:VAL:HG21	1:45:A:ARG:H	4	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,533)	1:40:A:VAL:HG22	1:45:A:ARG:H	4	0.34
(1,533)	1:40:A:VAL:HG23	1:45:A:ARG:H	4	0.34
(1,408)	1:27:A:ARG:HG3	1:28:A:VAL:H	8	0.34
(1,338)	1:20:A:LEU:HD11	1:26:A:PHE:HB2	10	0.34
(1,338)	1:20:A:LEU:HD11	1:26:A:PHE:HB3	10	0.34
(1,338)	1:20:A:LEU:HD12	1:26:A:PHE:HB2	10	0.34
(1,338)	1:20:A:LEU:HD12	1:26:A:PHE:HB3	10	0.34
(1,338)	1:20:A:LEU:HD13	1:26:A:PHE:HB2	10	0.34
(1,338)	1:20:A:LEU:HD13	1:26:A:PHE:HB3	10	0.34
(1,338)	1:20:A:LEU:HD21	1:26:A:PHE:HB2	10	0.34
(1,338)	1:20:A:LEU:HD21	1:26:A:PHE:HB3	10	0.34
(1,338)	1:20:A:LEU:HD22	1:26:A:PHE:HB2	10	0.34
(1,338)	1:20:A:LEU:HD22	1:26:A:PHE:HB3	10	0.34
(1,338)	1:20:A:LEU:HD23	1:26:A:PHE:HB2	10	0.34
(1,338)	1:20:A:LEU:HD23	1:26:A:PHE:HB3	10	0.34
(1,336)	1:20:A:LEU:HD21	1:27:A:ARG:H	1	0.34
(1,336)	1:20:A:LEU:HD22	1:27:A:ARG:H	1	0.34
(1,336)	1:20:A:LEU:HD23	1:27:A:ARG:H	1	0.34
(1,327)	1:20:A:LEU:HG	1:21:A:LEU:HB2	2	0.34
(1,327)	1:20:A:LEU:HG	1:21:A:LEU:HB3	2	0.34
(1,286)	1:18:A:THR:HG21	1:28:A:VAL:HA	4	0.34
(1,286)	1:18:A:THR:HG22	1:28:A:VAL:HA	4	0.34
(1,286)	1:18:A:THR:HG23	1:28:A:VAL:HA	4	0.34
(1,283)	1:18:A:THR:HB	1:53:A:ILE:HG21	4	0.34
(1,283)	1:18:A:THR:HB	1:53:A:ILE:HG22	4	0.34
(1,283)	1:18:A:THR:HB	1:53:A:ILE:HG23	4	0.34
(3,55)	1:44:A:VAL:O	1:47:A:SER:N	8	0.33
(3,52)	1:43:A:LYS:O	1:46:A:ARG:H	5	0.33
(3,36)	1:30:A:LEU:O	1:34:A:HIS:H	7	0.33
(3,17)	1:16:A:ALA:N	1:29:A:LYS:O	3	0.33
(1,1006)	1:83:A:ARG:HD2	1:84:A:THR:H	4	0.33
(1,1006)	1:83:A:ARG:HD3	1:84:A:THR:H	4	0.33
(1,740)	1:58:A:LEU:HD11	1:60:A:GLU:HG2	2	0.33
(1,740)	1:58:A:LEU:HD11	1:60:A:GLU:HG3	2	0.33
(1,740)	1:58:A:LEU:HD12	1:60:A:GLU:HG2	2	0.33
(1,740)	1:58:A:LEU:HD12	1:60:A:GLU:HG3	2	0.33
(1,740)	1:58:A:LEU:HD13	1:60:A:GLU:HG2	2	0.33
(1,740)	1:58:A:LEU:HD13	1:60:A:GLU:HG3	2	0.33
(1,740)	1:58:A:LEU:HD21	1:60:A:GLU:HG2	2	0.33
(1,740)	1:58:A:LEU:HD21	1:60:A:GLU:HG3	2	0.33
(1,740)	1:58:A:LEU:HD22	1:60:A:GLU:HG2	2	0.33
(1,740)	1:58:A:LEU:HD22	1:60:A:GLU:HG3	2	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,740)	1:58:A:LEU:HD23	1:60:A:GLU:HG2	2	0.33
(1,740)	1:58:A:LEU:HD23	1:60:A:GLU:HG3	2	0.33
(1,690)	1:52:A:ILE:HG21	1:75:A:ARG:HB2	4	0.33
(1,690)	1:52:A:ILE:HG22	1:75:A:ARG:HB2	4	0.33
(1,690)	1:52:A:ILE:HG23	1:75:A:ARG:HB2	4	0.33
(1,638)	1:49:A:ILE:HD11	1:75:A:ARG:HD2	6	0.33
(1,638)	1:49:A:ILE:HD12	1:75:A:ARG:HD2	6	0.33
(1,638)	1:49:A:ILE:HD13	1:75:A:ARG:HD2	6	0.33
(1,638)	1:49:A:ILE:HD11	1:75:A:ARG:HD3	6	0.33
(1,638)	1:49:A:ILE:HD12	1:75:A:ARG:HD3	6	0.33
(1,638)	1:49:A:ILE:HD13	1:75:A:ARG:HD3	6	0.33
(1,477)	1:36:A:ILE:HD11	1:37:A:ILE:H	8	0.33
(1,477)	1:36:A:ILE:HD12	1:37:A:ILE:H	8	0.33
(1,477)	1:36:A:ILE:HD13	1:37:A:ILE:H	8	0.33
(1,360)	1:23:A:ALA:HA	1:25:A:GLU:HB2	6	0.33
(1,360)	1:23:A:ALA:HA	1:25:A:GLU:HB3	6	0.33
(1,338)	1:20:A:LEU:HD11	1:26:A:PHE:HB2	7	0.33
(1,338)	1:20:A:LEU:HD11	1:26:A:PHE:HB3	7	0.33
(1,338)	1:20:A:LEU:HD12	1:26:A:PHE:HB2	7	0.33
(1,338)	1:20:A:LEU:HD12	1:26:A:PHE:HB3	7	0.33
(1,338)	1:20:A:LEU:HD13	1:26:A:PHE:HB2	7	0.33
(1,338)	1:20:A:LEU:HD13	1:26:A:PHE:HB3	7	0.33
(1,338)	1:20:A:LEU:HD21	1:26:A:PHE:HB2	7	0.33
(1,338)	1:20:A:LEU:HD21	1:26:A:PHE:HB3	7	0.33
(1,338)	1:20:A:LEU:HD22	1:26:A:PHE:HB2	7	0.33
(1,338)	1:20:A:LEU:HD22	1:26:A:PHE:HB3	7	0.33
(1,338)	1:20:A:LEU:HD23	1:26:A:PHE:HB2	7	0.33
(1,338)	1:20:A:LEU:HD23	1:26:A:PHE:HB3	7	0.33
(1,337)	1:20:A:LEU:HD11	1:21:A:LEU:HB2	2	0.33
(1,337)	1:20:A:LEU:HD11	1:21:A:LEU:HB3	2	0.33
(1,337)	1:20:A:LEU:HD12	1:21:A:LEU:HB2	2	0.33
(1,337)	1:20:A:LEU:HD12	1:21:A:LEU:HB3	2	0.33
(1,337)	1:20:A:LEU:HD13	1:21:A:LEU:HB2	2	0.33
(1,337)	1:20:A:LEU:HD13	1:21:A:LEU:HB3	2	0.33
(1,337)	1:20:A:LEU:HD21	1:21:A:LEU:HB2	2	0.33
(1,337)	1:20:A:LEU:HD21	1:21:A:LEU:HB3	2	0.33
(1,337)	1:20:A:LEU:HD22	1:21:A:LEU:HB2	2	0.33
(1,337)	1:20:A:LEU:HD22	1:21:A:LEU:HB3	2	0.33
(1,337)	1:20:A:LEU:HD23	1:21:A:LEU:HB2	2	0.33
(1,337)	1:20:A:LEU:HD23	1:21:A:LEU:HB3	2	0.33
(1,332)	1:20:A:LEU:HD11	1:27:A:ARG:H	5	0.33
(1,332)	1:20:A:LEU:HD12	1:27:A:ARG:H	5	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,332)	1:20:A:LEU:HD13	1:27:A:ARG:H	5	0.33
(1,332)	1:20:A:LEU:HD11	1:27:A:ARG:H	7	0.33
(1,332)	1:20:A:LEU:HD12	1:27:A:ARG:H	7	0.33
(1,332)	1:20:A:LEU:HD13	1:27:A:ARG:H	7	0.33
(1,122)	1:10:A:LEU:HB2	1:61:A:MET:HB2	9	0.33
(1,122)	1:10:A:LEU:HB2	1:61:A:MET:HB3	9	0.33
(1,122)	1:10:A:LEU:HB3	1:61:A:MET:HB2	9	0.33
(1,122)	1:10:A:LEU:HB3	1:61:A:MET:HB3	9	0.33
(1,35)	1:5:A:GLU:H	1:5:A:GLU:HB2	2	0.33
(1,35)	1:5:A:GLU:H	1:5:A:GLU:HB3	2	0.33
(1,35)	1:5:A:GLU:H	1:5:A:GLU:HB2	9	0.33
(1,35)	1:5:A:GLU:H	1:5:A:GLU:HB3	9	0.33
(3,37)	1:30:A:LEU:O	1:34:A:HIS:N	10	0.32
(2,2)	1:11:A:PHE:H	1:61:A:MET:HB3	2	0.32
(1,739)	1:58:A:LEU:HD11	1:60:A:GLU:HB2	3	0.32
(1,739)	1:58:A:LEU:HD11	1:60:A:GLU:HB3	3	0.32
(1,739)	1:58:A:LEU:HD12	1:60:A:GLU:HB2	3	0.32
(1,739)	1:58:A:LEU:HD12	1:60:A:GLU:HB3	3	0.32
(1,739)	1:58:A:LEU:HD13	1:60:A:GLU:HB2	3	0.32
(1,739)	1:58:A:LEU:HD13	1:60:A:GLU:HB3	3	0.32
(1,739)	1:58:A:LEU:HD21	1:60:A:GLU:HB2	3	0.32
(1,739)	1:58:A:LEU:HD21	1:60:A:GLU:HB3	3	0.32
(1,739)	1:58:A:LEU:HD22	1:60:A:GLU:HB2	3	0.32
(1,739)	1:58:A:LEU:HD22	1:60:A:GLU:HB3	3	0.32
(1,739)	1:58:A:LEU:HD23	1:60:A:GLU:HB2	3	0.32
(1,739)	1:58:A:LEU:HD23	1:60:A:GLU:HB3	3	0.32
(1,735)	1:58:A:LEU:HG	1:73:A:ILE:HA	5	0.32
(1,719)	1:56:A:ARG:HB3	1:57:A:VAL:H	3	0.32
(1,691)	1:52:A:ILE:HG21	1:75:A:ARG:HG2	10	0.32
(1,691)	1:52:A:ILE:HG21	1:75:A:ARG:HG3	10	0.32
(1,691)	1:52:A:ILE:HG22	1:75:A:ARG:HG2	10	0.32
(1,691)	1:52:A:ILE:HG22	1:75:A:ARG:HG3	10	0.32
(1,691)	1:52:A:ILE:HG23	1:75:A:ARG:HG2	10	0.32
(1,691)	1:52:A:ILE:HG23	1:75:A:ARG:HG3	10	0.32
(1,530)	1:40:A:VAL:HG11	1:44:A:VAL:HA	7	0.32
(1,530)	1:40:A:VAL:HG12	1:44:A:VAL:HA	7	0.32
(1,530)	1:40:A:VAL:HG13	1:44:A:VAL:HA	7	0.32
(1,530)	1:40:A:VAL:HG21	1:44:A:VAL:HA	7	0.32
(1,530)	1:40:A:VAL:HG22	1:44:A:VAL:HA	7	0.32
(1,530)	1:40:A:VAL:HG23	1:44:A:VAL:HA	7	0.32
(1,485)	1:37:A:ILE:H	1:70:A:LYS:H	3	0.32
(1,312)	1:20:A:LEU:HA	1:25:A:GLU:H	9	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,311)	1:20:A:LEU:HA	1:21:A:LEU:HB2	5	0.32
(1,311)	1:20:A:LEU:HA	1:21:A:LEU:HB3	5	0.32
(1,311)	1:20:A:LEU:HA	1:21:A:LEU:HB2	10	0.32
(1,311)	1:20:A:LEU:HA	1:21:A:LEU:HB3	10	0.32
(1,226)	1:16:A:ALA:H	1:30:A:LEU:HA	2	0.32
(1,203)	1:14:A:GLU:HB2	1:58:A:LEU:HD11	4	0.32
(1,203)	1:14:A:GLU:HB2	1:58:A:LEU:HD12	4	0.32
(1,203)	1:14:A:GLU:HB2	1:58:A:LEU:HD13	4	0.32
(1,203)	1:14:A:GLU:HB2	1:58:A:LEU:HD21	4	0.32
(1,203)	1:14:A:GLU:HB2	1:58:A:LEU:HD22	4	0.32
(1,203)	1:14:A:GLU:HB2	1:58:A:LEU:HD23	4	0.32
(1,203)	1:14:A:GLU:HB3	1:58:A:LEU:HD11	4	0.32
(1,203)	1:14:A:GLU:HB3	1:58:A:LEU:HD12	4	0.32
(1,203)	1:14:A:GLU:HB3	1:58:A:LEU:HD13	4	0.32
(1,203)	1:14:A:GLU:HB3	1:58:A:LEU:HD21	4	0.32
(1,203)	1:14:A:GLU:HB3	1:58:A:LEU:HD22	4	0.32
(1,203)	1:14:A:GLU:HB3	1:58:A:LEU:HD23	4	0.32
(1,74)	1:8:A:LYS:H	1:9:A:THR:H	7	0.32
(1,17)	1:3:A:LYS:H	1:4:A:ASP:H	7	0.32
(3,43)	1:37:A:ILE:N	1:69:A:LYS:O	1	0.31
(1,1019)	1:84:A:THR:HB	1:85:A:ILE:H	5	0.31
(1,990)	1:82:A:ASP:HB2	1:85:A:ILE:HD11	3	0.31
(1,990)	1:82:A:ASP:HB2	1:85:A:ILE:HD12	3	0.31
(1,990)	1:82:A:ASP:HB2	1:85:A:ILE:HD13	3	0.31
(1,990)	1:82:A:ASP:HB3	1:85:A:ILE:HD11	3	0.31
(1,990)	1:82:A:ASP:HB3	1:85:A:ILE:HD12	3	0.31
(1,990)	1:82:A:ASP:HB3	1:85:A:ILE:HD13	3	0.31
(1,735)	1:58:A:LEU:HG	1:73:A:ILE:HA	1	0.31
(1,659)	1:50:A:ARG:HB2	1:52:A:ILE:HG12	6	0.31
(1,659)	1:50:A:ARG:HB2	1:52:A:ILE:HG13	6	0.31
(1,659)	1:50:A:ARG:HB3	1:52:A:ILE:HG12	6	0.31
(1,659)	1:50:A:ARG:HB3	1:52:A:ILE:HG13	6	0.31
(1,638)	1:49:A:ILE:HD11	1:75:A:ARG:HD2	7	0.31
(1,638)	1:49:A:ILE:HD12	1:75:A:ARG:HD2	7	0.31
(1,638)	1:49:A:ILE:HD13	1:75:A:ARG:HD2	7	0.31
(1,638)	1:49:A:ILE:HD11	1:75:A:ARG:HD3	7	0.31
(1,638)	1:49:A:ILE:HD12	1:75:A:ARG:HD3	7	0.31
(1,638)	1:49:A:ILE:HD13	1:75:A:ARG:HD3	7	0.31
(1,574)	1:44:A:VAL:HG11	1:51:A:ILE:HG21	1	0.31
(1,574)	1:44:A:VAL:HG11	1:51:A:ILE:HG22	1	0.31
(1,574)	1:44:A:VAL:HG11	1:51:A:ILE:HG23	1	0.31
(1,574)	1:44:A:VAL:HG12	1:51:A:ILE:HG21	1	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,574)	1:44:A:VAL:HG12	1:51:A:ILE:HG22	1	0.31
(1,574)	1:44:A:VAL:HG12	1:51:A:ILE:HG23	1	0.31
(1,574)	1:44:A:VAL:HG13	1:51:A:ILE:HG21	1	0.31
(1,574)	1:44:A:VAL:HG13	1:51:A:ILE:HG22	1	0.31
(1,574)	1:44:A:VAL:HG13	1:51:A:ILE:HG23	1	0.31
(1,574)	1:44:A:VAL:HG21	1:51:A:ILE:HG21	1	0.31
(1,574)	1:44:A:VAL:HG21	1:51:A:ILE:HG22	1	0.31
(1,574)	1:44:A:VAL:HG21	1:51:A:ILE:HG23	1	0.31
(1,574)	1:44:A:VAL:HG22	1:51:A:ILE:HG21	1	0.31
(1,574)	1:44:A:VAL:HG22	1:51:A:ILE:HG22	1	0.31
(1,574)	1:44:A:VAL:HG22	1:51:A:ILE:HG23	1	0.31
(1,574)	1:44:A:VAL:HG23	1:51:A:ILE:HG21	1	0.31
(1,574)	1:44:A:VAL:HG23	1:51:A:ILE:HG22	1	0.31
(1,574)	1:44:A:VAL:HG23	1:51:A:ILE:HG23	1	0.31
(1,409)	1:27:A:ARG:HG2	1:38:A:CYS:HB2	10	0.31
(1,409)	1:27:A:ARG:HG2	1:38:A:CYS:HB3	10	0.31
(1,409)	1:27:A:ARG:HG3	1:38:A:CYS:HB2	10	0.31
(1,409)	1:27:A:ARG:HG3	1:38:A:CYS:HB3	10	0.31
(1,405)	1:27:A:ARG:HB2	1:38:A:CYS:H	9	0.31
(1,405)	1:27:A:ARG:HB3	1:38:A:CYS:H	9	0.31
(1,311)	1:20:A:LEU:HA	1:21:A:LEU:HB2	2	0.31
(1,311)	1:20:A:LEU:HA	1:21:A:LEU:HB3	2	0.31
(1,311)	1:20:A:LEU:HA	1:21:A:LEU:HB2	7	0.31
(1,311)	1:20:A:LEU:HA	1:21:A:LEU:HB3	7	0.31
(1,299)	1:19:A:ALA:HA	1:53:A:ILE:HA	7	0.31
(1,266)	1:17:A:VAL:HG11	1:53:A:ILE:HB	5	0.31
(1,266)	1:17:A:VAL:HG12	1:53:A:ILE:HB	5	0.31
(1,266)	1:17:A:VAL:HG13	1:53:A:ILE:HB	5	0.31
(1,266)	1:17:A:VAL:HG21	1:53:A:ILE:HB	5	0.31
(1,266)	1:17:A:VAL:HG22	1:53:A:ILE:HB	5	0.31
(1,266)	1:17:A:VAL:HG23	1:53:A:ILE:HB	5	0.31
(1,188)	1:13:A:VAL:HG11	1:30:A:LEU:HA	7	0.31
(1,188)	1:13:A:VAL:HG12	1:30:A:LEU:HA	7	0.31
(1,188)	1:13:A:VAL:HG13	1:30:A:LEU:HA	7	0.31
(1,188)	1:13:A:VAL:HG21	1:30:A:LEU:HA	7	0.31
(1,188)	1:13:A:VAL:HG22	1:30:A:LEU:HA	7	0.31
(1,188)	1:13:A:VAL:HG23	1:30:A:LEU:HA	7	0.31
(1,169)	1:12:A:GLU:HG3	1:61:A:MET:H	10	0.31
(1,118)	1:10:A:LEU:HG	1:61:A:MET:HG2	8	0.31
(1,118)	1:10:A:LEU:HG	1:61:A:MET:HG3	8	0.31
(1,1005)	1:83:A:ARG:HB3	1:84:A:THR:H	5	0.3
(1,972)	1:78:A:LYS:HA	1:78:A:LYS:HD2	4	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,972)	1:78:A:LYS:HA	1:78:A:LYS:HD3	4	0.3
(1,926)	1:75:A:ARG:HB2	1:76:A:ARG:H	4	0.3
(1,713)	1:56:A:ARG:H	1:76:A:ARG:H	5	0.3
(1,713)	1:56:A:ARG:H	1:76:A:ARG:H	9	0.3
(1,611)	1:48:A:LYS:HA	1:48:A:LYS:HE2	8	0.3
(1,611)	1:48:A:LYS:HA	1:48:A:LYS:HE3	8	0.3
(1,574)	1:44:A:VAL:HG11	1:51:A:ILE:HG21	5	0.3
(1,574)	1:44:A:VAL:HG11	1:51:A:ILE:HG22	5	0.3
(1,574)	1:44:A:VAL:HG11	1:51:A:ILE:HG23	5	0.3
(1,574)	1:44:A:VAL:HG12	1:51:A:ILE:HG21	5	0.3
(1,574)	1:44:A:VAL:HG12	1:51:A:ILE:HG22	5	0.3
(1,574)	1:44:A:VAL:HG12	1:51:A:ILE:HG23	5	0.3
(1,574)	1:44:A:VAL:HG13	1:51:A:ILE:HG21	5	0.3
(1,574)	1:44:A:VAL:HG13	1:51:A:ILE:HG22	5	0.3
(1,574)	1:44:A:VAL:HG13	1:51:A:ILE:HG23	5	0.3
(1,574)	1:44:A:VAL:HG21	1:51:A:ILE:HG21	5	0.3
(1,574)	1:44:A:VAL:HG21	1:51:A:ILE:HG22	5	0.3
(1,574)	1:44:A:VAL:HG21	1:51:A:ILE:HG23	5	0.3
(1,574)	1:44:A:VAL:HG22	1:51:A:ILE:HG21	5	0.3
(1,574)	1:44:A:VAL:HG22	1:51:A:ILE:HG22	5	0.3
(1,574)	1:44:A:VAL:HG22	1:51:A:ILE:HG23	5	0.3
(1,574)	1:44:A:VAL:HG23	1:51:A:ILE:HG21	5	0.3
(1,574)	1:44:A:VAL:HG23	1:51:A:ILE:HG22	5	0.3
(1,574)	1:44:A:VAL:HG23	1:51:A:ILE:HG23	5	0.3
(1,566)	1:44:A:VAL:H	1:47:A:SER:H	4	0.3
(1,419)	1:28:A:VAL:HB	1:29:A:LYS:H	7	0.3
(1,346)	1:21:A:LEU:HA	1:23:A:ALA:H	9	0.3
(1,312)	1:20:A:LEU:HA	1:25:A:GLU:H	2	0.3
(1,311)	1:20:A:LEU:HA	1:21:A:LEU:HB2	9	0.3
(1,311)	1:20:A:LEU:HA	1:21:A:LEU:HB3	9	0.3
(1,292)	1:18:A:THR:HG21	1:53:A:ILE:HG21	1	0.3
(1,292)	1:18:A:THR:HG21	1:53:A:ILE:HG22	1	0.3
(1,292)	1:18:A:THR:HG21	1:53:A:ILE:HG23	1	0.3
(1,292)	1:18:A:THR:HG22	1:53:A:ILE:HG21	1	0.3
