



Full wwPDB NMR Structure Validation Report ⓘ

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

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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

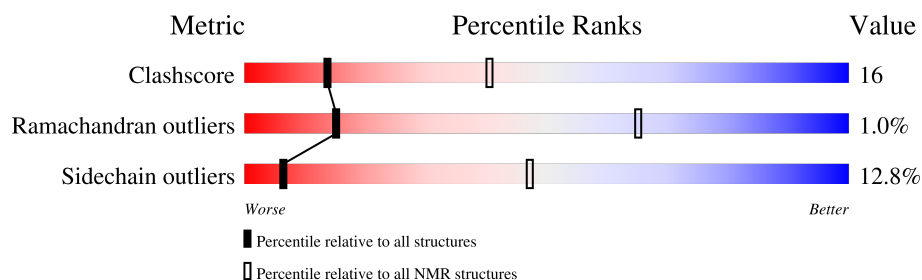
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 88%.

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	76	

2 Ensemble composition and analysis

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

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:1-A:71 (71)	0.38	1

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

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

NmrClust was unable to cluster the ensemble.

Error message: Inconsistent models

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1232 atoms, of which 632 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Polyubiquitin-B.

Mol	Chain	Residues	Atoms						Trace
1	A	76	Total	C	H	N	O	S	0
			1232	378	632	103	118	1	

There are 4 discrepancies between the modelled and reference sequences:

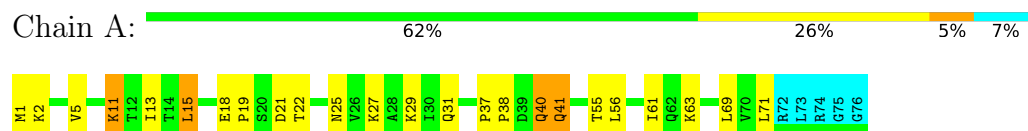
Chain	Residue	Modelled	Actual	Comment	Reference
A	2	LYS	GLN	conflict	UNP J3QS39
A	33	GLU	LYS	conflict	UNP J3QS39
A	49	LYS	GLN	conflict	UNP J3QS39
A	60	SER	ASN	conflict	UNP J3QS39

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: Polyubiquitin-B

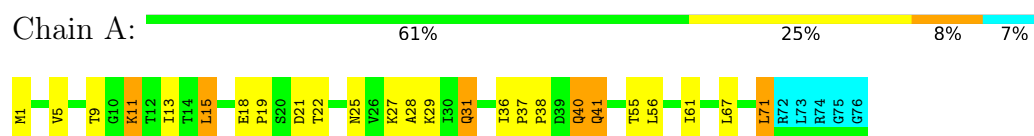


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

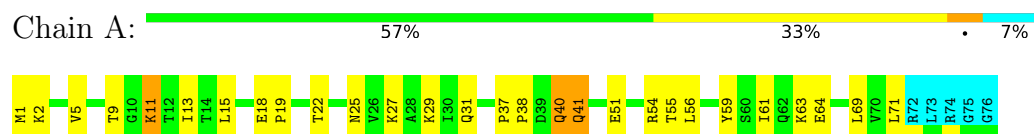
4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Polyubiquitin-B



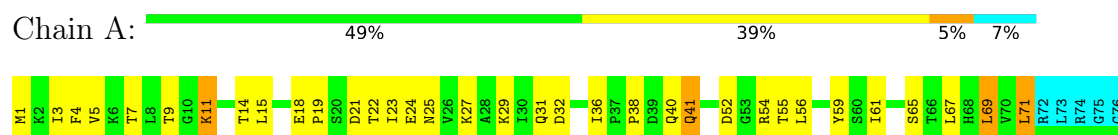
4.2.2 Score per residue for model 2

- Molecule 1: Polyubiquitin-B



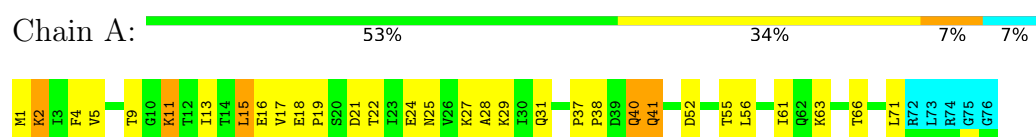
4.2.3 Score per residue for model 3

- Molecule 1: Polyubiquitin-B



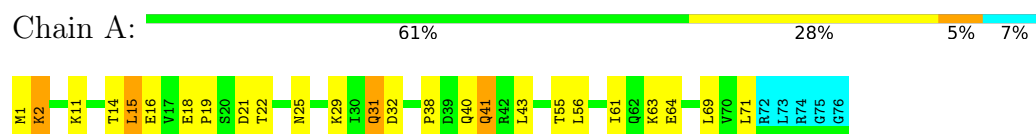
4.2.4 Score per residue for model 4

- Molecule 1: Polyubiquitin-B



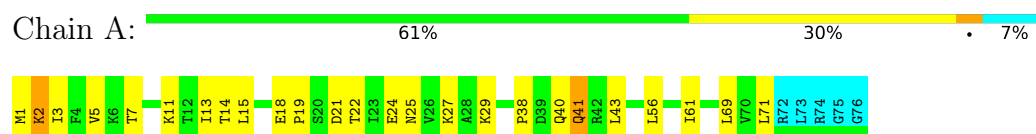
4.2.5 Score per residue for model 5

- Molecule 1: Polyubiquitin-B



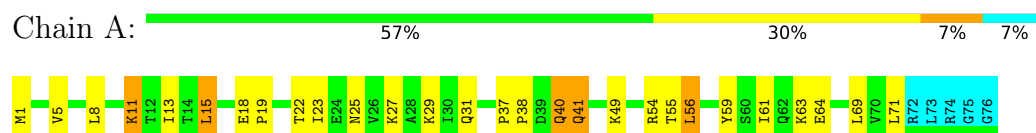
4.2.6 Score per residue for model 6

- Molecule 1: Polyubiquitin-B



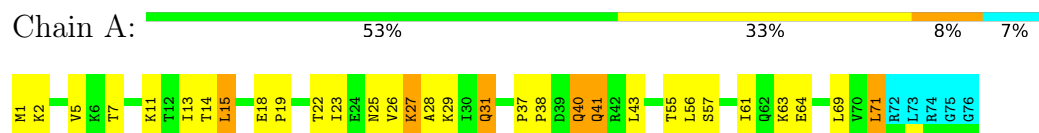
4.2.7 Score per residue for model 7

- Molecule 1: Polyubiquitin-B



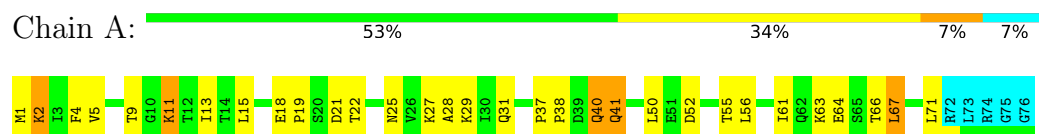
4.2.8 Score per residue for model 8

- Molecule 1: Polyubiquitin-B



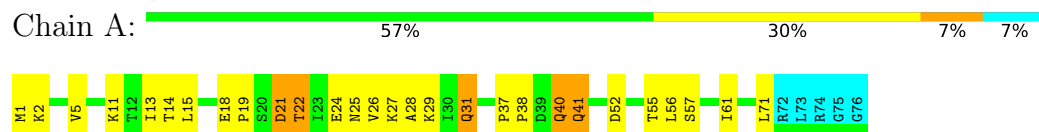
4.2.9 Score per residue for model 9

- Molecule 1: Polyubiquitin-B



4.2.10 Score per residue for model 10

- Molecule 1: Polyubiquitin-B



5 Refinement protocol and experimental data overview

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

Of the 500 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
ARIA2alpha	structure calculation	

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	921
Number of shifts mapped to atoms	921
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	88%

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	561	589	588	18±3
All	All	5610	5890	5880	183

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 16.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:19:PRO:HA	1:A:56:LEU:HB2	0.62	1.71	9	10
1:A:38:PRO:HA	1:A:41:GLN:CG	0.61	2.26	1	10
1:A:19:PRO:HB3	1:A:61:ILE:O	0.61	1.95	7	2
1:A:37:PRO:HB2	1:A:40:GLN:NE2	0.60	2.11	9	7
1:A:22:THR:OG1	1:A:55:THR:HG22	0.60	1.97	2	1
1:A:19:PRO:HA	1:A:56:LEU:CB	0.59	2.27	7	1
1:A:1:MET:HE2	1:A:18:GLU:HG2	0.56	1.78	9	8
1:A:28:ALA:O	1:A:31:GLN:HG2	0.56	2.01	4	1
1:A:1:MET:HE3	1:A:63:LYS:HB2	0.56	1.77	4	1
1:A:9:THR:OG1	1:A:11:LYS:HG3	0.55	2.02	9	5
1:A:28:ALA:HA	1:A:31:GLN:HG2	0.55	1.79	10	3
1:A:19:PRO:HA	1:A:56:LEU:HD12	0.54	1.80	2	1
1:A:1:MET:SD	1:A:63:LYS:HD2	0.54	2.43	4	1
1:A:38:PRO:HA	1:A:41:GLN:HG3	0.54	1.78	6	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:3:ILE:O	1:A:14:THR:HA	0.53	2.03	3	2
1:A:8:LEU:HG	1:A:69:LEU:O	0.53	2.04	7	1
1:A:25:ASN:OD1	1:A:29:LYS:HE2	0.53	2.04	10	2
1:A:25:ASN:O	1:A:29:LYS:HG2	0.52	2.05	9	10
1:A:1:MET:SD	1:A:18:GLU:HG2	0.52	2.45	8	1
1:A:31:GLN:CD	1:A:38:PRO:HD3	0.52	2.30	3	1
1:A:1:MET:HG3	1:A:18:GLU:HG2	0.52	1.82	9	7
1:A:19:PRO:CA	1:A:56:LEU:HB2	0.51	2.36	10	5
1:A:23:ILE:HD13	1:A:56:LEU:HD23	0.51	1.83	8	2
1:A:22:THR:HA	1:A:55:THR:HA	0.51	1.83	1	9
1:A:5:VAL:CG1	1:A:13:ILE:HB	0.49	2.38	4	8
1:A:36:ILE:HG23	1:A:71:LEU:HD11	0.49	1.84	3	2
1:A:7:THR:OG1	1:A:11:LYS:HG2	0.49	2.07	8	1
1:A:28:ALA:O	1:A:31:GLN:HB2	0.48	2.08	9	1
1:A:56:LEU:HB3	1:A:61:ILE:HB	0.48	1.86	5	9
1:A:21:ASP:O	1:A:56:LEU:HG	0.48	2.09	9	5
1:A:26:VAL:HG21	1:A:56:LEU:HD21	0.48	1.85	8	1
1:A:1:MET:HG3	1:A:18:GLU:CG	0.47	2.39	5	2
1:A:63:LYS:HG2	1:A:64:GLU:N	0.47	2.24	2	5
1:A:15:LEU:CD1	1:A:29:LYS:HB3	0.46	2.40	7	2
1:A:22:THR:OG1	1:A:24:GLU:HG2	0.46	2.10	4	1
1:A:22:THR:HG23	1:A:54:ARG:C	0.46	2.35	7	2
1:A:15:LEU:HD11	1:A:29:LYS:CB	0.46	2.40	8	1
1:A:4:PHE:HB2	1:A:65:SER:O	0.46	2.10	3	1
1:A:37:PRO:HB2	1:A:40:GLN:HE22	0.46	1.71	2	4
1:A:43:LEU:HD12	1:A:43:LEU:N	0.45	2.25	8	3
1:A:22:THR:HB	1:A:24:GLU:OE1	0.45	2.12	6	1
1:A:15:LEU:HD13	1:A:16:GLU:N	0.45	2.27	4	1
1:A:22:THR:O	1:A:26:VAL:HG23	0.45	2.11	10	1
1:A:22:THR:HG23	1:A:54:ARG:O	0.45	2.12	2	2
1:A:21:ASP:O	1:A:25:ASN:HB3	0.45	2.12	10	1
1:A:23:ILE:HD13	1:A:54:ARG:O	0.45	2.12	7	1
1:A:18:GLU:O	1:A:21:ASP:HB2	0.44	2.13	1	2
1:A:38:PRO:HA	1:A:41:GLN:HG2	0.44	1.88	9	1
1:A:15:LEU:HD13	1:A:16:GLU:H	0.44	1.70	5	1
1:A:19:PRO:HA	1:A:56:LEU:HB3	0.43	1.89	7	1
1:A:2:LYS:CD	1:A:14:THR:HG22	0.43	2.43	5	1
1:A:4:PHE:O	1:A:66:THR:HA	0.43	2.13	4	2
1:A:19:PRO:O	1:A:56:LEU:HB2	0.43	2.14	2	1
1:A:1:MET:HG2	1:A:17:VAL:O	0.43	2.14	4	1
1:A:7:THR:HA	1:A:69:LEU:CB	0.42	2.44	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:54:ARG:HD2	1:A:59:TYR:CE2	0.42	2.49	7	2
1:A:29:LYS:O	1:A:32:ASP:HB3	0.42	2.15	3	1
1:A:50:LEU:HD11	1:A:67:LEU:HD11	0.42	1.92	9	1
1:A:5:VAL:HG13	1:A:13:ILE:HB	0.41	1.92	4	1
1:A:31:GLN:HG3	1:A:32:ASP:N	0.41	2.29	5	1
1:A:24:GLU:HB3	1:A:52:ASP:HB2	0.41	1.93	3	1
1:A:2:LYS:HD2	1:A:14:THR:HG22	0.41	1.90	5	1
1:A:41:GLN:HG3	1:A:41:GLN:O	0.41	2.16	3	1
1:A:23:ILE:O	1:A:27:LYS:HG3	0.41	2.16	8	1
1:A:7:THR:HA	1:A:69:LEU:HB3	0.41	1.92	3	1
1:A:51:GLU:HG2	1:A:59:TYR:OH	0.40	2.16	2	1
1:A:5:VAL:HA	1:A:67:LEU:O	0.40	2.16	3	1
1:A:24:GLU:HB3	1:A:52:ASP:CB	0.40	2.46	10	1
1:A:11:LYS:HE2	1:A:13:ILE:HG12	0.40	1.93	7	1
1:A:27:LYS:HB3	1:A:41:GLN:NE2	0.40	2.31	8	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	70/76 (92%)	67±1 (96±2%)	2±1 (3±2%)	1±1 (1±1%)	15	65
All	All	700/760 (92%)	673 (96%)	20 (3%)	7 (1%)	15	65

All 2 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	2	LYS	6
1	A	22	THR	1

6.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR

entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	65/68 (96%)	57±1 (87±2%)	8±1 (13±2%)	6	47
All	All	650/680 (96%)	567 (87%)	83 (13%)	6	47

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	15	LEU	10
1	A	40	GLN	10
1	A	41	GLN	10
1	A	71	LEU	10
1	A	11	LYS	9
1	A	27	LYS	9
1	A	31	GLN	6
1	A	69	LEU	4
1	A	2	LYS	4
1	A	67	LEU	2
1	A	52	ASP	2
1	A	14	THR	2
1	A	57	SER	2
1	A	49	LYS	1
1	A	56	LEU	1
1	A	21	ASP	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry

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 88% for the well-defined parts and 86% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list*

7.1.1 Bookkeeping

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

Total number of shifts	921
Number of shifts mapped to atoms	921
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	74	-0.08 ± 0.15	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	68	0.21 ± 0.14	None needed (< 0.5 ppm)
$^{13}\text{C}'$	70	-0.13 ± 0.23	None needed (< 0.5 ppm)
^{15}N	70	0.63 ± 0.54	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 88%, i.e. 877 atoms were assigned a chemical shift out of a possible 992. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	342/353 (97%)	140/143 (98%)	136/142 (96%)	66/68 (97%)
Sidechain	531/602 (88%)	360/390 (92%)	166/193 (86%)	5/19 (26%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	4/37 (11%)	4/18 (22%)	0/17 (0%)	0/2 (0%)
Overall	877/992 (88%)	504/551 (91%)	302/352 (86%)	71/89 (80%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 86%, i.e. 921 atoms were assigned a chemical shift out of a possible 1068. 0 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	364/380 (96%)	150/155 (97%)	144/152 (95%)	70/73 (96%)
Sidechain	553/651 (85%)	375/421 (89%)	173/205 (84%)	5/25 (20%)
Aromatic	4/37 (11%)	4/18 (22%)	0/17 (0%)	0/2 (0%)
Overall	921/1068 (86%)	529/594 (89%)	317/374 (85%)	75/100 (75%)

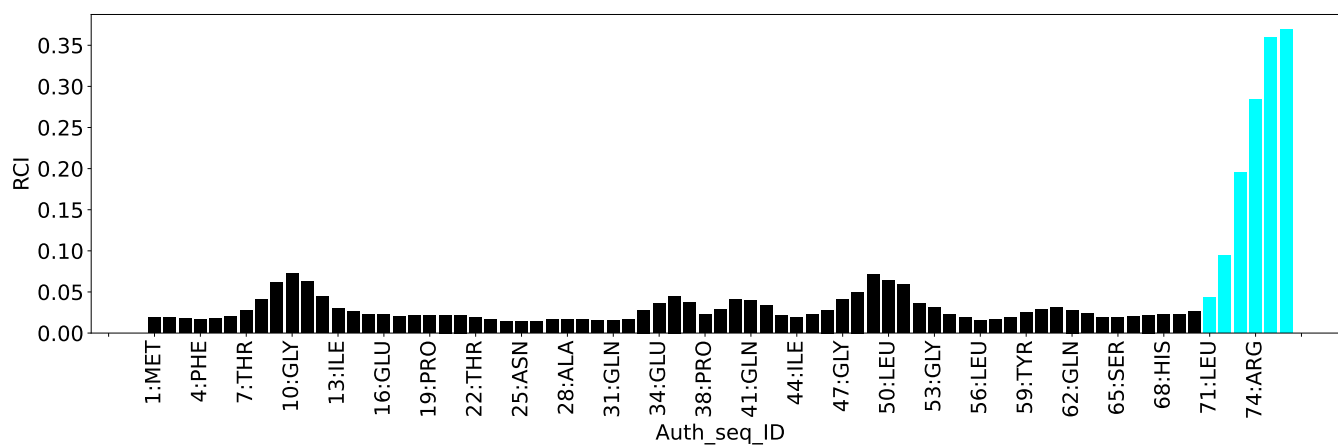
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	1282
Intra-residue ($ i-j =0$)	565
Sequential ($ i-j =1$)	240
Medium range ($ i-j >1$ and $ i-j <5$)	173
Long range ($ i-j \geq 5$)	304
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	16.9
Number of long range restraints per residue ¹	4.0

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)	34.3	0.2
0.2-0.5 (Medium)	32.2	0.5
>0.5 (Large)	47.5	2.63

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

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

9 Distance violation analysis ⓘ

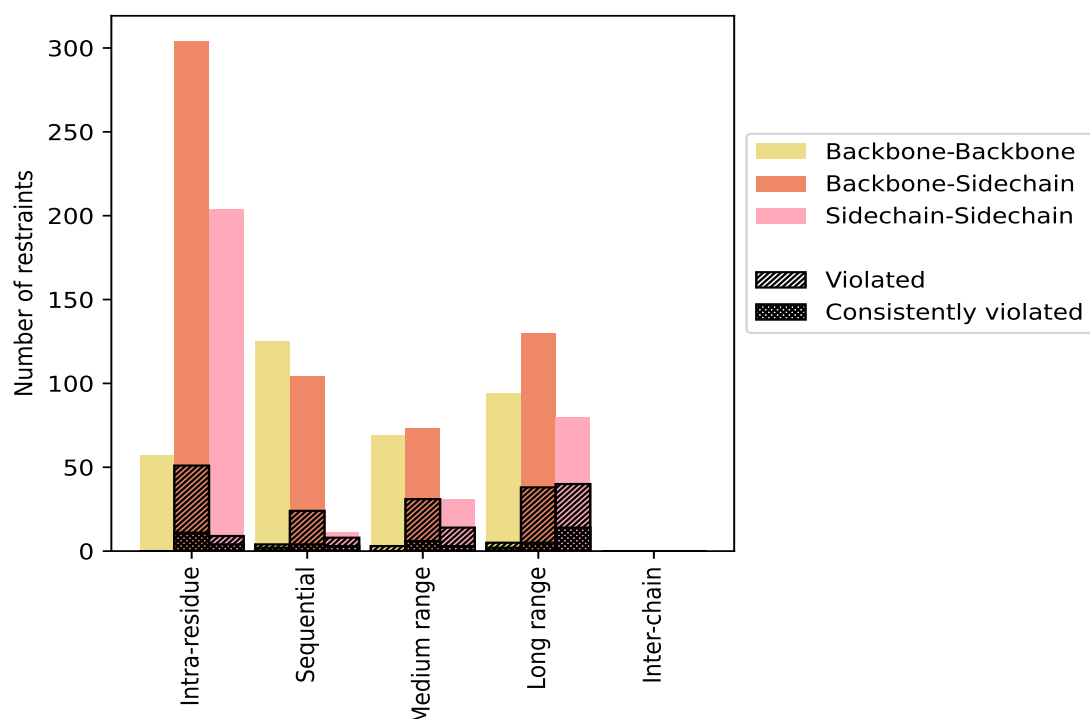
9.1 Summary of distance violations ⓘ

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

Restraints type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	565	44.1	60	10.6	4.7	15	2.7	1.2
Backbone-Backbone	57	4.4	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	304	23.7	51	16.8	4.0	11	3.6	0.9
Sidechain-Sidechain	204	15.9	9	4.4	0.7	4	2.0	0.3
Sequential ($i-j =1$)	240	18.7	36	15.0	2.8	9	3.8	0.7
Backbone-Backbone	125	9.8	4	3.2	0.3	2	1.6	0.2
Backbone-Sidechain	104	8.1	24	23.1	1.9	4	3.8	0.3
Sidechain-Sidechain	11	0.9	8	72.7	0.6	3	27.3	0.2
Medium range ($i-j >1$ & $i-j <5$)	173	13.5	48	27.7	3.7	9	5.2	0.7
Backbone-Backbone	69	5.4	3	4.3	0.2	0	0.0	0.0
Backbone-Sidechain	73	5.7	31	42.5	2.4	6	8.2	0.5
Sidechain-Sidechain	31	2.4	14	45.2	1.1	3	9.7	0.2
Long range ($i-j \geq 5$)	304	23.7	83	27.3	6.5	21	6.9	1.6
Backbone-Backbone	94	7.3	5	5.3	0.4	2	2.1	0.2
Backbone-Sidechain	130	10.1	38	29.2	3.0	5	3.8	0.4
Sidechain-Sidechain	80	6.2	40	50.0	3.1	14	17.5	1.1
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1282	100.0	227	17.7	17.7	54	4.2	4.2
Backbone-Backbone	345	26.9	12	3.5	0.9	4	1.2	0.3
Backbone-Sidechain	611	47.7	144	23.6	11.2	26	4.3	2.0
Sidechain-Sidechain	326	25.4	71	21.8	5.5	24	7.4	1.9

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

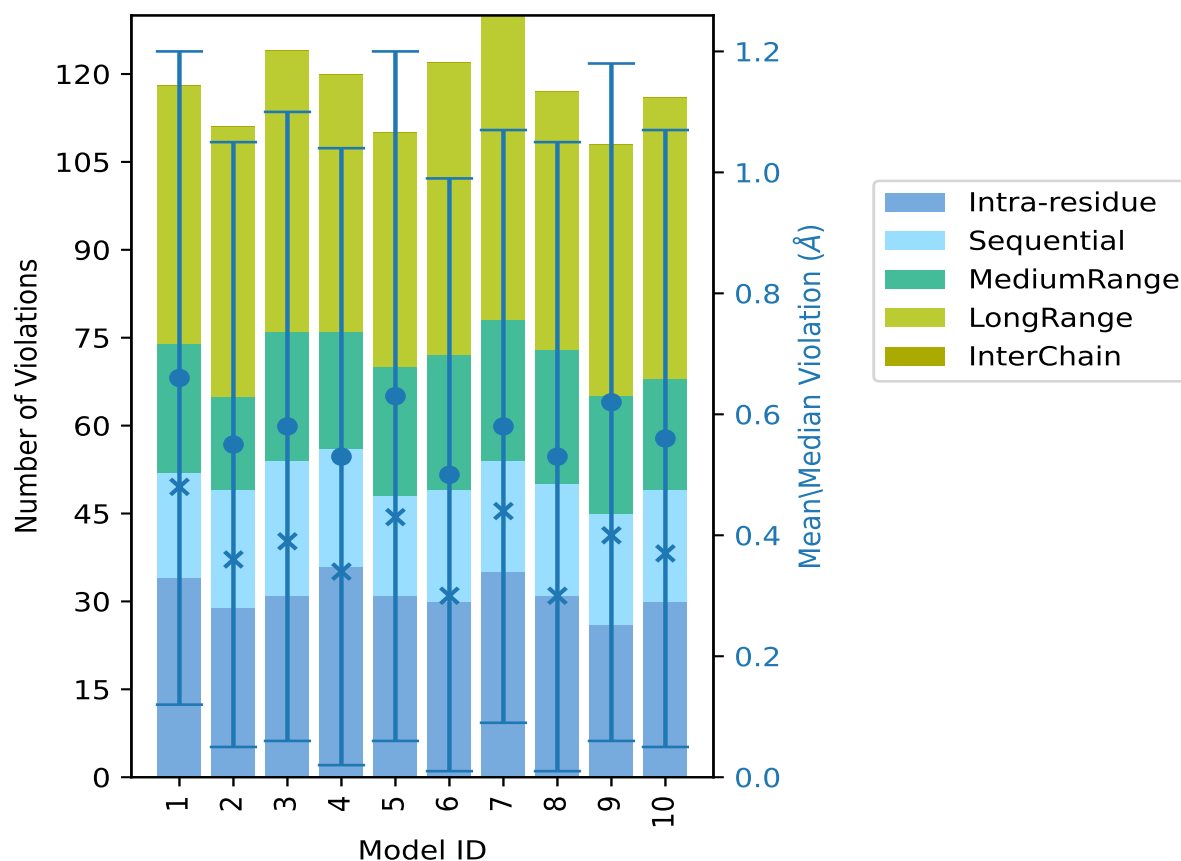
9.2 Distance violation statistics for each model [i](#)

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	34	18	22	44	0	118	0.66	2.37	0.54	0.48
2	29	20	16	46	0	111	0.55	2.43	0.5	0.36
3	31	23	22	48	0	124	0.58	2.32	0.52	0.39
4	36	20	20	44	0	120	0.53	2.54	0.51	0.34
5	31	17	22	40	0	110	0.63	2.63	0.57	0.43
6	30	19	23	50	0	122	0.5	2.37	0.49	0.3
7	35	19	24	52	0	130	0.58	2.27	0.49	0.44
8	31	19	23	44	0	117	0.53	2.44	0.52	0.3
9	26	19	20	43	0	108	0.62	2.37	0.56	0.4
10	30	19	19	48	0	116	0.56	2.34	0.51	0.37

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

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



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

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

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1055(IR:505, SQ:204, MR:125, LR:221, 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	7	10	22	0	51	1	10.0
9	5	9	8	0	31	2	20.0
9	3	3	5	0	20	3	30.0

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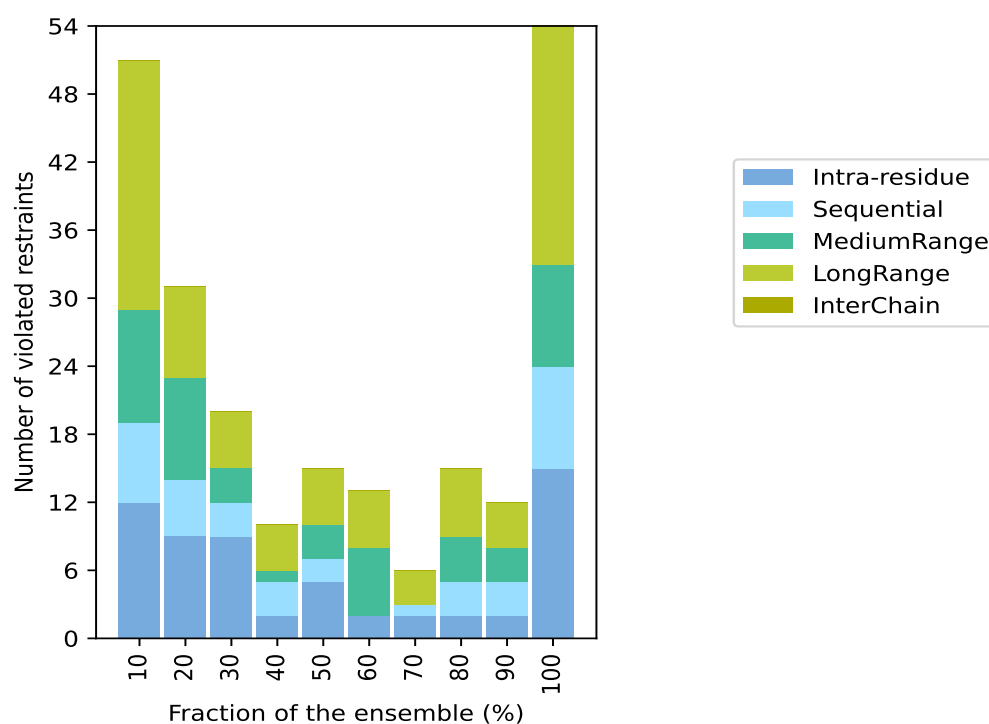
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
2	3	1	4	0	10	4	40.0
5	2	3	5	0	15	5	50.0
2	0	6	5	0	13	6	60.0
2	1	0	3	0	6	7	70.0
2	3	4	6	0	15	8	80.0
2	3	3	4	0	12	9	90.0
15	9	9	21	0	54	10	100.0

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

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

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

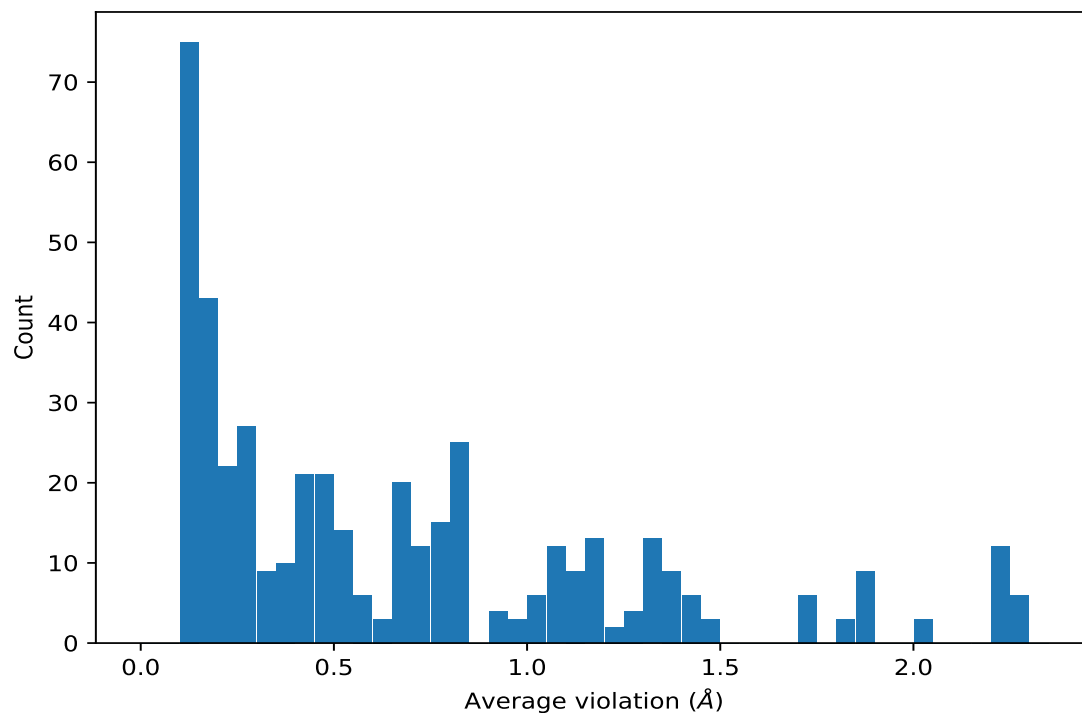


9.4 Most violated distance restraints in the ensemble [i](#)

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

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

in the ensemble



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,118)	1:17:A:VAL:HG21	1:29:A:LYS:HD2	10	2.3	0.09	2.3
(1,118)	1:17:A:VAL:HG21	1:29:A:LYS:HD3	10	2.3	0.09	2.3
(1,118)	1:17:A:VAL:HG22	1:29:A:LYS:HD2	10	2.3	0.09	2.3
(1,118)	1:17:A:VAL:HG22	1:29:A:LYS:HD3	10	2.3	0.09	2.3
(1,118)	1:17:A:VAL:HG23	1:29:A:LYS:HD2	10	2.3	0.09	2.3
(1,118)	1:17:A:VAL:HG23	1:29:A:LYS:HD3	10	2.3	0.09	2.3
(1,594)	1:3:A:ILE:HD11	1:56:A:LEU:HD21	10	2.23	0.46	2.37
(1,594)	1:3:A:ILE:HD11	1:56:A:LEU:HD22	10	2.23	0.46	2.37
(1,594)	1:3:A:ILE:HD11	1:56:A:LEU:HD23	10	2.23	0.46	2.37
(1,594)	1:3:A:ILE:HD12	1:56:A:LEU:HD21	10	2.23	0.46	2.37
(1,594)	1:3:A:ILE:HD12	1:56:A:LEU:HD22	10	2.23	0.46	2.37
(1,594)	1:3:A:ILE:HD12	1:56:A:LEU:HD23	10	2.23	0.46	2.37
(1,594)	1:3:A:ILE:HD13	1:56:A:LEU:HD21	10	2.23	0.46	2.37
(1,594)	1:3:A:ILE:HD13	1:56:A:LEU:HD22	10	2.23	0.46	2.37
(1,594)	1:3:A:ILE:HD13	1:56:A:LEU:HD23	10	2.23	0.46	2.37

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1167)	1:50:A:LEU:HD21	1:68:A:HIS:H	10	2.0	0.12	1.98
(1,1167)	1:50:A:LEU:HD22	1:68:A:HIS:H	10	2.0	0.12	1.98
(1,1167)	1:50:A:LEU:HD23	1:68:A:HIS:H	10	2.0	0.12	1.98
(1,28)	1:23:A:ILE:HD13	1:50:A:LEU:HB2	10	1.8	0.42	2.0
(1,28)	1:23:A:ILE:HD11	1:50:A:LEU:HB2	10	1.8	0.42	2.0
(1,28)	1:23:A:ILE:HD12	1:50:A:LEU:HB2	10	1.8	0.42	2.0
(1,106)	1:26:A:VAL:HG21	1:27:A:LYS:HA	10	1.74	0.02	1.74
(1,106)	1:26:A:VAL:HG22	1:27:A:LYS:HA	10	1.74	0.02	1.74
(1,106)	1:26:A:VAL:HG23	1:27:A:LYS:HA	10	1.74	0.02	1.74
(1,346)	1:17:A:VAL:HG21	1:29:A:LYS:HE2	10	1.45	0.17	1.48
(1,346)	1:17:A:VAL:HG21	1:29:A:LYS:HE3	10	1.45	0.17	1.48
(1,346)	1:17:A:VAL:HG22	1:29:A:LYS:HE2	10	1.45	0.17	1.48
(1,346)	1:17:A:VAL:HG22	1:29:A:LYS:HE3	10	1.45	0.17	1.48
(1,346)	1:17:A:VAL:HG23	1:29:A:LYS:HE2	10	1.45	0.17	1.48
(1,346)	1:17:A:VAL:HG23	1:29:A:LYS:HE3	10	1.45	0.17	1.48
(1,77)	1:17:A:VAL:HG11	1:3:A:ILE:HG21	10	1.35	0.2	1.29
(1,77)	1:17:A:VAL:HG11	1:3:A:ILE:HG22	10	1.35	0.2	1.29
(1,77)	1:17:A:VAL:HG11	1:3:A:ILE:HG23	10	1.35	0.2	1.29
(1,77)	1:17:A:VAL:HG12	1:3:A:ILE:HG21	10	1.35	0.2	1.29
(1,77)	1:17:A:VAL:HG12	1:3:A:ILE:HG22	10	1.35	0.2	1.29
(1,77)	1:17:A:VAL:HG12	1:3:A:ILE:HG23	10	1.35	0.2	1.29
(1,77)	1:17:A:VAL:HG13	1:3:A:ILE:HG21	10	1.35	0.2	1.29
(1,77)	1:17:A:VAL:HG13	1:3:A:ILE:HG22	10	1.35	0.2	1.29
(1,77)	1:17:A:VAL:HG13	1:3:A:ILE:HG23	10	1.35	0.2	1.29
(1,92)	1:17:A:VAL:HG11	1:1:A:MET:HE1	10	1.33	0.17	1.31
(1,92)	1:17:A:VAL:HG11	1:1:A:MET:HE2	10	1.33	0.17	1.31
(1,92)	1:17:A:VAL:HG11	1:1:A:MET:HE3	10	1.33	0.17	1.31
(1,92)	1:17:A:VAL:HG12	1:1:A:MET:HE1	10	1.33	0.17	1.31
(1,92)	1:17:A:VAL:HG12	1:1:A:MET:HE2	10	1.33	0.17	1.31
(1,92)	1:17:A:VAL:HG12	1:1:A:MET:HE3	10	1.33	0.17	1.31
(1,92)	1:17:A:VAL:HG13	1:1:A:MET:HE1	10	1.33	0.17	1.31
(1,92)	1:17:A:VAL:HG13	1:1:A:MET:HE2	10	1.33	0.17	1.31
(1,92)	1:17:A:VAL:HG13	1:1:A:MET:HE3	10	1.33	0.17	1.31
(1,1170)	1:26:A:VAL:HG11	1:18:A:GLU:H	10	1.31	0.3	1.32
(1,1170)	1:26:A:VAL:HG12	1:18:A:GLU:H	10	1.31	0.3	1.32
(1,1170)	1:26:A:VAL:HG13	1:18:A:GLU:H	10	1.31	0.3	1.32
(1,1268)	1:71:A:LEU:HG	1:40:A:GLN:HE22	10	1.3	0.16	1.3
(1,1123)	1:50:A:LEU:HD21	1:43:A:LEU:H	10	1.27	0.11	1.31
(1,1123)	1:50:A:LEU:HD22	1:43:A:LEU:H	10	1.27	0.11	1.31
(1,1123)	1:50:A:LEU:HD23	1:43:A:LEU:H	10	1.27	0.11	1.31
(1,322)	1:10:A:GLY:HA3	1:6:A:LYS:HE2	10	1.23	0.4	1.38
(1,322)	1:10:A:GLY:HA3	1:6:A:LYS:HE3	10	1.23	0.4	1.38

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,374)	1:26:A:VAL:HG11	1:21:A:ASP:HB3	10	1.2	0.23	1.16
(1,374)	1:26:A:VAL:HG12	1:21:A:ASP:HB3	10	1.2	0.23	1.16
(1,374)	1:26:A:VAL:HG13	1:21:A:ASP:HB3	10	1.2	0.23	1.16
(1,516)	1:26:A:VAL:HG11	1:56:A:LEU:HD11	10	1.18	0.19	1.08
(1,516)	1:26:A:VAL:HG11	1:56:A:LEU:HD12	10	1.18	0.19	1.08
(1,516)	1:26:A:VAL:HG11	1:56:A:LEU:HD13	10	1.18	0.19	1.08
(1,516)	1:26:A:VAL:HG12	1:56:A:LEU:HD11	10	1.18	0.19	1.08
(1,516)	1:26:A:VAL:HG12	1:56:A:LEU:HD12	10	1.18	0.19	1.08
(1,516)	1:26:A:VAL:HG12	1:56:A:LEU:HD13	10	1.18	0.19	1.08
(1,516)	1:26:A:VAL:HG13	1:56:A:LEU:HD11	10	1.18	0.19	1.08
(1,516)	1:26:A:VAL:HG13	1:56:A:LEU:HD12	10	1.18	0.19	1.08
(1,516)	1:26:A:VAL:HG13	1:56:A:LEU:HD13	10	1.18	0.19	1.08
(1,435)	1:33:A:GLU:HG2	1:15:A:LEU:HD11	10	1.13	0.26	1.04
(1,435)	1:33:A:GLU:HG2	1:15:A:LEU:HD12	10	1.13	0.26	1.04
(1,435)	1:33:A:GLU:HG2	1:15:A:LEU:HD13	10	1.13	0.26	1.04
(1,39)	1:3:A:ILE:HD11	1:17:A:VAL:HG11	10	1.09	0.23	1.07
(1,39)	1:3:A:ILE:HD11	1:17:A:VAL:HG12	10	1.09	0.23	1.07
(1,39)	1:3:A:ILE:HD11	1:17:A:VAL:HG13	10	1.09	0.23	1.07
(1,39)	1:3:A:ILE:HD12	1:17:A:VAL:HG11	10	1.09	0.23	1.07
(1,39)	1:3:A:ILE:HD12	1:17:A:VAL:HG12	10	1.09	0.23	1.07
(1,39)	1:3:A:ILE:HD12	1:17:A:VAL:HG13	10	1.09	0.23	1.07
(1,39)	1:3:A:ILE:HD13	1:17:A:VAL:HG11	10	1.09	0.23	1.07
(1,39)	1:3:A:ILE:HD13	1:17:A:VAL:HG12	10	1.09	0.23	1.07
(1,39)	1:3:A:ILE:HD13	1:17:A:VAL:HG13	10	1.09	0.23	1.07
(1,720)	1:26:A:VAL:HG11	1:26:A:VAL:H	10	0.85	0.0	0.85
(1,720)	1:26:A:VAL:HG12	1:26:A:VAL:H	10	0.85	0.0	0.85
(1,720)	1:26:A:VAL:HG13	1:26:A:VAL:H	10	0.85	0.0	0.85
(1,1143)	1:70:A:VAL:HG13	1:71:A:LEU:H	10	0.84	0.38	0.7
(1,1143)	1:70:A:VAL:HG11	1:71:A:LEU:H	10	0.84	0.38	0.7
(1,1143)	1:70:A:VAL:HG12	1:71:A:LEU:H	10	0.84	0.38	0.7
(1,580)	1:41:A:GLN:HG3	1:69:A:LEU:HD21	10	0.83	0.15	0.82
(1,580)	1:41:A:GLN:HG3	1:69:A:LEU:HD23	10	0.83	0.15	0.82
(1,580)	1:41:A:GLN:HG2	1:71:A:LEU:HD23	10	0.83	0.15	0.82
(1,580)	1:41:A:GLN:HG2	1:71:A:LEU:HD21	10	0.83	0.15	0.82
(1,282)	1:50:A:LEU:HD11	1:50:A:LEU:HA	10	0.82	0.03	0.82
(1,282)	1:50:A:LEU:HD12	1:50:A:LEU:HA	10	0.82	0.03	0.82
(1,282)	1:50:A:LEU:HD13	1:50:A:LEU:HA	10	0.82	0.03	0.82
(1,931)	1:17:A:VAL:HG11	1:3:A:ILE:H	10	0.81	0.25	0.78
(1,931)	1:17:A:VAL:HG12	1:3:A:ILE:H	10	0.81	0.25	0.78
(1,931)	1:17:A:VAL:HG13	1:3:A:ILE:H	10	0.81	0.25	0.78
(1,1013)	1:62:A:GLN:HB2	1:65:A:SER:H	10	0.78	0.16	0.82
(1,1013)	1:63:A:LYS:HB3	1:65:A:SER:H	10	0.78	0.16	0.82

