



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 06:21 PM UTC

PDB ID : 6G81 / pdb_00006g81
BMRB ID : 34257
Title : Solution structure of the Ni metallochaperone HypA from *Helicobacter pylori*
Authors : Spronk, C.A.E.M.; Zerko, S.; Gorka, M.; Kozminski, W.; Bardiaux, B.; Zambelli, B.; Musiani, F.; Piccioli, M.; Hu, H.; Maroney, M.; Ciurli, S.
Deposited on : 2018-04-07

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<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

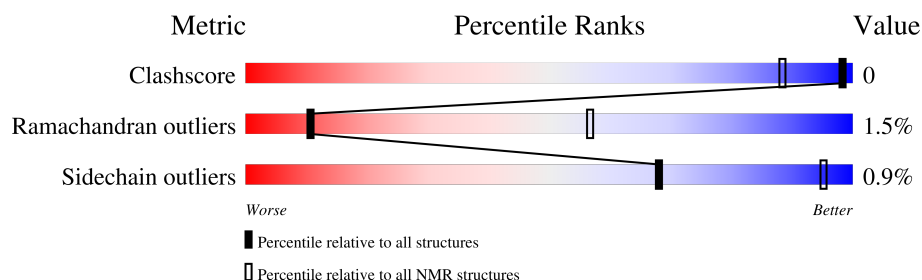
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 91%.

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	117	 95%

2 Ensemble composition and analysis

This entry contains 20 models. Model 7 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:117 (117)	0.93	7

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

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

The models can be grouped into 4 clusters and 1 single-model cluster was found.

Cluster number	Models
1	1, 4, 6, 7, 11, 12, 16, 19
2	3, 8, 13, 18
3	2, 9, 17, 20
4	10, 14, 15
Single-model clusters	5

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1843 atoms, of which 923 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Hydrogenase maturation factor HypA.

Mol	Chain	Residues	Atoms						Trace
1	A	117	Total	C	H	N	O	S	0
			1842	574	923	155	180	10	

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

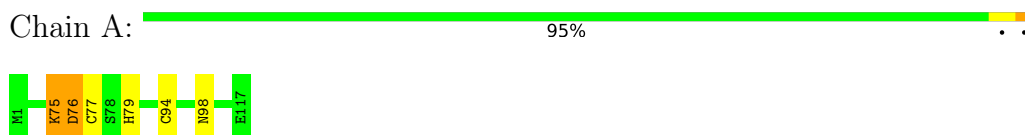
Mol	Chain	Residues	Atoms	
2	A	1	Total	Zn
			1	1

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: Hydrogenase maturation factor HypA

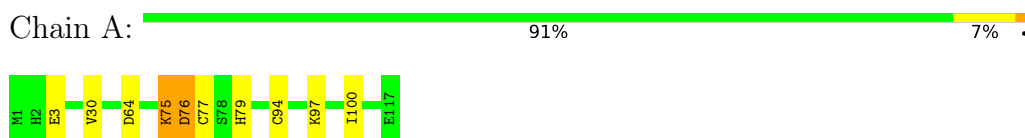


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

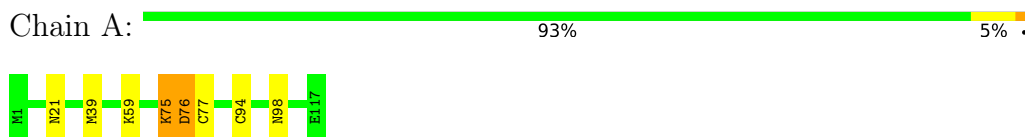
4.2.1 Score per residue for model 1

- Molecule 1: Hydrogenase maturation factor HypA



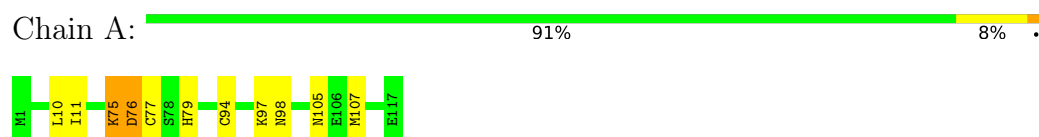
4.2.2 Score per residue for model 2

- Molecule 1: Hydrogenase maturation factor HypA



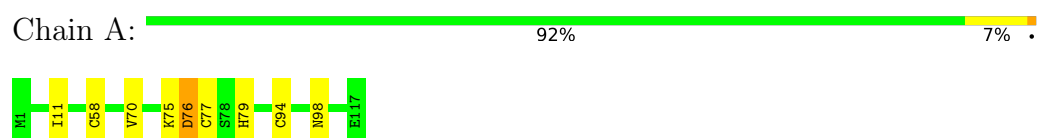
4.2.3 Score per residue for model 3

- Molecule 1: Hydrogenase maturation factor HypA



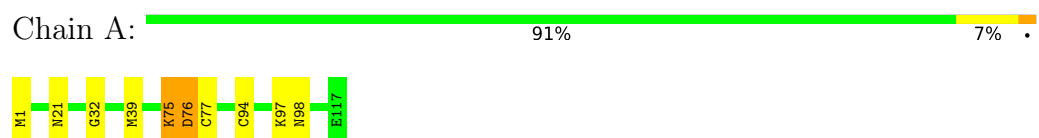
4.2.4 Score per residue for model 4

- Molecule 1: Hydrogenase maturation factor HypA



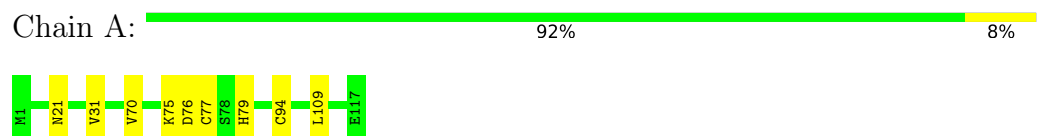
4.2.5 Score per residue for model 5

- Molecule 1: Hydrogenase maturation factor HypA



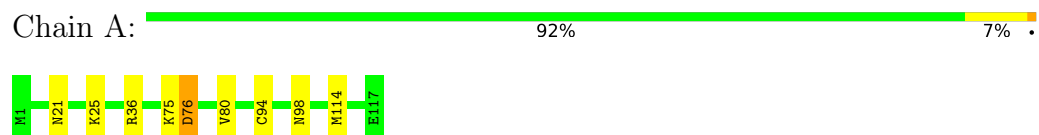
4.2.6 Score per residue for model 6

- Molecule 1: Hydrogenase maturation factor HypA



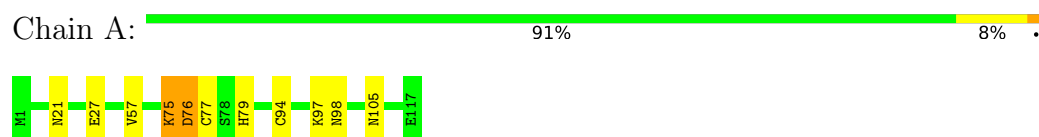
4.2.7 Score per residue for model 7 (medoid)

- Molecule 1: Hydrogenase maturation factor HypA



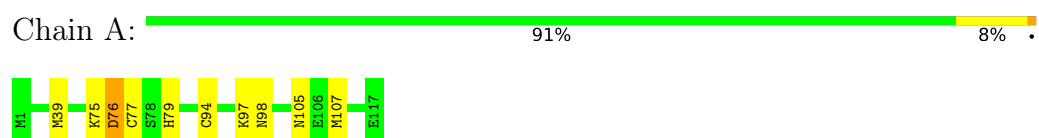
4.2.8 Score per residue for model 8

- Molecule 1: Hydrogenase maturation factor HypA



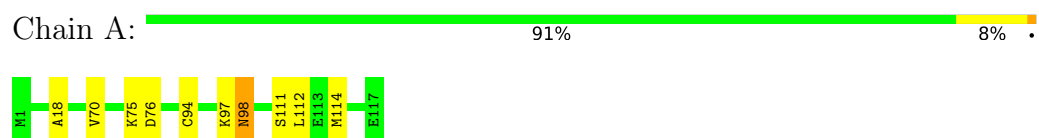
4.2.9 Score per residue for model 9

- Molecule 1: Hydrogenase maturation factor HypA



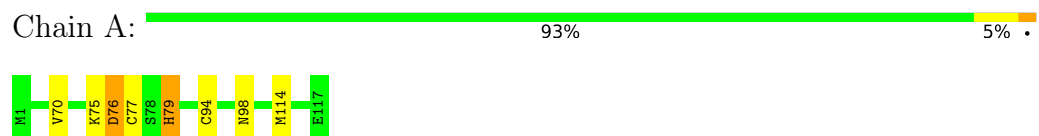
4.2.10 Score per residue for model 10

- Molecule 1: Hydrogenase maturation factor HypA



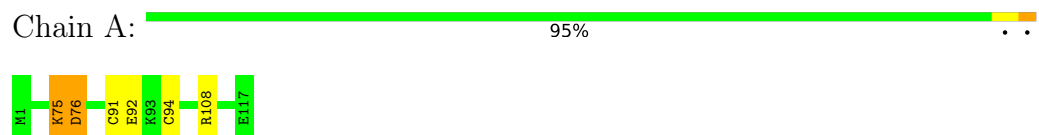
4.2.11 Score per residue for model 11

- Molecule 1: Hydrogenase maturation factor HypA



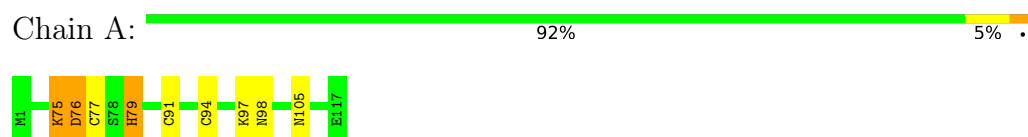
4.2.12 Score per residue for model 12

- Molecule 1: Hydrogenase maturation factor HypA



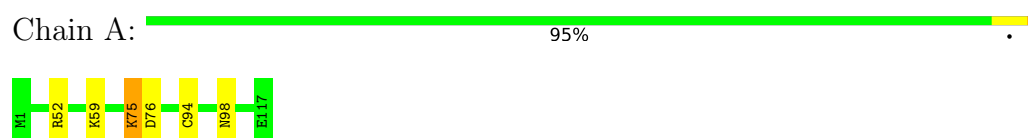
4.2.13 Score per residue for model 13

- Molecule 1: Hydrogenase maturation factor HypA



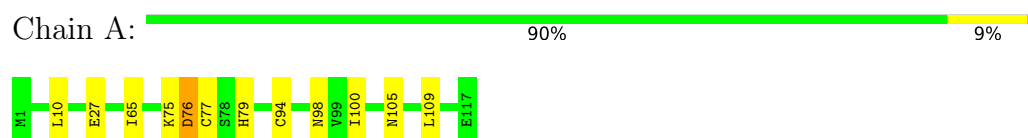
4.2.14 Score per residue for model 14

- Molecule 1: Hydrogenase maturation factor HypA



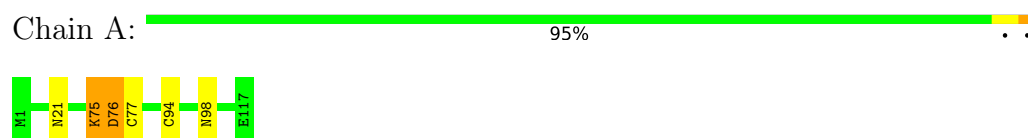
4.2.15 Score per residue for model 15

- Molecule 1: Hydrogenase maturation factor HypA



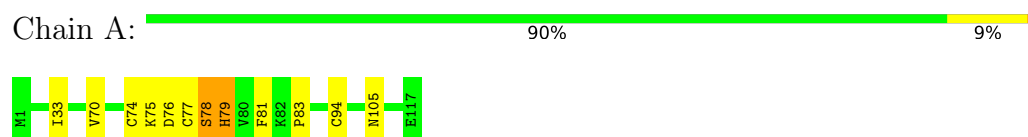
4.2.16 Score per residue for model 16

- Molecule 1: Hydrogenase maturation factor HypA



4.2.17 Score per residue for model 17

- Molecule 1: Hydrogenase maturation factor HypA



4.2.18 Score per residue for model 18

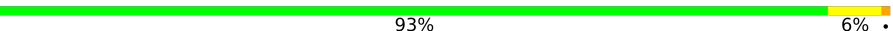
- Molecule 1: Hydrogenase maturation factor HypA

Chain A:  91% 9% .



4.2.19 Score per residue for model 19

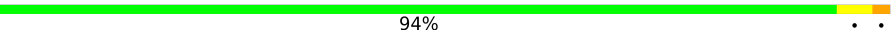
- Molecule 1: Hydrogenase maturation factor HypA

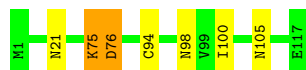
Chain A:  93% 6% .



4.2.20 Score per residue for model 20

- Molecule 1: Hydrogenase maturation factor HypA

Chain A:  94% . .



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 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
YARIA	structure calculation	
ARIA	structure calculation	
YASARA	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1443
Number of shifts mapped to atoms	1443
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	91%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.04±0.03	1±1/930 (0.1± 0.1%)	1.25±0.03	7±2/1246 (0.5± 0.2%)
All	All	1.04	11/18600 (0.1%)	1.25	134/24920 (0.5%)

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.7±0.5
All	All	0	13

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	114	MET	SD-CE	-6.57	1.63	1.79	11	4
1	A	65	ILE	CA-CB	5.83	1.61	1.54	15	1
1	A	107	MET	SD-CE	5.60	1.93	1.79	9	1
1	A	57	VAL	CA-CB	5.43	1.61	1.54	8	1
1	A	98	ASN	N-CA	5.33	1.53	1.46	10	1
1	A	39	MET	SD-CE	-5.29	1.66	1.79	9	3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	79	HIS	N-CA-C	10.53	129.82	113.19	8	9
1	A	77	CYS	N-CA-C	-9.88	94.52	109.83	17	14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	94	CYS	N-CA-C	-9.77	94.38	109.52	18	20
1	A	75	LYS	N-CA-C	-7.72	99.03	110.23	7	19
1	A	59	LYS	N-CA-C	7.07	118.99	111.28	19	3
1	A	76	ASP	CA-C-N	6.92	132.80	121.86	5	12
1	A	76	ASP	C-N-CA	6.92	132.80	121.86	5	12
1	A	105	ASN	N-CA-C	-6.67	105.28	113.41	20	8
1	A	97	LYS	N-CA-C	-6.31	102.03	110.55	3	7
1	A	76	ASP	CA-C-O	6.22	129.41	120.51	9	3
1	A	108	ARG	NE-CZ-NH2	6.21	124.79	119.20	12	1
1	A	75	LYS	CB-CA-C	6.08	119.82	109.72	7	2
1	A	91	CYS	N-CA-C	-5.66	103.06	110.53	12	2
1	A	70	VAL	N-CA-C	5.65	116.59	110.21	4	4
1	A	80	VAL	N-CA-C	5.62	116.32	109.30	7	1
1	A	50	THR	N-CA-C	5.52	117.38	111.36	19	1
1	A	70	VAL	CB-CA-C	-5.51	105.27	111.45	10	1
1	A	33	ILE	N-CA-C	-5.44	100.28	108.12	17	1
1	A	76	ASP	N-CA-C	5.38	122.26	110.80	15	6
1	A	32	GLY	N-CA-C	-5.38	102.48	110.71	5	1
1	A	18	ALA	N-CA-C	-5.36	105.44	111.28	10	1
1	A	78	SER	N-CA-C	5.34	117.98	110.23	17	1
1	A	52	ARG	NE-CZ-NH2	5.33	123.99	119.20	14	1
1	A	36	ARG	NE-CZ-NH2	5.29	123.96	119.20	7	1
1	A	11	ILE	N-CA-C	-5.19	105.32	110.62	3	1
1	A	94	CYS	CA-C-O	-5.14	115.76	121.51	8	1
1	A	3	GLU	N-CA-C	5.04	116.78	111.28	1	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	75	LYS	Peptide	11
1	A	79	HIS	Peptide	2

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	919	923	918	1±1
All	All	18400	18460	18360	12

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 0.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:10:LEU:HD13	1:A:107:MET:HE1	0.49	1.85	18	2
1:A:31:VAL:HG12	1:A:109:LEU:HD23	0.46	1.88	6	1
1:A:10:LEU:HD11	1:A:109:LEU:HD21	0.45	1.87	15	2
1:A:77:CYS:SG	1:A:79:HIS:ND1	0.44	2.90	18	1
1:A:111:SER:C	1:A:112:LEU:HD12	0.43	2.39	10	1
1:A:74:CYS:SG	1:A:78:SER:HA	0.42	2.55	17	1
1:A:30:VAL:HG12	1:A:64:ASP:HB2	0.42	1.92	1	1
1:A:11:ILE:HD12	1:A:58:CYS:SG	0.41	2.56	4	1
1:A:74:CYS:SG	1:A:79:HIS:ND1	0.40	2.85	17	1
1:A:81:PHE:CE2	1:A:83:PRO:HA	0.40	2.51	17	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	115/117 (98%)	110±1 (96±1%)	3±1 (3±1%)	2±0 (2±0%)	11	57
All	All	2300/2340 (98%)	2200 (96%)	65 (3%)	35 (2%)	11	57

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	76	ASP	20
1	A	98	ASN	15

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	105/105 (100%)	104±1 (99±1%)	1±1 (1±1%)	68 95
All	All	2100/2100 (100%)	2081 (99%)	19 (1%)	68 95

All 9 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	21	ASN	7
1	A	100	ILE	3
1	A	27	GLU	2
1	A	79	HIS	2
1	A	1	MET	1
1	A	25	LYS	1
1	A	92	GLU	1
1	A	76	ASP	1
1	A	105	ASN	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 91% for the well-defined parts and 91% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *D_1200009528_cs-upload_P1.str.V2*

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	1443
Number of shifts mapped to atoms	1443
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	115	-0.45 ± 0.17	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	110	0.17 ± 0.26	None needed (< 0.5 ppm)
$^{13}\text{C}'$	116	-0.06 ± 0.14	None needed (< 0.5 ppm)
^{15}N	114	-0.16 ± 0.41	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 91%, i.e. 1443 atoms were assigned a chemical shift out of a possible 1592. 0 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	578/587 (98%)	233/237 (98%)	231/234 (99%)	114/116 (98%)
Sidechain	801/907 (88%)	548/590 (93%)	253/289 (88%)	0/28 (0%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	64/98 (65%)	32/48 (67%)	32/40 (80%)	0/10 (0%)
Overall	1443/1592 (91%)	813/875 (93%)	516/563 (92%)	114/154 (74%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 91%, i.e. 1443 atoms were assigned a chemical shift out of a possible 1592. 0 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	578/587 (98%)	233/237 (98%)	231/234 (99%)	114/116 (98%)
Sidechain	801/907 (88%)	548/590 (93%)	253/289 (88%)	0/28 (0%)
Aromatic	64/98 (65%)	32/48 (67%)	32/40 (80%)	0/10 (0%)
Overall	1443/1592 (91%)	813/875 (93%)	516/563 (92%)	114/154 (74%)

7.1.4 Statistically unusual chemical shifts [i](#)

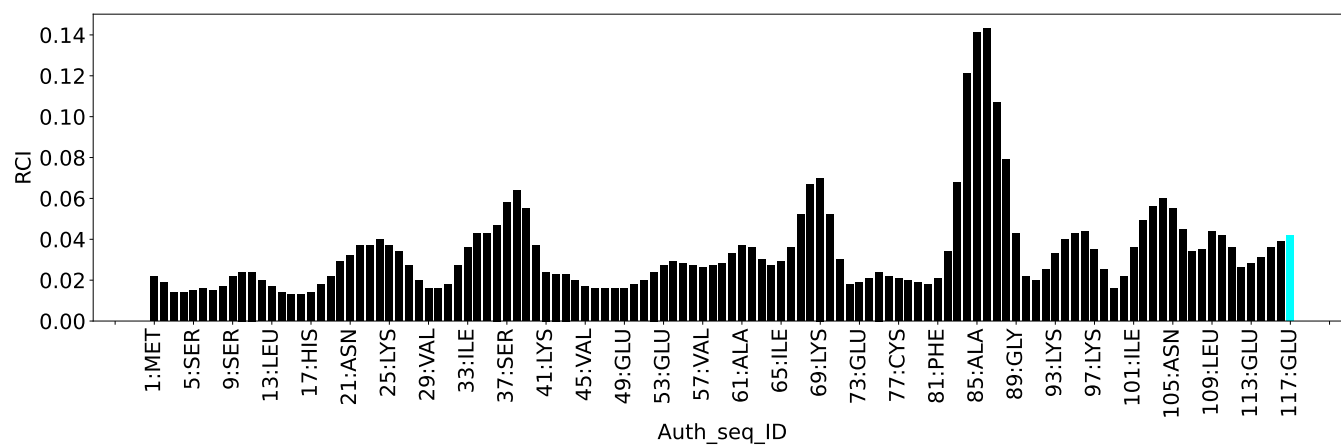
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	92	GLU	HG3	1.04	1.20 – 3.30	-5.7

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

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	2704
Intra-residue ($ i-j =0$)	1326
Sequential ($ i-j =1$)	402
Medium range ($ i-j >1$ and $ i-j <5$)	320
Long range ($ i-j \geq 5$)	652
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	191
Number of unmapped restraints	0
Number of restraints per residue	24.5
Number of long range restraints per residue ¹	5.5

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)	82.6	0.2
0.2-0.5 (Medium)	180.4	0.5
>0.5 (Large)	205.3	4.33

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

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

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	1.2	5.88
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

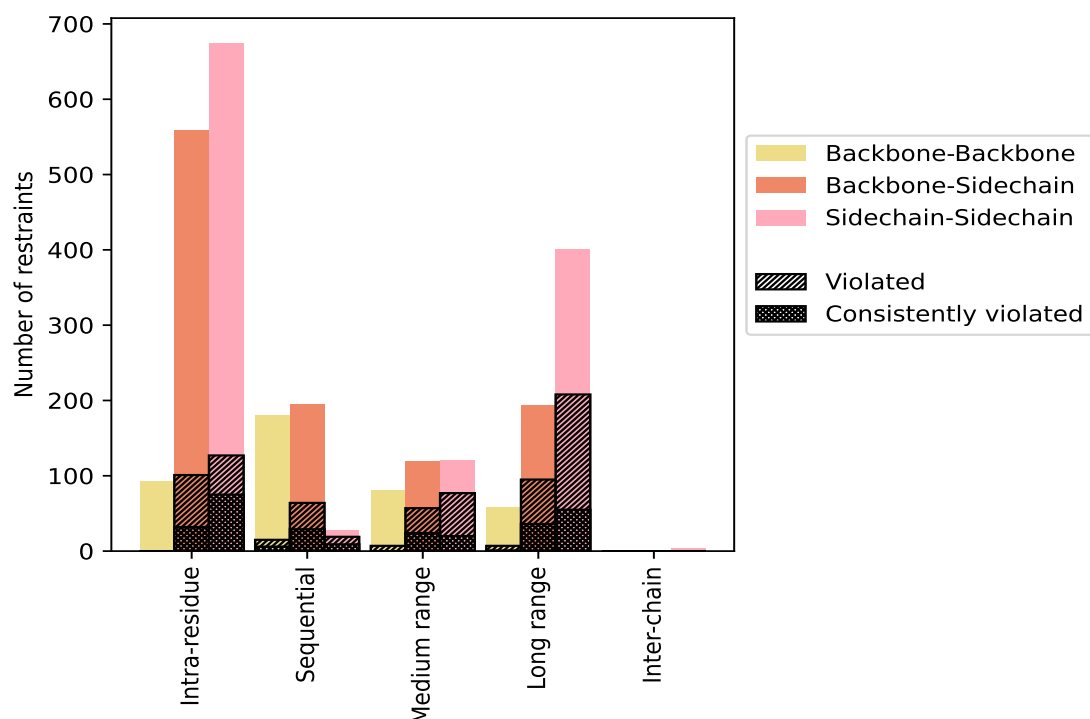
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue (i-j =0)	1326	49.0	228	17.2	8.4	107	8.1	4.0
Backbone-Backbone	93	3.4	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	559	20.7	101	18.1	3.7	32	5.7	1.2
Sidechain-Sidechain	674	24.9	127	18.8	4.7	75	11.1	2.8
Sequential (i-j =1)	402	14.9	98	24.4	3.6	44	10.9	1.6
Backbone-Backbone	180	6.7	15	8.3	0.6	6	3.3	0.2
Backbone-Sidechain	195	7.2	64	32.8	2.4	29	14.9	1.1
Sidechain-Sidechain	27	1.0	19	70.4	0.7	9	33.3	0.3
Medium range (i-j >1 & i-j <5)	320	11.8	141	44.1	5.2	44	13.8	1.6
Backbone-Backbone	80	3.0	7	8.8	0.3	0	0.0	0.0
Backbone-Sidechain	119	4.4	57	47.9	2.1	24	20.2	0.9
Sidechain-Sidechain	121	4.5	77	63.6	2.8	20	16.5	0.7
Long range (i-j ≥5)	652	24.1	310	47.5	11.5	92	14.1	3.4
Backbone-Backbone	58	2.1	7	12.1	0.3	1	1.7	0.0
Backbone-Sidechain	193	7.1	95	49.2	3.5	36	18.7	1.3
Sidechain-Sidechain	401	14.8	208	51.9	7.7	55	13.7	2.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	2704	100.0	777	28.7	28.7	287	10.6	10.6
Backbone-Backbone	411	15.2	29	7.1	1.1	7	1.7	0.3
Backbone-Sidechain	1066	39.4	317	29.7	11.7	121	11.4	4.5
Sidechain-Sidechain	1227	45.4	431	35.1	15.9	159	13.0	5.9

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	158	68	81	154	0	461	0.6	3.28	0.56	0.44
2	167	64	77	159	0	467	0.6	3.54	0.56	0.43
3	161	68	73	161	0	463	0.61	3.43	0.57	0.45
4	160	66	77	162	0	465	0.6	3.42	0.56	0.44
5	163	65	79	173	0	480	0.62	3.48	0.57	0.47
6	159	70	77	172	0	478	0.6	3.23	0.55	0.42
7	170	67	81	176	0	494	0.6	3.6	0.57	0.42
8	164	66	82	172	0	484	0.6	3.46	0.54	0.43
9	158	65	75	161	0	459	0.62	3.69	0.58	0.46
10	156	67	72	172	0	467	0.63	3.3	0.57	0.46

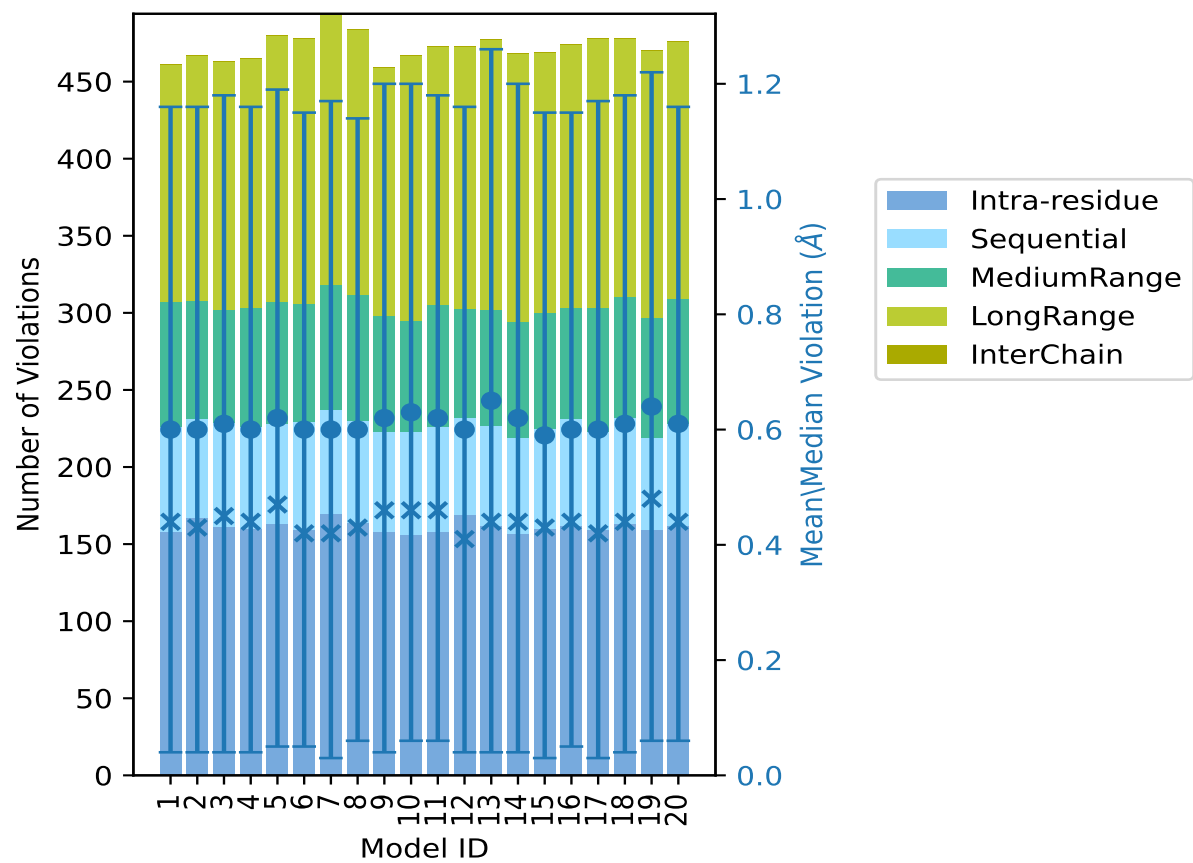
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	158	68	79	168	0	473	0.62	3.57	0.56	0.46
12	169	63	71	170	0	473	0.6	3.36	0.56	0.41
13	162	65	75	175	0	477	0.65	4.33	0.61	0.44
14	157	62	75	174	0	468	0.62	3.58	0.58	0.44
15	160	65	75	169	0	469	0.59	3.65	0.56	0.43
16	162	69	72	171	0	474	0.6	3.33	0.55	0.44
17	159	64	80	175	0	478	0.6	3.2	0.57	0.42
18	163	69	78	168	0	478	0.61	3.67	0.57	0.44
19	159	60	78	173	0	470	0.64	3.82	0.58	0.48
20	162	66	81	167	0	476	0.61	3.5	0.55	0.44

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

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



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

9.3 Distance violation statistics for the ensemble

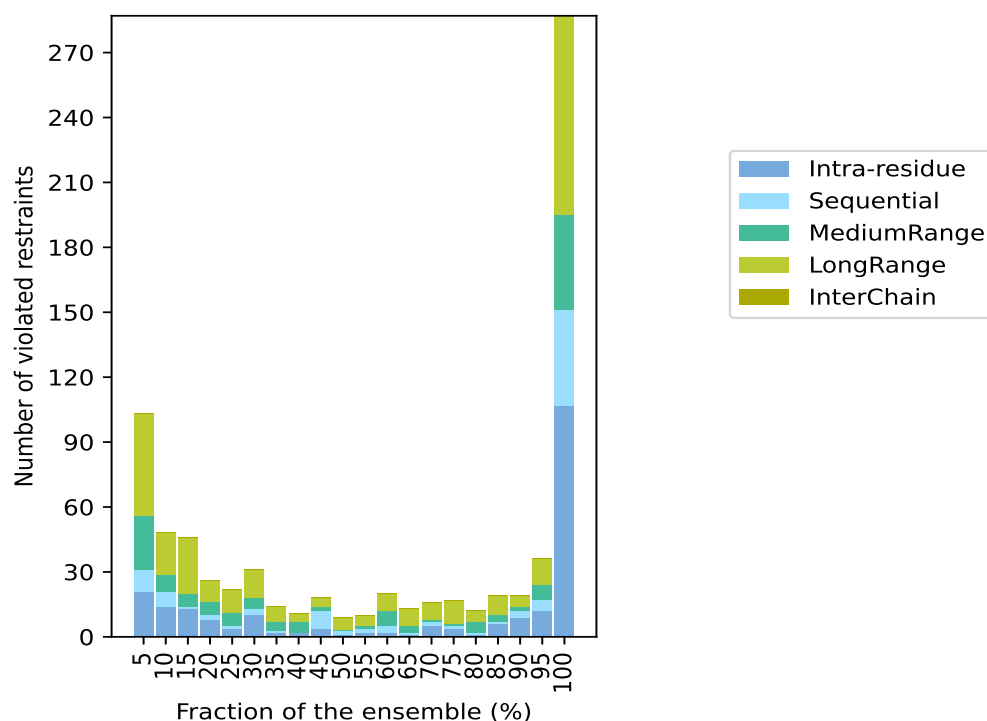
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1923(IR:1098, SQ:304, MR:179, LR:342, IC:0) restraints are 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	%
21	10	25	47	0	103	1	5.0
14	7	8	19	0	48	2	10.0
13	1	6	26	0	46	3	15.0
8	2	6	10	0	26	4	20.0
4	1	6	11	0	22	5	25.0
10	3	5	13	0	31	6	30.0
2	1	4	7	0	14	7	35.0
2	0	5	4	0	11	8	40.0
4	8	2	4	0	18	9	45.0
1	2	0	6	0	9	10	50.0
2	2	1	5	0	10	11	55.0
2	3	7	8	0	20	12	60.0
1	1	3	8	0	13	13	65.0
5	2	1	8	0	16	14	70.0
4	1	1	11	0	17	15	75.0
1	1	5	5	0	12	16	80.0
6	1	3	9	0	19	17	85.0
9	3	2	5	0	19	18	90.0
12	5	7	12	0	36	19	95.0
107	44	44	92	0	287	20	100.0

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

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

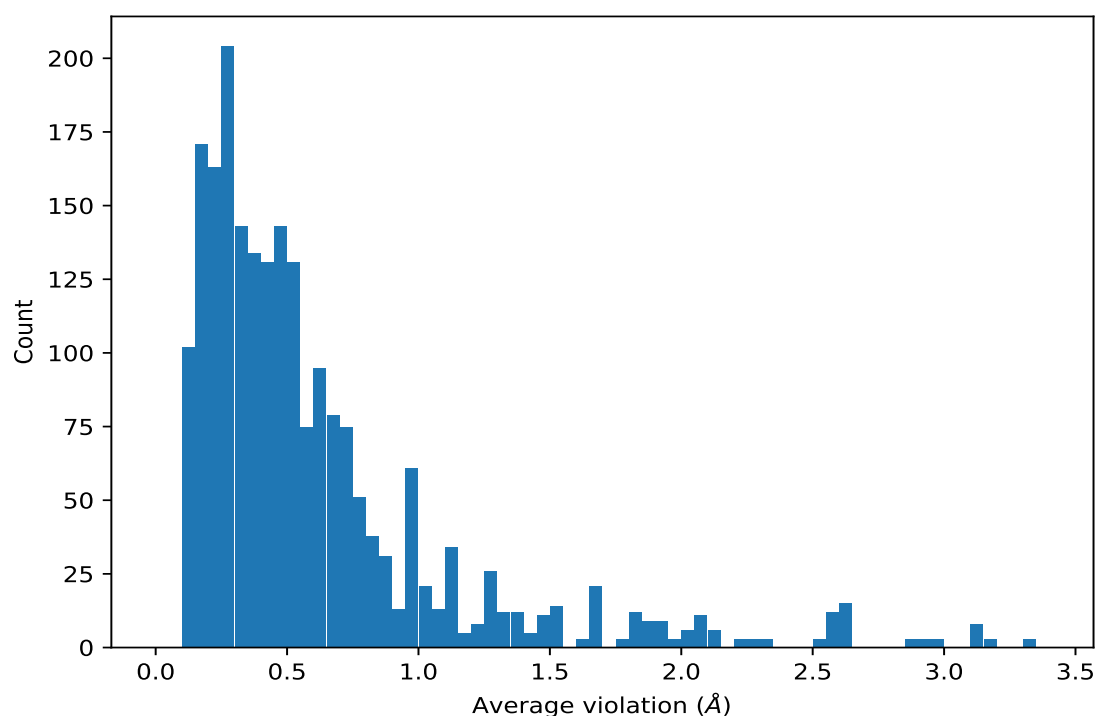
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(1,1432)	1:99:A:VAL:HG23	1:74:A:CYS:HB3	20	3.34	0.48	3.44
(1,1432)	1:99:A:VAL:HG22	1:74:A:CYS:HB3	20	3.34	0.48	3.44
(1,1432)	1:99:A:VAL:HG21	1:74:A:CYS:HB3	20	3.34	0.48	3.44
(1,1801)	1:29:A:VAL:HG11	1:61:A:ALA:HA	20	3.16	0.12	3.18
(1,1801)	1:29:A:VAL:HG12	1:61:A:ALA:HA	20	3.16	0.12	3.18
(1,1801)	1:29:A:VAL:HG13	1:61:A:ALA:HA	20	3.16	0.12	3.18
(1,799)	1:11:A:ILE:HD11	1:7:A:VAL:HG23	20	3.13	0.28	3.12
(1,799)	1:11:A:ILE:HD11	1:7:A:VAL:HG22	20	3.13	0.28	3.12
(1,799)	1:11:A:ILE:HD13	1:7:A:VAL:HG22	20	3.13	0.28	3.12
(1,799)	1:11:A:ILE:HD12	1:7:A:VAL:HG21	20	3.13	0.28	3.12
(1,799)	1:11:A:ILE:HD12	1:7:A:VAL:HG23	20	3.13	0.28	3.12
(1,799)	1:11:A:ILE:HD11	1:7:A:VAL:HG21	20	3.13	0.28	3.12
(1,799)	1:11:A:ILE:HD12	1:7:A:VAL:HG22	20	3.13	0.28	3.12
(1,799)	1:11:A:ILE:HD13	1:7:A:VAL:HG21	20	3.13	0.28	3.12
(1,2619)	1:109:A:LEU:HB2	1:30:A:VAL:HG21	20	2.97	0.16	2.96
(1,2619)	1:109:A:LEU:HB2	1:30:A:VAL:HG23	20	2.97	0.16	2.96

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2619)	1:109:A:LEU:HB2	1:30:A:VAL:HG22	20	2.97	0.16	2.96
(1,797)	1:7:A:VAL:HG21	1:51:A:PHE:HB3	20	2.9	0.2	2.92
(1,797)	1:7:A:VAL:HG23	1:51:A:PHE:HB3	20	2.9	0.2	2.92
(1,797)	1:7:A:VAL:HG22	1:51:A:PHE:HB3	20	2.9	0.2	2.92
(1,2663)	1:33:A:ILE:HA	1:31:A:VAL:HG11	20	2.89	0.16	2.87
(1,2663)	1:33:A:ILE:HA	1:31:A:VAL:HG12	20	2.89	0.16	2.87
(1,2663)	1:33:A:ILE:HA	1:31:A:VAL:HG13	20	2.89	0.16	2.87
(1,985)	1:29:A:VAL:HG11	1:61:A:ALA:HB2	20	2.64	0.13	2.64
(1,985)	1:29:A:VAL:HG12	1:61:A:ALA:HB1	20	2.64	0.13	2.64
(1,985)	1:29:A:VAL:HG13	1:61:A:ALA:HB1	20	2.64	0.13	2.64
(1,985)	1:29:A:VAL:HG11	1:61:A:ALA:HB3	20	2.64	0.13	2.64
(1,985)	1:29:A:VAL:HG12	1:61:A:ALA:HB3	20	2.64	0.13	2.64
(1,985)	1:29:A:VAL:HG11	1:61:A:ALA:HB1	20	2.64	0.13	2.64
(1,985)	1:29:A:VAL:HG13	1:61:A:ALA:HB3	20	2.64	0.13	2.64
(1,985)	1:29:A:VAL:HG13	1:61:A:ALA:HB2	20	2.64	0.13	2.64
(1,985)	1:29:A:VAL:HG12	1:61:A:ALA:HB2	20	2.64	0.13	2.64
(1,782)	1:99:A:VAL:HG12	1:89:A:GLY:HA3	20	2.62	0.26	2.6
(1,782)	1:99:A:VAL:HG11	1:89:A:GLY:HA3	20	2.62	0.26	2.6
(1,782)	1:99:A:VAL:HG13	1:89:A:GLY:HA3	20	2.62	0.26	2.6
(1,85)	1:99:A:VAL:HG23	1:74:A:CYS:H	20	2.6	0.11	2.63
(1,85)	1:99:A:VAL:HG22	1:74:A:CYS:H	20	2.6	0.11	2.63
(1,85)	1:99:A:VAL:HG21	1:74:A:CYS:H	20	2.6	0.11	2.63
(1,1763)	1:7:A:VAL:HG23	1:11:A:ILE:HG13	20	2.57	0.3	2.54
(1,1763)	1:7:A:VAL:HG22	1:11:A:ILE:HG13	20	2.57	0.3	2.54
(1,1763)	1:7:A:VAL:HG21	1:11:A:ILE:HG13	20	2.57	0.3	2.54
(1,738)	1:7:A:VAL:HG11	1:6:A:VAL:HG12	20	2.55	0.11	2.55
(1,738)	1:7:A:VAL:HG13	1:6:A:VAL:HG11	20	2.55	0.11	2.55
(1,738)	1:7:A:VAL:HG12	1:6:A:VAL:HG12	20	2.55	0.11	2.55
(1,738)	1:7:A:VAL:HG11	1:6:A:VAL:HG11	20	2.55	0.11	2.55
(1,738)	1:7:A:VAL:HG13	1:6:A:VAL:HG12	20	2.55	0.11	2.55
(1,738)	1:7:A:VAL:HG13	1:6:A:VAL:HG13	20	2.55	0.11	2.55
(1,738)	1:7:A:VAL:HG12	1:6:A:VAL:HG11	20	2.55	0.11	2.55
(1,738)	1:7:A:VAL:HG12	1:6:A:VAL:HG13	20	2.55	0.11	2.55
(1,738)	1:7:A:VAL:HG11	1:6:A:VAL:HG13	20	2.55	0.11	2.55
(1,1813)	1:26:A:ILE:HG12	1:57:A:VAL:HG23	20	2.5	0.14	2.48
(1,1813)	1:26:A:ILE:HG12	1:57:A:VAL:HG21	20	2.5	0.14	2.48
(1,1813)	1:26:A:ILE:HG12	1:57:A:VAL:HG22	20	2.5	0.14	2.48
(1,2115)	1:28:A:ARG:HA	1:29:A:VAL:HG12	20	2.34	0.05	2.34
(1,2115)	1:28:A:ARG:HA	1:29:A:VAL:HG13	20	2.34	0.05	2.34
(1,2115)	1:28:A:ARG:HA	1:29:A:VAL:HG11	20	2.34	0.05	2.34
(1,80)	1:99:A:VAL:HG21	1:75:A:LYS:H	20	2.29	0.16	2.32
(1,80)	1:99:A:VAL:HG23	1:75:A:LYS:H	20	2.29	0.16	2.32

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,80)	1:99:A:VAL:HG22	1:75:A:LYS:H	20	2.29	0.16	2.32
(1,1863)	1:12:A:ALA:HB3	1:15:A:GLU:HG2	20	2.2	0.19	2.2
(1,1863)	1:12:A:ALA:HB1	1:15:A:GLU:HG2	20	2.2	0.19	2.2
(1,1863)	1:12:A:ALA:HB2	1:15:A:GLU:HG2	20	2.2	0.19	2.2
(1,2598)	1:7:A:VAL:HG22	1:8:A:SER:HA	20	2.11	0.06	2.1
(1,2598)	1:7:A:VAL:HG23	1:8:A:SER:HA	20	2.11	0.06	2.1
(1,2598)	1:7:A:VAL:HG21	1:8:A:SER:HA	20	2.11	0.06	2.1
(1,2003)	1:99:A:VAL:HG23	1:91:A:CYS:HB3	20	2.11	0.26	2.04
(1,2003)	1:99:A:VAL:HG22	1:91:A:CYS:HB3	20	2.11	0.26	2.04
(1,2003)	1:99:A:VAL:HG21	1:91:A:CYS:HB3	20	2.11	0.26	2.04
(1,2591)	1:7:A:VAL:HG11	1:107:A:MET:HE3	20	2.09	0.24	2.1
(1,2591)	1:7:A:VAL:HG13	1:107:A:MET:HE2	20	2.09	0.24	2.1
(1,2591)	1:7:A:VAL:HG13	1:107:A:MET:HE3	20	2.09	0.24	2.1
(1,2591)	1:7:A:VAL:HG13	1:107:A:MET:HE1	20	2.09	0.24	2.1
(1,2591)	1:7:A:VAL:HG12	1:107:A:MET:HE1	20	2.09	0.24	2.1
(1,2591)	1:7:A:VAL:HG11	1:107:A:MET:HE2	20	2.09	0.24	2.1
(1,2591)	1:7:A:VAL:HG12	1:107:A:MET:HE2	20	2.09	0.24	2.1
(1,2591)	1:7:A:VAL:HG11	1:107:A:MET:HE1	20	2.09	0.24	2.1
(1,1654)	1:74:A:CYS:HA	1:99:A:VAL:HG23	20	2.07	0.11	2.08
(1,1654)	1:74:A:CYS:HA	1:99:A:VAL:HG22	20	2.07	0.11	2.08
(1,1654)	1:74:A:CYS:HA	1:99:A:VAL:HG21	20	2.07	0.11	2.08
(1,2615)	1:50:A:THR:HG23	1:49:A:GLU:HB3	20	2.03	0.1	2.02
(1,2615)	1:50:A:THR:HG22	1:49:A:GLU:HB3	20	2.03	0.1	2.02
(1,2615)	1:50:A:THR:HG21	1:49:A:GLU:HB3	20	2.03	0.1	2.02
(1,1493)	1:7:A:VAL:HG13	1:44:A:PHE:HA	20	2.03	0.2	2.02
(1,1493)	1:7:A:VAL:HG12	1:44:A:PHE:HA	20	2.03	0.2	2.02
(1,1493)	1:7:A:VAL:HG11	1:44:A:PHE:HA	20	2.03	0.2	2.02
(1,1729)	1:6:A:VAL:HB	1:7:A:VAL:HG11	20	1.98	0.08	1.98
(1,1729)	1:6:A:VAL:HB	1:7:A:VAL:HG13	20	1.98	0.08	1.98
(1,1729)	1:6:A:VAL:HB	1:7:A:VAL:HG12	20	1.98	0.08	1.98
(1,872)	1:26:A:ILE:HG21	1:29:A:VAL:HG13	20	1.91	0.13	1.92
(1,872)	1:26:A:ILE:HG22	1:29:A:VAL:HG11	20	1.91	0.13	1.92
(1,872)	1:26:A:ILE:HG23	1:29:A:VAL:HG11	20	1.91	0.13	1.92
(1,872)	1:26:A:ILE:HG23	1:29:A:VAL:HG13	20	1.91	0.13	1.92
(1,872)	1:26:A:ILE:HG23	1:29:A:VAL:HG12	20	1.91	0.13	1.92
(1,872)	1:26:A:ILE:HG22	1:29:A:VAL:HG13	20	1.91	0.13	1.92
(1,872)	1:26:A:ILE:HG22	1:29:A:VAL:HG12	20	1.91	0.13	1.92
(1,872)	1:26:A:ILE:HG21	1:29:A:VAL:HG12	20	1.91	0.13	1.92
(1,872)	1:26:A:ILE:HG21	1:29:A:VAL:HG11	20	1.91	0.13	1.92
(1,812)	1:29:A:VAL:HG23	1:109:A:LEU:HD23	20	1.86	0.16	1.81
(1,812)	1:29:A:VAL:HG21	1:109:A:LEU:HD22	20	1.86	0.16	1.81
(1,812)	1:29:A:VAL:HG22	1:109:A:LEU:HD23	20	1.86	0.16	1.81