(1,292)	1:18:A:THR:HG22	1:53:A:ILE:HG22	1	0.3
(1,292)	1:18:A:THR:HG22	1:53:A:ILE:HG23	1	0.3
(1,292)	1:18:A:THR:HG23	1:53:A:ILE:HG21	1	0.3
(1,292)	1:18:A:THR:HG23	1:53:A:ILE:HG22	1	0.3
(1,292)	1:18:A:THR:HG23	1:53:A:ILE:HG23	1	0.3
(1,246)	1:17:A:VAL:HA	1:27:A:ARG:HB3	6	0.3
(1,179)	1:13:A:VAL:H	1:60:A:GLU:HB2	6	0.3
(1,179)	1:13:A:VAL:H	1:60:A:GLU:HB3	6	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,154)	1:12:A:GLU:H	1:13:A:VAL:H	2	0.3
(1,87)	1:8:A:LYS:HD3	1:9:A:THR:H	4	0.3
(1,87)	1:8:A:LYS:HD3	1:9:A:THR:H	6	0.3
(1,1019)	1:84:A:THR:HB	1:85:A:ILE:H	6	0.29
(1,871)	1:70:A:LYS:HG2	1:71:A:GLY:H	8	0.29
(1,637)	1:49:A:ILE:HD11	1:74:A:ILE:HG12	6	0.29
(1,637)	1:49:A:ILE:HD12	1:74:A:ILE:HG12	6	0.29
(1,637)	1:49:A:ILE:HD13	1:74:A:ILE:HG12	6	0.29
(1,637)	1:49:A:ILE:HD11	1:74:A:ILE:HG13	6	0.29
(1,637)	1:49:A:ILE:HD12	1:74:A:ILE:HG13	6	0.29
(1,637)	1:49:A:ILE:HD13	1:74:A:ILE:HG13	6	0.29
(1,485)	1:37:A:ILE:H	1:70:A:LYS:H	5	0.29
(1,409)	1:27:A:ARG:HG2	1:38:A:CYS:HB2	2	0.29
(1,409)	1:27:A:ARG:HG2	1:38:A:CYS:HB3	2	0.29
(1,409)	1:27:A:ARG:HG3	1:38:A:CYS:HB2	2	0.29
(1,409)	1:27:A:ARG:HG3	1:38:A:CYS:HB3	2	0.29
(1,408)	1:27:A:ARG:HG3	1:28:A:VAL:H	5	0.29
(1,266)	1:17:A:VAL:HG11	1:53:A:ILE:HB	7	0.29
(1,266)	1:17:A:VAL:HG12	1:53:A:ILE:HB	7	0.29
(1,266)	1:17:A:VAL:HG13	1:53:A:ILE:HB	7	0.29
(1,266)	1:17:A:VAL:HG21	1:53:A:ILE:HB	7	0.29
(1,266)	1:17:A:VAL:HG22	1:53:A:ILE:HB	7	0.29
(1,266)	1:17:A:VAL:HG23	1:53:A:ILE:HB	7	0.29
(1,250)	1:17:A:VAL:HB	1:53:A:ILE:HA	7	0.29
(1,18)	1:3:A:LYS:HA	1:3:A:LYS:HD2	5	0.29
(1,18)	1:3:A:LYS:HA	1:3:A:LYS:HD3	5	0.29
(3,36)	1:30:A:LEU:O	1:34:A:HIS:H	5	0.28
(2,20)	1:49:A:ILE:HA	1:74:A:ILE:HG12	7	0.28
(1,847)	1:69:A:LYS:HD2	1:70:A:LYS:H	3	0.28
(1,847)	1:69:A:LYS:HD3	1:70:A:LYS:H	3	0.28
(1,810)	1:64:A:TYR:HB3	1:66:A:ARG:H	10	0.28
(1,756)	1:60:A:GLU:H	1:73:A:ILE:HG21	8	0.28
(1,756)	1:60:A:GLU:H	1:73:A:ILE:HG22	8	0.28
(1,756)	1:60:A:GLU:H	1:73:A:ILE:HG23	8	0.28
(1,544)	1:41:A:SER:HB2	1:72:A:ARG:HD2	6	0.28
(1,544)	1:41:A:SER:HB2	1:72:A:ARG:HD3	6	0.28
(1,544)	1:41:A:SER:HB3	1:72:A:ARG:HD2	6	0.28
(1,544)	1:41:A:SER:HB3	1:72:A:ARG:HD3	6	0.28
(1,517)	1:40:A:VAL:HA	1:72:A:ARG:HA	3	0.28
(1,419)	1:28:A:VAL:HB	1:29:A:LYS:H	2	0.28
(1,409)	1:27:A:ARG:HG2	1:38:A:CYS:HB2	3	0.28
(1,409)	1:27:A:ARG:HG2	1:38:A:CYS:HB3	3	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,409)	1:27:A:ARG:HG3	1:38:A:CYS:HB2	3	0.28
(1,409)	1:27:A:ARG:HG3	1:38:A:CYS:HB3	3	0.28
(1,335)	1:20:A:LEU:HD21	1:26:A:PHE:HA	1	0.28
(1,335)	1:20:A:LEU:HD22	1:26:A:PHE:HA	1	0.28
(1,335)	1:20:A:LEU:HD23	1:26:A:PHE:HA	1	0.28
(1,291)	1:18:A:THR:HG21	1:53:A:ILE:HD11	6	0.28
(1,291)	1:18:A:THR:HG21	1:53:A:ILE:HD12	6	0.28
(1,291)	1:18:A:THR:HG21	1:53:A:ILE:HD13	6	0.28
(1,291)	1:18:A:THR:HG22	1:53:A:ILE:HD11	6	0.28
(1,291)	1:18:A:THR:HG22	1:53:A:ILE:HD12	6	0.28
(1,291)	1:18:A:THR:HG22	1:53:A:ILE:HD13	6	0.28
(1,291)	1:18:A:THR:HG23	1:53:A:ILE:HD11	6	0.28
(1,291)	1:18:A:THR:HG23	1:53:A:ILE:HD12	6	0.28
(1,291)	1:18:A:THR:HG23	1:53:A:ILE:HD13	6	0.28
(1,266)	1:17:A:VAL:HG11	1:53:A:ILE:HB	6	0.28
(1,266)	1:17:A:VAL:HG12	1:53:A:ILE:HB	6	0.28
(1,266)	1:17:A:VAL:HG13	1:53:A:ILE:HB	6	0.28
(1,266)	1:17:A:VAL:HG21	1:53:A:ILE:HB	6	0.28
(1,266)	1:17:A:VAL:HG22	1:53:A:ILE:HB	6	0.28
(1,266)	1:17:A:VAL:HG23	1:53:A:ILE:HB	6	0.28
(1,206)	1:15:A:GLY:H	1:56:A:ARG:HA	6	0.28
(1,188)	1:13:A:VAL:HG11	1:30:A:LEU:HA	3	0.28
(1,188)	1:13:A:VAL:HG12	1:30:A:LEU:HA	3	0.28
(1,188)	1:13:A:VAL:HG13	1:30:A:LEU:HA	3	0.28
(1,188)	1:13:A:VAL:HG21	1:30:A:LEU:HA	3	0.28
(1,188)	1:13:A:VAL:HG22	1:30:A:LEU:HA	3	0.28
(1,188)	1:13:A:VAL:HG23	1:30:A:LEU:HA	3	0.28
(1,167)	1:12:A:GLU:HG2	1:61:A:MET:H	4	0.28
(1,155)	1:12:A:GLU:H	1:13:A:VAL:HG11	2	0.28
(1,155)	1:12:A:GLU:H	1:13:A:VAL:HG12	2	0.28
(1,155)	1:12:A:GLU:H	1:13:A:VAL:HG13	2	0.28
(1,155)	1:12:A:GLU:H	1:13:A:VAL:HG21	2	0.28
(1,155)	1:12:A:GLU:H	1:13:A:VAL:HG22	2	0.28
(1,155)	1:12:A:GLU:H	1:13:A:VAL:HG23	2	0.28
(1,87)	1:8:A:LYS:HD3	1:9:A:THR:H	1	0.28
(1,68)	1:7:A:SER:H	1:8:A:LYS:H	7	0.28
(1,30)	1:3:A:LYS:HG3	1:4:A:ASP:H	1	0.28
(3,17)	1:16:A:ALA:N	1:29:A:LYS:O	2	0.27
(3,17)	1:16:A:ALA:N	1:29:A:LYS:O	8	0.27
(1,1021)	1:84:A:THR:HG21	1:85:A:ILE:HA	5	0.27
(1,1021)	1:84:A:THR:HG22	1:85:A:ILE:HA	5	0.27
(1,1021)	1:84:A:THR:HG23	1:85:A:ILE:HA	5	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,989)	1:82:A:ASP:HA	1:85:A:ILE:HG21	7	0.27
(1,989)	1:82:A:ASP:HA	1:85:A:ILE:HG22	7	0.27
(1,989)	1:82:A:ASP:HA	1:85:A:ILE:HG23	7	0.27
(1,858)	1:70:A:LYS:H	1:70:A:LYS:HD2	2	0.27
(1,858)	1:70:A:LYS:H	1:70:A:LYS:HD3	2	0.27
(1,849)	1:69:A:LYS:HG2	1:69:A:LYS:HE2	2	0.27
(1,849)	1:69:A:LYS:HG2	1:69:A:LYS:HE3	2	0.27
(1,811)	1:64:A:TYR:HB3	1:68:A:ALA:HB1	4	0.27
(1,811)	1:64:A:TYR:HB3	1:68:A:ALA:HB2	4	0.27
(1,811)	1:64:A:TYR:HB3	1:68:A:ALA:HB3	4	0.27
(1,760)	1:60:A:GLU:HG2	1:61:A:MET:H	6	0.27
(1,760)	1:60:A:GLU:HG3	1:61:A:MET:H	6	0.27
(1,760)	1:60:A:GLU:HG2	1:61:A:MET:H	6	0.27
(1,760)	1:60:A:GLU:HG3	1:61:A:MET:H	6	0.27
(1,611)	1:48:A:LYS:HA	1:48:A:LYS:HE2	9	0.27
(1,611)	1:48:A:LYS:HA	1:48:A:LYS:HE3	9	0.27
(1,607)	1:48:A:LYS:H	1:48:A:LYS:HE2	7	0.27
(1,607)	1:48:A:LYS:H	1:48:A:LYS:HE3	7	0.27
(1,604)	1:47:A:SER:HA	1:49:A:ILE:H	5	0.27
(1,583)	1:45:A:ARG:HB2	1:46:A:ARG:H	6	0.27
(1,540)	1:41:A:SER:H	1:72:A:ARG:H	2	0.27
(1,530)	1:40:A:VAL:HG11	1:44:A:VAL:HA	9	0.27
(1,530)	1:40:A:VAL:HG12	1:44:A:VAL:HA	9	0.27
(1,530)	1:40:A:VAL:HG13	1:44:A:VAL:HA	9	0.27
(1,530)	1:40:A:VAL:HG21	1:44:A:VAL:HA	9	0.27
(1,530)	1:40:A:VAL:HG22	1:44:A:VAL:HA	9	0.27
(1,530)	1:40:A:VAL:HG23	1:44:A:VAL:HA	9	0.27
(1,525)	1:40:A:VAL:HG11	1:45:A:ARG:HA	6	0.27
(1,525)	1:40:A:VAL:HG12	1:45:A:ARG:HA	6	0.27
(1,525)	1:40:A:VAL:HG13	1:45:A:ARG:HA	6	0.27
(1,376)	1:25:A:GLU:HG2	1:39:A:HIS:HA	9	0.27
(1,327)	1:20:A:LEU:HG	1:21:A:LEU:HB2	4	0.27
(1,327)	1:20:A:LEU:HG	1:21:A:LEU:HB3	4	0.27
(1,292)	1:18:A:THR:HG21	1:53:A:ILE:HG21	3	0.27
(1,292)	1:18:A:THR:HG21	1:53:A:ILE:HG22	3	0.27
(1,292)	1:18:A:THR:HG21	1:53:A:ILE:HG23	3	0.27
(1,292)	1:18:A:THR:HG22	1:53:A:ILE:HG21	3	0.27
(1,292)	1:18:A:THR:HG22	1:53:A:ILE:HG22	3	0.27
(1,292)	1:18:A:THR:HG22	1:53:A:ILE:HG23	3	0.27
(1,292)	1:18:A:THR:HG23	1:53:A:ILE:HG21	3	0.27
(1,292)	1:18:A:THR:HG23	1:53:A:ILE:HG22	3	0.27
(1,292)	1:18:A:THR:HG23	1:53:A:ILE:HG23	3	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,269)	1:17:A:VAL:HG11	1:55:A:ASP:HA	1	0.27
(1,269)	1:17:A:VAL:HG12	1:55:A:ASP:HA	1	0.27
(1,269)	1:17:A:VAL:HG13	1:55:A:ASP:HA	1	0.27
(1,269)	1:17:A:VAL:HG21	1:55:A:ASP:HA	1	0.27
(1,269)	1:17:A:VAL:HG22	1:55:A:ASP:HA	1	0.27
(1,269)	1:17:A:VAL:HG23	1:55:A:ASP:HA	1	0.27
(1,226)	1:16:A:ALA:H	1:30:A:LEU:HA	4	0.27
(1,191)	1:13:A:VAL:HG11	1:59:A:VAL:HB	3	0.27
(1,191)	1:13:A:VAL:HG12	1:59:A:VAL:HB	3	0.27
(1,191)	1:13:A:VAL:HG13	1:59:A:VAL:HB	3	0.27
(1,191)	1:13:A:VAL:HG21	1:59:A:VAL:HB	3	0.27
(1,191)	1:13:A:VAL:HG22	1:59:A:VAL:HB	3	0.27
(1,191)	1:13:A:VAL:HG23	1:59:A:VAL:HB	3	0.27
(1,167)	1:12:A:GLU:HG2	1:61:A:MET:H	10	0.27
(1,128)	1:10:A:LEU:HD11	1:61:A:MET:HB2	10	0.27
(1,128)	1:10:A:LEU:HD11	1:61:A:MET:HB3	10	0.27
(1,128)	1:10:A:LEU:HD12	1:61:A:MET:HB2	10	0.27
(1,128)	1:10:A:LEU:HD12	1:61:A:MET:HB3	10	0.27
(1,128)	1:10:A:LEU:HD13	1:61:A:MET:HB2	10	0.27
(1,128)	1:10:A:LEU:HD13	1:61:A:MET:HB3	10	0.27
(1,128)	1:10:A:LEU:HD21	1:61:A:MET:HB2	10	0.27
(1,128)	1:10:A:LEU:HD21	1:61:A:MET:HB3	10	0.27
(1,128)	1:10:A:LEU:HD22	1:61:A:MET:HB2	10	0.27
(1,128)	1:10:A:LEU:HD22	1:61:A:MET:HB3	10	0.27
(1,128)	1:10:A:LEU:HD23	1:61:A:MET:HB2	10	0.27
(1,128)	1:10:A:LEU:HD23	1:61:A:MET:HB3	10	0.27
(1,112)	1:10:A:LEU:HB2	1:61:A:MET:HA	9	0.27
(1,44)	1:5:A:GLU:HB3	1:6:A:LYS:H	8	0.27
(3,53)	1:43:A:LYS:O	1:46:A:ARG:N	10	0.26
(3,22)	1:21:A:LEU:O	1:25:A:GLU:H	7	0.26
(2,1)	1:8:A:LYS:HB2	1:10:A:LEU:H	5	0.26
(1,1019)	1:84:A:THR:HB	1:85:A:ILE:H	10	0.26
(1,973)	1:78:A:LYS:HA	1:78:A:LYS:HE2	4	0.26
(1,973)	1:78:A:LYS:HA	1:78:A:LYS:HE3	4	0.26
(1,937)	1:76:A:ARG:HA	1:76:A:ARG:HD2	4	0.26
(1,937)	1:76:A:ARG:HA	1:76:A:ARG:HD3	4	0.26
(1,860)	1:70:A:LYS:H	1:70:A:LYS:HD2	10	0.26
(1,860)	1:70:A:LYS:H	1:70:A:LYS:HD3	10	0.26
(1,827)	1:67:A:ASN:HA	1:68:A:ALA:HB1	7	0.26
(1,827)	1:67:A:ASN:HA	1:68:A:ALA:HB2	7	0.26
(1,827)	1:67:A:ASN:HA	1:68:A:ALA:HB3	7	0.26
(1,713)	1:56:A:ARG:H	1:76:A:ARG:H	7	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,712)	1:56:A:ARG:H	1:75:A:ARG:HG2	1	0.26
(1,587)	1:45:A:ARG:HG2	1:46:A:ARG:H	10	0.26
(1,587)	1:45:A:ARG:HG3	1:46:A:ARG:H	10	0.26
(1,338)	1:20:A:LEU:HD11	1:26:A:PHE:HB2	3	0.26
(1,338)	1:20:A:LEU:HD11	1:26:A:PHE:HB3	3	0.26
(1,338)	1:20:A:LEU:HD12	1:26:A:PHE:HB2	3	0.26
(1,338)	1:20:A:LEU:HD12	1:26:A:PHE:HB3	3	0.26
(1,338)	1:20:A:LEU:HD13	1:26:A:PHE:HB2	3	0.26
(1,338)	1:20:A:LEU:HD13	1:26:A:PHE:HB3	3	0.26
(1,338)	1:20:A:LEU:HD21	1:26:A:PHE:HB2	3	0.26
(1,338)	1:20:A:LEU:HD21	1:26:A:PHE:HB3	3	0.26
(1,338)	1:20:A:LEU:HD22	1:26:A:PHE:HB2	3	0.26
(1,338)	1:20:A:LEU:HD22	1:26:A:PHE:HB3	3	0.26
(1,338)	1:20:A:LEU:HD23	1:26:A:PHE:HB2	3	0.26
(1,338)	1:20:A:LEU:HD23	1:26:A:PHE:HB3	3	0.26
(1,327)	1:20:A:LEU:HG	1:21:A:LEU:HB2	8	0.26
(1,327)	1:20:A:LEU:HG	1:21:A:LEU:HB3	8	0.26
(1,291)	1:18:A:THR:HG21	1:53:A:ILE:HD11	9	0.26
(1,291)	1:18:A:THR:HG21	1:53:A:ILE:HD12	9	0.26
(1,291)	1:18:A:THR:HG21	1:53:A:ILE:HD13	9	0.26
(1,291)	1:18:A:THR:HG22	1:53:A:ILE:HD11	9	0.26
(1,291)	1:18:A:THR:HG22	1:53:A:ILE:HD12	9	0.26
(1,291)	1:18:A:THR:HG22	1:53:A:ILE:HD13	9	0.26
(1,291)	1:18:A:THR:HG23	1:53:A:ILE:HD11	9	0.26
(1,291)	1:18:A:THR:HG23	1:53:A:ILE:HD12	9	0.26
(1,291)	1:18:A:THR:HG23	1:53:A:ILE:HD13	9	0.26
(1,218)	1:15:A:GLY:HA2	1:29:A:LYS:HD2	2	0.26
(1,218)	1:15:A:GLY:HA2	1:29:A:LYS:HD3	2	0.26
(1,218)	1:15:A:GLY:HA3	1:29:A:LYS:HD2	2	0.26
(1,218)	1:15:A:GLY:HA3	1:29:A:LYS:HD3	2	0.26
(1,216)	1:15:A:GLY:HA3	1:30:A:LEU:HA	4	0.26
(1,185)	1:13:A:VAL:HB	1:14:A:GLU:H	1	0.26
(1,136)	1:11:A:PHE:H	1:61:A:MET:HB2	10	0.26
(1,120)	1:10:A:LEU:HB2	1:11:A:PHE:H	1	0.26
(1,120)	1:10:A:LEU:HB3	1:11:A:PHE:H	1	0.26
(1,26)	1:3:A:LYS:HD2	1:4:A:ASP:H	1	0.26
(1,26)	1:3:A:LYS:HD3	1:4:A:ASP:H	1	0.26
(1,17)	1:3:A:LYS:H	1:4:A:ASP:H	4	0.26
(1,17)	1:3:A:LYS:H	1:4:A:ASP:H	9	0.26
(3,46)	1:39:A:HIS:O	1:73:A:ILE:H	3	0.25
(1,850)	1:69:A:LYS:HG2	1:70:A:LYS:H	1	0.25
(1,773)	1:62:A:SER:H	1:66:A:ARG:HG2	9	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,338)	1:20:A:LEU:HD11	1:26:A:PHE:HB2	9	0.25
(1,338)	1:20:A:LEU:HD11	1:26:A:PHE:HB3	9	0.25
(1,338)	1:20:A:LEU:HD12	1:26:A:PHE:HB2	9	0.25
(1,338)	1:20:A:LEU:HD12	1:26:A:PHE:HB3	9	0.25
(1,338)	1:20:A:LEU:HD13	1:26:A:PHE:HB2	9	0.25
(1,338)	1:20:A:LEU:HD13	1:26:A:PHE:HB3	9	0.25
(1,338)	1:20:A:LEU:HD21	1:26:A:PHE:HB2	9	0.25
(1,338)	1:20:A:LEU:HD21	1:26:A:PHE:HB3	9	0.25
(1,338)	1:20:A:LEU:HD22	1:26:A:PHE:HB2	9	0.25
(1,338)	1:20:A:LEU:HD22	1:26:A:PHE:HB3	9	0.25
(1,338)	1:20:A:LEU:HD23	1:26:A:PHE:HB2	9	0.25
(1,338)	1:20:A:LEU:HD23	1:26:A:PHE:HB3	9	0.25
(1,336)	1:20:A:LEU:HD21	1:27:A:ARG:H	4	0.25
(1,336)	1:20:A:LEU:HD22	1:27:A:ARG:H	4	0.25
(1,336)	1:20:A:LEU:HD23	1:27:A:ARG:H	4	0.25
(1,291)	1:18:A:THR:HG21	1:53:A:ILE:HD11	7	0.25
(1,291)	1:18:A:THR:HG21	1:53:A:ILE:HD12	7	0.25
(1,291)	1:18:A:THR:HG21	1:53:A:ILE:HD13	7	0.25
(1,291)	1:18:A:THR:HG22	1:53:A:ILE:HD11	7	0.25
(1,291)	1:18:A:THR:HG22	1:53:A:ILE:HD12	7	0.25
(1,291)	1:18:A:THR:HG22	1:53:A:ILE:HD13	7	0.25
(1,291)	1:18:A:THR:HG23	1:53:A:ILE:HD11	7	0.25
(1,291)	1:18:A:THR:HG23	1:53:A:ILE:HD12	7	0.25
(1,291)	1:18:A:THR:HG23	1:53:A:ILE:HD13	7	0.25
(1,250)	1:17:A:VAL:HB	1:53:A:ILE:HA	2	0.25
(1,201)	1:14:A:GLU:HG2	1:59:A:VAL:H	8	0.25
(1,191)	1:13:A:VAL:HG11	1:59:A:VAL:HB	9	0.25
(1,191)	1:13:A:VAL:HG12	1:59:A:VAL:HB	9	0.25