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,430)	1:15:A:LEU:HD21	1:16:A:GLU:HG3	10	0.78	0.5	0.91
(1,430)	1:15:A:LEU:HD22	1:16:A:GLU:HG3	10	0.78	0.5	0.91
(1,430)	1:15:A:LEU:HD23	1:16:A:GLU:HG3	10	0.78	0.5	0.91
(1,729)	1:27:A:LYS:HB3	1:28:A:ALA:H	10	0.76	0.09	0.8
(1,513)	1:17:A:VAL:HG21	1:17:A:VAL:HA	10	0.74	0.01	0.74
(1,513)	1:17:A:VAL:HG22	1:17:A:VAL:HA	10	0.74	0.01	0.74
(1,513)	1:17:A:VAL:HG23	1:17:A:VAL:HA	10	0.74	0.01	0.74
(1,593)	1:3:A:ILE:HD11	1:15:A:LEU:HB2	10	0.68	0.13	0.72
(1,593)	1:3:A:ILE:HD12	1:15:A:LEU:HB2	10	0.68	0.13	0.72
(1,593)	1:3:A:ILE:HD13	1:15:A:LEU:HB2	10	0.68	0.13	0.72
(1,582)	1:55:A:THR:HB	1:19:A:PRO:HA	10	0.67	0.14	0.7
(1,582)	1:55:A:THR:HB	1:20:A:SER:HB3	10	0.67	0.14	0.7
(1,448)	1:30:A:ILE:HD11	1:27:A:LYS:HB2	10	0.66	0.26	0.65
(1,448)	1:30:A:ILE:HD12	1:27:A:LYS:HB2	10	0.66	0.26	0.65
(1,448)	1:30:A:ILE:HD13	1:27:A:LYS:HB2	10	0.66	0.26	0.65
(1,134)	1:26:A:VAL:HG11	1:23:A:ILE:HA	10	0.55	0.12	0.51
(1,134)	1:26:A:VAL:HG12	1:23:A:ILE:HA	10	0.55	0.12	0.51
(1,134)	1:26:A:VAL:HG13	1:23:A:ILE:HA	10	0.55	0.12	0.51
(1,188)	1:26:A:VAL:HG11	1:23:A:ILE:HA	10	0.52	0.12	0.47
(1,188)	1:26:A:VAL:HG12	1:23:A:ILE:HA	10	0.52	0.12	0.47
(1,188)	1:26:A:VAL:HG13	1:23:A:ILE:HA	10	0.52	0.12	0.47
(1,743)	1:30:A:ILE:HG12	1:30:A:ILE:H	10	0.51	0.04	0.5
(1,120)	1:17:A:VAL:HG21	1:17:A:VAL:HA	10	0.46	0.01	0.46
(1,120)	1:17:A:VAL:HG22	1:17:A:VAL:HA	10	0.46	0.01	0.46
(1,120)	1:17:A:VAL:HG23	1:17:A:VAL:HA	10	0.46	0.01	0.46
(1,125)	1:26:A:VAL:HG11	1:56:A:LEU:HD11	10	0.44	0.2	0.35
(1,125)	1:26:A:VAL:HG11	1:56:A:LEU:HD12	10	0.44	0.2	0.35
(1,125)	1:26:A:VAL:HG11	1:56:A:LEU:HD13	10	0.44	0.2	0.35
(1,125)	1:26:A:VAL:HG12	1:56:A:LEU:HD11	10	0.44	0.2	0.35
(1,125)	1:26:A:VAL:HG12	1:56:A:LEU:HD12	10	0.44	0.2	0.35
(1,125)	1:26:A:VAL:HG12	1:56:A:LEU:HD13	10	0.44	0.2	0.35
(1,125)	1:26:A:VAL:HG13	1:56:A:LEU:HD11	10	0.44	0.2	0.35
(1,125)	1:26:A:VAL:HG13	1:56:A:LEU:HD12	10	0.44	0.2	0.35
(1,125)	1:26:A:VAL:HG13	1:56:A:LEU:HD13	10	0.44	0.2	0.35
(1,966)	1:26:A:VAL:HG12	1:29:A:LYS:H	10	0.44	0.07	0.45
(1,966)	1:26:A:VAL:HG11	1:29:A:LYS:H	10	0.44	0.07	0.45
(1,966)	1:26:A:VAL:HG13	1:29:A:LYS:H	10	0.44	0.07	0.45
(1,532)	1:6:A:LYS:HE2	1:6:A:LYS:HE3	10	0.4	0.0	0.4
(1,499)	1:25:A:ASN:HA	1:25:A:ASN:HB2	10	0.38	0.23	0.38
(1,559)	1:56:A:LEU:HD21	1:22:A:THR:HA	10	0.36	0.47	0.22
(1,559)	1:56:A:LEU:HD22	1:22:A:THR:HA	10	0.36	0.47	0.22
(1,559)	1:56:A:LEU:HD23	1:22:A:THR:HA	10	0.36	0.47	0.22

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,744)	1:29:A:LYS:HG2	1:30:A:ILE:H	10	0.36	0.05	0.36
(1,573)	1:40:A:GLN:HG2	1:40:A:GLN:HA	10	0.33	0.03	0.34
(1,573)	1:40:A:GLN:HG3	1:40:A:GLN:HA	10	0.33	0.03	0.34
(1,539)	1:10:A:GLY:HA3	1:11:A:LYS:HA	10	0.33	0.04	0.33
(1,444)	1:6:A:LYS:HD2	1:6:A:LYS:HB3	10	0.31	0.03	0.3
(1,1280)	1:15:A:LEU:HB2	1:17:A:VAL:H	10	0.29	0.14	0.28
(1,545)	1:63:A:LYS:HA	1:18:A:GLU:HA	10	0.28	0.04	0.27
(1,696)	1:18:A:GLU:HB3	1:18:A:GLU:H	10	0.26	0.03	0.26
(1,1254)	1:41:A:GLN:HB2	1:40:A:GLN:HE22	10	0.22	0.04	0.24
(1,1254)	1:41:A:GLN:HB3	1:40:A:GLN:HE22	10	0.22	0.04	0.24
(1,541)	1:12:A:THR:HA	1:11:A:LYS:HA	10	0.22	0.02	0.22
(1,575)	1:41:A:GLN:HB2	1:40:A:GLN:HG2	10	0.19	0.04	0.2
(1,575)	1:41:A:GLN:HB2	1:40:A:GLN:HG3	10	0.19	0.04	0.2
(1,575)	1:41:A:GLN:HB3	1:40:A:GLN:HG2	10	0.19	0.04	0.2
(1,575)	1:41:A:GLN:HB3	1:40:A:GLN:HG3	10	0.19	0.04	0.2
(1,517)	1:7:A:THR:HB	1:7:A:THR:HA	10	0.18	0.04	0.18
(1,568)	1:29:A:LYS:HE2	1:29:A:LYS:HE3	10	0.18	0.0	0.18
(1,579)	1:38:A:PRO:HG3	1:41:A:GLN:HG2	10	0.17	0.02	0.18
(1,579)	1:38:A:PRO:HG3	1:41:A:GLN:HG3	10	0.17	0.02	0.18
(1,596)	1:30:A:ILE:HA	1:30:A:ILE:HD11	10	0.14	0.02	0.13
(1,596)	1:30:A:ILE:HA	1:30:A:ILE:HD12	10	0.14	0.02	0.13
(1,596)	1:30:A:ILE:HA	1:30:A:ILE:HD13	10	0.14	0.02	0.13
(1,1001)	1:56:A:LEU:HA	1:57:A:SER:H	10	0.13	0.01	0.13
(1,504)	1:58:A:ASP:HB2	1:58:A:ASP:HA	10	0.12	0.01	0.12
(1,542)	1:11:A:LYS:HD2	1:11:A:LYS:HD3	10	0.11	0.0	0.11
(1,328)	1:69:A:LEU:HB2	1:69:A:LEU:HD11	9	0.53	0.01	0.53
(1,328)	1:69:A:LEU:HB2	1:69:A:LEU:HD12	9	0.53	0.01	0.53
(1,328)	1:69:A:LEU:HB2	1:69:A:LEU:HD13	9	0.53	0.01	0.53
(1,704)	1:18:A:GLU:HB3	1:21:A:ASP:H	9	0.48	0.25	0.48
(1,56)	1:30:A:ILE:HD12	1:69:A:LEU:HB2	9	0.34	0.14	0.32
(1,56)	1:30:A:ILE:HD13	1:69:A:LEU:HB2	9	0.34	0.14	0.32
(1,56)	1:67:A:LEU:HB2	1:30:A:ILE:HD11	9	0.34	0.14	0.32
(1,549)	1:56:A:LEU:HD21	1:19:A:PRO:HA	9	0.3	0.05	0.3
(1,549)	1:56:A:LEU:HD22	1:19:A:PRO:HA	9	0.3	0.05	0.3
(1,549)	1:56:A:LEU:HD23	1:19:A:PRO:HA	9	0.3	0.05	0.3
(1,825)	1:50:A:LEU:HD11	1:51:A:GLU:H	9	0.26	0.09	0.32
(1,825)	1:50:A:LEU:HD12	1:51:A:GLU:H	9	0.26	0.09	0.32
(1,825)	1:50:A:LEU:HD13	1:51:A:GLU:H	9	0.26	0.09	0.32
(1,1035)	1:23:A:ILE:HD11	1:57:A:SER:H	9	0.19	0.03	0.2
(1,1035)	1:23:A:ILE:HD12	1:57:A:SER:H	9	0.19	0.03	0.2
(1,1035)	1:23:A:ILE:HD13	1:57:A:SER:H	9	0.19	0.03	0.2
(1,249)	1:36:A:ILE:HA	1:71:A:LEU:HD11	9	0.16	0.04	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,249)	1:36:A:ILE:HA	1:71:A:LEU:HD12	9	0.16	0.04	0.14
(1,249)	1:36:A:ILE:HA	1:71:A:LEU:HD13	9	0.16	0.04	0.14
(1,590)	1:73:A:LEU:HG	1:73:A:LEU:HA	9	0.15	0.04	0.14
(1,536)	1:11:A:LYS:HD2	1:9:A:THR:HG21	9	0.15	0.03	0.15
(1,536)	1:11:A:LYS:HD2	1:9:A:THR:HG22	9	0.15	0.03	0.15
(1,536)	1:11:A:LYS:HD2	1:9:A:THR:HG23	9	0.15	0.03	0.15
(1,536)	1:11:A:LYS:HD3	1:9:A:THR:HG21	9	0.15	0.03	0.15
(1,536)	1:11:A:LYS:HD3	1:9:A:THR:HG22	9	0.15	0.03	0.15
(1,536)	1:11:A:LYS:HD3	1:9:A:THR:HG23	9	0.15	0.03	0.15
(1,847)	1:56:A:LEU:HB3	1:56:A:LEU:H	9	0.14	0.01	0.13
(1,899)	1:64:A:GLU:HG2	1:65:A:SER:H	9	0.13	0.01	0.12
(1,899)	1:64:A:GLU:HG3	1:65:A:SER:H	9	0.13	0.01	0.12
(1,54)	1:61:A:ILE:HD11	1:59:A:TYR:H	9	0.11	0.01	0.12
(1,54)	1:61:A:ILE:HD12	1:59:A:TYR:H	9	0.11	0.01	0.12
(1,54)	1:61:A:ILE:HD13	1:59:A:TYR:H	9	0.11	0.01	0.12
(1,1166)	1:44:A:ILE:HG22	1:68:A:HIS:H	8	0.71	0.08	0.74
(1,1166)	1:67:A:LEU:HD12	1:68:A:HIS:H	8	0.71	0.08	0.74
(1,1166)	1:67:A:LEU:HD11	1:68:A:HIS:H	8	0.71	0.08	0.74
(1,1166)	1:67:A:LEU:HD13	1:68:A:HIS:H	8	0.71	0.08	0.74
(1,447)	1:27:A:LYS:HB2	1:27:A:LYS:HD2	8	0.71	0.06	0.72
(1,447)	1:27:A:LYS:HB2	1:27:A:LYS:HD3	8	0.71	0.06	0.72
(1,798)	1:43:A:LEU:HD21	1:44:A:ILE:H	8	0.7	0.35	0.71
(1,798)	1:44:A:ILE:HG21	1:44:A:ILE:H	8	0.7	0.35	0.71
(1,798)	1:44:A:ILE:HG22	1:44:A:ILE:H	8	0.7	0.35	0.71
(1,798)	1:43:A:LEU:HD22	1:44:A:ILE:H	8	0.7	0.35	0.71
(1,163)	1:27:A:LYS:HB3	1:38:A:PRO:HA	8	0.63	0.05	0.64
(1,1091)	1:34:A:GLU:HB2	1:36:A:ILE:H	8	0.55	0.11	0.5
(1,1279)	1:21:A:ASP:HB2	1:22:A:THR:H	8	0.52	0.12	0.52
(1,207)	1:23:A:ILE:HB	1:24:A:GLU:HA	8	0.48	0.21	0.54
(1,207)	1:27:A:LYS:HE3	1:24:A:GLU:HA	8	0.48	0.21	0.54
(1,207)	1:27:A:LYS:HE2	1:24:A:GLU:HA	8	0.48	0.21	0.54
(1,514)	1:72:A:ARG:HB3	1:72:A:ARG:HA	8	0.43	0.01	0.44
(1,1089)	1:64:A:GLU:HB2	1:4:A:PHE:H	8	0.2	0.05	0.22
(1,547)	1:1:A:MET:HB2	1:18:A:GLU:HG2	8	0.19	0.03	0.18
(1,547)	1:1:A:MET:HB2	1:18:A:GLU:HG3	8	0.19	0.03	0.18
(1,547)	1:1:A:MET:HB3	1:18:A:GLU:HG2	8	0.19	0.03	0.18
(1,547)	1:1:A:MET:HB3	1:18:A:GLU:HG3	8	0.19	0.03	0.18
(1,79)	1:3:A:ILE:HG21	1:1:A:MET:HB2	8	0.16	0.02	0.15
(1,79)	1:3:A:ILE:HG21	1:1:A:MET:HB3	8	0.16	0.02	0.15
(1,79)	1:3:A:ILE:HG22	1:1:A:MET:HB2	8	0.16	0.02	0.15
(1,79)	1:3:A:ILE:HG22	1:1:A:MET:HB3	8	0.16	0.02	0.15
(1,79)	1:3:A:ILE:HG23	1:1:A:MET:HB2	8	0.16	0.02	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,79)	1:3:A:ILE:HG23	1:1:A:MET:HB3	8	0.16	0.02	0.15
(1,577)	1:71:A:LEU:HG	1:41:A:GLN:HA	8	0.15	0.03	0.15
(1,560)	1:55:A:THR:HB	1:22:A:THR:HA	8	0.15	0.05	0.14
(1,398)	1:56:A:LEU:HB2	1:19:A:PRO:HA	8	0.14	0.02	0.14
(1,1132)	1:16:A:GLU:HA	1:2:A:LYS:H	8	0.14	0.04	0.12
(1,572)	1:31:A:GLN:HA	1:31:A:GLN:HG2	7	1.16	0.13	1.18
(1,25)	1:50:A:LEU:HD11	1:23:A:ILE:HG12	7	1.03	0.8	1.51
(1,25)	1:50:A:LEU:HD12	1:23:A:ILE:HG12	7	1.03	0.8	1.51
(1,25)	1:50:A:LEU:HD13	1:23:A:ILE:HG12	7	1.03	0.8	1.51
(1,630)	1:21:A:ASP:HB3	1:20:A:SER:H	7	0.54	0.05	0.55
(1,703)	1:21:A:ASP:HB3	1:21:A:ASP:H	7	0.49	0.05	0.52
(1,488)	1:30:A:ILE:HD12	1:43:A:LEU:HG	7	0.47	0.19	0.4
(1,488)	1:30:A:ILE:HD13	1:43:A:LEU:HG	7	0.47	0.19	0.4
(1,488)	1:30:A:ILE:HD11	1:43:A:LEU:HG	7	0.47	0.19	0.4
(1,212)	1:5:A:VAL:HA	1:67:A:LEU:HA	7	0.17	0.06	0.15
(1,212)	1:5:A:VAL:HA	1:68:A:HIS:HA	7	0.17	0.06	0.15
(1,727)	1:43:A:LEU:HD21	1:27:A:LYS:H	6	1.74	0.13	1.72
(1,727)	1:43:A:LEU:HD22	1:27:A:LYS:H	6	1.74	0.13	1.72
(1,727)	1:43:A:LEU:HD23	1:27:A:LYS:H	6	1.74	0.13	1.72
(1,1218)	1:20:A:SER:HB3	1:22:A:THR:H	6	1.27	0.3	1.37
(1,292)	1:43:A:LEU:HD11	1:43:A:LEU:HA	6	0.98	0.01	0.98
(1,292)	1:43:A:LEU:HD12	1:43:A:LEU:HA	6	0.98	0.01	0.98
(1,292)	1:43:A:LEU:HD13	1:43:A:LEU:HA	6	0.98	0.01	0.98
(1,23)	1:23:A:ILE:HD11	1:50:A:LEU:HD11	6	0.76	0.07	0.78
(1,23)	1:23:A:ILE:HD11	1:50:A:LEU:HD12	6	0.76	0.07	0.78
(1,23)	1:23:A:ILE:HD11	1:50:A:LEU:HD13	6	0.76	0.07	0.78
(1,23)	1:23:A:ILE:HD12	1:50:A:LEU:HD11	6	0.76	0.07	0.78
(1,23)	1:23:A:ILE:HD12	1:50:A:LEU:HD12	6	0.76	0.07	0.78
(1,23)	1:23:A:ILE:HD12	1:50:A:LEU:HD13	6	0.76	0.07	0.78
(1,23)	1:23:A:ILE:HD13	1:50:A:LEU:HD11	6	0.76	0.07	0.78
(1,23)	1:23:A:ILE:HD13	1:50:A:LEU:HD12	6	0.76	0.07	0.78
(1,23)	1:23:A:ILE:HD13	1:50:A:LEU:HD13	6	0.76	0.07	0.78
(1,234)	1:27:A:LYS:HA	1:43:A:LEU:HD21	6	0.65	0.1	0.63
(1,234)	1:27:A:LYS:HA	1:43:A:LEU:HD22	6	0.65	0.1	0.63
(1,234)	1:27:A:LYS:HA	1:43:A:LEU:HD23	6	0.65	0.1	0.63
(1,1070)	1:25:A:ASN:HB3	1:21:A:ASP:H	6	0.62	0.44	0.55
(1,845)	1:59:A:TYR:HB2	1:56:A:LEU:H	6	0.46	0.22	0.48
(1,845)	1:21:A:ASP:HB2	1:56:A:LEU:H	6	0.46	0.22	0.48
(1,405)	1:59:A:TYR:HB2	1:56:A:LEU:HD21	6	0.43	0.65	0.15
(1,405)	1:59:A:TYR:HB2	1:56:A:LEU:HD22	6	0.43	0.65	0.15
(1,405)	1:59:A:TYR:HB2	1:56:A:LEU:HD23	6	0.43	0.65	0.15
(1,567)	1:29:A:LYS:HB3	1:15:A:LEU:HD23	6	0.26	0.12	0.22

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,567)	1:29:A:LYS:HB3	1:15:A:LEU:HD21	6	0.26	0.12	0.22
(1,567)	1:29:A:LYS:HB3	1:15:A:LEU:HD22	6	0.26	0.12	0.22
(1,1016)	1:4:A:PHE:HB3	1:66:A:THR:H	6	0.17	0.02	0.18
(1,1081)	1:32:A:ASP:HB2	1:34:A:GLU:H	6	0.17	0.03	0.18
(1,204)	1:57:A:SER:HA	1:60:A:SER:HA	6	0.11	0.02	0.11
(1,510)	1:65:A:SER:HA	1:65:A:SER:HB3	6	0.11	0.0	0.11
(1,1095)	1:23:A:ILE:HG13	1:52:A:ASP:H	5	0.57	0.23	0.66
(1,717)	1:25:A:ASN:HB3	1:25:A:ASN:H	5	0.49	0.01	0.48
(1,111)	1:2:A:LYS:HD3	1:14:A:THR:HG21	5	0.48	0.36	0.23
(1,111)	1:2:A:LYS:HD3	1:14:A:THR:HG22	5	0.48	0.36	0.23
(1,111)	1:2:A:LYS:HD3	1:14:A:THR:HG23	5	0.48	0.36	0.23
(1,449)	1:27:A:LYS:HB2	1:43:A:LEU:HD11	5	0.46	0.42	0.3
(1,449)	1:27:A:LYS:HB2	1:43:A:LEU:HD12	5	0.46	0.42	0.3
(1,449)	1:27:A:LYS:HB2	1:43:A:LEU:HD13	5	0.46	0.42	0.3
(1,154)	1:9:A:THR:HB	1:11:A:LYS:HG2	5	0.34	0.03	0.33
(1,844)	1:21:A:ASP:HB3	1:56:A:LEU:H	5	0.3	0.19	0.23
(1,749)	1:31:A:GLN:HG2	1:31:A:GLN:H	5	0.29	0.15	0.22
(1,1057)	1:72:A:ARG:HD2	1:72:A:ARG:H	5	0.25	0.06	0.29
(1,1057)	1:72:A:ARG:HD3	1:72:A:ARG:H	5	0.25	0.06	0.29
(1,276)	1:69:A:LEU:HA	1:69:A:LEU:HD11	5	0.24	0.1	0.17
(1,276)	1:69:A:LEU:HA	1:69:A:LEU:HD12	5	0.24	0.1	0.17
(1,276)	1:69:A:LEU:HA	1:69:A:LEU:HD13	5	0.24	0.1	0.17
(1,486)	1:69:A:LEU:HA	1:69:A:LEU:HD11	5	0.21	0.1	0.14
(1,486)	1:69:A:LEU:HA	1:69:A:LEU:HD12	5	0.21	0.1	0.14
(1,486)	1:69:A:LEU:HA	1:69:A:LEU:HD13	5	0.21	0.1	0.14
(1,121)	1:4:A:PHE:HB2	1:12:A:THR:HG21	5	0.21	0.17	0.13
(1,121)	1:4:A:PHE:HB2	1:12:A:THR:HG22	5	0.21	0.17	0.13
(1,121)	1:4:A:PHE:HB2	1:12:A:THR:HG23	5	0.21	0.17	0.13
(1,1204)	1:64:A:GLU:H	1:63:A:LYS:HD2	5	0.15	0.04	0.13
(1,1204)	1:64:A:GLU:H	1:63:A:LYS:HD3	5	0.15	0.04	0.13
(1,1136)	1:50:A:LEU:HA	1:49:A:LYS:H	5	0.14	0.04	0.13
(1,1136)	1:47:A:GLY:HA2	1:49:A:LYS:H	5	0.14	0.04	0.13
(1,570)	1:25:A:ASN:HB3	1:29:A:LYS:HG2	5	0.14	0.03	0.13
(1,570)	1:25:A:ASN:HB3	1:29:A:LYS:HG3	5	0.14	0.03	0.13
(1,755)	1:28:A:ALA:HB1	1:32:A:ASP:H	5	0.11	0.02	0.1
(1,755)	1:28:A:ALA:HB2	1:32:A:ASP:H	5	0.11	0.02	0.1
(1,755)	1:28:A:ALA:HB3	1:32:A:ASP:H	5	0.11	0.02	0.1
(1,754)	1:31:A:GLN:HG2	1:32:A:ASP:H	4	0.9	0.34	1.02
(1,427)	1:15:A:LEU:HD21	1:16:A:GLU:HG2	4	0.67	0.13	0.62
(1,427)	1:15:A:LEU:HD22	1:16:A:GLU:HG2	4	0.67	0.13	0.62
(1,427)	1:15:A:LEU:HD23	1:16:A:GLU:HG2	4	0.67	0.13	0.62
(1,945)	1:16:A:GLU:HB3	1:16:A:GLU:H	4	0.54	0.01	0.54

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,592)	1:44:A:ILE:HD11	1:49:A:LYS:HB2	4	0.26	0.13	0.22
(1,592)	1:44:A:ILE:HD11	1:49:A:LYS:HB3	4	0.26	0.13	0.22
(1,592)	1:44:A:ILE:HD12	1:49:A:LYS:HB2	4	0.26	0.13	0.22
(1,592)	1:44:A:ILE:HD12	1:49:A:LYS:HB3	4	0.26	0.13	0.22
(1,592)	1:44:A:ILE:HD13	1:49:A:LYS:HB2	4	0.26	0.13	0.22
(1,592)	1:44:A:ILE:HD13	1:49:A:LYS:HB3	4	0.26	0.13	0.22
(1,563)	1:55:A:THR:HA	1:22:A:THR:HB	4	0.24	0.14	0.24
(1,962)	1:25:A:ASN:HB3	1:26:A:VAL:H	4	0.21	0.07	0.2
(1,905)	1:3:A:ILE:HD11	1:66:A:THR:H	4	0.15	0.03	0.15
(1,905)	1:3:A:ILE:HD12	1:66:A:THR:H	4	0.15	0.03	0.15
(1,905)	1:3:A:ILE:HD13	1:66:A:THR:H	4	0.15	0.03	0.15
(1,268)	1:16:A:GLU:HA	1:16:A:GLU:HB2	4	0.12	0.0	0.12
(1,1068)	1:43:A:LEU:H	1:51:A:GLU:H	4	0.12	0.02	0.11
(1,1164)	1:31:A:GLN:HB2	1:29:A:LYS:H	4	0.11	0.01	0.1
(1,1164)	1:31:A:GLN:HB3	1:29:A:LYS:H	4	0.11	0.01	0.1
(1,926)	1:70:A:VAL:HG11	1:73:A:LEU:H	3	1.13	0.19	1.06
(1,926)	1:70:A:VAL:HG12	1:73:A:LEU:H	3	1.13	0.19	1.06
(1,926)	1:70:A:VAL:HG13	1:73:A:LEU:H	3	1.13	0.19	1.06
(1,81)	1:65:A:SER:HB3	1:3:A:ILE:HG21	3	1.08	0.1	1.02
(1,81)	1:65:A:SER:HB3	1:3:A:ILE:HG22	3	1.08	0.1	1.02
(1,81)	1:65:A:SER:HB3	1:3:A:ILE:HG23	3	1.08	0.1	1.02
(1,1278)	1:70:A:VAL:HG21	1:70:A:VAL:H	3	0.72	0.02	0.71
(1,1278)	1:70:A:VAL:HG22	1:70:A:VAL:H	3	0.72	0.02	0.71
(1,1278)	1:70:A:VAL:HG23	1:70:A:VAL:H	3	0.72	0.02	0.71
(1,1059)	1:72:A:ARG:HB2	1:72:A:ARG:H	3	0.67	0.4	0.94
(1,1255)	1:39:A:ASP:HA	1:40:A:GLN:HE22	3	0.65	0.15	0.61
(1,1282)	1:57:A:SER:HB3	1:57:A:SER:H	3	0.52	0.0	0.52
(1,55)	1:69:A:LEU:HG	1:30:A:ILE:HD12	3	0.49	0.16	0.43
(1,137)	1:43:A:LEU:HB3	1:43:A:LEU:HD11	3	0.43	0.0	0.43
(1,137)	1:43:A:LEU:HB3	1:43:A:LEU:HD12	3	0.43	0.0	0.43
(1,137)	1:43:A:LEU:HB3	1:43:A:LEU:HD13	3	0.43	0.0	0.43
(1,216)	1:70:A:VAL:HG11	1:70:A:VAL:HA	3	0.36	0.0	0.36
(1,216)	1:70:A:VAL:HG12	1:70:A:VAL:HA	3	0.36	0.0	0.36
(1,216)	1:70:A:VAL:HG13	1:70:A:VAL:HA	3	0.36	0.0	0.36
(1,1275)	1:39:A:ASP:HB2	1:39:A:ASP:H	3	0.32	0.02	0.32
(1,937)	1:4:A:PHE:HB2	1:6:A:LYS:H	3	0.3	0.25	0.13
(1,561)	1:69:A:LEU:HB2	1:7:A:THR:HB	3	0.27	0.23	0.12
(1,529)	1:57:A:SER:HB2	1:57:A:SER:HA	3	0.25	0.0	0.25
(1,1270)	1:24:A:GLU:HG3	1:25:A:ASN:HD21	3	0.23	0.11	0.16
(1,82)	1:50:A:LEU:HB2	1:23:A:ILE:HG21	3	0.23	0.12	0.15
(1,82)	1:50:A:LEU:HB2	1:23:A:ILE:HG22	3	0.23	0.12	0.15
(1,82)	1:50:A:LEU:HB2	1:23:A:ILE:HG23	3	0.23	0.12	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,20)	1:65:A:SER:HA	1:65:A:SER:HB2	3	0.19	0.0	0.19
(1,1075)	1:56:A:LEU:HB3	1:20:A:SER:H	3	0.16	0.05	0.14
(1,591)	1:73:A:LEU:HB2	1:72:A:ARG:HD2	3	0.13	0.01	0.12
(1,591)	1:73:A:LEU:HB2	1:72:A:ARG:HD3	3	0.13	0.01	0.12
(1,591)	1:73:A:LEU:HB3	1:72:A:ARG:HD2	3	0.13	0.01	0.12
(1,591)	1:73:A:LEU:HB3	1:72:A:ARG:HD3	3	0.13	0.01	0.12
(1,1151)	1:13:A:ILE:HG13	1:5:A:VAL:H	3	0.12	0.0	0.12
(1,688)	1:15:A:LEU:HD11	1:15:A:LEU:H	3	0.12	0.01	0.12
(1,688)	1:15:A:LEU:HD12	1:15:A:LEU:H	3	0.12	0.01	0.12
(1,688)	1:15:A:LEU:HD13	1:15:A:LEU:H	3	0.12	0.01	0.12
(1,688)	1:15:A:LEU:HD21	1:15:A:LEU:H	3	0.12	0.01	0.12
(1,688)	1:15:A:LEU:HD22	1:15:A:LEU:H	3	0.12	0.01	0.12
(1,688)	1:15:A:LEU:HD23	1:15:A:LEU:H	3	0.12	0.01	0.12
(1,177)	1:65:A:SER:HB2	1:67:A:LEU:HD11	2	2.21	0.16	2.21
(1,177)	1:65:A:SER:HB2	1:67:A:LEU:HD12	2	2.21	0.16	2.21
(1,177)	1:65:A:SER:HB2	1:67:A:LEU:HD13	2	2.21	0.16	2.21
(1,66)	1:61:A:ILE:HG21	1:67:A:LEU:HD11	2	1.88	0.0	1.88
(1,66)	1:61:A:ILE:HG21	1:67:A:LEU:HD12	2	1.88	0.0	1.88
(1,66)	1:61:A:ILE:HG21	1:67:A:LEU:HD13	2	1.88	0.0	1.88
(1,66)	1:61:A:ILE:HG22	1:67:A:LEU:HD11	2	1.88	0.0	1.88
(1,66)	1:61:A:ILE:HG22	1:67:A:LEU:HD12	2	1.88	0.0	1.88
(1,66)	1:61:A:ILE:HG22	1:67:A:LEU:HD13	2	1.88	0.0	1.88
(1,66)	1:61:A:ILE:HG23	1:67:A:LEU:HD11	2	1.88	0.0	1.88
(1,66)	1:61:A:ILE:HG23	1:67:A:LEU:HD12	2	1.88	0.0	1.88
(1,66)	1:61:A:ILE:HG23	1:67:A:LEU:HD13	2	1.88	0.0	1.88
(1,194)	1:67:A:LEU:HD11	1:66:A:THR:HA	2	1.48	0.01	1.48
(1,194)	1:67:A:LEU:HD12	1:66:A:THR:HA	2	1.48	0.01	1.48
(1,194)	1:67:A:LEU:HD13	1:66:A:THR:HA	2	1.48	0.01	1.48
(1,175)	1:65:A:SER:HB3	1:67:A:LEU:HD11	2	1.12	0.01	1.12
(1,175)	1:65:A:SER:HB3	1:67:A:LEU:HD12	2	1.12	0.01	1.12
(1,175)	1:65:A:SER:HB3	1:67:A:LEU:HD13	2	1.12	0.01	1.12
(1,289)	1:73:A:LEU:HD11	1:73:A:LEU:HA	2	1.0	0.03	1.0
(1,289)	1:73:A:LEU:HD12	1:73:A:LEU:HA	2	1.0	0.03	1.0
(1,289)	1:73:A:LEU:HD13	1:73:A:LEU:HA	2	1.0	0.03	1.0
(1,131)	1:73:A:LEU:HD11	1:73:A:LEU:HA	2	0.94	0.02	0.94
(1,131)	1:73:A:LEU:HD12	1:73:A:LEU:HA	2	0.94	0.02	0.94
(1,131)	1:73:A:LEU:HD13	1:73:A:LEU:HA	2	0.94	0.02	0.94
(1,130)	1:73:A:LEU:HD11	1:75:A:GLY:HA2	2	0.82	0.38	0.82
(1,130)	1:73:A:LEU:HD11	1:75:A:GLY:HA3	2	0.82	0.38	0.82
(1,130)	1:73:A:LEU:HD12	1:75:A:GLY:HA2	2	0.82	0.38	0.82
(1,130)	1:73:A:LEU:HD12	1:75:A:GLY:HA3	2	0.82	0.38	0.82
(1,130)	1:73:A:LEU:HD13	1:75:A:GLY:HA2	2	0.82	0.38	0.82

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,130)	1:73:A:LEU:HD13	1:75:A:GLY:HA3	2	0.82	0.38	0.82
(1,909)	1:67:A:LEU:HD11	1:67:A:LEU:H	2	0.82	0.03	0.82
(1,909)	1:67:A:LEU:HD12	1:67:A:LEU:H	2	0.82	0.03	0.82
(1,909)	1:67:A:LEU:HD13	1:67:A:LEU:H	2	0.82	0.03	0.82
(1,1223)	1:34:A:GLU:HB3	1:34:A:GLU:H	2	0.61	0.01	0.61
(1,1174)	1:27:A:LYS:HD2	1:27:A:LYS:H	2	0.58	0.29	0.58
(1,1196)	1:5:A:VAL:HG22	1:7:A:THR:H	2	0.54	0.25	0.54
(1,1196)	1:13:A:ILE:HD11	1:7:A:THR:H	2	0.54	0.25	0.54
(1,707)	1:21:A:ASP:HA	1:22:A:THR:H	2	0.52	0.15	0.52
(1,982)	1:49:A:LYS:HG2	1:49:A:LYS:H	2	0.44	0.02	0.44
(1,284)	1:28:A:ALA:HA	1:31:A:GLN:HG2	2	0.38	0.01	0.38
(1,524)	1:20:A:SER:HA	1:20:A:SER:HB2	2	0.36	0.0	0.36
(1,1168)	1:67:A:LEU:HG	1:68:A:HIS:H	2	0.28	0.01	0.28
(1,1191)	1:35:A:GLY:H	1:33:A:GLU:H	2	0.26	0.14	0.26
(1,1140)	1:31:A:GLN:HB2	1:28:A:ALA:H	2	0.24	0.01	0.24
(1,1140)	1:31:A:GLN:HB3	1:28:A:ALA:H	2	0.24	0.01	0.24
(1,1154)	1:15:A:LEU:HG	1:30:A:ILE:H	2	0.21	0.04	0.21
(1,788)	1:41:A:GLN:HG2	1:41:A:GLN:H	2	0.19	0.02	0.19
(1,85)	1:23:A:ILE:HG21	1:27:A:LYS:HE2	2	0.16	0.02	0.16
(1,85)	1:23:A:ILE:HG21	1:27:A:LYS:HE3	2	0.16	0.02	0.16
(1,85)	1:23:A:ILE:HG22	1:27:A:LYS:HE2	2	0.16	0.02	0.16
(1,85)	1:23:A:ILE:HG22	1:27:A:LYS:HE3	2	0.16	0.02	0.16
(1,85)	1:23:A:ILE:HG23	1:27:A:LYS:HE2	2	0.16	0.02	0.16
(1,85)	1:23:A:ILE:HG23	1:27:A:LYS:HE3	2	0.16	0.02	0.16
(1,17)	1:44:A:ILE:HD11	1:49:A:LYS:HE2	2	0.16	0.05	0.16
(1,17)	1:44:A:ILE:HD11	1:49:A:LYS:HE3	2	0.16	0.05	0.16
(1,17)	1:44:A:ILE:HD12	1:49:A:LYS:HE2	2	0.16	0.05	0.16
(1,17)	1:44:A:ILE:HD12	1:49:A:LYS:HE3	2	0.16	0.05	0.16
(1,17)	1:44:A:ILE:HD13	1:49:A:LYS:HE2	2	0.16	0.05	0.16
(1,17)	1:44:A:ILE:HD13	1:49:A:LYS:HE3	2	0.16	0.05	0.16
(1,492)	1:28:A:ALA:HB1	1:38:A:PRO:HG2	2	0.15	0.03	0.15
(1,492)	1:28:A:ALA:HB2	1:38:A:PRO:HG2	2	0.15	0.03	0.15
(1,492)	1:28:A:ALA:HB3	1:38:A:PRO:HG2	2	0.15	0.03	0.15
(1,1058)	1:40:A:GLN:HG2	1:72:A:ARG:H	2	0.15	0.03	0.15
(1,144)	1:7:A:THR:HB	1:8:A:LEU:HB2	2	0.14	0.04	0.14
(1,144)	1:7:A:THR:HB	1:8:A:LEU:HB3	2	0.14	0.04	0.14
(1,1120)	1:33:A:GLU:HG2	1:15:A:LEU:H	2	0.14	0.02	0.14
(1,319)	1:22:A:THR:HG21	1:53:A:GLY:HA2	2	0.12	0.01	0.12
(1,319)	1:22:A:THR:HG21	1:53:A:GLY:HA3	2	0.12	0.01	0.12
(1,319)	1:22:A:THR:HG22	1:53:A:GLY:HA2	2	0.12	0.01	0.12
(1,319)	1:22:A:THR:HG22	1:53:A:GLY:HA3	2	0.12	0.01	0.12
(1,319)	1:22:A:THR:HG23	1:53:A:GLY:HA2	2	0.12	0.01	0.12

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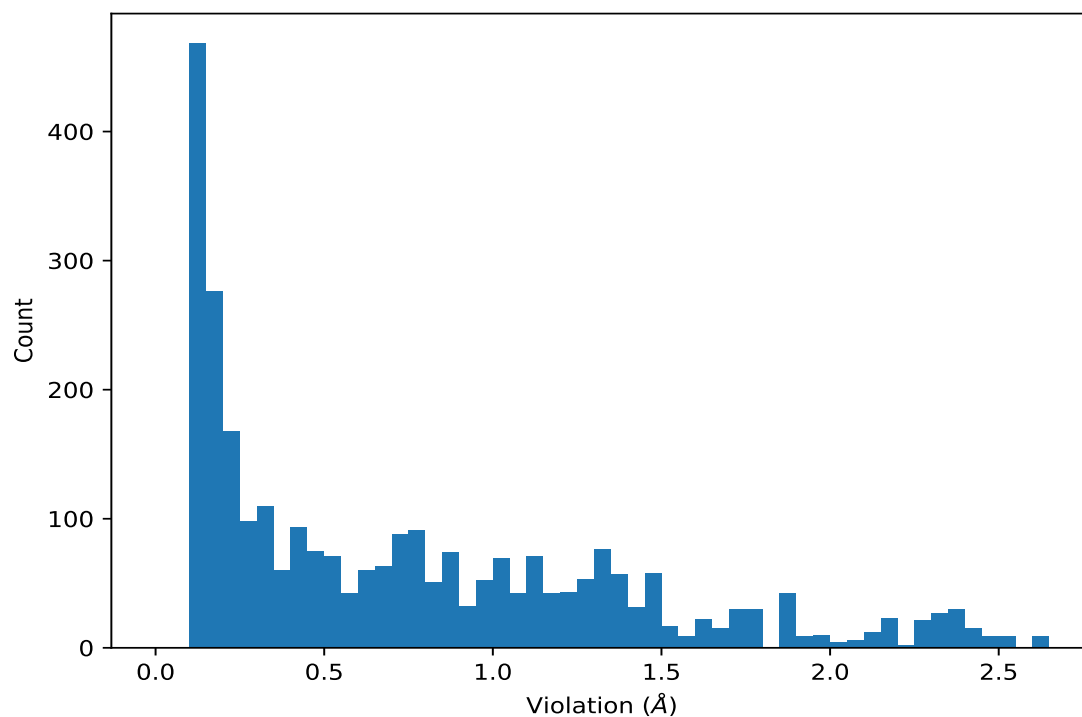
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,319)	1:22:A:THR:HG23	1:53:A:GLY:HA3	2	0.12	0.01	0.12
(1,1106)	1:50:A:LEU:HD11	1:49:A:LYS:H	2	0.12	0.02	0.12
(1,1106)	1:50:A:LEU:HD12	1:49:A:LYS:H	2	0.12	0.02	0.12
(1,1106)	1:50:A:LEU:HD13	1:49:A:LYS:H	2	0.12	0.02	0.12
(1,667)	1:6:A:LYS:HD2	1:6:A:LYS:H	2	0.11	0.0	0.11
(1,667)	1:6:A:LYS:HD3	1:6:A:LYS:H	2	0.11	0.0	0.11
(1,1094)	1:27:A:LYS:HG2	1:52:A:ASP:H	2	0.11	0.01	0.11
(1,1094)	1:27:A:LYS:HG3	1:52:A:ASP:H	2	0.11	0.01	0.11
(1,12)	1:23:A:ILE:HD11	1:54:A:ARG:HG2	2	0.1	0.0	0.1
(1,12)	1:23:A:ILE:HD12	1:54:A:ARG:HG2	2	0.1	0.0	0.1
(1,12)	1:23:A:ILE:HD13	1:54:A:ARG:HG2	2	0.1	0.0	0.1