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,812)	1:29:A:VAL:HG22	1:109:A:LEU:HD22	20	1.86	0.16	1.81
(1,812)	1:29:A:VAL:HG21	1:109:A:LEU:HD21	20	1.86	0.16	1.81
(1,812)	1:29:A:VAL:HG21	1:109:A:LEU:HD23	20	1.86	0.16	1.81
(1,812)	1:29:A:VAL:HG22	1:109:A:LEU:HD21	20	1.86	0.16	1.81
(1,812)	1:29:A:VAL:HG23	1:109:A:LEU:HD21	20	1.86	0.16	1.81
(1,812)	1:29:A:VAL:HG23	1:109:A:LEU:HD22	20	1.86	0.16	1.81
(1,2466)	1:29:A:VAL:HG21	1:10:A:LEU:HD23	20	1.81	0.2	1.81
(1,2466)	1:31:A:VAL:HG22	1:10:A:LEU:HD21	20	1.81	0.2	1.81
(1,2466)	1:31:A:VAL:HG23	1:10:A:LEU:HD22	20	1.81	0.2	1.81
(1,2466)	1:31:A:VAL:HG22	1:10:A:LEU:HD23	20	1.81	0.2	1.81
(1,2466)	1:31:A:VAL:HG23	1:10:A:LEU:HD23	20	1.81	0.2	1.81
(1,2466)	1:29:A:VAL:HG22	1:10:A:LEU:HD22	20	1.81	0.2	1.81
(1,2466)	1:31:A:VAL:HG22	1:10:A:LEU:HD22	20	1.81	0.2	1.81
(1,2466)	1:31:A:VAL:HG21	1:10:A:LEU:HD21	20	1.81	0.2	1.81
(1,2466)	1:29:A:VAL:HG23	1:10:A:LEU:HD22	20	1.81	0.2	1.81
(1,2466)	1:29:A:VAL:HG22	1:10:A:LEU:HD23	20	1.81	0.2	1.81
(1,2466)	1:29:A:VAL:HG23	1:10:A:LEU:HD23	20	1.81	0.2	1.81
(1,2466)	1:29:A:VAL:HG21	1:10:A:LEU:HD21	20	1.81	0.2	1.81
(1,855)	1:99:A:VAL:HG23	1:74:A:CYS:HB2	20	1.78	0.17	1.76
(1,855)	1:99:A:VAL:HG22	1:74:A:CYS:HB2	20	1.78	0.17	1.76
(1,855)	1:99:A:VAL:HG21	1:74:A:CYS:HB2	20	1.78	0.17	1.76
(1,811)	1:29:A:VAL:HG23	1:109:A:LEU:HD13	20	1.69	0.33	1.81
(1,811)	1:29:A:VAL:HG21	1:109:A:LEU:HD13	20	1.69	0.33	1.81
(1,811)	1:29:A:VAL:HG22	1:109:A:LEU:HD13	20	1.69	0.33	1.81
(1,811)	1:29:A:VAL:HG22	1:109:A:LEU:HD12	20	1.69	0.33	1.81
(1,811)	1:29:A:VAL:HG22	1:109:A:LEU:HD11	20	1.69	0.33	1.81
(1,811)	1:29:A:VAL:HG21	1:109:A:LEU:HD11	20	1.69	0.33	1.81
(1,811)	1:29:A:VAL:HG23	1:109:A:LEU:HD11	20	1.69	0.33	1.81
(1,811)	1:29:A:VAL:HG23	1:109:A:LEU:HD12	20	1.69	0.33	1.81
(1,2441)	1:29:A:VAL:HG21	1:10:A:LEU:HD23	20	1.67	0.17	1.67
(1,2441)	1:31:A:VAL:HG22	1:10:A:LEU:HD21	20	1.67	0.17	1.67
(1,2441)	1:31:A:VAL:HG23	1:10:A:LEU:HD22	20	1.67	0.17	1.67
(1,2441)	1:31:A:VAL:HG22	1:10:A:LEU:HD23	20	1.67	0.17	1.67
(1,2441)	1:31:A:VAL:HG23	1:10:A:LEU:HD23	20	1.67	0.17	1.67
(1,2441)	1:29:A:VAL:HG21	1:112:A:LEU:HD11	20	1.67	0.17	1.67
(1,2441)	1:31:A:VAL:HG22	1:10:A:LEU:HD22	20	1.67	0.17	1.67
(1,2441)	1:31:A:VAL:HG21	1:10:A:LEU:HD21	20	1.67	0.17	1.67
(1,2441)	1:29:A:VAL:HG23	1:10:A:LEU:HD22	20	1.67	0.17	1.67
(1,2441)	1:29:A:VAL:HG22	1:10:A:LEU:HD23	20	1.67	0.17	1.67
(1,2441)	1:29:A:VAL:HG21	1:112:A:LEU:HD13	20	1.67	0.17	1.67
(1,2441)	1:29:A:VAL:HG22	1:112:A:LEU:HD13	20	1.67	0.17	1.67
(1,2441)	1:29:A:VAL:HG21	1:10:A:LEU:HD21	20	1.67	0.17	1.67

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2599)	1:28:A:ARG:HG3	1:30:A:VAL:HG22	20	1.62	0.16	1.6
(1,2599)	1:28:A:ARG:HG3	1:30:A:VAL:HG21	20	1.62	0.16	1.6
(1,2599)	1:28:A:ARG:HG3	1:30:A:VAL:HG23	20	1.62	0.16	1.6
(1,48)	1:7:A:VAL:HG23	1:11:A:ILE:H	20	1.54	0.17	1.52
(1,48)	1:7:A:VAL:HG22	1:11:A:ILE:H	20	1.54	0.17	1.52
(1,48)	1:7:A:VAL:HG21	1:11:A:ILE:H	20	1.54	0.17	1.52
(1,2595)	1:110:A:LEU:HD21	1:66:A:VAL:HG13	20	1.52	0.21	1.57
(1,2595)	1:110:A:LEU:HD21	1:66:A:VAL:HG11	20	1.52	0.21	1.57
(1,2595)	1:110:A:LEU:HD23	1:66:A:VAL:HG13	20	1.52	0.21	1.57
(1,2595)	1:110:A:LEU:HD22	1:66:A:VAL:HG11	20	1.52	0.21	1.57
(1,2595)	1:110:A:LEU:HD22	1:66:A:VAL:HG12	20	1.52	0.21	1.57
(1,2595)	1:110:A:LEU:HD21	1:66:A:VAL:HG12	20	1.52	0.21	1.57
(1,2595)	1:110:A:LEU:HD23	1:66:A:VAL:HG12	20	1.52	0.21	1.57
(1,2595)	1:110:A:LEU:HD23	1:66:A:VAL:HG11	20	1.52	0.21	1.57
(1,772)	1:66:A:VAL:HG21	1:64:A:ASP:HB2	20	1.5	0.69	1.88
(1,772)	1:66:A:VAL:HG23	1:64:A:ASP:HB2	20	1.5	0.69	1.88
(1,772)	1:66:A:VAL:HG22	1:64:A:ASP:HB2	20	1.5	0.69	1.88
(1,2616)	1:50:A:THR:HG22	1:47:A:ALA:HB3	20	1.46	0.14	1.46
(1,2616)	1:50:A:THR:HG21	1:47:A:ALA:HB2	20	1.46	0.14	1.46
(1,2616)	1:50:A:THR:HG22	1:47:A:ALA:HB2	20	1.46	0.14	1.46
(1,2616)	1:50:A:THR:HG21	1:47:A:ALA:HB3	20	1.46	0.14	1.46
(1,2616)	1:50:A:THR:HG21	1:47:A:ALA:HB1	20	1.46	0.14	1.46
(1,2616)	1:50:A:THR:HG22	1:47:A:ALA:HB1	20	1.46	0.14	1.46
(1,2616)	1:50:A:THR:HG23	1:47:A:ALA:HB2	20	1.46	0.14	1.46
(1,2616)	1:50:A:THR:HG23	1:47:A:ALA:HB1	20	1.46	0.14	1.46
(1,106)	1:29:A:VAL:HG13	1:113:A:GLU:H	20	1.46	0.16	1.46
(1,106)	1:29:A:VAL:HG11	1:113:A:GLU:H	20	1.46	0.16	1.46
(1,106)	1:29:A:VAL:HG12	1:113:A:GLU:H	20	1.46	0.16	1.46
(1,2126)	1:7:A:VAL:HG11	1:44:A:PHE:HE1	20	1.4	0.16	1.38
(1,2126)	1:7:A:VAL:HG13	1:44:A:PHE:HE2	20	1.4	0.16	1.38
(1,2126)	1:7:A:VAL:HG13	1:44:A:PHE:HE1	20	1.4	0.16	1.38
(1,2126)	1:7:A:VAL:HG12	1:44:A:PHE:HE1	20	1.4	0.16	1.38
(1,2126)	1:7:A:VAL:HG12	1:44:A:PHE:HE2	20	1.4	0.16	1.38
(1,1737)	1:33:A:ILE:HG13	1:39:A:MET:HE2	20	1.39	0.5	1.4
(1,1737)	1:33:A:ILE:HG13	1:39:A:MET:HE1	20	1.39	0.5	1.4
(1,1737)	1:33:A:ILE:HG13	1:39:A:MET:HE3	20	1.39	0.5	1.4
(1,742)	1:72:A:LEU:HD11	1:99:A:VAL:HG13	20	1.36	0.73	1.25
(1,742)	1:72:A:LEU:HD11	1:99:A:VAL:HG12	20	1.36	0.73	1.25
(1,742)	1:72:A:LEU:HD12	1:99:A:VAL:HG11	20	1.36	0.73	1.25
(1,742)	1:72:A:LEU:HD12	1:99:A:VAL:HG13	20	1.36	0.73	1.25
(1,742)	1:72:A:LEU:HD12	1:99:A:VAL:HG12	20	1.36	0.73	1.25
(1,742)	1:72:A:LEU:HD11	1:99:A:VAL:HG11	20	1.36	0.73	1.25

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,742)	1:72:A:LEU:HD13	1:99:A:VAL:HG12	20	1.36	0.73	1.25
(1,742)	1:72:A:LEU:HD13	1:99:A:VAL:HG13	20	1.36	0.73	1.25
(1,742)	1:72:A:LEU:HD13	1:99:A:VAL:HG11	20	1.36	0.73	1.25
(1,1776)	1:80:A:VAL:HG11	1:73:A:GLU:HG2	20	1.34	0.32	1.33
(1,1776)	1:80:A:VAL:HG13	1:73:A:GLU:HG2	20	1.34	0.32	1.33
(1,1776)	1:80:A:VAL:HG12	1:73:A:GLU:HG2	20	1.34	0.32	1.33
(1,14)	1:7:A:VAL:HG12	1:7:A:VAL:H	20	1.33	0.03	1.33
(1,14)	1:7:A:VAL:HG11	1:7:A:VAL:H	20	1.33	0.03	1.33
(1,14)	1:7:A:VAL:HG13	1:7:A:VAL:H	20	1.33	0.03	1.33
(1,1289)	1:57:A:VAL:HG22	1:15:A:GLU:HG3	20	1.31	0.24	1.3
(1,1289)	1:57:A:VAL:HG21	1:15:A:GLU:HG3	20	1.31	0.24	1.3
(1,1289)	1:57:A:VAL:HG23	1:15:A:GLU:HG3	20	1.31	0.24	1.3
(1,1421)	1:51:A:PHE:HB2	1:7:A:VAL:HG21	20	1.3	0.19	1.33
(1,1421)	1:51:A:PHE:HB2	1:7:A:VAL:HG23	20	1.3	0.19	1.33
(1,1421)	1:51:A:PHE:HB2	1:7:A:VAL:HG22	20	1.3	0.19	1.33
(1,2443)	1:30:A:VAL:HG21	1:109:A:LEU:HA	20	1.29	0.15	1.3
(1,2443)	1:30:A:VAL:HG23	1:109:A:LEU:HA	20	1.29	0.15	1.3
(1,2443)	1:30:A:VAL:HG22	1:109:A:LEU:HA	20	1.29	0.15	1.3
(1,774)	1:66:A:VAL:HG21	1:32:A:GLY:HA3	20	1.29	0.23	1.32
(1,774)	1:66:A:VAL:HG23	1:32:A:GLY:HA3	20	1.29	0.23	1.32
(1,774)	1:66:A:VAL:HG22	1:32:A:GLY:HA3	20	1.29	0.23	1.32
(1,1743)	1:90:A:VAL:HG21	1:99:A:VAL:HG23	20	1.29	0.16	1.28
(1,1743)	1:90:A:VAL:HG21	1:99:A:VAL:HG22	20	1.29	0.16	1.28
(1,1743)	1:90:A:VAL:HG22	1:99:A:VAL:HG21	20	1.29	0.16	1.28
(1,1743)	1:90:A:VAL:HG23	1:99:A:VAL:HG21	20	1.29	0.16	1.28
(1,1743)	1:90:A:VAL:HG23	1:99:A:VAL:HG22	20	1.29	0.16	1.28
(1,1743)	1:90:A:VAL:HG22	1:99:A:VAL:HG22	20	1.29	0.16	1.28
(1,1743)	1:90:A:VAL:HG22	1:99:A:VAL:HG23	20	1.29	0.16	1.28
(1,1743)	1:90:A:VAL:HG23	1:99:A:VAL:HG23	20	1.29	0.16	1.28
(1,730)	1:33:A:ILE:HD11	1:45:A:VAL:HG12	20	1.25	0.19	1.24
(1,730)	1:33:A:ILE:HD13	1:45:A:VAL:HG11	20	1.25	0.19	1.24
(1,730)	1:33:A:ILE:HD12	1:45:A:VAL:HG13	20	1.25	0.19	1.24
(1,730)	1:33:A:ILE:HD13	1:45:A:VAL:HG13	20	1.25	0.19	1.24
(1,730)	1:33:A:ILE:HD12	1:45:A:VAL:HG11	20	1.25	0.19	1.24
(1,730)	1:33:A:ILE:HD13	1:45:A:VAL:HG12	20	1.25	0.19	1.24
(1,730)	1:33:A:ILE:HD12	1:45:A:VAL:HG12	20	1.25	0.19	1.24
(1,730)	1:33:A:ILE:HD11	1:45:A:VAL:HG11	20	1.25	0.19	1.24
(1,730)	1:33:A:ILE:HD11	1:45:A:VAL:HG13	20	1.25	0.19	1.24
(1,1418)	1:91:A:CYS:HB2	1:99:A:VAL:HG23	20	1.25	0.41	1.17
(1,1418)	1:91:A:CYS:HB2	1:99:A:VAL:HG22	20	1.25	0.41	1.17
(1,1418)	1:91:A:CYS:HB2	1:99:A:VAL:HG21	20	1.25	0.41	1.17
(1,827)	1:101:A:ILE:HG21	1:102:A:THR:HG23	20	1.24	0.08	1.23

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,827)	1:101:A:ILE:HG21	1:102:A:THR:HG21	20	1.24	0.08	1.23
(1,827)	1:101:A:ILE:HG22	1:102:A:THR:HG21	20	1.24	0.08	1.23
(1,827)	1:101:A:ILE:HG23	1:102:A:THR:HG21	20	1.24	0.08	1.23
(1,827)	1:101:A:ILE:HG23	1:102:A:THR:HG22	20	1.24	0.08	1.23
(1,827)	1:101:A:ILE:HG21	1:102:A:THR:HG22	20	1.24	0.08	1.23
(1,827)	1:101:A:ILE:HG22	1:102:A:THR:HG23	20	1.24	0.08	1.23
(1,2420)	1:101:A:ILE:HD13	1:102:A:THR:H	20	1.19	0.13	1.2
(1,2420)	1:100:A:ILE:HD13	1:102:A:THR:H	20	1.19	0.13	1.2
(1,2420)	1:100:A:ILE:HD12	1:102:A:THR:H	20	1.19	0.13	1.2
(1,2420)	1:100:A:ILE:HD11	1:102:A:THR:H	20	1.19	0.13	1.2
(1,2420)	1:101:A:ILE:HD11	1:102:A:THR:H	20	1.19	0.13	1.2
(1,2576)	1:66:A:VAL:HA	1:110:A:LEU:HD13	20	1.13	0.21	1.18
(1,2576)	1:66:A:VAL:HA	1:110:A:LEU:HD11	20	1.13	0.21	1.18
(1,2576)	1:66:A:VAL:HA	1:110:A:LEU:HD12	20	1.13	0.21	1.18
(1,2576)	1:91:A:CYS:HA	1:72:A:LEU:HD23	20	1.13	0.21	1.18
(1,854)	1:101:A:ILE:HG13	1:70:A:VAL:HG22	20	1.13	0.39	1.14
(1,854)	1:101:A:ILE:HG13	1:70:A:VAL:HG21	20	1.13	0.39	1.14
(1,854)	1:101:A:ILE:HG13	1:70:A:VAL:HG23	20	1.13	0.39	1.14
(1,1779)	1:31:A:VAL:HG11	1:33:A:ILE:HG12	20	1.12	0.2	1.08
(1,1779)	1:31:A:VAL:HG12	1:33:A:ILE:HG12	20	1.12	0.2	1.08
(1,1779)	1:31:A:VAL:HG13	1:33:A:ILE:HG12	20	1.12	0.2	1.08
(1,788)	1:65:A:ILE:HD12	1:45:A:VAL:HG23	20	1.1	0.12	1.08
(1,788)	1:65:A:ILE:HD13	1:45:A:VAL:HG23	20	1.1	0.12	1.08
(1,788)	1:65:A:ILE:HD11	1:45:A:VAL:HG21	20	1.1	0.12	1.08
(1,788)	1:65:A:ILE:HD11	1:45:A:VAL:HG23	20	1.1	0.12	1.08
(1,788)	1:65:A:ILE:HD13	1:45:A:VAL:HG22	20	1.1	0.12	1.08
(1,788)	1:65:A:ILE:HD12	1:45:A:VAL:HG21	20	1.1	0.12	1.08
(1,788)	1:65:A:ILE:HD11	1:45:A:VAL:HG22	20	1.1	0.12	1.08
(1,2144)	1:7:A:VAL:HG21	1:4:A:TYR:HD2	20	1.1	0.22	1.08
(1,2144)	1:7:A:VAL:HG23	1:4:A:TYR:HD2	20	1.1	0.22	1.08
(1,2144)	1:7:A:VAL:HG23	1:4:A:TYR:HD1	20	1.1	0.22	1.08
(1,2144)	1:7:A:VAL:HG22	1:4:A:TYR:HD1	20	1.1	0.22	1.08
(1,2144)	1:7:A:VAL:HG21	1:4:A:TYR:HD1	20	1.1	0.22	1.08
(1,2144)	1:7:A:VAL:HG22	1:4:A:TYR:HD2	20	1.1	0.22	1.08
(1,1717)	1:99:A:VAL:HG21	1:99:A:VAL:HA	20	1.08	0.03	1.08
(1,1717)	1:99:A:VAL:HG22	1:99:A:VAL:HA	20	1.08	0.03	1.08
(1,1717)	1:99:A:VAL:HG23	1:99:A:VAL:HA	20	1.08	0.03	1.08
(1,1538)	1:99:A:VAL:HG23	1:91:A:CYS:HA	20	1.02	0.23	1.0
(1,1538)	1:99:A:VAL:HG22	1:91:A:CYS:HA	20	1.02	0.23	1.0
(1,1538)	1:99:A:VAL:HG21	1:91:A:CYS:HA	20	1.02	0.23	1.0
(1,1363)	1:23:A:ALA:HB2	1:114:A:MET:HG2	20	1.02	0.13	1.04
(1,1363)	1:23:A:ALA:HB1	1:114:A:MET:HG2	20	1.02	0.13	1.04

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1363)	1:23:A:ALA:HB3	1:114:A:MET:HG2	20	1.02	0.13	1.04
(1,1265)	1:102:A:THR:HG22	1:73:A:GLU:HG2	20	1.02	0.16	1.0
(1,1265)	1:102:A:THR:HG23	1:73:A:GLU:HG2	20	1.02	0.16	1.0
(1,1265)	1:102:A:THR:HG21	1:73:A:GLU:HG2	20	1.02	0.16	1.0
(1,40)	1:99:A:VAL:HG13	1:89:A:GLY:H	20	1.01	0.31	1.02
(1,40)	1:99:A:VAL:HG12	1:89:A:GLY:H	20	1.01	0.31	1.02
(1,40)	1:99:A:VAL:HG11	1:89:A:GLY:H	20	1.01	0.31	1.02
(1,2588)	1:31:A:VAL:HG23	1:30:A:VAL:HA	20	1.01	0.04	1.01
(1,2588)	1:30:A:VAL:HG23	1:30:A:VAL:HA	20	1.01	0.04	1.01
(1,2588)	1:31:A:VAL:HG22	1:30:A:VAL:HA	20	1.01	0.04	1.01
(1,2588)	1:31:A:VAL:HG21	1:30:A:VAL:HA	20	1.01	0.04	1.01
(1,2588)	1:30:A:VAL:HG21	1:30:A:VAL:HA	20	1.01	0.04	1.01
(1,2588)	1:30:A:VAL:HG22	1:30:A:VAL:HA	20	1.01	0.04	1.01
(1,943)	1:6:A:VAL:HG11	1:107:A:MET:HG2	20	1.0	0.22	0.92
(1,943)	1:6:A:VAL:HG12	1:107:A:MET:HG2	20	1.0	0.22	0.92
(1,943)	1:6:A:VAL:HG13	1:107:A:MET:HG2	20	1.0	0.22	0.92
(1,38)	1:99:A:VAL:HG12	1:90:A:VAL:H	20	0.99	0.21	1.02
(1,38)	1:99:A:VAL:HG11	1:90:A:VAL:H	20	0.99	0.21	1.02
(1,38)	1:99:A:VAL:HG13	1:90:A:VAL:H	20	0.99	0.21	1.02
(1,1778)	1:112:A:LEU:HD23	1:18:A:ALA:HB2	20	0.98	0.26	1.04
(1,1778)	1:112:A:LEU:HD23	1:18:A:ALA:HB1	20	0.98	0.26	1.04
(1,1778)	1:112:A:LEU:HD22	1:18:A:ALA:HB1	20	0.98	0.26	1.04
(1,1778)	1:112:A:LEU:HD22	1:18:A:ALA:HB2	20	0.98	0.26	1.04
(1,1778)	1:112:A:LEU:HD21	1:18:A:ALA:HB1	20	0.98	0.26	1.04
(1,1778)	1:112:A:LEU:HD22	1:18:A:ALA:HB3	20	0.98	0.26	1.04
(1,1778)	1:112:A:LEU:HD21	1:18:A:ALA:HB2	20	0.98	0.26	1.04
(1,1778)	1:112:A:LEU:HD23	1:18:A:ALA:HB3	20	0.98	0.26	1.04
(1,84)	1:99:A:VAL:HG23	1:91:A:CYS:H	20	0.98	0.28	0.98
(1,84)	1:99:A:VAL:HG22	1:91:A:CYS:H	20	0.98	0.28	0.98
(1,84)	1:99:A:VAL:HG21	1:91:A:CYS:H	20	0.98	0.28	0.98
(1,1732)	1:72:A:LEU:HD11	1:89:A:GLY:HA3	20	0.97	0.43	0.88
(1,1732)	1:72:A:LEU:HD12	1:89:A:GLY:HA3	20	0.97	0.43	0.88
(1,1732)	1:72:A:LEU:HD13	1:89:A:GLY:HA3	20	0.97	0.43	0.88
(1,2127)	1:7:A:VAL:HG13	1:4:A:TYR:HD2	20	0.97	0.15	0.94
(1,2127)	1:7:A:VAL:HG12	1:4:A:TYR:HD1	20	0.97	0.15	0.94
(1,2127)	1:7:A:VAL:HG12	1:4:A:TYR:HD2	20	0.97	0.15	0.94
(1,2127)	1:7:A:VAL:HG11	1:4:A:TYR:HD1	20	0.97	0.15	0.94
(1,2127)	1:7:A:VAL:HG13	1:4:A:TYR:HD1	20	0.97	0.15	0.94
(1,2127)	1:7:A:VAL:HG11	1:4:A:TYR:HD2	20	0.97	0.15	0.94
(1,2633)	1:115:A:LEU:HD23	1:27:A:GLU:HB3	20	0.96	0.28	0.88
(1,2633)	1:115:A:LEU:HD21	1:27:A:GLU:HB3	20	0.96	0.28	0.88
(1,2633)	1:115:A:LEU:HD11	1:27:A:GLU:HB3	20	0.96	0.28	0.88

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2633)	1:115:A:LEU:HD12	1:27:A:GLU:HB3	20	0.96	0.28	0.88
(1,2633)	1:115:A:LEU:HD13	1:27:A:GLU:HB3	20	0.96	0.28	0.88
(1,2633)	1:115:A:LEU:HD22	1:27:A:GLU:HB3	20	0.96	0.28	0.88
(1,2563)	1:45:A:VAL:HA	1:63:A:LEU:HD21	20	0.96	0.13	0.97
(1,2563)	1:45:A:VAL:HA	1:63:A:LEU:HD23	20	0.96	0.13	0.97
(1,2563)	1:45:A:VAL:HA	1:63:A:LEU:HD22	20	0.96	0.13	0.97
(1,1805)	1:10:A:LEU:HD12	1:63:A:LEU:HD21	20	0.96	0.35	0.92
(1,1805)	1:10:A:LEU:HD12	1:63:A:LEU:HD23	20	0.96	0.35	0.92
(1,1805)	1:10:A:LEU:HD11	1:63:A:LEU:HD21	20	0.96	0.35	0.92
(1,1805)	1:10:A:LEU:HD13	1:63:A:LEU:HD23	20	0.96	0.35	0.92
(1,1805)	1:10:A:LEU:HD13	1:63:A:LEU:HD22	20	0.96	0.35	0.92
(1,1805)	1:10:A:LEU:HD13	1:63:A:LEU:HD21	20	0.96	0.35	0.92
(1,1805)	1:10:A:LEU:HD11	1:63:A:LEU:HD22	20	0.96	0.35	0.92
(1,1805)	1:10:A:LEU:HD11	1:63:A:LEU:HD23	20	0.96	0.35	0.92
(1,1805)	1:10:A:LEU:HD12	1:63:A:LEU:HD22	20	0.96	0.35	0.92
(1,914)	1:72:A:LEU:HD21	1:70:A:VAL:HG13	20	0.96	0.56	0.84
(1,914)	1:72:A:LEU:HD23	1:70:A:VAL:HG13	20	0.96	0.56	0.84
(1,914)	1:72:A:LEU:HD21	1:70:A:VAL:HG11	20	0.96	0.56	0.84
(1,914)	1:72:A:LEU:HD22	1:70:A:VAL:HG13	20	0.96	0.56	0.84
(1,914)	1:72:A:LEU:HD22	1:70:A:VAL:HG11	20	0.96	0.56	0.84
(1,914)	1:72:A:LEU:HD23	1:70:A:VAL:HG11	20	0.96	0.56	0.84
(1,914)	1:72:A:LEU:HD21	1:70:A:VAL:HG12	20	0.96	0.56	0.84
(1,914)	1:72:A:LEU:HD23	1:70:A:VAL:HG12	20	0.96	0.56	0.84
(1,914)	1:72:A:LEU:HD22	1:70:A:VAL:HG12	20	0.96	0.56	0.84
(1,881)	1:93:A:LYS:HB3	1:93:A:LYS:HE2	20	0.92	0.12	0.94
(1,1823)	1:45:A:VAL:HG12	1:41:A:LYS:HE2	20	0.91	0.25	0.93
(1,1823)	1:45:A:VAL:HG13	1:41:A:LYS:HE2	20	0.91	0.25	0.93
(1,1823)	1:45:A:VAL:HG11	1:41:A:LYS:HE2	20	0.91	0.25	0.93
(1,1517)	1:7:A:VAL:HG13	1:4:A:TYR:HA	20	0.91	0.09	0.91
(1,1517)	1:7:A:VAL:HG12	1:4:A:TYR:HA	20	0.91	0.09	0.91
(1,1517)	1:7:A:VAL:HG11	1:4:A:TYR:HA	20	0.91	0.09	0.91
(1,2512)	1:56:A:LEU:HD21	1:56:A:LEU:HB3	20	0.9	0.04	0.9
(1,2512)	1:56:A:LEU:HD22	1:56:A:LEU:HB3	20	0.9	0.04	0.9
(1,2512)	1:10:A:LEU:HD13	1:10:A:LEU:HB3	20	0.9	0.04	0.9
(1,2512)	1:10:A:LEU:HD11	1:10:A:LEU:HB3	20	0.9	0.04	0.9
(1,2512)	1:10:A:LEU:HD12	1:10:A:LEU:HB3	20	0.9	0.04	0.9
(1,2512)	1:56:A:LEU:HD23	1:56:A:LEU:HB3	20	0.9	0.04	0.9
(1,1723)	1:45:A:VAL:HG11	1:63:A:LEU:HD21	20	0.88	0.18	0.89
(1,1723)	1:45:A:VAL:HG11	1:63:A:LEU:HD23	20	0.88	0.18	0.89
(1,1723)	1:45:A:VAL:HG13	1:63:A:LEU:HD21	20	0.88	0.18	0.89
(1,1723)	1:45:A:VAL:HG13	1:63:A:LEU:HD23	20	0.88	0.18	0.89
(1,1723)	1:45:A:VAL:HG12	1:63:A:LEU:HD21	20	0.88	0.18	0.89

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1723)	1:45:A:VAL:HG12	1:63:A:LEU:HD23	20	0.88	0.18	0.89
(1,1723)	1:45:A:VAL:HG11	1:63:A:LEU:HD22	20	0.88	0.18	0.89
(1,1723)	1:45:A:VAL:HG12	1:63:A:LEU:HD22	20	0.88	0.18	0.89
(1,1723)	1:45:A:VAL:HG13	1:63:A:LEU:HD22	20	0.88	0.18	0.89
(1,1738)	1:65:A:ILE:HG22	1:63:A:LEU:HD12	20	0.87	0.11	0.9
(1,1738)	1:65:A:ILE:HG22	1:63:A:LEU:HD13	20	0.87	0.11	0.9
(1,1738)	1:65:A:ILE:HG23	1:63:A:LEU:HD11	20	0.87	0.11	0.9
(1,1738)	1:65:A:ILE:HG21	1:63:A:LEU:HD11	20	0.87	0.11	0.9
(1,1738)	1:65:A:ILE:HG22	1:63:A:LEU:HD11	20	0.87	0.11	0.9
(1,1738)	1:65:A:ILE:HG23	1:63:A:LEU:HD13	20	0.87	0.11	0.9
(1,1738)	1:65:A:ILE:HG21	1:63:A:LEU:HD12	20	0.87	0.11	0.9
(1,1738)	1:65:A:ILE:HG23	1:63:A:LEU:HD12	20	0.87	0.11	0.9
(1,1870)	1:20:A:LYS:HG2	1:16:A:GLU:HG3	20	0.87	0.17	0.82
(1,2672)	1:70:A:VAL:HG11	1:88:A:TYR:HD1	20	0.85	0.26	0.82
(1,2672)	1:10:A:LEU:HD12	1:48:A:PHE:HD1	20	0.85	0.26	0.82
(1,2672)	1:70:A:VAL:HG11	1:88:A:TYR:HD2	20	0.85	0.26	0.82
(1,2672)	1:70:A:VAL:HG13	1:88:A:TYR:HD1	20	0.85	0.26	0.82
(1,2672)	1:70:A:VAL:HG12	1:88:A:TYR:HD1	20	0.85	0.26	0.82
(1,2672)	1:70:A:VAL:HG12	1:88:A:TYR:HD2	20	0.85	0.26	0.82
(1,2177)	1:6:A:VAL:HG11	1:44:A:PHE:HD1	20	0.85	0.19	0.84
(1,2177)	1:6:A:VAL:HG12	1:44:A:PHE:HD1	20	0.85	0.19	0.84
(1,2177)	1:6:A:VAL:HG12	1:44:A:PHE:HD2	20	0.85	0.19	0.84
(1,2177)	1:6:A:VAL:HG13	1:44:A:PHE:HD2	20	0.85	0.19	0.84
(1,2177)	1:6:A:VAL:HG13	1:44:A:PHE:HD1	20	0.85	0.19	0.84
(1,725)	1:33:A:ILE:HD13	1:33:A:ILE:HA	20	0.83	0.04	0.84
(1,725)	1:33:A:ILE:HD12	1:33:A:ILE:HA	20	0.83	0.04	0.84
(1,725)	1:33:A:ILE:HD11	1:33:A:ILE:HA	20	0.83	0.04	0.84
(1,55)	1:80:A:VAL:HG12	1:80:A:VAL:H	20	0.83	0.04	0.83
(1,55)	1:80:A:VAL:HG13	1:80:A:VAL:H	20	0.83	0.04	0.83
(1,55)	1:80:A:VAL:HG11	1:80:A:VAL:H	20	0.83	0.04	0.83
(1,2654)	1:6:A:VAL:HA	1:107:A:MET:HE2	20	0.83	0.28	0.78
(1,2654)	1:6:A:VAL:HA	1:39:A:MET:HE3	20	0.83	0.28	0.78
(1,2654)	1:6:A:VAL:HA	1:107:A:MET:HE1	20	0.83	0.28	0.78
(1,2654)	1:6:A:VAL:HA	1:107:A:MET:HE3	20	0.83	0.28	0.78
(1,2654)	1:6:A:VAL:HA	1:39:A:MET:HE1	20	0.83	0.28	0.78
(1,1803)	1:10:A:LEU:HD12	1:109:A:LEU:HB2	20	0.82	0.29	0.72
(1,1803)	1:10:A:LEU:HD11	1:109:A:LEU:HB2	20	0.82	0.29	0.72
(1,1803)	1:10:A:LEU:HD13	1:109:A:LEU:HB2	20	0.82	0.29	0.72
(1,1840)	1:75:A:LYS:HG3	1:100:A:ILE:HG13	20	0.82	0.41	0.75
(1,15)	1:7:A:VAL:HG13	1:47:A:ALA:H	20	0.82	0.14	0.82
(1,15)	1:7:A:VAL:HG12	1:47:A:ALA:H	20	0.82	0.14	0.82
(1,15)	1:7:A:VAL:HG11	1:47:A:ALA:H	20	0.82	0.14	0.82

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,330)	1:68:A:GLU:HG2	1:33:A:ILE:H	20	0.82	0.16	0.8
(1,148)	1:6:A:VAL:HG12	1:9:A:SER:H	20	0.82	0.09	0.82
(1,148)	1:6:A:VAL:HG11	1:9:A:SER:H	20	0.82	0.09	0.82
(1,148)	1:6:A:VAL:HG13	1:9:A:SER:H	20	0.82	0.09	0.82
(1,805)	1:7:A:VAL:HG21	1:48:A:PHE:HB3	20	0.8	0.17	0.86
(1,805)	1:7:A:VAL:HG23	1:48:A:PHE:HB3	20	0.8	0.17	0.86
(1,805)	1:7:A:VAL:HG22	1:48:A:PHE:HB3	20	0.8	0.17	0.86
(1,100)	1:57:A:VAL:HG12	1:57:A:VAL:H	20	0.8	0.03	0.8
(1,100)	1:57:A:VAL:HG11	1:57:A:VAL:H	20	0.8	0.03	0.8
(1,100)	1:57:A:VAL:HG13	1:57:A:VAL:H	20	0.8	0.03	0.8
(1,804)	1:66:A:VAL:HG12	1:32:A:GLY:HA3	20	0.79	0.15	0.81
(1,804)	1:66:A:VAL:HG13	1:32:A:GLY:HA3	20	0.79	0.15	0.81
(1,804)	1:66:A:VAL:HG11	1:32:A:GLY:HA3	20	0.79	0.15	0.81
(1,2590)	1:33:A:ILE:HD13	1:39:A:MET:HG2	20	0.79	0.4	0.89
(1,2590)	1:33:A:ILE:HD12	1:39:A:MET:HG2	20	0.79	0.4	0.89
(1,2590)	1:33:A:ILE:HD13	1:39:A:MET:HG3	20	0.79	0.4	0.89
(1,2590)	1:33:A:ILE:HD11	1:39:A:MET:HG2	20	0.79	0.4	0.89
(1,2606)	1:57:A:VAL:HG12	1:26:A:ILE:HA	20	0.79	0.11	0.81
(1,2606)	1:57:A:VAL:HG13	1:26:A:ILE:HA	20	0.79	0.11	0.81
(1,2606)	1:57:A:VAL:HG11	1:26:A:ILE:HA	20	0.79	0.11	0.81
(1,760)	1:110:A:LEU:HD11	1:110:A:LEU:HA	20	0.79	0.04	0.78
(1,760)	1:110:A:LEU:HD13	1:110:A:LEU:HA	20	0.79	0.04	0.78
(1,760)	1:110:A:LEU:HD12	1:110:A:LEU:HA	20	0.79	0.04	0.78
(1,2023)	1:7:A:VAL:HA	1:11:A:ILE:HD12	20	0.78	0.15	0.81
(1,2023)	1:7:A:VAL:HA	1:11:A:ILE:HD11	20	0.78	0.15	0.81
(1,2023)	1:7:A:VAL:HA	1:11:A:ILE:HD13	20	0.78	0.15	0.81
(1,44)	1:99:A:VAL:HG13	1:73:A:GLU:H	20	0.78	0.16	0.8
(1,44)	1:99:A:VAL:HG12	1:73:A:GLU:H	20	0.78	0.16	0.8
(1,44)	1:99:A:VAL:HG11	1:73:A:GLU:H	20	0.78	0.16	0.8
(1,2047)	1:33:A:ILE:HG22	1:37:A:SER:HA	20	0.77	0.15	0.78
(1,2047)	1:33:A:ILE:HG23	1:37:A:SER:HA	20	0.77	0.15	0.78
(1,2047)	1:33:A:ILE:HG21	1:37:A:SER:HA	20	0.77	0.15	0.78
(1,2657)	1:20:A:LYS:HE2	1:20:A:LYS:HA	20	0.77	0.18	0.82
(1,2657)	1:20:A:LYS:HE3	1:20:A:LYS:HA	20	0.77	0.18	0.82
(1,2657)	1:56:A:LEU:HA	1:25:A:LYS:HE3	20	0.77	0.18	0.82
(1,253)	1:68:A:GLU:HG3	1:69:A:LYS:H	20	0.77	0.06	0.78
(1,2638)	1:107:A:MET:HA	1:107:A:MET:HE2	20	0.77	0.22	0.8
(1,2638)	1:107:A:MET:HA	1:39:A:MET:HE1	20	0.77	0.22	0.8
(1,2638)	1:107:A:MET:HA	1:107:A:MET:HE1	20	0.77	0.22	0.8
(1,2638)	1:107:A:MET:HA	1:39:A:MET:HE2	20	0.77	0.22	0.8
(1,2638)	1:107:A:MET:HA	1:107:A:MET:HE3	20	0.77	0.22	0.8
(1,2638)	1:107:A:MET:HA	1:39:A:MET:HE3	20	0.77	0.22	0.8

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1606)	1:10:A:LEU:HD21	1:10:A:LEU:HA	20	0.76	0.05	0.75
(1,1606)	1:10:A:LEU:HD23	1:10:A:LEU:HA	20	0.76	0.05	0.75
(1,1606)	1:10:A:LEU:HD22	1:10:A:LEU:HA	20	0.76	0.05	0.75
(1,1907)	1:25:A:LYS:HB2	1:57:A:VAL:HG12	20	0.73	0.17	0.75
(1,1907)	1:25:A:LYS:HB2	1:57:A:VAL:HG11	20	0.73	0.17	0.75
(1,1907)	1:25:A:LYS:HB2	1:57:A:VAL:HG13	20	0.73	0.17	0.75
(1,1739)	1:33:A:ILE:HG23	1:65:A:ILE:HG21	20	0.73	0.11	0.73
(1,1739)	1:33:A:ILE:HG21	1:65:A:ILE:HG21	20	0.73	0.11	0.73
(1,1739)	1:33:A:ILE:HG23	1:65:A:ILE:HG22	20	0.73	0.11	0.73
(1,1739)	1:33:A:ILE:HG22	1:65:A:ILE:HG23	20	0.73	0.11	0.73
(1,1739)	1:33:A:ILE:HG22	1:65:A:ILE:HG22	20	0.73	0.11	0.73
(1,1739)	1:33:A:ILE:HG22	1:65:A:ILE:HG21	20	0.73	0.11	0.73
(1,1739)	1:33:A:ILE:HG23	1:65:A:ILE:HG23	20	0.73	0.11	0.73
(1,1739)	1:33:A:ILE:HG21	1:65:A:ILE:HG22	20	0.73	0.11	0.73
(1,1739)	1:33:A:ILE:HG21	1:65:A:ILE:HG23	20	0.73	0.11	0.73
(1,2163)	1:45:A:VAL:HG23	1:44:A:PHE:HD2	20	0.72	0.11	0.7
(1,2163)	1:45:A:VAL:HG21	1:44:A:PHE:HD1	20	0.72	0.11	0.7
(1,2163)	1:45:A:VAL:HG22	1:44:A:PHE:HD2	20	0.72	0.11	0.7
(1,2163)	1:45:A:VAL:HG23	1:44:A:PHE:HD1	20	0.72	0.11	0.7
(1,2163)	1:45:A:VAL:HG21	1:44:A:PHE:HD2	20	0.72	0.11	0.7
(1,2463)	1:56:A:LEU:HD23	1:56:A:LEU:HD13	20	0.72	0.05	0.72
(1,2463)	1:56:A:LEU:HD22	1:56:A:LEU:HD11	20	0.72	0.05	0.72
(1,2463)	1:56:A:LEU:HD23	1:56:A:LEU:HD12	20	0.72	0.05	0.72
(1,2463)	1:56:A:LEU:HD21	1:56:A:LEU:HD12	20	0.72	0.05	0.72
(1,2463)	1:43:A:LEU:HD22	1:43:A:LEU:HD13	20	0.72	0.05	0.72
(1,2463)	1:43:A:LEU:HD22	1:43:A:LEU:HD12	20	0.72	0.05	0.72
(1,2463)	1:43:A:LEU:HD23	1:43:A:LEU:HD13	20	0.72	0.05	0.72
(1,2463)	1:43:A:LEU:HD21	1:43:A:LEU:HD12	20	0.72	0.05	0.72
(1,2463)	1:43:A:LEU:HD21	1:43:A:LEU:HD13	20	0.72	0.05	0.72
(1,2463)	1:43:A:LEU:HD22	1:43:A:LEU:HD11	20	0.72	0.05	0.72
(1,176)	1:18:A:ALA:HB1	1:16:A:GLU:H	20	0.72	0.08	0.74
(1,176)	1:18:A:ALA:HB2	1:16:A:GLU:H	20	0.72	0.08	0.74
(1,176)	1:18:A:ALA:HB3	1:16:A:GLU:H	20	0.72	0.08	0.74
(1,1482)	1:7:A:VAL:HG21	1:48:A:PHE:HA	20	0.72	0.21	0.72
(1,1482)	1:7:A:VAL:HG23	1:48:A:PHE:HA	20	0.72	0.21	0.72
(1,1482)	1:7:A:VAL:HG22	1:48:A:PHE:HA	20	0.72	0.21	0.72
(1,110)	1:43:A:LEU:HD22	1:44:A:PHE:H	20	0.72	0.06	0.7
(1,110)	1:43:A:LEU:HD21	1:44:A:PHE:H	20	0.72	0.06	0.7
(1,110)	1:43:A:LEU:HD23	1:44:A:PHE:H	20	0.72	0.06	0.7
(1,2457)	1:43:A:LEU:HD22	1:43:A:LEU:HD23	20	0.71	0.01	0.71
(1,2457)	1:43:A:LEU:HD22	1:43:A:LEU:HD21	20	0.71	0.01	0.71
(1,2457)	1:10:A:LEU:HD11	1:10:A:LEU:HD13	20	0.71	0.01	0.71

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2457)	1:10:A:LEU:HD12	1:10:A:LEU:HD13	20	0.71	0.01	0.71
(1,2457)	1:10:A:LEU:HD12	1:10:A:LEU:HD11	20	0.71	0.01	0.71
(1,2457)	1:43:A:LEU:HD21	1:43:A:LEU:HD23	20	0.71	0.01	0.71
(1,2457)	1:56:A:LEU:HD22	1:56:A:LEU:HD23	20	0.71	0.01	0.71
(1,2457)	1:56:A:LEU:HD22	1:56:A:LEU:HD21	20	0.71	0.01	0.71
(1,195)	1:12:A:ALA:HB1	1:15:A:GLU:H	20	0.71	0.09	0.7
(1,195)	1:12:A:ALA:HB3	1:15:A:GLU:H	20	0.71	0.09	0.7
(1,195)	1:12:A:ALA:HB2	1:15:A:GLU:H	20	0.71	0.09	0.7
(1,921)	1:45:A:VAL:HG21	1:45:A:VAL:HA	20	0.71	0.03	0.72
(1,921)	1:45:A:VAL:HG22	1:45:A:VAL:HA	20	0.71	0.03	0.72
(1,921)	1:45:A:VAL:HG23	1:45:A:VAL:HA	20	0.71	0.03	0.72
(1,1825)	1:62:A:ILE:HG21	1:62:A:ILE:HG13	20	0.71	0.03	0.71
(1,1825)	1:62:A:ILE:HG23	1:62:A:ILE:HG13	20	0.71	0.03	0.71
(1,1825)	1:62:A:ILE:HG22	1:62:A:ILE:HG13	20	0.71	0.03	0.71
(1,120)	1:13:A:LEU:HD12	1:13:A:LEU:H	20	0.7	0.09	0.71
(1,120)	1:13:A:LEU:HD11	1:13:A:LEU:H	20	0.7	0.09	0.71
(1,120)	1:13:A:LEU:HD13	1:13:A:LEU:H	20	0.7	0.09	0.71
(1,123)	1:13:A:LEU:HD13	1:14:A:CYS:H	20	0.7	0.06	0.7
(1,123)	1:13:A:LEU:HD12	1:14:A:CYS:H	20	0.7	0.06	0.7
(1,123)	1:13:A:LEU:HD11	1:14:A:CYS:H	20	0.7	0.06	0.7
(1,2091)	1:65:A:ILE:HA	1:31:A:VAL:HG12	20	0.7	0.14	0.72
(1,2091)	1:65:A:ILE:HA	1:31:A:VAL:HG13	20	0.7	0.14	0.72
(1,2091)	1:65:A:ILE:HA	1:31:A:VAL:HG11	20	0.7	0.14	0.72
(1,1597)	1:109:A:LEU:HD11	1:109:A:LEU:HA	20	0.69	0.04	0.68
(1,1597)	1:109:A:LEU:HD13	1:109:A:LEU:HA	20	0.69	0.04	0.68
(1,1597)	1:109:A:LEU:HD12	1:109:A:LEU:HA	20	0.69	0.04	0.68
(1,2597)	1:72:A:LEU:HB2	1:99:A:VAL:HG23	20	0.69	0.18	0.62
(1,2597)	1:72:A:LEU:HB2	1:99:A:VAL:HG22	20	0.69	0.18	0.62
(1,2597)	1:72:A:LEU:HB2	1:99:A:VAL:HG21	20	0.69	0.18	0.62
(1,2597)	1:72:A:LEU:HB2	1:80:A:VAL:HG11	20	0.69	0.18	0.62
(1,1514)	1:43:A:LEU:HD22	1:42:A:SER:HB3	20	0.69	0.19	0.66
(1,1514)	1:43:A:LEU:HD21	1:42:A:SER:HB2	20	0.69	0.19	0.66
(1,1514)	1:43:A:LEU:HD23	1:42:A:SER:HB2	20	0.69	0.19	0.66
(1,1514)	1:43:A:LEU:HD23	1:42:A:SER:HB3	20	0.69	0.19	0.66
(1,1514)	1:43:A:LEU:HD22	1:42:A:SER:HB2	20	0.69	0.19	0.66
(1,1514)	1:43:A:LEU:HD21	1:42:A:SER:HB3	20	0.69	0.19	0.66
(1,2651)	1:7:A:VAL:HA	1:48:A:PHE:HA	20	0.69	0.09	0.7
(1,2651)	1:45:A:VAL:HA	1:48:A:PHE:HA	20	0.69	0.09	0.7
(1,862)	1:109:A:LEU:HD23	1:13:A:LEU:HD21	20	0.68	0.27	0.72
(1,862)	1:109:A:LEU:HD21	1:13:A:LEU:HD23	20	0.68	0.27	0.72
(1,862)	1:109:A:LEU:HD23	1:13:A:LEU:HD22	20	0.68	0.27	0.72
(1,862)	1:109:A:LEU:HD23	1:13:A:LEU:HD23	20	0.68	0.27	0.72