(1,191)	1:13:A:VAL:HG13	1:59:A:VAL:HB	9	0.25
(1,191)	1:13:A:VAL:HG21	1:59:A:VAL:HB	9	0.25
(1,191)	1:13:A:VAL:HG22	1:59:A:VAL:HB	9	0.25
(1,191)	1:13:A:VAL:HG23	1:59:A:VAL:HB	9	0.25
(3,23)	1:21:A:LEU:O	1:25:A:GLU:N	6	0.24
(3,16)	1:16:A:ALA:H	1:29:A:LYS:O	4	0.24
(3,12)	1:17:A:VAL:H	1:55:A:ASP:O	9	0.24
(1,773)	1:62:A:SER:H	1:66:A:ARG:HG2	10	0.24
(1,772)	1:62:A:SER:H	1:64:A:TYR:HB2	9	0.24
(1,772)	1:62:A:SER:H	1:64:A:TYR:HB2	9	0.24
(1,772)	1:62:A:SER:H	1:64:A:TYR:HB3	9	0.24
(1,693)	1:53:A:ILE:H	1:53:A:ILE:HD11	4	0.24
(1,693)	1:53:A:ILE:H	1:53:A:ILE:HD12	4	0.24
(1,693)	1:53:A:ILE:H	1:53:A:ILE:HD13	4	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,419)	1:28:A:VAL:HB	1:29:A:LYS:H	3	0.24
(1,336)	1:20:A:LEU:HD21	1:27:A:ARG:H	9	0.24
(1,336)	1:20:A:LEU:HD22	1:27:A:ARG:H	9	0.24
(1,336)	1:20:A:LEU:HD23	1:27:A:ARG:H	9	0.24
(1,312)	1:20:A:LEU:HA	1:25:A:GLU:H	6	0.24
(1,312)	1:20:A:LEU:HA	1:25:A:GLU:H	8	0.24
(1,202)	1:14:A:GLU:HG3	1:15:A:GLY:H	2	0.24
(1,169)	1:12:A:GLU:HG3	1:61:A:MET:H	1	0.24
(1,147)	1:11:A:PHE:HB3	1:12:A:GLU:H	2	0.24
(1,118)	1:10:A:LEU:HG	1:61:A:MET:HG2	9	0.24
(1,118)	1:10:A:LEU:HG	1:61:A:MET:HG3	9	0.24
(1,30)	1:3:A:LYS:HG3	1:4:A:ASP:H	10	0.24
(3,47)	1:39:A:HIS:O	1:73:A:ILE:N	3	0.23
(3,44)	1:37:A:ILE:O	1:71:A:GLY:H	3	0.23
(1,965)	1:77:A:LEU:HD11	1:78:A:LYS:HE2	10	0.23
(1,965)	1:77:A:LEU:HD11	1:78:A:LYS:HE3	10	0.23
(1,965)	1:77:A:LEU:HD12	1:78:A:LYS:HE2	10	0.23
(1,965)	1:77:A:LEU:HD12	1:78:A:LYS:HE3	10	0.23
(1,965)	1:77:A:LEU:HD13	1:78:A:LYS:HE2	10	0.23
(1,965)	1:77:A:LEU:HD13	1:78:A:LYS:HE3	10	0.23
(1,965)	1:77:A:LEU:HD21	1:78:A:LYS:HE2	10	0.23
(1,965)	1:77:A:LEU:HD21	1:78:A:LYS:HE3	10	0.23
(1,965)	1:77:A:LEU:HD22	1:78:A:LYS:HE2	10	0.23
(1,965)	1:77:A:LEU:HD22	1:78:A:LYS:HE3	10	0.23
(1,965)	1:77:A:LEU:HD23	1:78:A:LYS:HE2	10	0.23
(1,965)	1:77:A:LEU:HD23	1:78:A:LYS:HE3	10	0.23
(1,871)	1:70:A:LYS:HG2	1:71:A:GLY:H	1	0.23
(1,847)	1:69:A:LYS:HD2	1:70:A:LYS:H	1	0.23
(1,847)	1:69:A:LYS:HD3	1:70:A:LYS:H	1	0.23
(1,772)	1:62:A:SER:H	1:64:A:TYR:HB2	3	0.23
(1,772)	1:62:A:SER:H	1:64:A:TYR:HB2	3	0.23
(1,772)	1:62:A:SER:H	1:64:A:TYR:HB3	3	0.23
(1,712)	1:56:A:ARG:H	1:75:A:ARG:HG2	9	0.23
(1,653)	1:50:A:ARG:HB2	1:52:A:ILE:HD11	6	0.23
(1,653)	1:50:A:ARG:HB2	1:52:A:ILE:HD12	6	0.23
(1,653)	1:50:A:ARG:HB2	1:52:A:ILE:HD13	6	0.23
(1,639)	1:49:A:ILE:HG12	1:74:A:ILE:HG12	4	0.23
(1,639)	1:49:A:ILE:HG12	1:74:A:ILE:HG13	4	0.23
(1,639)	1:49:A:ILE:HG13	1:74:A:ILE:HG12	4	0.23
(1,639)	1:49:A:ILE:HG13	1:74:A:ILE:HG13	4	0.23
(1,596)	1:46:A:ARG:HB2	1:47:A:SER:H	10	0.23
(1,572)	1:44:A:VAL:HG11	1:51:A:ILE:HG21	3	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,572)	1:44:A:VAL:HG11	1:51:A:ILE:HG22	3	0.23
(1,572)	1:44:A:VAL:HG11	1:51:A:ILE:HG23	3	0.23
(1,572)	1:44:A:VAL:HG12	1:51:A:ILE:HG21	3	0.23
(1,572)	1:44:A:VAL:HG12	1:51:A:ILE:HG22	3	0.23
(1,572)	1:44:A:VAL:HG12	1:51:A:ILE:HG23	3	0.23
(1,572)	1:44:A:VAL:HG13	1:51:A:ILE:HG21	3	0.23
(1,572)	1:44:A:VAL:HG13	1:51:A:ILE:HG22	3	0.23
(1,572)	1:44:A:VAL:HG13	1:51:A:ILE:HG23	3	0.23
(1,572)	1:44:A:VAL:HG11	1:51:A:ILE:HG21	9	0.23
(1,572)	1:44:A:VAL:HG11	1:51:A:ILE:HG22	9	0.23
(1,572)	1:44:A:VAL:HG11	1:51:A:ILE:HG23	9	0.23
(1,572)	1:44:A:VAL:HG12	1:51:A:ILE:HG21	9	0.23
(1,572)	1:44:A:VAL:HG12	1:51:A:ILE:HG22	9	0.23
(1,572)	1:44:A:VAL:HG12	1:51:A:ILE:HG23	9	0.23
(1,572)	1:44:A:VAL:HG13	1:51:A:ILE:HG21	9	0.23
(1,572)	1:44:A:VAL:HG13	1:51:A:ILE:HG22	9	0.23
(1,572)	1:44:A:VAL:HG13	1:51:A:ILE:HG23	9	0.23
(1,531)	1:40:A:VAL:HG11	1:44:A:VAL:HB	2	0.23
(1,531)	1:40:A:VAL:HG12	1:44:A:VAL:HB	2	0.23
(1,531)	1:40:A:VAL:HG13	1:44:A:VAL:HB	2	0.23
(1,531)	1:40:A:VAL:HG21	1:44:A:VAL:HB	2	0.23
(1,531)	1:40:A:VAL:HG22	1:44:A:VAL:HB	2	0.23
(1,531)	1:40:A:VAL:HG23	1:44:A:VAL:HB	2	0.23
(1,530)	1:40:A:VAL:HG11	1:44:A:VAL:HA	2	0.23
(1,530)	1:40:A:VAL:HG12	1:44:A:VAL:HA	2	0.23
(1,530)	1:40:A:VAL:HG13	1:44:A:VAL:HA	2	0.23
(1,530)	1:40:A:VAL:HG21	1:44:A:VAL:HA	2	0.23
(1,530)	1:40:A:VAL:HG22	1:44:A:VAL:HA	2	0.23
(1,530)	1:40:A:VAL:HG23	1:44:A:VAL:HA	2	0.23
(1,499)	1:38:A:CYS:HA	1:70:A:LYS:HD2	5	0.23
(1,499)	1:38:A:CYS:HA	1:70:A:LYS:HD3	5	0.23
(1,354)	1:22:A:PRO:HG2	1:23:A:ALA:H	10	0.23
(1,300)	1:19:A:ALA:HA	1:53:A:ILE:HB	5	0.23
(1,286)	1:18:A:THR:HG21	1:28:A:VAL:HA	10	0.23
(1,286)	1:18:A:THR:HG22	1:28:A:VAL:HA	10	0.23
(1,286)	1:18:A:THR:HG23	1:28:A:VAL:HA	10	0.23
(1,266)	1:17:A:VAL:HG11	1:53:A:ILE:HB	8	0.23
(1,266)	1:17:A:VAL:HG12	1:53:A:ILE:HB	8	0.23
(1,266)	1:17:A:VAL:HG13	1:53:A:ILE:HB	8	0.23
(1,266)	1:17:A:VAL:HG21	1:53:A:ILE:HB	8	0.23
(1,266)	1:17:A:VAL:HG22	1:53:A:ILE:HB	8	0.23
(1,266)	1:17:A:VAL:HG23	1:53:A:ILE:HB	8	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,250)	1:17:A:VAL:HB	1:53:A:ILE:HA	6	0.23
(1,206)	1:15:A:GLY:H	1:56:A:ARG:HA	9	0.23
(1,191)	1:13:A:VAL:HG11	1:59:A:VAL:HB	4	0.23
(1,191)	1:13:A:VAL:HG12	1:59:A:VAL:HB	4	0.23
(1,191)	1:13:A:VAL:HG13	1:59:A:VAL:HB	4	0.23
(1,191)	1:13:A:VAL:HG21	1:59:A:VAL:HB	4	0.23
(1,191)	1:13:A:VAL:HG22	1:59:A:VAL:HB	4	0.23
(1,191)	1:13:A:VAL:HG23	1:59:A:VAL:HB	4	0.23
(1,167)	1:12:A:GLU:HG2	1:61:A:MET:H	1	0.23
(1,149)	1:11:A:PHE:HB2	1:12:A:GLU:H	2	0.23
(1,149)	1:11:A:PHE:HB3	1:12:A:GLU:H	2	0.23
(1,118)	1:10:A:LEU:HG	1:61:A:MET:HG2	6	0.23
(1,118)	1:10:A:LEU:HG	1:61:A:MET:HG3	6	0.23
(1,34)	1:4:A:ASP:HB2	1:5:A:GLU:H	7	0.23
(1,34)	1:4:A:ASP:HB3	1:5:A:GLU:H	7	0.23
(1,1038)	1:87:A:LYS:H	1:87:A:LYS:HE2	3	0.22
(1,1038)	1:87:A:LYS:H	1:87:A:LYS:HE3	3	0.22
(1,860)	1:70:A:LYS:H	1:70:A:LYS:HD2	3	0.22
(1,860)	1:70:A:LYS:H	1:70:A:LYS:HD3	3	0.22
(1,806)	1:64:A:TYR:HB2	1:68:A:ALA:HA	6	0.22
(1,763)	1:61:A:MET:H	1:62:A:SER:H	4	0.22
(1,720)	1:56:A:ARG:HD2	1:57:A:VAL:H	8	0.22
(1,720)	1:56:A:ARG:HD3	1:57:A:VAL:H	8	0.22
(1,706)	1:55:A:ASP:H	1:56:A:ARG:H	10	0.22
(1,690)	1:52:A:ILE:HG21	1:75:A:ARG:HB2	10	0.22
(1,690)	1:52:A:ILE:HG22	1:75:A:ARG:HB2	10	0.22
(1,690)	1:52:A:ILE:HG23	1:75:A:ARG:HB2	10	0.22
(1,617)	1:48:A:LYS:HB3	1:48:A:LYS:HD2	2	0.22
(1,617)	1:48:A:LYS:HB3	1:48:A:LYS:HD3	2	0.22
(1,607)	1:48:A:LYS:H	1:48:A:LYS:HE2	4	0.22
(1,607)	1:48:A:LYS:H	1:48:A:LYS:HE3	4	0.22
(1,505)	1:39:A:HIS:H	1:72:A:ARG:H	3	0.22
(1,408)	1:27:A:ARG:HG3	1:28:A:VAL:H	6	0.22
(1,358)	1:23:A:ALA:H	1:24:A:ALA:HA	6	0.22
(1,337)	1:20:A:LEU:HD11	1:21:A:LEU:HB2	4	0.22
(1,337)	1:20:A:LEU:HD11	1:21:A:LEU:HB3	4	0.22
(1,337)	1:20:A:LEU:HD12	1:21:A:LEU:HB2	4	0.22
(1,337)	1:20:A:LEU:HD12	1:21:A:LEU:HB3	4	0.22
(1,337)	1:20:A:LEU:HD13	1:21:A:LEU:HB2	4	0.22
(1,337)	1:20:A:LEU:HD13	1:21:A:LEU:HB3	4	0.22
(1,337)	1:20:A:LEU:HD21	1:21:A:LEU:HB2	4	0.22
(1,337)	1:20:A:LEU:HD21	1:21:A:LEU:HB3	4	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,337)	1:20:A:LEU:HD22	1:21:A:LEU:HB2	4	0.22
(1,337)	1:20:A:LEU:HD22	1:21:A:LEU:HB3	4	0.22
(1,337)	1:20:A:LEU:HD23	1:21:A:LEU:HB2	4	0.22
(1,337)	1:20:A:LEU:HD23	1:21:A:LEU:HB3	4	0.22
(1,337)	1:20:A:LEU:HD11	1:21:A:LEU:HB2	8	0.22
(1,337)	1:20:A:LEU:HD11	1:21:A:LEU:HB3	8	0.22
(1,337)	1:20:A:LEU:HD12	1:21:A:LEU:HB2	8	0.22
(1,337)	1:20:A:LEU:HD12	1:21:A:LEU:HB3	8	0.22
(1,337)	1:20:A:LEU:HD13	1:21:A:LEU:HB2	8	0.22
(1,337)	1:20:A:LEU:HD13	1:21:A:LEU:HB3	8	0.22
(1,337)	1:20:A:LEU:HD21	1:21:A:LEU:HB2	8	0.22
(1,337)	1:20:A:LEU:HD21	1:21:A:LEU:HB3	8	0.22
(1,337)	1:20:A:LEU:HD22	1:21:A:LEU:HB2	8	0.22
(1,337)	1:20:A:LEU:HD22	1:21:A:LEU:HB3	8	0.22
(1,337)	1:20:A:LEU:HD23	1:21:A:LEU:HB2	8	0.22
(1,337)	1:20:A:LEU:HD23	1:21:A:LEU:HB3	8	0.22
(1,327)	1:20:A:LEU:HG	1:21:A:LEU:HB2	3	0.22
(1,327)	1:20:A:LEU:HG	1:21:A:LEU:HB3	3	0.22
(1,311)	1:20:A:LEU:HA	1:21:A:LEU:HB2	6	0.22
(1,311)	1:20:A:LEU:HA	1:21:A:LEU:HB3	6	0.22
(1,257)	1:17:A:VAL:HG21	1:53:A:ILE:HB	9	0.22
(1,257)	1:17:A:VAL:HG22	1:53:A:ILE:HB	9	0.22
(1,257)	1:17:A:VAL:HG23	1:53:A:ILE:HB	9	0.22
(1,191)	1:13:A:VAL:HG11	1:59:A:VAL:HB	2	0.22
(1,191)	1:13:A:VAL:HG12	1:59:A:VAL:HB	2	0.22
(1,191)	1:13:A:VAL:HG13	1:59:A:VAL:HB	2	0.22
(1,191)	1:13:A:VAL:HG21	1:59:A:VAL:HB	2	0.22
(1,191)	1:13:A:VAL:HG22	1:59:A:VAL:HB	2	0.22
(1,191)	1:13:A:VAL:HG23	1:59:A:VAL:HB	2	0.22
(1,162)	1:12:A:GLU:HB2	1:13:A:VAL:H	3	0.22
(1,128)	1:10:A:LEU:HD11	1:61:A:MET:HB2	8	0.22
(1,128)	1:10:A:LEU:HD11	1:61:A:MET:HB3	8	0.22
(1,128)	1:10:A:LEU:HD12	1:61:A:MET:HB2	8	0.22
(1,128)	1:10:A:LEU:HD12	1:61:A:MET:HB3	8	0.22
(1,128)	1:10:A:LEU:HD13	1:61:A:MET:HB2	8	0.22
(1,128)	1:10:A:LEU:HD13	1:61:A:MET:HB3	8	0.22
(1,128)	1:10:A:LEU:HD21	1:61:A:MET:HB2	8	0.22
(1,128)	1:10:A:LEU:HD21	1:61:A:MET:HB3	8	0.22
(1,128)	1:10:A:LEU:HD22	1:61:A:MET:HB2	8	0.22
(1,128)	1:10:A:LEU:HD22	1:61:A:MET:HB3	8	0.22
(1,128)	1:10:A:LEU:HD23	1:61:A:MET:HB2	8	0.22
(1,128)	1:10:A:LEU:HD23	1:61:A:MET:HB3	8	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,118)	1:10:A:LEU:HG	1:61:A:MET:HG2	4	0.22
(1,118)	1:10:A:LEU:HG	1:61:A:MET:HG3	4	0.22
(1,87)	1:8:A:LYS:HD3	1:9:A:THR:H	10	0.22
(1,60)	1:6:A:LYS:HD3	1:7:A:SER:H	5	0.22
(1,30)	1:3:A:LYS:HG3	1:4:A:ASP:H	4	0.22
(1,30)	1:3:A:LYS:HG3	1:4:A:ASP:H	6	0.22
(3,23)	1:21:A:LEU:O	1:25:A:GLU:N	2	0.21
(3,13)	1:17:A:VAL:N	1:55:A:ASP:O	9	0.21
(1,963)	1:77:A:LEU:HD11	1:78:A:LYS:HB2	10	0.21
(1,963)	1:77:A:LEU:HD11	1:78:A:LYS:HB3	10	0.21
(1,963)	1:77:A:LEU:HD12	1:78:A:LYS:HB2	10	0.21
(1,963)	1:77:A:LEU:HD12	1:78:A:LYS:HB3	10	0.21
(1,963)	1:77:A:LEU:HD13	1:78:A:LYS:HB2	10	0.21
(1,963)	1:77:A:LEU:HD13	1:78:A:LYS:HB3	10	0.21
(1,963)	1:77:A:LEU:HD21	1:78:A:LYS:HB2	10	0.21
(1,963)	1:77:A:LEU:HD21	1:78:A:LYS:HB3	10	0.21
(1,963)	1:77:A:LEU:HD22	1:78:A:LYS:HB2	10	0.21
(1,963)	1:77:A:LEU:HD22	1:78:A:LYS:HB3	10	0.21
(1,963)	1:77:A:LEU:HD23	1:78:A:LYS:HB2	10	0.21
(1,963)	1:77:A:LEU:HD23	1:78:A:LYS:HB3	10	0.21
(1,923)	1:75:A:ARG:HA	1:75:A:ARG:HB2	2	0.21
(1,923)	1:75:A:ARG:HA	1:75:A:ARG:HB3	2	0.21
(1,871)	1:70:A:LYS:HG2	1:71:A:GLY:H	2	0.21
(1,847)	1:69:A:LYS:HD2	1:70:A:LYS:H	5	0.21
(1,847)	1:69:A:LYS:HD3	1:70:A:LYS:H	5	0.21
(1,836)	1:69:A:LYS:H	1:69:A:LYS:HD2	2	0.21
(1,836)	1:69:A:LYS:H	1:69:A:LYS:HD3	2	0.21
(1,814)	1:64:A:TYR:HB2	1:66:A:ARG:H	10	0.21
(1,814)	1:64:A:TYR:HB3	1:66:A:ARG:H	10	0.21
(1,408)	1:27:A:ARG:HG3	1:28:A:VAL:H	1	0.21
(1,354)	1:22:A:PRO:HG2	1:23:A:ALA:H	4	0.21
(1,332)	1:20:A:LEU:HD11	1:27:A:ARG:H	9	0.21
(1,332)	1:20:A:LEU:HD12	1:27:A:ARG:H	9	0.21
(1,332)	1:20:A:LEU:HD13	1:27:A:ARG:H	9	0.21
(1,307)	1:20:A:LEU:HA	1:20:A:LEU:HG	6	0.21
(1,259)	1:17:A:VAL:HG11	1:19:A:ALA:HA	6	0.21
(1,259)	1:17:A:VAL:HG12	1:19:A:ALA:HA	6	0.21
(1,259)	1:17:A:VAL:HG13	1:19:A:ALA:HA	6	0.21
(1,259)	1:17:A:VAL:HG21	1:19:A:ALA:HA	6	0.21
(1,259)	1:17:A:VAL:HG22	1:19:A:ALA:HA	6	0.21
(1,259)	1:17:A:VAL:HG23	1:19:A:ALA:HA	6	0.21
(1,246)	1:17:A:VAL:HA	1:27:A:ARG:HB3	9	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,220)	1:15:A:GLY:HA2	1:56:A:ARG:HB2	1	0.21
(1,220)	1:15:A:GLY:HA2	1:56:A:ARG:HB3	1	0.21
(1,220)	1:15:A:GLY:HA3	1:56:A:ARG:HB2	1	0.21
(1,220)	1:15:A:GLY:HA3	1:56:A:ARG:HB3	1	0.21
(1,191)	1:13:A:VAL:HG11	1:59:A:VAL:HB	5	0.21
(1,191)	1:13:A:VAL:HG12	1:59:A:VAL:HB	5	0.21
(1,191)	1:13:A:VAL:HG13	1:59:A:VAL:HB	5	0.21
(1,191)	1:13:A:VAL:HG21	1:59:A:VAL:HB	5	0.21
(1,191)	1:13:A:VAL:HG22	1:59:A:VAL:HB	5	0.21
(1,191)	1:13:A:VAL:HG23	1:59:A:VAL:HB	5	0.21
(1,191)	1:13:A:VAL:HG11	1:59:A:VAL:HB	6	0.21
(1,191)	1:13:A:VAL:HG12	1:59:A:VAL:HB	6	0.21
(1,191)	1:13:A:VAL:HG13	1:59:A:VAL:HB	6	0.21
(1,191)	1:13:A:VAL:HG21	1:59:A:VAL:HB	6	0.21
(1,191)	1:13:A:VAL:HG22	1:59:A:VAL:HB	6	0.21
(1,191)	1:13:A:VAL:HG23	1:59:A:VAL:HB	6	0.21
(1,122)	1:10:A:LEU:HB2	1:61:A:MET:HB2	4	0.21
(1,122)	1:10:A:LEU:HB2	1:61:A:MET:HB3	4	0.21
(1,122)	1:10:A:LEU:HB3	1:61:A:MET:HB2	4	0.21
(1,122)	1:10:A:LEU:HB3	1:61:A:MET:HB3	4	0.21
(1,116)	1:10:A:LEU:HG	1:61:A:MET:HA	6	0.21
(1,60)	1:6:A:LYS:HD3	1:7:A:SER:H	1	0.21