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,594)	1:3:A:ILE:HD11	1:56:A:LEU:HD21	5	2.63
(1,594)	1:3:A:ILE:HD11	1:56:A:LEU:HD22	5	2.63
(1,594)	1:3:A:ILE:HD11	1:56:A:LEU:HD23	5	2.63
(1,594)	1:3:A:ILE:HD12	1:56:A:LEU:HD21	5	2.63
(1,594)	1:3:A:ILE:HD12	1:56:A:LEU:HD22	5	2.63
(1,594)	1:3:A:ILE:HD12	1:56:A:LEU:HD23	5	2.63
(1,594)	1:3:A:ILE:HD13	1:56:A:LEU:HD21	5	2.63
(1,594)	1:3:A:ILE:HD13	1:56:A:LEU:HD22	5	2.63
(1,594)	1:3:A:ILE:HD13	1:56:A:LEU:HD23	5	2.63
(1,594)	1:3:A:ILE:HD11	1:56:A:LEU:HD21	4	2.54
(1,594)	1:3:A:ILE:HD11	1:56:A:LEU:HD22	4	2.54
(1,594)	1:3:A:ILE:HD11	1:56:A:LEU:HD23	4	2.54
(1,594)	1:3:A:ILE:HD12	1:56:A:LEU:HD21	4	2.54
(1,594)	1:3:A:ILE:HD12	1:56:A:LEU:HD22	4	2.54
(1,594)	1:3:A:ILE:HD12	1:56:A:LEU:HD23	4	2.54
(1,594)	1:3:A:ILE:HD13	1:56:A:LEU:HD21	4	2.54
(1,594)	1:3:A:ILE:HD13	1:56:A:LEU:HD22	4	2.54
(1,594)	1:3:A:ILE:HD13	1:56:A:LEU:HD23	4	2.54
(1,118)	1:17:A:VAL:HG21	1:29:A:LYS:HD2	5	2.46
(1,118)	1:17:A:VAL:HG21	1:29:A:LYS:HD3	5	2.46
(1,118)	1:17:A:VAL:HG22	1:29:A:LYS:HD2	5	2.46
(1,118)	1:17:A:VAL:HG22	1:29:A:LYS:HD3	5	2.46
(1,118)	1:17:A:VAL:HG23	1:29:A:LYS:HD2	5	2.46
(1,118)	1:17:A:VAL:HG23	1:29:A:LYS:HD3	5	2.46
(1,1230)	1:5:A:VAL:HG21	1:69:A:LEU:H	5	2.45
(1,1230)	1:5:A:VAL:HG22	1:69:A:LEU:H	5	2.45
(1,1230)	1:5:A:VAL:HG23	1:69:A:LEU:H	5	2.45
(1,594)	1:3:A:ILE:HD11	1:56:A:LEU:HD21	8	2.44
(1,594)	1:3:A:ILE:HD11	1:56:A:LEU:HD22	8	2.44
(1,594)	1:3:A:ILE:HD11	1:56:A:LEU:HD23	8	2.44
(1,594)	1:3:A:ILE:HD12	1:56:A:LEU:HD21	8	2.44
(1,594)	1:3:A:ILE:HD12	1:56:A:LEU:HD22	8	2.44
(1,594)	1:3:A:ILE:HD12	1:56:A:LEU:HD23	8	2.44
(1,594)	1:3:A:ILE:HD13	1:56:A:LEU:HD21	8	2.44
(1,594)	1:3:A:ILE:HD13	1:56:A:LEU:HD22	8	2.44
(1,594)	1:3:A:ILE:HD13	1:56:A:LEU:HD23	8	2.44
(1,118)	1:17:A:VAL:HG21	1:29:A:LYS:HD2	2	2.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,118)	1:17:A:VAL:HG21	1:29:A:LYS:HD3	2	2.43
(1,118)	1:17:A:VAL:HG22	1:29:A:LYS:HD2	2	2.43
(1,118)	1:17:A:VAL:HG22	1:29:A:LYS:HD3	2	2.43
(1,118)	1:17:A:VAL:HG23	1:29:A:LYS:HD2	2	2.43
(1,118)	1:17:A:VAL:HG23	1:29:A:LYS:HD3	2	2.43
(1,594)	1:3:A:ILE:HD11	1:56:A:LEU:HD21	1	2.37
(1,594)	1:3:A:ILE:HD11	1:56:A:LEU:HD22	1	2.37
(1,594)	1:3:A:ILE:HD11	1:56:A:LEU:HD23	1	2.37
(1,594)	1:3:A:ILE:HD12	1:56:A:LEU:HD21	1	2.37
(1,594)	1:3:A:ILE:HD12	1:56:A:LEU:HD22	1	2.37
(1,594)	1:3:A:ILE:HD12	1:56:A:LEU:HD23	1	2.37
(1,594)	1:3:A:ILE:HD13	1:56:A:LEU:HD21	1	2.37
(1,594)	1:3:A:ILE:HD13	1:56:A:LEU:HD22	1	2.37
(1,594)	1:3:A:ILE:HD13	1:56:A:LEU:HD23	1	2.37
(1,594)	1:3:A:ILE:HD11	1:56:A:LEU:HD21	2	2.37
(1,594)	1:3:A:ILE:HD11	1:56:A:LEU:HD22	2	2.37
(1,594)	1:3:A:ILE:HD11	1:56:A:LEU:HD23	2	2.37
(1,594)	1:3:A:ILE:HD12	1:56:A:LEU:HD21	2	2.37
(1,594)	1:3:A:ILE:HD12	1:56:A:LEU:HD22	2	2.37
(1,594)	1:3:A:ILE:HD12	1:56:A:LEU:HD23	2	2.37
(1,594)	1:3:A:ILE:HD13	1:56:A:LEU:HD21	2	2.37
(1,594)	1:3:A:ILE:HD13	1:56:A:LEU:HD22	2	2.37
(1,594)	1:3:A:ILE:HD13	1:56:A:LEU:HD23	2	2.37
(1,594)	1:3:A:ILE:HD11	1:56:A:LEU:HD21	6	2.37
(1,594)	1:3:A:ILE:HD11	1:56:A:LEU:HD22	6	2.37
(1,594)	1:3:A:ILE:HD11	1:56:A:LEU:HD23	6	2.37
(1,594)	1:3:A:ILE:HD12	1:56:A:LEU:HD21	6	2.37
(1,594)	1:3:A:ILE:HD12	1:56:A:LEU:HD22	6	2.37
(1,594)	1:3:A:ILE:HD12	1:56:A:LEU:HD23	6	2.37
(1,594)	1:3:A:ILE:HD13	1:56:A:LEU:HD21	6	2.37
(1,594)	1:3:A:ILE:HD13	1:56:A:LEU:HD22	6	2.37
(1,594)	1:3:A:ILE:HD13	1:56:A:LEU:HD23	6	2.37
(1,177)	1:65:A:SER:HB2	1:67:A:LEU:HD11	9	2.37
(1,177)	1:65:A:SER:HB2	1:67:A:LEU:HD12	9	2.37
(1,177)	1:65:A:SER:HB2	1:67:A:LEU:HD13	9	2.37
(1,594)	1:3:A:ILE:HD11	1:56:A:LEU:HD21	10	2.34
(1,594)	1:3:A:ILE:HD11	1:56:A:LEU:HD22	10	2.34
(1,594)	1:3:A:ILE:HD11	1:56:A:LEU:HD23	10	2.34
(1,594)	1:3:A:ILE:HD12	1:56:A:LEU:HD21	10	2.34
(1,594)	1:3:A:ILE:HD12	1:56:A:LEU:HD22	10	2.34
(1,594)	1:3:A:ILE:HD12	1:56:A:LEU:HD23	10	2.34
(1,594)	1:3:A:ILE:HD13	1:56:A:LEU:HD21	10	2.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,594)	1:3:A:ILE:HD13	1:56:A:LEU:HD22	10	2.34
(1,594)	1:3:A:ILE:HD13	1:56:A:LEU:HD23	10	2.34
(1,118)	1:17:A:VAL:HG21	1:29:A:LYS:HD2	10	2.34
(1,118)	1:17:A:VAL:HG21	1:29:A:LYS:HD3	10	2.34
(1,118)	1:17:A:VAL:HG22	1:29:A:LYS:HD2	10	2.34
(1,118)	1:17:A:VAL:HG22	1:29:A:LYS:HD3	10	2.34
(1,118)	1:17:A:VAL:HG23	1:29:A:LYS:HD2	10	2.34
(1,118)	1:17:A:VAL:HG23	1:29:A:LYS:HD3	10	2.34
(1,118)	1:17:A:VAL:HG21	1:29:A:LYS:HD2	3	2.32
(1,118)	1:17:A:VAL:HG21	1:29:A:LYS:HD3	3	2.32
(1,118)	1:17:A:VAL:HG22	1:29:A:LYS:HD2	3	2.32
(1,118)	1:17:A:VAL:HG22	1:29:A:LYS:HD3	3	2.32
(1,118)	1:17:A:VAL:HG23	1:29:A:LYS:HD2	3	2.32
(1,118)	1:17:A:VAL:HG23	1:29:A:LYS:HD3	3	2.32
(1,118)	1:17:A:VAL:HG21	1:29:A:LYS:HD2	6	2.31
(1,118)	1:17:A:VAL:HG21	1:29:A:LYS:HD3	6	2.31
(1,118)	1:17:A:VAL:HG22	1:29:A:LYS:HD2	6	2.31
(1,118)	1:17:A:VAL:HG22	1:29:A:LYS:HD3	6	2.31
(1,118)	1:17:A:VAL:HG23	1:29:A:LYS:HD2	6	2.31
(1,118)	1:17:A:VAL:HG23	1:29:A:LYS:HD3	6	2.31
(1,118)	1:17:A:VAL:HG21	1:29:A:LYS:HD2	9	2.29
(1,118)	1:17:A:VAL:HG21	1:29:A:LYS:HD3	9	2.29
(1,118)	1:17:A:VAL:HG22	1:29:A:LYS:HD2	9	2.29
(1,118)	1:17:A:VAL:HG22	1:29:A:LYS:HD3	9	2.29
(1,118)	1:17:A:VAL:HG23	1:29:A:LYS:HD2	9	2.29
(1,118)	1:17:A:VAL:HG23	1:29:A:LYS:HD3	9	2.29
(1,1167)	1:50:A:LEU:HD21	1:68:A:HIS:H	4	2.27
(1,1167)	1:50:A:LEU:HD22	1:68:A:HIS:H	4	2.27
(1,1167)	1:50:A:LEU:HD23	1:68:A:HIS:H	4	2.27
(1,118)	1:17:A:VAL:HG21	1:29:A:LYS:HD2	4	2.27
(1,118)	1:17:A:VAL:HG21	1:29:A:LYS:HD3	4	2.27
(1,118)	1:17:A:VAL:HG22	1:29:A:LYS:HD2	4	2.27
(1,118)	1:17:A:VAL:HG22	1:29:A:LYS:HD3	4	2.27
(1,118)	1:17:A:VAL:HG23	1:29:A:LYS:HD2	4	2.27
(1,118)	1:17:A:VAL:HG23	1:29:A:LYS:HD3	4	2.27
(1,118)	1:17:A:VAL:HG21	1:29:A:LYS:HD2	7	2.27
(1,118)	1:17:A:VAL:HG21	1:29:A:LYS:HD3	7	2.27
(1,118)	1:17:A:VAL:HG22	1:29:A:LYS:HD2	7	2.27
(1,118)	1:17:A:VAL:HG22	1:29:A:LYS:HD3	7	2.27
(1,118)	1:17:A:VAL:HG23	1:29:A:LYS:HD2	7	2.27
(1,118)	1:17:A:VAL:HG23	1:29:A:LYS:HD3	7	2.27
(1,28)	1:23:A:ILE:HD11	1:50:A:LEU:HB2	5	2.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,28)	1:23:A:ILE:HD12	1:50:A:LEU:HB2	4	2.2
(1,118)	1:17:A:VAL:HG21	1:29:A:LYS:HD2	1	2.19
(1,118)	1:17:A:VAL:HG21	1:29:A:LYS:HD3	1	2.19
(1,118)	1:17:A:VAL:HG22	1:29:A:LYS:HD2	1	2.19
(1,118)	1:17:A:VAL:HG22	1:29:A:LYS:HD3	1	2.19
(1,118)	1:17:A:VAL:HG23	1:29:A:LYS:HD2	1	2.19
(1,118)	1:17:A:VAL:HG23	1:29:A:LYS:HD3	1	2.19
(1,594)	1:3:A:ILE:HD11	1:56:A:LEU:HD21	9	2.18
(1,594)	1:3:A:ILE:HD11	1:56:A:LEU:HD22	9	2.18
(1,594)	1:3:A:ILE:HD11	1:56:A:LEU:HD23	9	2.18
(1,594)	1:3:A:ILE:HD12	1:56:A:LEU:HD21	9	2.18
(1,594)	1:3:A:ILE:HD12	1:56:A:LEU:HD22	9	2.18
(1,594)	1:3:A:ILE:HD12	1:56:A:LEU:HD23	9	2.18
(1,594)	1:3:A:ILE:HD13	1:56:A:LEU:HD21	9	2.18
(1,594)	1:3:A:ILE:HD13	1:56:A:LEU:HD22	9	2.18
(1,594)	1:3:A:ILE:HD13	1:56:A:LEU:HD23	9	2.18
(1,28)	1:23:A:ILE:HD11	1:50:A:LEU:HB2	10	2.18
(1,118)	1:17:A:VAL:HG21	1:29:A:LYS:HD2	8	2.16
(1,118)	1:17:A:VAL:HG21	1:29:A:LYS:HD3	8	2.16
(1,118)	1:17:A:VAL:HG22	1:29:A:LYS:HD2	8	2.16
(1,118)	1:17:A:VAL:HG22	1:29:A:LYS:HD3	8	2.16
(1,118)	1:17:A:VAL:HG23	1:29:A:LYS:HD2	8	2.16
(1,118)	1:17:A:VAL:HG23	1:29:A:LYS:HD3	8	2.16
(1,28)	1:23:A:ILE:HD13	1:50:A:LEU:HB2	7	2.16
(1,1167)	1:50:A:LEU:HD21	1:68:A:HIS:H	8	2.13
(1,1167)	1:50:A:LEU:HD22	1:68:A:HIS:H	8	2.13
(1,1167)	1:50:A:LEU:HD23	1:68:A:HIS:H	8	2.13
(1,594)	1:3:A:ILE:HD11	1:56:A:LEU:HD21	3	2.12
(1,594)	1:3:A:ILE:HD11	1:56:A:LEU:HD22	3	2.12
(1,594)	1:3:A:ILE:HD11	1:56:A:LEU:HD23	3	2.12
(1,594)	1:3:A:ILE:HD12	1:56:A:LEU:HD21	3	2.12
(1,594)	1:3:A:ILE:HD12	1:56:A:LEU:HD22	3	2.12
(1,594)	1:3:A:ILE:HD12	1:56:A:LEU:HD23	3	2.12
(1,594)	1:3:A:ILE:HD13	1:56:A:LEU:HD21	3	2.12
(1,594)	1:3:A:ILE:HD13	1:56:A:LEU:HD22	3	2.12
(1,594)	1:3:A:ILE:HD13	1:56:A:LEU:HD23	3	2.12
(1,1167)	1:50:A:LEU:HD21	1:68:A:HIS:H	1	2.05
(1,1167)	1:50:A:LEU:HD22	1:68:A:HIS:H	1	2.05
(1,1167)	1:50:A:LEU:HD23	1:68:A:HIS:H	1	2.05
(1,177)	1:65:A:SER:HB2	1:67:A:LEU:HD11	1	2.05
(1,177)	1:65:A:SER:HB2	1:67:A:LEU:HD12	1	2.05
(1,177)	1:65:A:SER:HB2	1:67:A:LEU:HD13	1	2.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1167)	1:50:A:LEU:HD21	1:68:A:HIS:H	2	2.03
(1,1167)	1:50:A:LEU:HD22	1:68:A:HIS:H	2	2.03
(1,1167)	1:50:A:LEU:HD23	1:68:A:HIS:H	2	2.03
(1,28)	1:23:A:ILE:HD13	1:50:A:LEU:HB2	6	2.02
(1,1167)	1:50:A:LEU:HD21	1:68:A:HIS:H	9	1.99
(1,1167)	1:50:A:LEU:HD22	1:68:A:HIS:H	9	1.99
(1,1167)	1:50:A:LEU:HD23	1:68:A:HIS:H	9	1.99
(1,1167)	1:50:A:LEU:HD21	1:68:A:HIS:H	7	1.97
(1,1167)	1:50:A:LEU:HD22	1:68:A:HIS:H	7	1.97
(1,1167)	1:50:A:LEU:HD23	1:68:A:HIS:H	7	1.97
(1,28)	1:23:A:ILE:HD11	1:50:A:LEU:HB2	2	1.97
(1,727)	1:43:A:LEU:HD21	1:27:A:LYS:H	9	1.96
(1,727)	1:43:A:LEU:HD22	1:27:A:LYS:H	9	1.96
(1,727)	1:43:A:LEU:HD23	1:27:A:LYS:H	9	1.96
(1,25)	1:50:A:LEU:HD11	1:23:A:ILE:HG12	8	1.94
(1,25)	1:50:A:LEU:HD12	1:23:A:ILE:HG12	8	1.94
(1,25)	1:50:A:LEU:HD13	1:23:A:ILE:HG12	8	1.94
(1,1167)	1:50:A:LEU:HD21	1:68:A:HIS:H	10	1.92
(1,1167)	1:50:A:LEU:HD22	1:68:A:HIS:H	10	1.92
(1,1167)	1:50:A:LEU:HD23	1:68:A:HIS:H	10	1.92
(1,1167)	1:50:A:LEU:HD21	1:68:A:HIS:H	3	1.9
(1,1167)	1:50:A:LEU:HD22	1:68:A:HIS:H	3	1.9
(1,1167)	1:50:A:LEU:HD23	1:68:A:HIS:H	3	1.9
(1,1167)	1:50:A:LEU:HD21	1:68:A:HIS:H	5	1.89
(1,1167)	1:50:A:LEU:HD22	1:68:A:HIS:H	5	1.89
(1,1167)	1:50:A:LEU:HD23	1:68:A:HIS:H	5	1.89
(1,405)	1:59:A:TYR:HB2	1:56:A:LEU:HD21	7	1.89
(1,405)	1:59:A:TYR:HB2	1:56:A:LEU:HD22	7	1.89
(1,405)	1:59:A:TYR:HB2	1:56:A:LEU:HD23	7	1.89
(1,66)	1:61:A:ILE:HG21	1:67:A:LEU:HD11	9	1.88
(1,66)	1:61:A:ILE:HG21	1:67:A:LEU:HD12	9	1.88
(1,66)	1:61:A:ILE:HG21	1:67:A:LEU:HD13	9	1.88
(1,66)	1:61:A:ILE:HG22	1:67:A:LEU:HD11	9	1.88
(1,66)	1:61:A:ILE:HG22	1:67:A:LEU:HD12	9	1.88
(1,66)	1:61:A:ILE:HG22	1:67:A:LEU:HD13	9	1.88
(1,66)	1:61:A:ILE:HG23	1:67:A:LEU:HD11	9	1.88
(1,66)	1:61:A:ILE:HG23	1:67:A:LEU:HD12	9	1.88
(1,66)	1:61:A:ILE:HG23	1:67:A:LEU:HD13	9	1.88
(1,257)	1:5:A:VAL:HG21	1:68:A:HIS:HA	5	1.87
(1,257)	1:5:A:VAL:HG22	1:68:A:HIS:HA	5	1.87
(1,257)	1:5:A:VAL:HG23	1:68:A:HIS:HA	5	1.87
(1,66)	1:61:A:ILE:HG21	1:67:A:LEU:HD11	1	1.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,66)	1:61:A:ILE:HG21	1:67:A:LEU:HD12	1	1.87
(1,66)	1:61:A:ILE:HG21	1:67:A:LEU:HD13	1	1.87
(1,66)	1:61:A:ILE:HG22	1:67:A:LEU:HD11	1	1.87
(1,66)	1:61:A:ILE:HG22	1:67:A:LEU:HD12	1	1.87
(1,66)	1:61:A:ILE:HG22	1:67:A:LEU:HD13	1	1.87
(1,66)	1:61:A:ILE:HG23	1:67:A:LEU:HD11	1	1.87
(1,66)	1:61:A:ILE:HG23	1:67:A:LEU:HD12	1	1.87
(1,66)	1:61:A:ILE:HG23	1:67:A:LEU:HD13	1	1.87
(1,1167)	1:50:A:LEU:HD21	1:68:A:HIS:H	6	1.86
(1,1167)	1:50:A:LEU:HD22	1:68:A:HIS:H	6	1.86
(1,1167)	1:50:A:LEU:HD23	1:68:A:HIS:H	6	1.86
(1,727)	1:43:A:LEU:HD21	1:27:A:LYS:H	1	1.86
(1,727)	1:43:A:LEU:HD22	1:27:A:LYS:H	1	1.86
(1,727)	1:43:A:LEU:HD23	1:27:A:LYS:H	1	1.86
(1,77)	1:17:A:VAL:HG11	1:3:A:ILE:HG21	8	1.86
(1,77)	1:17:A:VAL:HG11	1:3:A:ILE:HG22	8	1.86
(1,77)	1:17:A:VAL:HG11	1:3:A:ILE:HG23	8	1.86
(1,77)	1:17:A:VAL:HG12	1:3:A:ILE:HG21	8	1.86
(1,77)	1:17:A:VAL:HG12	1:3:A:ILE:HG22	8	1.86
(1,77)	1:17:A:VAL:HG12	1:3:A:ILE:HG23	8	1.86
(1,77)	1:17:A:VAL:HG13	1:3:A:ILE:HG21	8	1.86
(1,77)	1:17:A:VAL:HG13	1:3:A:ILE:HG22	8	1.86
(1,77)	1:17:A:VAL:HG13	1:3:A:ILE:HG23	8	1.86
(1,92)	1:17:A:VAL:HG11	1:1:A:MET:HE1	4	1.79
(1,92)	1:17:A:VAL:HG11	1:1:A:MET:HE2	4	1.79
(1,92)	1:17:A:VAL:HG11	1:1:A:MET:HE3	4	1.79
(1,92)	1:17:A:VAL:HG12	1:1:A:MET:HE1	4	1.79
(1,92)	1:17:A:VAL:HG12	1:1:A:MET:HE2	4	1.79
(1,92)	1:17:A:VAL:HG12	1:1:A:MET:HE3	4	1.79
(1,92)	1:17:A:VAL:HG13	1:1:A:MET:HE1	4	1.79
(1,92)	1:17:A:VAL:HG13	1:1:A:MET:HE2	4	1.79
(1,92)	1:17:A:VAL:HG13	1:1:A:MET:HE3	4	1.79
(1,25)	1:50:A:LEU:HD11	1:23:A:ILE:HG12	3	1.79
(1,25)	1:50:A:LEU:HD12	1:23:A:ILE:HG12	3	1.79
(1,25)	1:50:A:LEU:HD13	1:23:A:ILE:HG12	3	1.79
(1,559)	1:56:A:LEU:HD21	1:22:A:THR:HA	7	1.78
(1,559)	1:56:A:LEU:HD22	1:22:A:THR:HA	7	1.78
(1,559)	1:56:A:LEU:HD23	1:22:A:THR:HA	7	1.78
(1,374)	1:26:A:VAL:HG11	1:21:A:ASP:HB3	3	1.78
(1,374)	1:26:A:VAL:HG12	1:21:A:ASP:HB3	3	1.78
(1,374)	1:26:A:VAL:HG13	1:21:A:ASP:HB3	3	1.78
(1,106)	1:26:A:VAL:HG21	1:27:A:LYS:HA	5	1.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,106)	1:26:A:VAL:HG22	1:27:A:LYS:HA	5	1.78
(1,106)	1:26:A:VAL:HG23	1:27:A:LYS:HA	5	1.78
(1,727)	1:43:A:LEU:HD21	1:27:A:LYS:H	7	1.75
(1,727)	1:43:A:LEU:HD22	1:27:A:LYS:H	7	1.75
(1,727)	1:43:A:LEU:HD23	1:27:A:LYS:H	7	1.75
(1,106)	1:26:A:VAL:HG21	1:27:A:LYS:HA	6	1.75
(1,106)	1:26:A:VAL:HG22	1:27:A:LYS:HA	6	1.75
(1,106)	1:26:A:VAL:HG23	1:27:A:LYS:HA	6	1.75
(1,106)	1:26:A:VAL:HG21	1:27:A:LYS:HA	8	1.75
(1,106)	1:26:A:VAL:HG22	1:27:A:LYS:HA	8	1.75
(1,106)	1:26:A:VAL:HG23	1:27:A:LYS:HA	8	1.75
(1,106)	1:26:A:VAL:HG21	1:27:A:LYS:HA	1	1.74
(1,106)	1:26:A:VAL:HG22	1:27:A:LYS:HA	1	1.74
(1,106)	1:26:A:VAL:HG23	1:27:A:LYS:HA	1	1.74
(1,106)	1:26:A:VAL:HG21	1:27:A:LYS:HA	2	1.74
(1,106)	1:26:A:VAL:HG22	1:27:A:LYS:HA	2	1.74
(1,106)	1:26:A:VAL:HG23	1:27:A:LYS:HA	2	1.74
(1,106)	1:26:A:VAL:HG21	1:27:A:LYS:HA	9	1.74
(1,106)	1:26:A:VAL:HG22	1:27:A:LYS:HA	9	1.74
(1,106)	1:26:A:VAL:HG23	1:27:A:LYS:HA	9	1.74
(1,106)	1:26:A:VAL:HG21	1:27:A:LYS:HA	10	1.74
(1,106)	1:26:A:VAL:HG22	1:27:A:LYS:HA	10	1.74
(1,106)	1:26:A:VAL:HG23	1:27:A:LYS:HA	10	1.74
(1,1170)	1:26:A:VAL:HG11	1:18:A:GLU:H	3	1.72
(1,1170)	1:26:A:VAL:HG12	1:18:A:GLU:H	3	1.72
(1,1170)	1:26:A:VAL:HG13	1:18:A:GLU:H	3	1.72
(1,106)	1:26:A:VAL:HG21	1:27:A:LYS:HA	3	1.72
(1,106)	1:26:A:VAL:HG22	1:27:A:LYS:HA	3	1.72
(1,106)	1:26:A:VAL:HG23	1:27:A:LYS:HA	3	1.72
(1,346)	1:17:A:VAL:HG21	1:29:A:LYS:HE2	1	1.71
(1,346)	1:17:A:VAL:HG21	1:29:A:LYS:HE3	1	1.71
(1,346)	1:17:A:VAL:HG22	1:29:A:LYS:HE2	1	1.71
(1,346)	1:17:A:VAL:HG22	1:29:A:LYS:HE3	1	1.71
(1,346)	1:17:A:VAL:HG23	1:29:A:LYS:HE2	1	1.71
(1,346)	1:17:A:VAL:HG23	1:29:A:LYS:HE3	1	1.71
(1,106)	1:26:A:VAL:HG21	1:27:A:LYS:HA	7	1.71
(1,106)	1:26:A:VAL:HG22	1:27:A:LYS:HA	7	1.71
(1,106)	1:26:A:VAL:HG23	1:27:A:LYS:HA	7	1.71
(1,106)	1:26:A:VAL:HG21	1:27:A:LYS:HA	4	1.7
(1,106)	1:26:A:VAL:HG22	1:27:A:LYS:HA	4	1.7
(1,106)	1:26:A:VAL:HG23	1:27:A:LYS:HA	4	1.7
(1,39)	1:3:A:ILE:HD11	1:17:A:VAL:HG11	8	1.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,39)	1:3:A:ILE:HD11	1:17:A:VAL:HG12	8	1.69
(1,39)	1:3:A:ILE:HD11	1:17:A:VAL:HG13	8	1.69
(1,39)	1:3:A:ILE:HD12	1:17:A:VAL:HG11	8	1.69
(1,39)	1:3:A:ILE:HD12	1:17:A:VAL:HG12	8	1.69
(1,39)	1:3:A:ILE:HD12	1:17:A:VAL:HG13	8	1.69
(1,39)	1:3:A:ILE:HD13	1:17:A:VAL:HG11	8	1.69
(1,39)	1:3:A:ILE:HD13	1:17:A:VAL:HG12	8	1.69
(1,39)	1:3:A:ILE:HD13	1:17:A:VAL:HG13	8	1.69
(1,1170)	1:26:A:VAL:HG11	1:18:A:GLU:H	4	1.68
(1,1170)	1:26:A:VAL:HG12	1:18:A:GLU:H	4	1.68
(1,1170)	1:26:A:VAL:HG13	1:18:A:GLU:H	4	1.68
(1,727)	1:43:A:LEU:HD21	1:27:A:LYS:H	2	1.68
(1,727)	1:43:A:LEU:HD22	1:27:A:LYS:H	2	1.68
(1,727)	1:43:A:LEU:HD23	1:27:A:LYS:H	2	1.68
(1,727)	1:43:A:LEU:HD21	1:27:A:LYS:H	3	1.63
(1,727)	1:43:A:LEU:HD22	1:27:A:LYS:H	3	1.63
(1,727)	1:43:A:LEU:HD23	1:27:A:LYS:H	3	1.63
(1,1143)	1:70:A:VAL:HG11	1:71:A:LEU:H	3	1.62
(1,346)	1:17:A:VAL:HG21	1:29:A:LYS:HE2	5	1.62
(1,346)	1:17:A:VAL:HG21	1:29:A:LYS:HE3	5	1.62
(1,346)	1:17:A:VAL:HG22	1:29:A:LYS:HE2	5	1.62
(1,346)	1:17:A:VAL:HG22	1:29:A:LYS:HE3	5	1.62
(1,346)	1:17:A:VAL:HG23	1:29:A:LYS:HE2	5	1.62
(1,346)	1:17:A:VAL:HG23	1:29:A:LYS:HE3	5	1.62
(1,25)	1:50:A:LEU:HD11	1:23:A:ILE:HG12	1	1.62
(1,25)	1:50:A:LEU:HD12	1:23:A:ILE:HG12	1	1.62
(1,25)	1:50:A:LEU:HD13	1:23:A:ILE:HG12	1	1.62
(1,3)	1:4:A:PHE:HA	1:5:A:VAL:HG11	5	1.61
(1,3)	1:4:A:PHE:HA	1:5:A:VAL:HG12	5	1.61
(1,3)	1:4:A:PHE:HA	1:5:A:VAL:HG13	5	1.61
(1,346)	1:17:A:VAL:HG21	1:29:A:LYS:HE2	7	1.6
(1,346)	1:17:A:VAL:HG21	1:29:A:LYS:HE3	7	1.6
(1,346)	1:17:A:VAL:HG22	1:29:A:LYS:HE2	7	1.6
(1,346)	1:17:A:VAL:HG22	1:29:A:LYS:HE3	7	1.6
(1,346)	1:17:A:VAL:HG23	1:29:A:LYS:HE2	7	1.6
(1,346)	1:17:A:VAL:HG23	1:29:A:LYS:HE3	7	1.6
(1,727)	1:43:A:LEU:HD21	1:27:A:LYS:H	10	1.59
(1,727)	1:43:A:LEU:HD22	1:27:A:LYS:H	10	1.59
(1,727)	1:43:A:LEU:HD23	1:27:A:LYS:H	10	1.59
(1,1268)	1:71:A:LEU:HG	1:40:A:GLN:HE22	8	1.58
(1,435)	1:33:A:GLU:HG2	1:15:A:LEU:HD11	6	1.55
(1,435)	1:33:A:GLU:HG2	1:15:A:LEU:HD12	6	1.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,435)	1:33:A:GLU:HG2	1:15:A:LEU:HD13	6	1.55
(1,322)	1:10:A:GLY:HA3	1:6:A:LYS:HE2	5	1.55
(1,322)	1:10:A:GLY:HA3	1:6:A:LYS:HE3	5	1.55
(1,1170)	1:26:A:VAL:HG11	1:18:A:GLU:H	7	1.54
(1,1170)	1:26:A:VAL:HG12	1:18:A:GLU:H	7	1.54
(1,1170)	1:26:A:VAL:HG13	1:18:A:GLU:H	7	1.54
(1,346)	1:17:A:VAL:HG21	1:29:A:LYS:HE2	2	1.54
(1,346)	1:17:A:VAL:HG21	1:29:A:LYS:HE3	2	1.54
(1,346)	1:17:A:VAL:HG22	1:29:A:LYS:HE2	2	1.54
(1,346)	1:17:A:VAL:HG22	1:29:A:LYS:HE3	2	1.54
(1,346)	1:17:A:VAL:HG23	1:29:A:LYS:HE2	2	1.54
(1,346)	1:17:A:VAL:HG23	1:29:A:LYS:HE3	2	1.54
(1,322)	1:10:A:GLY:HA3	1:6:A:LYS:HE2	9	1.54
(1,322)	1:10:A:GLY:HA3	1:6:A:LYS:HE3	9	1.54
(1,435)	1:33:A:GLU:HG2	1:15:A:LEU:HD11	9	1.52
(1,435)	1:33:A:GLU:HG2	1:15:A:LEU:HD12	9	1.52
(1,435)	1:33:A:GLU:HG2	1:15:A:LEU:HD13	9	1.52
(1,25)	1:50:A:LEU:HD11	1:23:A:ILE:HG12	9	1.51
(1,25)	1:50:A:LEU:HD12	1:23:A:ILE:HG12	9	1.51
(1,25)	1:50:A:LEU:HD13	1:23:A:ILE:HG12	9	1.51
(1,1268)	1:71:A:LEU:HG	1:40:A:GLN:HE22	3	1.49
(1,1170)	1:26:A:VAL:HG11	1:18:A:GLU:H	9	1.49
(1,1170)	1:26:A:VAL:HG12	1:18:A:GLU:H	9	1.49
(1,1170)	1:26:A:VAL:HG13	1:18:A:GLU:H	9	1.49
(1,516)	1:26:A:VAL:HG11	1:56:A:LEU:HD11	3	1.48
(1,516)	1:26:A:VAL:HG11	1:56:A:LEU:HD12	3	1.48
(1,516)	1:26:A:VAL:HG11	1:56:A:LEU:HD13	3	1.48
(1,516)	1:26:A:VAL:HG12	1:56:A:LEU:HD11	3	1.48
(1,516)	1:26:A:VAL:HG12	1:56:A:LEU:HD12	3	1.48
(1,516)	1:26:A:VAL:HG12	1:56:A:LEU:HD13	3	1.48
(1,516)	1:26:A:VAL:HG13	1:56:A:LEU:HD11	3	1.48
(1,516)	1:26:A:VAL:HG13	1:56:A:LEU:HD12	3	1.48
(1,516)	1:26:A:VAL:HG13	1:56:A:LEU:HD13	3	1.48
(1,346)	1:17:A:VAL:HG21	1:29:A:LYS:HE2	8	1.48
(1,346)	1:17:A:VAL:HG21	1:29:A:LYS:HE3	8	1.48
(1,346)	1:17:A:VAL:HG22	1:29:A:LYS:HE2	8	1.48
(1,346)	1:17:A:VAL:HG22	1:29:A:LYS:HE3	8	1.48
(1,346)	1:17:A:VAL:HG23	1:29:A:LYS:HE2	8	1.48
(1,346)	1:17:A:VAL:HG23	1:29:A:LYS:HE3	8	1.48
(1,194)	1:67:A:LEU:HD11	1:66:A:THR:HA	9	1.48
(1,194)	1:67:A:LEU:HD12	1:66:A:THR:HA	9	1.48
(1,194)	1:67:A:LEU:HD13	1:66:A:THR:HA	9	1.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,931)	1:17:A:VAL:HG11	1:3:A:ILE:H	8	1.47
(1,931)	1:17:A:VAL:HG12	1:3:A:ILE:H	8	1.47
(1,931)	1:17:A:VAL:HG13	1:3:A:ILE:H	8	1.47
(1,346)	1:17:A:VAL:HG21	1:29:A:LYS:HE2	10	1.47
(1,346)	1:17:A:VAL:HG21	1:29:A:LYS:HE3	10	1.47
(1,346)	1:17:A:VAL:HG22	1:29:A:LYS:HE2	10	1.47
(1,346)	1:17:A:VAL:HG22	1:29:A:LYS:HE3	10	1.47
(1,346)	1:17:A:VAL:HG23	1:29:A:LYS:HE2	10	1.47
(1,346)	1:17:A:VAL:HG23	1:29:A:LYS:HE3	10	1.47
(1,194)	1:67:A:LEU:HD11	1:66:A:THR:HA	1	1.47
(1,194)	1:67:A:LEU:HD12	1:66:A:THR:HA	1	1.47
(1,194)	1:67:A:LEU:HD13	1:66:A:THR:HA	1	1.47
(1,1195)	1:5:A:VAL:HG21	1:7:A:THR:H	5	1.46
(1,1195)	1:5:A:VAL:HG22	1:7:A:THR:H	5	1.46
(1,1195)	1:5:A:VAL:HG23	1:7:A:THR:H	5	1.46
(1,77)	1:17:A:VAL:HG11	1:3:A:ILE:HG21	6	1.46
(1,77)	1:17:A:VAL:HG11	1:3:A:ILE:HG22	6	1.46
(1,77)	1:17:A:VAL:HG11	1:3:A:ILE:HG23	6	1.46
(1,77)	1:17:A:VAL:HG12	1:3:A:ILE:HG21	6	1.46
(1,77)	1:17:A:VAL:HG12	1:3:A:ILE:HG22	6	1.46
(1,77)	1:17:A:VAL:HG12	1:3:A:ILE:HG23	6	1.46
(1,77)	1:17:A:VAL:HG13	1:3:A:ILE:HG21	6	1.46
(1,77)	1:17:A:VAL:HG13	1:3:A:ILE:HG22	6	1.46
(1,77)	1:17:A:VAL:HG13	1:3:A:ILE:HG23	6	1.46
(1,1268)	1:71:A:LEU:HG	1:40:A:GLN:HE22	1	1.45
(1,1218)	1:20:A:SER:HB3	1:22:A:THR:H	5	1.45
(1,1218)	1:20:A:SER:HB3	1:22:A:THR:H	8	1.45
(1,516)	1:26:A:VAL:HG11	1:56:A:LEU:HD11	4	1.45
(1,516)	1:26:A:VAL:HG11	1:56:A:LEU:HD12	4	1.45
(1,516)	1:26:A:VAL:HG11	1:56:A:LEU:HD13	4	1.45
(1,516)	1:26:A:VAL:HG12	1:56:A:LEU:HD11	4	1.45
(1,516)	1:26:A:VAL:HG12	1:56:A:LEU:HD12	4	1.45
(1,516)	1:26:A:VAL:HG12	1:56:A:LEU:HD13	4	1.45
(1,516)	1:26:A:VAL:HG13	1:56:A:LEU:HD11	4	1.45
(1,516)	1:26:A:VAL:HG13	1:56:A:LEU:HD12	4	1.45
(1,516)	1:26:A:VAL:HG13	1:56:A:LEU:HD13	4	1.45
(1,28)	1:23:A:ILE:HD13	1:50:A:LEU:HB2	3	1.44
(1,1123)	1:50:A:LEU:HD21	1:43:A:LEU:H	4	1.43
(1,1123)	1:50:A:LEU:HD22	1:43:A:LEU:H	4	1.43
(1,1123)	1:50:A:LEU:HD23	1:43:A:LEU:H	4	1.43
(1,322)	1:10:A:GLY:HA3	1:6:A:LYS:HE2	10	1.43
(1,322)	1:10:A:GLY:HA3	1:6:A:LYS:HE3	10	1.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,77)	1:17:A:VAL:HG11	1:3:A:ILE:HG21	10	1.43
(1,77)	1:17:A:VAL:HG11	1:3:A:ILE:HG22	10	1.43
(1,77)	1:17:A:VAL:HG11	1:3:A:ILE:HG23	10	1.43
(1,77)	1:17:A:VAL:HG12	1:3:A:ILE:HG21	10	1.43
(1,77)	1:17:A:VAL:HG12	1:3:A:ILE:HG22	10	1.43
(1,77)	1:17:A:VAL:HG12	1:3:A:ILE:HG23	10	1.43
(1,77)	1:17:A:VAL:HG13	1:3:A:ILE:HG21	10	1.43
(1,77)	1:17:A:VAL:HG13	1:3:A:ILE:HG22	10	1.43
(1,77)	1:17:A:VAL:HG13	1:3:A:ILE:HG23	10	1.43
(1,1123)	1:50:A:LEU:HD21	1:43:A:LEU:H	10	1.42
(1,1123)	1:50:A:LEU:HD22	1:43:A:LEU:H	10	1.42
(1,1123)	1:50:A:LEU:HD23	1:43:A:LEU:H	10	1.42
(1,28)	1:23:A:ILE:HD13	1:50:A:LEU:HB2	1	1.42
(1,92)	1:17:A:VAL:HG11	1:1:A:MET:HE1	9	1.41
(1,92)	1:17:A:VAL:HG11	1:1:A:MET:HE2	9	1.41
(1,92)	1:17:A:VAL:HG11	1:1:A:MET:HE3	9	1.41
(1,92)	1:17:A:VAL:HG12	1:1:A:MET:HE1	9	1.41
(1,92)	1:17:A:VAL:HG12	1:1:A:MET:HE2	9	1.41
(1,92)	1:17:A:VAL:HG12	1:1:A:MET:HE3	9	1.41
(1,92)	1:17:A:VAL:HG13	1:1:A:MET:HE1	9	1.41
(1,92)	1:17:A:VAL:HG13	1:1:A:MET:HE2	9	1.41
(1,92)	1:17:A:VAL:HG13	1:1:A:MET:HE3	9	1.41
(1,926)	1:70:A:VAL:HG11	1:73:A:LEU:H	3	1.4
(1,926)	1:70:A:VAL:HG12	1:73:A:LEU:H	3	1.4
(1,926)	1:70:A:VAL:HG13	1:73:A:LEU:H	3	1.4
(1,430)	1:15:A:LEU:HD21	1:16:A:GLU:HG3	7	1.38
(1,430)	1:15:A:LEU:HD22	1:16:A:GLU:HG3	7	1.38
(1,430)	1:15:A:LEU:HD23	1:16:A:GLU:HG3	7	1.38
(1,346)	1:17:A:VAL:HG21	1:29:A:LYS:HE2	3	1.38
(1,346)	1:17:A:VAL:HG21	1:29:A:LYS:HE3	3	1.38
(1,346)	1:17:A:VAL:HG22	1:29:A:LYS:HE2	3	1.38
(1,346)	1:17:A:VAL:HG22	1:29:A:LYS:HE3	3	1.38
(1,346)	1:17:A:VAL:HG23	1:29:A:LYS:HE2	3	1.38
(1,346)	1:17:A:VAL:HG23	1:29:A:LYS:HE3	3	1.38
(1,322)	1:10:A:GLY:HA3	1:6:A:LYS:HE2	6	1.38
(1,322)	1:10:A:GLY:HA3	1:6:A:LYS:HE3	6	1.38
(1,322)	1:10:A:GLY:HA3	1:6:A:LYS:HE2	7	1.38
(1,322)	1:10:A:GLY:HA3	1:6:A:LYS:HE3	7	1.38
(1,1218)	1:20:A:SER:HB3	1:22:A:THR:H	1	1.37
(1,1218)	1:20:A:SER:HB3	1:22:A:THR:H	3	1.37
(1,516)	1:26:A:VAL:HG11	1:56:A:LEU:HD11	1	1.37
(1,516)	1:26:A:VAL:HG11	1:56:A:LEU:HD12	1	1.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,516)	1:26:A:VAL:HG11	1:56:A:LEU:HD13	1	1.37
(1,516)	1:26:A:VAL:HG12	1:56:A:LEU:HD11	1	1.37
(1,516)	1:26:A:VAL:HG12	1:56:A:LEU:HD12	1	1.37
(1,516)	1:26:A:VAL:HG12	1:56:A:LEU:HD13	1	1.37
(1,516)	1:26:A:VAL:HG13	1:56:A:LEU:HD11	1	1.37
(1,516)	1:26:A:VAL:HG13	1:56:A:LEU:HD12	1	1.37
(1,516)	1:26:A:VAL:HG13	1:56:A:LEU:HD13	1	1.37
(1,489)	1:23:A:ILE:HD11	1:56:A:LEU:HD21	7	1.37
(1,489)	1:23:A:ILE:HD11	1:56:A:LEU:HD22	7	1.37
(1,489)	1:23:A:ILE:HD11	1:56:A:LEU:HD23	7	1.37
(1,489)	1:23:A:ILE:HD12	1:56:A:LEU:HD21	7	1.37
(1,489)	1:23:A:ILE:HD12	1:56:A:LEU:HD22	7	1.37