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,862)	1:109:A:LEU:HD21	1:13:A:LEU:HD21	20	0.68	0.27	0.72
(1,862)	1:109:A:LEU:HD22	1:13:A:LEU:HD21	20	0.68	0.27	0.72
(1,862)	1:109:A:LEU:HD21	1:13:A:LEU:HD22	20	0.68	0.27	0.72
(1,862)	1:109:A:LEU:HD22	1:13:A:LEU:HD22	20	0.68	0.27	0.72
(1,862)	1:109:A:LEU:HD22	1:13:A:LEU:HD23	20	0.68	0.27	0.72
(1,7)	1:72:A:LEU:HD11	1:73:A:GLU:H	20	0.67	0.1	0.67
(1,7)	1:72:A:LEU:HD12	1:73:A:GLU:H	20	0.67	0.1	0.67
(1,7)	1:72:A:LEU:HD13	1:73:A:GLU:H	20	0.67	0.1	0.67
(1,144)	1:47:A:ALA:HB2	1:50:A:THR:H	20	0.67	0.07	0.66
(1,144)	1:47:A:ALA:HB3	1:50:A:THR:H	20	0.67	0.07	0.66
(1,144)	1:47:A:ALA:HB1	1:50:A:THR:H	20	0.67	0.07	0.66
(1,50)	1:7:A:VAL:HG22	1:8:A:SER:H	20	0.66	0.05	0.65
(1,50)	1:7:A:VAL:HG21	1:8:A:SER:H	20	0.66	0.05	0.65
(1,50)	1:7:A:VAL:HG23	1:8:A:SER:H	20	0.66	0.05	0.65
(1,2605)	1:115:A:LEU:HD12	1:115:A:LEU:HD13	20	0.66	0.01	0.66
(1,2605)	1:86:A:LEU:HD11	1:86:A:LEU:HD13	20	0.66	0.01	0.66
(1,2605)	1:86:A:LEU:HD12	1:86:A:LEU:HD13	20	0.66	0.01	0.66
(1,2605)	1:86:A:LEU:HD12	1:86:A:LEU:HD11	20	0.66	0.01	0.66
(1,2605)	1:115:A:LEU:HD11	1:115:A:LEU:HD13	20	0.66	0.01	0.66
(1,2605)	1:115:A:LEU:HD12	1:115:A:LEU:HD11	20	0.66	0.01	0.66
(1,2613)	1:43:A:LEU:HD11	1:43:A:LEU:HD13	20	0.65	0.01	0.65
(1,2613)	1:56:A:LEU:HD12	1:56:A:LEU:HD11	20	0.65	0.01	0.65
(1,2613)	1:56:A:LEU:HD12	1:56:A:LEU:HD13	20	0.65	0.01	0.65
(1,2613)	1:43:A:LEU:HD12	1:43:A:LEU:HD13	20	0.65	0.01	0.65
(1,2613)	1:56:A:LEU:HD11	1:56:A:LEU:HD13	20	0.65	0.01	0.65
(1,2613)	1:43:A:LEU:HD12	1:43:A:LEU:HD11	20	0.65	0.01	0.65
(1,1753)	1:65:A:ILE:HD11	1:41:A:LYS:HD3	20	0.65	0.13	0.65
(1,1753)	1:65:A:ILE:HD13	1:41:A:LYS:HD3	20	0.65	0.13	0.65
(1,1753)	1:65:A:ILE:HD12	1:41:A:LYS:HD3	20	0.65	0.13	0.65
(1,1751)	1:65:A:ILE:HD11	1:33:A:ILE:HG23	20	0.65	0.14	0.61
(1,1751)	1:65:A:ILE:HD12	1:33:A:ILE:HG21	20	0.65	0.14	0.61
(1,1751)	1:65:A:ILE:HD13	1:33:A:ILE:HG23	20	0.65	0.14	0.61
(1,1751)	1:65:A:ILE:HD13	1:33:A:ILE:HG22	20	0.65	0.14	0.61
(1,1751)	1:65:A:ILE:HD11	1:33:A:ILE:HG21	20	0.65	0.14	0.61
(1,1751)	1:65:A:ILE:HD12	1:33:A:ILE:HG23	20	0.65	0.14	0.61
(1,1751)	1:65:A:ILE:HD12	1:33:A:ILE:HG22	20	0.65	0.14	0.61
(1,1751)	1:65:A:ILE:HD13	1:33:A:ILE:HG21	20	0.65	0.14	0.61
(1,2089)	1:79:A:HIS:HA	1:80:A:VAL:HG22	20	0.65	0.12	0.64
(1,2089)	1:79:A:HIS:HA	1:80:A:VAL:HG23	20	0.65	0.12	0.64
(1,2089)	1:79:A:HIS:HA	1:80:A:VAL:HG21	20	0.65	0.12	0.64
(1,2618)	1:6:A:VAL:HG23	1:2:A:HIS:HB2	20	0.64	0.18	0.63
(1,2618)	1:6:A:VAL:HG22	1:2:A:HIS:HB2	20	0.64	0.18	0.63

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2618)	1:6:A:VAL:HG21	1:2:A:HIS:HB2	20	0.64	0.18	0.63
(1,1420)	1:25:A:LYS:HE2	1:25:A:LYS:HB3	20	0.64	0.23	0.54
(1,1420)	1:25:A:LYS:HE3	1:25:A:LYS:HB3	20	0.64	0.23	0.54
(1,1420)	1:25:A:LYS:HE3	1:25:A:LYS:HB2	20	0.64	0.23	0.54
(1,2639)	1:107:A:MET:HE2	1:107:A:MET:HE1	20	0.64	0.01	0.64
(1,2639)	1:114:A:MET:HE2	1:114:A:MET:HE1	20	0.64	0.01	0.64
(1,2639)	1:114:A:MET:HE2	1:114:A:MET:HE3	20	0.64	0.01	0.64
(1,2639)	1:107:A:MET:HE2	1:107:A:MET:HE3	20	0.64	0.01	0.64
(1,2639)	1:39:A:MET:HE2	1:39:A:MET:HE1	20	0.64	0.01	0.64
(1,2639)	1:107:A:MET:HE1	1:107:A:MET:HE3	20	0.64	0.01	0.64
(1,2639)	1:39:A:MET:HE1	1:39:A:MET:HE3	20	0.64	0.01	0.64
(1,2639)	1:114:A:MET:HE1	1:114:A:MET:HE3	20	0.64	0.01	0.64
(1,2639)	1:39:A:MET:HE2	1:39:A:MET:HE3	20	0.64	0.01	0.64
(1,1248)	1:13:A:LEU:HD12	1:13:A:LEU:HB3	20	0.64	0.04	0.64
(1,1248)	1:13:A:LEU:HD11	1:13:A:LEU:HB3	20	0.64	0.04	0.64
(1,1248)	1:13:A:LEU:HD13	1:13:A:LEU:HB3	20	0.64	0.04	0.64
(1,828)	1:101:A:ILE:HG23	1:101:A:ILE:HG13	20	0.63	0.03	0.63
(1,828)	1:101:A:ILE:HG22	1:101:A:ILE:HG13	20	0.63	0.03	0.63
(1,828)	1:101:A:ILE:HG21	1:101:A:ILE:HG13	20	0.63	0.03	0.63
(1,70)	1:112:A:LEU:HD22	1:17:A:HIS:H	20	0.62	0.21	0.6
(1,70)	1:112:A:LEU:HD21	1:17:A:HIS:H	20	0.62	0.21	0.6
(1,70)	1:112:A:LEU:HD23	1:17:A:HIS:H	20	0.62	0.21	0.6
(1,937)	1:102:A:THR:HG23	1:73:A:GLU:HA	20	0.62	0.12	0.58
(1,937)	1:102:A:THR:HG21	1:73:A:GLU:HA	20	0.62	0.12	0.58
(1,937)	1:102:A:THR:HG22	1:73:A:GLU:HA	20	0.62	0.12	0.58
(1,2642)	1:39:A:MET:HE2	1:39:A:MET:HE1	20	0.62	0.01	0.62
(1,2642)	1:114:A:MET:HE2	1:114:A:MET:HE1	20	0.62	0.01	0.62
(1,2642)	1:114:A:MET:HE2	1:114:A:MET:HE3	20	0.62	0.01	0.62
(1,2642)	1:39:A:MET:HE2	1:39:A:MET:HE3	20	0.62	0.01	0.62
(1,2642)	1:39:A:MET:HE1	1:39:A:MET:HE3	20	0.62	0.01	0.62
(1,2642)	1:114:A:MET:HE1	1:114:A:MET:HE3	20	0.62	0.01	0.62
(1,2158)	1:29:A:VAL:HG11	1:48:A:PHE:HZ	20	0.62	0.26	0.57
(1,2158)	1:29:A:VAL:HG12	1:48:A:PHE:HZ	20	0.62	0.26	0.57
(1,2158)	1:29:A:VAL:HG13	1:48:A:PHE:HZ	20	0.62	0.26	0.57
(1,2586)	1:31:A:VAL:HA	1:31:A:VAL:HG22	20	0.62	0.04	0.61
(1,2586)	1:31:A:VAL:HA	1:31:A:VAL:HG21	20	0.62	0.04	0.61
(1,2586)	1:31:A:VAL:HA	1:31:A:VAL:HG23	20	0.62	0.04	0.61
(1,130)	1:10:A:LEU:HD22	1:10:A:LEU:H	20	0.61	0.08	0.63
(1,130)	1:10:A:LEU:HD23	1:10:A:LEU:H	20	0.61	0.08	0.63
(1,130)	1:10:A:LEU:HD21	1:10:A:LEU:H	20	0.61	0.08	0.63
(1,1697)	1:112:A:LEU:HD23	1:112:A:LEU:HA	20	0.61	0.04	0.61
(1,1697)	1:112:A:LEU:HD22	1:112:A:LEU:HA	20	0.61	0.04	0.61

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1697)	1:112:A:LEU:HD21	1:112:A:LEU:HA	20	0.61	0.04	0.61
(1,1020)	1:85:A:ALA:HB2	1:86:A:LEU:HA	20	0.61	0.1	0.62
(1,1020)	1:85:A:ALA:HB3	1:86:A:LEU:HA	20	0.61	0.1	0.62
(1,1020)	1:85:A:ALA:HB1	1:86:A:LEU:HA	20	0.61	0.1	0.62
(1,2652)	1:45:A:VAL:HA	1:47:A:ALA:HB1	20	0.59	0.1	0.57
(1,2652)	1:45:A:VAL:HA	1:47:A:ALA:HB3	20	0.59	0.1	0.57
(1,2652)	1:45:A:VAL:HA	1:47:A:ALA:HB2	20	0.59	0.1	0.57
(1,2459)	1:115:A:LEU:HD22	1:115:A:LEU:HD21	20	0.59	0.01	0.59
(1,2459)	1:86:A:LEU:HD11	1:86:A:LEU:HD13	20	0.59	0.01	0.59
(1,2459)	1:86:A:LEU:HD12	1:86:A:LEU:HD13	20	0.59	0.01	0.59
(1,2459)	1:115:A:LEU:HD21	1:115:A:LEU:HD23	20	0.59	0.01	0.59
(1,2459)	1:115:A:LEU:HD11	1:115:A:LEU:HD13	20	0.59	0.01	0.59
(1,2459)	1:115:A:LEU:HD22	1:115:A:LEU:HD23	20	0.59	0.01	0.59
(1,2459)	1:86:A:LEU:HD12	1:86:A:LEU:HD11	20	0.59	0.01	0.59
(1,2459)	1:115:A:LEU:HD12	1:115:A:LEU:HD11	20	0.59	0.01	0.59
(1,2459)	1:115:A:LEU:HD12	1:115:A:LEU:HD13	20	0.59	0.01	0.59
(1,923)	1:57:A:VAL:HG21	1:56:A:LEU:HB2	20	0.57	0.09	0.57
(1,923)	1:57:A:VAL:HG23	1:56:A:LEU:HB2	20	0.57	0.09	0.57
(1,923)	1:57:A:VAL:HG22	1:56:A:LEU:HB2	20	0.57	0.09	0.57
(1,2133)	1:65:A:ILE:HG21	1:44:A:PHE:HD2	20	0.56	0.09	0.58
(1,2133)	1:65:A:ILE:HG22	1:44:A:PHE:HD1	20	0.56	0.09	0.58
(1,2133)	1:65:A:ILE:HG23	1:44:A:PHE:HD2	20	0.56	0.09	0.58
(1,2133)	1:65:A:ILE:HG22	1:44:A:PHE:HD2	20	0.56	0.09	0.58
(1,2133)	1:65:A:ILE:HG21	1:44:A:PHE:HD1	20	0.56	0.09	0.58
(1,2133)	1:65:A:ILE:HG23	1:44:A:PHE:HD1	20	0.56	0.09	0.58
(1,1939)	1:39:A:MET:HE1	1:39:A:MET:HA	20	0.56	0.11	0.57
(1,1939)	1:39:A:MET:HE2	1:39:A:MET:HA	20	0.56	0.11	0.57
(1,1939)	1:39:A:MET:HE3	1:39:A:MET:HA	20	0.56	0.11	0.57
(1,2069)	1:112:A:LEU:HD23	1:29:A:VAL:HA	20	0.56	0.17	0.6
(1,2069)	1:112:A:LEU:HD22	1:29:A:VAL:HA	20	0.56	0.17	0.6
(1,2069)	1:112:A:LEU:HD21	1:29:A:VAL:HA	20	0.56	0.17	0.6
(1,2594)	1:66:A:VAL:HG12	1:66:A:VAL:HG13	20	0.56	0.01	0.56
(1,2594)	1:66:A:VAL:HG22	1:66:A:VAL:HG23	20	0.56	0.01	0.56
(1,2594)	1:66:A:VAL:HG21	1:66:A:VAL:HG23	20	0.56	0.01	0.56
(1,2594)	1:90:A:VAL:HG12	1:90:A:VAL:HG11	20	0.56	0.01	0.56
(1,2594)	1:66:A:VAL:HG12	1:66:A:VAL:HG11	20	0.56	0.01	0.56
(1,2594)	1:90:A:VAL:HG12	1:90:A:VAL:HG13	20	0.56	0.01	0.56
(1,2594)	1:66:A:VAL:HG22	1:66:A:VAL:HG21	20	0.56	0.01	0.56
(1,37)	1:99:A:VAL:HG12	1:99:A:VAL:H	20	0.56	0.06	0.56
(1,37)	1:99:A:VAL:HG11	1:99:A:VAL:H	20	0.56	0.06	0.56
(1,37)	1:99:A:VAL:HG13	1:99:A:VAL:H	20	0.56	0.06	0.56
(1,1708)	1:107:A:MET:HA	1:33:A:ILE:HD13	20	0.55	0.19	0.52

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1708)	1:107:A:MET:HA	1:33:A:ILE:HD12	20	0.55	0.19	0.52
(1,1708)	1:107:A:MET:HA	1:33:A:ILE:HD11	20	0.55	0.19	0.52
(1,197)	1:12:A:ALA:HB1	1:16:A:GLU:H	20	0.55	0.11	0.54
(1,197)	1:12:A:ALA:HB3	1:16:A:GLU:H	20	0.55	0.11	0.54
(1,197)	1:12:A:ALA:HB2	1:16:A:GLU:H	20	0.55	0.11	0.54
(1,1026)	1:116:A:ALA:HB2	1:116:A:ALA:HB3	20	0.55	0.01	0.55
(1,1026)	1:116:A:ALA:HB2	1:116:A:ALA:HB1	20	0.55	0.01	0.55
(1,1026)	1:116:A:ALA:HB1	1:116:A:ALA:HB3	20	0.55	0.01	0.55
(1,1793)	1:15:A:GLU:HG2	1:11:A:ILE:HG21	20	0.54	0.12	0.53
(1,1793)	1:15:A:GLU:HG2	1:11:A:ILE:HG23	20	0.54	0.12	0.53
(1,1793)	1:15:A:GLU:HG2	1:11:A:ILE:HG22	20	0.54	0.12	0.53
(1,2079)	1:71:A:GLU:HB2	1:103:A:GLN:HA	20	0.54	0.2	0.48
(1,765)	1:90:A:VAL:HG22	1:90:A:VAL:HG23	20	0.53	0.02	0.54
(1,765)	1:90:A:VAL:HG22	1:90:A:VAL:HG21	20	0.53	0.02	0.54
(1,765)	1:90:A:VAL:HG21	1:90:A:VAL:HG23	20	0.53	0.02	0.54
(1,2180)	1:61:A:ALA:HB1	1:48:A:PHE:HD2	20	0.53	0.25	0.55
(1,2180)	1:61:A:ALA:HB2	1:48:A:PHE:HD2	20	0.53	0.25	0.55
(1,2180)	1:61:A:ALA:HB1	1:48:A:PHE:HD1	20	0.53	0.25	0.55
(1,2180)	1:61:A:ALA:HB3	1:48:A:PHE:HD2	20	0.53	0.25	0.55
(1,2180)	1:61:A:ALA:HB3	1:48:A:PHE:HD1	20	0.53	0.25	0.55
(1,2445)	1:80:A:VAL:HG11	1:80:A:VAL:HG13	20	0.53	0.01	0.53
(1,2445)	1:31:A:VAL:HG22	1:31:A:VAL:HG23	20	0.53	0.01	0.53
(1,2445)	1:30:A:VAL:HG22	1:30:A:VAL:HG21	20	0.53	0.01	0.53
(1,2445)	1:29:A:VAL:HG22	1:29:A:VAL:HG21	20	0.53	0.01	0.53
(1,2445)	1:29:A:VAL:HG21	1:29:A:VAL:HG23	20	0.53	0.01	0.53
(1,2445)	1:80:A:VAL:HG12	1:80:A:VAL:HG13	20	0.53	0.01	0.53
(1,2445)	1:30:A:VAL:HG22	1:30:A:VAL:HG23	20	0.53	0.01	0.53
(1,2445)	1:80:A:VAL:HG12	1:80:A:VAL:HG11	20	0.53	0.01	0.53
(1,2445)	1:31:A:VAL:HG21	1:31:A:VAL:HG23	20	0.53	0.01	0.53
(1,2464)	1:45:A:VAL:HG21	1:45:A:VAL:HG23	20	0.53	0.01	0.53
(1,2464)	1:50:A:THR:HG21	1:50:A:THR:HG22	20	0.53	0.01	0.53
(1,2464)	1:45:A:VAL:HG22	1:45:A:VAL:HG21	20	0.53	0.01	0.53
(1,2464)	1:57:A:VAL:HG21	1:57:A:VAL:HG23	20	0.53	0.01	0.53
(1,2464)	1:50:A:THR:HG21	1:50:A:THR:HG23	20	0.53	0.01	0.53
(1,2464)	1:57:A:VAL:HG22	1:57:A:VAL:HG21	20	0.53	0.01	0.53
(1,2464)	1:57:A:VAL:HG22	1:57:A:VAL:HG23	20	0.53	0.01	0.53
(1,2464)	1:45:A:VAL:HG22	1:45:A:VAL:HG23	20	0.53	0.01	0.53
(1,2464)	1:50:A:THR:HG22	1:50:A:THR:HG23	20	0.53	0.01	0.53
(1,2206)	1:83:A:PRO:HB2	1:81:A:PHE:HD1	20	0.53	0.2	0.51
(1,2206)	1:83:A:PRO:HB2	1:81:A:PHE:HD2	20	0.53	0.2	0.51
(1,1842)	1:18:A:ALA:HB3	1:21:A:ASN:HB3	20	0.52	0.17	0.5
(1,1842)	1:18:A:ALA:HB2	1:21:A:ASN:HB3	20	0.52	0.17	0.5

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1842)	1:18:A:ALA:HB1	1:21:A:ASN:HB3	20	0.52	0.17	0.5
(1,1021)	1:85:A:ALA:HB1	1:85:A:ALA:HB3	20	0.52	0.02	0.52
(1,1021)	1:85:A:ALA:HB2	1:85:A:ALA:HB1	20	0.52	0.02	0.52
(1,1021)	1:85:A:ALA:HB2	1:85:A:ALA:HB3	20	0.52	0.02	0.52
(1,126)	1:45:A:VAL:HG21	1:47:A:ALA:H	20	0.52	0.08	0.53
(1,126)	1:45:A:VAL:HG22	1:47:A:ALA:H	20	0.52	0.08	0.53
(1,126)	1:45:A:VAL:HG23	1:47:A:ALA:H	20	0.52	0.08	0.53
(1,2474)	1:18:A:ALA:HB1	1:19:A:LYS:HA	20	0.52	0.08	0.55
(1,2474)	1:18:A:ALA:HB2	1:19:A:LYS:HA	20	0.52	0.08	0.55
(1,2474)	1:18:A:ALA:HB3	1:19:A:LYS:HA	20	0.52	0.08	0.55
(1,910)	1:109:A:LEU:HD12	1:13:A:LEU:HD11	20	0.51	0.17	0.5
(1,910)	1:109:A:LEU:HD11	1:13:A:LEU:HD13	20	0.51	0.17	0.5
(1,910)	1:109:A:LEU:HD12	1:13:A:LEU:HD12	20	0.51	0.17	0.5
(1,910)	1:109:A:LEU:HD13	1:13:A:LEU:HD11	20	0.51	0.17	0.5
(1,910)	1:109:A:LEU:HD12	1:13:A:LEU:HD13	20	0.51	0.17	0.5
(1,910)	1:109:A:LEU:HD11	1:13:A:LEU:HD12	20	0.51	0.17	0.5
(1,910)	1:109:A:LEU:HD11	1:13:A:LEU:HD11	20	0.51	0.17	0.5
(1,910)	1:109:A:LEU:HD13	1:13:A:LEU:HD13	20	0.51	0.17	0.5
(1,910)	1:109:A:LEU:HD13	1:13:A:LEU:HD12	20	0.51	0.17	0.5
(1,2426)	1:97:A:LYS:HD3	1:97:A:LYS:H	20	0.51	0.19	0.46
(1,2426)	1:25:A:LYS:HD2	1:115:A:LEU:H	20	0.51	0.19	0.46
(1,2426)	1:25:A:LYS:HD3	1:115:A:LEU:H	20	0.51	0.19	0.46
(1,2084)	1:58:A:CYS:HA	1:26:A:ILE:HG23	20	0.51	0.16	0.52
(1,2084)	1:58:A:CYS:HA	1:26:A:ILE:HG22	20	0.51	0.16	0.52
(1,2084)	1:58:A:CYS:HA	1:26:A:ILE:HG21	20	0.51	0.16	0.52
(1,1269)	1:80:A:VAL:HG23	1:73:A:GLU:HG2	20	0.51	0.16	0.47
(1,1269)	1:80:A:VAL:HG22	1:73:A:GLU:HG2	20	0.51	0.16	0.47
(1,1269)	1:80:A:VAL:HG21	1:73:A:GLU:HG2	20	0.51	0.16	0.47
(1,208)	1:41:A:LYS:HG2	1:42:A:SER:H	20	0.51	0.05	0.51
(1,53)	1:66:A:VAL:HG12	1:33:A:ILE:H	20	0.51	0.11	0.52
(1,53)	1:66:A:VAL:HG13	1:33:A:ILE:H	20	0.51	0.11	0.52
(1,53)	1:66:A:VAL:HG11	1:33:A:ILE:H	20	0.51	0.11	0.52
(1,809)	1:110:A:LEU:HD13	1:66:A:VAL:HG13	20	0.51	0.12	0.52
(1,809)	1:110:A:LEU:HD11	1:66:A:VAL:HG11	20	0.51	0.12	0.52
(1,809)	1:110:A:LEU:HD12	1:66:A:VAL:HG13	20	0.51	0.12	0.52
(1,809)	1:110:A:LEU:HD13	1:66:A:VAL:HG11	20	0.51	0.12	0.52
(1,809)	1:110:A:LEU:HD11	1:66:A:VAL:HG12	20	0.51	0.12	0.52
(1,809)	1:110:A:LEU:HD12	1:66:A:VAL:HG11	20	0.51	0.12	0.52
(1,809)	1:110:A:LEU:HD13	1:66:A:VAL:HG12	20	0.51	0.12	0.52
(1,809)	1:110:A:LEU:HD12	1:66:A:VAL:HG12	20	0.51	0.12	0.52
(1,809)	1:110:A:LEU:HD11	1:66:A:VAL:HG13	20	0.51	0.12	0.52
(1,116)	1:13:A:LEU:HD21	1:14:A:CYS:H	20	0.51	0.06	0.51

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,116)	1:13:A:LEU:HD23	1:14:A:CYS:H	20	0.51	0.06	0.51
(1,116)	1:13:A:LEU:HD22	1:14:A:CYS:H	20	0.51	0.06	0.51
(1,1806)	1:10:A:LEU:HD13	1:7:A:VAL:HA	20	0.5	0.12	0.5
(1,1806)	1:10:A:LEU:HD11	1:7:A:VAL:HA	20	0.5	0.12	0.5
(1,1806)	1:10:A:LEU:HD12	1:7:A:VAL:HA	20	0.5	0.12	0.5
(1,1812)	1:50:A:THR:HG22	1:47:A:ALA:HA	20	0.5	0.14	0.48
(1,1812)	1:50:A:THR:HG21	1:47:A:ALA:HA	20	0.5	0.14	0.48
(1,1812)	1:50:A:THR:HG23	1:47:A:ALA:HA	20	0.5	0.14	0.48
(1,996)	1:26:A:ILE:HG12	1:57:A:VAL:HG11	20	0.49	0.14	0.47
(1,996)	1:26:A:ILE:HG12	1:57:A:VAL:HG13	20	0.49	0.14	0.47
(1,996)	1:26:A:ILE:HG12	1:57:A:VAL:HG12	20	0.49	0.14	0.47
(1,912)	1:13:A:LEU:HD11	1:13:A:LEU:HD13	20	0.49	0.02	0.49
(1,912)	1:13:A:LEU:HD12	1:13:A:LEU:HD13	20	0.49	0.02	0.49
(1,912)	1:13:A:LEU:HD12	1:13:A:LEU:HD11	20	0.49	0.02	0.49
(1,2679)	1:7:A:VAL:HB	1:48:A:PHE:HD1	20	0.49	0.12	0.51
(1,2679)	1:7:A:VAL:HB	1:44:A:PHE:HD1	20	0.49	0.12	0.51
(1,2679)	1:7:A:VAL:HB	1:44:A:PHE:HD2	20	0.49	0.12	0.51
(1,2679)	1:7:A:VAL:HB	1:48:A:PHE:HD2	20	0.49	0.12	0.51
(1,200)	1:12:A:ALA:HB2	1:11:A:ILE:H	20	0.49	0.07	0.5
(1,200)	1:12:A:ALA:HB1	1:11:A:ILE:H	20	0.49	0.07	0.5
(1,200)	1:12:A:ALA:HB3	1:11:A:ILE:H	20	0.49	0.07	0.5
(1,23)	1:110:A:LEU:HD12	1:111:A:SER:H	20	0.49	0.1	0.49
(1,23)	1:110:A:LEU:HD11	1:111:A:SER:H	20	0.49	0.1	0.49
(1,23)	1:110:A:LEU:HD13	1:111:A:SER:H	20	0.49	0.1	0.49
(1,1794)	1:11:A:ILE:HG21	1:12:A:ALA:HB3	20	0.48	0.07	0.48
(1,1794)	1:11:A:ILE:HG23	1:12:A:ALA:HB2	20	0.48	0.07	0.48
(1,1794)	1:11:A:ILE:HG23	1:12:A:ALA:HB3	20	0.48	0.07	0.48
(1,1794)	1:11:A:ILE:HG22	1:12:A:ALA:HB2	20	0.48	0.07	0.48
(1,1794)	1:11:A:ILE:HG22	1:12:A:ALA:HB1	20	0.48	0.07	0.48
(1,1794)	1:11:A:ILE:HG21	1:12:A:ALA:HB1	20	0.48	0.07	0.48
(1,1794)	1:11:A:ILE:HG23	1:12:A:ALA:HB1	20	0.48	0.07	0.48
(1,1794)	1:11:A:ILE:HG21	1:12:A:ALA:HB2	20	0.48	0.07	0.48
(1,1794)	1:11:A:ILE:HG22	1:12:A:ALA:HB3	20	0.48	0.07	0.48
(1,2453)	1:62:A:ILE:HG22	1:62:A:ILE:HG21	20	0.48	0.01	0.48
(1,2453)	1:62:A:ILE:HG22	1:62:A:ILE:HG23	20	0.48	0.01	0.48
(1,2453)	1:100:A:ILE:HG21	1:100:A:ILE:HG23	20	0.48	0.01	0.48
(1,2453)	1:100:A:ILE:HG22	1:100:A:ILE:HG21	20	0.48	0.01	0.48
(1,2453)	1:100:A:ILE:HG22	1:100:A:ILE:HG23	20	0.48	0.01	0.48
(1,2453)	1:62:A:ILE:HG21	1:62:A:ILE:HG23	20	0.48	0.01	0.48
(1,2475)	1:18:A:ALA:HB2	1:18:A:ALA:HB1	20	0.48	0.02	0.48
(1,2475)	1:38:A:ALA:HB2	1:38:A:ALA:HB1	20	0.48	0.02	0.48
(1,2475)	1:18:A:ALA:HB2	1:18:A:ALA:HB3	20	0.48	0.02	0.48

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2475)	1:18:A:ALA:HB1	1:18:A:ALA:HB3	20	0.48	0.02	0.48
(1,2475)	1:38:A:ALA:HB1	1:38:A:ALA:HB3	20	0.48	0.02	0.48
(1,2475)	1:38:A:ALA:HB2	1:38:A:ALA:HB3	20	0.48	0.02	0.48
(1,1263)	1:11:A:ILE:HD13	1:11:A:ILE:HB	20	0.48	0.03	0.48
(1,1263)	1:11:A:ILE:HD12	1:11:A:ILE:HB	20	0.48	0.03	0.48
(1,1263)	1:11:A:ILE:HD11	1:11:A:ILE:HB	20	0.48	0.03	0.48
(1,136)	1:102:A:THR:HG23	1:100:A:ILE:H	20	0.48	0.18	0.48
(1,136)	1:102:A:THR:HG21	1:100:A:ILE:H	20	0.48	0.18	0.48
(1,136)	1:102:A:THR:HG22	1:100:A:ILE:H	20	0.48	0.18	0.48
(1,764)	1:70:A:VAL:HG23	1:70:A:VAL:HA	20	0.48	0.03	0.48
(1,764)	1:70:A:VAL:HG21	1:70:A:VAL:HA	20	0.48	0.03	0.48
(1,764)	1:70:A:VAL:HG22	1:70:A:VAL:HA	20	0.48	0.03	0.48
(1,2516)	1:25:A:LYS:HD2	1:25:A:LYS:HD3	20	0.47	0.01	0.47
(1,2516)	1:59:A:LYS:HD2	1:59:A:LYS:HD3	20	0.47	0.01	0.47
(1,2516)	1:19:A:LYS:HD2	1:19:A:LYS:HD3	20	0.47	0.01	0.47
(1,300)	1:107:A:MET:HE2	1:108:A:ARG:H	20	0.47	0.15	0.48
(1,300)	1:107:A:MET:HE1	1:108:A:ARG:H	20	0.47	0.15	0.48
(1,300)	1:107:A:MET:HE3	1:108:A:ARG:H	20	0.47	0.15	0.48
(1,1975)	1:12:A:ALA:HB1	1:15:A:GLU:HB2	20	0.46	0.1	0.48
(1,1975)	1:12:A:ALA:HB3	1:15:A:GLU:HB2	20	0.46	0.1	0.48
(1,1975)	1:12:A:ALA:HB2	1:15:A:GLU:HB2	20	0.46	0.1	0.48
(1,2447)	1:100:A:ILE:HD12	1:100:A:ILE:HD13	20	0.46	0.02	0.46
(1,2447)	1:101:A:ILE:HD12	1:101:A:ILE:HD11	20	0.46	0.02	0.46
(1,2447)	1:101:A:ILE:HD12	1:101:A:ILE:HD13	20	0.46	0.02	0.46
(1,2447)	1:100:A:ILE:HD12	1:100:A:ILE:HD11	20	0.46	0.02	0.46
(1,2447)	1:100:A:ILE:HD11	1:100:A:ILE:HD13	20	0.46	0.02	0.46
(1,2447)	1:101:A:ILE:HD11	1:101:A:ILE:HD13	20	0.46	0.02	0.46
(1,2160)	1:80:A:VAL:HG23	1:81:A:PHE:HD2	20	0.45	0.15	0.46
(1,2160)	1:80:A:VAL:HG22	1:81:A:PHE:HD1	20	0.45	0.15	0.46
(1,2160)	1:80:A:VAL:HG21	1:81:A:PHE:HD1	20	0.45	0.15	0.46
(1,2160)	1:80:A:VAL:HG21	1:81:A:PHE:HD2	20	0.45	0.15	0.46
(1,2160)	1:80:A:VAL:HG22	1:81:A:PHE:HD2	20	0.45	0.15	0.46
(1,2160)	1:80:A:VAL:HG23	1:81:A:PHE:HD1	20	0.45	0.15	0.46
(1,103)	1:43:A:LEU:HD22	1:46:A:SER:H	20	0.45	0.14	0.42
(1,103)	1:43:A:LEU:HD21	1:46:A:SER:H	20	0.45	0.14	0.42
(1,103)	1:43:A:LEU:HD23	1:46:A:SER:H	20	0.45	0.14	0.42
(1,146)	1:6:A:VAL:HG12	1:7:A:VAL:H	20	0.44	0.05	0.44
(1,146)	1:6:A:VAL:HG11	1:7:A:VAL:H	20	0.44	0.05	0.44
(1,146)	1:6:A:VAL:HG13	1:7:A:VAL:H	20	0.44	0.05	0.44
(1,1140)	1:59:A:LYS:HD3	1:59:A:LYS:HA	20	0.44	0.21	0.4
(1,1140)	1:59:A:LYS:HD2	1:59:A:LYS:HA	20	0.44	0.21	0.4
(1,118)	1:13:A:LEU:HD13	1:16:A:GLU:H	20	0.44	0.11	0.44

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,118)	1:13:A:LEU:HD12	1:16:A:GLU:H	20	0.44	0.11	0.44
(1,118)	1:13:A:LEU:HD11	1:16:A:GLU:H	20	0.44	0.11	0.44
(1,1830)	1:112:A:LEU:HD11	1:112:A:LEU:HB3	20	0.44	0.05	0.44
(1,1830)	1:112:A:LEU:HD13	1:112:A:LEU:HB3	20	0.44	0.05	0.44
(1,1830)	1:112:A:LEU:HD12	1:112:A:LEU:HB3	20	0.44	0.05	0.44
(1,2552)	1:81:A:PHE:HB2	1:81:A:PHE:HB3	20	0.43	0.01	0.43
(1,2552)	1:41:A:LYS:HE2	1:41:A:LYS:HE3	20	0.43	0.01	0.43
(1,1795)	1:86:A:LEU:HD23	1:86:A:LEU:HD11	20	0.43	0.05	0.44
(1,1795)	1:86:A:LEU:HD22	1:86:A:LEU:HD12	20	0.43	0.05	0.44
(1,1795)	1:86:A:LEU:HD23	1:86:A:LEU:HD13	20	0.43	0.05	0.44
(1,1795)	1:86:A:LEU:HD21	1:86:A:LEU:HD13	20	0.43	0.05	0.44
(1,1795)	1:86:A:LEU:HD23	1:86:A:LEU:HD12	20	0.43	0.05	0.44
(1,1795)	1:86:A:LEU:HD21	1:86:A:LEU:HD12	20	0.43	0.05	0.44
(1,1795)	1:86:A:LEU:HD21	1:86:A:LEU:HD11	20	0.43	0.05	0.44
(1,1795)	1:86:A:LEU:HD22	1:86:A:LEU:HD13	20	0.43	0.05	0.44
(1,905)	1:80:A:VAL:HG22	1:80:A:VAL:HG21	20	0.43	0.01	0.43
(1,905)	1:80:A:VAL:HG22	1:80:A:VAL:HG23	20	0.43	0.01	0.43
(1,905)	1:80:A:VAL:HG21	1:80:A:VAL:HG23	20	0.43	0.01	0.43
(1,1056)	1:69:A:LYS:HB3	1:69:A:LYS:HD3	20	0.43	0.04	0.43
(1,1056)	1:69:A:LYS:HB3	1:69:A:LYS:HD2	20	0.43	0.04	0.43
(1,891)	1:62:A:ILE:HD11	1:62:A:ILE:HD13	20	0.43	0.02	0.43
(1,891)	1:62:A:ILE:HD12	1:62:A:ILE:HD11	20	0.43	0.02	0.43
(1,891)	1:62:A:ILE:HD12	1:62:A:ILE:HD13	20	0.43	0.02	0.43
(1,1499)	1:6:A:VAL:HG23	1:3:A:GLU:HA	20	0.43	0.15	0.38
(1,1499)	1:6:A:VAL:HG21	1:3:A:GLU:HA	20	0.43	0.15	0.38
(1,1499)	1:6:A:VAL:HG22	1:3:A:GLU:HA	20	0.43	0.15	0.38
(1,906)	1:13:A:LEU:HD22	1:13:A:LEU:HD21	20	0.43	0.02	0.43
(1,906)	1:13:A:LEU:HD21	1:13:A:LEU:HD23	20	0.43	0.02	0.43
(1,906)	1:13:A:LEU:HD22	1:13:A:LEU:HD23	20	0.43	0.02	0.43
(1,2676)	1:47:A:ALA:HB1	1:44:A:PHE:HD1	20	0.42	0.14	0.46
(1,2676)	1:47:A:ALA:HB3	1:44:A:PHE:HD1	20	0.42	0.14	0.46
(1,2676)	1:47:A:ALA:HB3	1:44:A:PHE:HD2	20	0.42	0.14	0.46
(1,2676)	1:47:A:ALA:HB2	1:44:A:PHE:HD1	20	0.42	0.14	0.46
(1,2676)	1:47:A:ALA:HB2	1:44:A:PHE:HD2	20	0.42	0.14	0.46
(1,2676)	1:47:A:ALA:HB1	1:44:A:PHE:HD2	20	0.42	0.14	0.46
(1,875)	1:86:A:LEU:HD21	1:85:A:ALA:HA	20	0.42	0.14	0.4
(1,875)	1:86:A:LEU:HD23	1:85:A:ALA:HA	20	0.42	0.14	0.4
(1,875)	1:86:A:LEU:HD22	1:85:A:ALA:HA	20	0.42	0.14	0.4
(1,213)	1:75:A:LYS:HD3	1:75:A:LYS:H	20	0.41	0.1	0.42
(1,31)	1:33:A:ILE:HG22	1:33:A:ILE:H	20	0.41	0.04	0.42
(1,31)	1:33:A:ILE:HG23	1:33:A:ILE:H	20	0.41	0.04	0.42
(1,31)	1:33:A:ILE:HG21	1:33:A:ILE:H	20	0.41	0.04	0.42

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2650)	1:66:A:VAL:HG12	1:32:A:GLY:HA3	20	0.41	0.15	0.42
(1,2650)	1:66:A:VAL:HG13	1:32:A:GLY:HA3	20	0.41	0.15	0.42
(1,2650)	1:66:A:VAL:HG11	1:32:A:GLY:HA3	20	0.41	0.15	0.42
(1,222)	1:101:A:ILE:HG12	1:101:A:ILE:H	20	0.41	0.06	0.42
(1,781)	1:99:A:VAL:HG12	1:99:A:VAL:HG13	20	0.4	0.01	0.4
(1,781)	1:99:A:VAL:HG11	1:99:A:VAL:HG13	20	0.4	0.01	0.4
(1,781)	1:99:A:VAL:HG12	1:99:A:VAL:HG11	20	0.4	0.01	0.4
(1,182)	1:18:A:ALA:HB1	1:20:A:LYS:H	20	0.4	0.05	0.38
(1,182)	1:18:A:ALA:HB2	1:20:A:LYS:H	20	0.4	0.05	0.38
(1,182)	1:18:A:ALA:HB3	1:20:A:LYS:H	20	0.4	0.05	0.38
(1,75)	1:101:A:ILE:HG13	1:102:A:THR:H	20	0.39	0.04	0.4
(1,948)	1:45:A:VAL:HG12	1:42:A:SER:HA	20	0.39	0.09	0.4
(1,948)	1:45:A:VAL:HG13	1:42:A:SER:HA	20	0.39	0.09	0.4
(1,948)	1:45:A:VAL:HG11	1:42:A:SER:HA	20	0.39	0.09	0.4
(1,1744)	1:90:A:VAL:HG12	1:90:A:VAL:HG23	20	0.39	0.05	0.38
(1,1744)	1:90:A:VAL:HG11	1:90:A:VAL:HG23	20	0.39	0.05	0.38
(1,1744)	1:90:A:VAL:HG13	1:90:A:VAL:HG21	20	0.39	0.05	0.38
(1,1744)	1:90:A:VAL:HG13	1:90:A:VAL:HG22	20	0.39	0.05	0.38
(1,1744)	1:90:A:VAL:HG12	1:90:A:VAL:HG21	20	0.39	0.05	0.38
(1,1744)	1:90:A:VAL:HG12	1:90:A:VAL:HG22	20	0.39	0.05	0.38
(1,1744)	1:90:A:VAL:HG11	1:90:A:VAL:HG21	20	0.39	0.05	0.38
(1,1744)	1:90:A:VAL:HG11	1:90:A:VAL:HG22	20	0.39	0.05	0.38
(1,1059)	1:12:A:ALA:HB2	1:12:A:ALA:HB1	20	0.39	0.01	0.39
(1,1059)	1:12:A:ALA:HB2	1:12:A:ALA:HB3	20	0.39	0.01	0.39
(1,1059)	1:12:A:ALA:HB1	1:12:A:ALA:HB3	20	0.39	0.01	0.39
(1,2455)	1:57:A:VAL:HG11	1:57:A:VAL:HG13	20	0.39	0.02	0.39
(1,2455)	1:29:A:VAL:HG12	1:29:A:VAL:HG13	20	0.39	0.02	0.39
(1,2455)	1:29:A:VAL:HG12	1:29:A:VAL:HG11	20	0.39	0.02	0.39
(1,2455)	1:57:A:VAL:HG12	1:57:A:VAL:HG11	20	0.39	0.02	0.39
(1,2455)	1:29:A:VAL:HG11	1:29:A:VAL:HG13	20	0.39	0.02	0.39
(1,2455)	1:57:A:VAL:HG12	1:57:A:VAL:HG13	20	0.39	0.02	0.39
(1,964)	1:41:A:LYS:HG3	1:41:A:LYS:HE3	20	0.39	0.04	0.39
(1,2246)	1:4:A:TYR:HA	1:4:A:TYR:HE2	20	0.38	0.07	0.39
(1,2246)	1:4:A:TYR:HA	1:4:A:TYR:HE1	20	0.38	0.07	0.39
(1,239)	1:19:A:LYS:HD2	1:20:A:LYS:H	20	0.38	0.09	0.36
(1,239)	1:19:A:LYS:HD3	1:20:A:LYS:H	20	0.38	0.09	0.36
(1,74)	1:99:A:VAL:HG22	1:73:A:GLU:H	20	0.38	0.14	0.38
(1,74)	1:99:A:VAL:HG21	1:73:A:GLU:H	20	0.38	0.14	0.38
(1,74)	1:99:A:VAL:HG23	1:73:A:GLU:H	20	0.38	0.14	0.38
(1,945)	1:109:A:LEU:HD21	1:109:A:LEU:HB2	20	0.38	0.04	0.37
(1,945)	1:109:A:LEU:HD22	1:109:A:LEU:HB2	20	0.38	0.04	0.37
(1,945)	1:109:A:LEU:HD23	1:109:A:LEU:HB2	20	0.38	0.04	0.37

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2422)	1:47:A:ALA:HB2	1:7:A:VAL:H	20	0.37	0.1	0.38
(1,2422)	1:47:A:ALA:HB3	1:7:A:VAL:H	20	0.37	0.1	0.38
(1,2422)	1:47:A:ALA:HB1	1:7:A:VAL:H	20	0.37	0.1	0.38
(1,944)	1:6:A:VAL:HG11	1:6:A:VAL:HG13	20	0.36	0.01	0.37
(1,944)	1:6:A:VAL:HG12	1:6:A:VAL:HG13	20	0.36	0.01	0.37
(1,944)	1:6:A:VAL:HG22	1:6:A:VAL:HG21	20	0.36	0.01	0.37
(1,944)	1:6:A:VAL:HG12	1:6:A:VAL:HG11	20	0.36	0.01	0.37
(1,944)	1:6:A:VAL:HG21	1:6:A:VAL:HG23	20	0.36	0.01	0.37
(1,944)	1:6:A:VAL:HG22	1:6:A:VAL:HG23	20	0.36	0.01	0.37
(1,1474)	1:41:A:LYS:HA	1:41:A:LYS:HE2	20	0.36	0.06	0.36
(1,2448)	1:100:A:ILE:HD12	1:100:A:ILE:HD13	20	0.36	0.01	0.36
(1,2448)	1:26:A:ILE:HD11	1:26:A:ILE:HD13	20	0.36	0.01	0.36
(1,2448)	1:26:A:ILE:HD12	1:26:A:ILE:HD13	20	0.36	0.01	0.36
(1,2448)	1:26:A:ILE:HD12	1:26:A:ILE:HD11	20	0.36	0.01	0.36
(1,2448)	1:100:A:ILE:HD12	1:100:A:ILE:HD11	20	0.36	0.01	0.36
(1,2448)	1:100:A:ILE:HD11	1:100:A:ILE:HD13	20	0.36	0.01	0.36
(1,2448)	1:101:A:ILE:HD12	1:101:A:ILE:HD13	20	0.36	0.01	0.36
(1,2448)	1:101:A:ILE:HD11	1:101:A:ILE:HD13	20	0.36	0.01	0.36
(1,36)	1:99:A:VAL:HG11	1:100:A:ILE:H	20	0.35	0.06	0.36
(1,36)	1:99:A:VAL:HG13	1:100:A:ILE:H	20	0.35	0.06	0.36
(1,36)	1:99:A:VAL:HG12	1:100:A:ILE:H	20	0.35	0.06	0.36
(1,2440)	1:30:A:VAL:HG12	1:30:A:VAL:HG13	20	0.35	0.01	0.35
(1,2440)	1:30:A:VAL:HG12	1:30:A:VAL:HG11	20	0.35	0.01	0.35
(1,2440)	1:30:A:VAL:HG11	1:30:A:VAL:HG13	20	0.35	0.01	0.35
(1,2440)	1:66:A:VAL:HG12	1:66:A:VAL:HG11	20	0.35	0.01	0.35
(1,2440)	1:90:A:VAL:HG12	1:90:A:VAL:HG11	20	0.35	0.01	0.35
(1,2440)	1:90:A:VAL:HG12	1:90:A:VAL:HG13	20	0.35	0.01	0.35
(1,2440)	1:90:A:VAL:HG11	1:90:A:VAL:HG13	20	0.35	0.01	0.35
(1,2419)	1:69:A:LYS:HG3	1:69:A:LYS:H	20	0.34	0.08	0.33
(1,112)	1:10:A:LEU:HD11	1:11:A:ILE:H	20	0.34	0.1	0.34
(1,112)	1:10:A:LEU:HD12	1:11:A:ILE:H	20	0.34	0.1	0.34
(1,112)	1:10:A:LEU:HD13	1:11:A:ILE:H	20	0.34	0.1	0.34
(1,121)	1:70:A:VAL:HG12	1:71:A:GLU:H	20	0.34	0.09	0.32
(1,121)	1:70:A:VAL:HG11	1:71:A:GLU:H	20	0.34	0.09	0.32
(1,121)	1:70:A:VAL:HG13	1:71:A:GLU:H	20	0.34	0.09	0.32
(1,935)	1:102:A:THR:HG22	1:102:A:THR:HG23	20	0.33	0.02	0.34
(1,935)	1:102:A:THR:HG21	1:102:A:THR:HG23	20	0.33	0.02	0.34
(1,935)	1:102:A:THR:HG21	1:102:A:THR:HG22	20	0.33	0.02	0.34
(1,1619)	1:85:A:ALA:HB2	1:85:A:ALA:HA	20	0.33	0.02	0.32
(1,1619)	1:85:A:ALA:HB3	1:85:A:ALA:HA	20	0.33	0.02	0.32
(1,1619)	1:85:A:ALA:HB1	1:85:A:ALA:HA	20	0.33	0.02	0.32
(1,105)	1:29:A:VAL:HG12	1:29:A:VAL:H	20	0.33	0.04	0.32

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,105)	1:29:A:VAL:HG13	1:29:A:VAL:H	20	0.33	0.04	0.32
(1,105)	1:29:A:VAL:HG11	1:29:A:VAL:H	20	0.33	0.04	0.32
(1,907)	1:13:A:LEU:HD22	1:13:A:LEU:HD11	20	0.33	0.05	0.32
(1,907)	1:13:A:LEU:HD22	1:13:A:LEU:HD13	20	0.33	0.05	0.32
(1,907)	1:13:A:LEU:HD21	1:13:A:LEU:HD12	20	0.33	0.05	0.32
(1,907)	1:13:A:LEU:HD21	1:13:A:LEU:HD11	20	0.33	0.05	0.32
(1,907)	1:13:A:LEU:HD23	1:13:A:LEU:HD13	20	0.33	0.05	0.32
(1,907)	1:13:A:LEU:HD22	1:13:A:LEU:HD12	20	0.33	0.05	0.32
(1,907)	1:13:A:LEU:HD21	1:13:A:LEU:HD13	20	0.33	0.05	0.32
(1,1984)	1:7:A:VAL:HG13	1:48:A:PHE:HB3	20	0.32	0.1	0.31
(1,1984)	1:7:A:VAL:HG12	1:48:A:PHE:HB3	20	0.32	0.1	0.31
(1,1984)	1:7:A:VAL:HG11	1:48:A:PHE:HB3	20	0.32	0.1	0.31
(1,826)	1:101:A:ILE:HG22	1:103:A:GLN:HA	20	0.32	0.12	0.3
(1,826)	1:101:A:ILE:HG21	1:103:A:GLN:HA	20	0.32	0.12	0.3
(1,826)	1:101:A:ILE:HG23	1:103:A:GLN:HA	20	0.32	0.12	0.3
(1,886)	1:57:A:VAL:HG13	1:57:A:VAL:HG22	20	0.32	0.05	0.31
(1,886)	1:57:A:VAL:HG12	1:57:A:VAL:HG22	20	0.32	0.05	0.31
(1,886)	1:57:A:VAL:HG11	1:57:A:VAL:HG22	20	0.32	0.05	0.31
(1,886)	1:57:A:VAL:HG13	1:57:A:VAL:HG21	20	0.32	0.05	0.31
(1,886)	1:57:A:VAL:HG12	1:57:A:VAL:HG23	20	0.32	0.05	0.31
(1,886)	1:57:A:VAL:HG12	1:57:A:VAL:HG21	20	0.32	0.05	0.31
(1,886)	1:57:A:VAL:HG11	1:57:A:VAL:HG23	20	0.32	0.05	0.31
(1,953)	1:65:A:ILE:HG22	1:33:A:ILE:HG12	20	0.32	0.09	0.3
(1,953)	1:65:A:ILE:HG23	1:33:A:ILE:HG12	20	0.32	0.09	0.3
(1,953)	1:65:A:ILE:HG21	1:33:A:ILE:HG12	20	0.32	0.09	0.3
(1,2276)	1:88:A:TYR:HE2	1:88:A:TYR:HD2	20	0.32	0.02	0.32
(1,2276)	1:88:A:TYR:HE1	1:88:A:TYR:HD1	20	0.32	0.02	0.32
(1,911)	1:56:A:LEU:HD13	1:56:A:LEU:HA	20	0.31	0.04	0.3
(1,911)	1:56:A:LEU:HD11	1:56:A:LEU:HA	20	0.31	0.04	0.3
(1,911)	1:56:A:LEU:HD12	1:56:A:LEU:HA	20	0.31	0.04	0.3
(1,2143)	1:7:A:VAL:HG21	1:51:A:PHE:HD1	20	0.31	0.1	0.28
(1,2143)	1:7:A:VAL:HG23	1:51:A:PHE:HD1	20	0.31	0.1	0.28
(1,2143)	1:7:A:VAL:HG22	1:51:A:PHE:HD1	20	0.31	0.1	0.28
(1,773)	1:66:A:VAL:HG21	1:66:A:VAL:HG23	20	0.3	0.02	0.3
(1,773)	1:66:A:VAL:HG22	1:66:A:VAL:HG23	20	0.3	0.02	0.3
(1,773)	1:66:A:VAL:HG22	1:66:A:VAL:HG21	20	0.3	0.02	0.3
(1,2435)	1:72:A:LEU:HD21	1:72:A:LEU:HD23	20	0.3	0.01	0.31
(1,2435)	1:7:A:VAL:HG12	1:7:A:VAL:HG13	20	0.3	0.01	0.31
(1,2435)	1:7:A:VAL:HG12	1:7:A:VAL:HG11	20	0.3	0.01	0.31
(1,2435)	1:72:A:LEU:HD22	1:72:A:LEU:HD21	20	0.3	0.01	0.31
(1,2435)	1:72:A:LEU:HD22	1:72:A:LEU:HD23	20	0.3	0.01	0.31
(1,2435)	1:7:A:VAL:HG11	1:7:A:VAL:HG13	20	0.3	0.01	0.31