(1,11)	1:2:A:VAL:HA	1:3:A:LYS:H	4	0.21
(3,50)	1:60:A:GLU:H	1:72:A:ARG:O	8	0.2
(3,37)	1:30:A:LEU:O	1:34:A:HIS:N	7	0.2
(1,1022)	1:84:A:THR:HG21	1:85:A:ILE:HB	6	0.2
(1,1022)	1:84:A:THR:HG22	1:85:A:ILE:HB	6	0.2
(1,1022)	1:84:A:THR:HG23	1:85:A:ILE:HB	6	0.2
(1,1002)	1:83:A:ARG:HB2	1:84:A:THR:H	5	0.2
(1,991)	1:82:A:ASP:HB2	1:85:A:ILE:HG21	2	0.2
(1,991)	1:82:A:ASP:HB2	1:85:A:ILE:HG22	2	0.2
(1,991)	1:82:A:ASP:HB2	1:85:A:ILE:HG23	2	0.2
(1,991)	1:82:A:ASP:HB3	1:85:A:ILE:HG21	2	0.2
(1,991)	1:82:A:ASP:HB3	1:85:A:ILE:HG22	2	0.2
(1,991)	1:82:A:ASP:HB3	1:85:A:ILE:HG23	2	0.2
(1,891)	1:73:A:ILE:H	1:73:A:ILE:HA	7	0.2
(1,891)	1:73:A:ILE:H	1:73:A:ILE:HA	8	0.2
(1,847)	1:69:A:LYS:HD2	1:70:A:LYS:H	9	0.2
(1,847)	1:69:A:LYS:HD3	1:70:A:LYS:H	9	0.2
(1,763)	1:61:A:MET:H	1:62:A:SER:H	3	0.2
(1,763)	1:61:A:MET:H	1:62:A:SER:H	9	0.2
(1,668)	1:51:A:ILE:H	1:52:A:ILE:H	5	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,618)	1:48:A:LYS:HB3	1:48:A:LYS:HE2	2	0.2
(1,618)	1:48:A:LYS:HB3	1:48:A:LYS:HE3	2	0.2
(1,611)	1:48:A:LYS:HA	1:48:A:LYS:HE2	2	0.2
(1,611)	1:48:A:LYS:HA	1:48:A:LYS:HE3	2	0.2
(1,611)	1:48:A:LYS:HA	1:48:A:LYS:HE2	6	0.2
(1,611)	1:48:A:LYS:HA	1:48:A:LYS:HE3	6	0.2
(1,593)	1:46:A:ARG:HA	1:46:A:ARG:HD2	5	0.2
(1,593)	1:46:A:ARG:HA	1:46:A:ARG:HD3	5	0.2
(1,572)	1:44:A:VAL:HG11	1:51:A:ILE:HG21	1	0.2
(1,572)	1:44:A:VAL:HG11	1:51:A:ILE:HG22	1	0.2
(1,572)	1:44:A:VAL:HG11	1:51:A:ILE:HG23	1	0.2
(1,572)	1:44:A:VAL:HG12	1:51:A:ILE:HG21	1	0.2
(1,572)	1:44:A:VAL:HG12	1:51:A:ILE:HG22	1	0.2
(1,572)	1:44:A:VAL:HG12	1:51:A:ILE:HG23	1	0.2
(1,572)	1:44:A:VAL:HG13	1:51:A:ILE:HG21	1	0.2
(1,572)	1:44:A:VAL:HG13	1:51:A:ILE:HG22	1	0.2
(1,572)	1:44:A:VAL:HG13	1:51:A:ILE:HG23	1	0.2
(1,544)	1:41:A:SER:HB2	1:72:A:ARG:HD2	4	0.2
(1,544)	1:41:A:SER:HB2	1:72:A:ARG:HD3	4	0.2
(1,544)	1:41:A:SER:HB3	1:72:A:ARG:HD2	4	0.2
(1,544)	1:41:A:SER:HB3	1:72:A:ARG:HD3	4	0.2
(1,531)	1:40:A:VAL:HG11	1:44:A:VAL:HB	3	0.2
(1,531)	1:40:A:VAL:HG12	1:44:A:VAL:HB	3	0.2
(1,531)	1:40:A:VAL:HG13	1:44:A:VAL:HB	3	0.2
(1,531)	1:40:A:VAL:HG21	1:44:A:VAL:HB	3	0.2
(1,531)	1:40:A:VAL:HG22	1:44:A:VAL:HB	3	0.2
(1,531)	1:40:A:VAL:HG23	1:44:A:VAL:HB	3	0.2
(1,530)	1:40:A:VAL:HG11	1:44:A:VAL:HA	5	0.2
(1,530)	1:40:A:VAL:HG12	1:44:A:VAL:HA	5	0.2
(1,530)	1:40:A:VAL:HG13	1:44:A:VAL:HA	5	0.2
(1,530)	1:40:A:VAL:HG21	1:44:A:VAL:HA	5	0.2
(1,530)	1:40:A:VAL:HG22	1:44:A:VAL:HA	5	0.2
(1,530)	1:40:A:VAL:HG23	1:44:A:VAL:HA	5	0.2
(1,485)	1:37:A:ILE:H	1:70:A:LYS:H	8	0.2
(1,430)	1:29:A:LYS:HA	1:29:A:LYS:HD2	9	0.2
(1,430)	1:29:A:LYS:HA	1:29:A:LYS:HD3	9	0.2
(1,378)	1:25:A:GLU:HG3	1:39:A:HIS:HA	5	0.2
(1,356)	1:22:A:PRO:HG3	1:23:A:ALA:H	2	0.2
(1,337)	1:20:A:LEU:HD11	1:21:A:LEU:HB2	3	0.2
(1,337)	1:20:A:LEU:HD11	1:21:A:LEU:HB3	3	0.2
(1,337)	1:20:A:LEU:HD12	1:21:A:LEU:HB2	3	0.2
(1,337)	1:20:A:LEU:HD12	1:21:A:LEU:HB3	3	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,337)	1:20:A:LEU:HD13	1:21:A:LEU:HB2	3	0.2
(1,337)	1:20:A:LEU:HD13	1:21:A:LEU:HB3	3	0.2
(1,337)	1:20:A:LEU:HD21	1:21:A:LEU:HB2	3	0.2
(1,337)	1:20:A:LEU:HD21	1:21:A:LEU:HB3	3	0.2
(1,337)	1:20:A:LEU:HD22	1:21:A:LEU:HB2	3	0.2
(1,337)	1:20:A:LEU:HD22	1:21:A:LEU:HB3	3	0.2
(1,337)	1:20:A:LEU:HD23	1:21:A:LEU:HB2	3	0.2
(1,337)	1:20:A:LEU:HD23	1:21:A:LEU:HB3	3	0.2
(1,335)	1:20:A:LEU:HD21	1:26:A:PHE:HA	4	0.2
(1,335)	1:20:A:LEU:HD22	1:26:A:PHE:HA	4	0.2
(1,335)	1:20:A:LEU:HD23	1:26:A:PHE:HA	4	0.2
(1,307)	1:20:A:LEU:HA	1:20:A:LEU:HG	4	0.2
(1,307)	1:20:A:LEU:HA	1:20:A:LEU:HG	5	0.2
(1,307)	1:20:A:LEU:HA	1:20:A:LEU:HG	10	0.2
(1,280)	1:18:A:THR:HA	1:53:A:ILE:HG21	2	0.2
(1,280)	1:18:A:THR:HA	1:53:A:ILE:HG22	2	0.2
(1,280)	1:18:A:THR:HA	1:53:A:ILE:HG23	2	0.2
(1,277)	1:18:A:THR:HA	1:18:A:THR:HB	5	0.2
(1,191)	1:13:A:VAL:HG11	1:59:A:VAL:HB	7	0.2
(1,191)	1:13:A:VAL:HG12	1:59:A:VAL:HB	7	0.2
(1,191)	1:13:A:VAL:HG13	1:59:A:VAL:HB	7	0.2
(1,191)	1:13:A:VAL:HG21	1:59:A:VAL:HB	7	0.2
(1,191)	1:13:A:VAL:HG22	1:59:A:VAL:HB	7	0.2
(1,191)	1:13:A:VAL:HG23	1:59:A:VAL:HB	7	0.2
(1,162)	1:12:A:GLU:HB2	1:13:A:VAL:H	9	0.2
(1,114)	1:10:A:LEU:HB3	1:61:A:MET:HA	1	0.2
(1,11)	1:2:A:VAL:HA	1:3:A:LYS:H	6	0.2
(1,11)	1:2:A:VAL:HA	1:3:A:LYS:H	9	0.2
(3,40)	1:39:A:HIS:H	1:71:A:GLY:O	3	0.19
(3,17)	1:16:A:ALA:N	1:29:A:LYS:O	4	0.19
(2,9)	1:17:A:VAL:H	1:56:A:ARG:HB3	1	0.19
(1,961)	1:77:A:LEU:HB2	1:78:A:LYS:H	6	0.19
(1,961)	1:77:A:LEU:HB3	1:78:A:LYS:H	6	0.19
(1,891)	1:73:A:ILE:H	1:73:A:ILE:HA	5	0.19
(1,891)	1:73:A:ILE:H	1:73:A:ILE:HA	6	0.19
(1,891)	1:73:A:ILE:H	1:73:A:ILE:HA	9	0.19
(1,891)	1:73:A:ILE:H	1:73:A:ILE:HA	10	0.19
(1,806)	1:64:A:TYR:HB2	1:68:A:ALA:HA	2	0.19
(1,791)	1:63:A:ILE:HD11	1:64:A:TYR:H	10	0.19
(1,791)	1:63:A:ILE:HD12	1:64:A:TYR:H	10	0.19
(1,791)	1:63:A:ILE:HD13	1:64:A:TYR:H	10	0.19
(1,776)	1:62:A:SER:HA	1:63:A:ILE:HD11	4	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,776)	1:62:A:SER:HA	1:63:A:ILE:HD12	4	0.19
(1,776)	1:62:A:SER:HA	1:63:A:ILE:HD13	4	0.19
(1,773)	1:62:A:SER:H	1:66:A:ARG:HG2	7	0.19
(1,739)	1:58:A:LEU:HD11	1:60:A:GLU:HB2	5	0.19
(1,739)	1:58:A:LEU:HD11	1:60:A:GLU:HB3	5	0.19
(1,739)	1:58:A:LEU:HD12	1:60:A:GLU:HB2	5	0.19
(1,739)	1:58:A:LEU:HD12	1:60:A:GLU:HB3	5	0.19
(1,739)	1:58:A:LEU:HD13	1:60:A:GLU:HB2	5	0.19
(1,739)	1:58:A:LEU:HD13	1:60:A:GLU:HB3	5	0.19
(1,739)	1:58:A:LEU:HD21	1:60:A:GLU:HB2	5	0.19
(1,739)	1:58:A:LEU:HD21	1:60:A:GLU:HB3	5	0.19
(1,739)	1:58:A:LEU:HD22	1:60:A:GLU:HB2	5	0.19
(1,739)	1:58:A:LEU:HD22	1:60:A:GLU:HB3	5	0.19
(1,739)	1:58:A:LEU:HD23	1:60:A:GLU:HB2	5	0.19
(1,739)	1:58:A:LEU:HD23	1:60:A:GLU:HB3	5	0.19
(1,706)	1:55:A:ASP:H	1:56:A:ARG:H	7	0.19
(1,616)	1:48:A:LYS:HB2	1:49:A:ILE:H	5	0.19
(1,595)	1:46:A:ARG:HB2	1:46:A:ARG:HD2	9	0.19
(1,595)	1:46:A:ARG:HB2	1:46:A:ARG:HD3	9	0.19
(1,447)	1:30:A:LEU:HG	1:33:A:GLU:H	4	0.19
(1,406)	1:27:A:ARG:HG2	1:28:A:VAL:H	6	0.19
(1,356)	1:22:A:PRO:HG3	1:23:A:ALA:H	3	0.19
(1,307)	1:20:A:LEU:HA	1:20:A:LEU:HG	7	0.19
(1,307)	1:20:A:LEU:HA	1:20:A:LEU:HG	8	0.19
(1,307)	1:20:A:LEU:HA	1:20:A:LEU:HG	9	0.19
(1,231)	1:16:A:ALA:HA	1:56:A:ARG:HD2	3	0.19
(1,231)	1:16:A:ALA:HA	1:56:A:ARG:HD3	3	0.19
(1,191)	1:13:A:VAL:HG11	1:59:A:VAL:HB	10	0.19
(1,191)	1:13:A:VAL:HG12	1:59:A:VAL:HB	10	0.19
(1,191)	1:13:A:VAL:HG13	1:59:A:VAL:HB	10	0.19
(1,191)	1:13:A:VAL:HG21	1:59:A:VAL:HB	10	0.19
(1,191)	1:13:A:VAL:HG22	1:59:A:VAL:HB	10	0.19
(1,191)	1:13:A:VAL:HG23	1:59:A:VAL:HB	10	0.19
(1,169)	1:12:A:GLU:HG3	1:61:A:MET:H	5	0.19
(1,149)	1:11:A:PHE:HB2	1:12:A:GLU:H	6	0.19
(1,149)	1:11:A:PHE:HB3	1:12:A:GLU:H	6	0.19
(1,119)	1:10:A:LEU:HB2	1:10:A:LEU:HG	1	0.19
(1,119)	1:10:A:LEU:HB3	1:10:A:LEU:HG	1	0.19
(1,66)	1:6:A:LYS:HG3	1:7:A:SER:H	1	0.19
(1,30)	1:3:A:LYS:HG3	1:4:A:ASP:H	5	0.19
(1,14)	1:3:A:LYS:H	1:3:A:LYS:HD2	4	0.19
(1,14)	1:3:A:LYS:H	1:3:A:LYS:HD3	4	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,11)	1:2:A:VAL:HA	1:3:A:LYS:H	10	0.19
(3,54)	1:44:A:VAL:O	1:47:A:SER:H	9	0.18
(2,17)	1:44:A:VAL:HA	1:47:A:SER:HA	6	0.18
(1,923)	1:75:A:ARG:HA	1:75:A:ARG:HB2	6	0.18
(1,923)	1:75:A:ARG:HA	1:75:A:ARG:HB3	6	0.18
(1,891)	1:73:A:ILE:H	1:73:A:ILE:HA	1	0.18
(1,891)	1:73:A:ILE:H	1:73:A:ILE:HA	2	0.18
(1,891)	1:73:A:ILE:H	1:73:A:ILE:HA	4	0.18
(1,860)	1:70:A:LYS:H	1:70:A:LYS:HD2	4	0.18
(1,860)	1:70:A:LYS:H	1:70:A:LYS:HD3	4	0.18
(1,852)	1:69:A:LYS:HG3	1:70:A:LYS:H	2	0.18
(1,763)	1:61:A:MET:H	1:62:A:SER:H	2	0.18
(1,752)	1:60:A:GLU:H	1:61:A:MET:H	3	0.18
(1,752)	1:60:A:GLU:H	1:61:A:MET:H	10	0.18
(1,693)	1:53:A:ILE:H	1:53:A:ILE:HD11	1	0.18
(1,693)	1:53:A:ILE:H	1:53:A:ILE:HD12	1	0.18
(1,693)	1:53:A:ILE:H	1:53:A:ILE:HD13	1	0.18
(1,657)	1:50:A:ARG:HD2	1:51:A:ILE:H	5	0.18
(1,657)	1:50:A:ARG:HD3	1:51:A:ILE:H	5	0.18
(1,657)	1:50:A:ARG:HD2	1:51:A:ILE:H	9	0.18
(1,657)	1:50:A:ARG:HD3	1:51:A:ILE:H	9	0.18
(1,653)	1:50:A:ARG:HB2	1:52:A:ILE:HD11	5	0.18
(1,653)	1:50:A:ARG:HB2	1:52:A:ILE:HD12	5	0.18
(1,653)	1:50:A:ARG:HB2	1:52:A:ILE:HD13	5	0.18
(1,619)	1:48:A:LYS:HB3	1:49:A:ILE:H	2	0.18
(1,618)	1:48:A:LYS:HB3	1:48:A:LYS:HE2	6	0.18
(1,618)	1:48:A:LYS:HB3	1:48:A:LYS:HE3	6	0.18
(1,618)	1:48:A:LYS:HB3	1:48:A:LYS:HE2	8	0.18
(1,618)	1:48:A:LYS:HB3	1:48:A:LYS:HE3	8	0.18
(1,611)	1:48:A:LYS:HA	1:48:A:LYS:HE2	1	0.18
(1,611)	1:48:A:LYS:HA	1:48:A:LYS:HE3	1	0.18
(1,447)	1:30:A:LEU:HG	1:33:A:GLU:H	7	0.18
(1,413)	1:28:A:VAL:H	1:35:A:GLU:HB2	2	0.18
(1,413)	1:28:A:VAL:H	1:35:A:GLU:HB3	2	0.18
(1,405)	1:27:A:ARG:HB2	1:38:A:CYS:H	4	0.18
(1,405)	1:27:A:ARG:HB3	1:38:A:CYS:H	4	0.18
(1,330)	1:20:A:LEU:HD11	1:21:A:LEU:HA	7	0.18
(1,330)	1:20:A:LEU:HD12	1:21:A:LEU:HA	7	0.18
(1,330)	1:20:A:LEU:HD13	1:21:A:LEU:HA	7	0.18
(1,307)	1:20:A:LEU:HA	1:20:A:LEU:HG	2	0.18
(1,307)	1:20:A:LEU:HA	1:20:A:LEU:HG	3	0.18
(1,277)	1:18:A:THR:HA	1:18:A:THR:HB	4	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,277)	1:18:A:THR:HA	1:18:A:THR:HB	10	0.18
(1,259)	1:17:A:VAL:HG11	1:19:A:ALA:HA	7	0.18
(1,259)	1:17:A:VAL:HG12	1:19:A:ALA:HA	7	0.18
(1,259)	1:17:A:VAL:HG13	1:19:A:ALA:HA	7	0.18
(1,259)	1:17:A:VAL:HG21	1:19:A:ALA:HA	7	0.18
(1,259)	1:17:A:VAL:HG22	1:19:A:ALA:HA	7	0.18
(1,259)	1:17:A:VAL:HG23	1:19:A:ALA:HA	7	0.18
(1,250)	1:17:A:VAL:HB	1:53:A:ILE:HA	5	0.18
(1,180)	1:13:A:VAL:H	1:60:A:GLU:HG2	2	0.18
(1,180)	1:13:A:VAL:H	1:60:A:GLU:HG3	2	0.18
(1,180)	1:13:A:VAL:H	1:60:A:GLU:HG2	4	0.18
(1,180)	1:13:A:VAL:H	1:60:A:GLU:HG3	4	0.18
(1,167)	1:12:A:GLU:HG2	1:61:A:MET:H	8	0.18
(1,126)	1:10:A:LEU:HD21	1:62:A:SER:HA	10	0.18
(1,126)	1:10:A:LEU:HD22	1:62:A:SER:HA	10	0.18
(1,126)	1:10:A:LEU:HD23	1:62:A:SER:HA	10	0.18
(1,66)	1:6:A:LYS:HG3	1:7:A:SER:H	9	0.18
(1,12)	1:2:A:VAL:HB	1:3:A:LYS:H	3	0.18
(3,55)	1:44:A:VAL:O	1:47:A:SER:N	4	0.17
(3,50)	1:60:A:GLU:H	1:72:A:ARG:O	10	0.17
(3,46)	1:39:A:HIS:O	1:73:A:ILE:H	2	0.17
(3,23)	1:21:A:LEU:O	1:25:A:GLU:N	7	0.17
(3,20)	1:19:A:ALA:H	1:27:A:ARG:O	2	0.17
(1,973)	1:78:A:LYS:HA	1:78:A:LYS:HE2	6	0.17
(1,973)	1:78:A:LYS:HA	1:78:A:LYS:HE3	6	0.17
(1,923)	1:75:A:ARG:HA	1:75:A:ARG:HB2	3	0.17
(1,923)	1:75:A:ARG:HA	1:75:A:ARG:HB3	3	0.17
(1,921)	1:75:A:ARG:HA	1:75:A:ARG:HD2	5	0.17
(1,921)	1:75:A:ARG:HA	1:75:A:ARG:HD3	5	0.17
(1,891)	1:73:A:ILE:H	1:73:A:ILE:HA	3	0.17
(1,850)	1:69:A:LYS:HG2	1:70:A:LYS:H	5	0.17
(1,752)	1:60:A:GLU:H	1:61:A:MET:H	2	0.17
(1,752)	1:60:A:GLU:H	1:61:A:MET:H	4	0.17
(1,736)	1:58:A:LEU:HD11	1:60:A:GLU:HA	4	0.17
(1,736)	1:58:A:LEU:HD12	1:60:A:GLU:HA	4	0.17
(1,736)	1:58:A:LEU:HD13	1:60:A:GLU:HA	4	0.17
(1,736)	1:58:A:LEU:HD11	1:60:A:GLU:HA	9	0.17
(1,736)	1:58:A:LEU:HD12	1:60:A:GLU:HA	9	0.17
(1,736)	1:58:A:LEU:HD13	1:60:A:GLU:HA	9	0.17
(1,690)	1:52:A:ILE:HG21	1:75:A:ARG:HB2	5	0.17
(1,690)	1:52:A:ILE:HG22	1:75:A:ARG:HB2	5	0.17
(1,690)	1:52:A:ILE:HG23	1:75:A:ARG:HB2	5	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,653)	1:50:A:ARG:HB2	1:52:A:ILE:HD11	2	0.17
(1,653)	1:50:A:ARG:HB2	1:52:A:ILE:HD12	2	0.17
(1,653)	1:50:A:ARG:HB2	1:52:A:ILE:HD13	2	0.17
(1,618)	1:48:A:LYS:HB3	1:48:A:LYS:HE2	3	0.17
(1,618)	1:48:A:LYS:HB3	1:48:A:LYS:HE3	3	0.17
(1,617)	1:48:A:LYS:HB3	1:48:A:LYS:HD2	3	0.17
(1,617)	1:48:A:LYS:HB3	1:48:A:LYS:HD3	3	0.17
(1,617)	1:48:A:LYS:HB3	1:48:A:LYS:HD2	10	0.17
(1,617)	1:48:A:LYS:HB3	1:48:A:LYS:HD3	10	0.17
(1,616)	1:48:A:LYS:HB2	1:49:A:ILE:H	1	0.17
(1,579)	1:45:A:ARG:H	1:47:A:SER:H	4	0.17
(1,537)	1:41:A:SER:H	1:42:A:GLY:H	9	0.17
(1,530)	1:40:A:VAL:HG11	1:44:A:VAL:HA	8	0.17
(1,530)	1:40:A:VAL:HG12	1:44:A:VAL:HA	8	0.17
(1,530)	1:40:A:VAL:HG13	1:44:A:VAL:HA	8	0.17
(1,530)	1:40:A:VAL:HG21	1:44:A:VAL:HA	8	0.17
(1,530)	1:40:A:VAL:HG22	1:44:A:VAL:HA	8	0.17
(1,530)	1:40:A:VAL:HG23	1:44:A:VAL:HA	8	0.17
(1,503)	1:39:A:HIS:H	1:70:A:LYS:HA	10	0.17
(1,430)	1:29:A:LYS:HA	1:29:A:LYS:HD2	2	0.17
(1,430)	1:29:A:LYS:HA	1:29:A:LYS:HD3	2	0.17
(1,355)	1:22:A:PRO:HG2	1:24:A:ALA:H	2	0.17