(1,489)	1:23:A:ILE:HD12	1:56:A:LEU:HD23	7	1.37
(1,489)	1:23:A:ILE:HD13	1:56:A:LEU:HD21	7	1.37
(1,489)	1:23:A:ILE:HD13	1:56:A:LEU:HD22	7	1.37
(1,489)	1:23:A:ILE:HD13	1:56:A:LEU:HD23	7	1.37
(1,435)	1:33:A:GLU:HG2	1:15:A:LEU:HD11	3	1.37
(1,435)	1:33:A:GLU:HG2	1:15:A:LEU:HD12	3	1.37
(1,435)	1:33:A:GLU:HG2	1:15:A:LEU:HD13	3	1.37
(1,322)	1:10:A:GLY:HA3	1:6:A:LYS:HE2	3	1.37
(1,322)	1:10:A:GLY:HA3	1:6:A:LYS:HE3	3	1.37
(1,77)	1:17:A:VAL:HG11	1:3:A:ILE:HG21	2	1.37
(1,77)	1:17:A:VAL:HG11	1:3:A:ILE:HG22	2	1.37
(1,77)	1:17:A:VAL:HG11	1:3:A:ILE:HG23	2	1.37
(1,77)	1:17:A:VAL:HG12	1:3:A:ILE:HG21	2	1.37
(1,77)	1:17:A:VAL:HG12	1:3:A:ILE:HG22	2	1.37
(1,77)	1:17:A:VAL:HG12	1:3:A:ILE:HG23	2	1.37
(1,77)	1:17:A:VAL:HG13	1:3:A:ILE:HG21	2	1.37
(1,77)	1:17:A:VAL:HG13	1:3:A:ILE:HG22	2	1.37
(1,77)	1:17:A:VAL:HG13	1:3:A:ILE:HG23	2	1.37
(1,1218)	1:20:A:SER:HB3	1:22:A:THR:H	9	1.36
(1,1170)	1:26:A:VAL:HG11	1:18:A:GLU:H	1	1.36
(1,1170)	1:26:A:VAL:HG12	1:18:A:GLU:H	1	1.36
(1,1170)	1:26:A:VAL:HG13	1:18:A:GLU:H	1	1.36
(1,572)	1:31:A:GLN:HA	1:31:A:GLN:HG2	7	1.35
(1,430)	1:15:A:LEU:HD21	1:16:A:GLU:HG3	1	1.35
(1,430)	1:15:A:LEU:HD22	1:16:A:GLU:HG3	1	1.35
(1,430)	1:15:A:LEU:HD23	1:16:A:GLU:HG3	1	1.35
(1,322)	1:10:A:GLY:HA3	1:6:A:LYS:HE2	1	1.35
(1,322)	1:10:A:GLY:HA3	1:6:A:LYS:HE3	1	1.35
(1,1268)	1:71:A:LEU:HG	1:40:A:GLN:HE22	9	1.34
(1,1070)	1:25:A:ASN:HB3	1:21:A:ASP:H	5	1.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,92)	1:17:A:VAL:HG11	1:1:A:MET:HE1	10	1.34
(1,92)	1:17:A:VAL:HG11	1:1:A:MET:HE2	10	1.34
(1,92)	1:17:A:VAL:HG11	1:1:A:MET:HE3	10	1.34
(1,92)	1:17:A:VAL:HG12	1:1:A:MET:HE1	10	1.34
(1,92)	1:17:A:VAL:HG12	1:1:A:MET:HE2	10	1.34
(1,92)	1:17:A:VAL:HG12	1:1:A:MET:HE3	10	1.34
(1,92)	1:17:A:VAL:HG13	1:1:A:MET:HE1	10	1.34
(1,92)	1:17:A:VAL:HG13	1:1:A:MET:HE2	10	1.34
(1,92)	1:17:A:VAL:HG13	1:1:A:MET:HE3	10	1.34
(1,1123)	1:50:A:LEU:HD21	1:43:A:LEU:H	7	1.33
(1,1123)	1:50:A:LEU:HD22	1:43:A:LEU:H	7	1.33
(1,1123)	1:50:A:LEU:HD23	1:43:A:LEU:H	7	1.33
(1,1123)	1:50:A:LEU:HD21	1:43:A:LEU:H	8	1.33
(1,1123)	1:50:A:LEU:HD22	1:43:A:LEU:H	8	1.33
(1,1123)	1:50:A:LEU:HD23	1:43:A:LEU:H	8	1.33
(1,346)	1:17:A:VAL:HG21	1:29:A:LYS:HE2	6	1.33
(1,346)	1:17:A:VAL:HG21	1:29:A:LYS:HE3	6	1.33
(1,346)	1:17:A:VAL:HG22	1:29:A:LYS:HE2	6	1.33
(1,346)	1:17:A:VAL:HG22	1:29:A:LYS:HE3	6	1.33
(1,346)	1:17:A:VAL:HG23	1:29:A:LYS:HE2	6	1.33
(1,346)	1:17:A:VAL:HG23	1:29:A:LYS:HE3	6	1.33
(1,28)	1:23:A:ILE:HD12	1:50:A:LEU:HB2	9	1.33
(1,1268)	1:71:A:LEU:HG	1:40:A:GLN:HE22	10	1.32
(1,1123)	1:50:A:LEU:HD21	1:43:A:LEU:H	2	1.32
(1,1123)	1:50:A:LEU:HD22	1:43:A:LEU:H	2	1.32
(1,1123)	1:50:A:LEU:HD23	1:43:A:LEU:H	2	1.32
(1,92)	1:17:A:VAL:HG11	1:1:A:MET:HE1	1	1.32
(1,92)	1:17:A:VAL:HG11	1:1:A:MET:HE2	1	1.32
(1,92)	1:17:A:VAL:HG11	1:1:A:MET:HE3	1	1.32
(1,92)	1:17:A:VAL:HG12	1:1:A:MET:HE1	1	1.32
(1,92)	1:17:A:VAL:HG12	1:1:A:MET:HE2	1	1.32
(1,92)	1:17:A:VAL:HG12	1:1:A:MET:HE3	1	1.32
(1,92)	1:17:A:VAL:HG13	1:1:A:MET:HE1	1	1.32
(1,92)	1:17:A:VAL:HG13	1:1:A:MET:HE2	1	1.32
(1,92)	1:17:A:VAL:HG13	1:1:A:MET:HE3	1	1.32
(1,92)	1:17:A:VAL:HG11	1:1:A:MET:HE1	2	1.32
(1,92)	1:17:A:VAL:HG11	1:1:A:MET:HE2	2	1.32
(1,92)	1:17:A:VAL:HG11	1:1:A:MET:HE3	2	1.32
(1,92)	1:17:A:VAL:HG12	1:1:A:MET:HE1	2	1.32
(1,92)	1:17:A:VAL:HG12	1:1:A:MET:HE2	2	1.32
(1,92)	1:17:A:VAL:HG12	1:1:A:MET:HE3	2	1.32
(1,92)	1:17:A:VAL:HG13	1:1:A:MET:HE1	2	1.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,92)	1:17:A:VAL:HG13	1:1:A:MET:HE2	2	1.32
(1,92)	1:17:A:VAL:HG13	1:1:A:MET:HE3	2	1.32
(1,1123)	1:50:A:LEU:HD21	1:43:A:LEU:H	5	1.3
(1,1123)	1:50:A:LEU:HD22	1:43:A:LEU:H	5	1.3
(1,1123)	1:50:A:LEU:HD23	1:43:A:LEU:H	5	1.3
(1,516)	1:26:A:VAL:HG11	1:56:A:LEU:HD11	9	1.3
(1,516)	1:26:A:VAL:HG11	1:56:A:LEU:HD12	9	1.3
(1,516)	1:26:A:VAL:HG11	1:56:A:LEU:HD13	9	1.3
(1,516)	1:26:A:VAL:HG12	1:56:A:LEU:HD11	9	1.3
(1,516)	1:26:A:VAL:HG12	1:56:A:LEU:HD12	9	1.3
(1,516)	1:26:A:VAL:HG12	1:56:A:LEU:HD13	9	1.3
(1,516)	1:26:A:VAL:HG13	1:56:A:LEU:HD11	9	1.3
(1,516)	1:26:A:VAL:HG13	1:56:A:LEU:HD12	9	1.3
(1,516)	1:26:A:VAL:HG13	1:56:A:LEU:HD13	9	1.3
(1,92)	1:17:A:VAL:HG11	1:1:A:MET:HE1	5	1.3
(1,92)	1:17:A:VAL:HG11	1:1:A:MET:HE2	5	1.3
(1,92)	1:17:A:VAL:HG11	1:1:A:MET:HE3	5	1.3
(1,92)	1:17:A:VAL:HG12	1:1:A:MET:HE1	5	1.3
(1,92)	1:17:A:VAL:HG12	1:1:A:MET:HE2	5	1.3
(1,92)	1:17:A:VAL:HG12	1:1:A:MET:HE3	5	1.3
(1,92)	1:17:A:VAL:HG13	1:1:A:MET:HE1	5	1.3
(1,92)	1:17:A:VAL:HG13	1:1:A:MET:HE2	5	1.3
(1,92)	1:17:A:VAL:HG13	1:1:A:MET:HE3	5	1.3
(1,77)	1:17:A:VAL:HG11	1:3:A:ILE:HG21	1	1.3
(1,77)	1:17:A:VAL:HG11	1:3:A:ILE:HG22	1	1.3
(1,77)	1:17:A:VAL:HG11	1:3:A:ILE:HG23	1	1.3
(1,77)	1:17:A:VAL:HG12	1:3:A:ILE:HG21	1	1.3
(1,77)	1:17:A:VAL:HG12	1:3:A:ILE:HG22	1	1.3
(1,77)	1:17:A:VAL:HG12	1:3:A:ILE:HG23	1	1.3
(1,77)	1:17:A:VAL:HG13	1:3:A:ILE:HG21	1	1.3
(1,77)	1:17:A:VAL:HG13	1:3:A:ILE:HG22	1	1.3
(1,77)	1:17:A:VAL:HG13	1:3:A:ILE:HG23	1	1.3
(1,374)	1:26:A:VAL:HG11	1:21:A:ASP:HB3	1	1.29
(1,374)	1:26:A:VAL:HG12	1:21:A:ASP:HB3	1	1.29
(1,374)	1:26:A:VAL:HG13	1:21:A:ASP:HB3	1	1.29
(1,322)	1:10:A:GLY:HA3	1:6:A:LYS:HE2	2	1.29
(1,322)	1:10:A:GLY:HA3	1:6:A:LYS:HE3	2	1.29
(1,1268)	1:71:A:LEU:HG	1:40:A:GLN:HE22	6	1.28
(1,1170)	1:26:A:VAL:HG11	1:18:A:GLU:H	6	1.28
(1,1170)	1:26:A:VAL:HG12	1:18:A:GLU:H	6	1.28
(1,1170)	1:26:A:VAL:HG13	1:18:A:GLU:H	6	1.28
(1,430)	1:15:A:LEU:HD21	1:16:A:GLU:HG3	9	1.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,430)	1:15:A:LEU:HD22	1:16:A:GLU:HG3	9	1.28
(1,430)	1:15:A:LEU:HD23	1:16:A:GLU:HG3	9	1.28
(1,374)	1:26:A:VAL:HG11	1:21:A:ASP:HB3	4	1.28
(1,374)	1:26:A:VAL:HG12	1:21:A:ASP:HB3	4	1.28
(1,374)	1:26:A:VAL:HG13	1:21:A:ASP:HB3	4	1.28
(1,92)	1:17:A:VAL:HG11	1:1:A:MET:HE1	6	1.28
(1,92)	1:17:A:VAL:HG11	1:1:A:MET:HE2	6	1.28
(1,92)	1:17:A:VAL:HG11	1:1:A:MET:HE3	6	1.28
(1,92)	1:17:A:VAL:HG12	1:1:A:MET:HE1	6	1.28
(1,92)	1:17:A:VAL:HG12	1:1:A:MET:HE2	6	1.28
(1,92)	1:17:A:VAL:HG12	1:1:A:MET:HE3	6	1.28
(1,92)	1:17:A:VAL:HG13	1:1:A:MET:HE1	6	1.28
(1,92)	1:17:A:VAL:HG13	1:1:A:MET:HE2	6	1.28
(1,92)	1:17:A:VAL:HG13	1:1:A:MET:HE3	6	1.28
(1,77)	1:17:A:VAL:HG11	1:3:A:ILE:HG21	7	1.28
(1,77)	1:17:A:VAL:HG11	1:3:A:ILE:HG22	7	1.28
(1,77)	1:17:A:VAL:HG11	1:3:A:ILE:HG23	7	1.28
(1,77)	1:17:A:VAL:HG12	1:3:A:ILE:HG21	7	1.28
(1,77)	1:17:A:VAL:HG12	1:3:A:ILE:HG22	7	1.28
(1,77)	1:17:A:VAL:HG12	1:3:A:ILE:HG23	7	1.28
(1,77)	1:17:A:VAL:HG13	1:3:A:ILE:HG21	7	1.28
(1,77)	1:17:A:VAL:HG13	1:3:A:ILE:HG22	7	1.28
(1,77)	1:17:A:VAL:HG13	1:3:A:ILE:HG23	7	1.28
(1,77)	1:17:A:VAL:HG11	1:3:A:ILE:HG21	9	1.28
(1,77)	1:17:A:VAL:HG11	1:3:A:ILE:HG22	9	1.28
(1,77)	1:17:A:VAL:HG11	1:3:A:ILE:HG23	9	1.28
(1,77)	1:17:A:VAL:HG12	1:3:A:ILE:HG21	9	1.28
(1,77)	1:17:A:VAL:HG12	1:3:A:ILE:HG22	9	1.28
(1,77)	1:17:A:VAL:HG12	1:3:A:ILE:HG23	9	1.28
(1,77)	1:17:A:VAL:HG13	1:3:A:ILE:HG21	9	1.28
(1,77)	1:17:A:VAL:HG13	1:3:A:ILE:HG22	9	1.28
(1,77)	1:17:A:VAL:HG13	1:3:A:ILE:HG23	9	1.28
(1,1170)	1:26:A:VAL:HG11	1:18:A:GLU:H	10	1.27
(1,1170)	1:26:A:VAL:HG12	1:18:A:GLU:H	10	1.27
(1,1170)	1:26:A:VAL:HG13	1:18:A:GLU:H	10	1.27
(1,449)	1:27:A:LYS:HB2	1:43:A:LEU:HD11	4	1.27
(1,449)	1:27:A:LYS:HB2	1:43:A:LEU:HD12	4	1.27
(1,449)	1:27:A:LYS:HB2	1:43:A:LEU:HD13	4	1.27
(1,374)	1:26:A:VAL:HG11	1:21:A:ASP:HB3	6	1.27
(1,374)	1:26:A:VAL:HG12	1:21:A:ASP:HB3	6	1.27
(1,374)	1:26:A:VAL:HG13	1:21:A:ASP:HB3	6	1.27
(1,1143)	1:70:A:VAL:HG13	1:71:A:LEU:H	10	1.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,572)	1:31:A:GLN:HA	1:31:A:GLN:HG2	5	1.25
(1,1143)	1:70:A:VAL:HG13	1:71:A:LEU:H	1	1.24
(1,77)	1:17:A:VAL:HG11	1:3:A:ILE:HG21	5	1.24
(1,77)	1:17:A:VAL:HG11	1:3:A:ILE:HG22	5	1.24
(1,77)	1:17:A:VAL:HG11	1:3:A:ILE:HG23	5	1.24
(1,77)	1:17:A:VAL:HG12	1:3:A:ILE:HG21	5	1.24
(1,77)	1:17:A:VAL:HG12	1:3:A:ILE:HG22	5	1.24
(1,77)	1:17:A:VAL:HG12	1:3:A:ILE:HG23	5	1.24
(1,77)	1:17:A:VAL:HG13	1:3:A:ILE:HG21	5	1.24
(1,77)	1:17:A:VAL:HG13	1:3:A:ILE:HG22	5	1.24
(1,77)	1:17:A:VAL:HG13	1:3:A:ILE:HG23	5	1.24
(1,572)	1:31:A:GLN:HA	1:31:A:GLN:HG2	2	1.23
(1,81)	1:65:A:SER:HB3	1:3:A:ILE:HG21	1	1.23
(1,81)	1:65:A:SER:HB3	1:3:A:ILE:HG22	1	1.23
(1,81)	1:65:A:SER:HB3	1:3:A:ILE:HG23	1	1.23
(1,346)	1:17:A:VAL:HG21	1:29:A:LYS:HE2	9	1.22
(1,346)	1:17:A:VAL:HG21	1:29:A:LYS:HE3	9	1.22
(1,346)	1:17:A:VAL:HG22	1:29:A:LYS:HE2	9	1.22
(1,346)	1:17:A:VAL:HG22	1:29:A:LYS:HE3	9	1.22
(1,346)	1:17:A:VAL:HG23	1:29:A:LYS:HE2	9	1.22
(1,346)	1:17:A:VAL:HG23	1:29:A:LYS:HE3	9	1.22
(1,92)	1:17:A:VAL:HG11	1:1:A:MET:HE1	3	1.22
(1,92)	1:17:A:VAL:HG11	1:1:A:MET:HE2	3	1.22
(1,92)	1:17:A:VAL:HG11	1:1:A:MET:HE3	3	1.22
(1,92)	1:17:A:VAL:HG12	1:1:A:MET:HE1	3	1.22
(1,92)	1:17:A:VAL:HG12	1:1:A:MET:HE2	3	1.22
(1,92)	1:17:A:VAL:HG12	1:1:A:MET:HE3	3	1.22
(1,92)	1:17:A:VAL:HG13	1:1:A:MET:HE1	3	1.22
(1,92)	1:17:A:VAL:HG13	1:1:A:MET:HE2	3	1.22
(1,92)	1:17:A:VAL:HG13	1:1:A:MET:HE3	3	1.22
(1,92)	1:17:A:VAL:HG11	1:1:A:MET:HE1	7	1.22
(1,92)	1:17:A:VAL:HG11	1:1:A:MET:HE2	7	1.22
(1,92)	1:17:A:VAL:HG11	1:1:A:MET:HE3	7	1.22
(1,92)	1:17:A:VAL:HG12	1:1:A:MET:HE1	7	1.22
(1,92)	1:17:A:VAL:HG12	1:1:A:MET:HE2	7	1.22
(1,92)	1:17:A:VAL:HG12	1:1:A:MET:HE3	7	1.22
(1,92)	1:17:A:VAL:HG13	1:1:A:MET:HE1	7	1.22
(1,92)	1:17:A:VAL:HG13	1:1:A:MET:HE2	7	1.22
(1,92)	1:17:A:VAL:HG13	1:1:A:MET:HE3	7	1.22
(1,754)	1:31:A:GLN:HG2	1:32:A:ASP:H	3	1.21
(1,374)	1:26:A:VAL:HG11	1:21:A:ASP:HB3	9	1.21
(1,374)	1:26:A:VAL:HG12	1:21:A:ASP:HB3	9	1.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,374)	1:26:A:VAL:HG13	1:21:A:ASP:HB3	9	1.21
(1,1268)	1:71:A:LEU:HG	1:40:A:GLN:HE22	2	1.2
(1,1123)	1:50:A:LEU:HD21	1:43:A:LEU:H	3	1.19
(1,1123)	1:50:A:LEU:HD22	1:43:A:LEU:H	3	1.19
(1,1123)	1:50:A:LEU:HD23	1:43:A:LEU:H	3	1.19
(1,130)	1:73:A:LEU:HD11	1:75:A:GLY:HA2	1	1.19
(1,130)	1:73:A:LEU:HD11	1:75:A:GLY:HA3	1	1.19
(1,130)	1:73:A:LEU:HD12	1:75:A:GLY:HA2	1	1.19
(1,130)	1:73:A:LEU:HD12	1:75:A:GLY:HA3	1	1.19
(1,130)	1:73:A:LEU:HD13	1:75:A:GLY:HA2	1	1.19
(1,130)	1:73:A:LEU:HD13	1:75:A:GLY:HA3	1	1.19
(1,572)	1:31:A:GLN:HA	1:31:A:GLN:HG2	8	1.18
(1,77)	1:17:A:VAL:HG11	1:3:A:ILE:HG21	3	1.18
(1,77)	1:17:A:VAL:HG11	1:3:A:ILE:HG22	3	1.18
(1,77)	1:17:A:VAL:HG11	1:3:A:ILE:HG23	3	1.18
(1,77)	1:17:A:VAL:HG12	1:3:A:ILE:HG21	3	1.18
(1,77)	1:17:A:VAL:HG12	1:3:A:ILE:HG22	3	1.18
(1,77)	1:17:A:VAL:HG12	1:3:A:ILE:HG23	3	1.18
(1,77)	1:17:A:VAL:HG13	1:3:A:ILE:HG21	3	1.18
(1,77)	1:17:A:VAL:HG13	1:3:A:ILE:HG22	3	1.18
(1,77)	1:17:A:VAL:HG13	1:3:A:ILE:HG23	3	1.18
(1,754)	1:31:A:GLN:HG2	1:32:A:ASP:H	6	1.17
(1,1123)	1:50:A:LEU:HD21	1:43:A:LEU:H	6	1.16
(1,1123)	1:50:A:LEU:HD22	1:43:A:LEU:H	6	1.16
(1,1123)	1:50:A:LEU:HD23	1:43:A:LEU:H	6	1.16
(1,430)	1:15:A:LEU:HD21	1:16:A:GLU:HG3	10	1.16
(1,430)	1:15:A:LEU:HD22	1:16:A:GLU:HG3	10	1.16
(1,430)	1:15:A:LEU:HD23	1:16:A:GLU:HG3	10	1.16
(1,572)	1:31:A:GLN:HA	1:31:A:GLN:HG2	1	1.15
(1,346)	1:17:A:VAL:HG21	1:29:A:LYS:HE2	4	1.15
(1,346)	1:17:A:VAL:HG21	1:29:A:LYS:HE3	4	1.15
(1,346)	1:17:A:VAL:HG22	1:29:A:LYS:HE2	4	1.15
(1,346)	1:17:A:VAL:HG22	1:29:A:LYS:HE3	4	1.15
(1,346)	1:17:A:VAL:HG23	1:29:A:LYS:HE2	4	1.15
(1,346)	1:17:A:VAL:HG23	1:29:A:LYS:HE3	4	1.15
(1,39)	1:3:A:ILE:HD11	1:17:A:VAL:HG11	6	1.15
(1,39)	1:3:A:ILE:HD11	1:17:A:VAL:HG12	6	1.15
(1,39)	1:3:A:ILE:HD11	1:17:A:VAL:HG13	6	1.15
(1,39)	1:3:A:ILE:HD12	1:17:A:VAL:HG11	6	1.15
(1,39)	1:3:A:ILE:HD12	1:17:A:VAL:HG12	6	1.15
(1,39)	1:3:A:ILE:HD12	1:17:A:VAL:HG13	6	1.15
(1,39)	1:3:A:ILE:HD13	1:17:A:VAL:HG11	6	1.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,39)	1:3:A:ILE:HD13	1:17:A:VAL:HG12	6	1.15
(1,39)	1:3:A:ILE:HD13	1:17:A:VAL:HG13	6	1.15
(1,435)	1:33:A:GLU:HG2	1:15:A:LEU:HD11	4	1.14
(1,435)	1:33:A:GLU:HG2	1:15:A:LEU:HD12	4	1.14
(1,435)	1:33:A:GLU:HG2	1:15:A:LEU:HD13	4	1.14
(1,39)	1:3:A:ILE:HD11	1:17:A:VAL:HG11	10	1.14
(1,39)	1:3:A:ILE:HD11	1:17:A:VAL:HG12	10	1.14
(1,39)	1:3:A:ILE:HD11	1:17:A:VAL:HG13	10	1.14
(1,39)	1:3:A:ILE:HD12	1:17:A:VAL:HG11	10	1.14
(1,39)	1:3:A:ILE:HD12	1:17:A:VAL:HG12	10	1.14
(1,39)	1:3:A:ILE:HD12	1:17:A:VAL:HG13	10	1.14
(1,39)	1:3:A:ILE:HD13	1:17:A:VAL:HG11	10	1.14
(1,39)	1:3:A:ILE:HD13	1:17:A:VAL:HG12	10	1.14
(1,39)	1:3:A:ILE:HD13	1:17:A:VAL:HG13	10	1.14
(1,1268)	1:71:A:LEU:HG	1:40:A:GLN:HE22	4	1.13
(1,1123)	1:50:A:LEU:HD21	1:43:A:LEU:H	9	1.13
(1,1123)	1:50:A:LEU:HD22	1:43:A:LEU:H	9	1.13
(1,1123)	1:50:A:LEU:HD23	1:43:A:LEU:H	9	1.13
(1,516)	1:26:A:VAL:HG11	1:56:A:LEU:HD11	6	1.13
(1,516)	1:26:A:VAL:HG11	1:56:A:LEU:HD12	6	1.13
(1,516)	1:26:A:VAL:HG11	1:56:A:LEU:HD13	6	1.13
(1,516)	1:26:A:VAL:HG12	1:56:A:LEU:HD11	6	1.13
(1,516)	1:26:A:VAL:HG12	1:56:A:LEU:HD12	6	1.13
(1,516)	1:26:A:VAL:HG12	1:56:A:LEU:HD13	6	1.13
(1,516)	1:26:A:VAL:HG13	1:56:A:LEU:HD11	6	1.13
(1,516)	1:26:A:VAL:HG13	1:56:A:LEU:HD12	6	1.13
(1,516)	1:26:A:VAL:HG13	1:56:A:LEU:HD13	6	1.13
(1,448)	1:30:A:ILE:HD11	1:27:A:LYS:HB2	8	1.13
(1,448)	1:30:A:ILE:HD12	1:27:A:LYS:HB2	8	1.13
(1,448)	1:30:A:ILE:HD13	1:27:A:LYS:HB2	8	1.13
(1,175)	1:65:A:SER:HB3	1:67:A:LEU:HD11	9	1.13
(1,175)	1:65:A:SER:HB3	1:67:A:LEU:HD12	9	1.13
(1,175)	1:65:A:SER:HB3	1:67:A:LEU:HD13	9	1.13
(1,580)	1:41:A:GLN:HG2	1:71:A:LEU:HD23	5	1.12
(1,1268)	1:71:A:LEU:HG	1:40:A:GLN:HE22	7	1.11
(1,798)	1:44:A:ILE:HG22	1:44:A:ILE:H	5	1.11
(1,430)	1:15:A:LEU:HD21	1:16:A:GLU:HG3	8	1.11
(1,430)	1:15:A:LEU:HD22	1:16:A:GLU:HG3	8	1.11
(1,430)	1:15:A:LEU:HD23	1:16:A:GLU:HG3	8	1.11
(1,92)	1:17:A:VAL:HG11	1:1:A:MET:HE1	8	1.11
(1,92)	1:17:A:VAL:HG11	1:1:A:MET:HE2	8	1.11
(1,92)	1:17:A:VAL:HG11	1:1:A:MET:HE3	8	1.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,92)	1:17:A:VAL:HG12	1:1:A:MET:HE1	8	1.11
(1,92)	1:17:A:VAL:HG12	1:1:A:MET:HE2	8	1.11
(1,92)	1:17:A:VAL:HG12	1:1:A:MET:HE3	8	1.11
(1,92)	1:17:A:VAL:HG13	1:1:A:MET:HE1	8	1.11
(1,92)	1:17:A:VAL:HG13	1:1:A:MET:HE2	8	1.11
(1,92)	1:17:A:VAL:HG13	1:1:A:MET:HE3	8	1.11
(1,39)	1:3:A:ILE:HD11	1:17:A:VAL:HG11	1	1.11
(1,39)	1:3:A:ILE:HD11	1:17:A:VAL:HG12	1	1.11
(1,39)	1:3:A:ILE:HD11	1:17:A:VAL:HG13	1	1.11
(1,39)	1:3:A:ILE:HD12	1:17:A:VAL:HG11	1	1.11
(1,39)	1:3:A:ILE:HD12	1:17:A:VAL:HG12	1	1.11
(1,39)	1:3:A:ILE:HD12	1:17:A:VAL:HG13	1	1.11
(1,39)	1:3:A:ILE:HD13	1:17:A:VAL:HG11	1	1.11
(1,39)	1:3:A:ILE:HD13	1:17:A:VAL:HG12	1	1.11
(1,39)	1:3:A:ILE:HD13	1:17:A:VAL:HG13	1	1.11
(1,1268)	1:71:A:LEU:HG	1:40:A:GLN:HE22	5	1.1
(1,1170)	1:26:A:VAL:HG11	1:18:A:GLU:H	8	1.1
(1,1170)	1:26:A:VAL:HG12	1:18:A:GLU:H	8	1.1
(1,1170)	1:26:A:VAL:HG13	1:18:A:GLU:H	8	1.1
(1,1123)	1:50:A:LEU:HD21	1:43:A:LEU:H	1	1.1
(1,1123)	1:50:A:LEU:HD22	1:43:A:LEU:H	1	1.1
(1,1123)	1:50:A:LEU:HD23	1:43:A:LEU:H	1	1.1
(1,374)	1:26:A:VAL:HG11	1:21:A:ASP:HB3	2	1.1
(1,374)	1:26:A:VAL:HG12	1:21:A:ASP:HB3	2	1.1
(1,374)	1:26:A:VAL:HG13	1:21:A:ASP:HB3	2	1.1
(1,374)	1:26:A:VAL:HG11	1:21:A:ASP:HB3	10	1.1
(1,374)	1:26:A:VAL:HG12	1:21:A:ASP:HB3	10	1.1
(1,374)	1:26:A:VAL:HG13	1:21:A:ASP:HB3	10	1.1
(1,175)	1:65:A:SER:HB3	1:67:A:LEU:HD11	1	1.1
(1,175)	1:65:A:SER:HB3	1:67:A:LEU:HD12	1	1.1
(1,175)	1:65:A:SER:HB3	1:67:A:LEU:HD13	1	1.1
(1,374)	1:26:A:VAL:HG11	1:21:A:ASP:HB3	5	1.09
(1,374)	1:26:A:VAL:HG12	1:21:A:ASP:HB3	5	1.09
(1,374)	1:26:A:VAL:HG13	1:21:A:ASP:HB3	5	1.09
(1,374)	1:26:A:VAL:HG11	1:21:A:ASP:HB3	7	1.09
(1,374)	1:26:A:VAL:HG12	1:21:A:ASP:HB3	7	1.09
(1,374)	1:26:A:VAL:HG13	1:21:A:ASP:HB3	7	1.09
(1,77)	1:17:A:VAL:HG11	1:3:A:ILE:HG21	4	1.09
(1,77)	1:17:A:VAL:HG11	1:3:A:ILE:HG22	4	1.09
(1,77)	1:17:A:VAL:HG11	1:3:A:ILE:HG23	4	1.09
(1,77)	1:17:A:VAL:HG12	1:3:A:ILE:HG21	4	1.09
(1,77)	1:17:A:VAL:HG12	1:3:A:ILE:HG22	4	1.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,77)	1:17:A:VAL:HG12	1:3:A:ILE:HG23	4	1.09
(1,77)	1:17:A:VAL:HG13	1:3:A:ILE:HG21	4	1.09
(1,77)	1:17:A:VAL:HG13	1:3:A:ILE:HG22	4	1.09
(1,77)	1:17:A:VAL:HG13	1:3:A:ILE:HG23	4	1.09
(1,39)	1:3:A:ILE:HD11	1:17:A:VAL:HG11	2	1.08
(1,39)	1:3:A:ILE:HD11	1:17:A:VAL:HG12	2	1.08
(1,39)	1:3:A:ILE:HD11	1:17:A:VAL:HG13	2	1.08
(1,39)	1:3:A:ILE:HD12	1:17:A:VAL:HG11	2	1.08
(1,39)	1:3:A:ILE:HD12	1:17:A:VAL:HG12	2	1.08
(1,39)	1:3:A:ILE:HD12	1:17:A:VAL:HG13	2	1.08
(1,39)	1:3:A:ILE:HD13	1:17:A:VAL:HG11	2	1.08
(1,39)	1:3:A:ILE:HD13	1:17:A:VAL:HG12	2	1.08
(1,39)	1:3:A:ILE:HD13	1:17:A:VAL:HG13	2	1.08
(1,798)	1:44:A:ILE:HG21	1:44:A:ILE:H	4	1.07
(1,704)	1:18:A:GLU:HB3	1:21:A:ASP:H	10	1.07
(1,926)	1:70:A:VAL:HG11	1:73:A:LEU:H	10	1.06
(1,926)	1:70:A:VAL:HG12	1:73:A:LEU:H	10	1.06
(1,926)	1:70:A:VAL:HG13	1:73:A:LEU:H	10	1.06
(1,39)	1:3:A:ILE:HD11	1:17:A:VAL:HG11	7	1.06
(1,39)	1:3:A:ILE:HD11	1:17:A:VAL:HG12	7	1.06
(1,39)	1:3:A:ILE:HD11	1:17:A:VAL:HG13	7	1.06
(1,39)	1:3:A:ILE:HD12	1:17:A:VAL:HG11	7	1.06
(1,39)	1:3:A:ILE:HD12	1:17:A:VAL:HG12	7	1.06
(1,39)	1:3:A:ILE:HD12	1:17:A:VAL:HG13	7	1.06
(1,39)	1:3:A:ILE:HD13	1:17:A:VAL:HG11	7	1.06
(1,39)	1:3:A:ILE:HD13	1:17:A:VAL:HG12	7	1.06
(1,39)	1:3:A:ILE:HD13	1:17:A:VAL:HG13	7	1.06
(1,28)	1:23:A:ILE:HD11	1:50:A:LEU:HB2	8	1.06
(1,435)	1:33:A:GLU:HG2	1:15:A:LEU:HD11	2	1.05
(1,435)	1:33:A:GLU:HG2	1:15:A:LEU:HD12	2	1.05
(1,435)	1:33:A:GLU:HG2	1:15:A:LEU:HD13	2	1.05
(1,516)	1:26:A:VAL:HG11	1:56:A:LEU:HD11	2	1.04
(1,516)	1:26:A:VAL:HG11	1:56:A:LEU:HD12	2	1.04
(1,516)	1:26:A:VAL:HG11	1:56:A:LEU:HD13	2	1.04
(1,516)	1:26:A:VAL:HG12	1:56:A:LEU:HD11	2	1.04
(1,516)	1:26:A:VAL:HG12	1:56:A:LEU:HD12	2	1.04
(1,516)	1:26:A:VAL:HG12	1:56:A:LEU:HD13	2	1.04
(1,516)	1:26:A:VAL:HG13	1:56:A:LEU:HD11	2	1.04
(1,516)	1:26:A:VAL:HG13	1:56:A:LEU:HD12	2	1.04
(1,516)	1:26:A:VAL:HG13	1:56:A:LEU:HD13	2	1.04
(1,516)	1:26:A:VAL:HG11	1:56:A:LEU:HD11	5	1.03
(1,516)	1:26:A:VAL:HG11	1:56:A:LEU:HD12	5	1.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,516)	1:26:A:VAL:HG11	1:56:A:LEU:HD13	5	1.03
(1,516)	1:26:A:VAL:HG12	1:56:A:LEU:HD11	5	1.03
(1,516)	1:26:A:VAL:HG12	1:56:A:LEU:HD12	5	1.03
(1,516)	1:26:A:VAL:HG12	1:56:A:LEU:HD13	5	1.03
(1,516)	1:26:A:VAL:HG13	1:56:A:LEU:HD11	5	1.03
(1,516)	1:26:A:VAL:HG13	1:56:A:LEU:HD12	5	1.03
(1,516)	1:26:A:VAL:HG13	1:56:A:LEU:HD13	5	1.03
(1,516)	1:26:A:VAL:HG11	1:56:A:LEU:HD11	7	1.03
(1,516)	1:26:A:VAL:HG11	1:56:A:LEU:HD12	7	1.03
(1,516)	1:26:A:VAL:HG11	1:56:A:LEU:HD13	7	1.03
(1,516)	1:26:A:VAL:HG12	1:56:A:LEU:HD11	7	1.03
(1,516)	1:26:A:VAL:HG12	1:56:A:LEU:HD12	7	1.03
(1,516)	1:26:A:VAL:HG12	1:56:A:LEU:HD13	7	1.03
(1,516)	1:26:A:VAL:HG13	1:56:A:LEU:HD11	7	1.03
(1,516)	1:26:A:VAL:HG13	1:56:A:LEU:HD12	7	1.03
(1,516)	1:26:A:VAL:HG13	1:56:A:LEU:HD13	7	1.03
(1,448)	1:30:A:ILE:HD11	1:27:A:LYS:HB2	5	1.03
(1,448)	1:30:A:ILE:HD12	1:27:A:LYS:HB2	5	1.03
(1,448)	1:30:A:ILE:HD13	1:27:A:LYS:HB2	5	1.03
(1,435)	1:33:A:GLU:HG2	1:15:A:LEU:HD11	1	1.03
(1,435)	1:33:A:GLU:HG2	1:15:A:LEU:HD12	1	1.03
(1,435)	1:33:A:GLU:HG2	1:15:A:LEU:HD13	1	1.03
(1,289)	1:73:A:LEU:HD11	1:73:A:LEU:HA	7	1.03
(1,289)	1:73:A:LEU:HD12	1:73:A:LEU:HA	7	1.03
(1,289)	1:73:A:LEU:HD13	1:73:A:LEU:HA	7	1.03
(1,798)	1:44:A:ILE:HG21	1:44:A:ILE:H	6	1.02
(1,798)	1:44:A:ILE:HG22	1:44:A:ILE:H	8	1.02
(1,572)	1:31:A:GLN:HA	1:31:A:GLN:HG2	10	1.02
(1,435)	1:33:A:GLU:HG2	1:15:A:LEU:HD11	8	1.02
(1,435)	1:33:A:GLU:HG2	1:15:A:LEU:HD12	8	1.02
(1,435)	1:33:A:GLU:HG2	1:15:A:LEU:HD13	8	1.02
(1,81)	1:65:A:SER:HB3	1:3:A:ILE:HG21	8	1.02
(1,81)	1:65:A:SER:HB3	1:3:A:ILE:HG22	8	1.02
(1,81)	1:65:A:SER:HB3	1:3:A:ILE:HG23	8	1.02
(1,39)	1:3:A:ILE:HD11	1:17:A:VAL:HG11	3	1.01
(1,39)	1:3:A:ILE:HD11	1:17:A:VAL:HG12	3	1.01
(1,39)	1:3:A:ILE:HD11	1:17:A:VAL:HG13	3	1.01
(1,39)	1:3:A:ILE:HD12	1:17:A:VAL:HG11	3	1.01
(1,39)	1:3:A:ILE:HD12	1:17:A:VAL:HG12	3	1.01
(1,39)	1:3:A:ILE:HD12	1:17:A:VAL:HG13	3	1.01
(1,39)	1:3:A:ILE:HD13	1:17:A:VAL:HG11	3	1.01
(1,39)	1:3:A:ILE:HD13	1:17:A:VAL:HG12	3	1.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,39)	1:3:A:ILE:HD13	1:17:A:VAL:HG13	3	1.01
(1,1170)	1:26:A:VAL:HG11	1:18:A:GLU:H	2	1.0
(1,1170)	1:26:A:VAL:HG12	1:18:A:GLU:H	2	1.0
(1,1170)	1:26:A:VAL:HG13	1:18:A:GLU:H	2	1.0
(1,81)	1:65:A:SER:HB3	1:3:A:ILE:HG21	5	1.0
(1,81)	1:65:A:SER:HB3	1:3:A:ILE:HG22	5	1.0
(1,81)	1:65:A:SER:HB3	1:3:A:ILE:HG23	5	1.0
(1,39)	1:3:A:ILE:HD11	1:17:A:VAL:HG11	9	1.0
(1,39)	1:3:A:ILE:HD11	1:17:A:VAL:HG12	9	1.0
(1,39)	1:3:A:ILE:HD11	1:17:A:VAL:HG13	9	1.0
(1,39)	1:3:A:ILE:HD12	1:17:A:VAL:HG11	9	1.0
(1,39)	1:3:A:ILE:HD12	1:17:A:VAL:HG12	9	1.0
(1,39)	1:3:A:ILE:HD12	1:17:A:VAL:HG13	9	1.0
(1,39)	1:3:A:ILE:HD13	1:17:A:VAL:HG11	9	1.0
(1,39)	1:3:A:ILE:HD13	1:17:A:VAL:HG12	9	1.0
(1,39)	1:3:A:ILE:HD13	1:17:A:VAL:HG13	9	1.0
(1,516)	1:26:A:VAL:HG11	1:56:A:LEU:HD11	10	0.99
(1,516)	1:26:A:VAL:HG11	1:56:A:LEU:HD12	10	0.99
(1,516)	1:26:A:VAL:HG11	1:56:A:LEU:HD13	10	0.99
(1,516)	1:26:A:VAL:HG12	1:56:A:LEU:HD11	10	0.99
(1,516)	1:26:A:VAL:HG12	1:56:A:LEU:HD12	10	0.99
(1,516)	1:26:A:VAL:HG12	1:56:A:LEU:HD13	10	0.99
(1,516)	1:26:A:VAL:HG13	1:56:A:LEU:HD11	10	0.99
(1,516)	1:26:A:VAL:HG13	1:56:A:LEU:HD12	10	0.99
(1,516)	1:26:A:VAL:HG13	1:56:A:LEU:HD13	10	0.99
(1,292)	1:43:A:LEU:HD11	1:43:A:LEU:HA	2	0.99
(1,292)	1:43:A:LEU:HD12	1:43:A:LEU:HA	2	0.99
(1,292)	1:43:A:LEU:HD13	1:43:A:LEU:HA	2	0.99
(1,292)	1:43:A:LEU:HD11	1:43:A:LEU:HA	3	0.99
(1,292)	1:43:A:LEU:HD12	1:43:A:LEU:HA	3	0.99
(1,292)	1:43:A:LEU:HD13	1:43:A:LEU:HA	3	0.99
(1,292)	1:43:A:LEU:HD11	1:43:A:LEU:HA	9	0.99
(1,292)	1:43:A:LEU:HD12	1:43:A:LEU:HA	9	0.99
(1,292)	1:43:A:LEU:HD13	1:43:A:LEU:HA	9	0.99
(1,292)	1:43:A:LEU:HD11	1:43:A:LEU:HA	7	0.98
(1,292)	1:43:A:LEU:HD12	1:43:A:LEU:HA	7	0.98
(1,292)	1:43:A:LEU:HD13	1:43:A:LEU:HA	7	0.98
(1,289)	1:73:A:LEU:HD11	1:73:A:LEU:HA	1	0.98
(1,289)	1:73:A:LEU:HD12	1:73:A:LEU:HA	1	0.98
(1,289)	1:73:A:LEU:HD13	1:73:A:LEU:HA	1	0.98
(1,1059)	1:72:A:ARG:HB2	1:72:A:ARG:H	2	0.97
(1,580)	1:41:A:GLN:HG3	1:69:A:LEU:HD21	7	0.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,292)	1:43:A:LEU:HD11	1:43:A:LEU:HA	1	0.97
(1,292)	1:43:A:LEU:HD12	1:43:A:LEU:HA	1	0.97
(1,292)	1:43:A:LEU:HD13	1:43:A:LEU:HA	1	0.97
(1,292)	1:43:A:LEU:HD11	1:43:A:LEU:HA	10	0.97
(1,292)	1:43:A:LEU:HD12	1:43:A:LEU:HA	10	0.97
(1,292)	1:43:A:LEU:HD13	1:43:A:LEU:HA	10	0.97
(1,111)	1:2:A:LYS:HD3	1:14:A:THR:HG21	2	0.97
(1,111)	1:2:A:LYS:HD3	1:14:A:THR:HG22	2	0.97
(1,111)	1:2:A:LYS:HD3	1:14:A:THR:HG23	2	0.97
(1,39)	1:3:A:ILE:HD11	1:17:A:VAL:HG11	5	0.97
(1,39)	1:3:A:ILE:HD11	1:17:A:VAL:HG12	5	0.97
(1,39)	1:3:A:ILE:HD11	1:17:A:VAL:HG13	5	0.97
(1,39)	1:3:A:ILE:HD12	1:17:A:VAL:HG11	5	0.97
(1,39)	1:3:A:ILE:HD12	1:17:A:VAL:HG12	5	0.97
(1,39)	1:3:A:ILE:HD12	1:17:A:VAL:HG13	5	0.97
(1,39)	1:3:A:ILE:HD13	1:17:A:VAL:HG11	5	0.97
(1,39)	1:3:A:ILE:HD13	1:17:A:VAL:HG12	5	0.97
(1,39)	1:3:A:ILE:HD13	1:17:A:VAL:HG13	5	0.97
(1,1013)	1:62:A:GLN:HB2	1:65:A:SER:H	6	0.96
(1,580)	1:41:A:GLN:HG3	1:69:A:LEU:HD23	2	0.96
(1,435)	1:33:A:GLU:HG2	1:15:A:LEU:HD11	10	0.96
(1,435)	1:33:A:GLU:HG2	1:15:A:LEU:HD12	10	0.96
(1,435)	1:33:A:GLU:HG2	1:15:A:LEU:HD13	10	0.96
(1,131)	1:73:A:LEU:HD11	1:73:A:LEU:HA	7	0.96