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,754)	1:33:A:ILE:HG13	1:33:A:ILE:HG21	20	0.3	0.04	0.3
(1,754)	1:33:A:ILE:HG13	1:33:A:ILE:HG22	20	0.3	0.04	0.3
(1,754)	1:33:A:ILE:HG13	1:33:A:ILE:HG23	20	0.3	0.04	0.3
(1,196)	1:12:A:ALA:HB2	1:14:A:CYS:H	20	0.29	0.07	0.29
(1,196)	1:12:A:ALA:HB1	1:14:A:CYS:H	20	0.29	0.07	0.29
(1,196)	1:12:A:ALA:HB3	1:14:A:CYS:H	20	0.29	0.07	0.29
(1,1415)	1:20:A:LYS:HE2	1:20:A:LYS:HE3	20	0.29	0.02	0.29
(1,845)	1:31:A:VAL:HG11	1:31:A:VAL:HG13	20	0.28	0.01	0.28
(1,845)	1:31:A:VAL:HG12	1:31:A:VAL:HG11	20	0.28	0.01	0.28
(1,845)	1:31:A:VAL:HG12	1:31:A:VAL:HG13	20	0.28	0.01	0.28
(1,2496)	1:36:A:ARG:HG3	1:36:A:ARG:HG2	20	0.28	0.02	0.28
(1,2496)	1:75:A:LYS:HD2	1:75:A:LYS:HD3	20	0.28	0.02	0.28
(1,138)	1:102:A:THR:HG23	1:103:A:GLN:H	20	0.28	0.12	0.28
(1,138)	1:102:A:THR:HG21	1:103:A:GLN:H	20	0.28	0.12	0.28
(1,138)	1:102:A:THR:HG22	1:103:A:GLN:H	20	0.28	0.12	0.28
(1,83)	1:112:A:LEU:HD21	1:112:A:LEU:H	20	0.28	0.06	0.29
(1,83)	1:112:A:LEU:HD23	1:112:A:LEU:H	20	0.28	0.06	0.29
(1,83)	1:112:A:LEU:HD22	1:112:A:LEU:H	20	0.28	0.06	0.29
(1,2279)	1:4:A:TYR:HE2	1:4:A:TYR:HD2	20	0.28	0.03	0.27
(1,2279)	1:4:A:TYR:HE1	1:4:A:TYR:HD1	20	0.28	0.03	0.27
(1,831)	1:101:A:ILE:HG21	1:101:A:ILE:HG23	20	0.27	0.01	0.28
(1,831)	1:101:A:ILE:HG22	1:101:A:ILE:HG21	20	0.27	0.01	0.28
(1,831)	1:101:A:ILE:HG22	1:101:A:ILE:HG23	20	0.27	0.01	0.28
(1,922)	1:45:A:VAL:HG22	1:45:A:VAL:HG13	20	0.27	0.04	0.26
(1,922)	1:45:A:VAL:HG23	1:45:A:VAL:HG12	20	0.27	0.04	0.26
(1,922)	1:45:A:VAL:HG22	1:45:A:VAL:HG11	20	0.27	0.04	0.26
(1,922)	1:45:A:VAL:HG23	1:45:A:VAL:HG13	20	0.27	0.04	0.26
(1,922)	1:45:A:VAL:HG23	1:45:A:VAL:HG11	20	0.27	0.04	0.26
(1,922)	1:45:A:VAL:HG21	1:45:A:VAL:HG11	20	0.27	0.04	0.26
(1,922)	1:45:A:VAL:HG21	1:45:A:VAL:HG13	20	0.27	0.04	0.26
(1,922)	1:45:A:VAL:HG21	1:45:A:VAL:HG12	20	0.27	0.04	0.26
(1,922)	1:45:A:VAL:HG22	1:45:A:VAL:HG12	20	0.27	0.04	0.26
(1,2239)	1:41:A:LYS:HA	1:44:A:PHE:HD2	20	0.27	0.12	0.28
(1,2239)	1:41:A:LYS:HA	1:44:A:PHE:HD1	20	0.27	0.12	0.28
(1,950)	1:45:A:VAL:HG11	1:45:A:VAL:HG13	20	0.27	0.02	0.27
(1,950)	1:45:A:VAL:HG12	1:45:A:VAL:HG11	20	0.27	0.02	0.27
(1,950)	1:45:A:VAL:HG12	1:45:A:VAL:HG13	20	0.27	0.02	0.27
(1,2507)	1:20:A:LYS:HD2	1:20:A:LYS:HD3	20	0.27	0.01	0.27
(1,2507)	1:82:A:LYS:HD2	1:82:A:LYS:HD3	20	0.27	0.01	0.27
(1,1081)	1:43:A:LEU:HG	1:43:A:LEU:HA	20	0.27	0.04	0.28
(1,2692)	1:4:A:TYR:HE2	1:4:A:TYR:HD2	20	0.27	0.02	0.27
(1,2692)	1:88:A:TYR:HE2	1:88:A:TYR:HD2	20	0.27	0.02	0.27

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2692)	1:4:A:TYR:HE1	1:4:A:TYR:HD1	20	0.27	0.02	0.27
(1,1561)	1:38:A:ALA:HB1	1:38:A:ALA:HA	20	0.26	0.03	0.26
(1,1561)	1:38:A:ALA:HB3	1:38:A:ALA:HA	20	0.26	0.03	0.26
(1,1561)	1:38:A:ALA:HB2	1:38:A:ALA:HA	20	0.26	0.03	0.26
(1,858)	1:109:A:LEU:HD22	1:109:A:LEU:HD23	20	0.26	0.02	0.26
(1,858)	1:109:A:LEU:HD21	1:109:A:LEU:HD23	20	0.26	0.02	0.26
(1,858)	1:109:A:LEU:HD22	1:109:A:LEU:HD21	20	0.26	0.02	0.26
(1,39)	1:90:A:VAL:HG12	1:90:A:VAL:H	20	0.26	0.09	0.23
(1,39)	1:90:A:VAL:HG13	1:90:A:VAL:H	20	0.26	0.09	0.23
(1,39)	1:90:A:VAL:HG11	1:90:A:VAL:H	20	0.26	0.09	0.23
(1,2503)	1:36:A:ARG:HG3	1:36:A:ARG:HG2	20	0.25	0.01	0.26
(1,2503)	1:69:A:LYS:HD2	1:69:A:LYS:HD3	20	0.25	0.01	0.26
(1,2503)	1:75:A:LYS:HD2	1:75:A:LYS:HD3	20	0.25	0.01	0.26
(1,358)	1:22:A:GLN:HB2	1:23:A:ALA:H	20	0.25	0.05	0.26
(1,2450)	1:99:A:VAL:HG22	1:99:A:VAL:HG23	20	0.25	0.01	0.25
(1,2450)	1:30:A:VAL:HG22	1:30:A:VAL:HG21	20	0.25	0.01	0.25
(1,2450)	1:99:A:VAL:HG21	1:99:A:VAL:HG23	20	0.25	0.01	0.25
(1,2450)	1:99:A:VAL:HG22	1:99:A:VAL:HG21	20	0.25	0.01	0.25
(1,2450)	1:30:A:VAL:HG22	1:30:A:VAL:HG23	20	0.25	0.01	0.25
(1,2378)	1:97:A:LYS:H	1:96:A:SER:H	20	0.25	0.04	0.24
(1,134)	1:57:A:VAL:HG21	1:58:A:CYS:H	20	0.25	0.06	0.26
(1,134)	1:57:A:VAL:HG23	1:58:A:CYS:H	20	0.25	0.06	0.26
(1,134)	1:57:A:VAL:HG22	1:58:A:CYS:H	20	0.25	0.06	0.26
(1,2058)	1:12:A:ALA:HB1	1:13:A:LEU:HA	20	0.25	0.09	0.28
(1,2058)	1:12:A:ALA:HB2	1:13:A:LEU:HA	20	0.25	0.09	0.28
(1,2058)	1:12:A:ALA:HB3	1:13:A:LEU:HA	20	0.25	0.09	0.28
(1,741)	1:72:A:LEU:HD12	1:72:A:LEU:HD13	20	0.25	0.02	0.24
(1,741)	1:72:A:LEU:HD11	1:72:A:LEU:HD13	20	0.25	0.02	0.24
(1,741)	1:72:A:LEU:HD12	1:72:A:LEU:HD11	20	0.25	0.02	0.24
(1,980)	1:23:A:ALA:HB1	1:23:A:ALA:HB3	20	0.24	0.02	0.24
(1,980)	1:23:A:ALA:HB2	1:23:A:ALA:HB1	20	0.24	0.02	0.24
(1,980)	1:23:A:ALA:HB2	1:23:A:ALA:HB3	20	0.24	0.02	0.24
(1,2614)	1:10:A:LEU:HD11	1:10:A:LEU:HD13	20	0.24	0.01	0.25
(1,2614)	1:70:A:VAL:HG12	1:70:A:VAL:HG13	20	0.24	0.01	0.25
(1,2614)	1:10:A:LEU:HD12	1:10:A:LEU:HD13	20	0.24	0.01	0.25
(1,2614)	1:70:A:VAL:HG12	1:70:A:VAL:HG11	20	0.24	0.01	0.25
(1,2614)	1:10:A:LEU:HD12	1:10:A:LEU:HD11	20	0.24	0.01	0.25
(1,2614)	1:70:A:VAL:HG11	1:70:A:VAL:HG13	20	0.24	0.01	0.25
(1,1411)	1:84:A:ASN:HB2	1:84:A:ASN:HB3	20	0.24	0.01	0.24
(1,842)	1:112:A:LEU:HD21	1:112:A:LEU:HD23	20	0.24	0.02	0.24
(1,842)	1:112:A:LEU:HD22	1:112:A:LEU:HD21	20	0.24	0.02	0.24
(1,842)	1:112:A:LEU:HD22	1:112:A:LEU:HD23	20	0.24	0.02	0.24

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2396)	1:101:A:ILE:H	1:100:A:ILE:H	20	0.23	0.04	0.22
(1,1847)	1:110:A:LEU:HD23	1:110:A:LEU:HB2	20	0.22	0.04	0.22
(1,1847)	1:110:A:LEU:HD22	1:110:A:LEU:HB2	20	0.22	0.04	0.22
(1,1847)	1:110:A:LEU:HD21	1:110:A:LEU:HB2	20	0.22	0.04	0.22
(1,2050)	1:17:A:HIS:HA	1:16:A:GLU:HB2	20	0.22	0.04	0.22
(1,2041)	1:16:A:GLU:HA	1:17:A:HIS:HA	20	0.22	0.04	0.22
(1,2451)	1:26:A:ILE:HD12	1:26:A:ILE:HD13	20	0.22	0.01	0.22
(1,2451)	1:26:A:ILE:HD11	1:26:A:ILE:HD13	20	0.22	0.01	0.22
(1,2451)	1:101:A:ILE:HD11	1:101:A:ILE:HD13	20	0.22	0.01	0.22
(1,2451)	1:26:A:ILE:HD12	1:26:A:ILE:HD11	20	0.22	0.01	0.22
(1,2451)	1:101:A:ILE:HD12	1:101:A:ILE:HD13	20	0.22	0.01	0.22
(1,2451)	1:101:A:ILE:HD12	1:101:A:ILE:HD11	20	0.22	0.01	0.22
(1,2294)	1:99:A:VAL:H	1:100:A:ILE:H	20	0.22	0.04	0.22
(1,736)	1:11:A:ILE:HD12	1:11:A:ILE:HD11	20	0.21	0.02	0.21
(1,736)	1:11:A:ILE:HD12	1:11:A:ILE:HD13	20	0.21	0.02	0.21
(1,736)	1:11:A:ILE:HD11	1:11:A:ILE:HD13	20	0.21	0.02	0.21
(1,2287)	1:80:A:VAL:H	1:81:A:PHE:H	20	0.21	0.03	0.2
(1,1352)	1:22:A:GLN:HG2	1:22:A:GLN:HG3	20	0.21	0.02	0.21
(1,1581)	1:35:A:GLU:HG3	1:35:A:GLU:HA	20	0.2	0.02	0.2
(1,2653)	1:41:A:LYS:HD3	1:41:A:LYS:HA	20	0.19	0.04	0.2
(1,2539)	1:113:A:GLU:HG3	1:113:A:GLU:HG2	20	0.19	0.01	0.19
(1,2539)	1:106:A:GLU:HG2	1:106:A:GLU:HG3	20	0.19	0.01	0.19
(1,437)	1:24:A:HIS:HB3	1:25:A:LYS:H	20	0.19	0.05	0.18
(1,437)	1:24:A:HIS:HB2	1:25:A:LYS:H	20	0.19	0.05	0.18
(1,2380)	1:34:A:GLY:H	1:35:A:GLU:H	20	0.19	0.03	0.19
(1,793)	1:109:A:LEU:HD12	1:109:A:LEU:HD13	20	0.18	0.02	0.18
(1,793)	1:109:A:LEU:HD12	1:109:A:LEU:HD11	20	0.18	0.02	0.18
(1,793)	1:109:A:LEU:HD11	1:109:A:LEU:HD13	20	0.18	0.02	0.18
(1,758)	1:110:A:LEU:HD11	1:110:A:LEU:HD13	20	0.16	0.02	0.16
(1,758)	1:110:A:LEU:HD12	1:110:A:LEU:HD11	20	0.16	0.02	0.16
(1,758)	1:110:A:LEU:HD12	1:110:A:LEU:HD13	20	0.16	0.02	0.16
(1,768)	1:70:A:VAL:HG22	1:70:A:VAL:HG21	20	0.14	0.01	0.14
(1,768)	1:70:A:VAL:HG22	1:70:A:VAL:HG23	20	0.14	0.01	0.14
(1,768)	1:70:A:VAL:HG21	1:70:A:VAL:HG23	20	0.14	0.01	0.14
(1,1832)	1:61:A:ALA:HB2	1:61:A:ALA:HB3	20	0.13	0.01	0.13
(1,1832)	1:61:A:ALA:HB2	1:61:A:ALA:HB1	20	0.13	0.01	0.13
(1,1832)	1:61:A:ALA:HB1	1:61:A:ALA:HB3	20	0.13	0.01	0.13
(1,776)	1:33:A:ILE:HG22	1:33:A:ILE:HG23	20	0.13	0.01	0.13
(1,776)	1:33:A:ILE:HG21	1:33:A:ILE:HG23	20	0.13	0.01	0.13
(1,776)	1:33:A:ILE:HG22	1:33:A:ILE:HG21	20	0.13	0.01	0.13
(1,458)	1:74:A:CYS:HB2	1:77:A:CYS:H	19	0.84	0.15	0.84
(1,745)	1:72:A:LEU:HD11	1:72:A:LEU:HA	19	0.78	0.04	0.79

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,745)	1:72:A:LEU:HD12	1:72:A:LEU:HA	19	0.78	0.04	0.79
(1,745)	1:72:A:LEU:HD13	1:72:A:LEU:HA	19	0.78	0.04	0.79
(1,1857)	1:75:A:LYS:HG2	1:98:A:ASN:HB2	19	0.76	0.23	0.77
(1,770)	1:72:A:LEU:HD12	1:70:A:VAL:HG23	19	0.63	0.14	0.62
(1,770)	1:72:A:LEU:HD13	1:70:A:VAL:HG22	19	0.63	0.14	0.62
(1,770)	1:72:A:LEU:HD11	1:70:A:VAL:HG21	19	0.63	0.14	0.62
(1,770)	1:72:A:LEU:HD13	1:70:A:VAL:HG21	19	0.63	0.14	0.62
(1,770)	1:72:A:LEU:HD12	1:70:A:VAL:HG21	19	0.63	0.14	0.62
(1,770)	1:72:A:LEU:HD11	1:70:A:VAL:HG23	19	0.63	0.14	0.62
(1,1628)	1:61:A:ALA:HB3	1:27:A:GLU:HA	19	0.56	0.18	0.61
(1,1628)	1:61:A:ALA:HB2	1:27:A:GLU:HA	19	0.56	0.18	0.61
(1,1628)	1:61:A:ALA:HB1	1:27:A:GLU:HA	19	0.56	0.18	0.61
(1,2669)	1:31:A:VAL:HG21	1:44:A:PHE:HD2	19	0.56	0.12	0.53
(1,2669)	1:31:A:VAL:HG22	1:44:A:PHE:HD2	19	0.56	0.12	0.53
(1,2669)	1:31:A:VAL:HG23	1:44:A:PHE:HD1	19	0.56	0.12	0.53
(1,2669)	1:31:A:VAL:HG23	1:44:A:PHE:HD2	19	0.56	0.12	0.53
(1,2669)	1:31:A:VAL:HG21	1:44:A:PHE:HD1	19	0.56	0.12	0.53
(1,2669)	1:31:A:VAL:HG22	1:44:A:PHE:HD1	19	0.56	0.12	0.53
(1,101)	1:57:A:VAL:HG13	1:15:A:GLU:H	19	0.49	0.21	0.51
(1,101)	1:57:A:VAL:HG12	1:15:A:GLU:H	19	0.49	0.21	0.51
(1,101)	1:57:A:VAL:HG11	1:15:A:GLU:H	19	0.49	0.21	0.51
(1,2433)	1:63:A:LEU:HD21	1:31:A:VAL:HG23	19	0.48	0.13	0.49
(1,2433)	1:63:A:LEU:HD23	1:31:A:VAL:HG23	19	0.48	0.13	0.49
(1,2433)	1:63:A:LEU:HD23	1:31:A:VAL:HG22	19	0.48	0.13	0.49
(1,2433)	1:63:A:LEU:HD21	1:31:A:VAL:HG21	19	0.48	0.13	0.49
(1,2433)	1:63:A:LEU:HD22	1:31:A:VAL:HG22	19	0.48	0.13	0.49
(1,2433)	1:63:A:LEU:HD23	1:31:A:VAL:HG21	19	0.48	0.13	0.49
(1,2433)	1:63:A:LEU:HD22	1:31:A:VAL:HG21	19	0.48	0.13	0.49
(1,2433)	1:63:A:LEU:HD21	1:31:A:VAL:HG22	19	0.48	0.13	0.49
(1,88)	1:26:A:ILE:HD13	1:15:A:GLU:H	19	0.46	0.17	0.49
(1,88)	1:26:A:ILE:HD12	1:15:A:GLU:H	19	0.46	0.17	0.49
(1,88)	1:26:A:ILE:HD11	1:15:A:GLU:H	19	0.46	0.17	0.49
(1,2056)	1:15:A:GLU:HG2	1:12:A:ALA:HA	19	0.46	0.13	0.42
(1,34)	1:33:A:ILE:HG21	1:39:A:MET:H	19	0.45	0.22	0.39
(1,34)	1:33:A:ILE:HG22	1:39:A:MET:H	19	0.45	0.22	0.39
(1,34)	1:33:A:ILE:HG23	1:39:A:MET:H	19	0.45	0.22	0.39
(1,1987)	1:23:A:ALA:HB3	1:21:A:ASN:HB2	19	0.44	0.11	0.43
(1,1987)	1:23:A:ALA:HB1	1:21:A:ASN:HB2	19	0.44	0.11	0.43
(1,1987)	1:23:A:ALA:HB2	1:21:A:ASN:HB2	19	0.44	0.11	0.43
(1,897)	1:29:A:VAL:HG13	1:112:A:LEU:HD22	19	0.43	0.17	0.4
(1,897)	1:29:A:VAL:HG11	1:112:A:LEU:HD23	19	0.43	0.17	0.4
(1,897)	1:29:A:VAL:HG13	1:112:A:LEU:HD21	19	0.43	0.17	0.4

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,897)	1:29:A:VAL:HG12	1:112:A:LEU:HD23	19	0.43	0.17	0.4
(1,897)	1:29:A:VAL:HG12	1:112:A:LEU:HD22	19	0.43	0.17	0.4
(1,897)	1:29:A:VAL:HG13	1:112:A:LEU:HD23	19	0.43	0.17	0.4
(1,897)	1:29:A:VAL:HG12	1:112:A:LEU:HD21	19	0.43	0.17	0.4
(1,897)	1:29:A:VAL:HG11	1:112:A:LEU:HD22	19	0.43	0.17	0.4
(1,2671)	1:115:A:LEU:HD12	1:24:A:HIS:HD2	19	0.41	0.19	0.38
(1,2671)	1:115:A:LEU:HD11	1:24:A:HIS:HD2	19	0.41	0.19	0.38
(1,2671)	1:115:A:LEU:HD13	1:24:A:HIS:HD2	19	0.41	0.19	0.38
(1,2105)	1:64:A:ASP:HA	1:62:A:ILE:HG23	19	0.4	0.17	0.34
(1,2105)	1:64:A:ASP:HA	1:62:A:ILE:HG22	19	0.4	0.17	0.34
(1,2105)	1:64:A:ASP:HA	1:62:A:ILE:HG21	19	0.4	0.17	0.34
(1,2438)	1:65:A:ILE:HD12	1:41:A:LYS:HD2	19	0.39	0.18	0.4
(1,2438)	1:65:A:ILE:HD13	1:41:A:LYS:HD2	19	0.39	0.18	0.4
(1,2438)	1:65:A:ILE:HD11	1:41:A:LYS:HD2	19	0.39	0.18	0.4
(1,1601)	1:12:A:ALA:HB2	1:9:A:SER:HA	19	0.39	0.14	0.38
(1,1601)	1:12:A:ALA:HB1	1:9:A:SER:HA	19	0.39	0.14	0.38
(1,1601)	1:12:A:ALA:HB3	1:9:A:SER:HA	19	0.39	0.14	0.38
(1,113)	1:10:A:LEU:HD13	1:10:A:LEU:H	19	0.39	0.12	0.43
(1,113)	1:10:A:LEU:HD11	1:10:A:LEU:H	19	0.39	0.12	0.43
(1,113)	1:10:A:LEU:HD12	1:10:A:LEU:H	19	0.39	0.12	0.43
(1,2454)	1:62:A:ILE:HG23	1:28:A:ARG:HG3	19	0.38	0.14	0.38
(1,2454)	1:62:A:ILE:HG21	1:28:A:ARG:HG3	19	0.38	0.14	0.38
(1,2454)	1:62:A:ILE:HG22	1:28:A:ARG:HG3	19	0.38	0.14	0.38
(1,2454)	1:62:A:ILE:HG21	1:62:A:ILE:HG13	19	0.38	0.14	0.38
(1,1385)	1:48:A:PHE:HB3	1:63:A:LEU:HD13	19	0.37	0.18	0.3
(1,1385)	1:48:A:PHE:HB3	1:63:A:LEU:HD12	19	0.37	0.18	0.3
(1,1385)	1:48:A:PHE:HB3	1:63:A:LEU:HD11	19	0.37	0.18	0.3
(1,371)	1:22:A:GLN:HG3	1:21:A:ASN:H	19	0.32	0.11	0.34
(1,803)	1:72:A:LEU:HD23	1:72:A:LEU:HB2	19	0.32	0.04	0.32
(1,803)	1:72:A:LEU:HD22	1:72:A:LEU:HB2	19	0.32	0.04	0.32
(1,803)	1:72:A:LEU:HD21	1:72:A:LEU:HB2	19	0.32	0.04	0.32
(1,162)	1:23:A:ALA:HB3	1:22:A:GLN:H	19	0.31	0.09	0.29
(1,162)	1:23:A:ALA:HB1	1:22:A:GLN:H	19	0.31	0.09	0.29
(1,162)	1:23:A:ALA:HB2	1:22:A:GLN:H	19	0.31	0.09	0.29
(1,1618)	1:50:A:THR:HG21	1:51:A:PHE:HA	19	0.28	0.07	0.27
(1,1618)	1:50:A:THR:HG23	1:51:A:PHE:HA	19	0.28	0.07	0.27
(1,1618)	1:50:A:THR:HG22	1:51:A:PHE:HA	19	0.28	0.07	0.27
(1,818)	1:80:A:VAL:HG13	1:80:A:VAL:HG21	19	0.24	0.05	0.25
(1,818)	1:80:A:VAL:HG11	1:80:A:VAL:HG21	19	0.24	0.05	0.25
(1,818)	1:80:A:VAL:HG12	1:80:A:VAL:HG23	19	0.24	0.05	0.25
(1,818)	1:80:A:VAL:HG12	1:80:A:VAL:HG22	19	0.24	0.05	0.25
(1,818)	1:80:A:VAL:HG11	1:80:A:VAL:HG23	19	0.24	0.05	0.25

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,818)	1:80:A:VAL:HG11	1:80:A:VAL:HG22	19	0.24	0.05	0.25
(1,818)	1:80:A:VAL:HG13	1:80:A:VAL:HG23	19	0.24	0.05	0.25
(1,818)	1:80:A:VAL:HG12	1:80:A:VAL:HG21	19	0.24	0.05	0.25
(1,818)	1:80:A:VAL:HG13	1:80:A:VAL:HG22	19	0.24	0.05	0.25
(1,2442)	1:31:A:VAL:HG21	1:31:A:VAL:HG11	19	0.22	0.04	0.23
(1,2442)	1:31:A:VAL:HG22	1:31:A:VAL:HG12	19	0.22	0.04	0.23
(1,2442)	1:31:A:VAL:HG23	1:31:A:VAL:HG11	19	0.22	0.04	0.23
(1,2442)	1:31:A:VAL:HG22	1:31:A:VAL:HG13	19	0.22	0.04	0.23
(1,2442)	1:31:A:VAL:HG21	1:31:A:VAL:HG13	19	0.22	0.04	0.23
(1,2442)	1:31:A:VAL:HG21	1:31:A:VAL:HG12	19	0.22	0.04	0.23
(1,2442)	1:31:A:VAL:HG22	1:31:A:VAL:HG11	19	0.22	0.04	0.23
(1,2442)	1:31:A:VAL:HG23	1:31:A:VAL:HG13	19	0.22	0.04	0.23
(1,2442)	1:31:A:VAL:HG23	1:31:A:VAL:HG12	19	0.22	0.04	0.23
(1,940)	1:112:A:LEU:HD12	1:112:A:LEU:HA	19	0.21	0.05	0.21
(1,940)	1:112:A:LEU:HD11	1:112:A:LEU:HA	19	0.21	0.05	0.21
(1,940)	1:112:A:LEU:HD13	1:112:A:LEU:HA	19	0.21	0.05	0.21
(1,2229)	1:4:A:TYR:HB3	1:4:A:TYR:HE2	19	0.2	0.03	0.21
(1,2229)	1:4:A:TYR:HB3	1:4:A:TYR:HE1	19	0.2	0.03	0.21
(1,1299)	1:117:A:GLU:HB2	1:117:A:GLU:HG3	19	0.19	0.02	0.19
(1,1053)	1:63:A:LEU:HD11	1:63:A:LEU:HB2	19	0.19	0.04	0.19
(1,1053)	1:63:A:LEU:HD13	1:63:A:LEU:HB2	19	0.19	0.04	0.19
(1,1053)	1:63:A:LEU:HD12	1:63:A:LEU:HB2	19	0.19	0.04	0.19
(1,1897)	1:41:A:LYS:HD3	1:41:A:LYS:HA	19	0.18	0.03	0.17
(1,71)	1:31:A:VAL:HG13	1:32:A:GLY:H	19	0.17	0.06	0.17
(1,71)	1:31:A:VAL:HG12	1:32:A:GLY:H	19	0.17	0.06	0.17
(1,71)	1:31:A:VAL:HG11	1:32:A:GLY:H	19	0.17	0.06	0.17
(1,97)	1:11:A:ILE:HG21	1:12:A:ALA:H	19	0.17	0.04	0.16
(1,97)	1:11:A:ILE:HG23	1:12:A:ALA:H	19	0.17	0.04	0.16
(1,97)	1:11:A:ILE:HG22	1:12:A:ALA:H	19	0.17	0.04	0.16
(1,277)	1:54:A:GLU:HB3	1:54:A:GLU:H	19	0.15	0.02	0.15
(1,1583)	1:35:A:GLU:HG2	1:35:A:GLU:HA	19	0.14	0.02	0.14
(1,784)	1:65:A:ILE:HD12	1:65:A:ILE:HD11	19	0.13	0.02	0.13
(1,784)	1:65:A:ILE:HD11	1:65:A:ILE:HD13	19	0.13	0.02	0.13
(1,784)	1:65:A:ILE:HD12	1:65:A:ILE:HD13	19	0.13	0.02	0.13
(1,2204)	1:83:A:PRO:HB3	1:88:A:TYR:HE1	18	0.67	0.19	0.7
(1,2204)	1:83:A:PRO:HB3	1:88:A:TYR:HE2	18	0.67	0.19	0.7
(1,1254)	1:20:A:LYS:HB2	1:20:A:LYS:HE3	18	0.64	0.06	0.62
(1,1254)	1:20:A:LYS:HB3	1:20:A:LYS:HE2	18	0.64	0.06	0.62
(1,1992)	1:20:A:LYS:HE2	1:20:A:LYS:HA	18	0.6	0.05	0.6
(1,27)	1:90:A:VAL:HG23	1:89:A:GLY:H	18	0.54	0.1	0.54
(1,27)	1:90:A:VAL:HG21	1:89:A:GLY:H	18	0.54	0.1	0.54
(1,27)	1:90:A:VAL:HG22	1:89:A:GLY:H	18	0.54	0.1	0.54

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2693)	1:48:A:PHE:HD1	1:44:A:PHE:HZ	18	0.52	0.08	0.55
(1,2693)	1:44:A:PHE:HD2	1:44:A:PHE:HZ	18	0.52	0.08	0.55
(1,2693)	1:44:A:PHE:HD1	1:44:A:PHE:HZ	18	0.52	0.08	0.55
(1,2693)	1:48:A:PHE:HD2	1:44:A:PHE:HZ	18	0.52	0.08	0.55
(1,2202)	1:83:A:PRO:HB3	1:88:A:TYR:HD1	18	0.5	0.23	0.5
(1,2202)	1:83:A:PRO:HB3	1:88:A:TYR:HD2	18	0.5	0.23	0.5
(1,1829)	1:26:A:ILE:HD12	1:23:A:ALA:HB3	18	0.49	0.24	0.47
(1,1829)	1:26:A:ILE:HD12	1:23:A:ALA:HB1	18	0.49	0.24	0.47
(1,1829)	1:26:A:ILE:HD11	1:23:A:ALA:HB2	18	0.49	0.24	0.47
(1,1829)	1:26:A:ILE:HD11	1:23:A:ALA:HB1	18	0.49	0.24	0.47
(1,1829)	1:26:A:ILE:HD13	1:23:A:ALA:HB1	18	0.49	0.24	0.47
(1,1829)	1:26:A:ILE:HD13	1:23:A:ALA:HB2	18	0.49	0.24	0.47
(1,1829)	1:26:A:ILE:HD11	1:23:A:ALA:HB3	18	0.49	0.24	0.47
(1,1829)	1:26:A:ILE:HD13	1:23:A:ALA:HB3	18	0.49	0.24	0.47
(1,746)	1:72:A:LEU:HD12	1:83:A:PRO:HB2	18	0.4	0.22	0.36
(1,746)	1:72:A:LEU:HD13	1:83:A:PRO:HB2	18	0.4	0.22	0.36
(1,746)	1:72:A:LEU:HD11	1:83:A:PRO:HB2	18	0.4	0.22	0.36
(1,1769)	1:66:A:VAL:HG12	1:68:A:GLU:HB2	18	0.4	0.23	0.34
(1,1769)	1:66:A:VAL:HG13	1:68:A:GLU:HB2	18	0.4	0.23	0.34
(1,1769)	1:66:A:VAL:HG11	1:68:A:GLU:HB2	18	0.4	0.23	0.34
(1,1769)	1:66:A:VAL:HG11	1:68:A:GLU:HB3	18	0.4	0.23	0.34
(1,1769)	1:66:A:VAL:HG13	1:68:A:GLU:HB3	18	0.4	0.23	0.34
(1,864)	1:110:A:LEU:HD12	1:30:A:VAL:HG21	18	0.25	0.11	0.28
(1,864)	1:110:A:LEU:HD12	1:30:A:VAL:HG22	18	0.25	0.11	0.28
(1,864)	1:110:A:LEU:HD13	1:30:A:VAL:HG22	18	0.25	0.11	0.28
(1,864)	1:110:A:LEU:HD11	1:30:A:VAL:HG22	18	0.25	0.11	0.28
(1,864)	1:110:A:LEU:HD13	1:30:A:VAL:HG23	18	0.25	0.11	0.28
(1,864)	1:110:A:LEU:HD12	1:30:A:VAL:HG23	18	0.25	0.11	0.28
(1,864)	1:110:A:LEU:HD13	1:30:A:VAL:HG21	18	0.25	0.11	0.28
(1,2148)	1:80:A:VAL:HG11	1:81:A:PHE:HD2	18	0.25	0.09	0.25
(1,2148)	1:80:A:VAL:HG11	1:81:A:PHE:HD1	18	0.25	0.09	0.25
(1,2148)	1:80:A:VAL:HG13	1:81:A:PHE:HD2	18	0.25	0.09	0.25
(1,2148)	1:80:A:VAL:HG12	1:81:A:PHE:HD2	18	0.25	0.09	0.25
(1,2148)	1:80:A:VAL:HG13	1:81:A:PHE:HD1	18	0.25	0.09	0.25
(1,2148)	1:80:A:VAL:HG12	1:81:A:PHE:HD1	18	0.25	0.09	0.25
(1,12)	1:72:A:LEU:HD13	1:72:A:LEU:H	18	0.23	0.07	0.22
(1,12)	1:72:A:LEU:HD12	1:72:A:LEU:H	18	0.23	0.07	0.22
(1,12)	1:72:A:LEU:HD11	1:72:A:LEU:H	18	0.23	0.07	0.22
(1,1410)	1:84:A:ASN:HB3	1:84:A:ASN:HA	18	0.21	0.03	0.2
(1,1410)	1:84:A:ASN:HB2	1:84:A:ASN:HA	18	0.21	0.03	0.2
(1,2061)	1:33:A:ILE:HA	1:65:A:ILE:HG22	18	0.21	0.07	0.2
(1,2061)	1:33:A:ILE:HA	1:65:A:ILE:HG23	18	0.21	0.07	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2061)	1:33:A:ILE:HA	1:65:A:ILE:HG21	18	0.21	0.07	0.2
(1,780)	1:99:A:VAL:HG12	1:99:A:VAL:HG21	18	0.18	0.05	0.18
(1,780)	1:99:A:VAL:HG11	1:99:A:VAL:HG23	18	0.18	0.05	0.18
(1,780)	1:99:A:VAL:HG11	1:99:A:VAL:HG21	18	0.18	0.05	0.18
(1,780)	1:99:A:VAL:HG11	1:99:A:VAL:HG22	18	0.18	0.05	0.18
(1,780)	1:99:A:VAL:HG13	1:99:A:VAL:HG22	18	0.18	0.05	0.18
(1,780)	1:99:A:VAL:HG13	1:99:A:VAL:HG21	18	0.18	0.05	0.18
(1,780)	1:99:A:VAL:HG12	1:99:A:VAL:HG23	18	0.18	0.05	0.18
(1,780)	1:99:A:VAL:HG13	1:99:A:VAL:HG23	18	0.18	0.05	0.18
(1,780)	1:99:A:VAL:HG12	1:99:A:VAL:HG22	18	0.18	0.05	0.18
(1,2298)	1:71:A:GLU:H	1:70:A:VAL:H	18	0.16	0.04	0.16
(1,1038)	1:20:A:LYS:HG3	1:20:A:LYS:HD2	18	0.16	0.02	0.16
(1,1559)	1:12:A:ALA:HB3	1:12:A:ALA:HA	18	0.15	0.03	0.15
(1,1559)	1:12:A:ALA:HB1	1:12:A:ALA:HA	18	0.15	0.03	0.15
(1,1559)	1:12:A:ALA:HB2	1:12:A:ALA:HA	18	0.15	0.03	0.15
(1,1230)	1:54:A:GLU:HB3	1:54:A:GLU:HG2	18	0.13	0.01	0.13
(1,1019)	1:102:A:THR:HG21	1:100:A:ILE:HG12	17	1.1	0.24	1.06
(1,1019)	1:102:A:THR:HG23	1:100:A:ILE:HG12	17	1.1	0.24	1.06
(1,1019)	1:102:A:THR:HG22	1:100:A:ILE:HG12	17	1.1	0.24	1.06
(1,2621)	1:38:A:ALA:HB3	1:105:A:ASN:HB2	17	1.07	0.37	1.1
(1,2621)	1:18:A:ALA:HB3	1:21:A:ASN:HB2	17	1.07	0.37	1.1
(1,2621)	1:18:A:ALA:HB1	1:21:A:ASN:HB2	17	1.07	0.37	1.1
(1,2621)	1:38:A:ALA:HB2	1:105:A:ASN:HB2	17	1.07	0.37	1.1
(1,2621)	1:38:A:ALA:HB1	1:105:A:ASN:HB2	17	1.07	0.37	1.1
(1,2621)	1:18:A:ALA:HB2	1:21:A:ASN:HB2	17	1.07	0.37	1.1
(1,1782)	1:109:A:LEU:HD22	1:107:A:MET:HE1	17	0.95	0.38	1.04
(1,1782)	1:109:A:LEU:HD21	1:107:A:MET:HE1	17	0.95	0.38	1.04
(1,1782)	1:109:A:LEU:HD21	1:107:A:MET:HE3	17	0.95	0.38	1.04
(1,1782)	1:109:A:LEU:HD23	1:107:A:MET:HE3	17	0.95	0.38	1.04
(1,1782)	1:109:A:LEU:HD23	1:107:A:MET:HE2	17	0.95	0.38	1.04
(1,1782)	1:109:A:LEU:HD22	1:107:A:MET:HE2	17	0.95	0.38	1.04
(1,1782)	1:109:A:LEU:HD23	1:107:A:MET:HE1	17	0.95	0.38	1.04
(1,1782)	1:109:A:LEU:HD22	1:107:A:MET:HE3	17	0.95	0.38	1.04
(1,1782)	1:109:A:LEU:HD21	1:107:A:MET:HE2	17	0.95	0.38	1.04
(1,2583)	1:100:A:ILE:HA	1:100:A:ILE:HD13	17	0.76	0.06	0.75
(1,2583)	1:100:A:ILE:HA	1:100:A:ILE:HD12	17	0.76	0.06	0.75
(1,2583)	1:100:A:ILE:HA	1:100:A:ILE:HD11	17	0.76	0.06	0.75
(1,929)	1:100:A:ILE:HG22	1:100:A:ILE:HG13	17	0.75	0.04	0.75
(1,929)	1:100:A:ILE:HG23	1:100:A:ILE:HG13	17	0.75	0.04	0.75
(1,929)	1:100:A:ILE:HG21	1:100:A:ILE:HG13	17	0.75	0.04	0.75
(1,1824)	1:25:A:LYS:HG3	1:56:A:LEU:HD13	17	0.66	0.42	0.57
(1,1824)	1:25:A:LYS:HG3	1:56:A:LEU:HD11	17	0.66	0.42	0.57

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1824)	1:25:A:LYS:HG3	1:56:A:LEU:HD12	17	0.66	0.42	0.57
(1,2153)	1:99:A:VAL:HG22	1:81:A:PHE:HE1	17	0.62	0.51	0.37
(1,2153)	1:99:A:VAL:HG21	1:81:A:PHE:HE1	17	0.62	0.51	0.37
(1,2153)	1:99:A:VAL:HG21	1:81:A:PHE:HE2	17	0.62	0.51	0.37
(1,2153)	1:99:A:VAL:HG23	1:81:A:PHE:HE2	17	0.62	0.51	0.37
(1,2153)	1:99:A:VAL:HG22	1:81:A:PHE:HE2	17	0.62	0.51	0.37
(1,2153)	1:99:A:VAL:HG23	1:81:A:PHE:HE1	17	0.62	0.51	0.37
(1,1887)	1:82:A:LYS:HD2	1:71:A:GLU:HB3	17	0.59	0.35	0.45
(1,1887)	1:82:A:LYS:HD3	1:71:A:GLU:HB3	17	0.59	0.35	0.45
(1,66)	1:100:A:ILE:HD12	1:100:A:ILE:H	17	0.57	0.04	0.57
(1,66)	1:100:A:ILE:HD11	1:100:A:ILE:H	17	0.57	0.04	0.57
(1,66)	1:100:A:ILE:HD13	1:100:A:ILE:H	17	0.57	0.04	0.57
(1,2070)	1:109:A:LEU:HD21	1:29:A:VAL:HA	17	0.34	0.15	0.26
(1,2070)	1:109:A:LEU:HD22	1:29:A:VAL:HA	17	0.34	0.15	0.26
(1,2070)	1:109:A:LEU:HD23	1:29:A:VAL:HA	17	0.34	0.15	0.26
(1,849)	1:72:A:LEU:HD21	1:101:A:ILE:HG13	17	0.33	0.28	0.24
(1,849)	1:72:A:LEU:HD23	1:101:A:ILE:HG13	17	0.33	0.28	0.24
(1,849)	1:72:A:LEU:HD22	1:101:A:ILE:HG13	17	0.33	0.28	0.24
(1,174)	1:100:A:ILE:HG12	1:101:A:ILE:H	17	0.31	0.08	0.3
(1,2262)	1:88:A:TYR:HA	1:88:A:TYR:HD1	17	0.3	0.09	0.33
(1,2262)	1:88:A:TYR:HA	1:88:A:TYR:HD2	17	0.3	0.09	0.33
(1,2024)	1:107:A:MET:HE3	1:7:A:VAL:HA	17	0.29	0.11	0.29
(1,2024)	1:107:A:MET:HE2	1:7:A:VAL:HA	17	0.29	0.11	0.29
(1,2024)	1:107:A:MET:HE1	1:7:A:VAL:HA	17	0.29	0.11	0.29
(1,1819)	1:7:A:VAL:HG13	1:47:A:ALA:HB2	17	0.28	0.12	0.28
(1,1819)	1:7:A:VAL:HG12	1:47:A:ALA:HB2	17	0.28	0.12	0.28
(1,1819)	1:7:A:VAL:HG12	1:47:A:ALA:HB3	17	0.28	0.12	0.28
(1,1819)	1:7:A:VAL:HG11	1:47:A:ALA:HB1	17	0.28	0.12	0.28
(1,1819)	1:7:A:VAL:HG13	1:47:A:ALA:HB1	17	0.28	0.12	0.28
(1,1819)	1:7:A:VAL:HG12	1:47:A:ALA:HB1	17	0.28	0.12	0.28
(1,1819)	1:7:A:VAL:HG11	1:47:A:ALA:HB2	17	0.28	0.12	0.28
(1,1819)	1:7:A:VAL:HG11	1:47:A:ALA:HB3	17	0.28	0.12	0.28
(1,1010)	1:115:A:LEU:HB3	1:25:A:LYS:HB3	17	0.24	0.12	0.2
(1,1010)	1:115:A:LEU:HB3	1:25:A:LYS:HB2	17	0.24	0.12	0.2
(1,2183)	1:116:A:ALA:HB3	1:24:A:HIS:HD2	17	0.2	0.06	0.19
(1,2183)	1:116:A:ALA:HB1	1:24:A:HIS:HD2	17	0.2	0.06	0.19
(1,2183)	1:116:A:ALA:HB2	1:24:A:HIS:HD2	17	0.2	0.06	0.19
(1,248)	1:97:A:LYS:HB3	1:97:A:LYS:H	17	0.15	0.02	0.14
(1,2518)	1:25:A:LYS:HD3	1:25:A:LYS:HE3	17	0.13	0.02	0.13
(1,2518)	1:25:A:LYS:HD2	1:25:A:LYS:HE3	17	0.13	0.02	0.13
(1,2518)	1:19:A:LYS:HD2	1:19:A:LYS:HE3	17	0.13	0.02	0.13
(1,2518)	1:25:A:LYS:HD3	1:25:A:LYS:HE2	17	0.13	0.02	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2518)	1:19:A:LYS:HD3	1:19:A:LYS:HE2	17	0.13	0.02	0.13
(1,2518)	1:25:A:LYS:HD2	1:25:A:LYS:HE2	17	0.13	0.02	0.13
(1,1276)	1:19:A:LYS:HB2	1:19:A:LYS:HE3	16	0.84	0.06	0.86
(1,1276)	1:19:A:LYS:HB2	1:19:A:LYS:HE2	16	0.84	0.06	0.86
(1,1831)	1:58:A:CYS:HB2	1:61:A:ALA:HB1	16	0.72	0.27	0.68
(1,1831)	1:58:A:CYS:HB2	1:61:A:ALA:HB2	16	0.72	0.27	0.68
(1,1831)	1:58:A:CYS:HB2	1:61:A:ALA:HB3	16	0.72	0.27	0.68
(1,2612)	1:59:A:LYS:HE3	1:56:A:LEU:HD13	16	0.64	0.24	0.64
(1,2612)	1:59:A:LYS:HE2	1:56:A:LEU:HD13	16	0.64	0.24	0.64
(1,2612)	1:59:A:LYS:HE2	1:56:A:LEU:HD11	16	0.64	0.24	0.64
(1,2612)	1:25:A:LYS:HE3	1:56:A:LEU:HD12	16	0.64	0.24	0.64
(1,2612)	1:59:A:LYS:HE2	1:56:A:LEU:HD12	16	0.64	0.24	0.64
(1,2612)	1:25:A:LYS:HE3	1:56:A:LEU:HD11	16	0.64	0.24	0.64
(1,2612)	1:25:A:LYS:HE2	1:56:A:LEU:HD13	16	0.64	0.24	0.64
(1,2612)	1:25:A:LYS:HE3	1:56:A:LEU:HD13	16	0.64	0.24	0.64
(1,2612)	1:25:A:LYS:HE2	1:56:A:LEU:HD12	16	0.64	0.24	0.64
(1,2134)	1:72:A:LEU:HD22	1:81:A:PHE:HE1	16	0.62	0.4	0.52
(1,2134)	1:72:A:LEU:HD23	1:81:A:PHE:HE2	16	0.62	0.4	0.52
(1,2134)	1:72:A:LEU:HD21	1:81:A:PHE:HE2	16	0.62	0.4	0.52
(1,2134)	1:72:A:LEU:HD22	1:81:A:PHE:HE2	16	0.62	0.4	0.52
(1,2134)	1:72:A:LEU:HD23	1:81:A:PHE:HE1	16	0.62	0.4	0.52
(1,2134)	1:72:A:LEU:HD21	1:81:A:PHE:HE1	16	0.62	0.4	0.52
(1,1746)	1:90:A:VAL:HG23	1:87:A:ASP:HB3	16	0.5	0.26	0.57
(1,1746)	1:90:A:VAL:HG21	1:87:A:ASP:HB3	16	0.5	0.26	0.57
(1,1746)	1:90:A:VAL:HG22	1:87:A:ASP:HB3	16	0.5	0.26	0.57
(1,898)	1:29:A:VAL:HG13	1:112:A:LEU:HA	16	0.36	0.16	0.38
(1,898)	1:29:A:VAL:HG11	1:112:A:LEU:HA	16	0.36	0.16	0.38
(1,898)	1:29:A:VAL:HG12	1:112:A:LEU:HA	16	0.36	0.16	0.38
(1,1211)	1:75:A:LYS:HB3	1:98:A:ASN:HB2	16	0.35	0.2	0.27
(1,998)	1:65:A:ILE:HG12	1:63:A:LEU:HD21	16	0.31	0.15	0.3
(1,998)	1:65:A:ILE:HG12	1:63:A:LEU:HD23	16	0.31	0.15	0.3
(1,998)	1:65:A:ILE:HG12	1:63:A:LEU:HD22	16	0.31	0.15	0.3
(1,29)	1:70:A:VAL:HG23	1:72:A:LEU:H	16	0.27	0.14	0.21
(1,29)	1:70:A:VAL:HG21	1:72:A:LEU:H	16	0.27	0.14	0.21
(1,29)	1:70:A:VAL:HG22	1:72:A:LEU:H	16	0.27	0.14	0.21
(1,2661)	1:75:A:LYS:HA	1:75:A:LYS:HE3	16	0.24	0.09	0.24
(1,1944)	1:57:A:VAL:HB	1:26:A:ILE:HD11	16	0.22	0.07	0.22
(1,1944)	1:57:A:VAL:HB	1:26:A:ILE:HD13	16	0.22	0.07	0.22
(1,1944)	1:57:A:VAL:HB	1:26:A:ILE:HD12	16	0.22	0.07	0.22
(1,25)	1:90:A:VAL:HG21	1:91:A:CYS:H	16	0.18	0.04	0.16
(1,25)	1:90:A:VAL:HG22	1:91:A:CYS:H	16	0.18	0.04	0.16
(1,25)	1:90:A:VAL:HG23	1:91:A:CYS:H	16	0.18	0.04	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1695)	1:64:A:ASP:HB2	1:30:A:VAL:HA	15	0.88	0.1	0.86
(1,2016)	1:93:A:LYS:HD2	1:79:A:HIS:HB2	15	0.54	0.29	0.48
(1,1302)	1:1:A:MET:HE1	1:1:A:MET:HA	15	0.52	0.09	0.53
(1,1302)	1:1:A:MET:HE2	1:1:A:MET:HA	15	0.52	0.09	0.53
(1,1302)	1:1:A:MET:HE3	1:1:A:MET:HA	15	0.52	0.09	0.53
(1,990)	1:59:A:LYS:HG3	1:59:A:LYS:HE3	15	0.52	0.06	0.52
(1,962)	1:33:A:ILE:HD11	1:41:A:LYS:HG3	15	0.43	0.23	0.46
(1,962)	1:33:A:ILE:HD12	1:41:A:LYS:HG3	15	0.43	0.23	0.46
(1,962)	1:33:A:ILE:HD13	1:41:A:LYS:HG3	15	0.43	0.23	0.46
(1,2670)	1:11:A:ILE:HG22	1:51:A:PHE:HD2	15	0.41	0.15	0.4
(1,2670)	1:11:A:ILE:HG21	1:51:A:PHE:HD2	15	0.41	0.15	0.4
(1,2670)	1:11:A:ILE:HG23	1:51:A:PHE:HD2	15	0.41	0.15	0.4
(1,1798)	1:62:A:ILE:HD13	1:28:A:ARG:HD3	15	0.31	0.14	0.27
(1,1798)	1:62:A:ILE:HD11	1:28:A:ARG:HD3	15	0.31	0.14	0.27
(1,1798)	1:62:A:ILE:HD12	1:28:A:ARG:HD3	15	0.31	0.14	0.27
(1,1452)	1:63:A:LEU:HD11	1:45:A:VAL:HA	15	0.31	0.14	0.28
(1,1452)	1:63:A:LEU:HD13	1:45:A:VAL:HA	15	0.31	0.14	0.28
(1,1452)	1:63:A:LEU:HD12	1:45:A:VAL:HA	15	0.31	0.14	0.28
(1,874)	1:26:A:ILE:HG21	1:61:A:ALA:HB3	15	0.28	0.13	0.26
(1,874)	1:26:A:ILE:HG22	1:61:A:ALA:HB2	15	0.28	0.13	0.26
(1,874)	1:26:A:ILE:HG21	1:61:A:ALA:HB1	15	0.28	0.13	0.26
(1,874)	1:26:A:ILE:HG22	1:61:A:ALA:HB3	15	0.28	0.13	0.26
(1,874)	1:26:A:ILE:HG23	1:61:A:ALA:HB3	15	0.28	0.13	0.26
(1,874)	1:26:A:ILE:HG23	1:61:A:ALA:HB2	15	0.28	0.13	0.26
(1,2469)	1:6:A:VAL:HG11	1:107:A:MET:HE2	15	0.26	0.06	0.26
(1,2469)	1:6:A:VAL:HG12	1:107:A:MET:HE2	15	0.26	0.06	0.26
(1,2469)	1:6:A:VAL:HG12	1:39:A:MET:HE1	15	0.26	0.06	0.26
(1,2469)	1:6:A:VAL:HG13	1:39:A:MET:HE2	15	0.26	0.06	0.26
(1,2469)	1:6:A:VAL:HG11	1:39:A:MET:HE2	15	0.26	0.06	0.26
(1,2469)	1:6:A:VAL:HG12	1:39:A:MET:HE2	15	0.26	0.06	0.26
(1,2469)	1:6:A:VAL:HG13	1:39:A:MET:HE1	15	0.26	0.06	0.26
(1,2469)	1:6:A:VAL:HG11	1:107:A:MET:HE1	15	0.26	0.06	0.26
(1,2469)	1:6:A:VAL:HG13	1:107:A:MET:HE3	15	0.26	0.06	0.26
(1,771)	1:110:A:LEU:HD12	1:66:A:VAL:HG22	15	0.23	0.11	0.18
(1,771)	1:110:A:LEU:HD11	1:66:A:VAL:HG23	15	0.23	0.11	0.18
(1,771)	1:110:A:LEU:HD12	1:66:A:VAL:HG21	15	0.23	0.11	0.18
(1,771)	1:110:A:LEU:HD12	1:66:A:VAL:HG23	15	0.23	0.11	0.18
(1,771)	1:110:A:LEU:HD13	1:66:A:VAL:HG23	15	0.23	0.11	0.18
(1,771)	1:110:A:LEU:HD11	1:66:A:VAL:HG21	15	0.23	0.11	0.18
(1,771)	1:110:A:LEU:HD11	1:66:A:VAL:HG22	15	0.23	0.11	0.18
(1,771)	1:110:A:LEU:HD13	1:66:A:VAL:HG22	15	0.23	0.11	0.18
(1,1477)	1:45:A:VAL:HG12	1:41:A:LYS:HA	15	0.22	0.08	0.21