(1,307)	1:20:A:LEU:HA	1:20:A:LEU:HG	1	0.17
(1,279)	1:18:A:THR:HA	1:28:A:VAL:HG11	3	0.17
(1,279)	1:18:A:THR:HA	1:28:A:VAL:HG12	3	0.17
(1,279)	1:18:A:THR:HA	1:28:A:VAL:HG13	3	0.17
(1,279)	1:18:A:THR:HA	1:28:A:VAL:HG21	3	0.17
(1,279)	1:18:A:THR:HA	1:28:A:VAL:HG22	3	0.17
(1,279)	1:18:A:THR:HA	1:28:A:VAL:HG23	3	0.17
(1,266)	1:17:A:VAL:HG11	1:53:A:ILE:HB	9	0.17
(1,266)	1:17:A:VAL:HG12	1:53:A:ILE:HB	9	0.17
(1,266)	1:17:A:VAL:HG13	1:53:A:ILE:HB	9	0.17
(1,266)	1:17:A:VAL:HG21	1:53:A:ILE:HB	9	0.17
(1,266)	1:17:A:VAL:HG22	1:53:A:ILE:HB	9	0.17
(1,266)	1:17:A:VAL:HG23	1:53:A:ILE:HB	9	0.17
(1,246)	1:17:A:VAL:HA	1:27:A:ARG:HB3	10	0.17
(1,167)	1:12:A:GLU:HG2	1:61:A:MET:H	6	0.17
(1,162)	1:12:A:GLU:HB2	1:13:A:VAL:H	6	0.17
(1,72)	1:8:A:LYS:H	1:8:A:LYS:HE2	9	0.17
(1,72)	1:8:A:LYS:H	1:8:A:LYS:HE3	9	0.17
(1,63)	1:6:A:LYS:HG2	1:7:A:SER:H	3	0.17
(1,44)	1:5:A:GLU:HB3	1:6:A:LYS:H	1	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,11)	1:2:A:VAL:HA	1:3:A:LYS:H	1	0.17
(3,52)	1:43:A:LYS:O	1:46:A:ARG:H	6	0.16
(1,1021)	1:84:A:THR:HG21	1:85:A:ILE:HA	8	0.16
(1,1021)	1:84:A:THR:HG22	1:85:A:ILE:HA	8	0.16
(1,1021)	1:84:A:THR:HG23	1:85:A:ILE:HA	8	0.16
(1,1011)	1:83:A:ARG:HB2	1:84:A:THR:H	9	0.16
(1,1011)	1:83:A:ARG:HB3	1:84:A:THR:H	9	0.16
(1,923)	1:75:A:ARG:HA	1:75:A:ARG:HB2	8	0.16
(1,923)	1:75:A:ARG:HA	1:75:A:ARG:HB3	8	0.16
(1,871)	1:70:A:LYS:HG2	1:71:A:GLY:H	10	0.16
(1,814)	1:64:A:TYR:HB2	1:66:A:ARG:H	6	0.16
(1,814)	1:64:A:TYR:HB3	1:66:A:ARG:H	6	0.16
(1,814)	1:64:A:TYR:HB2	1:66:A:ARG:H	8	0.16
(1,814)	1:64:A:TYR:HB3	1:66:A:ARG:H	8	0.16
(1,763)	1:61:A:MET:H	1:62:A:SER:H	10	0.16
(1,752)	1:60:A:GLU:H	1:61:A:MET:H	1	0.16
(1,752)	1:60:A:GLU:H	1:61:A:MET:H	6	0.16
(1,712)	1:56:A:ARG:H	1:75:A:ARG:HG2	7	0.16
(1,693)	1:53:A:ILE:H	1:53:A:ILE:HD11	10	0.16
(1,693)	1:53:A:ILE:H	1:53:A:ILE:HD12	10	0.16
(1,693)	1:53:A:ILE:H	1:53:A:ILE:HD13	10	0.16
(1,657)	1:50:A:ARG:HD2	1:51:A:ILE:H	10	0.16
(1,657)	1:50:A:ARG:HD3	1:51:A:ILE:H	10	0.16
(1,618)	1:48:A:LYS:HB3	1:48:A:LYS:HE2	5	0.16
(1,618)	1:48:A:LYS:HB3	1:48:A:LYS:HE3	5	0.16
(1,618)	1:48:A:LYS:HB3	1:48:A:LYS:HE2	9	0.16
(1,618)	1:48:A:LYS:HB3	1:48:A:LYS:HE3	9	0.16
(1,616)	1:48:A:LYS:HB2	1:49:A:ILE:H	8	0.16
(1,616)	1:48:A:LYS:HB2	1:49:A:ILE:H	10	0.16
(1,530)	1:40:A:VAL:HG11	1:44:A:VAL:HA	1	0.16
(1,530)	1:40:A:VAL:HG12	1:44:A:VAL:HA	1	0.16
(1,530)	1:40:A:VAL:HG13	1:44:A:VAL:HA	1	0.16
(1,530)	1:40:A:VAL:HG21	1:44:A:VAL:HA	1	0.16
(1,530)	1:40:A:VAL:HG22	1:44:A:VAL:HA	1	0.16
(1,530)	1:40:A:VAL:HG23	1:44:A:VAL:HA	1	0.16
(1,447)	1:30:A:LEU:HG	1:33:A:GLU:H	6	0.16
(1,422)	1:28:A:VAL:HB	1:29:A:LYS:HD2	8	0.16
(1,422)	1:28:A:VAL:HB	1:29:A:LYS:HD3	8	0.16
(1,419)	1:28:A:VAL:HB	1:29:A:LYS:H	5	0.16
(1,348)	1:22:A:PRO:HA	1:23:A:ALA:H	6	0.16
(1,344)	1:21:A:LEU:H	1:26:A:PHE:HB2	1	0.16
(1,344)	1:21:A:LEU:H	1:26:A:PHE:HB3	1	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,332)	1:20:A:LEU:HD11	1:27:A:ARG:H	10	0.16
(1,332)	1:20:A:LEU:HD12	1:27:A:ARG:H	10	0.16
(1,332)	1:20:A:LEU:HD13	1:27:A:ARG:H	10	0.16
(1,315)	1:20:A:LEU:HB2	1:20:A:LEU:HG	10	0.16
(1,149)	1:11:A:PHE:HB2	1:12:A:GLU:H	9	0.16
(1,149)	1:11:A:PHE:HB3	1:12:A:GLU:H	9	0.16
(1,149)	1:11:A:PHE:HB2	1:12:A:GLU:H	10	0.16
(1,149)	1:11:A:PHE:HB3	1:12:A:GLU:H	10	0.16
(1,122)	1:10:A:LEU:HB2	1:61:A:MET:HB2	5	0.16
(1,122)	1:10:A:LEU:HB2	1:61:A:MET:HB3	5	0.16
(1,122)	1:10:A:LEU:HB3	1:61:A:MET:HB2	5	0.16
(1,122)	1:10:A:LEU:HB3	1:61:A:MET:HB3	5	0.16
(1,111)	1:10:A:LEU:HB2	1:11:A:PHE:H	1	0.16
(1,72)	1:8:A:LYS:H	1:8:A:LYS:HE2	4	0.16
(1,72)	1:8:A:LYS:H	1:8:A:LYS:HE3	4	0.16
(1,51)	1:6:A:LYS:HA	1:6:A:LYS:HE2	3	0.16
(1,51)	1:6:A:LYS:HA	1:6:A:LYS:HE3	3	0.16
(1,33)	1:4:A:ASP:HA	1:5:A:GLU:H	2	0.16
(3,51)	1:60:A:GLU:N	1:72:A:ARG:O	8	0.15
(3,51)	1:60:A:GLU:N	1:72:A:ARG:O	10	0.15
(3,36)	1:30:A:LEU:O	1:34:A:HIS:H	3	0.15
(3,12)	1:17:A:VAL:H	1:55:A:ASP:O	4	0.15
(3,12)	1:17:A:VAL:H	1:55:A:ASP:O	7	0.15
(1,985)	1:80:A:THR:HA	1:80:A:THR:HB	1	0.15
(1,953)	1:77:A:LEU:HB2	1:77:A:LEU:HG	2	0.15
(1,953)	1:77:A:LEU:HB2	1:77:A:LEU:HG	6	0.15
(1,950)	1:77:A:LEU:HA	1:77:A:LEU:HG	3	0.15
(1,923)	1:75:A:ARG:HA	1:75:A:ARG:HB2	5	0.15
(1,923)	1:75:A:ARG:HA	1:75:A:ARG:HB3	5	0.15
(1,923)	1:75:A:ARG:HA	1:75:A:ARG:HB2	9	0.15
(1,923)	1:75:A:ARG:HA	1:75:A:ARG:HB3	9	0.15
(1,923)	1:75:A:ARG:HA	1:75:A:ARG:HB2	10	0.15
(1,923)	1:75:A:ARG:HA	1:75:A:ARG:HB3	10	0.15
(1,921)	1:75:A:ARG:HA	1:75:A:ARG:HD2	2	0.15
(1,921)	1:75:A:ARG:HA	1:75:A:ARG:HD3	2	0.15
(1,772)	1:62:A:SER:H	1:64:A:TYR:HB2	2	0.15
(1,772)	1:62:A:SER:H	1:64:A:TYR:HB2	2	0.15
(1,772)	1:62:A:SER:H	1:64:A:TYR:HB3	2	0.15
(1,706)	1:55:A:ASP:H	1:56:A:ARG:H	1	0.15
(1,693)	1:53:A:ILE:H	1:53:A:ILE:HD11	3	0.15
(1,693)	1:53:A:ILE:H	1:53:A:ILE:HD12	3	0.15
(1,693)	1:53:A:ILE:H	1:53:A:ILE:HD13	3	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,693)	1:53:A:ILE:H	1:53:A:ILE:HD11	5	0.15
(1,693)	1:53:A:ILE:H	1:53:A:ILE:HD12	5	0.15
(1,693)	1:53:A:ILE:H	1:53:A:ILE:HD13	5	0.15
(1,668)	1:51:A:ILE:H	1:52:A:ILE:H	2	0.15
(1,618)	1:48:A:LYS:HB3	1:48:A:LYS:HE2	10	0.15
(1,618)	1:48:A:LYS:HB3	1:48:A:LYS:HE3	10	0.15
(1,587)	1:45:A:ARG:HG2	1:46:A:ARG:H	8	0.15
(1,587)	1:45:A:ARG:HG3	1:46:A:ARG:H	8	0.15
(1,503)	1:39:A:HIS:H	1:70:A:LYS:HA	1	0.15
(1,485)	1:37:A:ILE:H	1:70:A:LYS:H	1	0.15
(1,476)	1:36:A:ILE:HG12	1:37:A:ILE:H	3	0.15
(1,476)	1:36:A:ILE:HG13	1:37:A:ILE:H	3	0.15
(1,354)	1:22:A:PRO:HG2	1:23:A:ALA:H	1	0.15
(1,330)	1:20:A:LEU:HD11	1:21:A:LEU:HA	6	0.15
(1,330)	1:20:A:LEU:HD12	1:21:A:LEU:HA	6	0.15
(1,330)	1:20:A:LEU:HD13	1:21:A:LEU:HA	6	0.15
(1,315)	1:20:A:LEU:HB2	1:20:A:LEU:HG	7	0.15
(1,312)	1:20:A:LEU:HA	1:25:A:GLU:H	7	0.15
(1,273)	1:18:A:THR:H	1:27:A:ARG:H	2	0.15
(1,266)	1:17:A:VAL:HG11	1:53:A:ILE:HB	10	0.15
(1,266)	1:17:A:VAL:HG12	1:53:A:ILE:HB	10	0.15
(1,266)	1:17:A:VAL:HG13	1:53:A:ILE:HB	10	0.15
(1,266)	1:17:A:VAL:HG21	1:53:A:ILE:HB	10	0.15
(1,266)	1:17:A:VAL:HG22	1:53:A:ILE:HB	10	0.15
(1,266)	1:17:A:VAL:HG23	1:53:A:ILE:HB	10	0.15
(1,250)	1:17:A:VAL:HB	1:53:A:ILE:HA	3	0.15
(1,149)	1:11:A:PHE:HB2	1:12:A:GLU:H	5	0.15
(1,149)	1:11:A:PHE:HB3	1:12:A:GLU:H	5	0.15
(1,119)	1:10:A:LEU:HB2	1:10:A:LEU:HG	5	0.15
(1,119)	1:10:A:LEU:HB3	1:10:A:LEU:HG	5	0.15
(1,81)	1:8:A:LYS:HB3	1:10:A:LEU:H	10	0.15
(1,17)	1:3:A:LYS:H	1:4:A:ASP:H	1	0.15
(3,54)	1:44:A:VAL:O	1:47:A:SER:H	5	0.14
(3,52)	1:43:A:LYS:O	1:46:A:ARG:H	8	0.14
(3,52)	1:43:A:LYS:O	1:46:A:ARG:H	9	0.14
(3,16)	1:16:A:ALA:H	1:29:A:LYS:O	1	0.14
(2,1)	1:8:A:LYS:HB2	1:10:A:LEU:H	10	0.14
(1,1022)	1:84:A:THR:HG21	1:85:A:ILE:HB	10	0.14
(1,1022)	1:84:A:THR:HG22	1:85:A:ILE:HB	10	0.14
(1,1022)	1:84:A:THR:HG23	1:85:A:ILE:HB	10	0.14
(1,1011)	1:83:A:ARG:HB2	1:84:A:THR:H	5	0.14
(1,1011)	1:83:A:ARG:HB3	1:84:A:THR:H	5	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,963)	1:77:A:LEU:HD11	1:78:A:LYS:HB2	7	0.14
(1,963)	1:77:A:LEU:HD11	1:78:A:LYS:HB3	7	0.14
(1,963)	1:77:A:LEU:HD12	1:78:A:LYS:HB2	7	0.14
(1,963)	1:77:A:LEU:HD12	1:78:A:LYS:HB3	7	0.14
(1,963)	1:77:A:LEU:HD13	1:78:A:LYS:HB2	7	0.14
(1,963)	1:77:A:LEU:HD13	1:78:A:LYS:HB3	7	0.14
(1,963)	1:77:A:LEU:HD21	1:78:A:LYS:HB2	7	0.14
(1,963)	1:77:A:LEU:HD21	1:78:A:LYS:HB3	7	0.14
(1,963)	1:77:A:LEU:HD22	1:78:A:LYS:HB2	7	0.14
(1,963)	1:77:A:LEU:HD22	1:78:A:LYS:HB3	7	0.14
(1,963)	1:77:A:LEU:HD23	1:78:A:LYS:HB2	7	0.14
(1,963)	1:77:A:LEU:HD23	1:78:A:LYS:HB3	7	0.14
(1,953)	1:77:A:LEU:HB2	1:77:A:LEU:HG	4	0.14
(1,950)	1:77:A:LEU:HA	1:77:A:LEU:HG	1	0.14
(1,950)	1:77:A:LEU:HA	1:77:A:LEU:HG	8	0.14
(1,923)	1:75:A:ARG:HA	1:75:A:ARG:HB2	1	0.14
(1,923)	1:75:A:ARG:HA	1:75:A:ARG:HB3	1	0.14
(1,923)	1:75:A:ARG:HA	1:75:A:ARG:HB2	7	0.14
(1,923)	1:75:A:ARG:HA	1:75:A:ARG:HB3	7	0.14
(1,875)	1:70:A:LYS:HD2	1:71:A:GLY:H	4	0.14
(1,875)	1:70:A:LYS:HD3	1:71:A:GLY:H	4	0.14
(1,814)	1:64:A:TYR:HB2	1:66:A:ARG:H	2	0.14
(1,814)	1:64:A:TYR:HB3	1:66:A:ARG:H	2	0.14
(1,763)	1:61:A:MET:H	1:62:A:SER:H	1	0.14
(1,706)	1:55:A:ASP:H	1:56:A:ARG:H	3	0.14
(1,668)	1:51:A:ILE:H	1:52:A:ILE:H	8	0.14
(1,627)	1:49:A:ILE:HA	1:49:A:ILE:HB	1	0.14
(1,627)	1:49:A:ILE:HA	1:49:A:ILE:HB	3	0.14
(1,627)	1:49:A:ILE:HA	1:49:A:ILE:HB	8	0.14
(1,619)	1:48:A:LYS:HB3	1:49:A:ILE:H	3	0.14
(1,618)	1:48:A:LYS:HB3	1:48:A:LYS:HE2	1	0.14
(1,618)	1:48:A:LYS:HB3	1:48:A:LYS:HE3	1	0.14
(1,618)	1:48:A:LYS:HB3	1:48:A:LYS:HE2	4	0.14
(1,618)	1:48:A:LYS:HB3	1:48:A:LYS:HE3	4	0.14
(1,616)	1:48:A:LYS:HB2	1:49:A:ILE:H	6	0.14
(1,611)	1:48:A:LYS:HA	1:48:A:LYS:HE2	5	0.14
(1,611)	1:48:A:LYS:HA	1:48:A:LYS:HE3	5	0.14
(1,530)	1:40:A:VAL:HG11	1:44:A:VAL:HA	6	0.14
(1,530)	1:40:A:VAL:HG12	1:44:A:VAL:HA	6	0.14
(1,530)	1:40:A:VAL:HG13	1:44:A:VAL:HA	6	0.14
(1,530)	1:40:A:VAL:HG21	1:44:A:VAL:HA	6	0.14
(1,530)	1:40:A:VAL:HG22	1:44:A:VAL:HA	6	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,530)	1:40:A:VAL:HG23	1:44:A:VAL:HA	6	0.14
(1,517)	1:40:A:VAL:HA	1:72:A:ARG:HA	9	0.14
(1,517)	1:40:A:VAL:HA	1:72:A:ARG:HA	10	0.14
(1,504)	1:39:A:HIS:H	1:71:A:GLY:HA2	9	0.14
(1,504)	1:39:A:HIS:H	1:71:A:GLY:HA3	9	0.14
(1,431)	1:29:A:LYS:HA	1:29:A:LYS:HE2	9	0.14
(1,431)	1:29:A:LYS:HA	1:29:A:LYS:HE3	9	0.14
(1,430)	1:29:A:LYS:HA	1:29:A:LYS:HD2	7	0.14
(1,430)	1:29:A:LYS:HA	1:29:A:LYS:HD3	7	0.14
(1,422)	1:28:A:VAL:HB	1:29:A:LYS:HD2	10	0.14
(1,422)	1:28:A:VAL:HB	1:29:A:LYS:HD3	10	0.14
(1,419)	1:28:A:VAL:HB	1:29:A:LYS:H	4	0.14
(1,419)	1:28:A:VAL:HB	1:29:A:LYS:H	6	0.14
(1,376)	1:25:A:GLU:HG2	1:39:A:HIS:HA	2	0.14
(1,338)	1:20:A:LEU:HD11	1:26:A:PHE:HB2	2	0.14
(1,338)	1:20:A:LEU:HD11	1:26:A:PHE:HB3	2	0.14
(1,338)	1:20:A:LEU:HD12	1:26:A:PHE:HB2	2	0.14
(1,338)	1:20:A:LEU:HD12	1:26:A:PHE:HB3	2	0.14
(1,338)	1:20:A:LEU:HD13	1:26:A:PHE:HB2	2	0.14
(1,338)	1:20:A:LEU:HD13	1:26:A:PHE:HB3	2	0.14
(1,338)	1:20:A:LEU:HD21	1:26:A:PHE:HB2	2	0.14
(1,338)	1:20:A:LEU:HD21	1:26:A:PHE:HB3	2	0.14
(1,338)	1:20:A:LEU:HD22	1:26:A:PHE:HB2	2	0.14
(1,338)	1:20:A:LEU:HD22	1:26:A:PHE:HB3	2	0.14
(1,338)	1:20:A:LEU:HD23	1:26:A:PHE:HB2	2	0.14
(1,338)	1:20:A:LEU:HD23	1:26:A:PHE:HB3	2	0.14
(1,315)	1:20:A:LEU:HB2	1:20:A:LEU:HG	6	0.14
(1,312)	1:20:A:LEU:HA	1:25:A:GLU:H	10	0.14
(1,311)	1:20:A:LEU:HA	1:21:A:LEU:HB2	1	0.14
(1,311)	1:20:A:LEU:HA	1:21:A:LEU:HB3	1	0.14
(1,266)	1:17:A:VAL:HG11	1:53:A:ILE:HB	3	0.14
(1,266)	1:17:A:VAL:HG12	1:53:A:ILE:HB	3	0.14
(1,266)	1:17:A:VAL:HG13	1:53:A:ILE:HB	3	0.14
(1,266)	1:17:A:VAL:HG21	1:53:A:ILE:HB	3	0.14
(1,266)	1:17:A:VAL:HG22	1:53:A:ILE:HB	3	0.14
(1,266)	1:17:A:VAL:HG23	1:53:A:ILE:HB	3	0.14
(1,250)	1:17:A:VAL:HB	1:53:A:ILE:HA	1	0.14
(1,218)	1:15:A:GLY:HA2	1:29:A:LYS:HD2	1	0.14
(1,218)	1:15:A:GLY:HA2	1:29:A:LYS:HD3	1	0.14
(1,218)	1:15:A:GLY:HA3	1:29:A:LYS:HD2	1	0.14
(1,218)	1:15:A:GLY:HA3	1:29:A:LYS:HD3	1	0.14
(1,185)	1:13:A:VAL:HB	1:14:A:GLU:H	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,179)	1:13:A:VAL:H	1:60:A:GLU:HB2	1	0.14
(1,179)	1:13:A:VAL:H	1:60:A:GLU:HB3	1	0.14
(1,162)	1:12:A:GLU:HB2	1:13:A:VAL:H	8	0.14
(1,136)	1:11:A:PHE:H	1:61:A:MET:HB2	8	0.14
(1,95)	1:9:A:THR:H	1:10:A:LEU:H	3	0.14
(1,33)	1:4:A:ASP:HA	1:5:A:GLU:H	3	0.14
(1,12)	1:2:A:VAL:HB	1:3:A:LYS:H	2	0.14
(1,8)	1:2:A:VAL:H	1:3:A:LYS:H	3	0.14
(2,12)	1:26:A:PHE:HE2	1:51:A:ILE:H	9	0.13
(1,1010)	1:83:A:ARG:HG3	1:84:A:THR:H	8	0.13
(1,1005)	1:83:A:ARG:HB3	1:84:A:THR:H	9	0.13
(1,953)	1:77:A:LEU:HB2	1:77:A:LEU:HG	5	0.13
(1,950)	1:77:A:LEU:HA	1:77:A:LEU:HG	9	0.13
(1,934)	1:76:A:ARG:H	1:76:A:ARG:HD2	4	0.13
(1,934)	1:76:A:ARG:H	1:76:A:ARG:HD3	4	0.13
(1,932)	1:75:A:ARG:HB2	1:76:A:ARG:H	4	0.13
(1,932)	1:75:A:ARG:HB3	1:76:A:ARG:H	4	0.13
(1,827)	1:67:A:ASN:HA	1:68:A:ALA:HB1	5	0.13
(1,827)	1:67:A:ASN:HA	1:68:A:ALA:HB2	5	0.13
(1,827)	1:67:A:ASN:HA	1:68:A:ALA:HB3	5	0.13
(1,827)	1:67:A:ASN:HA	1:68:A:ALA:HB1	6	0.13
(1,827)	1:67:A:ASN:HA	1:68:A:ALA:HB2	6	0.13