(1,131)	1:73:A:LEU:HD12	1:73:A:LEU:HA	7	0.96
(1,131)	1:73:A:LEU:HD13	1:73:A:LEU:HA	7	0.96
(1,1070)	1:25:A:ASN:HB3	1:21:A:ASP:H	3	0.94
(1,1059)	1:72:A:ARG:HB2	1:72:A:ARG:H	3	0.94
(1,926)	1:70:A:VAL:HG11	1:73:A:LEU:H	1	0.94
(1,926)	1:70:A:VAL:HG12	1:73:A:LEU:H	1	0.94
(1,926)	1:70:A:VAL:HG13	1:73:A:LEU:H	1	0.94
(1,516)	1:26:A:VAL:HG11	1:56:A:LEU:HD11	8	0.94
(1,516)	1:26:A:VAL:HG11	1:56:A:LEU:HD12	8	0.94
(1,516)	1:26:A:VAL:HG11	1:56:A:LEU:HD13	8	0.94
(1,516)	1:26:A:VAL:HG12	1:56:A:LEU:HD11	8	0.94
(1,516)	1:26:A:VAL:HG12	1:56:A:LEU:HD12	8	0.94
(1,516)	1:26:A:VAL:HG12	1:56:A:LEU:HD13	8	0.94
(1,516)	1:26:A:VAL:HG13	1:56:A:LEU:HD11	8	0.94
(1,516)	1:26:A:VAL:HG13	1:56:A:LEU:HD12	8	0.94
(1,516)	1:26:A:VAL:HG13	1:56:A:LEU:HD13	8	0.94
(1,435)	1:33:A:GLU:HG2	1:15:A:LEU:HD11	7	0.93
(1,435)	1:33:A:GLU:HG2	1:15:A:LEU:HD12	7	0.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,435)	1:33:A:GLU:HG2	1:15:A:LEU:HD13	7	0.93
(1,1013)	1:63:A:LYS:HB3	1:65:A:SER:H	2	0.92
(1,594)	1:3:A:ILE:HD11	1:56:A:LEU:HD21	7	0.92
(1,594)	1:3:A:ILE:HD11	1:56:A:LEU:HD22	7	0.92
(1,594)	1:3:A:ILE:HD11	1:56:A:LEU:HD23	7	0.92
(1,594)	1:3:A:ILE:HD12	1:56:A:LEU:HD21	7	0.92
(1,594)	1:3:A:ILE:HD12	1:56:A:LEU:HD22	7	0.92
(1,594)	1:3:A:ILE:HD12	1:56:A:LEU:HD23	7	0.92
(1,594)	1:3:A:ILE:HD13	1:56:A:LEU:HD21	7	0.92
(1,594)	1:3:A:ILE:HD13	1:56:A:LEU:HD22	7	0.92
(1,594)	1:3:A:ILE:HD13	1:56:A:LEU:HD23	7	0.92
(1,580)	1:41:A:GLN:HG2	1:71:A:LEU:HD21	8	0.92
(1,572)	1:31:A:GLN:HA	1:31:A:GLN:HG2	4	0.92
(1,131)	1:73:A:LEU:HD11	1:73:A:LEU:HA	1	0.91
(1,131)	1:73:A:LEU:HD12	1:73:A:LEU:HA	1	0.91
(1,131)	1:73:A:LEU:HD13	1:73:A:LEU:HA	1	0.91
(1,427)	1:15:A:LEU:HD21	1:16:A:GLU:HG2	5	0.89
(1,427)	1:15:A:LEU:HD22	1:16:A:GLU:HG2	5	0.89
(1,427)	1:15:A:LEU:HD23	1:16:A:GLU:HG2	5	0.89
(1,931)	1:17:A:VAL:HG11	1:3:A:ILE:H	7	0.88
(1,931)	1:17:A:VAL:HG12	1:3:A:ILE:H	7	0.88
(1,931)	1:17:A:VAL:HG13	1:3:A:ILE:H	7	0.88
(1,111)	1:2:A:LYS:HD3	1:14:A:THR:HG21	1	0.88
(1,111)	1:2:A:LYS:HD3	1:14:A:THR:HG22	1	0.88
(1,111)	1:2:A:LYS:HD3	1:14:A:THR:HG23	1	0.88
(1,1174)	1:27:A:LYS:HD2	1:27:A:LYS:H	5	0.87
(1,931)	1:17:A:VAL:HG11	1:3:A:ILE:H	6	0.87
(1,931)	1:17:A:VAL:HG12	1:3:A:ILE:H	6	0.87
(1,931)	1:17:A:VAL:HG13	1:3:A:ILE:H	6	0.87
(1,754)	1:31:A:GLN:HG2	1:32:A:ASP:H	9	0.87
(1,593)	1:3:A:ILE:HD11	1:15:A:LEU:HB2	4	0.87
(1,593)	1:3:A:ILE:HD12	1:15:A:LEU:HB2	4	0.87
(1,593)	1:3:A:ILE:HD13	1:15:A:LEU:HB2	4	0.87
(1,582)	1:55:A:THR:HB	1:20:A:SER:HB3	8	0.87
(1,1255)	1:39:A:ASP:HA	1:40:A:GLN:HE22	4	0.86
(1,931)	1:17:A:VAL:HG11	1:3:A:ILE:H	3	0.86
(1,931)	1:17:A:VAL:HG12	1:3:A:ILE:H	3	0.86
(1,931)	1:17:A:VAL:HG13	1:3:A:ILE:H	3	0.86
(1,729)	1:27:A:LYS:HB3	1:28:A:ALA:H	3	0.86
(1,282)	1:50:A:LEU:HD11	1:50:A:LEU:HA	4	0.86
(1,282)	1:50:A:LEU:HD12	1:50:A:LEU:HA	4	0.86
(1,282)	1:50:A:LEU:HD13	1:50:A:LEU:HA	4	0.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,282)	1:50:A:LEU:HD11	1:50:A:LEU:HA	5	0.86
(1,282)	1:50:A:LEU:HD12	1:50:A:LEU:HA	5	0.86
(1,282)	1:50:A:LEU:HD13	1:50:A:LEU:HA	5	0.86
(1,254)	1:49:A:LYS:HA	1:49:A:LYS:HG2	7	0.86
(1,1013)	1:63:A:LYS:HB3	1:65:A:SER:H	10	0.85
(1,909)	1:67:A:LEU:HD11	1:67:A:LEU:H	1	0.85
(1,909)	1:67:A:LEU:HD12	1:67:A:LEU:H	1	0.85
(1,909)	1:67:A:LEU:HD13	1:67:A:LEU:H	1	0.85
(1,720)	1:26:A:VAL:HG11	1:26:A:VAL:H	1	0.85
(1,720)	1:26:A:VAL:HG12	1:26:A:VAL:H	1	0.85
(1,720)	1:26:A:VAL:HG13	1:26:A:VAL:H	1	0.85
(1,720)	1:26:A:VAL:HG11	1:26:A:VAL:H	2	0.85
(1,720)	1:26:A:VAL:HG12	1:26:A:VAL:H	2	0.85
(1,720)	1:26:A:VAL:HG13	1:26:A:VAL:H	2	0.85
(1,720)	1:26:A:VAL:HG11	1:26:A:VAL:H	3	0.85
(1,720)	1:26:A:VAL:HG12	1:26:A:VAL:H	3	0.85
(1,720)	1:26:A:VAL:HG13	1:26:A:VAL:H	3	0.85
(1,720)	1:26:A:VAL:HG11	1:26:A:VAL:H	4	0.85
(1,720)	1:26:A:VAL:HG12	1:26:A:VAL:H	4	0.85
(1,720)	1:26:A:VAL:HG13	1:26:A:VAL:H	4	0.85
(1,720)	1:26:A:VAL:HG11	1:26:A:VAL:H	5	0.85
(1,720)	1:26:A:VAL:HG12	1:26:A:VAL:H	5	0.85
(1,720)	1:26:A:VAL:HG13	1:26:A:VAL:H	5	0.85
(1,720)	1:26:A:VAL:HG11	1:26:A:VAL:H	6	0.85
(1,720)	1:26:A:VAL:HG12	1:26:A:VAL:H	6	0.85
(1,720)	1:26:A:VAL:HG13	1:26:A:VAL:H	6	0.85
(1,720)	1:26:A:VAL:HG11	1:26:A:VAL:H	8	0.85
(1,720)	1:26:A:VAL:HG12	1:26:A:VAL:H	8	0.85
(1,720)	1:26:A:VAL:HG13	1:26:A:VAL:H	8	0.85
(1,720)	1:26:A:VAL:HG11	1:26:A:VAL:H	9	0.85
(1,720)	1:26:A:VAL:HG12	1:26:A:VAL:H	9	0.85
(1,720)	1:26:A:VAL:HG13	1:26:A:VAL:H	9	0.85
(1,720)	1:26:A:VAL:HG11	1:26:A:VAL:H	10	0.85
(1,720)	1:26:A:VAL:HG12	1:26:A:VAL:H	10	0.85
(1,720)	1:26:A:VAL:HG13	1:26:A:VAL:H	10	0.85
(1,488)	1:30:A:ILE:HD12	1:43:A:LEU:HG	4	0.85
(1,282)	1:50:A:LEU:HD11	1:50:A:LEU:HA	8	0.85
(1,282)	1:50:A:LEU:HD12	1:50:A:LEU:HA	8	0.85
(1,282)	1:50:A:LEU:HD13	1:50:A:LEU:HA	8	0.85
(1,23)	1:23:A:ILE:HD11	1:50:A:LEU:HD11	5	0.85
(1,23)	1:23:A:ILE:HD11	1:50:A:LEU:HD12	5	0.85
(1,23)	1:23:A:ILE:HD11	1:50:A:LEU:HD13	5	0.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,23)	1:23:A:ILE:HD12	1:50:A:LEU:HD11	5	0.85
(1,23)	1:23:A:ILE:HD12	1:50:A:LEU:HD12	5	0.85
(1,23)	1:23:A:ILE:HD12	1:50:A:LEU:HD13	5	0.85
(1,23)	1:23:A:ILE:HD13	1:50:A:LEU:HD11	5	0.85
(1,23)	1:23:A:ILE:HD13	1:50:A:LEU:HD12	5	0.85
(1,23)	1:23:A:ILE:HD13	1:50:A:LEU:HD13	5	0.85
(1,1013)	1:63:A:LYS:HB3	1:65:A:SER:H	8	0.84
(1,729)	1:27:A:LYS:HB3	1:28:A:ALA:H	9	0.84
(1,720)	1:26:A:VAL:HG11	1:26:A:VAL:H	7	0.84
(1,720)	1:26:A:VAL:HG12	1:26:A:VAL:H	7	0.84
(1,720)	1:26:A:VAL:HG13	1:26:A:VAL:H	7	0.84
(1,282)	1:50:A:LEU:HD11	1:50:A:LEU:HA	2	0.84
(1,282)	1:50:A:LEU:HD12	1:50:A:LEU:HA	2	0.84
(1,282)	1:50:A:LEU:HD13	1:50:A:LEU:HA	2	0.84
(1,1013)	1:63:A:LYS:HB3	1:65:A:SER:H	9	0.83
(1,729)	1:27:A:LYS:HB3	1:28:A:ALA:H	10	0.83
(1,582)	1:55:A:THR:HB	1:20:A:SER:HB3	5	0.83
(1,282)	1:50:A:LEU:HD11	1:50:A:LEU:HA	6	0.83
(1,282)	1:50:A:LEU:HD12	1:50:A:LEU:HA	6	0.83
(1,282)	1:50:A:LEU:HD13	1:50:A:LEU:HA	6	0.83
(1,1013)	1:62:A:GLN:HB2	1:65:A:SER:H	3	0.82
(1,729)	1:27:A:LYS:HB3	1:28:A:ALA:H	4	0.82
(1,580)	1:41:A:GLN:HG2	1:71:A:LEU:HD21	6	0.82
(1,580)	1:41:A:GLN:HG3	1:69:A:LEU:HD21	9	0.82
(1,484)	1:56:A:LEU:HD11	1:19:A:PRO:HA	7	0.82
(1,484)	1:56:A:LEU:HD12	1:19:A:PRO:HA	7	0.82
(1,484)	1:56:A:LEU:HD13	1:19:A:PRO:HA	7	0.82
(1,322)	1:10:A:GLY:HA3	1:6:A:LYS:HE2	4	0.82
(1,322)	1:10:A:GLY:HA3	1:6:A:LYS:HE3	4	0.82
(1,282)	1:50:A:LEU:HD11	1:50:A:LEU:HA	3	0.82
(1,282)	1:50:A:LEU:HD12	1:50:A:LEU:HA	3	0.82
(1,282)	1:50:A:LEU:HD13	1:50:A:LEU:HA	3	0.82
(1,282)	1:50:A:LEU:HD11	1:50:A:LEU:HA	7	0.82
(1,282)	1:50:A:LEU:HD12	1:50:A:LEU:HA	7	0.82
(1,282)	1:50:A:LEU:HD13	1:50:A:LEU:HA	7	0.82
(1,729)	1:27:A:LYS:HB3	1:28:A:ALA:H	1	0.81
(1,374)	1:26:A:VAL:HG11	1:21:A:ASP:HB3	8	0.81
(1,374)	1:26:A:VAL:HG12	1:21:A:ASP:HB3	8	0.81
(1,374)	1:26:A:VAL:HG13	1:21:A:ASP:HB3	8	0.81
(1,282)	1:50:A:LEU:HD11	1:50:A:LEU:HA	10	0.81
(1,282)	1:50:A:LEU:HD12	1:50:A:LEU:HA	10	0.81
(1,282)	1:50:A:LEU:HD13	1:50:A:LEU:HA	10	0.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,234)	1:27:A:LYS:HA	1:43:A:LEU:HD21	9	0.81
(1,234)	1:27:A:LYS:HA	1:43:A:LEU:HD22	9	0.81
(1,234)	1:27:A:LYS:HA	1:43:A:LEU:HD23	9	0.81
(1,23)	1:23:A:ILE:HD11	1:50:A:LEU:HD11	10	0.81
(1,23)	1:23:A:ILE:HD11	1:50:A:LEU:HD12	10	0.81
(1,23)	1:23:A:ILE:HD11	1:50:A:LEU:HD13	10	0.81
(1,23)	1:23:A:ILE:HD12	1:50:A:LEU:HD11	10	0.81
(1,23)	1:23:A:ILE:HD12	1:50:A:LEU:HD12	10	0.81
(1,23)	1:23:A:ILE:HD12	1:50:A:LEU:HD13	10	0.81
(1,23)	1:23:A:ILE:HD13	1:50:A:LEU:HD11	10	0.81
(1,23)	1:23:A:ILE:HD13	1:50:A:LEU:HD12	10	0.81
(1,23)	1:23:A:ILE:HD13	1:50:A:LEU:HD13	10	0.81
(1,1166)	1:67:A:LEU:HD13	1:68:A:HIS:H	8	0.8
(1,1070)	1:25:A:ASN:HB3	1:21:A:ASP:H	1	0.8
(1,1013)	1:62:A:GLN:HB2	1:65:A:SER:H	4	0.8
(1,1166)	1:67:A:LEU:HD12	1:68:A:HIS:H	10	0.79
(1,1013)	1:63:A:LYS:HB3	1:65:A:SER:H	7	0.79
(1,729)	1:27:A:LYS:HB3	1:28:A:ALA:H	2	0.79
(1,593)	1:3:A:ILE:HD11	1:15:A:LEU:HB2	6	0.79
(1,593)	1:3:A:ILE:HD12	1:15:A:LEU:HB2	6	0.79
(1,593)	1:3:A:ILE:HD13	1:15:A:LEU:HB2	6	0.79
(1,282)	1:50:A:LEU:HD11	1:50:A:LEU:HA	1	0.79
(1,282)	1:50:A:LEU:HD12	1:50:A:LEU:HA	1	0.79
(1,282)	1:50:A:LEU:HD13	1:50:A:LEU:HA	1	0.79
(1,134)	1:26:A:VAL:HG11	1:23:A:ILE:HA	1	0.79
(1,134)	1:26:A:VAL:HG12	1:23:A:ILE:HA	1	0.79
(1,134)	1:26:A:VAL:HG13	1:23:A:ILE:HA	1	0.79
(1,23)	1:23:A:ILE:HD11	1:50:A:LEU:HD11	4	0.79
(1,23)	1:23:A:ILE:HD11	1:50:A:LEU:HD12	4	0.79
(1,23)	1:23:A:ILE:HD11	1:50:A:LEU:HD13	4	0.79
(1,23)	1:23:A:ILE:HD12	1:50:A:LEU:HD11	4	0.79
(1,23)	1:23:A:ILE:HD12	1:50:A:LEU:HD12	4	0.79
(1,23)	1:23:A:ILE:HD12	1:50:A:LEU:HD13	4	0.79
(1,23)	1:23:A:ILE:HD13	1:50:A:LEU:HD11	4	0.79
(1,23)	1:23:A:ILE:HD13	1:50:A:LEU:HD12	4	0.79
(1,23)	1:23:A:ILE:HD13	1:50:A:LEU:HD13	4	0.79
(1,1196)	1:13:A:ILE:HD11	1:7:A:THR:H	5	0.78
(1,1095)	1:23:A:ILE:HG13	1:52:A:ASP:H	10	0.78
(1,931)	1:17:A:VAL:HG11	1:3:A:ILE:H	2	0.78
(1,931)	1:17:A:VAL:HG12	1:3:A:ILE:H	2	0.78
(1,931)	1:17:A:VAL:HG13	1:3:A:ILE:H	2	0.78
(1,909)	1:67:A:LEU:HD11	1:67:A:LEU:H	9	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,909)	1:67:A:LEU:HD12	1:67:A:LEU:H	9	0.78
(1,909)	1:67:A:LEU:HD13	1:67:A:LEU:H	9	0.78
(1,582)	1:55:A:THR:HB	1:19:A:PRO:HA	1	0.78
(1,23)	1:23:A:ILE:HD11	1:50:A:LEU:HD11	6	0.78
(1,23)	1:23:A:ILE:HD11	1:50:A:LEU:HD12	6	0.78
(1,23)	1:23:A:ILE:HD11	1:50:A:LEU:HD13	6	0.78
(1,23)	1:23:A:ILE:HD12	1:50:A:LEU:HD11	6	0.78
(1,23)	1:23:A:ILE:HD12	1:50:A:LEU:HD12	6	0.78
(1,23)	1:23:A:ILE:HD12	1:50:A:LEU:HD13	6	0.78
(1,23)	1:23:A:ILE:HD13	1:50:A:LEU:HD11	6	0.78
(1,23)	1:23:A:ILE:HD13	1:50:A:LEU:HD12	6	0.78
(1,23)	1:23:A:ILE:HD13	1:50:A:LEU:HD13	6	0.78
(1,1091)	1:34:A:GLU:HB2	1:36:A:ILE:H	7	0.77
(1,931)	1:17:A:VAL:HG11	1:3:A:ILE:H	1	0.77
(1,931)	1:17:A:VAL:HG12	1:3:A:ILE:H	1	0.77
(1,931)	1:17:A:VAL:HG13	1:3:A:ILE:H	1	0.77
(1,582)	1:55:A:THR:HB	1:19:A:PRO:HA	3	0.77
(1,447)	1:27:A:LYS:HB2	1:27:A:LYS:HD2	9	0.77
(1,447)	1:27:A:LYS:HB2	1:27:A:LYS:HD3	9	0.77
(1,282)	1:50:A:LEU:HD11	1:50:A:LEU:HA	9	0.77
(1,282)	1:50:A:LEU:HD12	1:50:A:LEU:HA	9	0.77
(1,282)	1:50:A:LEU:HD13	1:50:A:LEU:HA	9	0.77
(1,593)	1:3:A:ILE:HD11	1:15:A:LEU:HB2	1	0.76
(1,593)	1:3:A:ILE:HD12	1:15:A:LEU:HB2	1	0.76
(1,593)	1:3:A:ILE:HD13	1:15:A:LEU:HB2	1	0.76
(1,448)	1:30:A:ILE:HD11	1:27:A:LYS:HB2	1	0.76
(1,448)	1:30:A:ILE:HD12	1:27:A:LYS:HB2	1	0.76
(1,448)	1:30:A:ILE:HD13	1:27:A:LYS:HB2	1	0.76
(1,207)	1:27:A:LYS:HE2	1:24:A:GLU:HA	6	0.76
(1,1166)	1:44:A:ILE:HG22	1:68:A:HIS:H	2	0.75
(1,1166)	1:67:A:LEU:HD11	1:68:A:HIS:H	4	0.75
(1,931)	1:17:A:VAL:HG11	1:3:A:ILE:H	10	0.75
(1,931)	1:17:A:VAL:HG12	1:3:A:ILE:H	10	0.75
(1,931)	1:17:A:VAL:HG13	1:3:A:ILE:H	10	0.75
(1,729)	1:27:A:LYS:HB3	1:28:A:ALA:H	7	0.75
(1,580)	1:41:A:GLN:HG3	1:69:A:LEU:HD21	10	0.75
(1,513)	1:17:A:VAL:HG21	1:17:A:VAL:HA	1	0.75
(1,513)	1:17:A:VAL:HG22	1:17:A:VAL:HA	1	0.75
(1,513)	1:17:A:VAL:HG23	1:17:A:VAL:HA	1	0.75
(1,513)	1:17:A:VAL:HG21	1:17:A:VAL:HA	3	0.75
(1,513)	1:17:A:VAL:HG22	1:17:A:VAL:HA	3	0.75
(1,513)	1:17:A:VAL:HG23	1:17:A:VAL:HA	3	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,513)	1:17:A:VAL:HG21	1:17:A:VAL:HA	5	0.75
(1,513)	1:17:A:VAL:HG22	1:17:A:VAL:HA	5	0.75
(1,513)	1:17:A:VAL:HG23	1:17:A:VAL:HA	5	0.75
(1,513)	1:17:A:VAL:HG21	1:17:A:VAL:HA	6	0.75
(1,513)	1:17:A:VAL:HG22	1:17:A:VAL:HA	6	0.75
(1,513)	1:17:A:VAL:HG23	1:17:A:VAL:HA	6	0.75
(1,447)	1:27:A:LYS:HB2	1:27:A:LYS:HD2	3	0.75
(1,447)	1:27:A:LYS:HB2	1:27:A:LYS:HD3	3	0.75
(1,447)	1:27:A:LYS:HB2	1:27:A:LYS:HD2	10	0.75
(1,447)	1:27:A:LYS:HB2	1:27:A:LYS:HD3	10	0.75
(1,188)	1:26:A:VAL:HG11	1:23:A:ILE:HA	1	0.75
(1,188)	1:26:A:VAL:HG12	1:23:A:ILE:HA	1	0.75
(1,188)	1:26:A:VAL:HG13	1:23:A:ILE:HA	1	0.75
(1,125)	1:26:A:VAL:HG11	1:56:A:LEU:HD11	3	0.75
(1,125)	1:26:A:VAL:HG11	1:56:A:LEU:HD12	3	0.75
(1,125)	1:26:A:VAL:HG11	1:56:A:LEU:HD13	3	0.75
(1,125)	1:26:A:VAL:HG12	1:56:A:LEU:HD11	3	0.75
(1,125)	1:26:A:VAL:HG12	1:56:A:LEU:HD12	3	0.75
(1,125)	1:26:A:VAL:HG12	1:56:A:LEU:HD13	3	0.75
(1,125)	1:26:A:VAL:HG13	1:56:A:LEU:HD11	3	0.75
(1,125)	1:26:A:VAL:HG13	1:56:A:LEU:HD12	3	0.75
(1,125)	1:26:A:VAL:HG13	1:56:A:LEU:HD13	3	0.75
(1,1278)	1:70:A:VAL:HG21	1:70:A:VAL:H	1	0.74
(1,1278)	1:70:A:VAL:HG22	1:70:A:VAL:H	1	0.74
(1,1278)	1:70:A:VAL:HG23	1:70:A:VAL:H	1	0.74
(1,1166)	1:44:A:ILE:HG22	1:68:A:HIS:H	5	0.74
(1,513)	1:17:A:VAL:HG21	1:17:A:VAL:HA	2	0.74
(1,513)	1:17:A:VAL:HG22	1:17:A:VAL:HA	2	0.74
(1,513)	1:17:A:VAL:HG23	1:17:A:VAL:HA	2	0.74
(1,513)	1:17:A:VAL:HG21	1:17:A:VAL:HA	7	0.74
(1,513)	1:17:A:VAL:HG22	1:17:A:VAL:HA	7	0.74
(1,513)	1:17:A:VAL:HG23	1:17:A:VAL:HA	7	0.74
(1,513)	1:17:A:VAL:HG21	1:17:A:VAL:HA	8	0.74
(1,513)	1:17:A:VAL:HG22	1:17:A:VAL:HA	8	0.74
(1,513)	1:17:A:VAL:HG23	1:17:A:VAL:HA	8	0.74
(1,513)	1:17:A:VAL:HG21	1:17:A:VAL:HA	9	0.74
(1,513)	1:17:A:VAL:HG22	1:17:A:VAL:HA	9	0.74
(1,513)	1:17:A:VAL:HG23	1:17:A:VAL:HA	9	0.74
(1,513)	1:17:A:VAL:HG21	1:17:A:VAL:HA	10	0.74
(1,513)	1:17:A:VAL:HG22	1:17:A:VAL:HA	10	0.74
(1,513)	1:17:A:VAL:HG23	1:17:A:VAL:HA	10	0.74
(1,448)	1:30:A:ILE:HD11	1:27:A:LYS:HB2	10	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,448)	1:30:A:ILE:HD12	1:27:A:LYS:HB2	10	0.74
(1,448)	1:30:A:ILE:HD13	1:27:A:LYS:HB2	10	0.74
(1,1143)	1:70:A:VAL:HG12	1:71:A:LEU:H	4	0.73
(1,729)	1:27:A:LYS:HB3	1:28:A:ALA:H	6	0.73
(1,593)	1:3:A:ILE:HD11	1:15:A:LEU:HB2	9	0.73
(1,593)	1:3:A:ILE:HD12	1:15:A:LEU:HB2	9	0.73
(1,593)	1:3:A:ILE:HD13	1:15:A:LEU:HB2	9	0.73
(1,582)	1:55:A:THR:HB	1:19:A:PRO:HA	9	0.73
(1,447)	1:27:A:LYS:HB2	1:27:A:LYS:HD2	6	0.73
(1,447)	1:27:A:LYS:HB2	1:27:A:LYS:HD3	6	0.73
(1,207)	1:27:A:LYS:HE3	1:24:A:GLU:HA	4	0.73
(1,593)	1:3:A:ILE:HD11	1:15:A:LEU:HB2	2	0.72
(1,593)	1:3:A:ILE:HD12	1:15:A:LEU:HB2	2	0.72
(1,593)	1:3:A:ILE:HD13	1:15:A:LEU:HB2	2	0.72
(1,513)	1:17:A:VAL:HG21	1:17:A:VAL:HA	4	0.72
(1,513)	1:17:A:VAL:HG22	1:17:A:VAL:HA	4	0.72
(1,513)	1:17:A:VAL:HG23	1:17:A:VAL:HA	4	0.72
(1,447)	1:27:A:LYS:HB2	1:27:A:LYS:HD2	4	0.72
(1,447)	1:27:A:LYS:HB2	1:27:A:LYS:HD3	4	0.72
(1,234)	1:27:A:LYS:HA	1:43:A:LEU:HD21	1	0.72
(1,234)	1:27:A:LYS:HA	1:43:A:LEU:HD22	1	0.72
(1,234)	1:27:A:LYS:HA	1:43:A:LEU:HD23	1	0.72
(1,163)	1:27:A:LYS:HB3	1:38:A:PRO:HA	6	0.72
(1,125)	1:26:A:VAL:HG11	1:56:A:LEU:HD11	4	0.72
(1,125)	1:26:A:VAL:HG11	1:56:A:LEU:HD12	4	0.72
(1,125)	1:26:A:VAL:HG11	1:56:A:LEU:HD13	4	0.72
(1,125)	1:26:A:VAL:HG12	1:56:A:LEU:HD11	4	0.72
(1,125)	1:26:A:VAL:HG12	1:56:A:LEU:HD12	4	0.72
(1,125)	1:26:A:VAL:HG12	1:56:A:LEU:HD13	4	0.72
(1,125)	1:26:A:VAL:HG13	1:56:A:LEU:HD11	4	0.72
(1,125)	1:26:A:VAL:HG13	1:56:A:LEU:HD12	4	0.72
(1,125)	1:26:A:VAL:HG13	1:56:A:LEU:HD13	4	0.72
(1,1278)	1:70:A:VAL:HG21	1:70:A:VAL:H	10	0.71
(1,1278)	1:70:A:VAL:HG22	1:70:A:VAL:H	10	0.71
(1,1278)	1:70:A:VAL:HG23	1:70:A:VAL:H	10	0.71
(1,1166)	1:67:A:LEU:HD12	1:68:A:HIS:H	7	0.71
(1,1143)	1:70:A:VAL:HG12	1:71:A:LEU:H	9	0.71
(1,845)	1:59:A:TYR:HB2	1:56:A:LEU:H	5	0.71
(1,593)	1:3:A:ILE:HD11	1:15:A:LEU:HB2	3	0.71
(1,593)	1:3:A:ILE:HD12	1:15:A:LEU:HB2	3	0.71
(1,593)	1:3:A:ILE:HD13	1:15:A:LEU:HB2	3	0.71
(1,580)	1:41:A:GLN:HG3	1:69:A:LEU:HD21	4	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,430)	1:15:A:LEU:HD21	1:16:A:GLU:HG3	3	0.71
(1,430)	1:15:A:LEU:HD22	1:16:A:GLU:HG3	3	0.71
(1,430)	1:15:A:LEU:HD23	1:16:A:GLU:HG3	3	0.71
(1,55)	1:69:A:LEU:HG	1:30:A:ILE:HD12	6	0.71
(1,1278)	1:70:A:VAL:HG21	1:70:A:VAL:H	3	0.7
(1,1278)	1:70:A:VAL:HG22	1:70:A:VAL:H	3	0.7
(1,1278)	1:70:A:VAL:HG23	1:70:A:VAL:H	3	0.7
(1,1143)	1:70:A:VAL:HG13	1:71:A:LEU:H	2	0.7
(1,845)	1:59:A:TYR:HB2	1:56:A:LEU:H	2	0.7
(1,447)	1:27:A:LYS:HB2	1:27:A:LYS:HD2	2	0.7
(1,447)	1:27:A:LYS:HB2	1:27:A:LYS:HD3	2	0.7
(1,435)	1:33:A:GLU:HG2	1:15:A:LEU:HD11	5	0.7
(1,435)	1:33:A:GLU:HG2	1:15:A:LEU:HD12	5	0.7
(1,435)	1:33:A:GLU:HG2	1:15:A:LEU:HD13	5	0.7
(1,134)	1:26:A:VAL:HG11	1:23:A:ILE:HA	3	0.7
(1,134)	1:26:A:VAL:HG12	1:23:A:ILE:HA	3	0.7
(1,134)	1:26:A:VAL:HG13	1:23:A:ILE:HA	3	0.7
(1,39)	1:3:A:ILE:HD11	1:17:A:VAL:HG11	4	0.7
(1,39)	1:3:A:ILE:HD11	1:17:A:VAL:HG12	4	0.7
(1,39)	1:3:A:ILE:HD11	1:17:A:VAL:HG13	4	0.7
(1,39)	1:3:A:ILE:HD12	1:17:A:VAL:HG11	4	0.7
(1,39)	1:3:A:ILE:HD12	1:17:A:VAL:HG12	4	0.7
(1,39)	1:3:A:ILE:HD12	1:17:A:VAL:HG13	4	0.7
(1,39)	1:3:A:ILE:HD13	1:17:A:VAL:HG11	4	0.7
(1,39)	1:3:A:ILE:HD13	1:17:A:VAL:HG12	4	0.7
(1,39)	1:3:A:ILE:HD13	1:17:A:VAL:HG13	4	0.7
(1,1170)	1:26:A:VAL:HG11	1:18:A:GLU:H	5	0.69
(1,1170)	1:26:A:VAL:HG12	1:18:A:GLU:H	5	0.69
(1,1170)	1:26:A:VAL:HG13	1:18:A:GLU:H	5	0.69
(1,447)	1:27:A:LYS:HB2	1:27:A:LYS:HD2	7	0.69
(1,447)	1:27:A:LYS:HB2	1:27:A:LYS:HD3	7	0.69
(1,1279)	1:21:A:ASP:HB2	1:22:A:THR:H	7	0.68
(1,1095)	1:23:A:ILE:HG13	1:52:A:ASP:H	5	0.68
(1,931)	1:17:A:VAL:HG11	1:3:A:ILE:H	5	0.68
(1,931)	1:17:A:VAL:HG12	1:3:A:ILE:H	5	0.68
(1,931)	1:17:A:VAL:HG13	1:3:A:ILE:H	5	0.68
(1,582)	1:55:A:THR:HB	1:19:A:PRO:HA	4	0.68
(1,448)	1:30:A:ILE:HD11	1:27:A:LYS:HB2	4	0.68
(1,448)	1:30:A:ILE:HD12	1:27:A:LYS:HB2	4	0.68
(1,448)	1:30:A:ILE:HD13	1:27:A:LYS:HB2	4	0.68
(1,23)	1:23:A:ILE:HD11	1:50:A:LEU:HD11	2	0.68
(1,23)	1:23:A:ILE:HD11	1:50:A:LEU:HD12	2	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,23)	1:23:A:ILE:HD11	1:50:A:LEU:HD13	2	0.68
(1,23)	1:23:A:ILE:HD12	1:50:A:LEU:HD11	2	0.68
(1,23)	1:23:A:ILE:HD12	1:50:A:LEU:HD12	2	0.68
(1,23)	1:23:A:ILE:HD12	1:50:A:LEU:HD13	2	0.68
(1,23)	1:23:A:ILE:HD13	1:50:A:LEU:HD11	2	0.68
(1,23)	1:23:A:ILE:HD13	1:50:A:LEU:HD12	2	0.68
(1,23)	1:23:A:ILE:HD13	1:50:A:LEU:HD13	2	0.68
(1,1091)	1:34:A:GLU:HB2	1:36:A:ILE:H	9	0.67
(1,844)	1:21:A:ASP:HB3	1:56:A:LEU:H	10	0.67
(1,707)	1:21:A:ASP:HA	1:22:A:THR:H	2	0.67
(1,580)	1:41:A:GLN:HG3	1:69:A:LEU:HD23	3	0.67
(1,163)	1:27:A:LYS:HB3	1:38:A:PRO:HA	3	0.67
(1,128)	1:17:A:VAL:HB	1:56:A:LEU:HD11	7	0.67
(1,128)	1:17:A:VAL:HB	1:56:A:LEU:HD12	7	0.67
(1,128)	1:17:A:VAL:HB	1:56:A:LEU:HD13	7	0.67
(1,23)	1:23:A:ILE:HD11	1:50:A:LEU:HD11	7	0.67
(1,23)	1:23:A:ILE:HD11	1:50:A:LEU:HD12	7	0.67
(1,23)	1:23:A:ILE:HD11	1:50:A:LEU:HD13	7	0.67
(1,23)	1:23:A:ILE:HD12	1:50:A:LEU:HD11	7	0.67
(1,23)	1:23:A:ILE:HD12	1:50:A:LEU:HD12	7	0.67
(1,23)	1:23:A:ILE:HD12	1:50:A:LEU:HD13	7	0.67
(1,23)	1:23:A:ILE:HD13	1:50:A:LEU:HD11	7	0.67
(1,23)	1:23:A:ILE:HD13	1:50:A:LEU:HD12	7	0.67
(1,23)	1:23:A:ILE:HD13	1:50:A:LEU:HD13	7	0.67
(1,1279)	1:21:A:ASP:HB2	1:22:A:THR:H	4	0.66
(1,1224)	1:56:A:LEU:HD11	1:21:A:ASP:H	7	0.66
(1,1224)	1:56:A:LEU:HD12	1:21:A:ASP:H	7	0.66
(1,1224)	1:56:A:LEU:HD13	1:21:A:ASP:H	7	0.66
(1,1095)	1:23:A:ILE:HG13	1:52:A:ASP:H	4	0.66
(1,937)	1:4:A:PHE:HB2	1:6:A:LYS:H	3	0.66
(1,706)	1:56:A:LEU:HD11	1:21:A:ASP:H	7	0.66
(1,706)	1:56:A:LEU:HD12	1:21:A:ASP:H	7	0.66
(1,706)	1:56:A:LEU:HD13	1:21:A:ASP:H	7	0.66
(1,593)	1:3:A:ILE:HD11	1:15:A:LEU:HB2	5	0.66
(1,593)	1:3:A:ILE:HD12	1:15:A:LEU:HB2	5	0.66
(1,593)	1:3:A:ILE:HD13	1:15:A:LEU:HB2	5	0.66
(1,188)	1:26:A:VAL:HG11	1:23:A:ILE:HA	3	0.66
(1,188)	1:26:A:VAL:HG12	1:23:A:ILE:HA	3	0.66
(1,188)	1:26:A:VAL:HG13	1:23:A:ILE:HA	3	0.66
(1,163)	1:27:A:LYS:HB3	1:38:A:PRO:HA	2	0.66
(1,134)	1:26:A:VAL:HG11	1:23:A:ILE:HA	8	0.66
(1,134)	1:26:A:VAL:HG12	1:23:A:ILE:HA	8	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,134)	1:26:A:VAL:HG13	1:23:A:ILE:HA	8	0.66
(1,234)	1:27:A:LYS:HA	1:43:A:LEU:HD21	2	0.65
(1,234)	1:27:A:LYS:HA	1:43:A:LEU:HD22	2	0.65
(1,234)	1:27:A:LYS:HA	1:43:A:LEU:HD23	2	0.65
(1,163)	1:27:A:LYS:HB3	1:38:A:PRO:HA	7	0.65
(1,663)	1:5:A:VAL:HG11	1:5:A:VAL:H	5	0.64
(1,663)	1:5:A:VAL:HG12	1:5:A:VAL:H	5	0.64
(1,663)	1:5:A:VAL:HG13	1:5:A:VAL:H	5	0.64
(1,323)	1:73:A:LEU:HG	1:76:A:GLY:HA3	1	0.64
(1,125)	1:26:A:VAL:HG11	1:56:A:LEU:HD11	1	0.64
(1,125)	1:26:A:VAL:HG11	1:56:A:LEU:HD12	1	0.64
(1,125)	1:26:A:VAL:HG11	1:56:A:LEU:HD13	1	0.64
(1,125)	1:26:A:VAL:HG12	1:56:A:LEU:HD11	1	0.64
(1,125)	1:26:A:VAL:HG12	1:56:A:LEU:HD12	1	0.64
(1,125)	1:26:A:VAL:HG12	1:56:A:LEU:HD13	1	0.64
(1,125)	1:26:A:VAL:HG13	1:56:A:LEU:HD11	1	0.64
(1,125)	1:26:A:VAL:HG13	1:56:A:LEU:HD12	1	0.64
(1,125)	1:26:A:VAL:HG13	1:56:A:LEU:HD13	1	0.64
(1,1280)	1:15:A:LEU:HB2	1:17:A:VAL:H	8	0.63
(1,1143)	1:70:A:VAL:HG11	1:71:A:LEU:H	7	0.63
(1,593)	1:3:A:ILE:HD11	1:15:A:LEU:HB2	10	0.63
(1,593)	1:3:A:ILE:HD12	1:15:A:LEU:HB2	10	0.63
(1,593)	1:3:A:ILE:HD13	1:15:A:LEU:HB2	10	0.63
(1,188)	1:26:A:VAL:HG11	1:23:A:ILE:HA	8	0.63
(1,188)	1:26:A:VAL:HG12	1:23:A:ILE:HA	8	0.63
(1,188)	1:26:A:VAL:HG13	1:23:A:ILE:HA	8	0.63
(1,1223)	1:34:A:GLU:HB3	1:34:A:GLU:H	3	0.62
(1,1091)	1:34:A:GLU:HB2	1:36:A:ILE:H	10	0.62
(1,1013)	1:62:A:GLN:HB2	1:65:A:SER:H	5	0.62
(1,931)	1:17:A:VAL:HG11	1:3:A:ILE:H	9	0.62
(1,931)	1:17:A:VAL:HG12	1:3:A:ILE:H	9	0.62
(1,931)	1:17:A:VAL:HG13	1:3:A:ILE:H	9	0.62
(1,448)	1:30:A:ILE:HD11	1:27:A:LYS:HB2	2	0.62
(1,448)	1:30:A:ILE:HD12	1:27:A:LYS:HB2	2	0.62
(1,448)	1:30:A:ILE:HD13	1:27:A:LYS:HB2	2	0.62
(1,427)	1:15:A:LEU:HD21	1:16:A:GLU:HG2	4	0.62
(1,427)	1:15:A:LEU:HD22	1:16:A:GLU:HG2	4	0.62
(1,427)	1:15:A:LEU:HD23	1:16:A:GLU:HG2	4	0.62
(1,163)	1:27:A:LYS:HB3	1:38:A:PRO:HA	10	0.62
(1,1255)	1:39:A:ASP:HA	1:40:A:GLN:HE22	10	0.61
(1,1218)	1:20:A:SER:HB3	1:22:A:THR:H	7	0.61
(1,1095)	1:23:A:ILE:HG13	1:52:A:ASP:H	7	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,743)	1:30:A:ILE:HG12	1:30:A:ILE:H	6	0.61
(1,729)	1:27:A:LYS:HB3	1:28:A:ALA:H	8	0.61
(1,630)	1:21:A:ASP:HB3	1:20:A:SER:H	10	0.61
(1,499)	1:25:A:ASN:HA	1:25:A:ASN:HB2	5	0.61
(1,427)	1:15:A:LEU:HD21	1:16:A:GLU:HG2	6	0.61
(1,427)	1:15:A:LEU:HD22	1:16:A:GLU:HG2	6	0.61
(1,427)	1:15:A:LEU:HD23	1:16:A:GLU:HG2	6	0.61
(1,234)	1:27:A:LYS:HA	1:43:A:LEU:HD21	10	0.61
(1,234)	1:27:A:LYS:HA	1:43:A:LEU:HD22	10	0.61
(1,234)	1:27:A:LYS:HA	1:43:A:LEU:HD23	10	0.61
(1,134)	1:26:A:VAL:HG11	1:23:A:ILE:HA	9	0.61
(1,134)	1:26:A:VAL:HG12	1:23:A:ILE:HA	9	0.61
(1,134)	1:26:A:VAL:HG13	1:23:A:ILE:HA	9	0.61
(1,1223)	1:34:A:GLU:HB3	1:34:A:GLU:H	4	0.6
(1,1166)	1:67:A:LEU:HD12	1:68:A:HIS:H	6	0.6
(1,580)	1:41:A:GLN:HG3	1:69:A:LEU:HD21	1	0.6
(1,499)	1:25:A:ASN:HA	1:25:A:ASN:HB2	1	0.6
(1,499)	1:25:A:ASN:HA	1:25:A:ASN:HB2	3	0.6
(1,499)	1:25:A:ASN:HA	1:25:A:ASN:HB2	4	0.6
(1,499)	1:25:A:ASN:HA	1:25:A:ASN:HB2	7	0.6
(1,234)	1:27:A:LYS:HA	1:43:A:LEU:HD21	7	0.6
(1,234)	1:27:A:LYS:HA	1:43:A:LEU:HD22	7	0.6
(1,234)	1:27:A:LYS:HA	1:43:A:LEU:HD23	7	0.6
(1,582)	1:55:A:THR:HB	1:19:A:PRO:HA	7	0.59
(1,561)	1:69:A:LEU:HB2	1:7:A:THR:HB	8	0.59
(1,488)	1:30:A:ILE:HD13	1:43:A:LEU:HG	3	0.59
(1,163)	1:27:A:LYS:HB3	1:38:A:PRO:HA	1	0.59
(1,1208)	1:56:A:LEU:HB2	1:60:A:SER:H	7	0.58
(1,749)	1:31:A:GLN:HG2	1:31:A:GLN:H	7	0.58
(1,447)	1:27:A:LYS:HB2	1:27:A:LYS:HD2	1	0.58
(1,447)	1:27:A:LYS:HB2	1:27:A:LYS:HD3	1	0.58
(1,188)	1:26:A:VAL:HG11	1:23:A:ILE:HA	9	0.58
(1,188)	1:26:A:VAL:HG12	1:23:A:ILE:HA	9	0.58
(1,188)	1:26:A:VAL:HG13	1:23:A:ILE:HA	9	0.58
(1,1166)	1:67:A:LEU:HD12	1:68:A:HIS:H	3	0.57
(1,743)	1:30:A:ILE:HG12	1:30:A:ILE:H	4	0.57
(1,729)	1:27:A:LYS:HB3	1:28:A:ALA:H	5	0.57
(1,630)	1:21:A:ASP:HB3	1:20:A:SER:H	7	0.57