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1477)	1:45:A:VAL:HG13	1:41:A:LYS:HA	15	0.22	0.08	0.21
(1,1477)	1:45:A:VAL:HG11	1:41:A:LYS:HA	15	0.22	0.08	0.21
(1,1361)	1:26:A:ILE:HD11	1:114:A:MET:HG2	15	0.22	0.09	0.2
(1,1361)	1:26:A:ILE:HD13	1:114:A:MET:HG2	15	0.22	0.09	0.2
(1,1361)	1:26:A:ILE:HD12	1:114:A:MET:HG2	15	0.22	0.09	0.2
(1,1771)	1:31:A:VAL:HG21	1:65:A:ILE:HB	15	0.21	0.08	0.21
(1,1771)	1:31:A:VAL:HG23	1:65:A:ILE:HB	15	0.21	0.08	0.21
(1,1771)	1:31:A:VAL:HG22	1:65:A:ILE:HB	15	0.21	0.08	0.21
(1,142)	1:47:A:ALA:HB3	1:46:A:SER:H	15	0.19	0.06	0.16
(1,142)	1:47:A:ALA:HB2	1:46:A:SER:H	15	0.19	0.06	0.16
(1,142)	1:47:A:ALA:HB1	1:46:A:SER:H	15	0.19	0.06	0.16
(1,2569)	1:92:A:GLU:HG2	1:92:A:GLU:HA	15	0.17	0.04	0.18
(1,2600)	1:30:A:VAL:HG12	1:30:A:VAL:HG11	15	0.12	0.01	0.12
(1,2600)	1:30:A:VAL:HG11	1:30:A:VAL:HG13	15	0.12	0.01	0.12
(1,2600)	1:66:A:VAL:HG12	1:66:A:VAL:HG11	15	0.12	0.01	0.12
(1,2600)	1:66:A:VAL:HG11	1:66:A:VAL:HG13	15	0.12	0.01	0.12
(1,2600)	1:30:A:VAL:HG12	1:30:A:VAL:HG13	15	0.12	0.01	0.12
(1,2600)	1:66:A:VAL:HG12	1:66:A:VAL:HG13	15	0.12	0.01	0.12
(1,2088)	1:105:A:ASN:HA	1:36:A:ARG:HB3	14	0.53	0.28	0.46
(1,834)	1:72:A:LEU:HD22	1:101:A:ILE:HG21	14	0.45	0.69	0.24
(1,834)	1:72:A:LEU:HD23	1:101:A:ILE:HG22	14	0.45	0.69	0.24
(1,834)	1:72:A:LEU:HD21	1:101:A:ILE:HG21	14	0.45	0.69	0.24
(1,834)	1:72:A:LEU:HD22	1:101:A:ILE:HG22	14	0.45	0.69	0.24
(1,834)	1:72:A:LEU:HD22	1:101:A:ILE:HG23	14	0.45	0.69	0.24
(1,834)	1:72:A:LEU:HD23	1:101:A:ILE:HG23	14	0.45	0.69	0.24
(1,834)	1:72:A:LEU:HD23	1:101:A:ILE:HG21	14	0.45	0.69	0.24
(1,1800)	1:115:A:LEU:HD13	1:25:A:LYS:HG2	14	0.44	0.21	0.44
(1,1800)	1:115:A:LEU:HD12	1:25:A:LYS:HG2	14	0.44	0.21	0.44
(1,1800)	1:115:A:LEU:HD11	1:25:A:LYS:HG2	14	0.44	0.21	0.44
(1,904)	1:31:A:VAL:HG13	1:10:A:LEU:HD12	14	0.4	0.24	0.36
(1,904)	1:31:A:VAL:HG12	1:10:A:LEU:HD11	14	0.4	0.24	0.36
(1,904)	1:31:A:VAL:HG12	1:10:A:LEU:HD13	14	0.4	0.24	0.36
(1,904)	1:31:A:VAL:HG11	1:10:A:LEU:HD13	14	0.4	0.24	0.36
(1,904)	1:31:A:VAL:HG11	1:10:A:LEU:HD11	14	0.4	0.24	0.36
(1,904)	1:31:A:VAL:HG13	1:10:A:LEU:HD11	14	0.4	0.24	0.36
(1,904)	1:31:A:VAL:HG12	1:10:A:LEU:HD12	14	0.4	0.24	0.36
(1,904)	1:31:A:VAL:HG11	1:10:A:LEU:HD12	14	0.4	0.24	0.36
(1,904)	1:31:A:VAL:HG13	1:10:A:LEU:HD13	14	0.4	0.24	0.36
(1,1324)	1:106:A:GLU:HG3	1:105:A:ASN:HB2	14	0.36	0.24	0.24
(1,1324)	1:106:A:GLU:HG2	1:105:A:ASN:HB2	14	0.36	0.24	0.24
(1,889)	1:57:A:VAL:HG13	1:15:A:GLU:HG3	14	0.33	0.16	0.32
(1,889)	1:57:A:VAL:HG12	1:15:A:GLU:HG3	14	0.33	0.16	0.32

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,889)	1:57:A:VAL:HG11	1:15:A:GLU:HG3	14	0.33	0.16	0.32
(1,1145)	1:41:A:LYS:HD2	1:33:A:ILE:HG21	14	0.31	0.2	0.26
(1,1145)	1:41:A:LYS:HD2	1:33:A:ILE:HG23	14	0.31	0.2	0.26
(1,1145)	1:41:A:LYS:HD2	1:33:A:ILE:HG22	14	0.31	0.2	0.26
(1,963)	1:41:A:LYS:HG3	1:65:A:ILE:HD12	14	0.31	0.11	0.27
(1,963)	1:41:A:LYS:HG3	1:65:A:ILE:HD13	14	0.31	0.11	0.27
(1,963)	1:41:A:LYS:HG3	1:65:A:ILE:HD11	14	0.31	0.11	0.27
(1,2100)	1:97:A:LYS:HA	1:97:A:LYS:HE2	14	0.3	0.25	0.18
(1,2100)	1:97:A:LYS:HA	1:97:A:LYS:HE3	14	0.3	0.25	0.18
(1,1749)	1:65:A:ILE:HG13	1:63:A:LEU:HD22	14	0.26	0.11	0.26
(1,1749)	1:65:A:ILE:HG13	1:63:A:LEU:HD23	14	0.26	0.11	0.26
(1,1749)	1:65:A:ILE:HG13	1:63:A:LEU:HD21	14	0.26	0.11	0.26
(1,2172)	1:47:A:ALA:HB3	1:4:A:TYR:HD2	14	0.25	0.14	0.18
(1,2172)	1:47:A:ALA:HB1	1:4:A:TYR:HD1	14	0.25	0.14	0.18
(1,2172)	1:47:A:ALA:HB2	1:4:A:TYR:HD1	14	0.25	0.14	0.18
(1,2172)	1:47:A:ALA:HB3	1:4:A:TYR:HD1	14	0.25	0.14	0.18
(1,2172)	1:47:A:ALA:HB1	1:4:A:TYR:HD2	14	0.25	0.14	0.18
(1,1384)	1:93:A:LYS:HE3	1:93:A:LYS:HA	14	0.22	0.15	0.15
(1,1384)	1:93:A:LYS:HE2	1:93:A:LYS:HA	14	0.22	0.15	0.15
(1,2401)	1:90:A:VAL:H	1:91:A:CYS:H	14	0.16	0.04	0.16
(1,767)	1:70:A:VAL:HG21	1:70:A:VAL:HG11	14	0.15	0.03	0.14
(1,767)	1:70:A:VAL:HG23	1:70:A:VAL:HG12	14	0.15	0.03	0.14
(1,767)	1:70:A:VAL:HG22	1:70:A:VAL:HG13	14	0.15	0.03	0.14
(1,767)	1:70:A:VAL:HG22	1:70:A:VAL:HG12	14	0.15	0.03	0.14
(1,767)	1:70:A:VAL:HG23	1:70:A:VAL:HG11	14	0.15	0.03	0.14
(1,767)	1:70:A:VAL:HG21	1:70:A:VAL:HG12	14	0.15	0.03	0.14
(1,767)	1:70:A:VAL:HG23	1:70:A:VAL:HG13	14	0.15	0.03	0.14
(1,767)	1:70:A:VAL:HG21	1:70:A:VAL:HG13	14	0.15	0.03	0.14
(1,767)	1:70:A:VAL:HG22	1:70:A:VAL:HG11	14	0.15	0.03	0.14
(1,744)	1:72:A:LEU:HD12	1:72:A:LEU:HD21	14	0.15	0.03	0.13
(1,744)	1:72:A:LEU:HD11	1:72:A:LEU:HD22	14	0.15	0.03	0.13
(1,744)	1:72:A:LEU:HD11	1:72:A:LEU:HD21	14	0.15	0.03	0.13
(1,744)	1:72:A:LEU:HD12	1:72:A:LEU:HD23	14	0.15	0.03	0.13
(1,744)	1:72:A:LEU:HD12	1:72:A:LEU:HD22	14	0.15	0.03	0.13
(1,744)	1:72:A:LEU:HD13	1:72:A:LEU:HD21	14	0.15	0.03	0.13
(1,744)	1:72:A:LEU:HD13	1:72:A:LEU:HD23	14	0.15	0.03	0.13
(1,1058)	1:11:A:ILE:HG22	1:11:A:ILE:HG12	14	0.14	0.02	0.14
(1,1058)	1:11:A:ILE:HG21	1:11:A:ILE:HG12	14	0.14	0.02	0.14
(1,1058)	1:11:A:ILE:HG23	1:11:A:ILE:HG12	14	0.14	0.02	0.14
(1,822)	1:80:A:VAL:HG11	1:102:A:THR:HG22	13	0.61	0.34	0.56
(1,822)	1:80:A:VAL:HG13	1:102:A:THR:HG23	13	0.61	0.34	0.56
(1,822)	1:80:A:VAL:HG11	1:102:A:THR:HG23	13	0.61	0.34	0.56

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,822)	1:80:A:VAL:HG13	1:102:A:THR:HG21	13	0.61	0.34	0.56
(1,822)	1:80:A:VAL:HG12	1:102:A:THR:HG22	13	0.61	0.34	0.56
(1,822)	1:80:A:VAL:HG12	1:102:A:THR:HG21	13	0.61	0.34	0.56
(1,822)	1:80:A:VAL:HG13	1:102:A:THR:HG22	13	0.61	0.34	0.56
(1,822)	1:80:A:VAL:HG11	1:102:A:THR:HG21	13	0.61	0.34	0.56
(1,1854)	1:75:A:LYS:HG2	1:100:A:ILE:HG13	13	0.57	0.44	0.39
(1,1391)	1:58:A:CYS:HB3	1:55:A:SER:HB3	13	0.55	0.18	0.56
(1,1391)	1:58:A:CYS:HB3	1:55:A:SER:HB2	13	0.55	0.18	0.56
(1,2678)	1:39:A:MET:HE1	1:44:A:PHE:HZ	13	0.54	0.3	0.44
(1,2678)	1:39:A:MET:HE2	1:44:A:PHE:HZ	13	0.54	0.3	0.44
(1,2678)	1:107:A:MET:HE2	1:44:A:PHE:HZ	13	0.54	0.3	0.44
(1,2678)	1:107:A:MET:HE1	1:44:A:PHE:HZ	13	0.54	0.3	0.44
(1,2678)	1:107:A:MET:HE3	1:44:A:PHE:HZ	13	0.54	0.3	0.44
(1,2678)	1:39:A:MET:HE3	1:44:A:PHE:HZ	13	0.54	0.3	0.44
(1,1748)	1:33:A:ILE:HG21	1:107:A:MET:HG3	13	0.46	0.22	0.44
(1,1748)	1:33:A:ILE:HG22	1:107:A:MET:HG3	13	0.46	0.22	0.44
(1,1748)	1:33:A:ILE:HG23	1:107:A:MET:HG3	13	0.46	0.22	0.44
(1,2555)	1:115:A:LEU:HD13	1:25:A:LYS:HE2	13	0.45	0.21	0.4
(1,2555)	1:115:A:LEU:HD13	1:25:A:LYS:HE3	13	0.45	0.21	0.4
(1,2555)	1:25:A:LYS:HE3	1:56:A:LEU:HD12	13	0.45	0.21	0.4
(1,2555)	1:115:A:LEU:HD12	1:25:A:LYS:HE2	13	0.45	0.21	0.4
(1,2555)	1:25:A:LYS:HE3	1:56:A:LEU:HD11	13	0.45	0.21	0.4
(1,2555)	1:25:A:LYS:HE3	1:56:A:LEU:HD13	13	0.45	0.21	0.4
(1,2555)	1:115:A:LEU:HD11	1:25:A:LYS:HE2	13	0.45	0.21	0.4
(1,1024)	1:57:A:VAL:HG12	1:18:A:ALA:HB1	13	0.36	0.24	0.24
(1,1024)	1:57:A:VAL:HG13	1:18:A:ALA:HB1	13	0.36	0.24	0.24
(1,1024)	1:57:A:VAL:HG11	1:18:A:ALA:HB2	13	0.36	0.24	0.24
(1,1024)	1:57:A:VAL:HG12	1:18:A:ALA:HB3	13	0.36	0.24	0.24
(1,1024)	1:57:A:VAL:HG11	1:18:A:ALA:HB3	13	0.36	0.24	0.24
(1,1024)	1:57:A:VAL:HG12	1:18:A:ALA:HB2	13	0.36	0.24	0.24
(1,1024)	1:57:A:VAL:HG13	1:18:A:ALA:HB3	13	0.36	0.24	0.24
(1,1777)	1:112:A:LEU:HD22	1:109:A:LEU:HD11	13	0.35	0.2	0.33
(1,1777)	1:112:A:LEU:HD23	1:109:A:LEU:HD11	13	0.35	0.2	0.33
(1,1777)	1:112:A:LEU:HD21	1:109:A:LEU:HD12	13	0.35	0.2	0.33
(1,1777)	1:112:A:LEU:HD21	1:109:A:LEU:HD11	13	0.35	0.2	0.33
(1,1777)	1:112:A:LEU:HD23	1:109:A:LEU:HD13	13	0.35	0.2	0.33
(1,1777)	1:112:A:LEU:HD21	1:109:A:LEU:HD13	13	0.35	0.2	0.33
(1,1777)	1:112:A:LEU:HD22	1:109:A:LEU:HD13	13	0.35	0.2	0.33
(1,1777)	1:112:A:LEU:HD22	1:109:A:LEU:HD12	13	0.35	0.2	0.33
(1,750)	1:72:A:LEU:HD23	1:99:A:VAL:HG13	13	0.33	0.13	0.33
(1,750)	1:72:A:LEU:HD22	1:99:A:VAL:HG12	13	0.33	0.13	0.33
(1,750)	1:72:A:LEU:HD21	1:99:A:VAL:HG13	13	0.33	0.13	0.33

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,750)	1:72:A:LEU:HD23	1:99:A:VAL:HG12	13	0.33	0.13	0.33
(1,750)	1:72:A:LEU:HD21	1:99:A:VAL:HG11	13	0.33	0.13	0.33
(1,750)	1:72:A:LEU:HD21	1:99:A:VAL:HG12	13	0.33	0.13	0.33
(1,2051)	1:114:A:MET:HE2	1:17:A:HIS:HA	13	0.27	0.11	0.26
(1,2051)	1:114:A:MET:HE1	1:17:A:HIS:HA	13	0.27	0.11	0.26
(1,2051)	1:114:A:MET:HE3	1:17:A:HIS:HA	13	0.27	0.11	0.26
(1,2067)	1:10:A:LEU:HA	1:13:A:LEU:HG	13	0.25	0.09	0.23
(1,448)	1:79:A:HIS:HB2	1:80:A:VAL:H	13	0.25	0.06	0.26
(1,1802)	1:29:A:VAL:HG21	1:29:A:VAL:HG11	13	0.15	0.02	0.15
(1,1802)	1:29:A:VAL:HG23	1:29:A:VAL:HG13	13	0.15	0.02	0.15
(1,1802)	1:29:A:VAL:HG23	1:29:A:VAL:HG11	13	0.15	0.02	0.15
(1,1802)	1:29:A:VAL:HG22	1:29:A:VAL:HG11	13	0.15	0.02	0.15
(1,1802)	1:29:A:VAL:HG21	1:29:A:VAL:HG13	13	0.15	0.02	0.15
(1,1802)	1:29:A:VAL:HG23	1:29:A:VAL:HG12	13	0.15	0.02	0.15
(1,1802)	1:29:A:VAL:HG22	1:29:A:VAL:HG13	13	0.15	0.02	0.15
(1,851)	1:101:A:ILE:HD11	1:105:A:ASN:HB3	12	1.14	0.31	1.21
(1,851)	1:101:A:ILE:HD12	1:105:A:ASN:HB3	12	1.14	0.31	1.21
(1,851)	1:101:A:ILE:HD13	1:105:A:ASN:HB3	12	1.14	0.31	1.21
(1,1864)	1:9:A:SER:HB2	1:12:A:ALA:HB2	12	0.73	0.45	0.92
(1,1864)	1:9:A:SER:HB3	1:12:A:ALA:HB1	12	0.73	0.45	0.92
(1,1864)	1:9:A:SER:HB2	1:12:A:ALA:HB3	12	0.73	0.45	0.92
(1,1864)	1:9:A:SER:HB2	1:12:A:ALA:HB1	12	0.73	0.45	0.92
(1,2645)	1:33:A:ILE:HG21	1:39:A:MET:HG3	12	0.45	0.19	0.44
(1,2645)	1:33:A:ILE:HG22	1:39:A:MET:HG3	12	0.45	0.19	0.44
(1,2645)	1:33:A:ILE:HG23	1:39:A:MET:HG3	12	0.45	0.19	0.44
(1,2035)	1:42:A:SER:HB2	1:45:A:VAL:HG23	12	0.43	0.15	0.4
(1,2035)	1:42:A:SER:HB3	1:45:A:VAL:HG23	12	0.43	0.15	0.4
(1,2035)	1:42:A:SER:HB2	1:45:A:VAL:HG21	12	0.43	0.15	0.4
(1,2035)	1:42:A:SER:HB2	1:45:A:VAL:HG22	12	0.43	0.15	0.4
(1,769)	1:72:A:LEU:HD21	1:70:A:VAL:HG22	12	0.38	0.37	0.24
(1,769)	1:72:A:LEU:HD21	1:70:A:VAL:HG21	12	0.38	0.37	0.24
(1,769)	1:72:A:LEU:HD22	1:70:A:VAL:HG21	12	0.38	0.37	0.24
(1,769)	1:72:A:LEU:HD22	1:70:A:VAL:HG23	12	0.38	0.37	0.24
(1,769)	1:72:A:LEU:HD22	1:70:A:VAL:HG22	12	0.38	0.37	0.24
(1,769)	1:72:A:LEU:HD21	1:70:A:VAL:HG23	12	0.38	0.37	0.24
(1,769)	1:72:A:LEU:HD23	1:70:A:VAL:HG23	12	0.38	0.37	0.24
(1,769)	1:72:A:LEU:HD23	1:70:A:VAL:HG22	12	0.38	0.37	0.24
(1,1159)	1:108:A:ARG:HB2	1:110:A:LEU:HD21	12	0.37	0.19	0.37
(1,1159)	1:108:A:ARG:HB2	1:110:A:LEU:HD22	12	0.37	0.19	0.37
(1,1159)	1:108:A:ARG:HB2	1:110:A:LEU:HD23	12	0.37	0.19	0.37
(1,1780)	1:112:A:LEU:HD21	1:17:A:HIS:HA	12	0.35	0.15	0.32
(1,1780)	1:112:A:LEU:HD23	1:17:A:HIS:HA	12	0.35	0.15	0.32

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1780)	1:112:A:LEU:HD22	1:17:A:HIS:HA	12	0.35	0.15	0.32
(1,887)	1:57:A:VAL:HG12	1:18:A:ALA:HA	12	0.33	0.22	0.22
(1,887)	1:57:A:VAL:HG13	1:18:A:ALA:HA	12	0.33	0.22	0.22
(1,887)	1:57:A:VAL:HG11	1:18:A:ALA:HA	12	0.33	0.22	0.22
(1,1677)	1:25:A:LYS:HA	1:57:A:VAL:HG21	12	0.29	0.1	0.26
(1,1677)	1:25:A:LYS:HA	1:57:A:VAL:HG23	12	0.29	0.1	0.26
(1,1677)	1:25:A:LYS:HA	1:57:A:VAL:HG22	12	0.29	0.1	0.26
(1,2166)	1:50:A:THR:HG21	1:51:A:PHE:HE1	12	0.29	0.14	0.26
(1,2166)	1:50:A:THR:HG23	1:51:A:PHE:HE2	12	0.29	0.14	0.26
(1,2166)	1:50:A:THR:HG23	1:51:A:PHE:HE1	12	0.29	0.14	0.26
(1,2166)	1:50:A:THR:HG22	1:51:A:PHE:HE1	12	0.29	0.14	0.26
(1,1774)	1:31:A:VAL:HG22	1:107:A:MET:HG2	12	0.28	0.12	0.24
(1,1774)	1:31:A:VAL:HG23	1:107:A:MET:HG2	12	0.28	0.12	0.24
(1,1774)	1:31:A:VAL:HG21	1:107:A:MET:HG2	12	0.28	0.12	0.24
(1,2052)	1:20:A:LYS:HG2	1:17:A:HIS:HA	12	0.26	0.09	0.26
(1,1249)	1:72:A:LEU:HD12	1:83:A:PRO:HG2	12	0.25	0.1	0.24
(1,1249)	1:72:A:LEU:HD13	1:83:A:PRO:HG2	12	0.25	0.1	0.24
(1,1249)	1:72:A:LEU:HD11	1:83:A:PRO:HG2	12	0.25	0.1	0.24
(1,131)	1:10:A:LEU:HD23	1:11:A:ILE:H	12	0.23	0.1	0.23
(1,131)	1:10:A:LEU:HD21	1:11:A:ILE:H	12	0.23	0.1	0.23
(1,131)	1:10:A:LEU:HD22	1:11:A:ILE:H	12	0.23	0.1	0.23
(1,1576)	1:35:A:GLU:HG3	1:69:A:LYS:HA	12	0.22	0.1	0.2
(1,1554)	1:20:A:LYS:HE2	1:17:A:HIS:HA	12	0.22	0.07	0.2
(1,1554)	1:20:A:LYS:HE3	1:17:A:HIS:HA	12	0.22	0.07	0.2
(1,2042)	1:16:A:GLU:HA	1:15:A:GLU:HB2	12	0.18	0.04	0.17
(1,107)	1:56:A:LEU:HD22	1:56:A:LEU:H	12	0.16	0.04	0.16
(1,107)	1:56:A:LEU:HD21	1:56:A:LEU:H	12	0.16	0.04	0.16
(1,107)	1:56:A:LEU:HD23	1:56:A:LEU:H	12	0.16	0.04	0.16
(1,125)	1:43:A:LEU:HD13	1:43:A:LEU:H	12	0.16	0.03	0.16
(1,125)	1:43:A:LEU:HD11	1:43:A:LEU:H	12	0.16	0.03	0.16
(1,125)	1:43:A:LEU:HD12	1:43:A:LEU:H	12	0.16	0.03	0.16
(1,2397)	1:100:A:ILE:H	1:74:A:CYS:H	12	0.15	0.05	0.14
(1,2643)	1:39:A:MET:HE3	1:106:A:GLU:HG2	11	0.68	0.47	0.51
(1,2643)	1:107:A:MET:HE1	1:106:A:GLU:HG3	11	0.68	0.47	0.51
(1,2643)	1:107:A:MET:HE3	1:106:A:GLU:HG3	11	0.68	0.47	0.51
(1,2643)	1:39:A:MET:HE2	1:106:A:GLU:HG2	11	0.68	0.47	0.51
(1,2643)	1:39:A:MET:HE1	1:106:A:GLU:HG2	11	0.68	0.47	0.51
(1,1814)	1:107:A:MET:HE3	1:10:A:LEU:HD21	11	0.67	0.26	0.67
(1,1814)	1:107:A:MET:HE3	1:10:A:LEU:HD23	11	0.67	0.26	0.67
(1,1814)	1:107:A:MET:HE2	1:10:A:LEU:HD23	11	0.67	0.26	0.67
(1,1814)	1:107:A:MET:HE1	1:10:A:LEU:HD23	11	0.67	0.26	0.67
(1,1814)	1:107:A:MET:HE1	1:10:A:LEU:HD22	11	0.67	0.26	0.67

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1814)	1:107:A:MET:HE2	1:10:A:LEU:HD22	11	0.67	0.26	0.67
(1,1814)	1:107:A:MET:HE2	1:10:A:LEU:HD21	11	0.67	0.26	0.67
(1,2622)	1:38:A:ALA:HB2	1:1:A:MET:HB2	11	0.48	0.29	0.45
(1,2622)	1:38:A:ALA:HB1	1:1:A:MET:HB2	11	0.48	0.29	0.45
(1,2622)	1:38:A:ALA:HB3	1:1:A:MET:HB2	11	0.48	0.29	0.45
(1,2142)	1:7:A:VAL:HG22	1:48:A:PHE:HD1	11	0.27	0.07	0.25
(1,2142)	1:7:A:VAL:HG21	1:48:A:PHE:HD1	11	0.27	0.07	0.25
(1,2142)	1:7:A:VAL:HG23	1:48:A:PHE:HD1	11	0.27	0.07	0.25
(1,2142)	1:7:A:VAL:HG23	1:48:A:PHE:HD2	11	0.27	0.07	0.25
(1,2142)	1:7:A:VAL:HG22	1:48:A:PHE:HD2	11	0.27	0.07	0.25
(1,2142)	1:7:A:VAL:HG21	1:48:A:PHE:HD2	11	0.27	0.07	0.25
(1,1727)	1:11:A:ILE:HD13	1:55:A:SER:HB3	11	0.26	0.14	0.27
(1,1727)	1:11:A:ILE:HD11	1:55:A:SER:HB3	11	0.26	0.14	0.27
(1,1727)	1:11:A:ILE:HD11	1:55:A:SER:HB2	11	0.26	0.14	0.27
(1,1727)	1:11:A:ILE:HD12	1:55:A:SER:HB3	11	0.26	0.14	0.27
(1,156)	1:23:A:ALA:HB2	1:21:A:ASN:H	11	0.22	0.07	0.24
(1,156)	1:23:A:ALA:HB1	1:21:A:ASN:H	11	0.22	0.07	0.24
(1,156)	1:23:A:ALA:HB3	1:21:A:ASN:H	11	0.22	0.07	0.24
(1,2104)	1:82:A:LYS:HA	1:83:A:PRO:HG3	11	0.15	0.03	0.14
(1,191)	1:93:A:LYS:HB2	1:94:A:CYS:H	11	0.14	0.04	0.12
(1,1332)	1:16:A:GLU:HB3	1:16:A:GLU:HG2	11	0.13	0.02	0.11
(1,752)	1:65:A:ILE:HG21	1:65:A:ILE:HG13	11	0.12	0.02	0.12
(1,752)	1:65:A:ILE:HG22	1:65:A:ILE:HG13	11	0.12	0.02	0.12
(1,752)	1:65:A:ILE:HG23	1:65:A:ILE:HG13	11	0.12	0.02	0.12
(1,1960)	1:113:A:GLU:HG3	1:27:A:GLU:HB3	10	0.53	0.43	0.38
(1,2170)	1:92:A:GLU:HG3	1:81:A:PHE:HD2	10	0.51	0.29	0.46
(1,2170)	1:92:A:GLU:HG3	1:81:A:PHE:HD1	10	0.51	0.29	0.46
(1,1217)	1:72:A:LEU:HD11	1:99:A:VAL:HB	10	0.42	0.69	0.17
(1,1217)	1:72:A:LEU:HD12	1:99:A:VAL:HB	10	0.42	0.69	0.17
(1,1888)	1:85:A:ALA:HB3	1:86:A:LEU:HG	10	0.38	0.17	0.39
(1,1888)	1:85:A:ALA:HB1	1:86:A:LEU:HG	10	0.38	0.17	0.39
(1,1888)	1:85:A:ALA:HB2	1:86:A:LEU:HG	10	0.38	0.17	0.39
(1,2427)	1:107:A:MET:HE2	1:107:A:MET:H	10	0.33	0.11	0.38
(1,2427)	1:107:A:MET:HE1	1:107:A:MET:H	10	0.33	0.11	0.38
(1,2427)	1:39:A:MET:HE2	1:107:A:MET:H	10	0.33	0.11	0.38
(1,2427)	1:107:A:MET:HE3	1:107:A:MET:H	10	0.33	0.11	0.38
(1,825)	1:101:A:ILE:HG22	1:72:A:LEU:HA	10	0.23	0.09	0.22
(1,825)	1:101:A:ILE:HG21	1:72:A:LEU:HA	10	0.23	0.09	0.22
(1,825)	1:101:A:ILE:HG23	1:72:A:LEU:HA	10	0.23	0.09	0.22
(1,2053)	1:17:A:HIS:HA	1:16:A:GLU:HG2	10	0.2	0.06	0.21
(1,1303)	1:23:A:ALA:HB1	1:114:A:MET:HB2	10	0.18	0.05	0.18
(1,1303)	1:23:A:ALA:HB3	1:114:A:MET:HB2	10	0.18	0.05	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1303)	1:23:A:ALA:HB2	1:114:A:MET:HB2	10	0.18	0.05	0.18
(1,344)	1:113:A:GLU:HG3	1:113:A:GLU:H	10	0.17	0.06	0.14
(1,185)	1:38:A:ALA:HB2	1:39:A:MET:H	9	0.5	0.13	0.56
(1,185)	1:38:A:ALA:HB1	1:39:A:MET:H	9	0.5	0.13	0.56
(1,185)	1:38:A:ALA:HB3	1:39:A:MET:H	9	0.5	0.13	0.56
(1,2130)	1:72:A:LEU:HD13	1:81:A:PHE:HE2	9	0.47	0.5	0.3
(1,2130)	1:72:A:LEU:HD13	1:81:A:PHE:HE1	9	0.47	0.5	0.3
(1,2130)	1:72:A:LEU:HD11	1:81:A:PHE:HE1	9	0.47	0.5	0.3
(1,2130)	1:72:A:LEU:HD11	1:81:A:PHE:HE2	9	0.47	0.5	0.3
(1,2130)	1:72:A:LEU:HD12	1:81:A:PHE:HE1	9	0.47	0.5	0.3
(1,2130)	1:72:A:LEU:HD12	1:81:A:PHE:HE2	9	0.47	0.5	0.3
(1,1820)	1:10:A:LEU:HD21	1:6:A:VAL:HG12	9	0.39	0.16	0.42
(1,1820)	1:10:A:LEU:HD23	1:6:A:VAL:HG11	9	0.39	0.16	0.42
(1,1820)	1:10:A:LEU:HD22	1:6:A:VAL:HG12	9	0.39	0.16	0.42
(1,1820)	1:10:A:LEU:HD21	1:6:A:VAL:HG13	9	0.39	0.16	0.42
(1,1820)	1:10:A:LEU:HD23	1:6:A:VAL:HG12	9	0.39	0.16	0.42
(1,1820)	1:10:A:LEU:HD22	1:6:A:VAL:HG13	9	0.39	0.16	0.42
(1,1845)	1:38:A:ALA:HB2	1:39:A:MET:HA	9	0.38	0.08	0.41
(1,1845)	1:38:A:ALA:HB3	1:39:A:MET:HA	9	0.38	0.08	0.41
(1,1845)	1:38:A:ALA:HB1	1:39:A:MET:HA	9	0.38	0.08	0.41
(1,2171)	1:47:A:ALA:HB1	1:4:A:TYR:HE2	9	0.32	0.1	0.32
(1,2171)	1:47:A:ALA:HB1	1:4:A:TYR:HE1	9	0.32	0.1	0.32
(1,2171)	1:47:A:ALA:HB2	1:4:A:TYR:HE1	9	0.32	0.1	0.32
(1,2171)	1:47:A:ALA:HB3	1:4:A:TYR:HE2	9	0.32	0.1	0.32
(1,2171)	1:47:A:ALA:HB2	1:4:A:TYR:HE2	9	0.32	0.1	0.32
(1,908)	1:56:A:LEU:HD11	1:57:A:VAL:HG23	9	0.22	0.06	0.21
(1,908)	1:56:A:LEU:HD12	1:57:A:VAL:HG23	9	0.22	0.06	0.21
(1,908)	1:56:A:LEU:HD13	1:57:A:VAL:HG23	9	0.22	0.06	0.21
(1,908)	1:56:A:LEU:HD11	1:57:A:VAL:HG22	9	0.22	0.06	0.21
(1,908)	1:56:A:LEU:HD13	1:57:A:VAL:HG21	9	0.22	0.06	0.21
(1,2647)	1:82:A:LYS:HE2	1:82:A:LYS:HB2	9	0.22	0.1	0.16
(1,2647)	1:59:A:LYS:HB3	1:25:A:LYS:HE3	9	0.22	0.1	0.16
(1,2647)	1:82:A:LYS:HE2	1:82:A:LYS:HB3	9	0.22	0.1	0.16
(1,1799)	1:29:A:VAL:HG13	1:109:A:LEU:HD13	9	0.2	0.05	0.2
(1,1799)	1:29:A:VAL:HG11	1:109:A:LEU:HD13	9	0.2	0.05	0.2
(1,1799)	1:29:A:VAL:HG13	1:109:A:LEU:HD11	9	0.2	0.05	0.2
(1,1799)	1:29:A:VAL:HG12	1:109:A:LEU:HD12	9	0.2	0.05	0.2
(1,1799)	1:29:A:VAL:HG11	1:109:A:LEU:HD11	9	0.2	0.05	0.2
(1,1799)	1:29:A:VAL:HG12	1:109:A:LEU:HD13	9	0.2	0.05	0.2
(1,33)	1:33:A:ILE:HG22	1:37:A:SER:H	9	0.18	0.04	0.2
(1,33)	1:33:A:ILE:HG23	1:37:A:SER:H	9	0.18	0.04	0.2
(1,33)	1:33:A:ILE:HG21	1:37:A:SER:H	9	0.18	0.04	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1280)	1:39:A:MET:HB2	1:39:A:MET:HE1	9	0.18	0.05	0.17
(1,1280)	1:39:A:MET:HB2	1:39:A:MET:HE2	9	0.18	0.05	0.17
(1,1280)	1:39:A:MET:HB2	1:39:A:MET:HE3	9	0.18	0.05	0.17
(1,2577)	1:54:A:GLU:HG2	1:54:A:GLU:HA	9	0.17	0.05	0.18
(1,1570)	1:102:A:THR:HA	1:101:A:ILE:HG22	9	0.16	0.04	0.15
(1,1570)	1:102:A:THR:HA	1:101:A:ILE:HG21	9	0.16	0.04	0.15
(1,1570)	1:102:A:THR:HA	1:101:A:ILE:HG23	9	0.16	0.04	0.15
(1,108)	1:115:A:LEU:HD21	1:116:A:ALA:H	9	0.15	0.03	0.15
(1,108)	1:115:A:LEU:HD23	1:116:A:ALA:H	9	0.15	0.03	0.15
(1,108)	1:115:A:LEU:HD22	1:116:A:ALA:H	9	0.15	0.03	0.15
(1,1491)	1:6:A:VAL:HG13	1:6:A:VAL:HA	9	0.14	0.03	0.16
(1,1491)	1:6:A:VAL:HG11	1:6:A:VAL:HA	9	0.14	0.03	0.16
(1,301)	1:69:A:LYS:HB2	1:70:A:VAL:H	9	0.14	0.03	0.13
(1,2386)	1:101:A:ILE:H	1:102:A:THR:H	9	0.14	0.03	0.13
(1,1534)	1:56:A:LEU:HB3	1:56:A:LEU:HA	9	0.12	0.01	0.12
(1,1127)	1:10:A:LEU:HD13	1:10:A:LEU:HB3	9	0.12	0.01	0.12
(1,1127)	1:10:A:LEU:HD11	1:10:A:LEU:HB3	9	0.12	0.01	0.12
(1,1127)	1:10:A:LEU:HD12	1:10:A:LEU:HB3	9	0.12	0.01	0.12
(1,2660)	1:69:A:LYS:HA	1:69:A:LYS:HE2	8	0.57	0.18	0.62
(1,2660)	1:69:A:LYS:HA	1:69:A:LYS:HE3	8	0.57	0.18	0.62
(1,2571)	1:59:A:LYS:HD2	1:56:A:LEU:HA	8	0.39	0.1	0.43
(1,2571)	1:59:A:LYS:HD3	1:56:A:LEU:HA	8	0.39	0.1	0.43
(1,72)	1:31:A:VAL:HG13	1:108:A:ARG:H	8	0.32	0.21	0.29
(1,72)	1:31:A:VAL:HG11	1:108:A:ARG:H	8	0.32	0.21	0.29
(1,72)	1:31:A:VAL:HG12	1:108:A:ARG:H	8	0.32	0.21	0.29
(1,844)	1:112:A:LEU:HD23	1:114:A:MET:HE3	8	0.26	0.11	0.24
(1,844)	1:112:A:LEU:HD21	1:114:A:MET:HE2	8	0.26	0.11	0.24
(1,844)	1:112:A:LEU:HD21	1:114:A:MET:HE1	8	0.26	0.11	0.24
(1,844)	1:112:A:LEU:HD21	1:114:A:MET:HE3	8	0.26	0.11	0.24
(1,844)	1:112:A:LEU:HD22	1:114:A:MET:HE1	8	0.26	0.11	0.24
(1,844)	1:112:A:LEU:HD23	1:114:A:MET:HE1	8	0.26	0.11	0.24
(1,1931)	1:65:A:ILE:HD12	1:41:A:LYS:HB2	8	0.25	0.1	0.22
(1,1931)	1:65:A:ILE:HD11	1:41:A:LYS:HB2	8	0.25	0.1	0.22
(1,1931)	1:65:A:ILE:HD13	1:41:A:LYS:HB2	8	0.25	0.1	0.22
(1,1914)	1:68:A:GLU:HB2	1:34:A:GLY:HA3	8	0.24	0.12	0.18
(1,1687)	1:31:A:VAL:HA	1:110:A:LEU:HD12	8	0.24	0.14	0.19
(1,1687)	1:31:A:VAL:HA	1:110:A:LEU:HD13	8	0.24	0.14	0.19
(1,1687)	1:31:A:VAL:HA	1:110:A:LEU:HD11	8	0.24	0.14	0.19
(1,821)	1:30:A:VAL:HG12	1:28:A:ARG:HG3	8	0.24	0.11	0.22
(1,821)	1:30:A:VAL:HG11	1:28:A:ARG:HG3	8	0.24	0.11	0.22
(1,821)	1:30:A:VAL:HG13	1:28:A:ARG:HG3	8	0.24	0.11	0.22
(1,2673)	1:43:A:LEU:HD11	1:4:A:TYR:HE1	8	0.17	0.08	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2673)	1:13:A:LEU:HD11	1:17:A:HIS:HD2	8	0.17	0.08	0.14
(1,2673)	1:13:A:LEU:HD12	1:17:A:HIS:HD2	8	0.17	0.08	0.14
(1,2673)	1:43:A:LEU:HD12	1:4:A:TYR:HE1	8	0.17	0.08	0.14
(1,2673)	1:13:A:LEU:HD13	1:17:A:HIS:HD2	8	0.17	0.08	0.14
(1,1283)	1:15:A:GLU:HB3	1:12:A:ALA:HA	8	0.17	0.04	0.16
(1,737)	1:7:A:VAL:HG12	1:7:A:VAL:HG13	8	0.11	0.01	0.1
(1,737)	1:7:A:VAL:HG12	1:7:A:VAL:HG11	8	0.11	0.01	0.1
(1,737)	1:7:A:VAL:HG11	1:7:A:VAL:HG13	8	0.11	0.01	0.1
(1,1988)	1:40:A:ASP:HB2	1:43:A:LEU:HB3	7	1.2	0.12	1.12
(1,823)	1:30:A:VAL:HG12	1:111:A:SER:HB2	7	0.84	0.04	0.86
(1,823)	1:30:A:VAL:HG11	1:111:A:SER:HB2	7	0.84	0.04	0.86
(1,823)	1:30:A:VAL:HG13	1:111:A:SER:HB2	7	0.84	0.04	0.86
(1,1994)	1:3:A:GLU:HG2	1:40:A:ASP:HB2	7	0.77	0.25	0.79
(1,1731)	1:72:A:LEU:HD12	1:91:A:CYS:HA	7	0.52	0.75	0.19
(1,1731)	1:72:A:LEU:HD11	1:91:A:CYS:HA	7	0.52	0.75	0.19
(1,1731)	1:72:A:LEU:HD13	1:91:A:CYS:HA	7	0.52	0.75	0.19
(1,299)	1:39:A:MET:HE3	1:6:A:VAL:H	7	0.49	0.2	0.47
(1,299)	1:39:A:MET:HE2	1:6:A:VAL:H	7	0.49	0.2	0.47
(1,299)	1:39:A:MET:HE1	1:6:A:VAL:H	7	0.49	0.2	0.47
(1,1093)	1:82:A:LYS:HD3	1:82:A:LYS:HA	7	0.4	0.05	0.38
(1,1093)	1:82:A:LYS:HD2	1:82:A:LYS:HA	7	0.4	0.05	0.38
(1,1490)	1:6:A:VAL:HA	1:9:A:SER:HB3	7	0.26	0.09	0.24
(1,710)	1:72:A:LEU:HA	1:103:A:GLN:H	7	0.26	0.11	0.27
(1,832)	1:101:A:ILE:HG23	1:105:A:ASN:HB2	7	0.22	0.08	0.2
(1,832)	1:101:A:ILE:HG22	1:105:A:ASN:HB2	7	0.22	0.08	0.2
(1,832)	1:101:A:ILE:HG21	1:105:A:ASN:HB2	7	0.22	0.08	0.2
(1,1507)	1:26:A:ILE:HD13	1:14:A:CYS:HA	7	0.2	0.06	0.19
(1,1507)	1:26:A:ILE:HD12	1:14:A:CYS:HA	7	0.2	0.06	0.19
(1,1507)	1:26:A:ILE:HD11	1:14:A:CYS:HA	7	0.2	0.06	0.19
(1,2068)	1:30:A:VAL:HG11	1:29:A:VAL:HA	7	0.17	0.06	0.15
(1,2068)	1:30:A:VAL:HG13	1:29:A:VAL:HA	7	0.17	0.06	0.15
(1,2068)	1:30:A:VAL:HG12	1:29:A:VAL:HA	7	0.17	0.06	0.15
(1,1949)	1:15:A:GLU:HB3	1:57:A:VAL:HG13	7	0.17	0.04	0.15
(1,1949)	1:15:A:GLU:HB3	1:57:A:VAL:HG11	7	0.17	0.04	0.15
(1,1949)	1:15:A:GLU:HB3	1:57:A:VAL:HG12	7	0.17	0.04	0.15
(1,2250)	1:4:A:TYR:HA	1:4:A:TYR:HD1	7	0.14	0.03	0.13
(1,2250)	1:4:A:TYR:HA	1:4:A:TYR:HD2	7	0.14	0.03	0.13
(1,1990)	1:17:A:HIS:HB3	1:14:A:CYS:HA	7	0.14	0.02	0.14
(1,1356)	1:107:A:MET:HG2	1:107:A:MET:HE3	6	0.82	0.07	0.82
(1,1356)	1:107:A:MET:HG2	1:107:A:MET:HE2	6	0.82	0.07	0.82
(1,2063)	1:33:A:ILE:HA	1:107:A:MET:HG3	6	0.69	0.2	0.67
(1,813)	1:29:A:VAL:HG23	1:10:A:LEU:HD12	6	0.61	0.26	0.62