(1,827)	1:67:A:ASN:HA	1:68:A:ALA:HB3	6	0.13
(1,784)	1:63:A:ILE:HA	1:63:A:ILE:HB	4	0.13
(1,784)	1:63:A:ILE:HA	1:63:A:ILE:HB	8	0.13
(1,763)	1:61:A:MET:H	1:62:A:SER:H	7	0.13
(1,763)	1:61:A:MET:H	1:62:A:SER:H	8	0.13
(1,668)	1:51:A:ILE:H	1:52:A:ILE:H	4	0.13
(1,627)	1:49:A:ILE:HA	1:49:A:ILE:HB	2	0.13
(1,627)	1:49:A:ILE:HA	1:49:A:ILE:HB	4	0.13
(1,627)	1:49:A:ILE:HA	1:49:A:ILE:HB	5	0.13
(1,627)	1:49:A:ILE:HA	1:49:A:ILE:HB	6	0.13
(1,627)	1:49:A:ILE:HA	1:49:A:ILE:HB	9	0.13
(1,627)	1:49:A:ILE:HA	1:49:A:ILE:HB	10	0.13
(1,616)	1:48:A:LYS:HB2	1:49:A:ILE:H	9	0.13
(1,611)	1:48:A:LYS:HA	1:48:A:LYS:HE2	4	0.13
(1,611)	1:48:A:LYS:HA	1:48:A:LYS:HE3	4	0.13
(1,574)	1:44:A:VAL:HG11	1:51:A:ILE:HG21	7	0.13
(1,574)	1:44:A:VAL:HG11	1:51:A:ILE:HG22	7	0.13
(1,574)	1:44:A:VAL:HG11	1:51:A:ILE:HG23	7	0.13
(1,574)	1:44:A:VAL:HG12	1:51:A:ILE:HG21	7	0.13
(1,574)	1:44:A:VAL:HG12	1:51:A:ILE:HG22	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,574)	1:44:A:VAL:HG12	1:51:A:ILE:HG23	7	0.13
(1,574)	1:44:A:VAL:HG13	1:51:A:ILE:HG21	7	0.13
(1,574)	1:44:A:VAL:HG13	1:51:A:ILE:HG22	7	0.13
(1,574)	1:44:A:VAL:HG13	1:51:A:ILE:HG23	7	0.13
(1,574)	1:44:A:VAL:HG21	1:51:A:ILE:HG21	7	0.13
(1,574)	1:44:A:VAL:HG21	1:51:A:ILE:HG22	7	0.13
(1,574)	1:44:A:VAL:HG21	1:51:A:ILE:HG23	7	0.13
(1,574)	1:44:A:VAL:HG22	1:51:A:ILE:HG21	7	0.13
(1,574)	1:44:A:VAL:HG22	1:51:A:ILE:HG22	7	0.13
(1,574)	1:44:A:VAL:HG22	1:51:A:ILE:HG23	7	0.13
(1,574)	1:44:A:VAL:HG23	1:51:A:ILE:HG21	7	0.13
(1,574)	1:44:A:VAL:HG23	1:51:A:ILE:HG22	7	0.13
(1,574)	1:44:A:VAL:HG23	1:51:A:ILE:HG23	7	0.13
(1,476)	1:36:A:ILE:HG12	1:37:A:ILE:H	8	0.13
(1,476)	1:36:A:ILE:HG13	1:37:A:ILE:H	8	0.13
(1,370)	1:25:A:GLU:H	1:26:A:PHE:H	5	0.13
(1,315)	1:20:A:LEU:HB2	1:20:A:LEU:HG	5	0.13
(1,282)	1:18:A:THR:HB	1:29:A:LYS:H	10	0.13
(1,246)	1:17:A:VAL:HA	1:27:A:ARG:HB3	3	0.13
(1,205)	1:15:A:GLY:H	1:16:A:ALA:H	6	0.13
(1,162)	1:12:A:GLU:HB2	1:13:A:VAL:H	7	0.13
(1,149)	1:11:A:PHE:HB2	1:12:A:GLU:H	7	0.13
(1,149)	1:11:A:PHE:HB3	1:12:A:GLU:H	7	0.13
(1,106)	1:10:A:LEU:H	1:62:A:SER:HA	10	0.13
(1,75)	1:8:A:LYS:HA	1:8:A:LYS:HD2	2	0.13
(1,75)	1:8:A:LYS:HA	1:8:A:LYS:HD3	2	0.13
(1,33)	1:4:A:ASP:HA	1:5:A:GLU:H	1	0.13
(1,33)	1:4:A:ASP:HA	1:5:A:GLU:H	5	0.13
(3,41)	1:39:A:HIS:N	1:71:A:GLY:O	3	0.12
(3,37)	1:30:A:LEU:O	1:34:A:HIS:N	5	0.12
(3,36)	1:30:A:LEU:O	1:34:A:HIS:H	2	0.12
(1,995)	1:83:A:ARG:H	1:83:A:ARG:HB2	2	0.12
(1,995)	1:83:A:ARG:H	1:83:A:ARG:HB3	2	0.12
(1,923)	1:75:A:ARG:HA	1:75:A:ARG:HB2	4	0.12
(1,923)	1:75:A:ARG:HA	1:75:A:ARG:HB3	4	0.12
(1,921)	1:75:A:ARG:HA	1:75:A:ARG:HD2	1	0.12
(1,921)	1:75:A:ARG:HA	1:75:A:ARG:HD3	1	0.12
(1,858)	1:70:A:LYS:H	1:70:A:LYS:HD2	10	0.12
(1,858)	1:70:A:LYS:H	1:70:A:LYS:HD3	10	0.12
(1,784)	1:63:A:ILE:HA	1:63:A:ILE:HB	1	0.12
(1,784)	1:63:A:ILE:HA	1:63:A:ILE:HB	2	0.12
(1,784)	1:63:A:ILE:HA	1:63:A:ILE:HB	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,784)	1:63:A:ILE:HA	1:63:A:ILE:HB	5	0.12
(1,784)	1:63:A:ILE:HA	1:63:A:ILE:HB	6	0.12
(1,784)	1:63:A:ILE:HA	1:63:A:ILE:HB	7	0.12
(1,784)	1:63:A:ILE:HA	1:63:A:ILE:HB	9	0.12
(1,784)	1:63:A:ILE:HA	1:63:A:ILE:HB	10	0.12
(1,760)	1:60:A:GLU:HG2	1:61:A:MET:H	1	0.12
(1,760)	1:60:A:GLU:HG3	1:61:A:MET:H	1	0.12
(1,760)	1:60:A:GLU:HG2	1:61:A:MET:H	1	0.12
(1,760)	1:60:A:GLU:HG3	1:61:A:MET:H	1	0.12
(1,706)	1:55:A:ASP:H	1:56:A:ARG:H	2	0.12
(1,706)	1:55:A:ASP:H	1:56:A:ARG:H	4	0.12
(1,693)	1:53:A:ILE:H	1:53:A:ILE:HD11	6	0.12
(1,693)	1:53:A:ILE:H	1:53:A:ILE:HD12	6	0.12
(1,693)	1:53:A:ILE:H	1:53:A:ILE:HD13	6	0.12
(1,668)	1:51:A:ILE:H	1:52:A:ILE:H	6	0.12
(1,659)	1:50:A:ARG:HB2	1:52:A:ILE:HG12	2	0.12
(1,659)	1:50:A:ARG:HB2	1:52:A:ILE:HG13	2	0.12
(1,659)	1:50:A:ARG:HB3	1:52:A:ILE:HG12	2	0.12
(1,659)	1:50:A:ARG:HB3	1:52:A:ILE:HG13	2	0.12
(1,653)	1:50:A:ARG:HB2	1:52:A:ILE:HD11	8	0.12
(1,653)	1:50:A:ARG:HB2	1:52:A:ILE:HD12	8	0.12
(1,653)	1:50:A:ARG:HB2	1:52:A:ILE:HD13	8	0.12
(1,611)	1:48:A:LYS:HA	1:48:A:LYS:HE2	3	0.12
(1,611)	1:48:A:LYS:HA	1:48:A:LYS:HE3	3	0.12
(1,596)	1:46:A:ARG:HB2	1:47:A:SER:H	5	0.12
(1,593)	1:46:A:ARG:HA	1:46:A:ARG:HD2	8	0.12
(1,593)	1:46:A:ARG:HA	1:46:A:ARG:HD3	8	0.12
(1,566)	1:44:A:VAL:H	1:47:A:SER:H	7	0.12
(1,447)	1:30:A:LEU:HG	1:33:A:GLU:H	5	0.12
(1,430)	1:29:A:LYS:HA	1:29:A:LYS:HD2	3	0.12
(1,430)	1:29:A:LYS:HA	1:29:A:LYS:HD3	3	0.12
(1,376)	1:25:A:GLU:HG2	1:39:A:HIS:HA	1	0.12
(1,351)	1:22:A:PRO:HB2	1:24:A:ALA:H	2	0.12
(1,315)	1:20:A:LEU:HB2	1:20:A:LEU:HG	1	0.12
(1,291)	1:18:A:THR:HG21	1:53:A:ILE:HD11	8	0.12
(1,291)	1:18:A:THR:HG21	1:53:A:ILE:HD12	8	0.12
(1,291)	1:18:A:THR:HG21	1:53:A:ILE:HD13	8	0.12
(1,291)	1:18:A:THR:HG22	1:53:A:ILE:HD11	8	0.12
(1,291)	1:18:A:THR:HG22	1:53:A:ILE:HD12	8	0.12
(1,291)	1:18:A:THR:HG22	1:53:A:ILE:HD13	8	0.12
(1,291)	1:18:A:THR:HG23	1:53:A:ILE:HD11	8	0.12
(1,291)	1:18:A:THR:HG23	1:53:A:ILE:HD12	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,291)	1:18:A:THR:HG23	1:53:A:ILE:HD13	8	0.12
(1,285)	1:18:A:THR:HG21	1:27:A:ARG:H	5	0.12
(1,285)	1:18:A:THR:HG22	1:27:A:ARG:H	5	0.12
(1,285)	1:18:A:THR:HG23	1:27:A:ARG:H	5	0.12
(1,279)	1:18:A:THR:HA	1:28:A:VAL:HG11	8	0.12
(1,279)	1:18:A:THR:HA	1:28:A:VAL:HG12	8	0.12
(1,279)	1:18:A:THR:HA	1:28:A:VAL:HG13	8	0.12
(1,279)	1:18:A:THR:HA	1:28:A:VAL:HG21	8	0.12
(1,279)	1:18:A:THR:HA	1:28:A:VAL:HG22	8	0.12
(1,279)	1:18:A:THR:HA	1:28:A:VAL:HG23	8	0.12
(1,224)	1:16:A:ALA:H	1:28:A:VAL:HG21	8	0.12
(1,224)	1:16:A:ALA:H	1:28:A:VAL:HG22	8	0.12
(1,224)	1:16:A:ALA:H	1:28:A:VAL:HG23	8	0.12
(1,224)	1:16:A:ALA:H	1:28:A:VAL:HG11	8	0.12
(1,224)	1:16:A:ALA:H	1:28:A:VAL:HG12	8	0.12
(1,224)	1:16:A:ALA:H	1:28:A:VAL:HG13	8	0.12
(1,224)	1:16:A:ALA:H	1:28:A:VAL:HG21	8	0.12
(1,224)	1:16:A:ALA:H	1:28:A:VAL:HG22	8	0.12
(1,224)	1:16:A:ALA:H	1:28:A:VAL:HG23	8	0.12
(1,175)	1:13:A:VAL:H	1:14:A:GLU:H	3	0.12
(1,162)	1:12:A:GLU:HB2	1:13:A:VAL:H	10	0.12
(1,147)	1:11:A:PHE:HB3	1:12:A:GLU:H	6	0.12
(1,136)	1:11:A:PHE:H	1:61:A:MET:HB2	2	0.12
(1,93)	1:8:A:LYS:HG3	1:9:A:THR:H	7	0.12
(1,51)	1:6:A:LYS:HA	1:6:A:LYS:HE2	6	0.12
(1,51)	1:6:A:LYS:HA	1:6:A:LYS:HE3	6	0.12
(1,33)	1:4:A:ASP:HA	1:5:A:GLU:H	4	0.12
(1,19)	1:3:A:LYS:HA	1:3:A:LYS:HE2	1	0.12
(1,19)	1:3:A:LYS:HA	1:3:A:LYS:HE3	1	0.12
(3,47)	1:39:A:HIS:O	1:73:A:ILE:N	2	0.11
(2,5)	1:12:A:GLU:HG2	1:62:A:SER:HA	9	0.11
(2,5)	1:12:A:GLU:HG3	1:62:A:SER:HA	9	0.11
(1,995)	1:83:A:ARG:H	1:83:A:ARG:HB2	10	0.11
(1,995)	1:83:A:ARG:H	1:83:A:ARG:HB3	10	0.11
(1,961)	1:77:A:LEU:HB2	1:78:A:LYS:H	4	0.11
(1,961)	1:77:A:LEU:HB3	1:78:A:LYS:H	4	0.11
(1,953)	1:77:A:LEU:HB2	1:77:A:LEU:HG	10	0.11
(1,926)	1:75:A:ARG:HB2	1:76:A:ARG:H	10	0.11
(1,921)	1:75:A:ARG:HA	1:75:A:ARG:HD2	6	0.11
(1,921)	1:75:A:ARG:HA	1:75:A:ARG:HD3	6	0.11
(1,921)	1:75:A:ARG:HA	1:75:A:ARG:HD2	7	0.11
(1,921)	1:75:A:ARG:HA	1:75:A:ARG:HD3	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,871)	1:70:A:LYS:HG2	1:71:A:GLY:H	7	0.11
(1,752)	1:60:A:GLU:H	1:61:A:MET:H	5	0.11
(1,739)	1:58:A:LEU:HD11	1:60:A:GLU:HB2	8	0.11
(1,739)	1:58:A:LEU:HD11	1:60:A:GLU:HB3	8	0.11
(1,739)	1:58:A:LEU:HD12	1:60:A:GLU:HB2	8	0.11
(1,739)	1:58:A:LEU:HD12	1:60:A:GLU:HB3	8	0.11
(1,739)	1:58:A:LEU:HD13	1:60:A:GLU:HB2	8	0.11
(1,739)	1:58:A:LEU:HD13	1:60:A:GLU:HB3	8	0.11
(1,739)	1:58:A:LEU:HD21	1:60:A:GLU:HB2	8	0.11
(1,739)	1:58:A:LEU:HD21	1:60:A:GLU:HB3	8	0.11
(1,739)	1:58:A:LEU:HD22	1:60:A:GLU:HB2	8	0.11
(1,739)	1:58:A:LEU:HD22	1:60:A:GLU:HB3	8	0.11
(1,739)	1:58:A:LEU:HD23	1:60:A:GLU:HB2	8	0.11
(1,739)	1:58:A:LEU:HD23	1:60:A:GLU:HB3	8	0.11
(1,732)	1:58:A:LEU:H	1:75:A:ARG:H	8	0.11
(1,695)	1:53:A:ILE:H	1:54:A:GLY:H	6	0.11
(1,693)	1:53:A:ILE:H	1:53:A:ILE:HD11	9	0.11
(1,693)	1:53:A:ILE:H	1:53:A:ILE:HD12	9	0.11
(1,693)	1:53:A:ILE:H	1:53:A:ILE:HD13	9	0.11
(1,659)	1:50:A:ARG:HB2	1:52:A:ILE:HG12	5	0.11
(1,659)	1:50:A:ARG:HB2	1:52:A:ILE:HG13	5	0.11
(1,659)	1:50:A:ARG:HB3	1:52:A:ILE:HG12	5	0.11
(1,659)	1:50:A:ARG:HB3	1:52:A:ILE:HG13	5	0.11
(1,657)	1:50:A:ARG:HD2	1:51:A:ILE:H	7	0.11
(1,657)	1:50:A:ARG:HD3	1:51:A:ILE:H	7	0.11
(1,583)	1:45:A:ARG:HB2	1:46:A:ARG:H	4	0.11
(1,569)	1:44:A:VAL:HA	1:47:A:SER:HB2	4	0.11
(1,569)	1:44:A:VAL:HA	1:47:A:SER:HB3	4	0.11
(1,538)	1:41:A:SER:H	1:44:A:VAL:H	2	0.11
(1,355)	1:22:A:PRO:HG2	1:24:A:ALA:H	3	0.11
(1,353)	1:22:A:PRO:HB3	1:24:A:ALA:H	2	0.11
(1,330)	1:20:A:LEU:HD11	1:21:A:LEU:HA	2	0.11
(1,330)	1:20:A:LEU:HD12	1:21:A:LEU:HA	2	0.11
(1,330)	1:20:A:LEU:HD13	1:21:A:LEU:HA	2	0.11
(1,315)	1:20:A:LEU:HB2	1:20:A:LEU:HG	2	0.11
(1,315)	1:20:A:LEU:HB2	1:20:A:LEU:HG	4	0.11
(1,296)	1:19:A:ALA:H	1:27:A:ARG:H	2	0.11
(1,266)	1:17:A:VAL:HG11	1:53:A:ILE:HB	4	0.11
(1,266)	1:17:A:VAL:HG12	1:53:A:ILE:HB	4	0.11
(1,266)	1:17:A:VAL:HG13	1:53:A:ILE:HB	4	0.11
(1,266)	1:17:A:VAL:HG21	1:53:A:ILE:HB	4	0.11
(1,266)	1:17:A:VAL:HG22	1:53:A:ILE:HB	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,266)	1:17:A:VAL:HG23	1:53:A:ILE:HB	4	0.11
(1,185)	1:13:A:VAL:HB	1:14:A:GLU:H	5	0.11
(1,175)	1:13:A:VAL:H	1:14:A:GLU:H	8	0.11
(1,175)	1:13:A:VAL:H	1:14:A:GLU:H	10	0.11
(1,149)	1:11:A:PHE:HB2	1:12:A:GLU:H	4	0.11
(1,149)	1:11:A:PHE:HB3	1:12:A:GLU:H	4	0.11
(1,119)	1:10:A:LEU:HB2	1:10:A:LEU:HG	9	0.11
(1,119)	1:10:A:LEU:HB3	1:10:A:LEU:HG	9	0.11
(1,85)	1:8:A:LYS:HD2	1:9:A:THR:H	9	0.11
(1,75)	1:8:A:LYS:HA	1:8:A:LYS:HD2	1	0.11
(1,75)	1:8:A:LYS:HA	1:8:A:LYS:HD3	1	0.11
(1,75)	1:8:A:LYS:HA	1:8:A:LYS:HD2	6	0.11
(1,75)	1:8:A:LYS:HA	1:8:A:LYS:HD3	6	0.11
(1,75)	1:8:A:LYS:HA	1:8:A:LYS:HD2	9	0.11
(1,75)	1:8:A:LYS:HA	1:8:A:LYS:HD3	9	0.11
(1,75)	1:8:A:LYS:HA	1:8:A:LYS:HD2	10	0.11
(1,75)	1:8:A:LYS:HA	1:8:A:LYS:HD3	10	0.11
(1,35)	1:5:A:GLU:H	1:5:A:GLU:HB2	7	0.11
(1,35)	1:5:A:GLU:H	1:5:A:GLU:HB3	7	0.11
(1,34)	1:4:A:ASP:HB2	1:5:A:GLU:H	6	0.11
(1,34)	1:4:A:ASP:HB3	1:5:A:GLU:H	6	0.11
(1,33)	1:4:A:ASP:HA	1:5:A:GLU:H	6	0.11
(1,814)	1:64:A:TYR:HB2	1:66:A:ARG:H	7	0.1
(1,814)	1:64:A:TYR:HB3	1:66:A:ARG:H	7	0.1
(1,760)	1:60:A:GLU:HG2	1:61:A:MET:H	10	0.1
(1,760)	1:60:A:GLU:HG3	1:61:A:MET:H	10	0.1
(1,760)	1:60:A:GLU:HG2	1:61:A:MET:H	10	0.1
(1,760)	1:60:A:GLU:HG3	1:61:A:MET:H	10	0.1
(1,695)	1:53:A:ILE:H	1:54:A:GLY:H	5	0.1
(1,668)	1:51:A:ILE:H	1:52:A:ILE:H	1	0.1
(1,657)	1:50:A:ARG:HD2	1:51:A:ILE:H	2	0.1
(1,657)	1:50:A:ARG:HD3	1:51:A:ILE:H	2	0.1
(1,618)	1:48:A:LYS:HB3	1:48:A:LYS:HE2	7	0.1
(1,618)	1:48:A:LYS:HB3	1:48:A:LYS:HE3	7	0.1
(1,617)	1:48:A:LYS:HB3	1:48:A:LYS:HD2	6	0.1
(1,617)	1:48:A:LYS:HB3	1:48:A:LYS:HD3	6	0.1
(1,611)	1:48:A:LYS:HA	1:48:A:LYS:HE2	7	0.1
(1,611)	1:48:A:LYS:HA	1:48:A:LYS:HE3	7	0.1
(1,482)	1:37:A:ILE:H	1:37:A:ILE:HG12	2	0.1
(1,482)	1:37:A:ILE:H	1:37:A:ILE:HG13	2	0.1
(1,350)	1:22:A:PRO:HB2	1:23:A:ALA:H	9	0.1
(1,338)	1:20:A:LEU:HD11	1:26:A:PHE:HB2	8	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,338)	1:20:A:LEU:HD11	1:26:A:PHE:HB3	8	0.1
(1,338)	1:20:A:LEU:HD12	1:26:A:PHE:HB2	8	0.1
(1,338)	1:20:A:LEU:HD12	1:26:A:PHE:HB3	8	0.1
(1,338)	1:20:A:LEU:HD13	1:26:A:PHE:HB2	8	0.1
(1,338)	1:20:A:LEU:HD13	1:26:A:PHE:HB3	8	0.1
(1,338)	1:20:A:LEU:HD21	1:26:A:PHE:HB2	8	0.1
(1,338)	1:20:A:LEU:HD21	1:26:A:PHE:HB3	8	0.1
(1,338)	1:20:A:LEU:HD22	1:26:A:PHE:HB2	8	0.1
(1,338)	1:20:A:LEU:HD22	1:26:A:PHE:HB3	8	0.1
(1,338)	1:20:A:LEU:HD23	1:26:A:PHE:HB2	8	0.1
(1,338)	1:20:A:LEU:HD23	1:26:A:PHE:HB3	8	0.1
(1,315)	1:20:A:LEU:HB2	1:20:A:LEU:HG	3	0.1
(1,306)	1:20:A:LEU:H	1:21:A:LEU:H	1	0.1
(1,96)	1:9:A:THR:H	1:10:A:LEU:HD11	1	0.1
(1,96)	1:9:A:THR:H	1:10:A:LEU:HD12	1	0.1
(1,96)	1:9:A:THR:H	1:10:A:LEU:HD13	1	0.1
(1,96)	1:9:A:THR:H	1:10:A:LEU:HD21	1	0.1
(1,96)	1:9:A:THR:H	1:10:A:LEU:HD22	1	0.1
(1,96)	1:9:A:THR:H	1:10:A:LEU:HD23	1	0.1
(1,75)	1:8:A:LYS:HA	1:8:A:LYS:HD2	8	0.1
(1,75)	1:8:A:LYS:HA	1:8:A:LYS:HD3	8	0.1
(1,33)	1:4:A:ASP:HA	1:5:A:GLU:H	10	0.1
(1,11)	1:2:A:VAL:HA	1:3:A:LYS:H	7	0.1