(1,448)	1:30:A:ILE:HD11	1:27:A:LYS:HB2	7	0.57
(1,448)	1:30:A:ILE:HD12	1:27:A:LYS:HB2	7	0.57
(1,448)	1:30:A:ILE:HD13	1:27:A:LYS:HB2	7	0.57
(1,163)	1:27:A:LYS:HB3	1:38:A:PRO:HA	9	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,125)	1:26:A:VAL:HG11	1:56:A:LEU:HD11	9	0.57
(1,125)	1:26:A:VAL:HG11	1:56:A:LEU:HD12	9	0.57
(1,125)	1:26:A:VAL:HG11	1:56:A:LEU:HD13	9	0.57
(1,125)	1:26:A:VAL:HG12	1:56:A:LEU:HD11	9	0.57
(1,125)	1:26:A:VAL:HG12	1:56:A:LEU:HD12	9	0.57
(1,125)	1:26:A:VAL:HG12	1:56:A:LEU:HD13	9	0.57
(1,125)	1:26:A:VAL:HG13	1:56:A:LEU:HD11	9	0.57
(1,125)	1:26:A:VAL:HG13	1:56:A:LEU:HD12	9	0.57
(1,125)	1:26:A:VAL:HG13	1:56:A:LEU:HD13	9	0.57
(1,704)	1:18:A:GLU:HB3	1:21:A:ASP:H	2	0.56
(1,630)	1:21:A:ASP:HB3	1:20:A:SER:H	3	0.56
(1,163)	1:27:A:LYS:HB3	1:38:A:PRO:HA	4	0.56
(1,703)	1:21:A:ASP:HB3	1:21:A:ASP:H	7	0.55
(1,630)	1:21:A:ASP:HB3	1:20:A:SER:H	9	0.55
(1,582)	1:55:A:THR:HB	1:20:A:SER:HB3	2	0.55
(1,427)	1:15:A:LEU:HD21	1:16:A:GLU:HG2	2	0.55
(1,427)	1:15:A:LEU:HD22	1:16:A:GLU:HG2	2	0.55
(1,427)	1:15:A:LEU:HD23	1:16:A:GLU:HG2	2	0.55
(1,207)	1:27:A:LYS:HE3	1:24:A:GLU:HA	5	0.55
(1,207)	1:23:A:ILE:HB	1:24:A:GLU:HA	10	0.55
(1,121)	1:4:A:PHE:HB2	1:12:A:THR:HG21	3	0.55
(1,121)	1:4:A:PHE:HB2	1:12:A:THR:HG22	3	0.55
(1,121)	1:4:A:PHE:HB2	1:12:A:THR:HG23	3	0.55
(1,966)	1:26:A:VAL:HG12	1:29:A:LYS:H	3	0.54
(1,945)	1:16:A:GLU:HB3	1:16:A:GLU:H	2	0.54
(1,945)	1:16:A:GLU:HB3	1:16:A:GLU:H	6	0.54
(1,56)	1:67:A:LEU:HB2	1:30:A:ILE:HD11	8	0.54
(1,1279)	1:21:A:ASP:HB2	1:22:A:THR:H	6	0.53
(1,945)	1:16:A:GLU:HB3	1:16:A:GLU:H	4	0.53
(1,945)	1:16:A:GLU:HB3	1:16:A:GLU:H	5	0.53
(1,704)	1:18:A:GLU:HB3	1:21:A:ASP:H	8	0.53
(1,328)	1:69:A:LEU:HB2	1:69:A:LEU:HD11	2	0.53
(1,328)	1:69:A:LEU:HB2	1:69:A:LEU:HD12	2	0.53
(1,328)	1:69:A:LEU:HB2	1:69:A:LEU:HD13	2	0.53
(1,328)	1:69:A:LEU:HB2	1:69:A:LEU:HD11	4	0.53
(1,328)	1:69:A:LEU:HB2	1:69:A:LEU:HD12	4	0.53
(1,328)	1:69:A:LEU:HB2	1:69:A:LEU:HD13	4	0.53
(1,328)	1:69:A:LEU:HB2	1:69:A:LEU:HD11	5	0.53
(1,328)	1:69:A:LEU:HB2	1:69:A:LEU:HD12	5	0.53
(1,328)	1:69:A:LEU:HB2	1:69:A:LEU:HD13	5	0.53
(1,328)	1:69:A:LEU:HB2	1:69:A:LEU:HD11	7	0.53
(1,328)	1:69:A:LEU:HB2	1:69:A:LEU:HD12	7	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,328)	1:69:A:LEU:HB2	1:69:A:LEU:HD13	7	0.53
(1,328)	1:69:A:LEU:HB2	1:69:A:LEU:HD11	8	0.53
(1,328)	1:69:A:LEU:HB2	1:69:A:LEU:HD12	8	0.53
(1,328)	1:69:A:LEU:HB2	1:69:A:LEU:HD13	8	0.53
(1,328)	1:69:A:LEU:HB2	1:69:A:LEU:HD11	9	0.53
(1,328)	1:69:A:LEU:HB2	1:69:A:LEU:HD12	9	0.53
(1,328)	1:69:A:LEU:HB2	1:69:A:LEU:HD13	9	0.53
(1,209)	1:24:A:GLU:HA	1:27:A:LYS:HG2	8	0.53
(1,1282)	1:57:A:SER:HB3	1:57:A:SER:H	1	0.52
(1,1282)	1:57:A:SER:HB3	1:57:A:SER:H	2	0.52
(1,1282)	1:57:A:SER:HB3	1:57:A:SER:H	4	0.52
(1,1279)	1:21:A:ASP:HB2	1:22:A:THR:H	1	0.52
(1,1279)	1:21:A:ASP:HB2	1:22:A:THR:H	8	0.52
(1,966)	1:26:A:VAL:HG11	1:29:A:LYS:H	4	0.52
(1,704)	1:18:A:GLU:HB3	1:21:A:ASP:H	3	0.52
(1,703)	1:21:A:ASP:HB3	1:21:A:ASP:H	3	0.52
(1,703)	1:21:A:ASP:HB3	1:21:A:ASP:H	6	0.52
(1,703)	1:21:A:ASP:HB3	1:21:A:ASP:H	9	0.52
(1,630)	1:21:A:ASP:HB3	1:20:A:SER:H	4	0.52
(1,328)	1:69:A:LEU:HB2	1:69:A:LEU:HD11	3	0.52
(1,328)	1:69:A:LEU:HB2	1:69:A:LEU:HD12	3	0.52
(1,328)	1:69:A:LEU:HB2	1:69:A:LEU:HD13	3	0.52
(1,328)	1:69:A:LEU:HB2	1:69:A:LEU:HD11	10	0.52
(1,328)	1:69:A:LEU:HB2	1:69:A:LEU:HD12	10	0.52
(1,328)	1:69:A:LEU:HB2	1:69:A:LEU:HD13	10	0.52
(1,207)	1:23:A:ILE:HB	1:24:A:GLU:HA	2	0.52
(1,134)	1:26:A:VAL:HG11	1:23:A:ILE:HA	6	0.52
(1,134)	1:26:A:VAL:HG12	1:23:A:ILE:HA	6	0.52
(1,134)	1:26:A:VAL:HG13	1:23:A:ILE:HA	6	0.52
(1,1143)	1:70:A:VAL:HG11	1:71:A:LEU:H	8	0.51
(1,743)	1:30:A:ILE:HG12	1:30:A:ILE:H	5	0.51
(1,328)	1:69:A:LEU:HB2	1:69:A:LEU:HD11	1	0.51
(1,328)	1:69:A:LEU:HB2	1:69:A:LEU:HD12	1	0.51
(1,328)	1:69:A:LEU:HB2	1:69:A:LEU:HD13	1	0.51
(1,1091)	1:34:A:GLU:HB2	1:36:A:ILE:H	1	0.5
(1,1091)	1:34:A:GLU:HB2	1:36:A:ILE:H	8	0.5
(1,845)	1:21:A:ASP:HB2	1:56:A:LEU:H	8	0.5
(1,743)	1:30:A:ILE:HG12	1:30:A:ILE:H	1	0.5
(1,743)	1:30:A:ILE:HG12	1:30:A:ILE:H	9	0.5
(1,717)	1:25:A:ASN:HB3	1:25:A:ASN:H	1	0.5
(1,717)	1:25:A:ASN:HB3	1:25:A:ASN:H	3	0.5
(1,630)	1:21:A:ASP:HB3	1:20:A:SER:H	6	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,593)	1:3:A:ILE:HD11	1:15:A:LEU:HB2	7	0.5
(1,593)	1:3:A:ILE:HD12	1:15:A:LEU:HB2	7	0.5
(1,593)	1:3:A:ILE:HD13	1:15:A:LEU:HB2	7	0.5
(1,567)	1:29:A:LYS:HB3	1:15:A:LEU:HD21	5	0.5
(1,234)	1:27:A:LYS:HA	1:43:A:LEU:HD21	3	0.5
(1,234)	1:27:A:LYS:HA	1:43:A:LEU:HD22	3	0.5
(1,234)	1:27:A:LYS:HA	1:43:A:LEU:HD23	3	0.5
(1,134)	1:26:A:VAL:HG11	1:23:A:ILE:HA	7	0.5
(1,134)	1:26:A:VAL:HG12	1:23:A:ILE:HA	7	0.5
(1,134)	1:26:A:VAL:HG13	1:23:A:ILE:HA	7	0.5
(1,1279)	1:21:A:ASP:HB2	1:22:A:THR:H	3	0.49
(1,1255)	1:39:A:ASP:HA	1:40:A:GLN:HE22	7	0.49
(1,1091)	1:34:A:GLU:HB2	1:36:A:ILE:H	6	0.49
(1,966)	1:26:A:VAL:HG11	1:29:A:LYS:H	5	0.49
(1,743)	1:30:A:ILE:HG12	1:30:A:ILE:H	2	0.49
(1,703)	1:21:A:ASP:HB3	1:21:A:ASP:H	4	0.49
(1,56)	1:30:A:ILE:HD12	1:69:A:LEU:HB2	6	0.49
(1,1143)	1:70:A:VAL:HG12	1:71:A:LEU:H	5	0.48
(1,743)	1:30:A:ILE:HG12	1:30:A:ILE:H	3	0.48
(1,743)	1:30:A:ILE:HG12	1:30:A:ILE:H	7	0.48
(1,743)	1:30:A:ILE:HG12	1:30:A:ILE:H	8	0.48
(1,743)	1:30:A:ILE:HG12	1:30:A:ILE:H	10	0.48
(1,717)	1:25:A:ASN:HB3	1:25:A:ASN:H	4	0.48
(1,717)	1:25:A:ASN:HB3	1:25:A:ASN:H	5	0.48
(1,704)	1:18:A:GLU:HB3	1:21:A:ASP:H	7	0.48
(1,188)	1:26:A:VAL:HG11	1:23:A:ILE:HA	6	0.48
(1,188)	1:26:A:VAL:HG12	1:23:A:ILE:HA	6	0.48
(1,188)	1:26:A:VAL:HG13	1:23:A:ILE:HA	6	0.48
(1,134)	1:26:A:VAL:HG11	1:23:A:ILE:HA	10	0.48
(1,134)	1:26:A:VAL:HG12	1:23:A:ILE:HA	10	0.48
(1,134)	1:26:A:VAL:HG13	1:23:A:ILE:HA	10	0.48
(1,1143)	1:70:A:VAL:HG13	1:71:A:LEU:H	6	0.47
(1,966)	1:26:A:VAL:HG11	1:29:A:LYS:H	7	0.47
(1,966)	1:26:A:VAL:HG11	1:29:A:LYS:H	8	0.47
(1,717)	1:25:A:ASN:HB3	1:25:A:ASN:H	7	0.47
(1,703)	1:21:A:ASP:HB3	1:21:A:ASP:H	1	0.47
(1,592)	1:44:A:ILE:HD11	1:49:A:LYS:HB2	10	0.47
(1,592)	1:44:A:ILE:HD11	1:49:A:LYS:HB3	10	0.47
(1,592)	1:44:A:ILE:HD12	1:49:A:LYS:HB2	10	0.47
(1,592)	1:44:A:ILE:HD12	1:49:A:LYS:HB3	10	0.47
(1,592)	1:44:A:ILE:HD13	1:49:A:LYS:HB2	10	0.47
(1,592)	1:44:A:ILE:HD13	1:49:A:LYS:HB3	10	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,582)	1:55:A:THR:HB	1:20:A:SER:HB3	10	0.47
(1,120)	1:17:A:VAL:HG21	1:17:A:VAL:HA	1	0.47
(1,120)	1:17:A:VAL:HG22	1:17:A:VAL:HA	1	0.47
(1,120)	1:17:A:VAL:HG23	1:17:A:VAL:HA	1	0.47
(1,56)	1:30:A:ILE:HD13	1:69:A:LEU:HB2	5	0.47
(1,1279)	1:21:A:ASP:HB2	1:22:A:THR:H	9	0.46
(1,982)	1:49:A:LYS:HG2	1:49:A:LYS:H	3	0.46
(1,845)	1:21:A:ASP:HB2	1:56:A:LEU:H	10	0.46
(1,488)	1:30:A:ILE:HD13	1:43:A:LEU:HG	9	0.46
(1,188)	1:26:A:VAL:HG11	1:23:A:ILE:HA	7	0.46
(1,188)	1:26:A:VAL:HG12	1:23:A:ILE:HA	7	0.46
(1,188)	1:26:A:VAL:HG13	1:23:A:ILE:HA	7	0.46
(1,120)	1:17:A:VAL:HG21	1:17:A:VAL:HA	2	0.46
(1,120)	1:17:A:VAL:HG22	1:17:A:VAL:HA	2	0.46
(1,120)	1:17:A:VAL:HG23	1:17:A:VAL:HA	2	0.46
(1,120)	1:17:A:VAL:HG21	1:17:A:VAL:HA	3	0.46
(1,120)	1:17:A:VAL:HG22	1:17:A:VAL:HA	3	0.46
(1,120)	1:17:A:VAL:HG23	1:17:A:VAL:HA	3	0.46
(1,120)	1:17:A:VAL:HG21	1:17:A:VAL:HA	5	0.46
(1,120)	1:17:A:VAL:HG22	1:17:A:VAL:HA	5	0.46
(1,120)	1:17:A:VAL:HG23	1:17:A:VAL:HA	5	0.46
(1,120)	1:17:A:VAL:HG21	1:17:A:VAL:HA	6	0.46
(1,120)	1:17:A:VAL:HG22	1:17:A:VAL:HA	6	0.46
(1,120)	1:17:A:VAL:HG23	1:17:A:VAL:HA	6	0.46
(1,120)	1:17:A:VAL:HG21	1:17:A:VAL:HA	7	0.46
(1,120)	1:17:A:VAL:HG22	1:17:A:VAL:HA	7	0.46
(1,120)	1:17:A:VAL:HG23	1:17:A:VAL:HA	7	0.46
(1,120)	1:17:A:VAL:HG21	1:17:A:VAL:HA	10	0.46
(1,120)	1:17:A:VAL:HG22	1:17:A:VAL:HA	10	0.46
(1,120)	1:17:A:VAL:HG23	1:17:A:VAL:HA	10	0.46
(1,1091)	1:34:A:GLU:HB2	1:36:A:ILE:H	2	0.45
(1,704)	1:18:A:GLU:HB3	1:21:A:ASP:H	6	0.45
(1,630)	1:21:A:ASP:HB3	1:20:A:SER:H	1	0.45
(1,526)	1:33:A:GLU:HA	1:33:A:GLU:HB2	8	0.45
(1,134)	1:26:A:VAL:HG11	1:23:A:ILE:HA	4	0.45
(1,134)	1:26:A:VAL:HG12	1:23:A:ILE:HA	4	0.45
(1,134)	1:26:A:VAL:HG13	1:23:A:ILE:HA	4	0.45
(1,120)	1:17:A:VAL:HG21	1:17:A:VAL:HA	8	0.45
(1,120)	1:17:A:VAL:HG22	1:17:A:VAL:HA	8	0.45
(1,120)	1:17:A:VAL:HG23	1:17:A:VAL:HA	8	0.45
(1,120)	1:17:A:VAL:HG21	1:17:A:VAL:HA	9	0.45
(1,120)	1:17:A:VAL:HG22	1:17:A:VAL:HA	9	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,120)	1:17:A:VAL:HG23	1:17:A:VAL:HA	9	0.45
(1,931)	1:17:A:VAL:HG11	1:3:A:ILE:H	4	0.44
(1,931)	1:17:A:VAL:HG12	1:3:A:ILE:H	4	0.44
(1,931)	1:17:A:VAL:HG13	1:3:A:ILE:H	4	0.44
(1,582)	1:55:A:THR:HB	1:20:A:SER:HB3	6	0.44
(1,515)	1:61:A:ILE:HB	1:56:A:LEU:HD11	7	0.44
(1,515)	1:61:A:ILE:HB	1:56:A:LEU:HD12	7	0.44
(1,515)	1:61:A:ILE:HB	1:56:A:LEU:HD13	7	0.44
(1,514)	1:72:A:ARG:HB3	1:72:A:ARG:HA	4	0.44
(1,514)	1:72:A:ARG:HB3	1:72:A:ARG:HA	5	0.44
(1,514)	1:72:A:ARG:HB3	1:72:A:ARG:HA	6	0.44
(1,514)	1:72:A:ARG:HB3	1:72:A:ARG:HA	7	0.44
(1,514)	1:72:A:ARG:HB3	1:72:A:ARG:HA	9	0.44
(1,188)	1:26:A:VAL:HG11	1:23:A:ILE:HA	10	0.44
(1,188)	1:26:A:VAL:HG12	1:23:A:ILE:HA	10	0.44
(1,188)	1:26:A:VAL:HG13	1:23:A:ILE:HA	10	0.44
(1,130)	1:73:A:LEU:HD11	1:75:A:GLY:HA2	7	0.44
(1,130)	1:73:A:LEU:HD11	1:75:A:GLY:HA3	7	0.44
(1,130)	1:73:A:LEU:HD12	1:75:A:GLY:HA2	7	0.44
(1,130)	1:73:A:LEU:HD12	1:75:A:GLY:HA3	7	0.44
(1,130)	1:73:A:LEU:HD13	1:75:A:GLY:HA2	7	0.44
(1,130)	1:73:A:LEU:HD13	1:75:A:GLY:HA3	7	0.44
(1,56)	1:30:A:ILE:HD12	1:69:A:LEU:HB2	7	0.44
(1,982)	1:49:A:LYS:HG2	1:49:A:LYS:H	7	0.43
(1,966)	1:26:A:VAL:HG12	1:29:A:LYS:H	2	0.43
(1,514)	1:72:A:ARG:HB3	1:72:A:ARG:HA	8	0.43
(1,514)	1:72:A:ARG:HB3	1:72:A:ARG:HA	10	0.43
(1,448)	1:30:A:ILE:HD11	1:27:A:LYS:HB2	3	0.43
(1,448)	1:30:A:ILE:HD12	1:27:A:LYS:HB2	3	0.43
(1,448)	1:30:A:ILE:HD13	1:27:A:LYS:HB2	3	0.43
(1,448)	1:30:A:ILE:HD11	1:27:A:LYS:HB2	9	0.43
(1,448)	1:30:A:ILE:HD12	1:27:A:LYS:HB2	9	0.43
(1,448)	1:30:A:ILE:HD13	1:27:A:LYS:HB2	9	0.43
(1,137)	1:43:A:LEU:HB3	1:43:A:LEU:HD11	6	0.43
(1,137)	1:43:A:LEU:HB3	1:43:A:LEU:HD12	6	0.43
(1,137)	1:43:A:LEU:HB3	1:43:A:LEU:HD13	6	0.43
(1,137)	1:43:A:LEU:HB3	1:43:A:LEU:HD11	8	0.43
(1,137)	1:43:A:LEU:HB3	1:43:A:LEU:HD12	8	0.43
(1,137)	1:43:A:LEU:HB3	1:43:A:LEU:HD13	8	0.43
(1,134)	1:26:A:VAL:HG11	1:23:A:ILE:HA	2	0.43
(1,134)	1:26:A:VAL:HG12	1:23:A:ILE:HA	2	0.43
(1,134)	1:26:A:VAL:HG13	1:23:A:ILE:HA	2	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,120)	1:17:A:VAL:HG21	1:17:A:VAL:HA	4	0.43
(1,120)	1:17:A:VAL:HG22	1:17:A:VAL:HA	4	0.43
(1,120)	1:17:A:VAL:HG23	1:17:A:VAL:HA	4	0.43
(1,55)	1:69:A:LEU:HG	1:30:A:ILE:HD12	8	0.43
(1,1206)	1:33:A:GLU:HG3	1:34:A:GLU:H	8	0.42
(1,1091)	1:34:A:GLU:HB2	1:36:A:ILE:H	5	0.42
(1,966)	1:26:A:VAL:HG12	1:29:A:LYS:H	1	0.42
(1,744)	1:29:A:LYS:HG2	1:30:A:ILE:H	1	0.42
(1,744)	1:29:A:LYS:HG2	1:30:A:ILE:H	3	0.42
(1,449)	1:27:A:LYS:HB2	1:43:A:LEU:HD11	1	0.42
(1,449)	1:27:A:LYS:HB2	1:43:A:LEU:HD12	1	0.42
(1,449)	1:27:A:LYS:HB2	1:43:A:LEU:HD13	1	0.42
(1,188)	1:26:A:VAL:HG11	1:23:A:ILE:HA	4	0.42
(1,188)	1:26:A:VAL:HG12	1:23:A:ILE:HA	4	0.42
(1,188)	1:26:A:VAL:HG13	1:23:A:ILE:HA	4	0.42
(1,137)	1:43:A:LEU:HB3	1:43:A:LEU:HD11	5	0.42
(1,137)	1:43:A:LEU:HB3	1:43:A:LEU:HD12	5	0.42
(1,137)	1:43:A:LEU:HB3	1:43:A:LEU:HD13	5	0.42
(1,563)	1:55:A:THR:HA	1:22:A:THR:HB	7	0.41
(1,539)	1:10:A:GLY:HA3	1:11:A:LYS:HA	6	0.41
(1,514)	1:72:A:ARG:HB3	1:72:A:ARG:HA	1	0.41
(1,798)	1:43:A:LEU:HD21	1:44:A:ILE:H	3	0.4
(1,593)	1:3:A:ILE:HD11	1:15:A:LEU:HB2	8	0.4
(1,593)	1:3:A:ILE:HD12	1:15:A:LEU:HB2	8	0.4
(1,593)	1:3:A:ILE:HD13	1:15:A:LEU:HB2	8	0.4
(1,532)	1:6:A:LYS:HE2	1:6:A:LYS:HE3	1	0.4
(1,532)	1:6:A:LYS:HE2	1:6:A:LYS:HE3	2	0.4
(1,532)	1:6:A:LYS:HE2	1:6:A:LYS:HE3	3	0.4
(1,532)	1:6:A:LYS:HE2	1:6:A:LYS:HE3	4	0.4
(1,532)	1:6:A:LYS:HE2	1:6:A:LYS:HE3	5	0.4
(1,532)	1:6:A:LYS:HE2	1:6:A:LYS:HE3	6	0.4
(1,532)	1:6:A:LYS:HE2	1:6:A:LYS:HE3	7	0.4
(1,532)	1:6:A:LYS:HE2	1:6:A:LYS:HE3	8	0.4
(1,532)	1:6:A:LYS:HE2	1:6:A:LYS:HE3	9	0.4
(1,532)	1:6:A:LYS:HE2	1:6:A:LYS:HE3	10	0.4
(1,488)	1:30:A:ILE:HD13	1:43:A:LEU:HG	7	0.4
(1,188)	1:26:A:VAL:HG11	1:23:A:ILE:HA	2	0.4
(1,188)	1:26:A:VAL:HG12	1:23:A:ILE:HA	2	0.4
(1,188)	1:26:A:VAL:HG13	1:23:A:ILE:HA	2	0.4
(1,154)	1:9:A:THR:HB	1:11:A:LYS:HG2	10	0.4
(1,134)	1:26:A:VAL:HG11	1:23:A:ILE:HA	5	0.4
(1,134)	1:26:A:VAL:HG12	1:23:A:ILE:HA	5	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,134)	1:26:A:VAL:HG13	1:23:A:ILE:HA	5	0.4
(1,125)	1:26:A:VAL:HG11	1:56:A:LEU:HD11	6	0.4
(1,125)	1:26:A:VAL:HG11	1:56:A:LEU:HD12	6	0.4
(1,125)	1:26:A:VAL:HG11	1:56:A:LEU:HD13	6	0.4
(1,125)	1:26:A:VAL:HG12	1:56:A:LEU:HD11	6	0.4
(1,125)	1:26:A:VAL:HG12	1:56:A:LEU:HD12	6	0.4
(1,125)	1:26:A:VAL:HG12	1:56:A:LEU:HD13	6	0.4
(1,125)	1:26:A:VAL:HG13	1:56:A:LEU:HD11	6	0.4
(1,125)	1:26:A:VAL:HG13	1:56:A:LEU:HD12	6	0.4
(1,125)	1:26:A:VAL:HG13	1:56:A:LEU:HD13	6	0.4
(1,1270)	1:24:A:GLU:HG3	1:25:A:ASN:HD21	6	0.39
(1,1191)	1:35:A:GLY:H	1:33:A:GLU:H	8	0.39
(1,1145)	1:33:A:GLU:HG2	1:14:A:THR:H	8	0.39
(1,1013)	1:62:A:GLN:HB2	1:65:A:SER:H	1	0.39
(1,966)	1:26:A:VAL:HG13	1:29:A:LYS:H	9	0.39
(1,744)	1:29:A:LYS:HG2	1:30:A:ILE:H	6	0.39
(1,744)	1:29:A:LYS:HG2	1:30:A:ILE:H	9	0.39
(1,488)	1:30:A:ILE:HD11	1:43:A:LEU:HG	10	0.39
(1,276)	1:69:A:LEU:HA	1:69:A:LEU:HD11	1	0.39
(1,276)	1:69:A:LEU:HA	1:69:A:LEU:HD12	1	0.39
(1,276)	1:69:A:LEU:HA	1:69:A:LEU:HD13	1	0.39
(1,82)	1:50:A:LEU:HB2	1:23:A:ILE:HG21	2	0.39
(1,82)	1:50:A:LEU:HB2	1:23:A:ILE:HG22	2	0.39
(1,82)	1:50:A:LEU:HB2	1:23:A:ILE:HG23	2	0.39
(1,798)	1:43:A:LEU:HD22	1:44:A:ILE:H	7	0.38
(1,744)	1:29:A:LYS:HG2	1:30:A:ILE:H	4	0.38
(1,707)	1:21:A:ASP:HA	1:22:A:THR:H	10	0.38
(1,703)	1:21:A:ASP:HB3	1:21:A:ASP:H	10	0.38
(1,573)	1:40:A:GLN:HG2	1:40:A:GLN:HA	8	0.38
(1,573)	1:40:A:GLN:HG3	1:40:A:GLN:HA	8	0.38
(1,284)	1:28:A:ALA:HA	1:31:A:GLN:HG2	3	0.38
(1,549)	1:56:A:LEU:HD21	1:19:A:PRO:HA	1	0.37
(1,549)	1:56:A:LEU:HD22	1:19:A:PRO:HA	1	0.37
(1,549)	1:56:A:LEU:HD23	1:19:A:PRO:HA	1	0.37
(1,539)	1:10:A:GLY:HA3	1:11:A:LYS:HA	7	0.37
(1,444)	1:6:A:LYS:HD2	1:6:A:LYS:HB3	2	0.37
(1,284)	1:28:A:ALA:HA	1:31:A:GLN:HG2	6	0.37
(1,188)	1:26:A:VAL:HG11	1:23:A:ILE:HA	5	0.37
(1,188)	1:26:A:VAL:HG12	1:23:A:ILE:HA	5	0.37
(1,188)	1:26:A:VAL:HG13	1:23:A:ILE:HA	5	0.37
(1,825)	1:50:A:LEU:HD11	1:51:A:GLU:H	4	0.36
(1,825)	1:50:A:LEU:HD12	1:51:A:GLU:H	4	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,825)	1:50:A:LEU:HD13	1:51:A:GLU:H	4	0.36
(1,573)	1:40:A:GLN:HG2	1:40:A:GLN:HA	2	0.36
(1,573)	1:40:A:GLN:HG3	1:40:A:GLN:HA	2	0.36
(1,563)	1:55:A:THR:HA	1:22:A:THR:HB	2	0.36
(1,524)	1:20:A:SER:HA	1:20:A:SER:HB2	4	0.36
(1,524)	1:20:A:SER:HA	1:20:A:SER:HB2	6	0.36
(1,486)	1:69:A:LEU:HA	1:69:A:LEU:HD11	1	0.36
(1,486)	1:69:A:LEU:HA	1:69:A:LEU:HD12	1	0.36
(1,486)	1:69:A:LEU:HA	1:69:A:LEU:HD13	1	0.36
(1,444)	1:6:A:LYS:HD2	1:6:A:LYS:HB3	6	0.36
(1,216)	1:70:A:VAL:HG11	1:70:A:VAL:HA	1	0.36
(1,216)	1:70:A:VAL:HG12	1:70:A:VAL:HA	1	0.36
(1,216)	1:70:A:VAL:HG13	1:70:A:VAL:HA	1	0.36
(1,216)	1:70:A:VAL:HG11	1:70:A:VAL:HA	3	0.36
(1,216)	1:70:A:VAL:HG12	1:70:A:VAL:HA	3	0.36
(1,216)	1:70:A:VAL:HG13	1:70:A:VAL:HA	3	0.36
(1,216)	1:70:A:VAL:HG11	1:70:A:VAL:HA	10	0.36
(1,216)	1:70:A:VAL:HG12	1:70:A:VAL:HA	10	0.36
(1,216)	1:70:A:VAL:HG13	1:70:A:VAL:HA	10	0.36
(1,966)	1:26:A:VAL:HG12	1:29:A:LYS:H	6	0.35
(1,798)	1:43:A:LEU:HD21	1:44:A:ILE:H	2	0.35
(1,754)	1:31:A:GLN:HG2	1:32:A:ASP:H	7	0.35
(1,744)	1:29:A:LYS:HG2	1:30:A:ILE:H	7	0.35
(1,744)	1:29:A:LYS:HG2	1:30:A:ILE:H	10	0.35
(1,549)	1:56:A:LEU:HD21	1:19:A:PRO:HA	9	0.35
(1,549)	1:56:A:LEU:HD22	1:19:A:PRO:HA	9	0.35
(1,549)	1:56:A:LEU:HD23	1:19:A:PRO:HA	9	0.35
(1,539)	1:10:A:GLY:HA3	1:11:A:LYS:HA	5	0.35
(1,1275)	1:39:A:ASP:HB2	1:39:A:ASP:H	10	0.34
(1,825)	1:50:A:LEU:HD11	1:51:A:GLU:H	2	0.34
(1,825)	1:50:A:LEU:HD12	1:51:A:GLU:H	2	0.34
(1,825)	1:50:A:LEU:HD13	1:51:A:GLU:H	2	0.34
(1,825)	1:50:A:LEU:HD11	1:51:A:GLU:H	6	0.34
(1,825)	1:50:A:LEU:HD12	1:51:A:GLU:H	6	0.34
(1,825)	1:50:A:LEU:HD13	1:51:A:GLU:H	6	0.34
(1,825)	1:50:A:LEU:HD11	1:51:A:GLU:H	8	0.34
(1,825)	1:50:A:LEU:HD12	1:51:A:GLU:H	8	0.34
(1,825)	1:50:A:LEU:HD13	1:51:A:GLU:H	8	0.34
(1,573)	1:40:A:GLN:HG2	1:40:A:GLN:HA	1	0.34
(1,573)	1:40:A:GLN:HG3	1:40:A:GLN:HA	1	0.34
(1,573)	1:40:A:GLN:HG2	1:40:A:GLN:HA	3	0.34
(1,573)	1:40:A:GLN:HG3	1:40:A:GLN:HA	3	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,573)	1:40:A:GLN:HG2	1:40:A:GLN:HA	5	0.34
(1,573)	1:40:A:GLN:HG3	1:40:A:GLN:HA	5	0.34
(1,573)	1:40:A:GLN:HG2	1:40:A:GLN:HA	9	0.34
(1,573)	1:40:A:GLN:HG3	1:40:A:GLN:HA	9	0.34
(1,545)	1:63:A:LYS:HA	1:18:A:GLU:HA	2	0.34
(1,545)	1:63:A:LYS:HA	1:18:A:GLU:HA	4	0.34
(1,539)	1:10:A:GLY:HA3	1:11:A:LYS:HA	10	0.34
(1,488)	1:30:A:ILE:HD13	1:43:A:LEU:HG	2	0.34
(1,83)	1:23:A:ILE:HG22	1:43:A:LEU:HB2	2	0.34
(1,1280)	1:15:A:LEU:HB2	1:17:A:VAL:H	10	0.33
(1,573)	1:40:A:GLN:HG2	1:40:A:GLN:HA	6	0.33
(1,573)	1:40:A:GLN:HG3	1:40:A:GLN:HA	6	0.33
(1,549)	1:56:A:LEU:HD21	1:19:A:PRO:HA	3	0.33
(1,549)	1:56:A:LEU:HD22	1:19:A:PRO:HA	3	0.33
(1,549)	1:56:A:LEU:HD23	1:19:A:PRO:HA	3	0.33
(1,539)	1:10:A:GLY:HA3	1:11:A:LYS:HA	3	0.33
(1,539)	1:10:A:GLY:HA3	1:11:A:LYS:HA	4	0.33
(1,444)	1:6:A:LYS:HD2	1:6:A:LYS:HB3	5	0.33
(1,444)	1:6:A:LYS:HD2	1:6:A:LYS:HB3	10	0.33
(1,207)	1:27:A:LYS:HE2	1:24:A:GLU:HA	7	0.33
(1,154)	1:9:A:THR:HB	1:11:A:LYS:HG2	3	0.33
(1,154)	1:9:A:THR:HB	1:11:A:LYS:HG2	6	0.33
(1,154)	1:9:A:THR:HB	1:11:A:LYS:HG2	7	0.33
(1,55)	1:69:A:LEU:HG	1:30:A:ILE:HD12	7	0.33
(1,1280)	1:15:A:LEU:HB2	1:17:A:VAL:H	1	0.32
(1,1275)	1:39:A:ASP:HB2	1:39:A:ASP:H	4	0.32
(1,825)	1:50:A:LEU:HD11	1:51:A:GLU:H	7	0.32
(1,825)	1:50:A:LEU:HD12	1:51:A:GLU:H	7	0.32
(1,825)	1:50:A:LEU:HD13	1:51:A:GLU:H	7	0.32
(1,704)	1:18:A:GLU:HB3	1:21:A:ASP:H	9	0.32
(1,549)	1:56:A:LEU:HD21	1:19:A:PRO:HA	5	0.32
(1,549)	1:56:A:LEU:HD22	1:19:A:PRO:HA	5	0.32
(1,549)	1:56:A:LEU:HD23	1:19:A:PRO:HA	5	0.32
(1,539)	1:10:A:GLY:HA3	1:11:A:LYS:HA	8	0.32
(1,359)	1:44:A:ILE:HB	1:68:A:HIS:HB2	3	0.32
(1,276)	1:69:A:LEU:HA	1:69:A:LEU:HD11	10	0.32
(1,276)	1:69:A:LEU:HA	1:69:A:LEU:HD12	10	0.32
(1,276)	1:69:A:LEU:HA	1:69:A:LEU:HD13	10	0.32
(1,56)	1:30:A:ILE:HD12	1:69:A:LEU:HB2	2	0.32
(1,962)	1:25:A:ASN:HB3	1:26:A:VAL:H	5	0.31
(1,744)	1:29:A:LYS:HG2	1:30:A:ILE:H	2	0.31
(1,573)	1:40:A:GLN:HG2	1:40:A:GLN:HA	7	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,573)	1:40:A:GLN:HG3	1:40:A:GLN:HA	7	0.31
(1,567)	1:29:A:LYS:HB3	1:15:A:LEU:HD23	4	0.31
(1,545)	1:63:A:LYS:HA	1:18:A:GLU:HA	5	0.31
(1,539)	1:10:A:GLY:HA3	1:11:A:LYS:HA	2	0.31
(1,154)	1:9:A:THR:HB	1:11:A:LYS:HG2	4	0.31
(1,1280)	1:15:A:LEU:HB2	1:17:A:VAL:H	3	0.3
(1,1275)	1:39:A:ASP:HB2	1:39:A:ASP:H	7	0.3
(1,1070)	1:25:A:ASN:HB3	1:21:A:ASP:H	7	0.3
(1,1057)	1:72:A:ARG:HD2	1:72:A:ARG:H	4	0.3
(1,573)	1:40:A:GLN:HG2	1:40:A:GLN:HA	10	0.3
(1,573)	1:40:A:GLN:HG3	1:40:A:GLN:HA	10	0.3
(1,549)	1:56:A:LEU:HD21	1:19:A:PRO:HA	6	0.3
(1,549)	1:56:A:LEU:HD22	1:19:A:PRO:HA	6	0.3
(1,549)	1:56:A:LEU:HD23	1:19:A:PRO:HA	6	0.3
(1,549)	1:56:A:LEU:HD21	1:19:A:PRO:HA	8	0.3
(1,549)	1:56:A:LEU:HD22	1:19:A:PRO:HA	8	0.3
(1,549)	1:56:A:LEU:HD23	1:19:A:PRO:HA	8	0.3
(1,548)	1:56:A:LEU:HG	1:19:A:PRO:HA	7	0.3
(1,545)	1:63:A:LYS:HA	1:18:A:GLU:HA	3	0.3
(1,486)	1:69:A:LEU:HA	1:69:A:LEU:HD11	10	0.3
(1,486)	1:69:A:LEU:HA	1:69:A:LEU:HD12	10	0.3
(1,486)	1:69:A:LEU:HA	1:69:A:LEU:HD13	10	0.3
(1,449)	1:27:A:LYS:HB2	1:43:A:LEU:HD11	9	0.3
(1,449)	1:27:A:LYS:HB2	1:43:A:LEU:HD12	9	0.3
(1,449)	1:27:A:LYS:HB2	1:43:A:LEU:HD13	9	0.3
(1,444)	1:6:A:LYS:HD2	1:6:A:LYS:HB3	1	0.3
(1,444)	1:6:A:LYS:HD2	1:6:A:LYS:HB3	9	0.3
(1,125)	1:26:A:VAL:HG11	1:56:A:LEU:HD11	2	0.3
(1,125)	1:26:A:VAL:HG11	1:56:A:LEU:HD12	2	0.3
(1,125)	1:26:A:VAL:HG11	1:56:A:LEU:HD13	2	0.3
(1,125)	1:26:A:VAL:HG12	1:56:A:LEU:HD11	2	0.3
(1,125)	1:26:A:VAL:HG12	1:56:A:LEU:HD12	2	0.3
(1,125)	1:26:A:VAL:HG12	1:56:A:LEU:HD13	2	0.3
(1,125)	1:26:A:VAL:HG13	1:56:A:LEU:HD11	2	0.3
(1,125)	1:26:A:VAL:HG13	1:56:A:LEU:HD12	2	0.3
(1,125)	1:26:A:VAL:HG13	1:56:A:LEU:HD13	2	0.3
(1,125)	1:26:A:VAL:HG11	1:56:A:LEU:HD11	5	0.3
(1,125)	1:26:A:VAL:HG11	1:56:A:LEU:HD12	5	0.3
(1,125)	1:26:A:VAL:HG11	1:56:A:LEU:HD13	5	0.3
(1,125)	1:26:A:VAL:HG12	1:56:A:LEU:HD11	5	0.3
(1,125)	1:26:A:VAL:HG12	1:56:A:LEU:HD12	5	0.3
(1,125)	1:26:A:VAL:HG12	1:56:A:LEU:HD13	5	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,125)	1:26:A:VAL:HG13	1:56:A:LEU:HD11	5	0.3
(1,125)	1:26:A:VAL:HG13	1:56:A:LEU:HD12	5	0.3
(1,125)	1:26:A:VAL:HG13	1:56:A:LEU:HD13	5	0.3
(1,125)	1:26:A:VAL:HG11	1:56:A:LEU:HD11	7	0.3
(1,125)	1:26:A:VAL:HG11	1:56:A:LEU:HD12	7	0.3
(1,125)	1:26:A:VAL:HG11	1:56:A:LEU:HD13	7	0.3
(1,125)	1:26:A:VAL:HG12	1:56:A:LEU:HD11	7	0.3
(1,125)	1:26:A:VAL:HG12	1:56:A:LEU:HD12	7	0.3
(1,125)	1:26:A:VAL:HG12	1:56:A:LEU:HD13	7	0.3
(1,125)	1:26:A:VAL:HG13	1:56:A:LEU:HD11	7	0.3
(1,125)	1:26:A:VAL:HG13	1:56:A:LEU:HD12	7	0.3
(1,125)	1:26:A:VAL:HG13	1:56:A:LEU:HD13	7	0.3
(1,1280)	1:15:A:LEU:HB2	1:17:A:VAL:H	6	0.29
(1,1196)	1:5:A:VAL:HG22	1:7:A:THR:H	9	0.29
(1,1174)	1:27:A:LYS:HD2	1:27:A:LYS:H	8	0.29
(1,1057)	1:72:A:ARG:HD3	1:72:A:ARG:H	5	0.29
(1,1057)	1:72:A:ARG:HD3	1:72:A:ARG:H	6	0.29
(1,966)	1:26:A:VAL:HG13	1:29:A:LYS:H	10	0.29
(1,798)	1:43:A:LEU:HD21	1:44:A:ILE:H	10	0.29
(1,696)	1:18:A:GLU:HB3	1:18:A:GLU:H	1	0.29
(1,696)	1:18:A:GLU:HB3	1:18:A:GLU:H	3	0.29
(1,696)	1:18:A:GLU:HB3	1:18:A:GLU:H	9	0.29
(1,549)	1:56:A:LEU:HD21	1:19:A:PRO:HA	4	0.29
(1,549)	1:56:A:LEU:HD22	1:19:A:PRO:HA	4	0.29
(1,549)	1:56:A:LEU:HD23	1:19:A:PRO:HA	4	0.29
(1,539)	1:10:A:GLY:HA3	1:11:A:LYS:HA	9	0.29
(1,444)	1:6:A:LYS:HD2	1:6:A:LYS:HB3	3	0.29
(1,444)	1:6:A:LYS:HD2	1:6:A:LYS:HB3	4	0.29
(1,444)	1:6:A:LYS:HD2	1:6:A:LYS:HB3	8	0.29
(1,212)	1:5:A:VAL:HA	1:68:A:HIS:HA	7	0.29
(1,1168)	1:67:A:LEU:HG	1:68:A:HIS:H	9	0.28
(1,744)	1:29:A:LYS:HG2	1:30:A:ILE:H	5	0.28
(1,744)	1:29:A:LYS:HG2	1:30:A:ILE:H	8	0.28
(1,696)	1:18:A:GLU:HB3	1:18:A:GLU:H	6	0.28
(1,573)	1:40:A:GLN:HG2	1:40:A:GLN:HA	4	0.28
(1,573)	1:40:A:GLN:HG3	1:40:A:GLN:HA	4	0.28
(1,517)	1:7:A:THR:HB	1:7:A:THR:HA	8	0.28
(1,1280)	1:15:A:LEU:HB2	1:17:A:VAL:H	9	0.27
(1,1279)	1:21:A:ASP:HB2	1:22:A:THR:H	5	0.27
(1,1168)	1:67:A:LEU:HG	1:68:A:HIS:H	1	0.27
(1,1073)	1:49:A:LYS:HE2	1:50:A:LEU:H	3	0.27
(1,1073)	1:49:A:LYS:HE3	1:50:A:LEU:H	3	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,844)	1:21:A:ASP:HB3	1:56:A:LEU:H	6	0.27
(1,704)	1:18:A:GLU:HB3	1:21:A:ASP:H	1	0.27
(1,696)	1:18:A:GLU:HB3	1:18:A:GLU:H	10	0.27
(1,575)	1:41:A:GLN:HB2	1:40:A:GLN:HG2	1	0.27
(1,575)	1:41:A:GLN:HB2	1:40:A:GLN:HG3	1	0.27
(1,575)	1:41:A:GLN:HB3	1:40:A:GLN:HG2	1	0.27
(1,575)	1:41:A:GLN:HB3	1:40:A:GLN:HG3	1	0.27
(1,547)	1:1:A:MET:HB2	1:18:A:GLU:HG2	8	0.27
(1,547)	1:1:A:MET:HB2	1:18:A:GLU:HG3	8	0.27
(1,547)	1:1:A:MET:HB3	1:18:A:GLU:HG2	8	0.27
(1,547)	1:1:A:MET:HB3	1:18:A:GLU:HG3	8	0.27
(1,545)	1:63:A:LYS:HA	1:18:A:GLU:HA	1	0.27
(1,545)	1:63:A:LYS:HA	1:18:A:GLU:HA	9	0.27
(1,444)	1:6:A:LYS:HD2	1:6:A:LYS:HB3	7	0.27
(1,231)	1:55:A:THR:HG21	1:22:A:THR:HA	2	0.27