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,813)	1:29:A:VAL:HG23	1:10:A:LEU:HD13	6	0.61	0.26	0.62
(1,813)	1:29:A:VAL:HG21	1:10:A:LEU:HD13	6	0.61	0.26	0.62
(1,813)	1:29:A:VAL:HG22	1:10:A:LEU:HD13	6	0.61	0.26	0.62
(1,813)	1:29:A:VAL:HG22	1:10:A:LEU:HD11	6	0.61	0.26	0.62
(1,1615)	1:10:A:LEU:HA	1:107:A:MET:HE1	6	0.5	0.17	0.44
(1,1615)	1:10:A:LEU:HA	1:107:A:MET:HE3	6	0.5	0.17	0.44
(1,1615)	1:10:A:LEU:HA	1:107:A:MET:HE2	6	0.5	0.17	0.44
(1,1006)	1:100:A:ILE:HD11	1:75:A:LYS:HG3	6	0.46	0.19	0.39
(1,1006)	1:100:A:ILE:HD13	1:75:A:LYS:HG3	6	0.46	0.19	0.39
(1,1688)	1:97:A:LYS:HA	1:99:A:VAL:HG21	6	0.42	0.22	0.48
(1,1688)	1:97:A:LYS:HA	1:99:A:VAL:HG23	6	0.42	0.22	0.48
(1,1688)	1:97:A:LYS:HA	1:99:A:VAL:HG22	6	0.42	0.22	0.48
(1,2132)	1:72:A:LEU:HB3	1:81:A:PHE:HD2	6	0.41	0.27	0.24
(1,2132)	1:72:A:LEU:HB3	1:81:A:PHE:HD1	6	0.41	0.27	0.24
(1,1665)	1:24:A:HIS:HA	1:57:A:VAL:HG22	6	0.32	0.14	0.31
(1,1665)	1:24:A:HIS:HA	1:57:A:VAL:HG21	6	0.32	0.14	0.31
(1,1665)	1:24:A:HIS:HA	1:57:A:VAL:HG23	6	0.32	0.14	0.31
(1,1982)	1:106:A:GLU:HG2	1:105:A:ASN:HB3	6	0.31	0.16	0.26
(1,1982)	1:106:A:GLU:HG3	1:105:A:ASN:HB3	6	0.31	0.16	0.26
(1,1445)	1:48:A:PHE:HB2	1:63:A:LEU:HD11	6	0.3	0.09	0.31
(1,1445)	1:48:A:PHE:HB2	1:63:A:LEU:HD12	6	0.3	0.09	0.31
(1,1445)	1:48:A:PHE:HB2	1:63:A:LEU:HD13	6	0.3	0.09	0.31
(1,1197)	1:80:A:VAL:HG13	1:71:A:GLU:HG3	6	0.29	0.1	0.26
(1,1197)	1:80:A:VAL:HG12	1:71:A:GLU:HG3	6	0.29	0.1	0.26
(1,1197)	1:80:A:VAL:HG11	1:71:A:GLU:HG3	6	0.29	0.1	0.26
(1,1707)	1:107:A:MET:HG3	1:107:A:MET:HA	6	0.28	0.03	0.27
(1,2608)	1:115:A:LEU:HD23	1:27:A:GLU:HB2	6	0.28	0.14	0.23
(1,2608)	1:115:A:LEU:HD22	1:27:A:GLU:HB2	6	0.28	0.14	0.23
(1,2608)	1:115:A:LEU:HD21	1:27:A:GLU:HB2	6	0.28	0.14	0.23
(1,860)	1:109:A:LEU:HD21	1:31:A:VAL:HA	6	0.27	0.05	0.28
(1,860)	1:109:A:LEU:HD23	1:31:A:VAL:HA	6	0.27	0.05	0.28
(1,860)	1:109:A:LEU:HD22	1:31:A:VAL:HA	6	0.27	0.05	0.28
(1,2040)	1:90:A:VAL:HG22	1:92:A:GLU:HA	6	0.26	0.13	0.24
(1,2040)	1:90:A:VAL:HG23	1:92:A:GLU:HA	6	0.26	0.13	0.24
(1,2040)	1:90:A:VAL:HG21	1:92:A:GLU:HA	6	0.26	0.13	0.24
(1,96)	1:11:A:ILE:HG23	1:15:A:GLU:H	6	0.25	0.11	0.26
(1,96)	1:11:A:ILE:HG22	1:15:A:GLU:H	6	0.25	0.11	0.26
(1,96)	1:11:A:ILE:HG21	1:15:A:GLU:H	6	0.25	0.11	0.26
(1,2030)	1:83:A:PRO:HD2	1:72:A:LEU:HD13	6	0.25	0.09	0.26
(1,2030)	1:83:A:PRO:HD2	1:72:A:LEU:HD11	6	0.25	0.09	0.26
(1,2030)	1:83:A:PRO:HD2	1:72:A:LEU:HD12	6	0.25	0.09	0.26
(1,2537)	1:115:A:LEU:HD11	1:27:A:GLU:HG2	6	0.24	0.04	0.23

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2537)	1:115:A:LEU:HD13	1:27:A:GLU:HG2	6	0.24	0.04	0.23
(1,2537)	1:115:A:LEU:HD21	1:27:A:GLU:HG2	6	0.24	0.04	0.23
(1,2537)	1:115:A:LEU:HD12	1:27:A:GLU:HG2	6	0.24	0.04	0.23
(1,952)	1:33:A:ILE:HG12	1:31:A:VAL:HG21	6	0.21	0.06	0.2
(1,952)	1:33:A:ILE:HG12	1:31:A:VAL:HG23	6	0.21	0.06	0.2
(1,952)	1:33:A:ILE:HG12	1:31:A:VAL:HG22	6	0.21	0.06	0.2
(1,18)	1:72:A:LEU:HD21	1:72:A:LEU:H	6	0.19	0.15	0.13
(1,18)	1:72:A:LEU:HD23	1:72:A:LEU:H	6	0.19	0.15	0.13
(1,18)	1:72:A:LEU:HD22	1:72:A:LEU:H	6	0.19	0.15	0.13
(1,787)	1:63:A:LEU:HD13	1:65:A:ILE:HD11	6	0.17	0.07	0.16
(1,787)	1:63:A:LEU:HD11	1:65:A:ILE:HD11	6	0.17	0.07	0.16
(1,787)	1:63:A:LEU:HD11	1:65:A:ILE:HD12	6	0.17	0.07	0.16
(1,787)	1:63:A:LEU:HD13	1:65:A:ILE:HD12	6	0.17	0.07	0.16
(1,787)	1:63:A:LEU:HD12	1:65:A:ILE:HD11	6	0.17	0.07	0.16
(1,1388)	1:11:A:ILE:HD11	1:51:A:PHE:HB3	6	0.16	0.07	0.14
(1,1388)	1:11:A:ILE:HD12	1:51:A:PHE:HB3	6	0.16	0.07	0.14
(1,234)	1:39:A:MET:HB3	1:39:A:MET:H	6	0.15	0.02	0.14
(1,759)	1:110:A:LEU:HD13	1:110:A:LEU:HD21	6	0.14	0.03	0.14
(1,759)	1:110:A:LEU:HD13	1:110:A:LEU:HD22	6	0.14	0.03	0.14
(1,759)	1:110:A:LEU:HD12	1:110:A:LEU:HD22	6	0.14	0.03	0.14
(1,759)	1:110:A:LEU:HD11	1:110:A:LEU:HD21	6	0.14	0.03	0.14
(1,759)	1:110:A:LEU:HD11	1:110:A:LEU:HD23	6	0.14	0.03	0.14
(1,214)	1:36:A:ARG:HB3	1:36:A:ARG:H	6	0.13	0.02	0.13
(1,1567)	1:102:A:THR:HG22	1:102:A:THR:HA	6	0.13	0.02	0.12
(1,1567)	1:102:A:THR:HG21	1:102:A:THR:HA	6	0.13	0.02	0.12
(1,1567)	1:102:A:THR:HG23	1:102:A:THR:HA	6	0.13	0.02	0.12
(1,407)	1:76:A:ASP:HB2	1:76:A:ASP:H	6	0.13	0.02	0.13
(1,2369)	1:82:A:LYS:H	1:81:A:PHE:H	6	0.12	0.02	0.12
(1,1541)	1:19:A:LYS:HB3	1:19:A:LYS:HA	6	0.12	0.02	0.11
(1,2487)	1:20:A:LYS:HG2	1:20:A:LYS:HD2	6	0.12	0.02	0.12
(1,2487)	1:82:A:LYS:HG2	1:82:A:LYS:HD3	6	0.12	0.02	0.12
(1,2487)	1:20:A:LYS:HG2	1:20:A:LYS:HD3	6	0.12	0.02	0.12
(1,152)	1:45:A:VAL:HG12	1:44:A:PHE:H	6	0.12	0.01	0.11
(1,152)	1:45:A:VAL:HG13	1:44:A:PHE:H	6	0.12	0.01	0.11
(1,152)	1:45:A:VAL:HG11	1:44:A:PHE:H	6	0.12	0.01	0.11
(1,2152)	1:99:A:VAL:HG23	1:81:A:PHE:HZ	5	1.07	0.35	1.06
(1,2152)	1:99:A:VAL:HG21	1:81:A:PHE:HZ	5	1.07	0.35	1.06
(1,1772)	1:64:A:ASP:HB3	1:30:A:VAL:HG12	5	0.59	0.06	0.58
(1,1772)	1:64:A:ASP:HB3	1:30:A:VAL:HG13	5	0.59	0.06	0.58
(1,1772)	1:64:A:ASP:HB3	1:30:A:VAL:HG11	5	0.59	0.06	0.58
(1,1775)	1:100:A:ILE:HD13	1:102:A:THR:HB	5	0.57	0.36	0.65
(1,1775)	1:100:A:ILE:HD12	1:102:A:THR:HB	5	0.57	0.36	0.65

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1775)	1:100:A:ILE:HD11	1:102:A:THR:HB	5	0.57	0.36	0.65
(1,1761)	1:110:A:LEU:HD22	1:108:A:ARG:HD2	5	0.54	0.26	0.61
(1,1761)	1:110:A:LEU:HD23	1:108:A:ARG:HD2	5	0.54	0.26	0.61
(1,420)	1:19:A:LYS:HE2	1:19:A:LYS:H	5	0.53	0.12	0.56
(1,1889)	1:82:A:LYS:HD3	1:71:A:GLU:HG3	5	0.5	0.24	0.43
(1,1889)	1:82:A:LYS:HD2	1:71:A:GLU:HG3	5	0.5	0.24	0.43
(1,869)	1:26:A:ILE:HD13	1:61:A:ALA:HB3	5	0.39	0.21	0.38
(1,869)	1:26:A:ILE:HD11	1:61:A:ALA:HB3	5	0.39	0.21	0.38
(1,869)	1:26:A:ILE:HD13	1:61:A:ALA:HB2	5	0.39	0.21	0.38
(1,449)	1:79:A:HIS:HB2	1:79:A:HIS:H	5	0.37	0.05	0.39
(1,415)	1:20:A:LYS:HE2	1:20:A:LYS:H	5	0.29	0.15	0.2
(1,415)	1:20:A:LYS:HE3	1:20:A:LYS:H	5	0.29	0.15	0.2
(1,1698)	1:80:A:VAL:HG11	1:73:A:GLU:HA	5	0.28	0.15	0.35
(1,1698)	1:80:A:VAL:HG13	1:73:A:GLU:HA	5	0.28	0.15	0.35
(1,1698)	1:80:A:VAL:HG12	1:73:A:GLU:HA	5	0.28	0.15	0.35
(1,1735)	1:72:A:LEU:HD21	1:88:A:TYR:HB3	5	0.28	0.21	0.15
(1,1735)	1:72:A:LEU:HD23	1:88:A:TYR:HB3	5	0.28	0.21	0.15
(1,2060)	1:35:A:GLU:HA	1:33:A:ILE:HG23	5	0.26	0.09	0.23
(1,2060)	1:35:A:GLU:HA	1:33:A:ILE:HG21	5	0.26	0.09	0.23
(1,2060)	1:35:A:GLU:HA	1:33:A:ILE:HG22	5	0.26	0.09	0.23
(1,1950)	1:57:A:VAL:HG22	1:15:A:GLU:HB3	5	0.22	0.15	0.15
(1,1950)	1:57:A:VAL:HG21	1:15:A:GLU:HB3	5	0.22	0.15	0.15
(1,1950)	1:57:A:VAL:HG23	1:15:A:GLU:HB3	5	0.22	0.15	0.15
(1,2675)	1:10:A:LEU:HD21	1:48:A:PHE:HZ	5	0.21	0.08	0.18
(1,2675)	1:63:A:LEU:HG	1:48:A:PHE:HZ	5	0.21	0.08	0.18
(1,2675)	1:10:A:LEU:HD22	1:48:A:PHE:HZ	5	0.21	0.08	0.18
(1,2675)	1:10:A:LEU:HD23	1:48:A:PHE:HZ	5	0.21	0.08	0.18
(1,1765)	1:72:A:LEU:HB2	1:99:A:VAL:HB	5	0.19	0.06	0.2
(1,457)	1:74:A:CYS:HB2	1:79:A:HIS:H	5	0.17	0.04	0.17
(1,2199)	1:7:A:VAL:HB	1:4:A:TYR:HD2	5	0.17	0.05	0.16
(1,2199)	1:7:A:VAL:HB	1:4:A:TYR:HD1	5	0.17	0.05	0.16
(1,690)	1:76:A:ASP:HA	1:77:A:CYS:H	5	0.17	0.06	0.13
(1,829)	1:101:A:ILE:HG21	1:105:A:ASN:HB3	5	0.16	0.03	0.15
(1,829)	1:101:A:ILE:HG22	1:105:A:ASN:HB3	5	0.16	0.03	0.15
(1,829)	1:101:A:ILE:HG23	1:105:A:ASN:HB3	5	0.16	0.03	0.15
(1,2138)	1:65:A:ILE:HD11	1:44:A:PHE:HE2	5	0.16	0.09	0.12
(1,2138)	1:65:A:ILE:HD13	1:44:A:PHE:HE1	5	0.16	0.09	0.12
(1,2655)	1:17:A:HIS:HB3	1:14:A:CYS:HA	5	0.14	0.02	0.15
(1,1331)	1:16:A:GLU:HB2	1:16:A:GLU:HG3	5	0.12	0.01	0.11
(1,1204)	1:75:A:LYS:HB3	1:98:A:ASN:HB3	4	0.78	0.54	0.66
(1,1430)	1:59:A:LYS:HG2	1:59:A:LYS:HE2	4	0.55	0.03	0.56
(1,2490)	1:82:A:LYS:HG2	1:82:A:LYS:HE2	4	0.55	0.02	0.55

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2490)	1:97:A:LYS:HG3	1:97:A:LYS:HE3	4	0.55	0.02	0.55
(1,857)	1:109:A:LEU:HD21	1:112:A:LEU:HD12	4	0.48	0.4	0.34
(1,857)	1:109:A:LEU:HD21	1:112:A:LEU:HD11	4	0.48	0.4	0.34
(1,857)	1:109:A:LEU:HD23	1:112:A:LEU:HD12	4	0.48	0.4	0.34
(1,857)	1:109:A:LEU:HD22	1:112:A:LEU:HD11	4	0.48	0.4	0.34
(1,1962)	1:97:A:LYS:HB2	1:90:A:VAL:HG13	4	0.45	0.24	0.34
(1,1962)	1:97:A:LYS:HB2	1:90:A:VAL:HG12	4	0.45	0.24	0.34
(1,2095)	1:25:A:LYS:HA	1:25:A:LYS:HD2	4	0.44	0.03	0.44
(1,1933)	1:38:A:ALA:HB3	1:1:A:MET:HB2	4	0.36	0.08	0.39
(1,2465)	1:31:A:VAL:HG11	1:10:A:LEU:HD23	4	0.34	0.2	0.28
(1,2465)	1:10:A:LEU:HD21	1:7:A:VAL:HG21	4	0.34	0.2	0.28
(1,2465)	1:31:A:VAL:HG12	1:10:A:LEU:HD23	4	0.34	0.2	0.28
(1,2010)	1:114:A:MET:HE2	1:17:A:HIS:HB2	4	0.27	0.15	0.19
(1,2010)	1:114:A:MET:HE1	1:17:A:HIS:HB2	4	0.27	0.15	0.19
(1,2157)	1:43:A:LEU:HD23	1:4:A:TYR:HE2	4	0.26	0.12	0.22
(1,2157)	1:43:A:LEU:HD23	1:4:A:TYR:HE1	4	0.26	0.12	0.22
(1,2157)	1:43:A:LEU:HD21	1:4:A:TYR:HE2	4	0.26	0.12	0.22
(1,1354)	1:1:A:MET:HG3	1:1:A:MET:HA	4	0.24	0.06	0.25
(1,1354)	1:1:A:MET:HG2	1:1:A:MET:HA	4	0.24	0.06	0.25
(1,428)	1:59:A:LYS:HE2	1:59:A:LYS:H	4	0.2	0.06	0.2
(1,2071)	1:26:A:ILE:HG22	1:29:A:VAL:HA	4	0.19	0.07	0.18
(1,2071)	1:26:A:ILE:HG23	1:29:A:VAL:HA	4	0.19	0.07	0.18
(1,77)	1:109:A:LEU:HD22	1:109:A:LEU:H	4	0.18	0.09	0.14
(1,77)	1:109:A:LEU:HD21	1:109:A:LEU:H	4	0.18	0.09	0.14
(1,82)	1:109:A:LEU:HD21	1:30:A:VAL:H	4	0.18	0.06	0.16
(1,82)	1:109:A:LEU:HD23	1:30:A:VAL:H	4	0.18	0.06	0.16
(1,82)	1:109:A:LEU:HD22	1:30:A:VAL:H	4	0.18	0.06	0.16
(1,1736)	1:65:A:ILE:HG21	1:41:A:LYS:HG3	4	0.18	0.04	0.16
(1,1736)	1:65:A:ILE:HG22	1:41:A:LYS:HG3	4	0.18	0.04	0.16
(1,172)	1:18:A:ALA:HB3	1:23:A:ALA:H	4	0.17	0.02	0.17
(1,172)	1:18:A:ALA:HB1	1:23:A:ALA:H	4	0.17	0.02	0.17
(1,353)	1:107:A:MET:HG3	1:108:A:ARG:H	4	0.17	0.01	0.17
(1,934)	1:102:A:THR:HG23	1:100:A:ILE:HB	4	0.16	0.06	0.14
(1,934)	1:102:A:THR:HG21	1:100:A:ILE:HB	4	0.16	0.06	0.14
(1,934)	1:102:A:THR:HG22	1:100:A:ILE:HB	4	0.16	0.06	0.14
(1,42)	1:109:A:LEU:HD12	1:109:A:LEU:H	4	0.15	0.04	0.15
(1,42)	1:109:A:LEU:HD13	1:109:A:LEU:H	4	0.15	0.04	0.15
(1,42)	1:109:A:LEU:HD11	1:109:A:LEU:H	4	0.15	0.04	0.15
(1,111)	1:10:A:LEU:HD13	1:13:A:LEU:H	4	0.14	0.03	0.14
(1,111)	1:10:A:LEU:HD11	1:13:A:LEU:H	4	0.14	0.03	0.14
(1,1796)	1:62:A:ILE:HD13	1:28:A:ARG:HA	4	0.14	0.01	0.14
(1,1796)	1:62:A:ILE:HD11	1:28:A:ARG:HA	4	0.14	0.01	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,893)	1:43:A:LEU:HD23	1:40:A:ASP:HB3	4	0.13	0.02	0.14
(1,893)	1:43:A:LEU:HD22	1:40:A:ASP:HB3	4	0.13	0.02	0.14
(1,1787)	1:26:A:ILE:HG21	1:112:A:LEU:HA	4	0.13	0.02	0.12
(1,203)	1:20:A:LYS:HG2	1:20:A:LYS:H	4	0.12	0.01	0.12
(1,2417)	1:39:A:MET:H	1:40:A:ASP:H	4	0.12	0.0	0.12
(1,13)	1:72:A:LEU:HD11	1:90:A:VAL:H	3	0.96	0.59	0.56
(1,13)	1:72:A:LEU:HD12	1:90:A:VAL:H	3	0.96	0.59	0.56
(1,1565)	1:100:A:ILE:HD13	1:102:A:THR:HA	3	0.78	0.12	0.87
(1,1565)	1:100:A:ILE:HD11	1:102:A:THR:HA	3	0.78	0.12	0.87
(1,351)	1:103:A:GLN:HG2	1:103:A:GLN:H	3	0.77	0.01	0.77
(1,351)	1:103:A:GLN:HG3	1:103:A:GLN:H	3	0.77	0.01	0.77
(1,1938)	1:71:A:GLU:HG2	1:103:A:GLN:HG2	3	0.72	0.31	0.86
(1,1788)	1:75:A:LYS:HE3	1:100:A:ILE:HG23	3	0.71	0.37	0.77
(1,1788)	1:75:A:LYS:HE3	1:100:A:ILE:HG21	3	0.71	0.37	0.77
(1,1018)	1:100:A:ILE:HG22	1:100:A:ILE:HG12	3	0.7	0.02	0.7
(1,1968)	1:113:A:GLU:HG2	1:27:A:GLU:HB3	3	0.67	0.69	0.22
(1,1328)	1:103:A:GLN:HG3	1:103:A:GLN:HA	3	0.65	0.05	0.67
(1,1792)	1:11:A:ILE:HG22	1:52:A:ARG:HA	3	0.63	0.32	0.82
(1,1792)	1:11:A:ILE:HG23	1:52:A:ARG:HA	3	0.63	0.32	0.82
(1,1791)	1:62:A:ILE:HG23	1:64:A:ASP:HB3	3	0.52	0.11	0.48
(1,1791)	1:62:A:ILE:HG22	1:64:A:ASP:HB3	3	0.52	0.11	0.48
(1,2156)	1:93:A:LYS:HB3	1:79:A:HIS:HD2	3	0.51	0.12	0.45
(1,1301)	1:1:A:MET:HE3	1:1:A:MET:HB2	3	0.49	0.33	0.26
(1,1301)	1:1:A:MET:HE2	1:1:A:MET:HB2	3	0.49	0.33	0.26
(1,1936)	1:114:A:MET:HE1	1:114:A:MET:HB3	3	0.48	0.51	0.12
(1,1936)	1:114:A:MET:HE2	1:114:A:MET:HB3	3	0.48	0.51	0.12
(1,1936)	1:114:A:MET:HE3	1:114:A:MET:HB3	3	0.48	0.51	0.12
(1,2225)	1:36:A:ARG:HD2	1:88:A:TYR:HD1	3	0.46	0.29	0.44
(1,1941)	1:107:A:MET:HE3	1:10:A:LEU:HB3	3	0.44	0.21	0.52
(1,1645)	1:72:A:LEU:HD13	1:88:A:TYR:HA	3	0.44	0.3	0.36
(1,1645)	1:72:A:LEU:HD12	1:88:A:TYR:HA	3	0.44	0.3	0.36
(1,1645)	1:72:A:LEU:HD11	1:88:A:TYR:HA	3	0.44	0.3	0.36
(1,846)	1:31:A:VAL:HG12	1:10:A:LEU:HD23	3	0.41	0.16	0.42
(1,846)	1:31:A:VAL:HG11	1:10:A:LEU:HD23	3	0.41	0.16	0.42
(1,846)	1:31:A:VAL:HG12	1:10:A:LEU:HD22	3	0.41	0.16	0.42
(1,2018)	1:90:A:VAL:HG11	1:95:A:HIS:HB3	3	0.4	0.14	0.33
(1,2018)	1:90:A:VAL:HG13	1:95:A:HIS:HB3	3	0.4	0.14	0.33
(1,2018)	1:90:A:VAL:HG12	1:95:A:HIS:HB3	3	0.4	0.14	0.33
(1,689)	1:97:A:LYS:HA	1:99:A:VAL:H	3	0.37	0.06	0.41
(1,135)	1:100:A:ILE:HG13	1:100:A:ILE:H	3	0.34	0.06	0.32
(1,2444)	1:80:A:VAL:HG13	1:73:A:GLU:HA	3	0.34	0.04	0.33
(1,2444)	1:80:A:VAL:HG12	1:73:A:GLU:HA	3	0.34	0.04	0.33

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2592)	1:41:A:LYS:HD2	1:33:A:ILE:HG22	3	0.32	0.12	0.24
(1,2592)	1:41:A:LYS:HD2	1:33:A:ILE:HG23	3	0.32	0.12	0.24
(1,1401)	1:41:A:LYS:HE3	1:33:A:ILE:HD12	3	0.3	0.14	0.24
(1,1401)	1:41:A:LYS:HE3	1:33:A:ILE:HD11	3	0.3	0.14	0.24
(1,1401)	1:41:A:LYS:HE3	1:33:A:ILE:HD13	3	0.3	0.14	0.24
(1,1930)	1:71:A:GLU:HB2	1:103:A:GLN:HB2	3	0.28	0.1	0.35
(1,2162)	1:43:A:LEU:HD12	1:4:A:TYR:HD2	3	0.26	0.15	0.18
(1,2162)	1:43:A:LEU:HD11	1:4:A:TYR:HD2	3	0.26	0.15	0.18
(1,2162)	1:43:A:LEU:HD13	1:4:A:TYR:HD2	3	0.26	0.15	0.18
(1,2620)	1:115:A:LEU:HD11	1:25:A:LYS:HG2	3	0.26	0.21	0.11
(1,2620)	1:25:A:LYS:HG2	1:56:A:LEU:HD13	3	0.26	0.21	0.11
(1,2620)	1:25:A:LYS:HG2	1:56:A:LEU:HD12	3	0.26	0.21	0.11
(1,1953)	1:68:A:GLU:HG2	1:32:A:GLY:HA3	3	0.24	0.09	0.21
(1,1644)	1:88:A:TYR:HA	1:72:A:LEU:HD21	3	0.23	0.07	0.25
(1,1644)	1:88:A:TYR:HA	1:72:A:LEU:HD22	3	0.23	0.07	0.25
(1,2078)	1:82:A:LYS:HD3	1:71:A:GLU:HA	3	0.22	0.07	0.19
(1,2078)	1:82:A:LYS:HD2	1:71:A:GLU:HA	3	0.22	0.07	0.19
(1,2001)	1:59:A:LYS:HE2	1:56:A:LEU:HB2	3	0.22	0.1	0.18
(1,2001)	1:59:A:LYS:HE3	1:56:A:LEU:HB2	3	0.22	0.1	0.18
(1,2121)	1:63:A:LEU:HD21	1:48:A:PHE:HD1	3	0.21	0.05	0.2
(1,2121)	1:63:A:LEU:HD22	1:48:A:PHE:HD1	3	0.21	0.05	0.2
(1,1755)	1:65:A:ILE:HD11	1:45:A:VAL:HA	3	0.19	0.01	0.2
(1,1755)	1:65:A:ILE:HD12	1:45:A:VAL:HA	3	0.19	0.01	0.2
(1,2436)	1:110:A:LEU:HD12	1:66:A:VAL:HG21	3	0.18	0.04	0.21
(1,2436)	1:110:A:LEU:HD13	1:66:A:VAL:HG22	3	0.18	0.04	0.21
(1,242)	1:19:A:LYS:HD3	1:19:A:LYS:H	3	0.17	0.05	0.16
(1,242)	1:19:A:LYS:HD2	1:19:A:LYS:H	3	0.17	0.05	0.16
(1,367)	1:54:A:GLU:HG2	1:55:A:SER:H	3	0.17	0.05	0.14
(1,755)	1:65:A:ILE:HG22	1:41:A:LYS:HD2	3	0.17	0.04	0.15
(1,755)	1:65:A:ILE:HG21	1:41:A:LYS:HD2	3	0.17	0.04	0.15
(1,853)	1:31:A:VAL:HG11	1:107:A:MET:HG2	3	0.16	0.02	0.15
(1,853)	1:31:A:VAL:HG13	1:107:A:MET:HG2	3	0.16	0.02	0.15
(1,1428)	1:56:A:LEU:HD22	1:59:A:LYS:HE3	3	0.15	0.02	0.16
(1,1428)	1:56:A:LEU:HD23	1:59:A:LYS:HE3	3	0.15	0.02	0.16
(1,1428)	1:56:A:LEU:HD21	1:59:A:LYS:HE3	3	0.15	0.02	0.16
(1,396)	1:76:A:ASP:HB3	1:76:A:ASP:H	3	0.14	0.02	0.15
(1,1374)	1:40:A:ASP:HB3	1:43:A:LEU:HD13	3	0.14	0.03	0.12
(1,1374)	1:40:A:ASP:HB3	1:43:A:LEU:HD11	3	0.14	0.03	0.12
(1,1959)	1:113:A:GLU:HG3	1:28:A:ARG:HB3	3	0.13	0.01	0.13
(1,1314)	1:53:A:GLU:HB2	1:53:A:GLU:HG2	3	0.13	0.01	0.12
(1,1528)	1:50:A:THR:HB	1:50:A:THR:HA	3	0.12	0.02	0.11
(1,2500)	1:97:A:LYS:HG2	1:97:A:LYS:HD2	3	0.11	0.01	0.11

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2500)	1:19:A:LYS:HG2	1:19:A:LYS:HD2	3	0.11	0.01	0.11
(1,398)	1:15:A:GLU:HG2	1:15:A:GLU:H	3	0.11	0.0	0.11
(1,1251)	1:75:A:LYS:HB3	1:75:A:LYS:HB2	3	0.1	0.0	0.1
(1,2019)	1:14:A:CYS:HB2	1:11:A:ILE:HG21	2	1.12	0.02	1.12
(1,2019)	1:14:A:CYS:HB2	1:11:A:ILE:HG22	2	1.12	0.02	1.12
(1,1816)	1:102:A:THR:HG22	1:72:A:LEU:HD22	2	1.11	0.88	1.11
(1,1816)	1:102:A:THR:HG23	1:72:A:LEU:HD23	2	1.11	0.88	1.11
(1,1443)	1:30:A:VAL:HG12	1:28:A:ARG:HD2	2	1.1	0.07	1.1
(1,2137)	1:70:A:VAL:HG22	1:88:A:TYR:HD2	2	1.06	0.07	1.06
(1,2137)	1:70:A:VAL:HG21	1:88:A:TYR:HD2	2	1.06	0.07	1.06
(1,1466)	1:14:A:CYS:HB2	1:11:A:ILE:HA	2	0.86	0.05	0.86
(1,1752)	1:90:A:VAL:HG11	1:97:A:LYS:HD2	2	0.8	0.13	0.8
(1,1752)	1:90:A:VAL:HG13	1:97:A:LYS:HD2	2	0.8	0.13	0.8
(1,865)	1:26:A:ILE:HD13	1:114:A:MET:HE3	2	0.73	0.07	0.73
(1,865)	1:26:A:ILE:HD12	1:114:A:MET:HE1	2	0.73	0.07	0.73
(1,1367)	1:26:A:ILE:HD12	1:14:A:CYS:HB3	2	0.63	0.03	0.63
(1,1367)	1:26:A:ILE:HD13	1:14:A:CYS:HB3	2	0.63	0.03	0.63
(1,1993)	1:20:A:LYS:HG3	1:20:A:LYS:HE3	2	0.55	0.05	0.55
(1,2209)	1:1:A:MET:HG2	1:2:A:HIS:HD2	2	0.52	0.17	0.52
(1,2209)	1:1:A:MET:HG3	1:2:A:HIS:HD2	2	0.52	0.17	0.52
(1,2665)	1:97:A:LYS:HA	1:90:A:VAL:HB	2	0.51	0.19	0.51
(1,1986)	1:82:A:LYS:HE3	1:71:A:GLU:HB3	2	0.48	0.22	0.48
(1,303)	1:107:A:MET:HE1	1:10:A:LEU:H	2	0.44	0.06	0.44
(1,303)	1:107:A:MET:HE3	1:10:A:LEU:H	2	0.44	0.06	0.44
(1,1525)	1:93:A:LYS:HD3	1:93:A:LYS:HA	2	0.42	0.08	0.42
(1,94)	1:93:A:LYS:HB3	1:94:A:CYS:H	2	0.42	0.01	0.42
(1,1734)	1:72:A:LEU:HD13	1:88:A:TYR:HB3	2	0.42	0.08	0.42
(1,1734)	1:72:A:LEU:HD11	1:88:A:TYR:HB3	2	0.42	0.08	0.42
(1,2136)	1:70:A:VAL:HG23	1:88:A:TYR:HE2	2	0.38	0.12	0.38
(1,2136)	1:70:A:VAL:HG22	1:88:A:TYR:HE2	2	0.38	0.12	0.38
(1,2192)	1:92:A:GLU:HB2	1:95:A:HIS:HD2	2	0.38	0.01	0.38
(1,933)	1:102:A:THR:HG21	1:100:A:ILE:HG13	2	0.34	0.05	0.34
(1,933)	1:102:A:THR:HG23	1:100:A:ILE:HG13	2	0.34	0.05	0.34
(1,1545)	1:114:A:MET:HE2	1:18:A:ALA:HA	2	0.32	0.1	0.32
(1,1545)	1:114:A:MET:HE1	1:18:A:ALA:HA	2	0.32	0.1	0.32
(1,2210)	1:107:A:MET:HG2	1:44:A:PHE:HZ	2	0.32	0.18	0.32
(1,1462)	1:11:A:ILE:HD13	1:52:A:ARG:HA	2	0.31	0.03	0.31
(1,1462)	1:11:A:ILE:HD12	1:52:A:ARG:HA	2	0.31	0.03	0.31
(1,141)	1:93:A:LYS:HD3	1:93:A:LYS:H	2	0.3	0.08	0.3
(1,2193)	1:25:A:LYS:HB3	1:24:A:HIS:HD2	2	0.28	0.12	0.28
(1,95)	1:93:A:LYS:HB3	1:93:A:LYS:H	2	0.26	0.03	0.26
(1,438)	1:79:A:HIS:HB3	1:79:A:HIS:H	2	0.23	0.06	0.23

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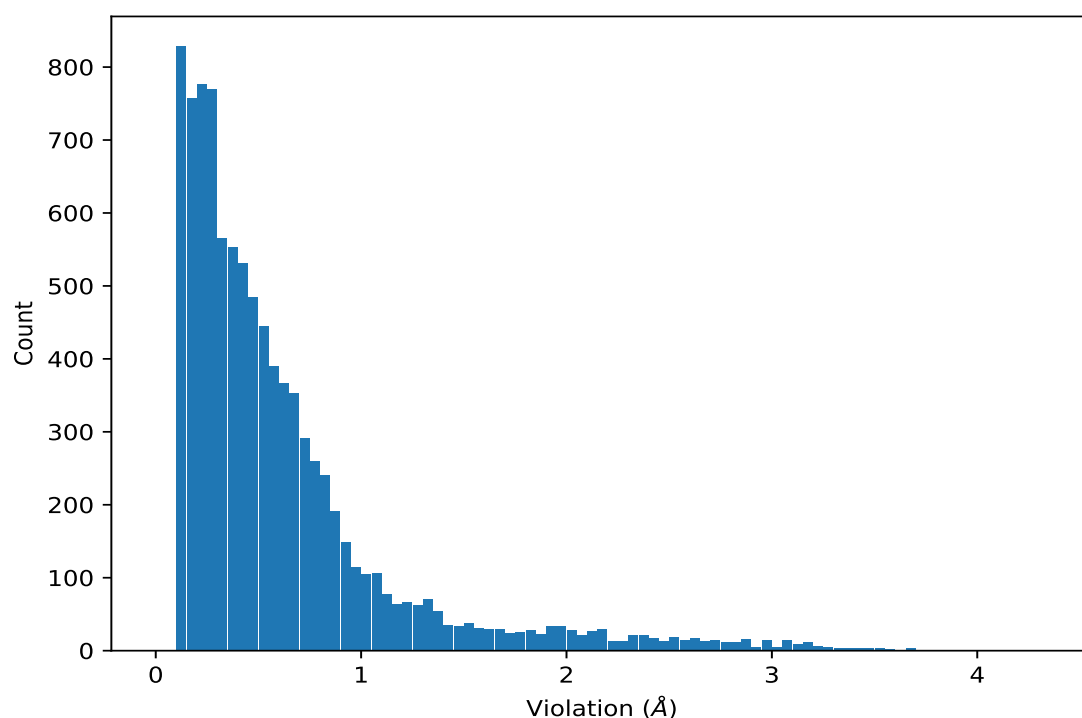
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1105)	1:69:A:LYS:HD3	1:69:A:LYS:HA	2	0.2	0.03	0.2
(1,1501)	1:3:A:GLU:HA	1:39:A:MET:HE1	2	0.2	0.01	0.2
(1,1115)	1:70:A:VAL:HG23	1:83:A:PRO:HG3	2	0.2	0.02	0.2
(1,1115)	1:70:A:VAL:HG22	1:83:A:PRO:HG3	2	0.2	0.02	0.2
(1,1880)	1:36:A:ARG:HA	1:36:A:ARG:HG3	2	0.2	0.08	0.2
(1,1786)	1:26:A:ILE:HG23	1:114:A:MET:HE3	2	0.18	0.06	0.18
(1,1786)	1:26:A:ILE:HG23	1:114:A:MET:HE1	2	0.18	0.06	0.18
(1,1957)	1:71:A:GLU:HB3	1:103:A:GLN:HB2	2	0.18	0.01	0.18
(1,1967)	1:20:A:LYS:HD2	1:16:A:GLU:HG3	2	0.18	0.0	0.18
(1,762)	1:70:A:VAL:HG23	1:71:A:GLU:HA	2	0.16	0.02	0.16
(1,762)	1:70:A:VAL:HG22	1:71:A:GLU:HA	2	0.16	0.02	0.16
(1,1273)	1:114:A:MET:HE3	1:112:A:LEU:HB3	2	0.16	0.06	0.16
(1,104)	1:43:A:LEU:HD22	1:43:A:LEU:H	2	0.15	0.01	0.15
(1,104)	1:43:A:LEU:HD23	1:43:A:LEU:H	2	0.15	0.01	0.15
(1,2150)	1:31:A:VAL:HG12	1:44:A:PHE:HE2	2	0.15	0.02	0.15
(1,794)	1:109:A:LEU:HD13	1:109:A:LEU:HD23	2	0.14	0.03	0.14
(1,794)	1:109:A:LEU:HD11	1:109:A:LEU:HD23	2	0.14	0.03	0.14
(1,1558)	1:86:A:LEU:HD22	1:86:A:LEU:HA	2	0.14	0.03	0.14
(1,1558)	1:86:A:LEU:HD21	1:86:A:LEU:HA	2	0.14	0.03	0.14
(1,2167)	1:50:A:THR:HG22	1:4:A:TYR:HD2	2	0.14	0.04	0.14
(1,2167)	1:50:A:THR:HG22	1:4:A:TYR:HD1	2	0.14	0.04	0.14
(1,228)	1:86:A:LEU:HB2	1:87:A:ASP:H	2	0.13	0.0	0.13
(1,2421)	1:115:A:LEU:HD21	1:115:A:LEU:H	2	0.13	0.0	0.13
(1,408)	1:76:A:ASP:HB2	1:77:A:CYS:H	2	0.12	0.02	0.12
(1,1548)	1:66:A:VAL:HG22	1:66:A:VAL:HA	2	0.12	0.0	0.12
(1,1901)	1:57:A:VAL:HG21	1:56:A:LEU:HB3	2	0.12	0.01	0.12
(1,1901)	1:57:A:VAL:HG23	1:56:A:LEU:HB3	2	0.12	0.01	0.12
(1,1405)	1:3:A:GLU:HG3	1:3:A:GLU:HG2	2	0.11	0.0	0.11
(1,2039)	1:26:A:ILE:HG21	1:61:A:ALA:HA	2	0.11	0.0	0.11
(1,2513)	1:59:A:LYS:HD3	1:59:A:LYS:HB3	2	0.11	0.0	0.11