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

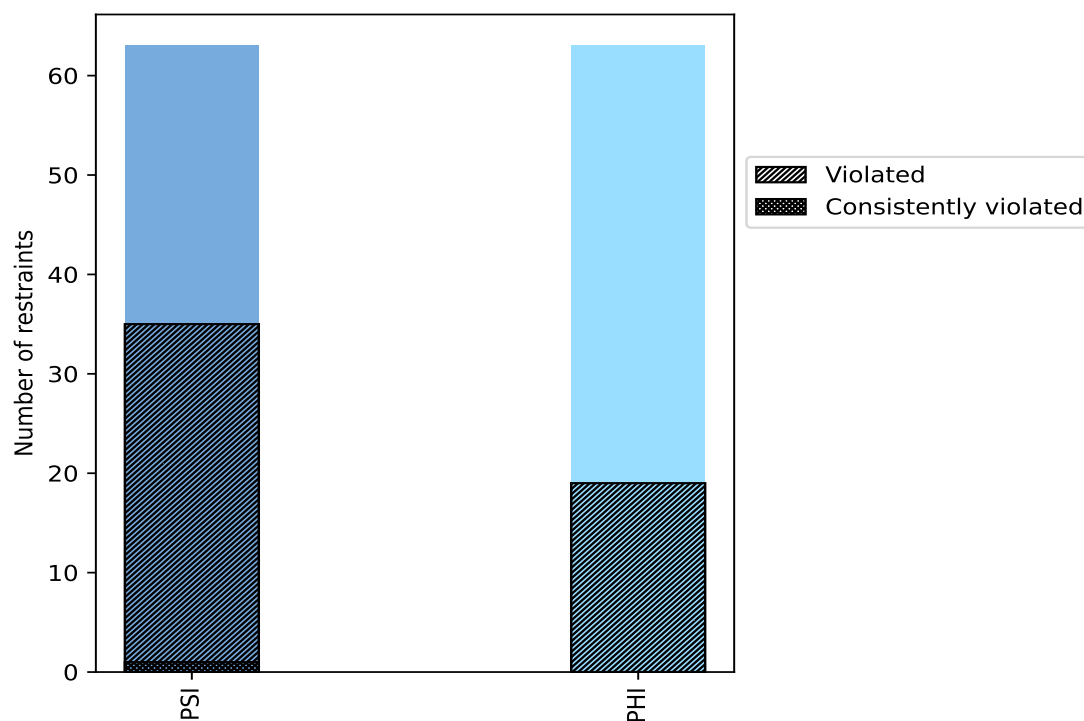
10.1 Summary of dihedral-angle violations [i](#)

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	63	50.0	35	55.6	27.8	1	1.6	0.8
PHI	63	50.0	19	30.2	15.1	0	0.0	0.0
Total	126	100.0	54	42.9	42.9	1	0.8	0.8

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](#)



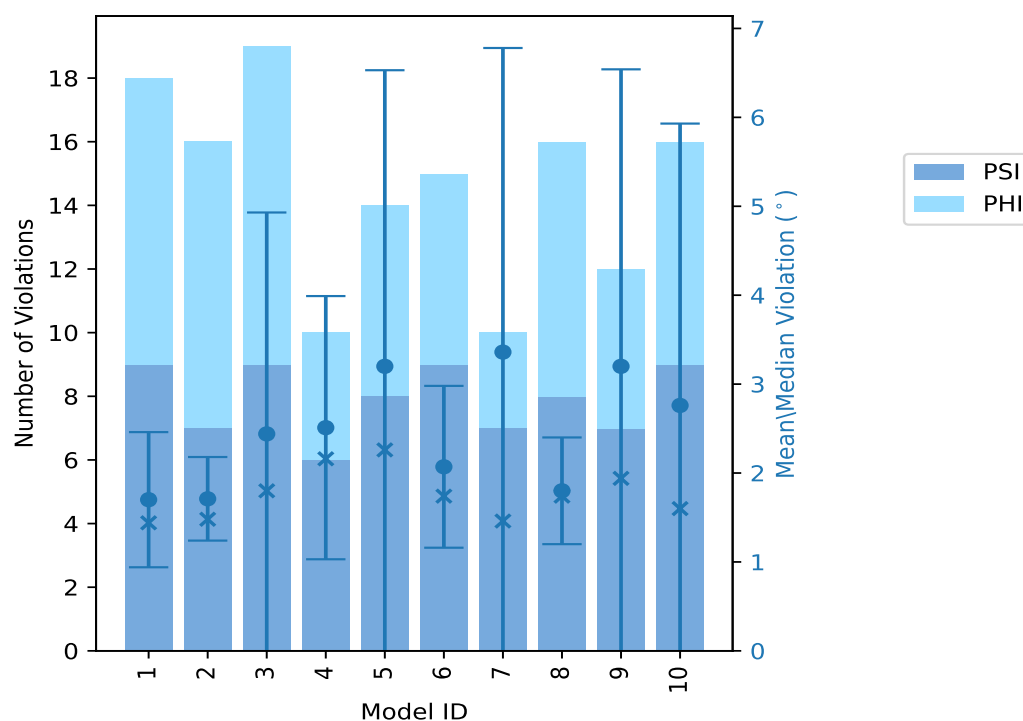
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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	9	9	18	1.7	3.71	0.76	1.44
2	7	9	16	1.71	2.97	0.47	1.48
3	9	10	19	2.44	12.5	2.49	1.8
4	6	4	10	2.51	6.38	1.48	2.16
5	8	6	14	3.2	14.4	3.33	2.26
6	9	6	15	2.07	4.33	0.91	1.74
7	7	3	10	3.36	11.75	3.42	1.46
8	8	8	16	1.8	2.8	0.6	1.74
9	7	5	12	3.2	13.33	3.34	1.94
10	9	7	16	2.76	13.51	3.17	1.6

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

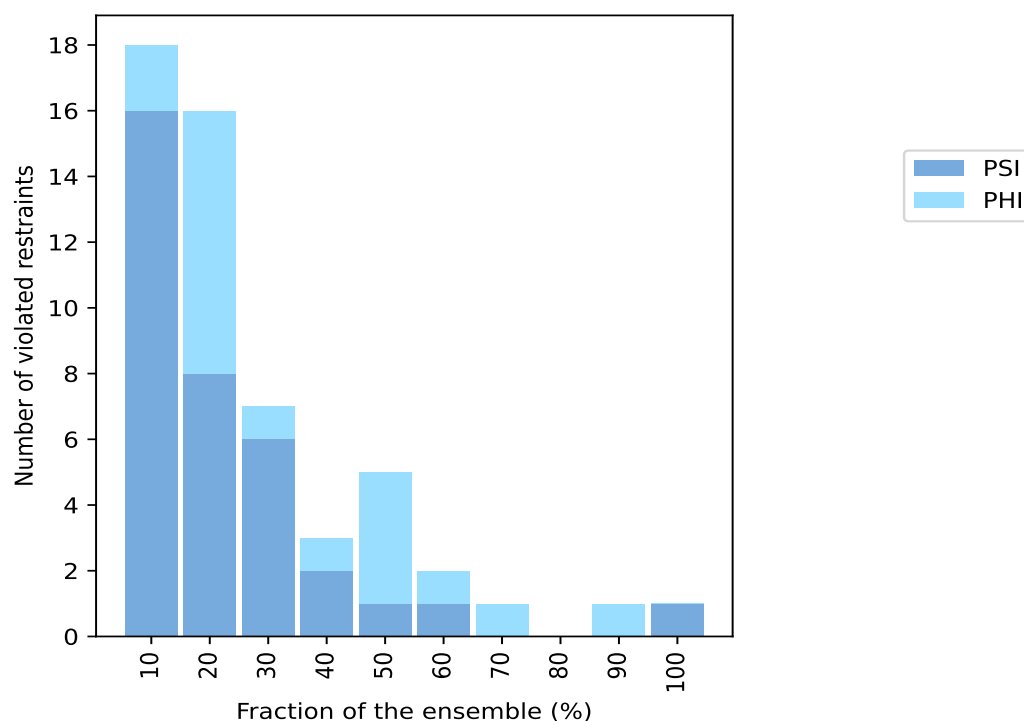
10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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	%
16	2	18	1	10.0
8	8	16	2	20.0
6	1	7	3	30.0
2	1	3	4	40.0
1	4	5	5	50.0
1	1	2	6	60.0
0	1	1	7	70.0
0	0	0	8	80.0
0	1	1	9	90.0
1	0	1	10	100.0

¹ Number of models with violations

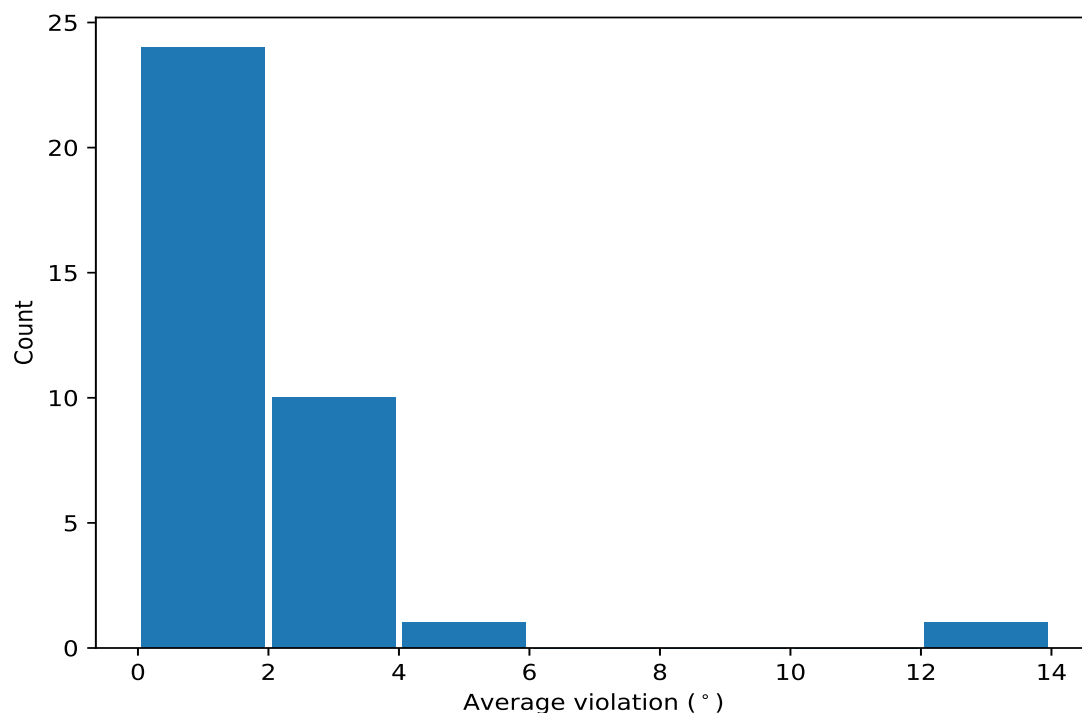
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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
(1,116)	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:C	1:75:A:ARG:N	10	4.16	1.7	3.9
(1,117)	1:74:A:ILE:C	1:75:A:ARG:N	1:75:A:ARG:CA	1:75:A:ARG:C	9	3.0	1.09	2.58
(1,43)	1:33:A:GLU:C	1:34:A:HIS:N	1:34:A:HIS:CA	1:34:A:HIS:C	7	1.65	0.3	1.5
(1,118)	1:75:A:ARG:N	1:75:A:ARG:CA	1:75:A:ARG:C	1:76:A:ARG:N	6	2.28	1.27	1.62
(1,79)	1:52:A:ILE:C	1:53:A:ILE:N	1:53:A:ILE:CA	1:53:A:ILE:C	6	1.59	0.56	1.39
(1,60)	1:42:A:GLY:N	1:42:A:GLY:CA	1:42:A:GLY:C	1:43:A:LYS:N	5	13.1	0.9	13.33
(1,111)	1:71:A:GLY:C	1:72:A:ARG:N	1:72:A:ARG:CA	1:72:A:ARG:C	5	2.31	1.15	1.86
(1,119)	1:75:A:ARG:C	1:76:A:ARG:N	1:76:A:ARG:CA	1:76:A:ARG:C	5	2.29	0.73	2.38
(1,99)	1:64:A:TYR:C	1:65:A:ASP:N	1:65:A:ASP:CA	1:65:A:ASP:C	5	1.69	0.53	1.52
(1,93)	1:61:A:MET:C	1:62:A:SER:N	1:62:A:SER:CA	1:62:A:SER:C	5	1.23	0.12	1.2
(1,100)	1:65:A:ASP:N	1:65:A:ASP:CA	1:65:A:ASP:C	1:66:A:ARG:N	4	2.17	0.45	2.16
(1,56)	1:40:A:VAL:N	1:40:A:VAL:CA	1:40:A:VAL:C	1:41:A:SER:N	4	1.76	0.36	1.82
(1,85)	1:57:A:VAL:C	1:58:A:LEU:N	1:58:A:LEU:CA	1:58:A:LEU:C	4	1.76	0.31	1.66

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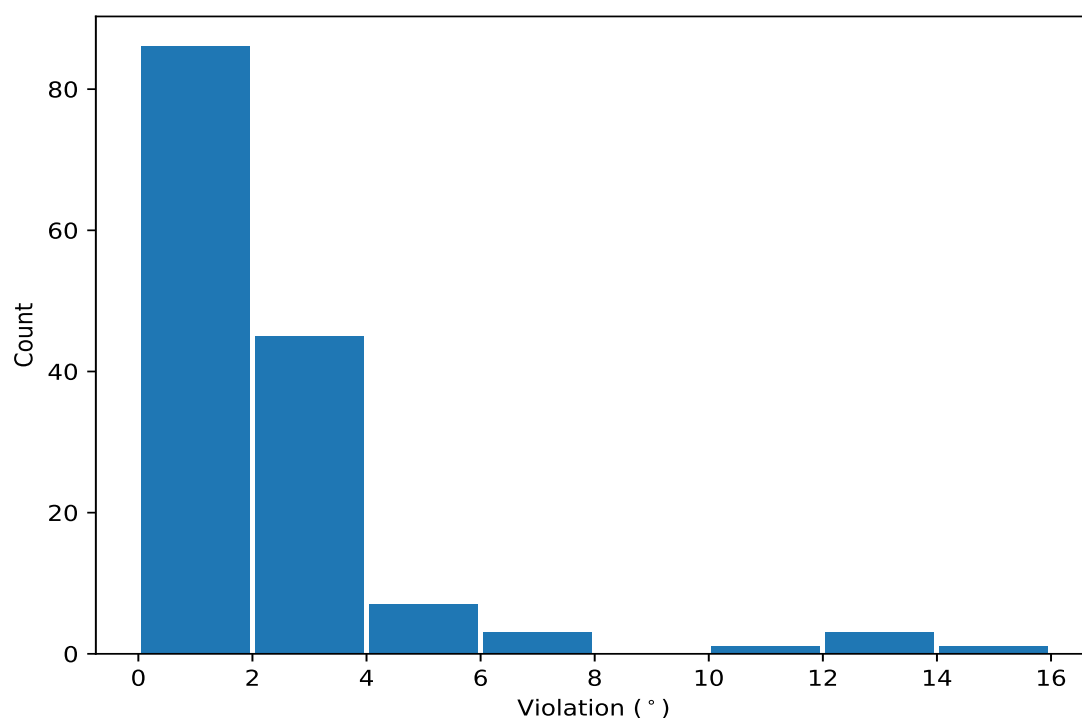
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,110)	1:71:A:GLY:N	1:71:A:GLY:CA	1:71:A:GLY:C	1:72:A:ARG:N	3	2.64	0.34	2.68
(1,59)	1:41:A:SER:C	1:42:A:GLY:N	1:42:A:GLY:CA	1:42:A:GLY:C	3	1.94	0.52	2.13
(1,78)	1:52:A:ILE:N	1:52:A:ILE:CA	1:52:A:ILE:C	1:53:A:ILE:N	3	1.61	0.72	1.2
(1,30)	1:25:A:GLU:N	1:25:A:GLU:CA	1:25:A:GLU:C	1:26:A:PHE:N	3	1.53	0.37	1.42
(1,104)	1:67:A:ASN:N	1:67:A:ASN:CA	1:67:A:ASN:C	1:68:A:ALA:N	3	1.52	0.46	1.4
(1,44)	1:34:A:HIS:N	1:34:A:HIS:CA	1:34:A:HIS:C	1:35:A:GLU:N	3	1.32	0.18	1.4
(1,26)	1:20:A:LEU:N	1:20:A:LEU:CA	1:20:A:LEU:C	1:21:A:LEU:N	3	1.18	0.16	1.14
(1,120)	1:76:A:ARG:N	1:76:A:ARG:CA	1:76:A:ARG:C	1:77:A:LEU:N	2	3.1	0.64	3.1
(1,103)	1:66:A:ARG:C	1:67:A:ASN:N	1:67:A:ASN:CA	1:67:A:ASN:C	2	2.74	0.66	2.74
(1,95)	1:62:A:SER:C	1:63:A:ILE:N	1:63:A:ILE:CA	1:63:A:ILE:C	2	2.08	0.44	2.08
(1,126)	1:82:A:ASP:N	1:82:A:ASP:CA	1:82:A:ASP:C	1:83:A:ARG:N	2	2.03	0.29	2.03
(1,83)	1:56:A:ARG:C	1:57:A:VAL:N	1:57:A:VAL:CA	1:57:A:VAL:C	2	1.88	0.2	1.88
(1,52)	1:38:A:CYS:N	1:38:A:CYS:CA	1:38:A:CYS:C	1:39:A:HIS:N	2	1.7	0.15	1.7
(1,15)	1:13:A:VAL:C	1:14:A:GLU:N	1:14:A:GLU:CA	1:14:A:GLU:C	2	1.64	0.6	1.64
(1,38)	1:29:A:LYS:N	1:29:A:LYS:CA	1:29:A:LYS:C	1:30:A:LEU:N	2	1.64	0.55	1.64
(1,109)	1:70:A:LYS:C	1:71:A:GLY:N	1:71:A:GLY:CA	1:71:A:GLY:C	2	1.32	0.08	1.32
(1,55)	1:39:A:HIS:C	1:40:A:VAL:N	1:40:A:VAL:CA	1:40:A:VAL:C	2	1.32	0.03	1.32
(1,10)	1:11:A:PHE:N	1:11:A:PHE:CA	1:11:A:PHE:C	1:12:A:GLU:N	2	1.3	0.04	1.3
(1,124)	1:78:A:LYS:N	1:78:A:LYS:CA	1:78:A:LYS:C	1:79:A:GLY:N	2	1.27	0.08	1.27
(1,53)	1:38:A:CYS:C	1:39:A:HIS:N	1:39:A:HIS:CA	1:39:A:HIS:C	2	1.24	0.16	1.24
(1,98)	1:64:A:TYR:N	1:64:A:TYR:CA	1:64:A:TYR:C	1:65:A:ASP:N	2	1.2	0.08	1.2
(1,96)	1:63:A:ILE:N	1:63:A:ILE:CA	1:63:A:ILE:C	1:64:A:TYR:N	2	1.19	0.15	1.19
(1,81)	1:55:A:ASP:C	1:56:A:ARG:N	1:56:A:ARG:CA	1:56:A:ARG:C	2	1.04	0.04	1.04