(1,231)	1:55:A:THR:HG22	1:22:A:THR:HA	2	0.27
(1,231)	1:55:A:THR:HG23	1:22:A:THR:HA	2	0.27
(1,1254)	1:41:A:GLN:HB2	1:40:A:GLN:HE22	6	0.26
(1,1254)	1:41:A:GLN:HB3	1:40:A:GLN:HE22	6	0.26
(1,1089)	1:64:A:GLU:HB2	1:4:A:PHE:H	1	0.26
(1,1089)	1:64:A:GLU:HB2	1:4:A:PHE:H	6	0.26
(1,559)	1:56:A:LEU:HD21	1:22:A:THR:HA	8	0.26
(1,559)	1:56:A:LEU:HD22	1:22:A:THR:HA	8	0.26
(1,559)	1:56:A:LEU:HD23	1:22:A:THR:HA	8	0.26
(1,545)	1:63:A:LYS:HA	1:18:A:GLU:HA	6	0.26
(1,541)	1:12:A:THR:HA	1:11:A:LYS:HA	8	0.26
(1,56)	1:30:A:ILE:HD13	1:69:A:LEU:HB2	10	0.26
(1,1280)	1:15:A:LEU:HB2	1:17:A:VAL:H	4	0.25
(1,1254)	1:41:A:GLN:HB2	1:40:A:GLN:HE22	2	0.25
(1,1254)	1:41:A:GLN:HB3	1:40:A:GLN:HE22	2	0.25
(1,1254)	1:41:A:GLN:HB2	1:40:A:GLN:HE22	7	0.25
(1,1254)	1:41:A:GLN:HB3	1:40:A:GLN:HE22	7	0.25
(1,1154)	1:15:A:LEU:HG	1:30:A:ILE:H	9	0.25
(1,1140)	1:31:A:GLN:HB2	1:28:A:ALA:H	3	0.25
(1,1140)	1:31:A:GLN:HB3	1:28:A:ALA:H	3	0.25
(1,1070)	1:25:A:ASN:HB3	1:21:A:ASP:H	4	0.25
(1,696)	1:18:A:GLU:HB3	1:18:A:GLU:H	2	0.25
(1,696)	1:18:A:GLU:HB3	1:18:A:GLU:H	5	0.25
(1,592)	1:44:A:ILE:HD11	1:49:A:LYS:HB2	3	0.25
(1,592)	1:44:A:ILE:HD11	1:49:A:LYS:HB3	3	0.25
(1,592)	1:44:A:ILE:HD12	1:49:A:LYS:HB2	3	0.25
(1,592)	1:44:A:ILE:HD12	1:49:A:LYS:HB3	3	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,592)	1:44:A:ILE:HD13	1:49:A:LYS:HB2	3	0.25
(1,592)	1:44:A:ILE:HD13	1:49:A:LYS:HB3	3	0.25
(1,567)	1:29:A:LYS:HB3	1:15:A:LEU:HD21	3	0.25
(1,560)	1:55:A:THR:HB	1:22:A:THR:HA	8	0.25
(1,549)	1:56:A:LEU:HD21	1:19:A:PRO:HA	2	0.25
(1,549)	1:56:A:LEU:HD22	1:19:A:PRO:HA	2	0.25
(1,549)	1:56:A:LEU:HD23	1:19:A:PRO:HA	2	0.25
(1,529)	1:57:A:SER:HB2	1:57:A:SER:HA	2	0.25
(1,529)	1:57:A:SER:HB2	1:57:A:SER:HA	4	0.25
(1,430)	1:15:A:LEU:HD21	1:16:A:GLU:HG3	5	0.25
(1,430)	1:15:A:LEU:HD22	1:16:A:GLU:HG3	5	0.25
(1,430)	1:15:A:LEU:HD23	1:16:A:GLU:HG3	5	0.25
(1,371)	1:4:A:PHE:HB2	1:12:A:THR:HG21	3	0.25
(1,371)	1:4:A:PHE:HB2	1:12:A:THR:HG22	3	0.25
(1,371)	1:4:A:PHE:HB2	1:12:A:THR:HG23	3	0.25
(1,207)	1:23:A:ILE:HB	1:24:A:GLU:HA	9	0.25
(1,125)	1:26:A:VAL:HG11	1:56:A:LEU:HD11	10	0.25
(1,125)	1:26:A:VAL:HG11	1:56:A:LEU:HD12	10	0.25
(1,125)	1:26:A:VAL:HG11	1:56:A:LEU:HD13	10	0.25
(1,125)	1:26:A:VAL:HG12	1:56:A:LEU:HD11	10	0.25
(1,125)	1:26:A:VAL:HG12	1:56:A:LEU:HD12	10	0.25
(1,125)	1:26:A:VAL:HG12	1:56:A:LEU:HD13	10	0.25
(1,125)	1:26:A:VAL:HG13	1:56:A:LEU:HD11	10	0.25
(1,125)	1:26:A:VAL:HG13	1:56:A:LEU:HD12	10	0.25
(1,125)	1:26:A:VAL:HG13	1:56:A:LEU:HD13	10	0.25
(1,56)	1:30:A:ILE:HD12	1:69:A:LEU:HB2	9	0.25
(1,1254)	1:41:A:GLN:HB2	1:40:A:GLN:HE22	5	0.24
(1,1254)	1:41:A:GLN:HB3	1:40:A:GLN:HE22	5	0.24
(1,1254)	1:41:A:GLN:HB2	1:40:A:GLN:HE22	10	0.24
(1,1254)	1:41:A:GLN:HB3	1:40:A:GLN:HE22	10	0.24
(1,1140)	1:31:A:GLN:HB2	1:28:A:ALA:H	6	0.24
(1,1140)	1:31:A:GLN:HB3	1:28:A:ALA:H	6	0.24
(1,1037)	1:56:A:LEU:HD21	1:56:A:LEU:H	7	0.24
(1,1037)	1:56:A:LEU:HD22	1:56:A:LEU:H	7	0.24
(1,1037)	1:56:A:LEU:HD23	1:56:A:LEU:H	7	0.24
(1,1035)	1:23:A:ILE:HD11	1:57:A:SER:H	4	0.24
(1,1035)	1:23:A:ILE:HD12	1:57:A:SER:H	4	0.24
(1,1035)	1:23:A:ILE:HD13	1:57:A:SER:H	4	0.24
(1,845)	1:21:A:ASP:HB2	1:56:A:LEU:H	4	0.24
(1,749)	1:31:A:GLN:HG2	1:31:A:GLN:H	6	0.24
(1,696)	1:18:A:GLU:HB3	1:18:A:GLU:H	7	0.24
(1,590)	1:73:A:LEU:HG	1:73:A:LEU:HA	9	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,559)	1:56:A:LEU:HD21	1:22:A:THR:HA	9	0.24
(1,559)	1:56:A:LEU:HD22	1:22:A:THR:HA	9	0.24
(1,559)	1:56:A:LEU:HD23	1:22:A:THR:HA	9	0.24
(1,545)	1:63:A:LYS:HA	1:18:A:GLU:HA	10	0.24
(1,539)	1:10:A:GLY:HA3	1:11:A:LYS:HA	1	0.24
(1,529)	1:57:A:SER:HB2	1:57:A:SER:HA	1	0.24
(1,488)	1:30:A:ILE:HD12	1:43:A:LEU:HG	1	0.24
(1,1280)	1:15:A:LEU:HB2	1:17:A:VAL:H	2	0.23
(1,1254)	1:41:A:GLN:HB2	1:40:A:GLN:HE22	1	0.23
(1,1254)	1:41:A:GLN:HB3	1:40:A:GLN:HE22	1	0.23
(1,1254)	1:41:A:GLN:HB2	1:40:A:GLN:HE22	4	0.23
(1,1254)	1:41:A:GLN:HB3	1:40:A:GLN:HE22	4	0.23
(1,1250)	1:31:A:GLN:H	1:41:A:GLN:HE22	6	0.23
(1,1089)	1:64:A:GLU:HB2	1:4:A:PHE:H	8	0.23
(1,1075)	1:56:A:LEU:HB3	1:20:A:SER:H	10	0.23
(1,1035)	1:23:A:ILE:HD11	1:57:A:SER:H	1	0.23
(1,1035)	1:23:A:ILE:HD12	1:57:A:SER:H	1	0.23
(1,1035)	1:23:A:ILE:HD13	1:57:A:SER:H	1	0.23
(1,1035)	1:23:A:ILE:HD11	1:57:A:SER:H	9	0.23
(1,1035)	1:23:A:ILE:HD12	1:57:A:SER:H	9	0.23
(1,1035)	1:23:A:ILE:HD13	1:57:A:SER:H	9	0.23
(1,844)	1:21:A:ASP:HB3	1:56:A:LEU:H	7	0.23
(1,825)	1:50:A:LEU:HD11	1:51:A:GLU:H	10	0.23
(1,825)	1:50:A:LEU:HD12	1:51:A:GLU:H	10	0.23
(1,825)	1:50:A:LEU:HD13	1:51:A:GLU:H	10	0.23
(1,575)	1:41:A:GLN:HB2	1:40:A:GLN:HG2	2	0.23
(1,575)	1:41:A:GLN:HB2	1:40:A:GLN:HG3	2	0.23
(1,575)	1:41:A:GLN:HB3	1:40:A:GLN:HG2	2	0.23
(1,575)	1:41:A:GLN:HB3	1:40:A:GLN:HG3	2	0.23
(1,559)	1:56:A:LEU:HD21	1:22:A:THR:HA	1	0.23
(1,559)	1:56:A:LEU:HD22	1:22:A:THR:HA	1	0.23
(1,559)	1:56:A:LEU:HD23	1:22:A:THR:HA	1	0.23
(1,559)	1:56:A:LEU:HD21	1:22:A:THR:HA	6	0.23
(1,559)	1:56:A:LEU:HD22	1:22:A:THR:HA	6	0.23
(1,559)	1:56:A:LEU:HD23	1:22:A:THR:HA	6	0.23
(1,545)	1:63:A:LYS:HA	1:18:A:GLU:HA	7	0.23
(1,541)	1:12:A:THR:HA	1:11:A:LYS:HA	2	0.23
(1,111)	1:2:A:LYS:HD3	1:14:A:THR:HG21	9	0.23
(1,111)	1:2:A:LYS:HD3	1:14:A:THR:HG22	9	0.23
(1,111)	1:2:A:LYS:HD3	1:14:A:THR:HG23	9	0.23
(1,1254)	1:41:A:GLN:HB2	1:40:A:GLN:HE22	9	0.22
(1,1254)	1:41:A:GLN:HB3	1:40:A:GLN:HE22	9	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1136)	1:50:A:LEU:HA	1:49:A:LYS:H	3	0.22
(1,1089)	1:64:A:GLU:HB2	1:4:A:PHE:H	2	0.22
(1,1089)	1:64:A:GLU:HB2	1:4:A:PHE:H	5	0.22
(1,844)	1:21:A:ASP:HB3	1:56:A:LEU:H	4	0.22
(1,749)	1:31:A:GLN:HG2	1:31:A:GLN:H	3	0.22
(1,749)	1:31:A:GLN:HG2	1:31:A:GLN:H	5	0.22
(1,560)	1:55:A:THR:HB	1:22:A:THR:HA	5	0.22
(1,559)	1:56:A:LEU:HD21	1:22:A:THR:HA	3	0.22
(1,559)	1:56:A:LEU:HD22	1:22:A:THR:HA	3	0.22
(1,559)	1:56:A:LEU:HD23	1:22:A:THR:HA	3	0.22
(1,545)	1:63:A:LYS:HA	1:18:A:GLU:HA	8	0.22
(1,541)	1:12:A:THR:HA	1:11:A:LYS:HA	1	0.22
(1,541)	1:12:A:THR:HA	1:11:A:LYS:HA	3	0.22
(1,541)	1:12:A:THR:HA	1:11:A:LYS:HA	10	0.22
(1,454)	1:2:A:LYS:HD2	1:2:A:LYS:HB2	5	0.22
(1,454)	1:2:A:LYS:HD3	1:2:A:LYS:HB2	5	0.22
(1,449)	1:27:A:LYS:HB2	1:43:A:LEU:HD11	2	0.22
(1,449)	1:27:A:LYS:HB2	1:43:A:LEU:HD12	2	0.22
(1,449)	1:27:A:LYS:HB2	1:43:A:LEU:HD13	2	0.22
(1,249)	1:36:A:ILE:HA	1:71:A:LEU:HD11	3	0.22
(1,249)	1:36:A:ILE:HA	1:71:A:LEU:HD12	3	0.22
(1,249)	1:36:A:ILE:HA	1:71:A:LEU:HD13	3	0.22
(1,1254)	1:41:A:GLN:HB2	1:40:A:GLN:HE22	8	0.21
(1,1254)	1:41:A:GLN:HB3	1:40:A:GLN:HE22	8	0.21
(1,1132)	1:16:A:GLU:HA	1:2:A:LYS:H	3	0.21
(1,1035)	1:23:A:ILE:HD11	1:57:A:SER:H	3	0.21
(1,1035)	1:23:A:ILE:HD12	1:57:A:SER:H	3	0.21
(1,1035)	1:23:A:ILE:HD13	1:57:A:SER:H	3	0.21
(1,962)	1:25:A:ASN:HB3	1:26:A:VAL:H	1	0.21
(1,788)	1:41:A:GLN:HG2	1:41:A:GLN:H	8	0.21
(1,696)	1:18:A:GLU:HB3	1:18:A:GLU:H	8	0.21
(1,577)	1:71:A:LEU:HG	1:41:A:GLN:HA	6	0.21
(1,575)	1:41:A:GLN:HB2	1:40:A:GLN:HG2	10	0.21
(1,575)	1:41:A:GLN:HB2	1:40:A:GLN:HG3	10	0.21
(1,575)	1:41:A:GLN:HB3	1:40:A:GLN:HG2	10	0.21
(1,575)	1:41:A:GLN:HB3	1:40:A:GLN:HG3	10	0.21
(1,559)	1:56:A:LEU:HD21	1:22:A:THR:HA	4	0.21
(1,559)	1:56:A:LEU:HD22	1:22:A:THR:HA	4	0.21
(1,559)	1:56:A:LEU:HD23	1:22:A:THR:HA	4	0.21
(1,541)	1:12:A:THR:HA	1:11:A:LYS:HA	7	0.21
(1,536)	1:11:A:LYS:HD2	1:9:A:THR:HG21	4	0.21
(1,536)	1:11:A:LYS:HD2	1:9:A:THR:HG22	4	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,536)	1:11:A:LYS:HD2	1:9:A:THR:HG23	4	0.21
(1,536)	1:11:A:LYS:HD3	1:9:A:THR:HG21	4	0.21
(1,536)	1:11:A:LYS:HD3	1:9:A:THR:HG22	4	0.21
(1,536)	1:11:A:LYS:HD3	1:9:A:THR:HG23	4	0.21
(1,448)	1:30:A:ILE:HD11	1:27:A:LYS:HB2	6	0.21
(1,448)	1:30:A:ILE:HD12	1:27:A:LYS:HB2	6	0.21
(1,448)	1:30:A:ILE:HD13	1:27:A:LYS:HB2	6	0.21
(1,27)	1:50:A:LEU:HD11	1:45:A:PHE:HB3	9	0.21
(1,27)	1:50:A:LEU:HD12	1:45:A:PHE:HB3	9	0.21
(1,27)	1:50:A:LEU:HD13	1:45:A:PHE:HB3	9	0.21
(1,17)	1:44:A:ILE:HD11	1:49:A:LYS:HE2	7	0.21
(1,17)	1:44:A:ILE:HD11	1:49:A:LYS:HE3	7	0.21
(1,17)	1:44:A:ILE:HD12	1:49:A:LYS:HE2	7	0.21
(1,17)	1:44:A:ILE:HD12	1:49:A:LYS:HE3	7	0.21
(1,17)	1:44:A:ILE:HD13	1:49:A:LYS:HE2	7	0.21
(1,17)	1:44:A:ILE:HD13	1:49:A:LYS:HE3	7	0.21
(1,1204)	1:64:A:GLU:H	1:63:A:LYS:HD2	3	0.2
(1,1204)	1:64:A:GLU:H	1:63:A:LYS:HD3	3	0.2
(1,1081)	1:32:A:ASP:HB2	1:34:A:GLU:H	8	0.2
(1,1035)	1:23:A:ILE:HD11	1:57:A:SER:H	6	0.2
(1,1035)	1:23:A:ILE:HD12	1:57:A:SER:H	6	0.2
(1,1035)	1:23:A:ILE:HD13	1:57:A:SER:H	6	0.2
(1,1016)	1:4:A:PHE:HB3	1:66:A:THR:H	4	0.2
(1,579)	1:38:A:PRO:HG3	1:41:A:GLN:HG2	7	0.2
(1,579)	1:38:A:PRO:HG3	1:41:A:GLN:HG3	7	0.2
(1,575)	1:41:A:GLN:HB2	1:40:A:GLN:HG2	5	0.2
(1,575)	1:41:A:GLN:HB2	1:40:A:GLN:HG3	5	0.2
(1,575)	1:41:A:GLN:HB3	1:40:A:GLN:HG2	5	0.2
(1,575)	1:41:A:GLN:HB3	1:40:A:GLN:HG3	5	0.2
(1,575)	1:41:A:GLN:HB2	1:40:A:GLN:HG2	8	0.2
(1,575)	1:41:A:GLN:HB2	1:40:A:GLN:HG3	8	0.2
(1,575)	1:41:A:GLN:HB3	1:40:A:GLN:HG2	8	0.2
(1,575)	1:41:A:GLN:HB3	1:40:A:GLN:HG3	8	0.2
(1,547)	1:1:A:MET:HB2	1:18:A:GLU:HG2	2	0.2
(1,547)	1:1:A:MET:HB2	1:18:A:GLU:HG3	2	0.2
(1,547)	1:1:A:MET:HB3	1:18:A:GLU:HG2	2	0.2
(1,547)	1:1:A:MET:HB3	1:18:A:GLU:HG3	2	0.2
(1,547)	1:1:A:MET:HB2	1:18:A:GLU:HG2	7	0.2
(1,547)	1:1:A:MET:HB2	1:18:A:GLU:HG3	7	0.2
(1,547)	1:1:A:MET:HB3	1:18:A:GLU:HG2	7	0.2
(1,547)	1:1:A:MET:HB3	1:18:A:GLU:HG3	7	0.2
(1,541)	1:12:A:THR:HA	1:11:A:LYS:HA	4	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,541)	1:12:A:THR:HA	1:11:A:LYS:HA	6	0.2
(1,541)	1:12:A:THR:HA	1:11:A:LYS:HA	9	0.2
(1,517)	1:7:A:THR:HB	1:7:A:THR:HA	9	0.2
(1,430)	1:15:A:LEU:HD21	1:16:A:GLU:HG3	2	0.2
(1,430)	1:15:A:LEU:HD22	1:16:A:GLU:HG3	2	0.2
(1,430)	1:15:A:LEU:HD23	1:16:A:GLU:HG3	2	0.2
(1,249)	1:36:A:ILE:HA	1:71:A:LEU:HD11	8	0.2
(1,249)	1:36:A:ILE:HA	1:71:A:LEU:HD12	8	0.2
(1,249)	1:36:A:ILE:HA	1:71:A:LEU:HD13	8	0.2
(1,212)	1:5:A:VAL:HA	1:67:A:LEU:HA	9	0.2
(1,125)	1:26:A:VAL:HG11	1:56:A:LEU:HD11	8	0.2
(1,125)	1:26:A:VAL:HG11	1:56:A:LEU:HD12	8	0.2
(1,125)	1:26:A:VAL:HG11	1:56:A:LEU:HD13	8	0.2
(1,125)	1:26:A:VAL:HG12	1:56:A:LEU:HD11	8	0.2
(1,125)	1:26:A:VAL:HG12	1:56:A:LEU:HD12	8	0.2
(1,125)	1:26:A:VAL:HG12	1:56:A:LEU:HD13	8	0.2
(1,125)	1:26:A:VAL:HG13	1:56:A:LEU:HD11	8	0.2
(1,125)	1:26:A:VAL:HG13	1:56:A:LEU:HD12	8	0.2
(1,125)	1:26:A:VAL:HG13	1:56:A:LEU:HD13	8	0.2
(1,79)	1:3:A:ILE:HG21	1:1:A:MET:HB2	4	0.2
(1,79)	1:3:A:ILE:HG21	1:1:A:MET:HB3	4	0.2
(1,79)	1:3:A:ILE:HG22	1:1:A:MET:HB2	4	0.2
(1,79)	1:3:A:ILE:HG22	1:1:A:MET:HB3	4	0.2
(1,79)	1:3:A:ILE:HG23	1:1:A:MET:HB2	4	0.2
(1,79)	1:3:A:ILE:HG23	1:1:A:MET:HB3	4	0.2
(1,56)	1:30:A:ILE:HD12	1:69:A:LEU:HB2	3	0.2
(1,1204)	1:64:A:GLU:H	1:63:A:LYS:HD2	6	0.19
(1,1204)	1:64:A:GLU:H	1:63:A:LYS:HD3	6	0.19
(1,1132)	1:16:A:GLU:HA	1:2:A:LYS:H	7	0.19
(1,1081)	1:32:A:ASP:HB2	1:34:A:GLU:H	2	0.19
(1,1081)	1:32:A:ASP:HB2	1:34:A:GLU:H	4	0.19
(1,1057)	1:72:A:ARG:HD2	1:72:A:ARG:H	7	0.19
(1,1035)	1:23:A:ILE:HD11	1:57:A:SER:H	8	0.19
(1,1035)	1:23:A:ILE:HD12	1:57:A:SER:H	8	0.19
(1,1035)	1:23:A:ILE:HD13	1:57:A:SER:H	8	0.19
(1,1016)	1:4:A:PHE:HB3	1:66:A:THR:H	2	0.19
(1,825)	1:50:A:LEU:HD11	1:51:A:GLU:H	5	0.19
(1,825)	1:50:A:LEU:HD12	1:51:A:GLU:H	5	0.19
(1,825)	1:50:A:LEU:HD13	1:51:A:GLU:H	5	0.19
(1,696)	1:18:A:GLU:HB3	1:18:A:GLU:H	4	0.19
(1,592)	1:44:A:ILE:HD11	1:49:A:LYS:HB2	7	0.19
(1,592)	1:44:A:ILE:HD11	1:49:A:LYS:HB3	7	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,592)	1:44:A:ILE:HD12	1:49:A:LYS:HB2	7	0.19
(1,592)	1:44:A:ILE:HD12	1:49:A:LYS:HB3	7	0.19
(1,592)	1:44:A:ILE:HD13	1:49:A:LYS:HB2	7	0.19
(1,592)	1:44:A:ILE:HD13	1:49:A:LYS:HB3	7	0.19
(1,590)	1:73:A:LEU:HG	1:73:A:LEU:HA	4	0.19
(1,583)	1:55:A:THR:HB	1:57:A:SER:HB2	8	0.19
(1,583)	1:55:A:THR:HB	1:57:A:SER:HB3	8	0.19
(1,575)	1:41:A:GLN:HB2	1:40:A:GLN:HG2	3	0.19
(1,575)	1:41:A:GLN:HB2	1:40:A:GLN:HG3	3	0.19
(1,575)	1:41:A:GLN:HB3	1:40:A:GLN:HG2	3	0.19
(1,575)	1:41:A:GLN:HB3	1:40:A:GLN:HG3	3	0.19
(1,570)	1:25:A:ASN:HB3	1:29:A:LYS:HG2	8	0.19
(1,570)	1:25:A:ASN:HB3	1:29:A:LYS:HG3	8	0.19
(1,567)	1:29:A:LYS:HB3	1:15:A:LEU:HD22	6	0.19
(1,559)	1:56:A:LEU:HD21	1:22:A:THR:HA	5	0.19
(1,559)	1:56:A:LEU:HD22	1:22:A:THR:HA	5	0.19
(1,559)	1:56:A:LEU:HD23	1:22:A:THR:HA	5	0.19
(1,547)	1:1:A:MET:HB2	1:18:A:GLU:HG2	10	0.19
(1,547)	1:1:A:MET:HB2	1:18:A:GLU:HG3	10	0.19
(1,547)	1:1:A:MET:HB3	1:18:A:GLU:HG2	10	0.19
(1,547)	1:1:A:MET:HB3	1:18:A:GLU:HG3	10	0.19
(1,541)	1:12:A:THR:HA	1:11:A:LYS:HA	5	0.19
(1,517)	1:7:A:THR:HB	1:7:A:THR:HA	2	0.19
(1,517)	1:7:A:THR:HB	1:7:A:THR:HA	5	0.19
(1,517)	1:7:A:THR:HB	1:7:A:THR:HA	7	0.19
(1,491)	1:15:A:LEU:HD11	1:16:A:GLU:HG3	8	0.19
(1,491)	1:15:A:LEU:HD12	1:16:A:GLU:HG3	8	0.19
(1,491)	1:15:A:LEU:HD13	1:16:A:GLU:HG3	8	0.19
(1,430)	1:15:A:LEU:HD21	1:16:A:GLU:HG3	6	0.19
(1,430)	1:15:A:LEU:HD22	1:16:A:GLU:HG3	6	0.19
(1,430)	1:15:A:LEU:HD23	1:16:A:GLU:HG3	6	0.19
(1,20)	1:65:A:SER:HA	1:65:A:SER:HB2	1	0.19
(1,20)	1:65:A:SER:HA	1:65:A:SER:HB2	5	0.19
(1,20)	1:65:A:SER:HA	1:65:A:SER:HB2	8	0.19
(1,1139)	1:27:A:LYS:HG2	1:28:A:ALA:H	8	0.18
(1,1139)	1:27:A:LYS:HG3	1:28:A:ALA:H	8	0.18
(1,1016)	1:4:A:PHE:HB3	1:66:A:THR:H	10	0.18
(1,962)	1:25:A:ASN:HB3	1:26:A:VAL:H	3	0.18
(1,905)	1:3:A:ILE:HD11	1:66:A:THR:H	1	0.18
(1,905)	1:3:A:ILE:HD12	1:66:A:THR:H	1	0.18
(1,905)	1:3:A:ILE:HD13	1:66:A:THR:H	1	0.18
(1,749)	1:31:A:GLN:HG2	1:31:A:GLN:H	2	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,596)	1:30:A:ILE:HA	1:30:A:ILE:HD11	5	0.18
(1,596)	1:30:A:ILE:HA	1:30:A:ILE:HD12	5	0.18
(1,596)	1:30:A:ILE:HA	1:30:A:ILE:HD13	5	0.18
(1,579)	1:38:A:PRO:HG3	1:41:A:GLN:HG2	1	0.18
(1,579)	1:38:A:PRO:HG3	1:41:A:GLN:HG3	1	0.18
(1,579)	1:38:A:PRO:HG3	1:41:A:GLN:HG2	3	0.18
(1,579)	1:38:A:PRO:HG3	1:41:A:GLN:HG3	3	0.18
(1,579)	1:38:A:PRO:HG3	1:41:A:GLN:HG2	5	0.18
(1,579)	1:38:A:PRO:HG3	1:41:A:GLN:HG3	5	0.18
(1,579)	1:38:A:PRO:HG3	1:41:A:GLN:HG2	8	0.18
(1,579)	1:38:A:PRO:HG3	1:41:A:GLN:HG3	8	0.18
(1,575)	1:41:A:GLN:HB2	1:40:A:GLN:HG2	9	0.18
(1,575)	1:41:A:GLN:HB2	1:40:A:GLN:HG3	9	0.18
(1,575)	1:41:A:GLN:HB3	1:40:A:GLN:HG2	9	0.18
(1,575)	1:41:A:GLN:HB3	1:40:A:GLN:HG3	9	0.18
(1,568)	1:29:A:LYS:HE2	1:29:A:LYS:HE3	1	0.18
(1,568)	1:29:A:LYS:HE2	1:29:A:LYS:HE3	2	0.18
(1,568)	1:29:A:LYS:HE2	1:29:A:LYS:HE3	3	0.18
(1,568)	1:29:A:LYS:HE2	1:29:A:LYS:HE3	4	0.18
(1,568)	1:29:A:LYS:HE2	1:29:A:LYS:HE3	5	0.18
(1,568)	1:29:A:LYS:HE2	1:29:A:LYS:HE3	6	0.18
(1,568)	1:29:A:LYS:HE2	1:29:A:LYS:HE3	7	0.18
(1,568)	1:29:A:LYS:HE2	1:29:A:LYS:HE3	8	0.18
(1,568)	1:29:A:LYS:HE2	1:29:A:LYS:HE3	9	0.18
(1,568)	1:29:A:LYS:HE2	1:29:A:LYS:HE3	10	0.18
(1,549)	1:56:A:LEU:HD21	1:19:A:PRO:HA	10	0.18
(1,549)	1:56:A:LEU:HD22	1:19:A:PRO:HA	10	0.18
(1,549)	1:56:A:LEU:HD23	1:19:A:PRO:HA	10	0.18
(1,536)	1:11:A:LYS:HD2	1:9:A:THR:HG21	7	0.18
(1,536)	1:11:A:LYS:HD2	1:9:A:THR:HG22	7	0.18
(1,536)	1:11:A:LYS:HD2	1:9:A:THR:HG23	7	0.18
(1,536)	1:11:A:LYS:HD3	1:9:A:THR:HG21	7	0.18
(1,536)	1:11:A:LYS:HD3	1:9:A:THR:HG22	7	0.18
(1,536)	1:11:A:LYS:HD3	1:9:A:THR:HG23	7	0.18
(1,511)	1:68:A:HIS:HA	1:68:A:HIS:HB3	3	0.18
(1,249)	1:36:A:ILE:HA	1:71:A:LEU:HD11	4	0.18
(1,249)	1:36:A:ILE:HA	1:71:A:LEU:HD12	4	0.18
(1,249)	1:36:A:ILE:HA	1:71:A:LEU:HD13	4	0.18
(1,144)	1:7:A:THR:HB	1:8:A:LEU:HB2	4	0.18
(1,144)	1:7:A:THR:HB	1:8:A:LEU:HB3	4	0.18
(1,85)	1:23:A:ILE:HG21	1:27:A:LYS:HE2	6	0.18
(1,85)	1:23:A:ILE:HG21	1:27:A:LYS:HE3	6	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,85)	1:23:A:ILE:HG22	1:27:A:LYS:HE2	6	0.18
(1,85)	1:23:A:ILE:HG22	1:27:A:LYS:HE3	6	0.18
(1,85)	1:23:A:ILE:HG23	1:27:A:LYS:HE2	6	0.18
(1,85)	1:23:A:ILE:HG23	1:27:A:LYS:HE3	6	0.18
(1,1277)	1:65:A:SER:HB2	1:65:A:SER:H	10	0.17
(1,1154)	1:15:A:LEU:HG	1:30:A:ILE:H	6	0.17
(1,1089)	1:64:A:GLU:HB2	1:4:A:PHE:H	4	0.17
(1,1058)	1:40:A:GLN:HG2	1:72:A:ARG:H	3	0.17
(1,1057)	1:72:A:ARG:HD3	1:72:A:ARG:H	8	0.17
(1,1016)	1:4:A:PHE:HB3	1:66:A:THR:H	6	0.17
(1,905)	1:3:A:ILE:HD11	1:66:A:THR:H	5	0.17
(1,905)	1:3:A:ILE:HD12	1:66:A:THR:H	5	0.17
(1,905)	1:3:A:ILE:HD13	1:66:A:THR:H	5	0.17
(1,788)	1:41:A:GLN:HG2	1:41:A:GLN:H	6	0.17
(1,661)	1:5:A:VAL:HB	1:5:A:VAL:H	3	0.17
(1,579)	1:38:A:PRO:HG3	1:41:A:GLN:HG2	2	0.17
(1,579)	1:38:A:PRO:HG3	1:41:A:GLN:HG3	2	0.17
(1,577)	1:71:A:LEU:HG	1:41:A:GLN:HA	2	0.17
(1,577)	1:71:A:LEU:HG	1:41:A:GLN:HA	3	0.17
(1,567)	1:29:A:LYS:HB3	1:15:A:LEU:HD23	2	0.17
(1,547)	1:1:A:MET:HB2	1:18:A:GLU:HG2	1	0.17
(1,547)	1:1:A:MET:HB2	1:18:A:GLU:HG3	1	0.17
(1,547)	1:1:A:MET:HB3	1:18:A:GLU:HG2	1	0.17
(1,547)	1:1:A:MET:HB3	1:18:A:GLU:HG3	1	0.17
(1,536)	1:11:A:LYS:HD2	1:9:A:THR:HG21	3	0.17
(1,536)	1:11:A:LYS:HD2	1:9:A:THR:HG22	3	0.17
(1,536)	1:11:A:LYS:HD2	1:9:A:THR:HG23	3	0.17
(1,536)	1:11:A:LYS:HD3	1:9:A:THR:HG21	3	0.17
(1,536)	1:11:A:LYS:HD3	1:9:A:THR:HG22	3	0.17
(1,536)	1:11:A:LYS:HD3	1:9:A:THR:HG23	3	0.17
(1,536)	1:11:A:LYS:HD2	1:9:A:THR:HG21	6	0.17
(1,536)	1:11:A:LYS:HD2	1:9:A:THR:HG22	6	0.17
(1,536)	1:11:A:LYS:HD2	1:9:A:THR:HG23	6	0.17
(1,536)	1:11:A:LYS:HD3	1:9:A:THR:HG21	6	0.17
(1,536)	1:11:A:LYS:HD3	1:9:A:THR:HG22	6	0.17
(1,536)	1:11:A:LYS:HD3	1:9:A:THR:HG23	6	0.17
(1,517)	1:7:A:THR:HB	1:7:A:THR:HA	1	0.17
(1,517)	1:7:A:THR:HB	1:7:A:THR:HA	4	0.17
(1,492)	1:28:A:ALA:HB1	1:38:A:PRO:HG2	3	0.17
(1,492)	1:28:A:ALA:HB2	1:38:A:PRO:HG2	3	0.17
(1,492)	1:28:A:ALA:HB3	1:38:A:PRO:HG2	3	0.17
(1,430)	1:15:A:LEU:HD21	1:16:A:GLU:HG3	4	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,430)	1:15:A:LEU:HD22	1:16:A:GLU:HG3	4	0.17
(1,430)	1:15:A:LEU:HD23	1:16:A:GLU:HG3	4	0.17
(1,322)	1:10:A:GLY:HA3	1:6:A:LYS:HE2	8	0.17
(1,322)	1:10:A:GLY:HA3	1:6:A:LYS:HE3	8	0.17
(1,276)	1:69:A:LEU:HA	1:69:A:LEU:HD11	4	0.17
(1,276)	1:69:A:LEU:HA	1:69:A:LEU:HD12	4	0.17
(1,276)	1:69:A:LEU:HA	1:69:A:LEU:HD13	4	0.17
(1,276)	1:69:A:LEU:HA	1:69:A:LEU:HD11	9	0.17
(1,276)	1:69:A:LEU:HA	1:69:A:LEU:HD12	9	0.17
(1,276)	1:69:A:LEU:HA	1:69:A:LEU:HD13	9	0.17
(1,261)	1:2:A:LYS:HD2	1:2:A:LYS:HA	8	0.17
(1,261)	1:2:A:LYS:HD3	1:2:A:LYS:HA	8	0.17
(1,249)	1:36:A:ILE:HA	1:71:A:LEU:HD11	6	0.17
(1,249)	1:36:A:ILE:HA	1:71:A:LEU:HD12	6	0.17
(1,249)	1:36:A:ILE:HA	1:71:A:LEU:HD13	6	0.17
(1,111)	1:2:A:LYS:HD3	1:14:A:THR:HG21	4	0.17
(1,111)	1:2:A:LYS:HD3	1:14:A:THR:HG22	4	0.17
(1,111)	1:2:A:LYS:HD3	1:14:A:THR:HG23	4	0.17
(1,111)	1:2:A:LYS:HD3	1:14:A:THR:HG21	6	0.17
(1,111)	1:2:A:LYS:HD3	1:14:A:THR:HG22	6	0.17
(1,111)	1:2:A:LYS:HD3	1:14:A:THR:HG23	6	0.17
(1,79)	1:3:A:ILE:HG21	1:1:A:MET:HB2	6	0.17
(1,79)	1:3:A:ILE:HG21	1:1:A:MET:HB3	6	0.17
(1,79)	1:3:A:ILE:HG22	1:1:A:MET:HB2	6	0.17
(1,79)	1:3:A:ILE:HG22	1:1:A:MET:HB3	6	0.17
(1,79)	1:3:A:ILE:HG23	1:1:A:MET:HB2	6	0.17
(1,79)	1:3:A:ILE:HG23	1:1:A:MET:HB3	6	0.17
(1,1270)	1:24:A:GLU:HG3	1:25:A:ASN:HD21	2	0.16
(1,1120)	1:33:A:GLU:HG2	1:15:A:LEU:H	8	0.16
(1,1089)	1:64:A:GLU:HB2	1:4:A:PHE:H	9	0.16
(1,1081)	1:32:A:ASP:HB2	1:34:A:GLU:H	5	0.16
(1,1035)	1:23:A:ILE:HD11	1:57:A:SER:H	7	0.16
(1,1035)	1:23:A:ILE:HD12	1:57:A:SER:H	7	0.16
(1,1035)	1:23:A:ILE:HD13	1:57:A:SER:H	7	0.16
(1,847)	1:56:A:LEU:HB3	1:56:A:LEU:H	8	0.16
(1,596)	1:30:A:ILE:HA	1:30:A:ILE:HD11	8	0.16
(1,596)	1:30:A:ILE:HA	1:30:A:ILE:HD12	8	0.16
(1,596)	1:30:A:ILE:HA	1:30:A:ILE:HD13	8	0.16
(1,590)	1:73:A:LEU:HG	1:73:A:LEU:HA	3	0.16
(1,579)	1:38:A:PRO:HG3	1:41:A:GLN:HG2	6	0.16
(1,579)	1:38:A:PRO:HG3	1:41:A:GLN:HG3	6	0.16
(1,579)	1:38:A:PRO:HG3	1:41:A:GLN:HG2	10	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,579)	1:38:A:PRO:HG3	1:41:A:GLN:HG3	10	0.16
(1,559)	1:56:A:LEU:HD21	1:22:A:THR:HA	10	0.16
(1,559)	1:56:A:LEU:HD22	1:22:A:THR:HA	10	0.16
(1,559)	1:56:A:LEU:HD23	1:22:A:THR:HA	10	0.16
(1,547)	1:1:A:MET:HB2	1:18:A:GLU:HG2	3	0.16
(1,547)	1:1:A:MET:HB2	1:18:A:GLU:HG3	3	0.16
(1,547)	1:1:A:MET:HB3	1:18:A:GLU:HG2	3	0.16
(1,547)	1:1:A:MET:HB3	1:18:A:GLU:HG3	3	0.16
(1,547)	1:1:A:MET:HB2	1:18:A:GLU:HG2	5	0.16
(1,547)	1:1:A:MET:HB2	1:18:A:GLU:HG3	5	0.16
(1,547)	1:1:A:MET:HB3	1:18:A:GLU:HG2	5	0.16
(1,547)	1:1:A:MET:HB3	1:18:A:GLU:HG3	5	0.16
(1,547)	1:1:A:MET:HB2	1:18:A:GLU:HG2	6	0.16
(1,547)	1:1:A:MET:HB2	1:18:A:GLU:HG3	6	0.16
(1,547)	1:1:A:MET:HB3	1:18:A:GLU:HG2	6	0.16
(1,547)	1:1:A:MET:HB3	1:18:A:GLU:HG3	6	0.16
(1,499)	1:25:A:ASN:HA	1:25:A:ASN:HB2	2	0.16
(1,499)	1:25:A:ASN:HA	1:25:A:ASN:HB2	10	0.16
(1,405)	1:59:A:TYR:HB2	1:56:A:LEU:HD21	3	0.16
(1,405)	1:59:A:TYR:HB2	1:56:A:LEU:HD22	3	0.16
(1,405)	1:59:A:TYR:HB2	1:56:A:LEU:HD23	3	0.16
(1,398)	1:56:A:LEU:HB2	1:19:A:PRO:HA	3	0.16
(1,398)	1:56:A:LEU:HB2	1:19:A:PRO:HA	9	0.16
(1,212)	1:5:A:VAL:HA	1:67:A:LEU:HA	1	0.16
(1,79)	1:3:A:ILE:HG21	1:1:A:MET:HB2	5	0.16
(1,79)	1:3:A:ILE:HG21	1:1:A:MET:HB3	5	0.16
(1,79)	1:3:A:ILE:HG22	1:1:A:MET:HB2	5	0.16
(1,79)	1:3:A:ILE:HG22	1:1:A:MET:HB3	5	0.16
(1,79)	1:3:A:ILE:HG23	1:1:A:MET:HB2	5	0.16
(1,79)	1:3:A:ILE:HG23	1:1:A:MET:HB3	5	0.16
(1,25)	1:50:A:LEU:HD11	1:23:A:ILE:HG12	6	0.16
(1,25)	1:50:A:LEU:HD12	1:23:A:ILE:HG12	6	0.16
(1,25)	1:50:A:LEU:HD13	1:23:A:ILE:HG12	6	0.16
(1,1270)	1:24:A:GLU:HG3	1:25:A:ASN:HD21	8	0.15
(1,1132)	1:16:A:GLU:HA	1:2:A:LYS:H	8	0.15
(1,1081)	1:32:A:ASP:HB2	1:34:A:GLU:H	7	0.15
(1,1035)	1:23:A:ILE:HD11	1:57:A:SER:H	2	0.15
(1,1035)	1:23:A:ILE:HD12	1:57:A:SER:H	2	0.15
(1,1035)	1:23:A:ILE:HD13	1:57:A:SER:H	2	0.15
(1,1016)	1:4:A:PHE:HB3	1:66:A:THR:H	7	0.15
(1,1001)	1:56:A:LEU:HA	1:57:A:SER:H	10	0.15
(1,899)	1:64:A:GLU:HG2	1:65:A:SER:H	2	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,899)	1:64:A:GLU:HG3	1:65:A:SER:H	2	0.15
(1,847)	1:56:A:LEU:HB3	1:56:A:LEU:H	2	0.15
(1,847)	1:56:A:LEU:HB3	1:56:A:LEU:H	5	0.15
(1,755)	1:28:A:ALA:HB1	1:32:A:ASP:H	10	0.15
(1,755)	1:28:A:ALA:HB2	1:32:A:ASP:H	10	0.15
(1,755)	1:28:A:ALA:HB3	1:32:A:ASP:H	10	0.15
(1,596)	1:30:A:ILE:HA	1:30:A:ILE:HD11	7	0.15
(1,596)	1:30:A:ILE:HA	1:30:A:ILE:HD12	7	0.15
(1,596)	1:30:A:ILE:HA	1:30:A:ILE:HD13	7	0.15
(1,591)	1:73:A:LEU:HB2	1:72:A:ARG:HD2	2	0.15
(1,591)	1:73:A:LEU:HB2	1:72:A:ARG:HD3	2	0.15
(1,591)	1:73:A:LEU:HB3	1:72:A:ARG:HD2	2	0.15
(1,591)	1:73:A:LEU:HB3	1:72:A:ARG:HD3	2	0.15
(1,579)	1:38:A:PRO:HG3	1:41:A:GLN:HG2	9	0.15
(1,579)	1:38:A:PRO:HG3	1:41:A:GLN:HG3	9	0.15
(1,577)	1:71:A:LEU:HG	1:41:A:GLN:HA	1	0.15
(1,577)	1:71:A:LEU:HG	1:41:A:GLN:HA	7	0.15
(1,570)	1:25:A:ASN:HB3	1:29:A:LYS:HG2	6	0.15
(1,570)	1:25:A:ASN:HB3	1:29:A:LYS:HG3	6	0.15
(1,536)	1:11:A:LYS:HD2	1:9:A:THR:HG21	5	0.15
(1,536)	1:11:A:LYS:HD2	1:9:A:THR:HG22	5	0.15
(1,536)	1:11:A:LYS:HD2	1:9:A:THR:HG23	5	0.15
(1,536)	1:11:A:LYS:HD3	1:9:A:THR:HG21	5	0.15
(1,536)	1:11:A:LYS:HD3	1:9:A:THR:HG22	5	0.15
(1,536)	1:11:A:LYS:HD3	1:9:A:THR:HG23	5	0.15
(1,517)	1:7:A:THR:HB	1:7:A:THR:HA	3	0.15
(1,517)	1:7:A:THR:HB	1:7:A:THR:HA	6	0.15
(1,499)	1:25:A:ASN:HA	1:25:A:ASN:HB2	9	0.15
(1,405)	1:59:A:TYR:HB2	1:56:A:LEU:HD21	1	0.15
(1,405)	1:59:A:TYR:HB2	1:56:A:LEU:HD22	1	0.15
(1,405)	1:59:A:TYR:HB2	1:56:A:LEU:HD23	1	0.15
(1,276)	1:69:A:LEU:HA	1:69:A:LEU:HD11	7	0.15
(1,276)	1:69:A:LEU:HA	1:69:A:LEU:HD12	7	0.15
(1,276)	1:69:A:LEU:HA	1:69:A:LEU:HD13	7	0.15