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,742)	1:72:A:LEU:HD11	1:99:A:VAL:HG13	13	4.33
(1,799)	1:11:A:ILE:HD12	1:7:A:VAL:HG21	19	3.82
(1,799)	1:11:A:ILE:HD11	1:7:A:VAL:HG22	9	3.69
(1,1432)	1:99:A:VAL:HG22	1:74:A:CYS:HB3	18	3.67
(1,1432)	1:99:A:VAL:HG21	1:74:A:CYS:HB3	15	3.65
(1,1432)	1:99:A:VAL:HG23	1:74:A:CYS:HB3	7	3.6
(1,1432)	1:99:A:VAL:HG23	1:74:A:CYS:HB3	14	3.58
(1,799)	1:11:A:ILE:HD11	1:7:A:VAL:HG21	11	3.57
(1,1432)	1:99:A:VAL:HG22	1:74:A:CYS:HB3	2	3.54
(1,1432)	1:99:A:VAL:HG22	1:74:A:CYS:HB3	11	3.5
(1,1432)	1:99:A:VAL:HG21	1:74:A:CYS:HB3	20	3.5
(1,1432)	1:99:A:VAL:HG21	1:74:A:CYS:HB3	5	3.48
(1,1432)	1:99:A:VAL:HG21	1:74:A:CYS:HB3	9	3.48
(1,1432)	1:99:A:VAL:HG22	1:74:A:CYS:HB3	8	3.46
(1,1763)	1:7:A:VAL:HG21	1:11:A:ILE:HG13	19	3.44
(1,1432)	1:99:A:VAL:HG21	1:74:A:CYS:HB3	3	3.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1432)	1:99:A:VAL:HG21	1:74:A:CYS:HB3	4	3.42
(1,1801)	1:29:A:VAL:HG12	1:61:A:ALA:HA	7	3.4
(1,1432)	1:99:A:VAL:HG23	1:74:A:CYS:HB3	13	3.38
(1,1432)	1:99:A:VAL:HG23	1:74:A:CYS:HB3	12	3.36
(1,1432)	1:99:A:VAL:HG23	1:74:A:CYS:HB3	19	3.36
(1,1432)	1:99:A:VAL:HG21	1:74:A:CYS:HB3	16	3.33
(1,1801)	1:29:A:VAL:HG13	1:61:A:ALA:HA	3	3.31
(1,1801)	1:29:A:VAL:HG13	1:61:A:ALA:HA	5	3.31
(1,1432)	1:99:A:VAL:HG21	1:74:A:CYS:HB3	10	3.3
(1,1801)	1:29:A:VAL:HG12	1:61:A:ALA:HA	19	3.29
(1,1801)	1:29:A:VAL:HG13	1:61:A:ALA:HA	18	3.28
(1,1432)	1:99:A:VAL:HG23	1:74:A:CYS:HB3	1	3.28
(1,2619)	1:109:A:LEU:HB2	1:30:A:VAL:HG22	3	3.26
(1,799)	1:11:A:ILE:HD11	1:7:A:VAL:HG23	10	3.26
(1,1432)	1:99:A:VAL:HG21	1:74:A:CYS:HB3	6	3.23
(1,782)	1:99:A:VAL:HG13	1:89:A:GLY:HA3	10	3.23
(1,797)	1:7:A:VAL:HG21	1:51:A:PHE:HB3	7	3.21
(1,797)	1:7:A:VAL:HG21	1:51:A:PHE:HB3	10	3.21
(1,2619)	1:109:A:LEU:HB2	1:30:A:VAL:HG22	14	3.2
(1,1801)	1:29:A:VAL:HG13	1:61:A:ALA:HA	17	3.2
(1,1801)	1:29:A:VAL:HG11	1:61:A:ALA:HA	6	3.19
(1,1801)	1:29:A:VAL:HG13	1:61:A:ALA:HA	14	3.19
(1,1801)	1:29:A:VAL:HG13	1:61:A:ALA:HA	15	3.19
(1,1801)	1:29:A:VAL:HG11	1:61:A:ALA:HA	1	3.18
(1,799)	1:11:A:ILE:HD12	1:7:A:VAL:HG23	7	3.18
(1,1801)	1:29:A:VAL:HG11	1:61:A:ALA:HA	12	3.17
(1,2663)	1:33:A:ILE:HA	1:31:A:VAL:HG13	14	3.16
(1,799)	1:11:A:ILE:HD11	1:7:A:VAL:HG22	16	3.16
(1,799)	1:11:A:ILE:HD11	1:7:A:VAL:HG21	17	3.16
(1,1801)	1:29:A:VAL:HG11	1:61:A:ALA:HA	10	3.15
(1,799)	1:11:A:ILE:HD13	1:7:A:VAL:HG22	3	3.15
(1,799)	1:11:A:ILE:HD11	1:7:A:VAL:HG21	6	3.14
(1,799)	1:11:A:ILE:HD12	1:7:A:VAL:HG23	5	3.13
(1,797)	1:7:A:VAL:HG22	1:51:A:PHE:HB3	19	3.13
(1,2663)	1:33:A:ILE:HA	1:31:A:VAL:HG12	17	3.12
(1,799)	1:11:A:ILE:HD12	1:7:A:VAL:HG22	18	3.12
(1,1801)	1:29:A:VAL:HG12	1:61:A:ALA:HA	8	3.11
(1,799)	1:11:A:ILE:HD13	1:7:A:VAL:HG21	14	3.11
(1,782)	1:99:A:VAL:HG12	1:89:A:GLY:HA3	4	3.11
(1,2663)	1:33:A:ILE:HA	1:31:A:VAL:HG11	13	3.1
(1,2663)	1:33:A:ILE:HA	1:31:A:VAL:HG12	20	3.09
(1,2619)	1:109:A:LEU:HB2	1:30:A:VAL:HG21	9	3.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2619)	1:109:A:LEU:HB2	1:30:A:VAL:HG23	18	3.09
(1,1801)	1:29:A:VAL:HG11	1:61:A:ALA:HA	9	3.09
(1,1801)	1:29:A:VAL:HG13	1:61:A:ALA:HA	16	3.09
(1,2619)	1:109:A:LEU:HB2	1:30:A:VAL:HG23	12	3.08
(1,2619)	1:109:A:LEU:HB2	1:30:A:VAL:HG23	17	3.08
(1,1801)	1:29:A:VAL:HG13	1:61:A:ALA:HA	20	3.08
(1,1801)	1:29:A:VAL:HG11	1:61:A:ALA:HA	4	3.07
(1,799)	1:11:A:ILE:HD13	1:7:A:VAL:HG21	15	3.07
(1,797)	1:7:A:VAL:HG23	1:51:A:PHE:HB3	17	3.07
(1,2663)	1:33:A:ILE:HA	1:31:A:VAL:HG11	1	3.06
(1,914)	1:72:A:LEU:HD22	1:70:A:VAL:HG11	13	3.06
(1,797)	1:7:A:VAL:HG21	1:51:A:PHE:HB3	5	3.06
(1,2663)	1:33:A:ILE:HA	1:31:A:VAL:HG13	12	3.03
(1,2619)	1:109:A:LEU:HB2	1:30:A:VAL:HG22	4	3.02
(1,2663)	1:33:A:ILE:HA	1:31:A:VAL:HG13	18	3.01
(1,799)	1:11:A:ILE:HD11	1:7:A:VAL:HG22	12	3.01
(1,2619)	1:109:A:LEU:HB2	1:30:A:VAL:HG23	20	3.0
(1,799)	1:11:A:ILE:HD11	1:7:A:VAL:HG21	13	2.98
(1,2619)	1:109:A:LEU:HB2	1:30:A:VAL:HG21	5	2.97
(1,2619)	1:109:A:LEU:HB2	1:30:A:VAL:HG21	16	2.97
(1,1801)	1:29:A:VAL:HG11	1:61:A:ALA:HA	13	2.97
(1,797)	1:7:A:VAL:HG23	1:51:A:PHE:HB3	2	2.97
(1,797)	1:7:A:VAL:HG22	1:51:A:PHE:HB3	4	2.97
(1,2619)	1:109:A:LEU:HB2	1:30:A:VAL:HG23	2	2.96
(1,1801)	1:29:A:VAL:HG11	1:61:A:ALA:HA	11	2.96
(1,1763)	1:7:A:VAL:HG22	1:11:A:ILE:HG13	9	2.96
(1,1763)	1:7:A:VAL:HG21	1:11:A:ILE:HG13	11	2.96
(1,797)	1:7:A:VAL:HG23	1:51:A:PHE:HB3	14	2.96
(1,2619)	1:109:A:LEU:HB2	1:30:A:VAL:HG22	15	2.95
(1,797)	1:7:A:VAL:HG21	1:51:A:PHE:HB3	1	2.95
(1,797)	1:7:A:VAL:HG23	1:51:A:PHE:HB3	15	2.95
(1,1801)	1:29:A:VAL:HG12	1:61:A:ALA:HA	2	2.93
(1,799)	1:11:A:ILE:HD11	1:7:A:VAL:HG22	2	2.93
(1,2619)	1:109:A:LEU:HB2	1:30:A:VAL:HG22	7	2.92
(1,2619)	1:109:A:LEU:HB2	1:30:A:VAL:HG22	6	2.91
(1,2619)	1:109:A:LEU:HB2	1:30:A:VAL:HG22	11	2.9
(1,2663)	1:33:A:ILE:HA	1:31:A:VAL:HG11	8	2.89
(1,834)	1:72:A:LEU:HD22	1:101:A:ILE:HG21	13	2.89
(1,797)	1:7:A:VAL:HG23	1:51:A:PHE:HB3	8	2.89
(1,2663)	1:33:A:ILE:HA	1:31:A:VAL:HG11	3	2.88
(1,2663)	1:33:A:ILE:HA	1:31:A:VAL:HG13	16	2.88
(1,2619)	1:109:A:LEU:HB2	1:30:A:VAL:HG21	1	2.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,985)	1:29:A:VAL:HG12	1:61:A:ALA:HB3	7	2.88
(1,2619)	1:109:A:LEU:HB2	1:30:A:VAL:HG22	10	2.87
(1,797)	1:7:A:VAL:HG23	1:51:A:PHE:HB3	3	2.87
(1,797)	1:7:A:VAL:HG21	1:51:A:PHE:HB3	9	2.87
(1,2663)	1:33:A:ILE:HA	1:31:A:VAL:HG13	9	2.86
(1,2619)	1:109:A:LEU:HB2	1:30:A:VAL:HG23	13	2.86
(1,2619)	1:109:A:LEU:HB2	1:30:A:VAL:HG22	8	2.85
(1,2003)	1:99:A:VAL:HG22	1:91:A:CYS:HB3	18	2.85
(1,799)	1:11:A:ILE:HD11	1:7:A:VAL:HG23	1	2.85
(1,797)	1:7:A:VAL:HG22	1:51:A:PHE:HB3	13	2.85
(1,782)	1:99:A:VAL:HG12	1:89:A:GLY:HA3	1	2.84
(1,782)	1:99:A:VAL:HG12	1:89:A:GLY:HA3	14	2.84
(1,985)	1:29:A:VAL:HG12	1:61:A:ALA:HB2	19	2.83
(1,2663)	1:33:A:ILE:HA	1:31:A:VAL:HG11	19	2.82
(1,1813)	1:26:A:ILE:HG12	1:57:A:VAL:HG21	5	2.82
(1,985)	1:29:A:VAL:HG13	1:61:A:ALA:HB1	5	2.82
(1,799)	1:11:A:ILE:HD11	1:7:A:VAL:HG21	20	2.82
(1,2663)	1:33:A:ILE:HA	1:31:A:VAL:HG12	5	2.8
(1,2663)	1:33:A:ILE:HA	1:31:A:VAL:HG11	11	2.8
(1,1763)	1:7:A:VAL:HG23	1:11:A:ILE:HG13	10	2.8
(1,797)	1:7:A:VAL:HG23	1:51:A:PHE:HB3	16	2.8
(1,782)	1:99:A:VAL:HG11	1:89:A:GLY:HA3	12	2.8
(1,985)	1:29:A:VAL:HG13	1:61:A:ALA:HB1	3	2.79
(1,797)	1:7:A:VAL:HG21	1:51:A:PHE:HB3	11	2.79
(1,2663)	1:33:A:ILE:HA	1:31:A:VAL:HG13	4	2.78
(1,1418)	1:91:A:CYS:HB2	1:99:A:VAL:HG21	17	2.78
(1,799)	1:11:A:ILE:HD12	1:7:A:VAL:HG21	4	2.78
(1,782)	1:99:A:VAL:HG11	1:89:A:GLY:HA3	9	2.77
(1,85)	1:99:A:VAL:HG22	1:74:A:CYS:H	2	2.77
(1,2663)	1:33:A:ILE:HA	1:31:A:VAL:HG13	15	2.76
(1,1813)	1:26:A:ILE:HG12	1:57:A:VAL:HG22	7	2.76
(1,799)	1:11:A:ILE:HD12	1:7:A:VAL:HG22	8	2.76
(1,782)	1:99:A:VAL:HG11	1:89:A:GLY:HA3	2	2.75
(1,85)	1:99:A:VAL:HG23	1:74:A:CYS:H	14	2.74
(1,85)	1:99:A:VAL:HG21	1:74:A:CYS:H	15	2.73
(1,2663)	1:33:A:ILE:HA	1:31:A:VAL:HG12	6	2.72
(1,2663)	1:33:A:ILE:HA	1:31:A:VAL:HG12	7	2.72
(1,985)	1:29:A:VAL:HG11	1:61:A:ALA:HB3	6	2.72
(1,985)	1:29:A:VAL:HG13	1:61:A:ALA:HB3	14	2.72
(1,782)	1:99:A:VAL:HG13	1:89:A:GLY:HA3	11	2.72
(1,85)	1:99:A:VAL:HG21	1:74:A:CYS:H	5	2.72
(1,738)	1:7:A:VAL:HG13	1:6:A:VAL:HG11	4	2.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,738)	1:7:A:VAL:HG11	1:6:A:VAL:HG11	18	2.71
(1,1763)	1:7:A:VAL:HG21	1:11:A:ILE:HG13	15	2.7
(1,985)	1:29:A:VAL:HG11	1:61:A:ALA:HB2	12	2.7
(1,797)	1:7:A:VAL:HG21	1:51:A:PHE:HB3	18	2.7
(1,738)	1:7:A:VAL:HG13	1:6:A:VAL:HG12	11	2.7
(1,985)	1:29:A:VAL:HG13	1:61:A:ALA:HB1	18	2.69
(1,797)	1:7:A:VAL:HG22	1:51:A:PHE:HB3	6	2.69
(1,85)	1:99:A:VAL:HG22	1:74:A:CYS:H	18	2.69
(1,85)	1:99:A:VAL:HG21	1:74:A:CYS:H	9	2.67
(1,2663)	1:33:A:ILE:HA	1:31:A:VAL:HG13	10	2.66
(1,985)	1:29:A:VAL:HG11	1:61:A:ALA:HB2	10	2.66
(1,985)	1:29:A:VAL:HG13	1:61:A:ALA:HB1	15	2.66
(1,782)	1:99:A:VAL:HG12	1:89:A:GLY:HA3	15	2.66
(1,738)	1:7:A:VAL:HG13	1:6:A:VAL:HG11	5	2.66
(1,85)	1:99:A:VAL:HG22	1:74:A:CYS:H	8	2.66
(1,80)	1:99:A:VAL:HG23	1:75:A:LYS:H	10	2.66
(1,1813)	1:26:A:ILE:HG12	1:57:A:VAL:HG21	16	2.65
(1,797)	1:7:A:VAL:HG23	1:51:A:PHE:HB3	12	2.65
(1,782)	1:99:A:VAL:HG11	1:89:A:GLY:HA3	16	2.64
(1,85)	1:99:A:VAL:HG21	1:74:A:CYS:H	3	2.64
(1,85)	1:99:A:VAL:HG23	1:74:A:CYS:H	7	2.64
(1,85)	1:99:A:VAL:HG21	1:74:A:CYS:H	20	2.64
(1,2663)	1:33:A:ILE:HA	1:31:A:VAL:HG12	2	2.63
(1,1763)	1:7:A:VAL:HG21	1:11:A:ILE:HG13	17	2.63
(1,985)	1:29:A:VAL:HG13	1:61:A:ALA:HB2	17	2.63
(1,1813)	1:26:A:ILE:HG12	1:57:A:VAL:HG22	12	2.62
(1,1763)	1:7:A:VAL:HG23	1:11:A:ILE:HG13	7	2.62
(1,85)	1:99:A:VAL:HG22	1:74:A:CYS:H	11	2.62
(1,738)	1:7:A:VAL:HG13	1:6:A:VAL:HG12	9	2.61
(1,738)	1:7:A:VAL:HG11	1:6:A:VAL:HG13	16	2.61
(1,85)	1:99:A:VAL:HG23	1:74:A:CYS:H	13	2.61
(1,1813)	1:26:A:ILE:HG12	1:57:A:VAL:HG21	17	2.6
(1,1763)	1:7:A:VAL:HG21	1:11:A:ILE:HG13	14	2.6
(1,985)	1:29:A:VAL:HG12	1:61:A:ALA:HB1	8	2.6
(1,985)	1:29:A:VAL:HG13	1:61:A:ALA:HB1	20	2.6
(1,1813)	1:26:A:ILE:HG12	1:57:A:VAL:HG22	3	2.59
(1,1763)	1:7:A:VAL:HG21	1:11:A:ILE:HG13	6	2.59
(1,985)	1:29:A:VAL:HG11	1:61:A:ALA:HB2	1	2.59
(1,985)	1:29:A:VAL:HG13	1:61:A:ALA:HB1	16	2.59
(1,738)	1:7:A:VAL:HG11	1:6:A:VAL:HG12	2	2.59
(1,738)	1:7:A:VAL:HG13	1:6:A:VAL:HG11	3	2.59
(1,2003)	1:99:A:VAL:HG21	1:91:A:CYS:HB3	17	2.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1813)	1:26:A:ILE:HG12	1:57:A:VAL:HG21	10	2.58
(1,738)	1:7:A:VAL:HG12	1:6:A:VAL:HG12	14	2.58
(1,1763)	1:7:A:VAL:HG23	1:11:A:ILE:HG13	5	2.57
(1,738)	1:7:A:VAL:HG11	1:6:A:VAL:HG11	8	2.57
(1,85)	1:99:A:VAL:HG21	1:74:A:CYS:H	17	2.56
(1,1813)	1:26:A:ILE:HG12	1:57:A:VAL:HG23	20	2.55
(1,782)	1:99:A:VAL:HG13	1:89:A:GLY:HA3	6	2.55
(1,85)	1:99:A:VAL:HG21	1:74:A:CYS:H	4	2.55
(1,80)	1:99:A:VAL:HG22	1:75:A:LYS:H	14	2.54
(1,985)	1:29:A:VAL:HG11	1:61:A:ALA:HB2	4	2.53
(1,985)	1:29:A:VAL:HG11	1:61:A:ALA:HB2	9	2.53
(1,782)	1:99:A:VAL:HG12	1:89:A:GLY:HA3	13	2.53
(1,738)	1:7:A:VAL:HG12	1:6:A:VAL:HG13	15	2.53
(1,85)	1:99:A:VAL:HG23	1:74:A:CYS:H	1	2.53
(1,1863)	1:12:A:ALA:HB1	1:15:A:GLU:HG2	9	2.52
(1,782)	1:99:A:VAL:HG11	1:89:A:GLY:HA3	5	2.52
(1,738)	1:7:A:VAL:HG12	1:6:A:VAL:HG12	7	2.52
(1,85)	1:99:A:VAL:HG23	1:74:A:CYS:H	12	2.52
(1,1763)	1:7:A:VAL:HG21	1:11:A:ILE:HG13	13	2.51
(1,782)	1:99:A:VAL:HG12	1:89:A:GLY:HA3	8	2.51
(1,738)	1:7:A:VAL:HG11	1:6:A:VAL:HG12	1	2.51
(1,85)	1:99:A:VAL:HG21	1:74:A:CYS:H	16	2.51
(1,1813)	1:26:A:ILE:HG12	1:57:A:VAL:HG22	4	2.5
(1,1763)	1:7:A:VAL:HG22	1:11:A:ILE:HG13	3	2.5
(1,738)	1:7:A:VAL:HG13	1:6:A:VAL:HG11	6	2.5
(1,738)	1:7:A:VAL:HG12	1:6:A:VAL:HG11	13	2.5
(1,1813)	1:26:A:ILE:HG12	1:57:A:VAL:HG22	6	2.49
(1,738)	1:7:A:VAL:HG13	1:6:A:VAL:HG13	10	2.49
(1,85)	1:99:A:VAL:HG23	1:74:A:CYS:H	19	2.49
(1,1763)	1:7:A:VAL:HG22	1:11:A:ILE:HG13	18	2.48
(1,738)	1:7:A:VAL:HG11	1:6:A:VAL:HG13	17	2.48
(1,1813)	1:26:A:ILE:HG12	1:57:A:VAL:HG23	11	2.47
(1,1217)	1:72:A:LEU:HD12	1:99:A:VAL:HB	13	2.47
(1,80)	1:99:A:VAL:HG23	1:75:A:LYS:H	17	2.47
(1,2591)	1:7:A:VAL:HG13	1:107:A:MET:HE3	4	2.46
(1,2619)	1:109:A:LEU:HB2	1:30:A:VAL:HG22	19	2.45
(1,2115)	1:28:A:ARG:HA	1:29:A:VAL:HG12	6	2.45
(1,985)	1:29:A:VAL:HG11	1:61:A:ALA:HB3	13	2.45
(1,782)	1:99:A:VAL:HG13	1:89:A:GLY:HA3	7	2.45
(1,2591)	1:7:A:VAL:HG11	1:107:A:MET:HE2	12	2.44
(1,1863)	1:12:A:ALA:HB3	1:15:A:GLU:HG2	19	2.44
(1,1813)	1:26:A:ILE:HG12	1:57:A:VAL:HG23	15	2.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1763)	1:7:A:VAL:HG22	1:11:A:ILE:HG13	16	2.44
(1,782)	1:99:A:VAL:HG12	1:89:A:GLY:HA3	3	2.44
(1,85)	1:99:A:VAL:HG21	1:74:A:CYS:H	10	2.44
(1,1813)	1:26:A:ILE:HG12	1:57:A:VAL:HG23	1	2.43
(1,1493)	1:7:A:VAL:HG12	1:44:A:PHE:HA	18	2.43
(1,985)	1:29:A:VAL:HG11	1:61:A:ALA:HB1	11	2.43
(1,738)	1:7:A:VAL:HG11	1:6:A:VAL:HG12	12	2.43
(1,80)	1:99:A:VAL:HG21	1:75:A:LYS:H	7	2.43
(1,2115)	1:28:A:ARG:HA	1:29:A:VAL:HG13	12	2.42
(1,738)	1:7:A:VAL:HG12	1:6:A:VAL:HG13	20	2.42
(1,1863)	1:12:A:ALA:HB1	1:15:A:GLU:HG2	11	2.41
(1,1813)	1:26:A:ILE:HG12	1:57:A:VAL:HG21	2	2.41
(1,2591)	1:7:A:VAL:HG12	1:107:A:MET:HE2	14	2.4
(1,2115)	1:28:A:ARG:HA	1:29:A:VAL:HG11	8	2.4
(1,2115)	1:28:A:ARG:HA	1:29:A:VAL:HG12	1	2.39
(1,2115)	1:28:A:ARG:HA	1:29:A:VAL:HG12	16	2.39
(1,1813)	1:26:A:ILE:HG12	1:57:A:VAL:HG22	19	2.39
(1,2115)	1:28:A:ARG:HA	1:29:A:VAL:HG13	9	2.38
(1,2115)	1:28:A:ARG:HA	1:29:A:VAL:HG11	15	2.38
(1,2003)	1:99:A:VAL:HG23	1:91:A:CYS:HB3	7	2.38
(1,1863)	1:12:A:ALA:HB1	1:15:A:GLU:HG2	10	2.38
(1,985)	1:29:A:VAL:HG12	1:61:A:ALA:HB1	2	2.38
(1,80)	1:99:A:VAL:HG23	1:75:A:LYS:H	8	2.38
(1,2115)	1:28:A:ARG:HA	1:29:A:VAL:HG11	3	2.37
(1,1863)	1:12:A:ALA:HB1	1:15:A:GLU:HG2	17	2.37
(1,1813)	1:26:A:ILE:HG12	1:57:A:VAL:HG22	14	2.37
(1,80)	1:99:A:VAL:HG21	1:75:A:LYS:H	19	2.37
(1,1863)	1:12:A:ALA:HB1	1:15:A:GLU:HG2	3	2.36
(1,1813)	1:26:A:ILE:HG12	1:57:A:VAL:HG22	13	2.36
(1,797)	1:7:A:VAL:HG22	1:51:A:PHE:HB3	20	2.36
(1,782)	1:99:A:VAL:HG13	1:89:A:GLY:HA3	17	2.36
(1,2115)	1:28:A:ARG:HA	1:29:A:VAL:HG11	19	2.35
(1,1813)	1:26:A:ILE:HG12	1:57:A:VAL:HG21	9	2.35
(1,782)	1:99:A:VAL:HG12	1:89:A:GLY:HA3	20	2.35
(1,85)	1:99:A:VAL:HG21	1:74:A:CYS:H	6	2.35
(1,2115)	1:28:A:ARG:HA	1:29:A:VAL:HG12	4	2.34
(1,2115)	1:28:A:ARG:HA	1:29:A:VAL:HG12	18	2.34
(1,1763)	1:7:A:VAL:HG22	1:11:A:ILE:HG13	2	2.34
(1,1763)	1:7:A:VAL:HG21	1:11:A:ILE:HG13	20	2.34
(1,1493)	1:7:A:VAL:HG11	1:44:A:PHE:HA	20	2.34
(1,2591)	1:7:A:VAL:HG13	1:107:A:MET:HE3	10	2.33
(1,1731)	1:72:A:LEU:HD11	1:91:A:CYS:HA	13	2.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,80)	1:99:A:VAL:HG22	1:75:A:LYS:H	6	2.33
(1,2115)	1:28:A:ARG:HA	1:29:A:VAL:HG12	5	2.32
(1,2115)	1:28:A:ARG:HA	1:29:A:VAL:HG12	20	2.32
(1,1737)	1:33:A:ILE:HG13	1:39:A:MET:HE1	3	2.32
(1,80)	1:99:A:VAL:HG23	1:75:A:LYS:H	11	2.32
(1,80)	1:99:A:VAL:HG23	1:75:A:LYS:H	15	2.32
(1,80)	1:99:A:VAL:HG21	1:75:A:LYS:H	18	2.32
(1,2591)	1:7:A:VAL:HG11	1:107:A:MET:HE2	16	2.31
(1,2115)	1:28:A:ARG:HA	1:29:A:VAL:HG13	2	2.31
(1,2115)	1:28:A:ARG:HA	1:29:A:VAL:HG11	14	2.31
(1,1813)	1:26:A:ILE:HG12	1:57:A:VAL:HG21	18	2.31
(1,80)	1:99:A:VAL:HG23	1:75:A:LYS:H	2	2.31
(1,2115)	1:28:A:ARG:HA	1:29:A:VAL:HG12	11	2.3
(1,1493)	1:7:A:VAL:HG13	1:44:A:PHE:HA	8	2.3
(1,2115)	1:28:A:ARG:HA	1:29:A:VAL:HG11	17	2.29
(1,1763)	1:7:A:VAL:HG21	1:11:A:ILE:HG13	4	2.29
(1,2115)	1:28:A:ARG:HA	1:29:A:VAL:HG13	10	2.28
(1,2115)	1:28:A:ARG:HA	1:29:A:VAL:HG12	13	2.28
(1,1813)	1:26:A:ILE:HG12	1:57:A:VAL:HG23	8	2.28
(1,855)	1:99:A:VAL:HG21	1:74:A:CYS:HB2	17	2.28
(1,2115)	1:28:A:ARG:HA	1:29:A:VAL:HG13	7	2.27
(1,2615)	1:50:A:THR:HG22	1:49:A:GLU:HB3	7	2.26
(1,872)	1:26:A:ILE:HG22	1:29:A:VAL:HG11	19	2.26
(1,80)	1:99:A:VAL:HG22	1:75:A:LYS:H	5	2.26
(1,2591)	1:7:A:VAL:HG13	1:107:A:MET:HE1	6	2.25
(1,1863)	1:12:A:ALA:HB3	1:15:A:GLU:HG2	7	2.25
(1,738)	1:7:A:VAL:HG12	1:6:A:VAL:HG12	19	2.25
(1,1654)	1:74:A:CYS:HA	1:99:A:VAL:HG23	15	2.24
(1,1493)	1:7:A:VAL:HG11	1:44:A:PHE:HA	6	2.24
(1,2003)	1:99:A:VAL:HG21	1:91:A:CYS:HB3	20	2.23
(1,782)	1:99:A:VAL:HG13	1:89:A:GLY:HA3	18	2.23
(1,2591)	1:7:A:VAL:HG13	1:107:A:MET:HE3	11	2.22
(1,1763)	1:7:A:VAL:HG23	1:11:A:ILE:HG13	1	2.22
(1,812)	1:29:A:VAL:HG23	1:109:A:LEU:HD21	19	2.22
(1,2591)	1:7:A:VAL:HG11	1:107:A:MET:HE3	2	2.21
(1,1863)	1:12:A:ALA:HB2	1:15:A:GLU:HG2	6	2.21
(1,1863)	1:12:A:ALA:HB3	1:15:A:GLU:HG2	8	2.21
(1,1863)	1:12:A:ALA:HB2	1:15:A:GLU:HG2	18	2.21
(1,1863)	1:12:A:ALA:HB2	1:15:A:GLU:HG2	13	2.2
(1,811)	1:29:A:VAL:HG21	1:109:A:LEU:HD13	17	2.2
(1,2615)	1:50:A:THR:HG22	1:49:A:GLU:HB3	15	2.19
(1,2598)	1:7:A:VAL:HG23	1:8:A:SER:HA	9	2.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2598)	1:7:A:VAL:HG23	1:8:A:SER:HA	19	2.19
(1,2466)	1:29:A:VAL:HG23	1:10:A:LEU:HD23	18	2.19
(1,2003)	1:99:A:VAL:HG22	1:91:A:CYS:HB3	8	2.19
(1,1763)	1:7:A:VAL:HG22	1:11:A:ILE:HG13	12	2.19
(1,1654)	1:74:A:CYS:HA	1:99:A:VAL:HG23	10	2.19
(1,1654)	1:74:A:CYS:HA	1:99:A:VAL:HG22	17	2.19
(1,782)	1:99:A:VAL:HG11	1:89:A:GLY:HA3	19	2.19
(1,2615)	1:50:A:THR:HG21	1:49:A:GLU:HB3	20	2.18
(1,2598)	1:7:A:VAL:HG22	1:8:A:SER:HA	3	2.18
(1,2598)	1:7:A:VAL:HG21	1:8:A:SER:HA	12	2.18
(1,1863)	1:12:A:ALA:HB3	1:15:A:GLU:HG2	1	2.18
(1,1863)	1:12:A:ALA:HB3	1:15:A:GLU:HG2	20	2.18
(1,1654)	1:74:A:CYS:HA	1:99:A:VAL:HG22	2	2.18
(1,1654)	1:74:A:CYS:HA	1:99:A:VAL:HG22	14	2.18
(1,80)	1:99:A:VAL:HG21	1:75:A:LYS:H	12	2.18
(1,2598)	1:7:A:VAL:HG22	1:8:A:SER:HA	14	2.17
(1,2598)	1:7:A:VAL:HG21	1:8:A:SER:HA	17	2.17
(1,2003)	1:99:A:VAL:HG21	1:91:A:CYS:HB3	15	2.17
(1,80)	1:99:A:VAL:HG22	1:75:A:LYS:H	20	2.17
(1,2598)	1:7:A:VAL:HG23	1:8:A:SER:HA	20	2.16
(1,2598)	1:7:A:VAL:HG22	1:8:A:SER:HA	15	2.15
(1,2003)	1:99:A:VAL:HG23	1:91:A:CYS:HB3	14	2.15
(1,1654)	1:74:A:CYS:HA	1:99:A:VAL:HG22	8	2.15
(1,1493)	1:7:A:VAL:HG12	1:44:A:PHE:HA	4	2.15
(1,1493)	1:7:A:VAL:HG13	1:44:A:PHE:HA	12	2.15
(1,812)	1:29:A:VAL:HG22	1:109:A:LEU:HD22	6	2.15
(1,80)	1:99:A:VAL:HG22	1:75:A:LYS:H	4	2.15
(1,80)	1:99:A:VAL:HG22	1:75:A:LYS:H	16	2.15
(1,2598)	1:7:A:VAL:HG22	1:8:A:SER:HA	8	2.14
(1,2003)	1:99:A:VAL:HG23	1:91:A:CYS:HB3	19	2.14
(1,1763)	1:7:A:VAL:HG22	1:11:A:ILE:HG13	8	2.14
(1,1729)	1:6:A:VAL:HB	1:7:A:VAL:HG11	2	2.14
(1,1654)	1:74:A:CYS:HA	1:99:A:VAL:HG22	18	2.14
(1,2466)	1:29:A:VAL:HG22	1:10:A:LEU:HD22	6	2.13
(1,1654)	1:74:A:CYS:HA	1:99:A:VAL:HG21	7	2.13
(1,1493)	1:7:A:VAL:HG12	1:44:A:PHE:HA	11	2.13
(1,1493)	1:7:A:VAL:HG13	1:44:A:PHE:HA	16	2.13
(1,80)	1:99:A:VAL:HG22	1:75:A:LYS:H	3	2.13
(1,2615)	1:50:A:THR:HG23	1:49:A:GLU:HB3	16	2.12
(1,2615)	1:50:A:THR:HG21	1:49:A:GLU:HB3	18	2.12
(1,2598)	1:7:A:VAL:HG21	1:8:A:SER:HA	16	2.12
(1,2591)	1:7:A:VAL:HG11	1:107:A:MET:HE1	17	2.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2466)	1:31:A:VAL:HG23	1:10:A:LEU:HD22	3	2.12
(1,2003)	1:99:A:VAL:HG21	1:91:A:CYS:HB3	5	2.12
(1,772)	1:66:A:VAL:HG23	1:64:A:ASP:HB2	15	2.12
(1,80)	1:99:A:VAL:HG21	1:75:A:LYS:H	1	2.12
(1,2615)	1:50:A:THR:HG22	1:49:A:GLU:HB3	17	2.11
(1,1729)	1:6:A:VAL:HB	1:7:A:VAL:HG13	9	2.11
(1,80)	1:99:A:VAL:HG23	1:75:A:LYS:H	9	2.11
(1,2591)	1:7:A:VAL:HG13	1:107:A:MET:HE2	5	2.1
(1,2591)	1:7:A:VAL:HG13	1:107:A:MET:HE1	9	2.1
(1,1863)	1:12:A:ALA:HB3	1:15:A:GLU:HG2	12	2.1
(1,1863)	1:12:A:ALA:HB3	1:15:A:GLU:HG2	16	2.1
(1,1654)	1:74:A:CYS:HA	1:99:A:VAL:HG21	3	2.1
(1,1654)	1:74:A:CYS:HA	1:99:A:VAL:HG21	5	2.1
(1,2598)	1:7:A:VAL:HG21	1:8:A:SER:HA	6	2.09
(1,1863)	1:12:A:ALA:HB2	1:15:A:GLU:HG2	14	2.09
(1,1729)	1:6:A:VAL:HB	1:7:A:VAL:HG13	11	2.09
(1,2615)	1:50:A:THR:HG23	1:49:A:GLU:HB3	14	2.08
(1,1737)	1:33:A:ILE:HG13	1:39:A:MET:HE2	18	2.08
(1,2598)	1:7:A:VAL:HG22	1:8:A:SER:HA	1	2.07
(1,1654)	1:74:A:CYS:HA	1:99:A:VAL:HG22	11	2.07
(1,1493)	1:7:A:VAL:HG13	1:44:A:PHE:HA	1	2.07
(1,1493)	1:7:A:VAL:HG11	1:44:A:PHE:HA	19	2.07
(1,872)	1:26:A:ILE:HG23	1:29:A:VAL:HG11	3	2.07
(1,2598)	1:7:A:VAL:HG22	1:8:A:SER:HA	2	2.06
(1,2598)	1:7:A:VAL:HG22	1:8:A:SER:HA	10	2.06
(1,2598)	1:7:A:VAL:HG21	1:8:A:SER:HA	13	2.06
(1,1863)	1:12:A:ALA:HB3	1:15:A:GLU:HG2	5	2.06
(1,1729)	1:6:A:VAL:HB	1:7:A:VAL:HG13	4	2.06
(1,812)	1:29:A:VAL:HG22	1:109:A:LEU:HD22	17	2.06
(1,2615)	1:50:A:THR:HG22	1:49:A:GLU:HB3	4	2.05
(1,2598)	1:7:A:VAL:HG22	1:8:A:SER:HA	7	2.05
(1,2598)	1:7:A:VAL:HG22	1:8:A:SER:HA	11	2.05
(1,2003)	1:99:A:VAL:HG22	1:91:A:CYS:HB3	11	2.05
(1,1654)	1:74:A:CYS:HA	1:99:A:VAL:HG23	20	2.05
(1,2615)	1:50:A:THR:HG23	1:49:A:GLU:HB3	9	2.04
(1,2615)	1:50:A:THR:HG23	1:49:A:GLU:HB3	11	2.04
(1,2598)	1:7:A:VAL:HG22	1:8:A:SER:HA	5	2.04
(1,2591)	1:7:A:VAL:HG13	1:107:A:MET:HE2	3	2.04
(1,2003)	1:99:A:VAL:HG22	1:91:A:CYS:HB3	2	2.04
(1,2003)	1:99:A:VAL:HG23	1:91:A:CYS:HB3	12	2.04
(1,1863)	1:12:A:ALA:HB3	1:15:A:GLU:HG2	2	2.04
(1,1729)	1:6:A:VAL:HB	1:7:A:VAL:HG11	18	2.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1654)	1:74:A:CYS:HA	1:99:A:VAL:HG21	9	2.04
(1,2598)	1:7:A:VAL:HG23	1:8:A:SER:HA	4	2.03
(1,872)	1:26:A:ILE:HG22	1:29:A:VAL:HG11	7	2.03
(1,80)	1:99:A:VAL:HG21	1:75:A:LYS:H	13	2.03
(1,2466)	1:29:A:VAL:HG22	1:10:A:LEU:HD23	15	2.02
(1,2003)	1:99:A:VAL:HG21	1:91:A:CYS:HB3	9	2.02
(1,1729)	1:6:A:VAL:HB	1:7:A:VAL:HG13	3	2.02
(1,1729)	1:6:A:VAL:HB	1:7:A:VAL:HG11	16	2.02
(1,2615)	1:50:A:THR:HG22	1:49:A:GLU:HB3	2	2.01
(1,2615)	1:50:A:THR:HG23	1:49:A:GLU:HB3	3	2.01
(1,2598)	1:7:A:VAL:HG22	1:8:A:SER:HA	18	2.01
(1,2003)	1:99:A:VAL:HG21	1:91:A:CYS:HB3	3	2.01
(1,1863)	1:12:A:ALA:HB1	1:15:A:GLU:HG2	4	2.01
(1,1737)	1:33:A:ILE:HG13	1:39:A:MET:HE3	9	2.01
(1,872)	1:26:A:ILE:HG23	1:29:A:VAL:HG12	17	2.01
(1,855)	1:99:A:VAL:HG22	1:74:A:CYS:HB2	18	2.01
(1,2441)	1:31:A:VAL:HG23	1:10:A:LEU:HD22	3	2.0
(1,1729)	1:6:A:VAL:HB	1:7:A:VAL:HG12	7	2.0
(1,1729)	1:6:A:VAL:HB	1:7:A:VAL:HG12	13	2.0
(1,812)	1:29:A:VAL:HG23	1:109:A:LEU:HD23	1	2.0
(1,2591)	1:7:A:VAL:HG11	1:107:A:MET:HE3	1	1.99
(1,2466)	1:29:A:VAL:HG21	1:10:A:LEU:HD23	1	1.99
(1,1816)	1:102:A:THR:HG23	1:72:A:LEU:HD23	13	1.99
(1,1729)	1:6:A:VAL:HB	1:7:A:VAL:HG11	1	1.99
(1,872)	1:26:A:ILE:HG21	1:29:A:VAL:HG13	6	1.99
(1,772)	1:66:A:VAL:HG23	1:64:A:ASP:HB2	7	1.99
(1,48)	1:7:A:VAL:HG21	1:11:A:ILE:H	19	1.99
(1,2615)	1:50:A:THR:HG22	1:49:A:GLU:HB3	6	1.98
(1,2003)	1:99:A:VAL:HG23	1:91:A:CYS:HB3	13	1.98
(1,1654)	1:74:A:CYS:HA	1:99:A:VAL:HG21	4	1.98
(1,1493)	1:7:A:VAL:HG12	1:44:A:PHE:HA	3	1.98
(1,872)	1:26:A:ILE:HG21	1:29:A:VAL:HG11	15	1.98
(1,812)	1:29:A:VAL:HG21	1:109:A:LEU:HD23	10	1.98
(1,812)	1:29:A:VAL:HG23	1:109:A:LEU:HD23	12	1.98
(1,772)	1:66:A:VAL:HG23	1:64:A:ASP:HB2	2	1.98
(1,2615)	1:50:A:THR:HG23	1:49:A:GLU:HB3	8	1.97
(1,1729)	1:6:A:VAL:HB	1:7:A:VAL:HG11	8	1.97
(1,1729)	1:6:A:VAL:HB	1:7:A:VAL:HG12	14	1.97
(1,872)	1:26:A:ILE:HG21	1:29:A:VAL:HG13	1	1.97
(1,811)	1:29:A:VAL:HG23	1:109:A:LEU:HD12	12	1.97
(1,2003)	1:99:A:VAL:HG21	1:91:A:CYS:HB3	16	1.96
(1,1654)	1:74:A:CYS:HA	1:99:A:VAL:HG21	6	1.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1654)	1:74:A:CYS:HA	1:99:A:VAL:HG23	12	1.96
(1,1654)	1:74:A:CYS:HA	1:99:A:VAL:HG23	19	1.96
(1,1493)	1:7:A:VAL:HG12	1:44:A:PHE:HA	5	1.96
(1,1493)	1:7:A:VAL:HG11	1:44:A:PHE:HA	13	1.96
(1,811)	1:29:A:VAL:HG23	1:109:A:LEU:HD13	1	1.96
(1,772)	1:66:A:VAL:HG23	1:64:A:ASP:HB2	14	1.96
(1,2615)	1:50:A:THR:HG23	1:49:A:GLU:HB3	1	1.95
(1,2615)	1:50:A:THR:HG21	1:49:A:GLU:HB3	10	1.95
(1,2595)	1:110:A:LEU:HD21	1:66:A:VAL:HG12	13	1.95
(1,2591)	1:7:A:VAL:HG12	1:107:A:MET:HE2	20	1.95
(1,872)	1:26:A:ILE:HG23	1:29:A:VAL:HG12	5	1.95
(1,811)	1:29:A:VAL:HG21	1:109:A:LEU:HD11	15	1.95
(1,2615)	1:50:A:THR:HG23	1:49:A:GLU:HB3	13	1.94
(1,1737)	1:33:A:ILE:HG13	1:39:A:MET:HE2	8	1.94
(1,1729)	1:6:A:VAL:HB	1:7:A:VAL:HG13	6	1.94
(1,1729)	1:6:A:VAL:HB	1:7:A:VAL:HG11	12	1.94
(1,1654)	1:74:A:CYS:HA	1:99:A:VAL:HG21	16	1.94
(1,1493)	1:7:A:VAL:HG13	1:44:A:PHE:HA	2	1.94
(1,872)	1:26:A:ILE:HG21	1:29:A:VAL:HG12	18	1.94
(1,772)	1:66:A:VAL:HG22	1:64:A:ASP:HB2	4	1.94
(1,772)	1:66:A:VAL:HG21	1:64:A:ASP:HB2	5	1.94
(1,772)	1:66:A:VAL:HG21	1:64:A:ASP:HB2	16	1.94
(1,2591)	1:7:A:VAL:HG12	1:107:A:MET:HE1	7	1.93
(1,1729)	1:6:A:VAL:HB	1:7:A:VAL:HG13	10	1.93
(1,872)	1:26:A:ILE:HG22	1:29:A:VAL:HG12	16	1.93
(1,855)	1:99:A:VAL:HG23	1:74:A:CYS:HB2	14	1.93
(1,855)	1:99:A:VAL:HG21	1:74:A:CYS:HB2	15	1.93
(1,2591)	1:7:A:VAL:HG12	1:107:A:MET:HE2	13	1.92
(1,2591)	1:7:A:VAL:HG11	1:107:A:MET:HE3	18	1.92
(1,1776)	1:80:A:VAL:HG12	1:73:A:GLU:HG2	14	1.92
(1,1776)	1:80:A:VAL:HG13	1:73:A:GLU:HG2	20	1.92
(1,1729)	1:6:A:VAL:HB	1:7:A:VAL:HG12	15	1.92
(1,872)	1:26:A:ILE:HG22	1:29:A:VAL:HG11	2	1.92
(1,872)	1:26:A:ILE:HG22	1:29:A:VAL:HG12	12	1.92
(1,2615)	1:50:A:THR:HG22	1:49:A:GLU:HB3	5	1.91
(1,2441)	1:29:A:VAL:HG22	1:10:A:LEU:HD23	15	1.91
(1,1729)	1:6:A:VAL:HB	1:7:A:VAL:HG13	5	1.91
(1,1493)	1:7:A:VAL:HG13	1:44:A:PHE:HA	14	1.91
(1,1418)	1:91:A:CYS:HB2	1:99:A:VAL:HG22	18	1.91
(1,812)	1:29:A:VAL:HG22	1:109:A:LEU:HD21	18	1.91
(1,772)	1:66:A:VAL:HG21	1:64:A:ASP:HB2	6	1.91
(1,772)	1:66:A:VAL:HG21	1:64:A:ASP:HB2	10	1.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2615)	1:50:A:THR:HG23	1:49:A:GLU:HB3	12	1.9
(1,2591)	1:7:A:VAL:HG11	1:107:A:MET:HE3	8	1.9
(1,1654)	1:74:A:CYS:HA	1:99:A:VAL:HG23	13	1.9
(1,772)	1:66:A:VAL:HG22	1:64:A:ASP:HB2	12	1.9
(1,2003)	1:99:A:VAL:HG21	1:91:A:CYS:HB3	10	1.89
(1,855)	1:99:A:VAL:HG23	1:74:A:CYS:HB2	7	1.89
(1,812)	1:29:A:VAL:HG22	1:109:A:LEU:HD23	3	1.89
(1,2466)	1:31:A:VAL:HG22	1:10:A:LEU:HD22	17	1.88
(1,2441)	1:29:A:VAL:HG21	1:10:A:LEU:HD23	1	1.88
(1,2003)	1:99:A:VAL:HG21	1:91:A:CYS:HB3	6	1.88
(1,1732)	1:72:A:LEU:HD11	1:89:A:GLY:HA3	2	1.88
(1,1732)	1:72:A:LEU:HD12	1:89:A:GLY:HA3	5	1.88
(1,1729)	1:6:A:VAL:HB	1:7:A:VAL:HG12	20	1.88
(1,1289)	1:57:A:VAL:HG22	1:15:A:GLU:HG3	17	1.88
(1,872)	1:26:A:ILE:HG21	1:29:A:VAL:HG12	14	1.87
(1,855)	1:99:A:VAL:HG21	1:74:A:CYS:HB2	5	1.87
(1,772)	1:66:A:VAL:HG21	1:64:A:ASP:HB2	17	1.87
(1,2615)	1:50:A:THR:HG23	1:49:A:GLU:HB3	19	1.86
(1,2599)	1:28:A:ARG:HG3	1:30:A:VAL:HG22	5	1.86
(1,2599)	1:28:A:ARG:HG3	1:30:A:VAL:HG23	8	1.86
(1,2466)	1:31:A:VAL:HG23	1:10:A:LEU:HD23	5	1.86
(1,2441)	1:29:A:VAL:HG22	1:112:A:LEU:HD13	18	1.86
(1,1729)	1:6:A:VAL:HB	1:7:A:VAL:HG11	17	1.86
(1,872)	1:26:A:ILE:HG21	1:29:A:VAL:HG13	11	1.86
(1,811)	1:29:A:VAL:HG23	1:109:A:LEU:HD11	9	1.86
(1,1654)	1:74:A:CYS:HA	1:99:A:VAL:HG23	1	1.85
(1,20)	1:72:A:LEU:HD23	1:102:A:THR:H	13	1.85
(1,2599)	1:28:A:ARG:HG3	1:30:A:VAL:HG23	6	1.84
(1,872)	1:26:A:ILE:HG22	1:29:A:VAL:HG13	10	1.84
(1,854)	1:101:A:ILE:HG13	1:70:A:VAL:HG21	5	1.84
(1,812)	1:29:A:VAL:HG22	1:109:A:LEU:HD23	4	1.84
(1,811)	1:29:A:VAL:HG22	1:109:A:LEU:HD13	3	1.84
(1,811)	1:29:A:VAL:HG23	1:109:A:LEU:HD13	7	1.84
(1,811)	1:29:A:VAL:HG21	1:109:A:LEU:HD11	8	1.84
(1,811)	1:29:A:VAL:HG22	1:109:A:LEU:HD12	18	1.84
(1,2466)	1:31:A:VAL:HG22	1:10:A:LEU:HD22	8	1.83
(1,2466)	1:29:A:VAL:HG21	1:10:A:LEU:HD21	19	1.83
(1,2130)	1:72:A:LEU:HD11	1:81:A:PHE:HE2	13	1.83
(1,855)	1:99:A:VAL:HG22	1:74:A:CYS:HB2	2	1.83
(1,855)	1:99:A:VAL:HG21	1:74:A:CYS:HB2	9	1.83
(1,855)	1:99:A:VAL:HG21	1:74:A:CYS:HB2	20	1.83
(1,2643)	1:107:A:MET:HE3	1:106:A:GLU:HG3	6	1.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2466)	1:29:A:VAL:HG23	1:10:A:LEU:HD22	11	1.82
(1,811)	1:29:A:VAL:HG23	1:109:A:LEU:HD11	20	1.82
(1,1737)	1:33:A:ILE:HG13	1:39:A:MET:HE2	1	1.81
(1,1729)	1:6:A:VAL:HB	1:7:A:VAL:HG12	19	1.81
(1,1493)	1:7:A:VAL:HG11	1:44:A:PHE:HA	15	1.81
(1,812)	1:29:A:VAL:HG21	1:109:A:LEU:HD22	2	1.81
(1,772)	1:66:A:VAL:HG21	1:64:A:ASP:HB2	3	1.81
(1,1493)	1:7:A:VAL:HG12	1:44:A:PHE:HA	9	1.8
(1,1493)	1:7:A:VAL:HG11	1:44:A:PHE:HA	10	1.8
(1,872)	1:26:A:ILE:HG23	1:29:A:VAL:HG13	4	1.8
(1,855)	1:99:A:VAL:HG22	1:74:A:CYS:HB2	11	1.8
(1,812)	1:29:A:VAL:HG22	1:109:A:LEU:HD23	14	1.8
(1,772)	1:66:A:VAL:HG23	1:64:A:ASP:HB2	11	1.8
(1,2466)	1:31:A:VAL:HG22	1:10:A:LEU:HD22	20	1.79
(1,872)	1:26:A:ILE:HG22	1:29:A:VAL:HG11	20	1.79
(1,812)	1:29:A:VAL:HG22	1:109:A:LEU:HD22	5	1.79
(1,812)	1:29:A:VAL:HG23	1:109:A:LEU:HD23	9	1.79
(1,812)	1:29:A:VAL:HG21	1:109:A:LEU:HD22	15	1.79
(1,812)	1:29:A:VAL:HG21	1:109:A:LEU:HD22	16	1.79
(1,811)	1:29:A:VAL:HG22	1:109:A:LEU:HD12	14	1.79
(1,106)	1:29:A:VAL:HG13	1:113:A:GLU:H	8	1.79
(1,13)	1:72:A:LEU:HD12	1:90:A:VAL:H	13	1.79
(1,2599)	1:28:A:ARG:HG3	1:30:A:VAL:HG21	12	1.78
(1,1776)	1:80:A:VAL:HG12	1:73:A:GLU:HG2	7	1.78
(1,2599)	1:28:A:ARG:HG3	1:30:A:VAL:HG23	7	1.77
(1,2466)	1:31:A:VAL:HG23	1:10:A:LEU:HD22	7	1.77
(1,1737)	1:33:A:ILE:HG13	1:39:A:MET:HE3	17	1.77
(1,1732)	1:72:A:LEU:HD12	1:89:A:GLY:HA3	13	1.77
(1,811)	1:29:A:VAL:HG21	1:109:A:LEU:HD13	16	1.77
(1,2466)	1:31:A:VAL:HG23	1:10:A:LEU:HD22	12	1.76
(1,2466)	1:31:A:VAL:HG22	1:10:A:LEU:HD23	13	1.76
(1,1840)	1:75:A:LYS:HG3	1:100:A:ILE:HG13	10	1.76
(1,1493)	1:7:A:VAL:HG12	1:44:A:PHE:HA	17	1.76
(1,2599)	1:28:A:ARG:HG3	1:30:A:VAL:HG23	11	1.75