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

10.5 All violated dihedral-angle restraints ⓘ

10.5.1 Histogram : Distribution of violations ⓘ

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



10.5.2 Table: All violated dihedral-angle restraints [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 (°)
(1,60)	1:42:A:GLY:N	1:42:A:GLY:CA	1:42:A:GLY:C	1:43:A:LYS:N	5	14.4
(1,60)	1:42:A:GLY:N	1:42:A:GLY:CA	1:42:A:GLY:C	1:43:A:LYS:N	10	13.51
(1,60)	1:42:A:GLY:N	1:42:A:GLY:CA	1:42:A:GLY:C	1:43:A:LYS:N	9	13.33
(1,60)	1:42:A:GLY:N	1:42:A:GLY:CA	1:42:A:GLY:C	1:43:A:LYS:N	3	12.5
(1,60)	1:42:A:GLY:N	1:42:A:GLY:CA	1:42:A:GLY:C	1:43:A:LYS:N	7	11.75
(1,2)	1:3:A:LYS:N	1:3:A:LYS:CA	1:3:A:LYS:C	1:4:A:ASP:N	10	7.39
(1,116)	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:C	1:75:A:ARG:N	7	7.21
(1,116)	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:C	1:75:A:ARG:N	4	6.38
(1,116)	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:C	1:75:A:ARG:N	9	5.68
(1,117)	1:74:A:ILE:C	1:75:A:ARG:N	1:75:A:ARG:CA	1:75:A:ARG:C	7	5.05
(1,117)	1:74:A:ILE:C	1:75:A:ARG:N	1:75:A:ARG:CA	1:75:A:ARG:C	9	4.43
(1,116)	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:C	1:75:A:ARG:N	3	4.35
(1,118)	1:75:A:ARG:N	1:75:A:ARG:CA	1:75:A:ARG:C	1:76:A:ARG:N	5	4.34
(1,111)	1:71:A:GLY:C	1:72:A:ARG:N	1:72:A:ARG:CA	1:72:A:ARG:C	6	4.33
(1,116)	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:C	1:75:A:ARG:N	5	4.04
(1,116)	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:C	1:75:A:ARG:N	6	3.75
(1,120)	1:76:A:ARG:N	1:76:A:ARG:CA	1:76:A:ARG:C	1:77:A:LEU:N	5	3.74
(1,118)	1:75:A:ARG:N	1:75:A:ARG:CA	1:75:A:ARG:C	1:76:A:ARG:N	1	3.71
(1,117)	1:74:A:ILE:C	1:75:A:ARG:N	1:75:A:ARG:CA	1:75:A:ARG:C	4	3.7
(1,116)	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:C	1:75:A:ARG:N	10	3.64
(1,103)	1:66:A:ARG:C	1:67:A:ASN:N	1:67:A:ASN:CA	1:67:A:ASN:C	5	3.41

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,117)	1:74:A:ILE:C	1:75:A:ARG:N	1:75:A:ARG:CA	1:75:A:ARG:C	5	3.12
(1,119)	1:75:A:ARG:C	1:76:A:ARG:N	1:76:A:ARG:CA	1:76:A:ARG:C	5	3.09
(1,110)	1:71:A:GLY:N	1:71:A:GLY:CA	1:71:A:GLY:C	1:72:A:ARG:N	6	3.04
(1,119)	1:75:A:ARG:C	1:76:A:ARG:N	1:76:A:ARG:CA	1:76:A:ARG:C	1	2.99
(1,58)	1:41:A:SER:N	1:41:A:SER:CA	1:41:A:SER:C	1:42:A:GLY:N	2	2.97
(1,111)	1:71:A:GLY:C	1:72:A:ARG:N	1:72:A:ARG:CA	1:72:A:ARG:C	3	2.8
(1,79)	1:52:A:ILE:C	1:53:A:ILE:N	1:53:A:ILE:CA	1:53:A:ILE:C	8	2.8
(1,100)	1:65:A:ASP:N	1:65:A:ASP:CA	1:65:A:ASP:C	1:66:A:ARG:N	8	2.74
(1,110)	1:71:A:GLY:N	1:71:A:GLY:CA	1:71:A:GLY:C	1:72:A:ARG:N	4	2.68
(1,78)	1:52:A:ILE:N	1:52:A:ILE:CA	1:52:A:ILE:C	1:53:A:ILE:N	8	2.62
(1,117)	1:74:A:ILE:C	1:75:A:ARG:N	1:75:A:ARG:CA	1:75:A:ARG:C	3	2.58
(1,95)	1:62:A:SER:C	1:63:A:ILE:N	1:63:A:ILE:CA	1:63:A:ILE:C	8	2.53
(1,100)	1:65:A:ASP:N	1:65:A:ASP:CA	1:65:A:ASP:C	1:66:A:ARG:N	10	2.49
(1,120)	1:76:A:ARG:N	1:76:A:ARG:CA	1:76:A:ARG:C	1:77:A:LEU:N	6	2.46
(1,99)	1:64:A:TYR:C	1:65:A:ASP:N	1:65:A:ASP:CA	1:65:A:ASP:C	4	2.46
(1,59)	1:41:A:SER:C	1:42:A:GLY:N	1:42:A:GLY:CA	1:42:A:GLY:C	2	2.46
(1,116)	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:C	1:75:A:ARG:N	1	2.42
(1,119)	1:75:A:ARG:C	1:76:A:ARG:N	1:76:A:ARG:CA	1:76:A:ARG:C	9	2.38
(1,126)	1:82:A:ASP:N	1:82:A:ASP:CA	1:82:A:ASP:C	1:83:A:ARG:N	9	2.32
(1,117)	1:74:A:ILE:C	1:75:A:ARG:N	1:75:A:ARG:CA	1:75:A:ARG:C	10	2.27
(1,116)	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:C	1:75:A:ARG:N	8	2.24
(1,85)	1:57:A:VAL:C	1:58:A:LEU:N	1:58:A:LEU:CA	1:58:A:LEU:C	9	2.24
(1,15)	1:13:A:VAL:C	1:14:A:GLU:N	1:14:A:GLU:CA	1:14:A:GLU:C	2	2.24
(1,110)	1:71:A:GLY:N	1:71:A:GLY:CA	1:71:A:GLY:C	1:72:A:ARG:N	3	2.21
(1,48)	1:36:A:ILE:N	1:36:A:ILE:CA	1:36:A:ILE:C	1:37:A:ILE:N	3	2.21
(1,38)	1:29:A:LYS:N	1:29:A:LYS:CA	1:29:A:LYS:C	1:30:A:LEU:N	7	2.19
(1,56)	1:40:A:VAL:N	1:40:A:VAL:CA	1:40:A:VAL:C	1:41:A:SER:N	4	2.17
(1,99)	1:64:A:TYR:C	1:65:A:ASP:N	1:65:A:ASP:CA	1:65:A:ASP:C	3	2.15
(1,104)	1:67:A:ASN:N	1:67:A:ASN:CA	1:67:A:ASN:C	1:68:A:ALA:N	4	2.14
(1,59)	1:41:A:SER:C	1:42:A:GLY:N	1:42:A:GLY:CA	1:42:A:GLY:C	1	2.13
(1,117)	1:74:A:ILE:C	1:75:A:ARG:N	1:75:A:ARG:CA	1:75:A:ARG:C	1	2.09
(1,83)	1:56:A:ARG:C	1:57:A:VAL:N	1:57:A:VAL:CA	1:57:A:VAL:C	3	2.09
(1,103)	1:66:A:ARG:C	1:67:A:ASN:N	1:67:A:ASN:CA	1:67:A:ASN:C	1	2.08
(1,43)	1:33:A:GLU:C	1:34:A:HIS:N	1:34:A:HIS:CA	1:34:A:HIS:C	1	2.08
(1,43)	1:33:A:GLU:C	1:34:A:HIS:N	1:34:A:HIS:CA	1:34:A:HIS:C	3	2.05
(1,30)	1:25:A:GLU:N	1:25:A:GLU:CA	1:25:A:GLU:C	1:26:A:PHE:N	2	2.02
(1,94)	1:62:A:SER:N	1:62:A:SER:CA	1:62:A:SER:C	1:63:A:ILE:N	10	2.01
(1,67)	1:45:A:ARG:C	1:46:A:ARG:N	1:46:A:ARG:CA	1:46:A:ARG:C	8	2.01
(1,56)	1:40:A:VAL:N	1:40:A:VAL:CA	1:40:A:VAL:C	1:41:A:SER:N	6	2.01
(1,117)	1:74:A:ILE:C	1:75:A:ARG:N	1:75:A:ARG:CA	1:75:A:ARG:C	6	1.99
(1,119)	1:75:A:ARG:C	1:76:A:ARG:N	1:76:A:ARG:CA	1:76:A:ARG:C	8	1.88
(1,116)	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:C	1:75:A:ARG:N	2	1.86
(1,111)	1:71:A:GLY:C	1:72:A:ARG:N	1:72:A:ARG:CA	1:72:A:ARG:C	4	1.86
(1,52)	1:38:A:CYS:N	1:38:A:CYS:CA	1:38:A:CYS:C	1:39:A:HIS:N	10	1.85
(1,100)	1:65:A:ASP:N	1:65:A:ASP:CA	1:65:A:ASP:C	1:66:A:ARG:N	6	1.83
(1,117)	1:74:A:ILE:C	1:75:A:ARG:N	1:75:A:ARG:CA	1:75:A:ARG:C	8	1.81
(1,85)	1:57:A:VAL:C	1:58:A:LEU:N	1:58:A:LEU:CA	1:58:A:LEU:C	3	1.8
(1,43)	1:33:A:GLU:C	1:34:A:HIS:N	1:34:A:HIS:CA	1:34:A:HIS:C	10	1.8
(1,62)	1:43:A:LYS:N	1:43:A:LYS:CA	1:43:A:LYS:C	1:44:A:VAL:N	1	1.78
(1,118)	1:75:A:ARG:N	1:75:A:ARG:CA	1:75:A:ARG:C	1:76:A:ARG:N	2	1.75
(1,126)	1:82:A:ASP:N	1:82:A:ASP:CA	1:82:A:ASP:C	1:83:A:ARG:N	6	1.74

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,83)	1:56:A:ARG:C	1:57:A:VAL:N	1:57:A:VAL:CA	1:57:A:VAL:C	8	1.68
(1,108)	1:70:A:LYS:N	1:70:A:LYS:CA	1:70:A:LYS:C	1:71:A:GLY:N	7	1.66
(1,100)	1:65:A:ASP:N	1:65:A:ASP:CA	1:65:A:ASP:C	1:66:A:ARG:N	9	1.64
(1,95)	1:62:A:SER:C	1:63:A:ILE:N	1:63:A:ILE:CA	1:63:A:ILE:C	3	1.64
(1,79)	1:52:A:ILE:C	1:53:A:ILE:N	1:53:A:ILE:CA	1:53:A:ILE:C	3	1.63
(1,56)	1:40:A:VAL:N	1:40:A:VAL:CA	1:40:A:VAL:C	1:41:A:SER:N	1	1.63
(1,52)	1:38:A:CYS:N	1:38:A:CYS:CA	1:38:A:CYS:C	1:39:A:HIS:N	2	1.56
(1,99)	1:64:A:TYR:C	1:65:A:ASP:N	1:65:A:ASP:CA	1:65:A:ASP:C	6	1.52
(1,85)	1:57:A:VAL:C	1:58:A:LEU:N	1:58:A:LEU:CA	1:58:A:LEU:C	6	1.52
(1,43)	1:33:A:GLU:C	1:34:A:HIS:N	1:34:A:HIS:CA	1:34:A:HIS:C	2	1.5
(1,118)	1:75:A:ARG:N	1:75:A:ARG:CA	1:75:A:ARG:C	1:76:A:ARG:N	6	1.48
(1,44)	1:34:A:HIS:N	1:34:A:HIS:CA	1:34:A:HIS:C	1:35:A:GLU:N	9	1.48
(1,93)	1:61:A:MET:C	1:62:A:SER:N	1:62:A:SER:CA	1:62:A:SER:C	2	1.46
(1,85)	1:57:A:VAL:C	1:58:A:LEU:N	1:58:A:LEU:CA	1:58:A:LEU:C	2	1.46
(1,43)	1:33:A:GLU:C	1:34:A:HIS:N	1:34:A:HIS:CA	1:34:A:HIS:C	9	1.45
(1,22)	1:18:A:THR:N	1:18:A:THR:CA	1:18:A:THR:C	1:19:A:ALA:N	5	1.44
(1,111)	1:71:A:GLY:C	1:72:A:ARG:N	1:72:A:ARG:CA	1:72:A:ARG:C	2	1.43
(1,30)	1:25:A:GLU:N	1:25:A:GLU:CA	1:25:A:GLU:C	1:26:A:PHE:N	6	1.42
(1,109)	1:70:A:LYS:C	1:71:A:GLY:N	1:71:A:GLY:CA	1:71:A:GLY:C	2	1.41
(1,104)	1:67:A:ASN:N	1:67:A:ASN:CA	1:67:A:ASN:C	1:68:A:ALA:N	10	1.4
(1,79)	1:52:A:ILE:C	1:53:A:ILE:N	1:53:A:ILE:CA	1:53:A:ILE:C	10	1.4
(1,53)	1:38:A:CYS:C	1:39:A:HIS:N	1:39:A:HIS:CA	1:39:A:HIS:C	5	1.4
(1,44)	1:34:A:HIS:N	1:34:A:HIS:CA	1:34:A:HIS:C	1:35:A:GLU:N	6	1.4
(1,26)	1:20:A:LEU:N	1:20:A:LEU:CA	1:20:A:LEU:C	1:21:A:LEU:N	8	1.4
(1,79)	1:52:A:ILE:C	1:53:A:ILE:N	1:53:A:ILE:CA	1:53:A:ILE:C	2	1.38
(1,124)	1:78:A:LYS:N	1:78:A:LYS:CA	1:78:A:LYS:C	1:79:A:GLY:N	4	1.35
(1,96)	1:63:A:ILE:N	1:63:A:ILE:CA	1:63:A:ILE:C	1:64:A:TYR:N	5	1.34
(1,55)	1:39:A:HIS:C	1:40:A:VAL:N	1:40:A:VAL:CA	1:40:A:VAL:C	2	1.34
(1,43)	1:33:A:GLU:C	1:34:A:HIS:N	1:34:A:HIS:CA	1:34:A:HIS:C	8	1.33
(1,10)	1:11:A:PHE:N	1:11:A:PHE:CA	1:11:A:PHE:C	1:12:A:GLU:N	9	1.33
(1,43)	1:33:A:GLU:C	1:34:A:HIS:N	1:34:A:HIS:CA	1:34:A:HIS:C	6	1.31
(1,55)	1:39:A:HIS:C	1:40:A:VAL:N	1:40:A:VAL:CA	1:40:A:VAL:C	3	1.29
(1,98)	1:64:A:TYR:N	1:64:A:TYR:CA	1:64:A:TYR:C	1:65:A:ASP:N	8	1.28
(1,10)	1:11:A:PHE:N	1:11:A:PHE:CA	1:11:A:PHE:C	1:12:A:GLU:N	2	1.26
(1,37)	1:28:A:VAL:C	1:29:A:LYS:N	1:29:A:LYS:CA	1:29:A:LYS:C	7	1.25
(1,109)	1:70:A:LYS:C	1:71:A:GLY:N	1:71:A:GLY:CA	1:71:A:GLY:C	1	1.24
(1,59)	1:41:A:SER:C	1:42:A:GLY:N	1:42:A:GLY:CA	1:42:A:GLY:C	4	1.24
(1,32)	1:26:A:PHE:N	1:26:A:PHE:CA	1:26:A:PHE:C	1:27:A:ARG:N	7	1.24
(1,56)	1:40:A:VAL:N	1:40:A:VAL:CA	1:40:A:VAL:C	1:41:A:SER:N	2	1.23
(1,99)	1:64:A:TYR:C	1:65:A:ASP:N	1:65:A:ASP:CA	1:65:A:ASP:C	7	1.22
(1,93)	1:61:A:MET:C	1:62:A:SER:N	1:62:A:SER:CA	1:62:A:SER:C	3	1.22
(1,12)	1:12:A:GLU:N	1:12:A:GLU:CA	1:12:A:GLU:C	1:13:A:VAL:N	3	1.22
(1,124)	1:78:A:LYS:N	1:78:A:LYS:CA	1:78:A:LYS:C	1:79:A:GLY:N	5	1.2
(1,93)	1:61:A:MET:C	1:62:A:SER:N	1:62:A:SER:CA	1:62:A:SER:C	1	1.2
(1,78)	1:52:A:ILE:N	1:52:A:ILE:CA	1:52:A:ILE:C	1:53:A:ILE:N	3	1.2
(1,118)	1:75:A:ARG:N	1:75:A:ARG:CA	1:75:A:ARG:C	1:76:A:ARG:N	3	1.19
(1,118)	1:75:A:ARG:N	1:75:A:ARG:CA	1:75:A:ARG:C	1:76:A:ARG:N	8	1.18
(1,79)	1:52:A:ILE:C	1:53:A:ILE:N	1:53:A:ILE:CA	1:53:A:ILE:C	6	1.18
(1,79)	1:52:A:ILE:C	1:53:A:ILE:N	1:53:A:ILE:CA	1:53:A:ILE:C	5	1.15
(1,111)	1:71:A:GLY:C	1:72:A:ARG:N	1:72:A:ARG:CA	1:72:A:ARG:C	1	1.14
(1,93)	1:61:A:MET:C	1:62:A:SER:N	1:62:A:SER:CA	1:62:A:SER:C	8	1.14

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,30)	1:25:A:GLU:N	1:25:A:GLU:CA	1:25:A:GLU:C	1:26:A:PHE:N	8	1.14
(1,26)	1:20:A:LEU:N	1:20:A:LEU:CA	1:20:A:LEU:C	1:21:A:LEU:N	4	1.14
(1,98)	1:64:A:TYR:N	1:64:A:TYR:CA	1:64:A:TYR:C	1:65:A:ASP:N	3	1.12
(1,82)	1:56:A:ARG:N	1:56:A:ARG:CA	1:56:A:ARG:C	1:57:A:VAL:N	3	1.12
(1,119)	1:75:A:ARG:C	1:76:A:ARG:N	1:76:A:ARG:CA	1:76:A:ARG:C	10	1.11
(1,93)	1:61:A:MET:C	1:62:A:SER:N	1:62:A:SER:CA	1:62:A:SER:C	10	1.11
(1,99)	1:64:A:TYR:C	1:65:A:ASP:N	1:65:A:ASP:CA	1:65:A:ASP:C	5	1.09
(1,53)	1:38:A:CYS:C	1:39:A:HIS:N	1:39:A:HIS:CA	1:39:A:HIS:C	10	1.08
(1,38)	1:29:A:LYS:N	1:29:A:LYS:CA	1:29:A:LYS:C	1:30:A:LEU:N	10	1.08
(1,81)	1:55:A:ASP:C	1:56:A:ARG:N	1:56:A:ARG:CA	1:56:A:ARG:C	10	1.07
(1,44)	1:34:A:HIS:N	1:34:A:HIS:CA	1:34:A:HIS:C	1:35:A:GLU:N	8	1.07
(1,24)	1:19:A:ALA:N	1:19:A:ALA:CA	1:19:A:ALA:C	1:20:A:LEU:N	5	1.05
(1,15)	1:13:A:VAL:C	1:14:A:GLU:N	1:14:A:GLU:CA	1:14:A:GLU:C	9	1.05
(1,14)	1:13:A:VAL:N	1:13:A:VAL:CA	1:13:A:VAL:C	1:14:A:GLU:N	1	1.05
(1,96)	1:63:A:ILE:N	1:63:A:ILE:CA	1:63:A:ILE:C	1:64:A:TYR:N	7	1.04
(1,104)	1:67:A:ASN:N	1:67:A:ASN:CA	1:67:A:ASN:C	1:68:A:ALA:N	1	1.03
(1,90)	1:60:A:GLU:N	1:60:A:GLU:CA	1:60:A:GLU:C	1:61:A:MET:N	1	1.02
(1,78)	1:52:A:ILE:N	1:52:A:ILE:CA	1:52:A:ILE:C	1:53:A:ILE:N	7	1.02
(1,112)	1:72:A:ARG:N	1:72:A:ARG:CA	1:72:A:ARG:C	1:73:A:ILE:N	10	1.01
(1,26)	1:20:A:LEU:N	1:20:A:LEU:CA	1:20:A:LEU:C	1:21:A:LEU:N	9	1.01
(1,16)	1:14:A:GLU:N	1:14:A:GLU:CA	1:14:A:GLU:C	1:15:A:GLY:N	1	1.01
(1,88)	1:59:A:VAL:N	1:59:A:VAL:CA	1:59:A:VAL:C	1:60:A:GLU:N	1	1.0
(1,81)	1:55:A:ASP:C	1:56:A:ARG:N	1:56:A:ARG:CA	1:56:A:ARG:C	1	1.0