(1,212)	1:5:A:VAL:HA	1:68:A:HIS:HA	2	0.15
(1,85)	1:23:A:ILE:HG21	1:27:A:LYS:HE2	7	0.15
(1,85)	1:23:A:ILE:HG21	1:27:A:LYS:HE3	7	0.15
(1,85)	1:23:A:ILE:HG22	1:27:A:LYS:HE2	7	0.15
(1,85)	1:23:A:ILE:HG22	1:27:A:LYS:HE3	7	0.15
(1,85)	1:23:A:ILE:HG23	1:27:A:LYS:HE2	7	0.15
(1,85)	1:23:A:ILE:HG23	1:27:A:LYS:HE3	7	0.15
(1,82)	1:50:A:LEU:HB2	1:23:A:ILE:HG21	4	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,82)	1:50:A:LEU:HB2	1:23:A:ILE:HG22	4	0.15
(1,82)	1:50:A:LEU:HB2	1:23:A:ILE:HG23	4	0.15
(1,79)	1:3:A:ILE:HG21	1:1:A:MET:HB2	3	0.15
(1,79)	1:3:A:ILE:HG21	1:1:A:MET:HB3	3	0.15
(1,79)	1:3:A:ILE:HG22	1:1:A:MET:HB2	3	0.15
(1,79)	1:3:A:ILE:HG22	1:1:A:MET:HB3	3	0.15
(1,79)	1:3:A:ILE:HG23	1:1:A:MET:HB2	3	0.15
(1,79)	1:3:A:ILE:HG23	1:1:A:MET:HB3	3	0.15
(1,1136)	1:50:A:LEU:HA	1:49:A:LYS:H	8	0.14
(1,1134)	1:72:A:ARG:HB2	1:73:A:LEU:H	2	0.14
(1,1106)	1:50:A:LEU:HD11	1:49:A:LYS:H	9	0.14
(1,1106)	1:50:A:LEU:HD12	1:49:A:LYS:H	9	0.14
(1,1106)	1:50:A:LEU:HD13	1:49:A:LYS:H	9	0.14
(1,1075)	1:56:A:LEU:HB3	1:20:A:SER:H	6	0.14
(1,1068)	1:43:A:LEU:H	1:51:A:GLU:H	3	0.14
(1,1035)	1:23:A:ILE:HD11	1:57:A:SER:H	5	0.14
(1,1035)	1:23:A:ILE:HD12	1:57:A:SER:H	5	0.14
(1,1035)	1:23:A:ILE:HD13	1:57:A:SER:H	5	0.14
(1,1016)	1:4:A:PHE:HB3	1:66:A:THR:H	9	0.14
(1,1001)	1:56:A:LEU:HA	1:57:A:SER:H	7	0.14
(1,899)	1:64:A:GLU:HG2	1:65:A:SER:H	4	0.14
(1,899)	1:64:A:GLU:HG3	1:65:A:SER:H	4	0.14
(1,704)	1:18:A:GLU:HB3	1:21:A:ASP:H	4	0.14
(1,596)	1:30:A:ILE:HA	1:30:A:ILE:HD11	3	0.14
(1,596)	1:30:A:ILE:HA	1:30:A:ILE:HD12	3	0.14
(1,596)	1:30:A:ILE:HA	1:30:A:ILE:HD13	3	0.14
(1,590)	1:73:A:LEU:HG	1:73:A:LEU:HA	7	0.14
(1,590)	1:73:A:LEU:HG	1:73:A:LEU:HA	8	0.14
(1,590)	1:73:A:LEU:HG	1:73:A:LEU:HA	10	0.14
(1,577)	1:71:A:LEU:HG	1:41:A:GLN:HA	10	0.14
(1,575)	1:41:A:GLN:HB2	1:40:A:GLN:HG2	4	0.14
(1,575)	1:41:A:GLN:HB2	1:40:A:GLN:HG3	4	0.14
(1,575)	1:41:A:GLN:HB3	1:40:A:GLN:HG2	4	0.14
(1,575)	1:41:A:GLN:HB3	1:40:A:GLN:HG3	4	0.14
(1,575)	1:41:A:GLN:HB2	1:40:A:GLN:HG2	6	0.14
(1,575)	1:41:A:GLN:HB2	1:40:A:GLN:HG3	6	0.14
(1,575)	1:41:A:GLN:HB3	1:40:A:GLN:HG2	6	0.14
(1,575)	1:41:A:GLN:HB3	1:40:A:GLN:HG3	6	0.14
(1,567)	1:29:A:LYS:HB3	1:15:A:LEU:HD22	9	0.14
(1,560)	1:55:A:THR:HB	1:22:A:THR:HA	1	0.14
(1,560)	1:55:A:THR:HB	1:22:A:THR:HA	4	0.14
(1,517)	1:7:A:THR:HB	1:7:A:THR:HA	10	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,499)	1:25:A:ASN:HA	1:25:A:ASN:HB2	6	0.14
(1,486)	1:69:A:LEU:HA	1:69:A:LEU:HD11	4	0.14
(1,486)	1:69:A:LEU:HA	1:69:A:LEU:HD12	4	0.14
(1,486)	1:69:A:LEU:HA	1:69:A:LEU:HD13	4	0.14
(1,486)	1:69:A:LEU:HA	1:69:A:LEU:HD11	9	0.14
(1,486)	1:69:A:LEU:HA	1:69:A:LEU:HD12	9	0.14
(1,486)	1:69:A:LEU:HA	1:69:A:LEU:HD13	9	0.14
(1,405)	1:59:A:TYR:HB2	1:56:A:LEU:HD21	8	0.14
(1,405)	1:59:A:TYR:HB2	1:56:A:LEU:HD22	8	0.14
(1,405)	1:59:A:TYR:HB2	1:56:A:LEU:HD23	8	0.14
(1,398)	1:56:A:LEU:HB2	1:19:A:PRO:HA	1	0.14
(1,398)	1:56:A:LEU:HB2	1:19:A:PRO:HA	5	0.14
(1,398)	1:56:A:LEU:HB2	1:19:A:PRO:HA	10	0.14
(1,249)	1:36:A:ILE:HA	1:71:A:LEU:HD11	1	0.14
(1,249)	1:36:A:ILE:HA	1:71:A:LEU:HD12	1	0.14
(1,249)	1:36:A:ILE:HA	1:71:A:LEU:HD13	1	0.14
(1,249)	1:36:A:ILE:HA	1:71:A:LEU:HD11	5	0.14
(1,249)	1:36:A:ILE:HA	1:71:A:LEU:HD12	5	0.14
(1,249)	1:36:A:ILE:HA	1:71:A:LEU:HD13	5	0.14
(1,212)	1:5:A:VAL:HA	1:68:A:HIS:HA	6	0.14
(1,212)	1:5:A:VAL:HA	1:68:A:HIS:HA	8	0.14
(1,204)	1:57:A:SER:HA	1:60:A:SER:HA	6	0.14
(1,121)	1:4:A:PHE:HB2	1:12:A:THR:HG21	10	0.14
(1,121)	1:4:A:PHE:HB2	1:12:A:THR:HG22	10	0.14
(1,121)	1:4:A:PHE:HB2	1:12:A:THR:HG23	10	0.14
(1,82)	1:50:A:LEU:HB2	1:23:A:ILE:HG21	7	0.14
(1,82)	1:50:A:LEU:HB2	1:23:A:ILE:HG22	7	0.14
(1,82)	1:50:A:LEU:HB2	1:23:A:ILE:HG23	7	0.14
(1,79)	1:3:A:ILE:HG21	1:1:A:MET:HB2	1	0.14
(1,79)	1:3:A:ILE:HG21	1:1:A:MET:HB3	1	0.14
(1,79)	1:3:A:ILE:HG22	1:1:A:MET:HB2	1	0.14
(1,79)	1:3:A:ILE:HG22	1:1:A:MET:HB3	1	0.14
(1,79)	1:3:A:ILE:HG23	1:1:A:MET:HB2	1	0.14
(1,79)	1:3:A:ILE:HG23	1:1:A:MET:HB3	1	0.14
(1,79)	1:3:A:ILE:HG21	1:1:A:MET:HB2	2	0.14
(1,79)	1:3:A:ILE:HG21	1:1:A:MET:HB3	2	0.14
(1,79)	1:3:A:ILE:HG22	1:1:A:MET:HB2	2	0.14
(1,79)	1:3:A:ILE:HG22	1:1:A:MET:HB3	2	0.14
(1,79)	1:3:A:ILE:HG23	1:1:A:MET:HB2	2	0.14
(1,79)	1:3:A:ILE:HG23	1:1:A:MET:HB3	2	0.14
(1,79)	1:3:A:ILE:HG21	1:1:A:MET:HB2	9	0.14
(1,79)	1:3:A:ILE:HG21	1:1:A:MET:HB3	9	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,79)	1:3:A:ILE:HG22	1:1:A:MET:HB2	9	0.14
(1,79)	1:3:A:ILE:HG22	1:1:A:MET:HB3	9	0.14
(1,79)	1:3:A:ILE:HG23	1:1:A:MET:HB2	9	0.14
(1,79)	1:3:A:ILE:HG23	1:1:A:MET:HB3	9	0.14
(1,79)	1:3:A:ILE:HG21	1:1:A:MET:HB2	10	0.14
(1,79)	1:3:A:ILE:HG21	1:1:A:MET:HB3	10	0.14
(1,79)	1:3:A:ILE:HG22	1:1:A:MET:HB2	10	0.14
(1,79)	1:3:A:ILE:HG22	1:1:A:MET:HB3	10	0.14
(1,79)	1:3:A:ILE:HG23	1:1:A:MET:HB2	10	0.14
(1,79)	1:3:A:ILE:HG23	1:1:A:MET:HB3	10	0.14
(1,1280)	1:15:A:LEU:HB2	1:17:A:VAL:H	5	0.13
(1,1204)	1:64:A:GLU:H	1:63:A:LYS:HD2	4	0.13
(1,1204)	1:64:A:GLU:H	1:63:A:LYS:HD3	4	0.13
(1,1164)	1:31:A:GLN:HB2	1:29:A:LYS:H	4	0.13
(1,1164)	1:31:A:GLN:HB3	1:29:A:LYS:H	4	0.13
(1,1151)	1:13:A:ILE:HG13	1:5:A:VAL:H	6	0.13
(1,1136)	1:50:A:LEU:HA	1:49:A:LYS:H	1	0.13
(1,1136)	1:47:A:GLY:HA2	1:49:A:LYS:H	7	0.13
(1,1132)	1:16:A:GLU:HA	1:2:A:LYS:H	1	0.13
(1,1114)	1:5:A:VAL:HG11	1:13:A:ILE:H	5	0.13
(1,1114)	1:5:A:VAL:HG12	1:13:A:ILE:H	5	0.13
(1,1114)	1:5:A:VAL:HG13	1:13:A:ILE:H	5	0.13
(1,1095)	1:23:A:ILE:HG13	1:52:A:ASP:H	2	0.13
(1,1081)	1:32:A:ASP:HB2	1:34:A:GLU:H	3	0.13
(1,1001)	1:56:A:LEU:HA	1:57:A:SER:H	2	0.13
(1,1001)	1:56:A:LEU:HA	1:57:A:SER:H	3	0.13
(1,1001)	1:56:A:LEU:HA	1:57:A:SER:H	4	0.13
(1,1001)	1:56:A:LEU:HA	1:57:A:SER:H	9	0.13
(1,962)	1:25:A:ASN:HB3	1:26:A:VAL:H	7	0.13
(1,937)	1:4:A:PHE:HB2	1:6:A:LYS:H	6	0.13
(1,905)	1:3:A:ILE:HD11	1:66:A:THR:H	3	0.13
(1,905)	1:3:A:ILE:HD12	1:66:A:THR:H	3	0.13
(1,905)	1:3:A:ILE:HD13	1:66:A:THR:H	3	0.13
(1,899)	1:64:A:GLU:HG2	1:65:A:SER:H	3	0.13
(1,899)	1:64:A:GLU:HG3	1:65:A:SER:H	3	0.13
(1,899)	1:64:A:GLU:HG2	1:65:A:SER:H	5	0.13
(1,899)	1:64:A:GLU:HG3	1:65:A:SER:H	5	0.13
(1,847)	1:56:A:LEU:HB3	1:56:A:LEU:H	1	0.13
(1,847)	1:56:A:LEU:HB3	1:56:A:LEU:H	6	0.13
(1,847)	1:56:A:LEU:HB3	1:56:A:LEU:H	9	0.13
(1,847)	1:56:A:LEU:HB3	1:56:A:LEU:H	10	0.13
(1,845)	1:21:A:ASP:HB2	1:56:A:LEU:H	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,844)	1:21:A:ASP:HB3	1:56:A:LEU:H	3	0.13
(1,825)	1:50:A:LEU:HD11	1:51:A:GLU:H	3	0.13
(1,825)	1:50:A:LEU:HD12	1:51:A:GLU:H	3	0.13
(1,825)	1:50:A:LEU:HD13	1:51:A:GLU:H	3	0.13
(1,688)	1:15:A:LEU:HD11	1:15:A:LEU:H	4	0.13
(1,688)	1:15:A:LEU:HD12	1:15:A:LEU:H	4	0.13
(1,688)	1:15:A:LEU:HD13	1:15:A:LEU:H	4	0.13
(1,688)	1:15:A:LEU:HD21	1:15:A:LEU:H	4	0.13
(1,688)	1:15:A:LEU:HD22	1:15:A:LEU:H	4	0.13
(1,688)	1:15:A:LEU:HD23	1:15:A:LEU:H	4	0.13
(1,596)	1:30:A:ILE:HA	1:30:A:ILE:HD11	1	0.13
(1,596)	1:30:A:ILE:HA	1:30:A:ILE:HD12	1	0.13
(1,596)	1:30:A:ILE:HA	1:30:A:ILE:HD13	1	0.13
(1,596)	1:30:A:ILE:HA	1:30:A:ILE:HD11	2	0.13
(1,596)	1:30:A:ILE:HA	1:30:A:ILE:HD12	2	0.13
(1,596)	1:30:A:ILE:HA	1:30:A:ILE:HD13	2	0.13
(1,596)	1:30:A:ILE:HA	1:30:A:ILE:HD11	4	0.13
(1,596)	1:30:A:ILE:HA	1:30:A:ILE:HD12	4	0.13
(1,596)	1:30:A:ILE:HA	1:30:A:ILE:HD13	4	0.13
(1,596)	1:30:A:ILE:HA	1:30:A:ILE:HD11	6	0.13
(1,596)	1:30:A:ILE:HA	1:30:A:ILE:HD12	6	0.13
(1,596)	1:30:A:ILE:HA	1:30:A:ILE:HD13	6	0.13
(1,596)	1:30:A:ILE:HA	1:30:A:ILE:HD11	10	0.13
(1,596)	1:30:A:ILE:HA	1:30:A:ILE:HD12	10	0.13
(1,596)	1:30:A:ILE:HA	1:30:A:ILE:HD13	10	0.13
(1,592)	1:44:A:ILE:HD11	1:49:A:LYS:HB2	1	0.13
(1,592)	1:44:A:ILE:HD11	1:49:A:LYS:HB3	1	0.13
(1,592)	1:44:A:ILE:HD12	1:49:A:LYS:HB2	1	0.13
(1,592)	1:44:A:ILE:HD12	1:49:A:LYS:HB3	1	0.13
(1,592)	1:44:A:ILE:HD13	1:49:A:LYS:HB2	1	0.13
(1,592)	1:44:A:ILE:HD13	1:49:A:LYS:HB3	1	0.13
(1,590)	1:73:A:LEU:HG	1:73:A:LEU:HA	2	0.13
(1,590)	1:73:A:LEU:HG	1:73:A:LEU:HA	5	0.13
(1,579)	1:38:A:PRO:HG3	1:41:A:GLN:HG2	4	0.13
(1,579)	1:38:A:PRO:HG3	1:41:A:GLN:HG3	4	0.13
(1,577)	1:71:A:LEU:HG	1:41:A:GLN:HA	8	0.13
(1,570)	1:25:A:ASN:HB3	1:29:A:LYS:HG2	9	0.13
(1,570)	1:25:A:ASN:HB3	1:29:A:LYS:HG3	9	0.13
(1,560)	1:55:A:THR:HB	1:22:A:THR:HA	3	0.13
(1,536)	1:11:A:LYS:HD2	1:9:A:THR:HG21	1	0.13
(1,536)	1:11:A:LYS:HD2	1:9:A:THR:HG22	1	0.13
(1,536)	1:11:A:LYS:HD2	1:9:A:THR:HG23	1	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,536)	1:11:A:LYS:HD3	1:9:A:THR:HG21	1	0.13
(1,536)	1:11:A:LYS:HD3	1:9:A:THR:HG22	1	0.13
(1,536)	1:11:A:LYS:HD3	1:9:A:THR:HG23	1	0.13
(1,504)	1:58:A:ASP:HB2	1:58:A:ASP:HA	3	0.13
(1,504)	1:58:A:ASP:HB2	1:58:A:ASP:HA	6	0.13
(1,504)	1:58:A:ASP:HB2	1:58:A:ASP:HA	9	0.13
(1,504)	1:58:A:ASP:HB2	1:58:A:ASP:HA	10	0.13
(1,499)	1:25:A:ASN:HA	1:25:A:ASN:HB2	8	0.13
(1,405)	1:59:A:TYR:HB2	1:56:A:LEU:HD21	9	0.13
(1,405)	1:59:A:TYR:HB2	1:56:A:LEU:HD22	9	0.13
(1,405)	1:59:A:TYR:HB2	1:56:A:LEU:HD23	9	0.13
(1,398)	1:56:A:LEU:HB2	1:19:A:PRO:HA	4	0.13
(1,398)	1:56:A:LEU:HB2	1:19:A:PRO:HA	8	0.13
(1,353)	1:27:A:LYS:HB3	1:27:A:LYS:HE2	8	0.13
(1,353)	1:27:A:LYS:HB3	1:27:A:LYS:HE3	8	0.13
(1,319)	1:22:A:THR:HG21	1:53:A:GLY:HA2	8	0.13
(1,319)	1:22:A:THR:HG21	1:53:A:GLY:HA3	8	0.13
(1,319)	1:22:A:THR:HG22	1:53:A:GLY:HA2	8	0.13
(1,319)	1:22:A:THR:HG22	1:53:A:GLY:HA3	8	0.13
(1,319)	1:22:A:THR:HG23	1:53:A:GLY:HA2	8	0.13
(1,319)	1:22:A:THR:HG23	1:53:A:GLY:HA3	8	0.13
(1,204)	1:57:A:SER:HA	1:60:A:SER:HA	8	0.13
(1,121)	1:4:A:PHE:HB2	1:12:A:THR:HG21	2	0.13
(1,121)	1:4:A:PHE:HB2	1:12:A:THR:HG22	2	0.13
(1,121)	1:4:A:PHE:HB2	1:12:A:THR:HG23	2	0.13
(1,54)	1:61:A:ILE:HD11	1:59:A:TYR:H	2	0.13
(1,54)	1:61:A:ILE:HD12	1:59:A:TYR:H	2	0.13
(1,54)	1:61:A:ILE:HD13	1:59:A:TYR:H	2	0.13
(1,1204)	1:64:A:GLU:H	1:63:A:LYS:HD2	2	0.12
(1,1204)	1:64:A:GLU:H	1:63:A:LYS:HD3	2	0.12
(1,1204)	1:64:A:GLU:H	1:63:A:LYS:HD2	9	0.12
(1,1204)	1:64:A:GLU:H	1:63:A:LYS:HD3	9	0.12
(1,1191)	1:35:A:GLY:H	1:33:A:GLU:H	6	0.12
(1,1151)	1:13:A:ILE:HG13	1:5:A:VAL:H	1	0.12
(1,1151)	1:13:A:ILE:HG13	1:5:A:VAL:H	2	0.12
(1,1094)	1:27:A:LYS:HG2	1:52:A:ASP:H	10	0.12
(1,1094)	1:27:A:LYS:HG3	1:52:A:ASP:H	10	0.12
(1,1089)	1:64:A:GLU:HB2	1:4:A:PHE:H	10	0.12
(1,1068)	1:43:A:LEU:H	1:51:A:GLU:H	7	0.12
(1,1058)	1:40:A:GLN:HG2	1:72:A:ARG:H	8	0.12
(1,1001)	1:56:A:LEU:HA	1:57:A:SER:H	1	0.12
(1,1001)	1:56:A:LEU:HA	1:57:A:SER:H	5	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,937)	1:4:A:PHE:HB2	1:6:A:LYS:H	7	0.12
(1,899)	1:64:A:GLU:HG2	1:65:A:SER:H	6	0.12
(1,899)	1:64:A:GLU:HG3	1:65:A:SER:H	6	0.12
(1,899)	1:64:A:GLU:HG2	1:65:A:SER:H	8	0.12
(1,899)	1:64:A:GLU:HG3	1:65:A:SER:H	8	0.12
(1,899)	1:64:A:GLU:HG2	1:65:A:SER:H	9	0.12
(1,899)	1:64:A:GLU:HG3	1:65:A:SER:H	9	0.12
(1,847)	1:56:A:LEU:HB3	1:56:A:LEU:H	3	0.12
(1,847)	1:56:A:LEU:HB3	1:56:A:LEU:H	4	0.12
(1,825)	1:50:A:LEU:HD11	1:51:A:GLU:H	1	0.12
(1,825)	1:50:A:LEU:HD12	1:51:A:GLU:H	1	0.12
(1,825)	1:50:A:LEU:HD13	1:51:A:GLU:H	1	0.12
(1,787)	1:72:A:ARG:HD2	1:41:A:GLN:H	10	0.12
(1,787)	1:72:A:ARG:HD3	1:41:A:GLN:H	10	0.12
(1,719)	1:28:A:ALA:HB1	1:25:A:ASN:H	5	0.12
(1,719)	1:28:A:ALA:HB2	1:25:A:ASN:H	5	0.12
(1,719)	1:28:A:ALA:HB3	1:25:A:ASN:H	5	0.12
(1,688)	1:15:A:LEU:HD11	1:15:A:LEU:H	8	0.12
(1,688)	1:15:A:LEU:HD12	1:15:A:LEU:H	8	0.12
(1,688)	1:15:A:LEU:HD13	1:15:A:LEU:H	8	0.12
(1,688)	1:15:A:LEU:HD21	1:15:A:LEU:H	8	0.12
(1,688)	1:15:A:LEU:HD22	1:15:A:LEU:H	8	0.12
(1,688)	1:15:A:LEU:HD23	1:15:A:LEU:H	8	0.12
(1,602)	1:23:A:ILE:H	1:26:A:VAL:H	1	0.12
(1,596)	1:30:A:ILE:HA	1:30:A:ILE:HD11	9	0.12
(1,596)	1:30:A:ILE:HA	1:30:A:ILE:HD12	9	0.12
(1,596)	1:30:A:ILE:HA	1:30:A:ILE:HD13	9	0.12
(1,591)	1:73:A:LEU:HB2	1:72:A:ARG:HD2	3	0.12
(1,591)	1:73:A:LEU:HB2	1:72:A:ARG:HD3	3	0.12
(1,591)	1:73:A:LEU:HB3	1:72:A:ARG:HD2	3	0.12
(1,591)	1:73:A:LEU:HB3	1:72:A:ARG:HD3	3	0.12
(1,591)	1:73:A:LEU:HB2	1:72:A:ARG:HD2	4	0.12
(1,591)	1:73:A:LEU:HB2	1:72:A:ARG:HD3	4	0.12
(1,591)	1:73:A:LEU:HB3	1:72:A:ARG:HD2	4	0.12
(1,591)	1:73:A:LEU:HB3	1:72:A:ARG:HD3	4	0.12
(1,590)	1:73:A:LEU:HG	1:73:A:LEU:HA	6	0.12
(1,575)	1:41:A:GLN:HB2	1:40:A:GLN:HG2	7	0.12
(1,575)	1:41:A:GLN:HB2	1:40:A:GLN:HG3	7	0.12
(1,575)	1:41:A:GLN:HB3	1:40:A:GLN:HG2	7	0.12
(1,575)	1:41:A:GLN:HB3	1:40:A:GLN:HG3	7	0.12
(1,570)	1:25:A:ASN:HB3	1:29:A:LYS:HG2	10	0.12
(1,570)	1:25:A:ASN:HB3	1:29:A:LYS:HG3	10	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,561)	1:69:A:LEU:HB2	1:7:A:THR:HB	6	0.12
(1,560)	1:55:A:THR:HB	1:22:A:THR:HA	10	0.12
(1,559)	1:56:A:LEU:HD21	1:22:A:THR:HA	2	0.12
(1,559)	1:56:A:LEU:HD22	1:22:A:THR:HA	2	0.12
(1,559)	1:56:A:LEU:HD23	1:22:A:THR:HA	2	0.12
(1,538)	1:7:A:THR:HB	1:9:A:THR:HG21	8	0.12
(1,538)	1:7:A:THR:HB	1:9:A:THR:HG22	8	0.12
(1,538)	1:7:A:THR:HB	1:9:A:THR:HG23	8	0.12
(1,504)	1:58:A:ASP:HB2	1:58:A:ASP:HA	1	0.12
(1,504)	1:58:A:ASP:HB2	1:58:A:ASP:HA	4	0.12
(1,504)	1:58:A:ASP:HB2	1:58:A:ASP:HA	5	0.12
(1,504)	1:58:A:ASP:HB2	1:58:A:ASP:HA	7	0.12
(1,504)	1:58:A:ASP:HB2	1:58:A:ASP:HA	8	0.12
(1,492)	1:28:A:ALA:HB1	1:38:A:PRO:HG2	6	0.12
(1,492)	1:28:A:ALA:HB2	1:38:A:PRO:HG2	6	0.12
(1,492)	1:28:A:ALA:HB3	1:38:A:PRO:HG2	6	0.12
(1,486)	1:69:A:LEU:HA	1:69:A:LEU:HD11	7	0.12
(1,486)	1:69:A:LEU:HA	1:69:A:LEU:HD12	7	0.12
(1,486)	1:69:A:LEU:HA	1:69:A:LEU:HD13	7	0.12
(1,321)	1:44:A:ILE:HG21	1:47:A:GLY:HA3	4	0.12
(1,321)	1:44:A:ILE:HG22	1:47:A:GLY:HA3	4	0.12
(1,321)	1:44:A:ILE:HG23	1:47:A:GLY:HA3	4	0.12
(1,319)	1:22:A:THR:HG21	1:53:A:GLY:HA2	10	0.12
(1,319)	1:22:A:THR:HG21	1:53:A:GLY:HA3	10	0.12
(1,319)	1:22:A:THR:HG22	1:53:A:GLY:HA2	10	0.12
(1,319)	1:22:A:THR:HG22	1:53:A:GLY:HA3	10	0.12
(1,319)	1:22:A:THR:HG23	1:53:A:GLY:HA2	10	0.12
(1,319)	1:22:A:THR:HG23	1:53:A:GLY:HA3	10	0.12
(1,268)	1:16:A:GLU:HA	1:16:A:GLU:HB2	5	0.12
(1,268)	1:16:A:GLU:HA	1:16:A:GLU:HB2	6	0.12
(1,249)	1:36:A:ILE:HA	1:71:A:LEU:HD11	7	0.12
(1,249)	1:36:A:ILE:HA	1:71:A:LEU:HD12	7	0.12
(1,249)	1:36:A:ILE:HA	1:71:A:LEU:HD13	7	0.12
(1,249)	1:36:A:ILE:HA	1:71:A:LEU:HD11	9	0.12
(1,249)	1:36:A:ILE:HA	1:71:A:LEU:HD12	9	0.12
(1,249)	1:36:A:ILE:HA	1:71:A:LEU:HD13	9	0.12
(1,207)	1:27:A:LYS:HE3	1:24:A:GLU:HA	3	0.12
(1,121)	1:4:A:PHE:HB2	1:12:A:THR:HG21	6	0.12
(1,121)	1:4:A:PHE:HB2	1:12:A:THR:HG22	6	0.12
(1,121)	1:4:A:PHE:HB2	1:12:A:THR:HG23	6	0.12
(1,54)	1:61:A:ILE:HD11	1:59:A:TYR:H	5	0.12
(1,54)	1:61:A:ILE:HD12	1:59:A:TYR:H	5	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,54)	1:61:A:ILE:HD13	1:59:A:TYR:H	5	0.12
(1,54)	1:61:A:ILE:HD11	1:59:A:TYR:H	6	0.12
(1,54)	1:61:A:ILE:HD12	1:59:A:TYR:H	6	0.12
(1,54)	1:61:A:ILE:HD13	1:59:A:TYR:H	6	0.12
(1,54)	1:61:A:ILE:HD11	1:59:A:TYR:H	8	0.12
(1,54)	1:61:A:ILE:HD12	1:59:A:TYR:H	8	0.12
(1,54)	1:61:A:ILE:HD13	1:59:A:TYR:H	8	0.12
(1,54)	1:61:A:ILE:HD11	1:59:A:TYR:H	10	0.12
(1,54)	1:61:A:ILE:HD12	1:59:A:TYR:H	10	0.12
(1,54)	1:61:A:ILE:HD13	1:59:A:TYR:H	10	0.12
(1,25)	1:50:A:LEU:HD11	1:23:A:ILE:HG12	7	0.12
(1,25)	1:50:A:LEU:HD12	1:23:A:ILE:HG12	7	0.12
(1,25)	1:50:A:LEU:HD13	1:23:A:ILE:HG12	7	0.12
(1,1132)	1:16:A:GLU:HA	1:2:A:LYS:H	6	0.11
(1,1132)	1:16:A:GLU:HA	1:2:A:LYS:H	9	0.11
(1,1120)	1:33:A:GLU:HG2	1:15:A:LEU:H	3	0.11
(1,1106)	1:50:A:LEU:HD11	1:49:A:LYS:H	1	0.11
(1,1106)	1:50:A:LEU:HD12	1:49:A:LYS:H	1	0.11
(1,1106)	1:50:A:LEU:HD13	1:49:A:LYS:H	1	0.11
(1,1075)	1:56:A:LEU:HB3	1:20:A:SER:H	8	0.11
(1,1070)	1:25:A:ASN:HB3	1:21:A:ASP:H	8	0.11
(1,1059)	1:72:A:ARG:HB2	1:72:A:ARG:H	1	0.11
(1,1001)	1:56:A:LEU:HA	1:57:A:SER:H	6	0.11
(1,1001)	1:56:A:LEU:HA	1:57:A:SER:H	8	0.11
(1,905)	1:3:A:ILE:HD11	1:66:A:THR:H	9	0.11
(1,905)	1:3:A:ILE:HD12	1:66:A:THR:H	9	0.11
(1,905)	1:3:A:ILE:HD13	1:66:A:THR:H	9	0.11
(1,899)	1:64:A:GLU:HG2	1:65:A:SER:H	7	0.11
(1,899)	1:64:A:GLU:HG3	1:65:A:SER:H	7	0.11
(1,899)	1:64:A:GLU:HG2	1:65:A:SER:H	10	0.11
(1,899)	1:64:A:GLU:HG3	1:65:A:SER:H	10	0.11
(1,773)	1:34:A:GLU:HG2	1:35:A:GLY:H	3	0.11
(1,773)	1:34:A:GLU:HG3	1:35:A:GLY:H	3	0.11
(1,755)	1:28:A:ALA:HB1	1:32:A:ASP:H	5	0.11
(1,755)	1:28:A:ALA:HB2	1:32:A:ASP:H	5	0.11
(1,755)	1:28:A:ALA:HB3	1:32:A:ASP:H	5	0.11
(1,705)	1:55:A:THR:HG21	1:21:A:ASP:H	7	0.11
(1,705)	1:55:A:THR:HG22	1:21:A:ASP:H	7	0.11
(1,705)	1:55:A:THR:HG23	1:21:A:ASP:H	7	0.11
(1,667)	1:6:A:LYS:HD2	1:6:A:LYS:H	8	0.11
(1,667)	1:6:A:LYS:HD3	1:6:A:LYS:H	8	0.11
(1,667)	1:6:A:LYS:HD2	1:6:A:LYS:H	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,667)	1:6:A:LYS:HD3	1:6:A:LYS:H	10	0.11
(1,581)	1:55:A:THR:HB	1:22:A:THR:HA	8	0.11
(1,577)	1:71:A:LEU:HG	1:41:A:GLN:HA	4	0.11
(1,570)	1:25:A:ASN:HB3	1:29:A:LYS:HG2	2	0.11
(1,570)	1:25:A:ASN:HB3	1:29:A:LYS:HG3	2	0.11
(1,563)	1:55:A:THR:HA	1:22:A:THR:HB	8	0.11
(1,560)	1:55:A:THR:HB	1:22:A:THR:HA	9	0.11
(1,542)	1:11:A:LYS:HD2	1:11:A:LYS:HD3	1	0.11
(1,542)	1:11:A:LYS:HD2	1:11:A:LYS:HD3	2	0.11
(1,542)	1:11:A:LYS:HD2	1:11:A:LYS:HD3	3	0.11
(1,542)	1:11:A:LYS:HD2	1:11:A:LYS:HD3	4	0.11
(1,542)	1:11:A:LYS:HD2	1:11:A:LYS:HD3	5	0.11
(1,542)	1:11:A:LYS:HD2	1:11:A:LYS:HD3	6	0.11
(1,542)	1:11:A:LYS:HD2	1:11:A:LYS:HD3	7	0.11
(1,542)	1:11:A:LYS:HD2	1:11:A:LYS:HD3	8	0.11
(1,542)	1:11:A:LYS:HD2	1:11:A:LYS:HD3	9	0.11
(1,542)	1:11:A:LYS:HD2	1:11:A:LYS:HD3	10	0.11
(1,536)	1:11:A:LYS:HD2	1:9:A:THR:HG21	2	0.11
(1,536)	1:11:A:LYS:HD2	1:9:A:THR:HG22	2	0.11
(1,536)	1:11:A:LYS:HD2	1:9:A:THR:HG23	2	0.11
(1,536)	1:11:A:LYS:HD3	1:9:A:THR:HG21	2	0.11
(1,536)	1:11:A:LYS:HD3	1:9:A:THR:HG22	2	0.11
(1,536)	1:11:A:LYS:HD3	1:9:A:THR:HG23	2	0.11
(1,536)	1:11:A:LYS:HD2	1:9:A:THR:HG21	8	0.11
(1,536)	1:11:A:LYS:HD2	1:9:A:THR:HG22	8	0.11
(1,536)	1:11:A:LYS:HD2	1:9:A:THR:HG23	8	0.11
(1,536)	1:11:A:LYS:HD3	1:9:A:THR:HG21	8	0.11
(1,536)	1:11:A:LYS:HD3	1:9:A:THR:HG22	8	0.11
(1,536)	1:11:A:LYS:HD3	1:9:A:THR:HG23	8	0.11
(1,536)	1:11:A:LYS:HD2	1:9:A:THR:HG21	10	0.11
(1,536)	1:11:A:LYS:HD2	1:9:A:THR:HG22	10	0.11
(1,536)	1:11:A:LYS:HD2	1:9:A:THR:HG23	10	0.11
(1,536)	1:11:A:LYS:HD3	1:9:A:THR:HG21	10	0.11
(1,536)	1:11:A:LYS:HD3	1:9:A:THR:HG22	10	0.11
(1,536)	1:11:A:LYS:HD3	1:9:A:THR:HG23	10	0.11
(1,510)	1:65:A:SER:HA	1:65:A:SER:HB3	2	0.11
(1,510)	1:65:A:SER:HA	1:65:A:SER:HB3	3	0.11
(1,510)	1:65:A:SER:HA	1:65:A:SER:HB3	4	0.11
(1,510)	1:65:A:SER:HA	1:65:A:SER:HB3	6	0.11
(1,510)	1:65:A:SER:HA	1:65:A:SER:HB3	7	0.11
(1,510)	1:65:A:SER:HA	1:65:A:SER:HB3	9	0.11
(1,505)	1:58:A:ASP:HB3	1:58:A:ASP:HA	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,504)	1:58:A:ASP:HB2	1:58:A:ASP:HA	2	0.11
(1,405)	1:59:A:TYR:HB2	1:56:A:LEU:HD21	6	0.11
(1,405)	1:59:A:TYR:HB2	1:56:A:LEU:HD22	6	0.11
(1,405)	1:59:A:TYR:HB2	1:56:A:LEU:HD23	6	0.11
(1,398)	1:56:A:LEU:HB2	1:19:A:PRO:HA	6	0.11
(1,268)	1:16:A:GLU:HA	1:16:A:GLU:HB2	2	0.11
(1,268)	1:16:A:GLU:HA	1:16:A:GLU:HB2	4	0.11
(1,249)	1:36:A:ILE:HA	1:71:A:LEU:HD11	10	0.11
(1,249)	1:36:A:ILE:HA	1:71:A:LEU:HD12	10	0.11
(1,249)	1:36:A:ILE:HA	1:71:A:LEU:HD13	10	0.11
(1,204)	1:57:A:SER:HA	1:60:A:SER:HA	9	0.11
(1,121)	1:4:A:PHE:HB2	1:12:A:THR:HG21	4	0.11
(1,121)	1:4:A:PHE:HB2	1:12:A:THR:HG22	4	0.11
(1,121)	1:4:A:PHE:HB2	1:12:A:THR:HG23	4	0.11
(1,54)	1:61:A:ILE:HD11	1:59:A:TYR:H	4	0.11
(1,54)	1:61:A:ILE:HD12	1:59:A:TYR:H	4	0.11
(1,54)	1:61:A:ILE:HD13	1:59:A:TYR:H	4	0.11
(1,1280)	1:15:A:LEU:HB2	1:17:A:VAL:H	7	0.1
(1,1254)	1:41:A:GLN:HB2	1:40:A:GLN:HE22	3	0.1
(1,1254)	1:41:A:GLN:HB3	1:40:A:GLN:HE22	3	0.1
(1,1164)	1:31:A:GLN:HB2	1:29:A:LYS:H	1	0.1
(1,1164)	1:31:A:GLN:HB3	1:29:A:LYS:H	1	0.1
(1,1164)	1:31:A:GLN:HB2	1:29:A:LYS:H	5	0.1
(1,1164)	1:31:A:GLN:HB3	1:29:A:LYS:H	5	0.1
(1,1164)	1:31:A:GLN:HB2	1:29:A:LYS:H	10	0.1
(1,1164)	1:31:A:GLN:HB3	1:29:A:LYS:H	10	0.1
(1,1136)	1:50:A:LEU:HA	1:49:A:LYS:H	5	0.1
(1,1132)	1:16:A:GLU:HA	1:2:A:LYS:H	4	0.1
(1,1132)	1:16:A:GLU:HA	1:2:A:LYS:H	10	0.1
(1,1094)	1:27:A:LYS:HG2	1:52:A:ASP:H	6	0.1
(1,1094)	1:27:A:LYS:HG3	1:52:A:ASP:H	6	0.1
(1,1088)	1:27:A:LYS:HE2	1:27:A:LYS:H	7	0.1
(1,1088)	1:27:A:LYS:HE3	1:27:A:LYS:H	7	0.1
(1,1068)	1:43:A:LEU:H	1:51:A:GLU:H	2	0.1
(1,1068)	1:43:A:LEU:H	1:51:A:GLU:H	10	0.1
(1,755)	1:28:A:ALA:HB1	1:32:A:ASP:H	4	0.1
(1,755)	1:28:A:ALA:HB2	1:32:A:ASP:H	4	0.1
(1,755)	1:28:A:ALA:HB3	1:32:A:ASP:H	4	0.1
(1,755)	1:28:A:ALA:HB1	1:32:A:ASP:H	7	0.1
(1,755)	1:28:A:ALA:HB2	1:32:A:ASP:H	7	0.1
(1,755)	1:28:A:ALA:HB3	1:32:A:ASP:H	7	0.1
(1,755)	1:28:A:ALA:HB1	1:32:A:ASP:H	9	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,755)	1:28:A:ALA:HB2	1:32:A:ASP:H	9	0.1
(1,755)	1:28:A:ALA:HB3	1:32:A:ASP:H	9	0.1
(1,688)	1:15:A:LEU:HD11	1:15:A:LEU:H	6	0.1
(1,688)	1:15:A:LEU:HD12	1:15:A:LEU:H	6	0.1
(1,688)	1:15:A:LEU:HD13	1:15:A:LEU:H	6	0.1
(1,688)	1:15:A:LEU:HD21	1:15:A:LEU:H	6	0.1
(1,688)	1:15:A:LEU:HD22	1:15:A:LEU:H	6	0.1
(1,688)	1:15:A:LEU:HD23	1:15:A:LEU:H	6	0.1
(1,616)	1:11:A:LYS:HE2	1:13:A:ILE:H	8	0.1
(1,616)	1:11:A:LYS:HE3	1:13:A:ILE:H	8	0.1
(1,563)	1:55:A:THR:HA	1:22:A:THR:HB	6	0.1
(1,561)	1:69:A:LEU:HB2	1:7:A:THR:HB	10	0.1
(1,560)	1:55:A:THR:HB	1:22:A:THR:HA	6	0.1
(1,449)	1:27:A:LYS:HB2	1:43:A:LEU:HD11	10	0.1
(1,449)	1:27:A:LYS:HB2	1:43:A:LEU:HD12	10	0.1
(1,449)	1:27:A:LYS:HB2	1:43:A:LEU:HD13	10	0.1
(1,212)	1:5:A:VAL:HA	1:68:A:HIS:HA	4	0.1
(1,204)	1:57:A:SER:HA	1:60:A:SER:HA	4	0.1
(1,204)	1:57:A:SER:HA	1:60:A:SER:HA	5	0.1
(1,204)	1:57:A:SER:HA	1:60:A:SER:HA	10	0.1
(1,144)	1:7:A:THR:HB	1:8:A:LEU:HB2	10	0.1
(1,144)	1:7:A:THR:HB	1:8:A:LEU:HB3	10	0.1
(1,112)	1:2:A:LYS:HE2	1:14:A:THR:HG21	5	0.1
(1,112)	1:2:A:LYS:HE2	1:14:A:THR:HG22	5	0.1
(1,112)	1:2:A:LYS:HE2	1:14:A:THR:HG23	5	0.1
(1,112)	1:2:A:LYS:HE3	1:14:A:THR:HG21	5	0.1
(1,112)	1:2:A:LYS:HE3	1:14:A:THR:HG22	5	0.1
(1,112)	1:2:A:LYS:HE3	1:14:A:THR:HG23	5	0.1
(1,56)	1:30:A:ILE:HD13	1:69:A:LEU:HB2	4	0.1
(1,54)	1:61:A:ILE:HD11	1:59:A:TYR:H	3	0.1
(1,54)	1:61:A:ILE:HD12	1:59:A:TYR:H	3	0.1
(1,54)	1:61:A:ILE:HD13	1:59:A:TYR:H	3	0.1
(1,54)	1:61:A:ILE:HD11	1:59:A:TYR:H	7	0.1
(1,54)	1:61:A:ILE:HD12	1:59:A:TYR:H	7	0.1
(1,54)	1:61:A:ILE:HD13	1:59:A:TYR:H	7	0.1
(1,54)	1:61:A:ILE:HD11	1:59:A:TYR:H	9	0.1
(1,54)	1:61:A:ILE:HD12	1:59:A:TYR:H	9	0.1
(1,54)	1:61:A:ILE:HD13	1:59:A:TYR:H	9	0.1
(1,34)	1:36:A:ILE:HD11	1:69:A:LEU:HG	6	0.1
(1,34)	1:36:A:ILE:HD12	1:69:A:LEU:HG	6	0.1
(1,34)	1:36:A:ILE:HD13	1:69:A:LEU:HG	6	0.1
(1,25)	1:50:A:LEU:HD11	1:23:A:ILE:HG12	4	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,25)	1:50:A:LEU:HD12	1:23:A:ILE:HG12	4	0.1
(1,25)	1:50:A:LEU:HD13	1:23:A:ILE:HG12	4	0.1
(1,17)	1:44:A:ILE:HD11	1:49:A:LYS:HE2	3	0.1
(1,17)	1:44:A:ILE:HD11	1:49:A:LYS:HE3	3	0.1
(1,17)	1:44:A:ILE:HD12	1:49:A:LYS:HE2	3	0.1
(1,17)	1:44:A:ILE:HD12	1:49:A:LYS:HE3	3	0.1
(1,17)	1:44:A:ILE:HD13	1:49:A:LYS:HE2	3	0.1
(1,17)	1:44:A:ILE:HD13	1:49:A:LYS:HE3	3	0.1
(1,12)	1:23:A:ILE:HD11	1:54:A:ARG:HG2	1	0.1
(1,12)	1:23:A:ILE:HD12	1:54:A:ARG:HG2	1	0.1
(1,12)	1:23:A:ILE:HD13	1:54:A:ARG:HG2	1	0.1
(1,12)	1:23:A:ILE:HD11	1:54:A:ARG:HG2	3	0.1
(1,12)	1:23:A:ILE:HD12	1:54:A:ARG:HG2	3	0.1
(1,12)	1:23:A:ILE:HD13	1:54:A:ARG:HG2	3	0.1

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found