(1,2595)	1:110:A:LEU:HD22	1:66:A:VAL:HG11	19	1.75
(1,2441)	1:31:A:VAL:HG23	1:10:A:LEU:HD23	5	1.75
(1,2441)	1:29:A:VAL:HG21	1:112:A:LEU:HD11	6	1.75
(1,2003)	1:99:A:VAL:HG21	1:91:A:CYS:HB3	4	1.75
(1,872)	1:26:A:ILE:HG22	1:29:A:VAL:HG13	13	1.75
(1,2599)	1:28:A:ARG:HG3	1:30:A:VAL:HG21	18	1.74
(1,48)	1:7:A:VAL:HG22	1:11:A:ILE:H	9	1.74
(1,2616)	1:50:A:THR:HG22	1:47:A:ALA:HB2	12	1.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2595)	1:110:A:LEU:HD21	1:66:A:VAL:HG13	15	1.73
(1,855)	1:99:A:VAL:HG21	1:74:A:CYS:HB2	3	1.73
(1,855)	1:99:A:VAL:HG22	1:74:A:CYS:HB2	8	1.73
(1,812)	1:29:A:VAL:HG21	1:109:A:LEU:HD21	7	1.73
(1,812)	1:29:A:VAL:HG21	1:109:A:LEU:HD21	8	1.73
(1,2441)	1:31:A:VAL:HG22	1:10:A:LEU:HD22	8	1.72
(1,2441)	1:29:A:VAL:HG21	1:10:A:LEU:HD21	19	1.72
(1,2153)	1:99:A:VAL:HG23	1:81:A:PHE:HE1	14	1.72
(1,772)	1:66:A:VAL:HG21	1:64:A:ASP:HB2	13	1.72
(1,2616)	1:50:A:THR:HG21	1:47:A:ALA:HB1	6	1.71
(1,2441)	1:29:A:VAL:HG23	1:10:A:LEU:HD22	11	1.71
(1,1703)	1:72:A:LEU:HD23	1:72:A:LEU:HA	13	1.71
(1,1289)	1:57:A:VAL:HG22	1:15:A:GLU:HG3	7	1.71
(1,872)	1:26:A:ILE:HG23	1:29:A:VAL:HG12	9	1.71
(1,855)	1:99:A:VAL:HG21	1:74:A:CYS:HB2	4	1.71
(1,855)	1:99:A:VAL:HG23	1:74:A:CYS:HB2	13	1.71
(1,812)	1:29:A:VAL:HG22	1:109:A:LEU:HD21	11	1.71
(1,2599)	1:28:A:ARG:HG3	1:30:A:VAL:HG21	20	1.7
(1,1737)	1:33:A:ILE:HG13	1:39:A:MET:HE2	6	1.7
(1,1493)	1:7:A:VAL:HG13	1:44:A:PHE:HA	7	1.7
(1,855)	1:99:A:VAL:HG23	1:74:A:CYS:HB2	19	1.7
(1,2591)	1:7:A:VAL:HG12	1:107:A:MET:HE1	15	1.69
(1,2153)	1:99:A:VAL:HG23	1:81:A:PHE:HE2	7	1.69
(1,48)	1:7:A:VAL:HG23	1:11:A:ILE:H	10	1.69
(1,2595)	1:110:A:LEU:HD22	1:66:A:VAL:HG11	4	1.68
(1,2441)	1:31:A:VAL:HG22	1:10:A:LEU:HD22	20	1.68
(1,2003)	1:99:A:VAL:HG23	1:91:A:CYS:HB3	1	1.68
(1,872)	1:26:A:ILE:HG23	1:29:A:VAL:HG13	8	1.68
(1,742)	1:72:A:LEU:HD11	1:99:A:VAL:HG13	1	1.68
(1,106)	1:29:A:VAL:HG11	1:113:A:GLU:H	2	1.68
(1,48)	1:7:A:VAL:HG21	1:11:A:ILE:H	15	1.68
(1,2466)	1:31:A:VAL:HG21	1:10:A:LEU:HD21	10	1.67
(1,1840)	1:75:A:LYS:HG3	1:100:A:ILE:HG13	14	1.67
(1,1805)	1:10:A:LEU:HD11	1:63:A:LEU:HD22	19	1.67
(1,851)	1:101:A:ILE:HD13	1:105:A:ASN:HB3	9	1.67
(1,730)	1:33:A:ILE:HD13	1:45:A:VAL:HG13	19	1.67
(1,48)	1:7:A:VAL:HG21	1:11:A:ILE:H	14	1.67
(1,2599)	1:28:A:ARG:HG3	1:30:A:VAL:HG23	3	1.66
(1,2441)	1:31:A:VAL:HG23	1:10:A:LEU:HD22	7	1.66
(1,2126)	1:7:A:VAL:HG11	1:44:A:PHE:HE1	1	1.66
(1,1831)	1:58:A:CYS:HB2	1:61:A:ALA:HB1	19	1.66
(1,855)	1:99:A:VAL:HG23	1:74:A:CYS:HB2	12	1.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,811)	1:29:A:VAL:HG21	1:109:A:LEU:HD13	10	1.66
(1,774)	1:66:A:VAL:HG23	1:32:A:GLY:HA3	19	1.66
(1,2466)	1:31:A:VAL:HG23	1:10:A:LEU:HD22	9	1.65
(1,2441)	1:31:A:VAL:HG23	1:10:A:LEU:HD22	12	1.65
(1,2441)	1:31:A:VAL:HG22	1:10:A:LEU:HD23	13	1.65
(1,2126)	1:7:A:VAL:HG12	1:44:A:PHE:HE2	14	1.65
(1,1968)	1:113:A:GLU:HG2	1:27:A:GLU:HB3	10	1.65
(1,1204)	1:75:A:LYS:HB3	1:98:A:ASN:HB3	10	1.65
(1,2621)	1:18:A:ALA:HB1	1:21:A:ASN:HB2	9	1.64
(1,812)	1:29:A:VAL:HG23	1:109:A:LEU:HD22	20	1.64
(1,774)	1:66:A:VAL:HG21	1:32:A:GLY:HA3	3	1.64
(1,742)	1:72:A:LEU:HD12	1:99:A:VAL:HG12	5	1.64
(1,106)	1:29:A:VAL:HG13	1:113:A:GLU:H	13	1.64
(1,48)	1:7:A:VAL:HG23	1:11:A:ILE:H	11	1.64
(1,2616)	1:50:A:THR:HG22	1:47:A:ALA:HB1	19	1.63
(1,2595)	1:110:A:LEU:HD21	1:66:A:VAL:HG11	2	1.63
(1,2595)	1:110:A:LEU:HD23	1:66:A:VAL:HG12	10	1.63
(1,1538)	1:99:A:VAL:HG22	1:91:A:CYS:HA	18	1.63
(1,1421)	1:51:A:PHE:HB2	1:7:A:VAL:HG21	10	1.63
(1,48)	1:7:A:VAL:HG23	1:11:A:ILE:H	7	1.63
(1,2595)	1:110:A:LEU:HD22	1:66:A:VAL:HG12	11	1.62
(1,2441)	1:29:A:VAL:HG21	1:112:A:LEU:HD13	17	1.62
(1,811)	1:29:A:VAL:HG22	1:109:A:LEU:HD11	5	1.62
(1,772)	1:66:A:VAL:HG23	1:64:A:ASP:HB2	19	1.62
(1,106)	1:29:A:VAL:HG13	1:113:A:GLU:H	10	1.62
(1,2595)	1:110:A:LEU:HD21	1:66:A:VAL:HG13	9	1.61
(1,2466)	1:31:A:VAL:HG21	1:10:A:LEU:HD21	16	1.61
(1,1863)	1:12:A:ALA:HB1	1:15:A:GLU:HG2	15	1.61
(1,106)	1:29:A:VAL:HG13	1:113:A:GLU:H	1	1.61
(1,2616)	1:50:A:THR:HG22	1:47:A:ALA:HB1	13	1.6
(1,2599)	1:28:A:ARG:HG3	1:30:A:VAL:HG23	15	1.6
(1,2443)	1:30:A:VAL:HG23	1:109:A:LEU:HA	18	1.6
(1,2126)	1:7:A:VAL:HG13	1:44:A:PHE:HE1	4	1.6
(1,1737)	1:33:A:ILE:HG13	1:39:A:MET:HE2	7	1.6
(1,855)	1:99:A:VAL:HG23	1:74:A:CYS:HB2	1	1.6
(1,742)	1:72:A:LEU:HD12	1:99:A:VAL:HG13	4	1.6
(1,84)	1:99:A:VAL:HG22	1:91:A:CYS:H	18	1.6
(1,48)	1:7:A:VAL:HG21	1:11:A:ILE:H	17	1.6
(1,2599)	1:28:A:ARG:HG3	1:30:A:VAL:HG22	9	1.59
(1,1854)	1:75:A:LYS:HG2	1:100:A:ILE:HG13	10	1.59
(1,1776)	1:80:A:VAL:HG11	1:73:A:GLU:HG2	1	1.59
(1,1743)	1:90:A:VAL:HG21	1:99:A:VAL:HG23	14	1.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1421)	1:51:A:PHE:HB2	1:7:A:VAL:HG21	7	1.59
(1,811)	1:29:A:VAL:HG21	1:109:A:LEU:HD13	2	1.59
(1,774)	1:66:A:VAL:HG21	1:32:A:GLY:HA3	5	1.59
(1,2616)	1:50:A:THR:HG22	1:47:A:ALA:HB3	1	1.58
(1,2599)	1:28:A:ARG:HG3	1:30:A:VAL:HG21	13	1.58
(1,2466)	1:31:A:VAL:HG22	1:10:A:LEU:HD23	4	1.58
(1,2126)	1:7:A:VAL:HG11	1:44:A:PHE:HE1	12	1.58
(1,1778)	1:112:A:LEU:HD21	1:18:A:ALA:HB2	19	1.58
(1,855)	1:99:A:VAL:HG21	1:74:A:CYS:HB2	16	1.58
(1,812)	1:29:A:VAL:HG23	1:109:A:LEU:HD21	13	1.58
(1,106)	1:29:A:VAL:HG13	1:113:A:GLU:H	4	1.58
(1,2595)	1:110:A:LEU:HD21	1:66:A:VAL:HG13	16	1.57
(1,2595)	1:110:A:LEU:HD22	1:66:A:VAL:HG12	17	1.57
(1,2595)	1:110:A:LEU:HD23	1:66:A:VAL:HG12	20	1.57
(1,1421)	1:51:A:PHE:HB2	1:7:A:VAL:HG22	19	1.57
(1,48)	1:7:A:VAL:HG22	1:11:A:ILE:H	18	1.57
(1,2621)	1:38:A:ALA:HB2	1:105:A:ASN:HB2	11	1.56
(1,2441)	1:31:A:VAL:HG21	1:10:A:LEU:HD21	10	1.56
(1,2126)	1:7:A:VAL:HG13	1:44:A:PHE:HE2	3	1.56
(1,1289)	1:57:A:VAL:HG21	1:15:A:GLU:HG3	13	1.56
(1,943)	1:6:A:VAL:HG12	1:107:A:MET:HG2	18	1.56
(1,2599)	1:28:A:ARG:HG3	1:30:A:VAL:HG21	2	1.55
(1,2591)	1:7:A:VAL:HG12	1:107:A:MET:HE2	19	1.55
(1,1743)	1:90:A:VAL:HG22	1:99:A:VAL:HG22	18	1.55
(1,914)	1:72:A:LEU:HD23	1:70:A:VAL:HG11	18	1.55
(1,811)	1:29:A:VAL:HG22	1:109:A:LEU:HD12	4	1.55
(1,774)	1:66:A:VAL:HG22	1:32:A:GLY:HA3	4	1.55
(1,2616)	1:50:A:THR:HG22	1:47:A:ALA:HB1	16	1.54
(1,2595)	1:110:A:LEU:HD22	1:66:A:VAL:HG12	5	1.54
(1,2595)	1:110:A:LEU:HD21	1:66:A:VAL:HG12	7	1.54
(1,2590)	1:33:A:ILE:HD13	1:39:A:MET:HG3	3	1.54
(1,2441)	1:31:A:VAL:HG23	1:10:A:LEU:HD22	9	1.54
(1,1824)	1:25:A:LYS:HG3	1:56:A:LEU:HD12	7	1.54
(1,1019)	1:102:A:THR:HG22	1:100:A:ILE:HG12	19	1.54
(1,855)	1:99:A:VAL:HG21	1:74:A:CYS:HB2	10	1.54
(1,106)	1:29:A:VAL:HG12	1:113:A:GLU:H	16	1.54
(1,2599)	1:28:A:ARG:HG3	1:30:A:VAL:HG22	16	1.53
(1,2466)	1:31:A:VAL:HG23	1:10:A:LEU:HD22	14	1.53
(1,2144)	1:7:A:VAL:HG23	1:4:A:TYR:HD1	12	1.53
(1,2126)	1:7:A:VAL:HG13	1:44:A:PHE:HE2	11	1.53
(1,1289)	1:57:A:VAL:HG22	1:15:A:GLU:HG3	20	1.53
(1,855)	1:99:A:VAL:HG21	1:74:A:CYS:HB2	6	1.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,730)	1:33:A:ILE:HD13	1:45:A:VAL:HG13	5	1.53
(1,106)	1:29:A:VAL:HG12	1:113:A:GLU:H	9	1.53
(1,48)	1:7:A:VAL:HG23	1:11:A:ILE:H	5	1.53
(1,40)	1:99:A:VAL:HG13	1:89:A:GLY:H	1	1.53
(1,40)	1:99:A:VAL:HG13	1:89:A:GLY:H	4	1.53
(1,2595)	1:110:A:LEU:HD23	1:66:A:VAL:HG13	3	1.52
(1,2595)	1:110:A:LEU:HD22	1:66:A:VAL:HG12	18	1.52
(1,1776)	1:80:A:VAL:HG13	1:73:A:GLU:HG2	4	1.52
(1,774)	1:66:A:VAL:HG23	1:32:A:GLY:HA3	7	1.52
(1,2126)	1:7:A:VAL:HG11	1:44:A:PHE:HE1	2	1.51
(1,1776)	1:80:A:VAL:HG12	1:73:A:GLU:HG2	10	1.51
(1,1743)	1:90:A:VAL:HG23	1:99:A:VAL:HG21	20	1.51
(1,1289)	1:57:A:VAL:HG23	1:15:A:GLU:HG3	14	1.51
(1,854)	1:101:A:ILE:HG13	1:70:A:VAL:HG22	2	1.51
(1,106)	1:29:A:VAL:HG13	1:113:A:GLU:H	11	1.51
(1,48)	1:7:A:VAL:HG22	1:11:A:ILE:H	16	1.51
(1,2599)	1:28:A:ARG:HG3	1:30:A:VAL:HG22	1	1.5
(1,2443)	1:30:A:VAL:HG22	1:109:A:LEU:HA	3	1.5
(1,2441)	1:31:A:VAL:HG21	1:10:A:LEU:HD21	16	1.5
(1,1776)	1:80:A:VAL:HG11	1:73:A:GLU:HG2	13	1.5
(1,854)	1:101:A:ILE:HG13	1:70:A:VAL:HG23	11	1.5
(1,811)	1:29:A:VAL:HG21	1:109:A:LEU:HD11	6	1.5
(1,48)	1:7:A:VAL:HG21	1:11:A:ILE:H	13	1.5
(1,2443)	1:30:A:VAL:HG23	1:109:A:LEU:HA	17	1.49
(1,2152)	1:99:A:VAL:HG23	1:81:A:PHE:HZ	7	1.49
(1,1805)	1:10:A:LEU:HD13	1:63:A:LEU:HD21	8	1.49
(1,1737)	1:33:A:ILE:HG13	1:39:A:MET:HE1	15	1.49
(1,851)	1:101:A:ILE:HD12	1:105:A:ASN:HB3	14	1.49
(1,48)	1:7:A:VAL:HG21	1:11:A:ILE:H	6	1.49
(1,2621)	1:18:A:ALA:HB1	1:21:A:ASN:HB2	19	1.48
(1,2616)	1:50:A:THR:HG22	1:47:A:ALA:HB3	14	1.48
(1,2599)	1:28:A:ARG:HG3	1:30:A:VAL:HG23	10	1.48
(1,2420)	1:101:A:ILE:HD11	1:102:A:THR:H	20	1.48
(1,2126)	1:7:A:VAL:HG12	1:44:A:PHE:HE1	13	1.48
(1,1779)	1:31:A:VAL:HG12	1:33:A:ILE:HG12	17	1.48
(1,106)	1:29:A:VAL:HG12	1:113:A:GLU:H	14	1.48
(1,48)	1:7:A:VAL:HG21	1:11:A:ILE:H	4	1.48
(1,40)	1:99:A:VAL:HG12	1:89:A:GLY:H	12	1.48
(1,2616)	1:50:A:THR:HG22	1:47:A:ALA:HB1	8	1.47
(1,2616)	1:50:A:THR:HG23	1:47:A:ALA:HB1	18	1.47
(1,2443)	1:30:A:VAL:HG22	1:109:A:LEU:HA	14	1.47
(1,2441)	1:31:A:VAL:HG22	1:10:A:LEU:HD23	4	1.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2134)	1:72:A:LEU:HD23	1:81:A:PHE:HE1	14	1.47
(1,811)	1:29:A:VAL:HG22	1:109:A:LEU:HD11	11	1.47
(1,769)	1:72:A:LEU:HD22	1:70:A:VAL:HG23	13	1.47
(1,2621)	1:18:A:ALA:HB3	1:21:A:ASN:HB2	12	1.46
(1,2616)	1:50:A:THR:HG21	1:47:A:ALA:HB2	2	1.46
(1,2599)	1:28:A:ARG:HG3	1:30:A:VAL:HG21	17	1.46
(1,2144)	1:7:A:VAL:HG23	1:4:A:TYR:HD1	8	1.46
(1,1840)	1:75:A:LYS:HG3	1:100:A:ILE:HG13	17	1.46
(1,1743)	1:90:A:VAL:HG21	1:99:A:VAL:HG23	7	1.46
(1,1743)	1:90:A:VAL:HG21	1:99:A:VAL:HG23	19	1.46
(1,1019)	1:102:A:THR:HG22	1:100:A:ILE:HG12	16	1.46
(1,2616)	1:50:A:THR:HG21	1:47:A:ALA:HB2	17	1.45
(1,1421)	1:51:A:PHE:HB2	1:7:A:VAL:HG23	17	1.45
(1,854)	1:101:A:ILE:HG13	1:70:A:VAL:HG21	7	1.45
(1,84)	1:99:A:VAL:HG21	1:91:A:CYS:H	17	1.45
(1,2599)	1:28:A:ARG:HG3	1:30:A:VAL:HG23	19	1.44
(1,1803)	1:10:A:LEU:HD13	1:109:A:LEU:HB2	6	1.44
(1,106)	1:29:A:VAL:HG11	1:113:A:GLU:H	20	1.44
(1,2616)	1:50:A:THR:HG23	1:47:A:ALA:HB2	10	1.43
(1,2144)	1:7:A:VAL:HG23	1:4:A:TYR:HD1	17	1.43
(1,1737)	1:33:A:ILE:HG13	1:39:A:MET:HE1	11	1.43
(1,1421)	1:51:A:PHE:HB2	1:7:A:VAL:HG21	5	1.43
(1,742)	1:72:A:LEU:HD12	1:99:A:VAL:HG12	12	1.43
(1,730)	1:33:A:ILE:HD12	1:45:A:VAL:HG13	7	1.43
(1,48)	1:7:A:VAL:HG21	1:11:A:ILE:H	20	1.43
(1,2616)	1:50:A:THR:HG21	1:47:A:ALA:HB2	5	1.42
(1,2441)	1:31:A:VAL:HG23	1:10:A:LEU:HD22	14	1.42
(1,2144)	1:7:A:VAL:HG21	1:4:A:TYR:HD2	5	1.42
(1,1805)	1:10:A:LEU:HD13	1:63:A:LEU:HD22	7	1.42
(1,1779)	1:31:A:VAL:HG13	1:33:A:ILE:HG12	14	1.42
(1,1779)	1:31:A:VAL:HG13	1:33:A:ILE:HG12	18	1.42
(1,1019)	1:102:A:THR:HG22	1:100:A:ILE:HG12	8	1.42
(1,854)	1:101:A:ILE:HG13	1:70:A:VAL:HG21	4	1.42
(1,854)	1:101:A:ILE:HG13	1:70:A:VAL:HG21	6	1.42
(1,2633)	1:115:A:LEU:HD23	1:27:A:GLU:HB3	10	1.41
(1,2443)	1:30:A:VAL:HG22	1:109:A:LEU:HA	6	1.41
(1,2126)	1:7:A:VAL:HG13	1:44:A:PHE:HE1	5	1.41
(1,2126)	1:7:A:VAL:HG13	1:44:A:PHE:HE2	10	1.41
(1,1776)	1:80:A:VAL:HG13	1:73:A:GLU:HG2	2	1.41
(1,1418)	1:91:A:CYS:HB2	1:99:A:VAL:HG23	7	1.41
(1,854)	1:101:A:ILE:HG13	1:70:A:VAL:HG22	20	1.41
(1,774)	1:66:A:VAL:HG21	1:32:A:GLY:HA3	18	1.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,48)	1:7:A:VAL:HG22	1:11:A:ILE:H	3	1.41
(1,2633)	1:115:A:LEU:HD13	1:27:A:GLU:HB3	13	1.4
(1,1289)	1:57:A:VAL:HG21	1:15:A:GLU:HG3	15	1.4
(1,943)	1:6:A:VAL:HG12	1:107:A:MET:HG2	3	1.4
(1,774)	1:66:A:VAL:HG23	1:32:A:GLY:HA3	2	1.4
(1,742)	1:72:A:LEU:HD11	1:99:A:VAL:HG11	11	1.4
(1,742)	1:72:A:LEU:HD12	1:99:A:VAL:HG12	16	1.4
(1,106)	1:29:A:VAL:HG11	1:113:A:GLU:H	3	1.4
(1,2616)	1:50:A:THR:HG21	1:47:A:ALA:HB3	11	1.39
(1,1805)	1:10:A:LEU:HD11	1:63:A:LEU:HD21	3	1.39
(1,1782)	1:109:A:LEU:HD22	1:107:A:MET:HE1	4	1.39
(1,827)	1:101:A:ILE:HG21	1:102:A:THR:HG21	15	1.39
(1,14)	1:7:A:VAL:HG11	1:7:A:VAL:H	9	1.39
(1,2616)	1:50:A:THR:HG22	1:47:A:ALA:HB2	3	1.38
(1,2616)	1:50:A:THR:HG23	1:47:A:ALA:HB1	20	1.38
(1,2466)	1:31:A:VAL:HG22	1:10:A:LEU:HD21	2	1.38
(1,1779)	1:31:A:VAL:HG12	1:33:A:ILE:HG12	20	1.38
(1,1538)	1:99:A:VAL:HG23	1:91:A:CYS:HA	7	1.38
(1,1421)	1:51:A:PHE:HB2	1:7:A:VAL:HG23	2	1.38
(1,1421)	1:51:A:PHE:HB2	1:7:A:VAL:HG23	14	1.38
(1,730)	1:33:A:ILE:HD12	1:45:A:VAL:HG13	4	1.38
(1,48)	1:7:A:VAL:HG23	1:11:A:ILE:H	1	1.38
(1,48)	1:7:A:VAL:HG22	1:11:A:ILE:H	2	1.38
(1,1960)	1:113:A:GLU:HG3	1:27:A:GLU:HB3	1	1.37
(1,1776)	1:80:A:VAL:HG12	1:73:A:GLU:HG2	9	1.37
(1,1737)	1:33:A:ILE:HG13	1:39:A:MET:HE1	5	1.37
(1,849)	1:72:A:LEU:HD22	1:101:A:ILE:HG13	13	1.37
(1,827)	1:101:A:ILE:HG23	1:102:A:THR:HG22	20	1.37
(1,774)	1:66:A:VAL:HG21	1:32:A:GLY:HA3	13	1.37
(1,742)	1:72:A:LEU:HD12	1:99:A:VAL:HG12	17	1.37
(1,106)	1:29:A:VAL:HG12	1:113:A:GLU:H	5	1.37
(1,14)	1:7:A:VAL:HG13	1:7:A:VAL:H	19	1.37
(1,2616)	1:50:A:THR:HG21	1:47:A:ALA:HB3	15	1.36
(1,2599)	1:28:A:ARG:HG3	1:30:A:VAL:HG23	14	1.36
(1,2443)	1:30:A:VAL:HG23	1:109:A:LEU:HA	12	1.36
(1,2126)	1:7:A:VAL:HG12	1:44:A:PHE:HE1	20	1.36
(1,1782)	1:109:A:LEU:HD22	1:107:A:MET:HE2	9	1.36
(1,1421)	1:51:A:PHE:HB2	1:7:A:VAL:HG22	4	1.36
(1,1421)	1:51:A:PHE:HB2	1:7:A:VAL:HG23	15	1.36
(1,1289)	1:57:A:VAL:HG23	1:15:A:GLU:HG3	5	1.36
(1,774)	1:66:A:VAL:HG21	1:32:A:GLY:HA3	6	1.36
(1,774)	1:66:A:VAL:HG22	1:32:A:GLY:HA3	9	1.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,742)	1:72:A:LEU:HD11	1:99:A:VAL:HG13	10	1.36
(1,730)	1:33:A:ILE:HD13	1:45:A:VAL:HG11	2	1.36
(1,730)	1:33:A:ILE:HD12	1:45:A:VAL:HG12	16	1.36
(1,38)	1:99:A:VAL:HG13	1:90:A:VAL:H	4	1.36
(1,14)	1:7:A:VAL:HG12	1:7:A:VAL:H	2	1.36
(1,14)	1:7:A:VAL:HG13	1:7:A:VAL:H	13	1.36
(1,2127)	1:7:A:VAL:HG13	1:4:A:TYR:HD1	12	1.35
(1,2126)	1:7:A:VAL:HG12	1:44:A:PHE:HE1	7	1.35
(1,2016)	1:93:A:LYS:HD2	1:79:A:HIS:HB2	13	1.35
(1,1864)	1:9:A:SER:HB2	1:12:A:ALA:HB2	20	1.35
(1,1824)	1:25:A:LYS:HG3	1:56:A:LEU:HD13	2	1.35
(1,1538)	1:99:A:VAL:HG23	1:91:A:CYS:HA	14	1.35
(1,1421)	1:51:A:PHE:HB2	1:7:A:VAL:HG21	1	1.35
(1,827)	1:101:A:ILE:HG21	1:102:A:THR:HG21	18	1.35
(1,730)	1:33:A:ILE:HD13	1:45:A:VAL:HG11	20	1.35
(1,40)	1:99:A:VAL:HG11	1:89:A:GLY:H	6	1.35
(1,17)	1:72:A:LEU:HD23	1:101:A:ILE:H	13	1.35
(1,14)	1:7:A:VAL:HG12	1:7:A:VAL:H	16	1.35
(1,14)	1:7:A:VAL:HG13	1:7:A:VAL:H	18	1.35
(1,14)	1:7:A:VAL:HG13	1:7:A:VAL:H	20	1.35
(1,2633)	1:115:A:LEU:HD21	1:27:A:GLU:HB3	18	1.34
(1,2595)	1:110:A:LEU:HD21	1:66:A:VAL:HG11	6	1.34
(1,2576)	1:66:A:VAL:HA	1:110:A:LEU:HD11	3	1.34
(1,2576)	1:66:A:VAL:HA	1:110:A:LEU:HD13	19	1.34
(1,2443)	1:30:A:VAL:HG22	1:109:A:LEU:HA	7	1.34
(1,2443)	1:30:A:VAL:HG22	1:109:A:LEU:HA	15	1.34
(1,2420)	1:101:A:ILE:HD13	1:102:A:THR:H	12	1.34
(1,2420)	1:101:A:ILE:HD11	1:102:A:THR:H	15	1.34
(1,1988)	1:40:A:ASP:HB2	1:43:A:LEU:HB3	14	1.34
(1,1776)	1:80:A:VAL:HG13	1:73:A:GLU:HG2	8	1.34
(1,851)	1:101:A:ILE:HD11	1:105:A:ASN:HB3	12	1.34
(1,14)	1:7:A:VAL:HG11	1:7:A:VAL:H	11	1.34
(1,2654)	1:6:A:VAL:HA	1:39:A:MET:HE1	18	1.33
(1,2616)	1:50:A:THR:HG21	1:47:A:ALA:HB3	4	1.33
(1,2134)	1:72:A:LEU:HD22	1:81:A:PHE:HE2	7	1.33
(1,2126)	1:7:A:VAL:HG13	1:44:A:PHE:HE1	9	1.33
(1,2126)	1:7:A:VAL:HG11	1:44:A:PHE:HE1	18	1.33
(1,1988)	1:40:A:ASP:HB2	1:43:A:LEU:HB3	4	1.33
(1,1782)	1:109:A:LEU:HD21	1:107:A:MET:HE1	2	1.33
(1,1743)	1:90:A:VAL:HG21	1:99:A:VAL:HG22	2	1.33
(1,1743)	1:90:A:VAL:HG22	1:99:A:VAL:HG21	5	1.33
(1,1289)	1:57:A:VAL:HG23	1:15:A:GLU:HG3	12	1.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,827)	1:101:A:ILE:HG22	1:102:A:THR:HG21	4	1.33
(1,730)	1:33:A:ILE:HD11	1:45:A:VAL:HG13	15	1.33
(1,106)	1:29:A:VAL:HG12	1:113:A:GLU:H	12	1.33
(1,106)	1:29:A:VAL:HG12	1:113:A:GLU:H	17	1.33
(1,106)	1:29:A:VAL:HG11	1:113:A:GLU:H	19	1.33
(1,14)	1:7:A:VAL:HG12	1:7:A:VAL:H	1	1.33
(1,14)	1:7:A:VAL:HG11	1:7:A:VAL:H	14	1.33
(1,2678)	1:39:A:MET:HE2	1:44:A:PHE:HZ	9	1.32
(1,2420)	1:101:A:ILE:HD13	1:102:A:THR:H	1	1.32
(1,2153)	1:99:A:VAL:HG21	1:81:A:PHE:HE1	20	1.32
(1,2126)	1:7:A:VAL:HG12	1:44:A:PHE:HE1	19	1.32
(1,1988)	1:40:A:ASP:HB2	1:43:A:LEU:HB3	13	1.32
(1,1864)	1:9:A:SER:HB2	1:12:A:ALA:HB3	13	1.32
(1,1776)	1:80:A:VAL:HG13	1:73:A:GLU:HG2	11	1.32
(1,1432)	1:99:A:VAL:HG21	1:74:A:CYS:HB3	17	1.32
(1,1289)	1:57:A:VAL:HG22	1:15:A:GLU:HG3	1	1.32
(1,1289)	1:57:A:VAL:HG23	1:15:A:GLU:HG3	19	1.32
(1,1265)	1:102:A:THR:HG22	1:73:A:GLU:HG2	19	1.32
(1,854)	1:101:A:ILE:HG13	1:70:A:VAL:HG22	1	1.32
(1,788)	1:65:A:ILE:HD13	1:45:A:VAL:HG23	9	1.32
(1,106)	1:29:A:VAL:HG13	1:113:A:GLU:H	6	1.32
(1,14)	1:7:A:VAL:HG11	1:7:A:VAL:H	4	1.32
(1,14)	1:7:A:VAL:HG11	1:7:A:VAL:H	7	1.32
(1,2633)	1:115:A:LEU:HD22	1:27:A:GLU:HB3	20	1.31
(1,2576)	1:66:A:VAL:HA	1:110:A:LEU:HD13	20	1.31
(1,2443)	1:30:A:VAL:HG21	1:109:A:LEU:HA	9	1.31
(1,1782)	1:109:A:LEU:HD21	1:107:A:MET:HE3	13	1.31
(1,1776)	1:80:A:VAL:HG11	1:73:A:GLU:HG2	5	1.31
(1,1776)	1:80:A:VAL:HG11	1:73:A:GLU:HG2	19	1.31
(1,851)	1:101:A:ILE:HD11	1:105:A:ASN:HB3	11	1.31
(1,827)	1:101:A:ILE:HG21	1:102:A:THR:HG21	2	1.31
(1,14)	1:7:A:VAL:HG12	1:7:A:VAL:H	6	1.31
(1,14)	1:7:A:VAL:HG13	1:7:A:VAL:H	17	1.31
(1,2672)	1:70:A:VAL:HG12	1:88:A:TYR:HD2	18	1.3
(1,2443)	1:30:A:VAL:HG21	1:109:A:LEU:HA	1	1.3
(1,2443)	1:30:A:VAL:HG23	1:109:A:LEU:HA	20	1.3
(1,2420)	1:100:A:ILE:HD13	1:102:A:THR:H	7	1.3
(1,2152)	1:99:A:VAL:HG21	1:81:A:PHE:HZ	20	1.3
(1,1823)	1:45:A:VAL:HG11	1:41:A:LYS:HE2	18	1.3
(1,1782)	1:109:A:LEU:HD23	1:107:A:MET:HE3	14	1.3
(1,1743)	1:90:A:VAL:HG22	1:99:A:VAL:HG21	9	1.3
(1,1421)	1:51:A:PHE:HB2	1:7:A:VAL:HG23	3	1.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1265)	1:102:A:THR:HG23	1:73:A:GLU:HG2	2	1.3
(1,106)	1:29:A:VAL:HG11	1:113:A:GLU:H	15	1.3
(1,84)	1:99:A:VAL:HG23	1:91:A:CYS:H	7	1.3
(1,38)	1:99:A:VAL:HG12	1:90:A:VAL:H	1	1.3
(1,14)	1:7:A:VAL:HG11	1:7:A:VAL:H	5	1.3
(1,14)	1:7:A:VAL:HG12	1:7:A:VAL:H	12	1.3
(1,2616)	1:50:A:THR:HG22	1:47:A:ALA:HB1	9	1.29
(1,2599)	1:28:A:ARG:HG3	1:30:A:VAL:HG23	4	1.29
(1,2126)	1:7:A:VAL:HG11	1:44:A:PHE:HE1	17	1.29
(1,1854)	1:75:A:LYS:HG2	1:100:A:ILE:HG13	17	1.29
(1,1743)	1:90:A:VAL:HG23	1:99:A:VAL:HG22	8	1.29
(1,1421)	1:51:A:PHE:HB2	1:7:A:VAL:HG21	9	1.29
(1,1019)	1:102:A:THR:HG22	1:100:A:ILE:HG12	18	1.29
(1,827)	1:101:A:ILE:HG23	1:102:A:THR:HG21	6	1.29
(1,827)	1:101:A:ILE:HG21	1:102:A:THR:HG23	9	1.29
(1,822)	1:80:A:VAL:HG12	1:102:A:THR:HG21	10	1.29
(1,742)	1:72:A:LEU:HD11	1:99:A:VAL:HG11	6	1.29
(1,730)	1:33:A:ILE:HD13	1:45:A:VAL:HG13	14	1.29
(1,40)	1:99:A:VAL:HG13	1:89:A:GLY:H	10	1.29
(1,14)	1:7:A:VAL:HG12	1:7:A:VAL:H	10	1.29
(1,14)	1:7:A:VAL:HG13	1:7:A:VAL:H	15	1.29
(1,2621)	1:18:A:ALA:HB1	1:21:A:ASN:HB2	5	1.28
(1,2420)	1:101:A:ILE:HD13	1:102:A:THR:H	8	1.28
(1,2144)	1:7:A:VAL:HG21	1:4:A:TYR:HD1	11	1.28
(1,1870)	1:20:A:LYS:HG2	1:16:A:GLU:HG3	7	1.28
(1,1743)	1:90:A:VAL:HG23	1:99:A:VAL:HG21	10	1.28
(1,1743)	1:90:A:VAL:HG23	1:99:A:VAL:HG21	17	1.28
(1,811)	1:29:A:VAL:HG23	1:109:A:LEU:HD13	13	1.28
(1,788)	1:65:A:ILE:HD11	1:45:A:VAL:HG23	14	1.28
(1,774)	1:66:A:VAL:HG23	1:32:A:GLY:HA3	11	1.28
(1,14)	1:7:A:VAL:HG11	1:7:A:VAL:H	3	1.28
(1,2633)	1:115:A:LEU:HD23	1:27:A:GLU:HB3	1	1.27
(1,2590)	1:33:A:ILE:HD11	1:39:A:MET:HG2	6	1.27
(1,2576)	1:66:A:VAL:HA	1:110:A:LEU:HD13	16	1.27
(1,1887)	1:82:A:LYS:HD3	1:71:A:GLU:HB3	19	1.27
(1,1823)	1:45:A:VAL:HG12	1:41:A:LYS:HE2	8	1.27
(1,1805)	1:10:A:LEU:HD11	1:63:A:LEU:HD23	15	1.27
(1,1803)	1:10:A:LEU:HD11	1:109:A:LEU:HB2	19	1.27
(1,1289)	1:57:A:VAL:HG22	1:15:A:GLU:HG3	2	1.27
(1,1289)	1:57:A:VAL:HG21	1:15:A:GLU:HG3	4	1.27
(1,1289)	1:57:A:VAL:HG22	1:15:A:GLU:HG3	16	1.27
(1,914)	1:72:A:LEU:HD21	1:70:A:VAL:HG13	1	1.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,851)	1:101:A:ILE:HD12	1:105:A:ASN:HB3	7	1.27
(1,827)	1:101:A:ILE:HG21	1:102:A:THR:HG23	1	1.27
(1,827)	1:101:A:ILE:HG21	1:102:A:THR:HG21	10	1.27
(1,788)	1:65:A:ILE:HD11	1:45:A:VAL:HG22	19	1.27
(1,730)	1:33:A:ILE:HD11	1:45:A:VAL:HG11	13	1.27
(1,14)	1:7:A:VAL:HG12	1:7:A:VAL:H	8	1.27
(1,2441)	1:31:A:VAL:HG22	1:10:A:LEU:HD21	2	1.26
(1,2420)	1:100:A:ILE:HD13	1:102:A:THR:H	16	1.26
(1,2126)	1:7:A:VAL:HG11	1:44:A:PHE:HE1	16	1.26
(1,1779)	1:31:A:VAL:HG13	1:33:A:ILE:HG12	9	1.26
(1,1778)	1:112:A:LEU:HD21	1:18:A:ALA:HB2	11	1.26
(1,1776)	1:80:A:VAL:HG13	1:73:A:GLU:HG2	16	1.26
(1,1737)	1:33:A:ILE:HG13	1:39:A:MET:HE3	13	1.26
(1,1421)	1:51:A:PHE:HB2	1:7:A:VAL:HG22	13	1.26
(1,1418)	1:91:A:CYS:HB2	1:99:A:VAL:HG21	5	1.26
(1,1418)	1:91:A:CYS:HB2	1:99:A:VAL:HG23	14	1.26
(1,851)	1:101:A:ILE:HD11	1:105:A:ASN:HB3	6	1.26
(1,48)	1:7:A:VAL:HG22	1:11:A:ILE:H	12	1.26
(1,2672)	1:70:A:VAL:HG11	1:88:A:TYR:HD1	8	1.25
(1,2621)	1:18:A:ALA:HB1	1:21:A:ASN:HB2	6	1.25
(1,2576)	1:66:A:VAL:HA	1:110:A:LEU:HD12	4	1.25
(1,1779)	1:31:A:VAL:HG11	1:33:A:ILE:HG12	8	1.25
(1,1743)	1:90:A:VAL:HG22	1:99:A:VAL:HG22	11	1.25
(1,1743)	1:90:A:VAL:HG22	1:99:A:VAL:HG21	15	1.25
(1,1418)	1:91:A:CYS:HB2	1:99:A:VAL:HG21	15	1.25
(1,943)	1:6:A:VAL:HG11	1:107:A:MET:HG2	8	1.25
(1,2590)	1:33:A:ILE:HD12	1:39:A:MET:HG2	18	1.24
(1,2129)	1:72:A:LEU:HD11	1:81:A:PHE:HZ	13	1.24
(1,1803)	1:10:A:LEU:HD13	1:109:A:LEU:HB2	17	1.24
(1,1779)	1:31:A:VAL:HG13	1:33:A:ILE:HG12	12	1.24
(1,1743)	1:90:A:VAL:HG22	1:99:A:VAL:HG21	3	1.24
(1,1737)	1:33:A:ILE:HG13	1:39:A:MET:HE2	20	1.24
(1,1538)	1:99:A:VAL:HG21	1:91:A:CYS:HA	20	1.24
(1,1265)	1:102:A:THR:HG22	1:73:A:GLU:HG2	1	1.24
(1,106)	1:29:A:VAL:HG11	1:113:A:GLU:H	7	1.24
(1,2420)	1:100:A:ILE:HD12	1:102:A:THR:H	19	1.23
(1,2144)	1:7:A:VAL:HG23	1:4:A:TYR:HD1	3	1.23
(1,1870)	1:20:A:LYS:HG2	1:16:A:GLU:HG3	17	1.23
(1,1779)	1:31:A:VAL:HG11	1:33:A:ILE:HG12	1	1.23
(1,1778)	1:112:A:LEU:HD23	1:18:A:ALA:HB2	10	1.23
(1,1421)	1:51:A:PHE:HB2	1:7:A:VAL:HG23	16	1.23
(1,1418)	1:91:A:CYS:HB2	1:99:A:VAL:HG21	20	1.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,827)	1:101:A:ILE:HG22	1:102:A:THR:HG21	7	1.23
(1,827)	1:101:A:ILE:HG23	1:102:A:THR:HG22	19	1.23
(1,788)	1:65:A:ILE:HD13	1:45:A:VAL:HG23	20	1.23
(1,2672)	1:10:A:LEU:HD12	1:48:A:PHE:HD1	5	1.22
(1,2654)	1:6:A:VAL:HA	1:39:A:MET:HE3	3	1.22
(1,2612)	1:25:A:LYS:HE2	1:56:A:LEU:HD13	13	1.22
(1,2590)	1:33:A:ILE:HD11	1:39:A:MET:HG2	9	1.22
(1,2576)	1:66:A:VAL:HA	1:110:A:LEU:HD12	9	1.22
(1,2576)	1:66:A:VAL:HA	1:110:A:LEU:HD12	15	1.22
(1,2443)	1:30:A:VAL:HG22	1:109:A:LEU:HA	4	1.22
(1,2443)	1:30:A:VAL:HG21	1:109:A:LEU:HA	5	1.22
(1,1769)	1:66:A:VAL:HG11	1:68:A:GLU:HB2	5	1.22
(1,1421)	1:51:A:PHE:HB2	1:7:A:VAL:HG23	8	1.22
(1,1363)	1:23:A:ALA:HB1	1:114:A:MET:HG2	5	1.22
(1,1289)	1:57:A:VAL:HG21	1:15:A:GLU:HG3	6	1.22
(1,1019)	1:102:A:THR:HG21	1:100:A:ILE:HG12	2	1.22
(1,1019)	1:102:A:THR:HG21	1:100:A:ILE:HG12	5	1.22
(1,1019)	1:102:A:THR:HG22	1:100:A:ILE:HG12	6	1.22
(1,943)	1:6:A:VAL:HG11	1:107:A:MET:HG2	1	1.22
(1,862)	1:109:A:LEU:HD23	1:13:A:LEU:HD22	14	1.22
(1,788)	1:65:A:ILE:HD12	1:45:A:VAL:HG23	1	1.22
(1,788)	1:65:A:ILE:HD13	1:45:A:VAL:HG22	7	1.22
(1,742)	1:72:A:LEU:HD11	1:99:A:VAL:HG12	19	1.22
(1,2643)	1:39:A:MET:HE3	1:106:A:GLU:HG2	4	1.21
(1,2595)	1:110:A:LEU:HD21	1:66:A:VAL:HG13	1	1.21
(1,2576)	1:66:A:VAL:HA	1:110:A:LEU:HD13	2	1.21
(1,2420)	1:100:A:ILE:HD12	1:102:A:THR:H	3	1.21
(1,2127)	1:7:A:VAL:HG12	1:4:A:TYR:HD1	17	1.21
(1,1936)	1:114:A:MET:HE1	1:114:A:MET:HB3	2	1.21
(1,1782)	1:109:A:LEU:HD22	1:107:A:MET:HE3	12	1.21
(1,914)	1:72:A:LEU:HD21	1:70:A:VAL:HG12	19	1.21
(1,854)	1:101:A:ILE:HG13	1:70:A:VAL:HG22	14	1.21
(1,774)	1:66:A:VAL:HG23	1:32:A:GLY:HA3	15	1.21
(1,730)	1:33:A:ILE:HD12	1:45:A:VAL:HG12	10	1.21
(1,2595)	1:110:A:LEU:HD23	1:66:A:VAL:HG13	12	1.2
(1,2590)	1:33:A:ILE:HD11	1:39:A:MET:HG2	8	1.2
(1,2576)	1:66:A:VAL:HA	1:110:A:LEU:HD11	11	1.2
(1,2443)	1:30:A:VAL:HG21	1:109:A:LEU:HA	16	1.2
(1,2420)	1:100:A:ILE:HD13	1:102:A:THR:H	6	1.2
(1,2420)	1:100:A:ILE:HD12	1:102:A:THR:H	11	1.2
(1,2144)	1:7:A:VAL:HG23	1:4:A:TYR:HD2	14	1.2
(1,1893)	1:110:A:LEU:HD22	1:108:A:ARG:HB3	16	1.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1824)	1:25:A:LYS:HG3	1:56:A:LEU:HD13	20	1.2
(1,1823)	1:45:A:VAL:HG13	1:41:A:LYS:HE2	5	1.2
(1,1782)	1:109:A:LEU:HD23	1:107:A:MET:HE3	20	1.2
(1,1743)	1:90:A:VAL:HG23	1:99:A:VAL:HG21	16	1.2
(1,914)	1:72:A:LEU:HD22	1:70:A:VAL:HG13	15	1.2
(1,827)	1:101:A:ILE:HG21	1:102:A:THR:HG21	5	1.2
(1,827)	1:101:A:ILE:HG23	1:102:A:THR:HG21	14	1.2
(1,774)	1:66:A:VAL:HG21	1:32:A:GLY:HA3	10	1.2
(1,48)	1:7:A:VAL:HG22	1:11:A:ILE:H	8	1.2
(1,2654)	1:6:A:VAL:HA	1:107:A:MET:HE2	8	1.19
(1,2633)	1:115:A:LEU:HD21	1:27:A:GLU:HB3	2	1.19
(1,2126)	1:7:A:VAL:HG13	1:44:A:PHE:HE1	6	1.19
(1,1960)	1:113:A:GLU:HG3	1:27:A:GLU:HB3	10	1.19
(1,1743)	1:90:A:VAL:HG22	1:99:A:VAL:HG23	12	1.19
(1,1732)	1:72:A:LEU:HD12	1:89:A:GLY:HA3	17	1.19
(1,1418)	1:91:A:CYS:HB2	1:99:A:VAL:HG22	8	1.19
(1,1418)	1:91:A:CYS:HB2	1:99:A:VAL:HG23	19	1.19
(1,1289)	1:57:A:VAL:HG21	1:15:A:GLU:HG3	3	1.19
(1,827)	1:101:A:ILE:HG21	1:102:A:THR:HG23	17	1.19
(1,2672)	1:70:A:VAL:HG12	1:88:A:TYR:HD2	14	1.18
(1,2595)	1:110:A:LEU:HD21	1:66:A:VAL:HG12	8	1.18
(1,2576)	1:66:A:VAL:HA	1:110:A:LEU:HD13	1	1.18
(1,2576)	1:66:A:VAL:HA	1:110:A:LEU:HD12	7	1.18
(1,2443)	1:30:A:VAL:HG22	1:109:A:LEU:HA	8	1.18
(1,1870)	1:20:A:LYS:HG2	1:16:A:GLU:HG3	8	1.18
(1,1779)	1:31:A:VAL:HG11	1:33:A:ILE:HG12	13	1.18
(1,1778)	1:112:A:LEU:HD22	1:18:A:ALA:HB2	4	1.18
(1,1421)	1:51:A:PHE:HB2	1:7:A:VAL:HG21	11	1.18
(1,1418)	1:91:A:CYS:HB2	1:99:A:VAL:HG22	11	1.18
(1,1289)	1:57:A:VAL:HG22	1:15:A:GLU:HG3	9	1.18
(1,827)	1:101:A:ILE:HG21	1:102:A:THR:HG21	16	1.18
(1,788)	1:65:A:ILE:HD11	1:45:A:VAL:HG21	10	1.18
(1,774)	1:66:A:VAL:HG23	1:32:A:GLY:HA3	16	1.18
(1,730)	1:33:A:ILE:HD13	1:45:A:VAL:HG12	11	1.18
(1,730)	1:33:A:ILE:HD13	1:45:A:VAL:HG12	12	1.18
(1,730)	1:33:A:ILE:HD11	1:45:A:VAL:HG13	17	1.18
(1,2633)	1:115:A:LEU:HD21	1:27:A:GLU:HB3	14	1.17
(1,2621)	1:18:A:ALA:HB2	1:21:A:ASN:HB2	20	1.17
(1,2563)	1:45:A:VAL:HA	1:63:A:LEU:HD22	9	1.17
(1,1778)	1:112:A:LEU:HD21	1:18:A:ALA:HB2	12	1.17
(1,1443)	1:30:A:VAL:HG12	1:28:A:ARG:HD2	5	1.17
(1,1363)	1:23:A:ALA:HB2	1:114:A:MET:HG2	12	1.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1265)	1:102:A:THR:HG23	1:73:A:GLU:HG2	5	1.17
(1,1265)	1:102:A:THR:HG21	1:73:A:GLU:HG2	18	1.17
(1,851)	1:101:A:ILE:HD12	1:105:A:ASN:HB3	13	1.17
(1,827)	1:101:A:ILE:HG23	1:102:A:THR:HG22	8	1.17
(1,730)	1:33:A:ILE:HD13	1:45:A:VAL:HG12	8	1.17
(1,40)	1:99:A:VAL:HG12	1:89:A:GLY:H	5	1.17
(1,2633)	1:115:A:LEU:HD22	1:27:A:GLU:HB3	19	1.16
(1,2576)	1:66:A:VAL:HA	1:110:A:LEU:HD12	17	1.16
(1,2443)	1:30:A:VAL:HG23	1:109:A:LEU:HA	2	1.16
(1,2443)	1:30:A:VAL:HG22	1:109:A:LEU:HA	19	1.16
(1,1823)	1:45:A:VAL:HG13	1:41:A:LYS:HE2	17	1.16
(1,1743)	1:90:A:VAL:HG23	1:99:A:VAL:HG21	4	1.16
(1,1418)	1:91:A:CYS:HB2	1:99:A:VAL:HG23	12	1.16
(1,827)	1:101:A:ILE:HG21	1:102:A:THR:HG23	3	1.16
(1,84)	1:99:A:VAL:HG21	1:91:A:CYS:H	20	1.16
(1,38)	1:99:A:VAL:HG11	1:90:A:VAL:H	5	1.16
(1,2621)	1:18:A:ALA:HB3	1:21:A:ASN:HB2	2	1.15
(1,2576)	1:66:A:VAL:HA	1:110:A:LEU:HD12	10	1.15
(1,2563)	1:45:A:VAL:HA	1:63:A:LEU:HD23	2	1.15
(1,2563)	1:45:A:VAL:HA	1:63:A:LEU:HD21	19	1.15
(1,2420)	1:100:A:ILE:HD13	1:102:A:THR:H	4	1.15
(1,2144)	1:7:A:VAL:HG22	1:4:A:TYR:HD2	19	1.15
(1,2088)	1:105:A:ASN:HA	1:36:A:ARG:HB3	13	1.15
(1,2023)	1:7:A:VAL:HA	1:11:A:ILE:HD12	9	1.15
(1,1778)	1:112:A:LEU:HD22	1:18:A:ALA:HB3	6	1.15
(1,1723)	1:45:A:VAL:HG12	1:63:A:LEU:HD22	9	1.15
(1,1723)	1:45:A:VAL:HG13	1:63:A:LEU:HD22	11	1.15
(1,1363)	1:23:A:ALA:HB3	1:114:A:MET:HG2	11	1.15
(1,827)	1:101:A:ILE:HG23	1:102:A:THR:HG22	12	1.15
(1,40)	1:99:A:VAL:HG12	1:89:A:GLY:H	16	1.15
(1,38)	1:99:A:VAL:HG12	1:90:A:VAL:H	12	1.15
(1,2443)	1:30:A:VAL:HG23	1:109:A:LEU:HA	13	1.14
(1,2420)	1:100:A:ILE:HD13	1:102:A:THR:H	14	1.14
(1,2177)	1:6:A:VAL:HG12	1:44:A:PHE:HD1	7	1.14
(1,2177)	1:6:A:VAL:HG13	1:44:A:PHE:HD1	17	1.14
(1,2019)	1:14:A:CYS:HB2	1:11:A:ILE:HG21	10	1.14
(1,1823)	1:45:A:VAL:HG12	1:41:A:LYS:HE2	3	1.14
(1,1717)	1:99:A:VAL:HG22	1:99:A:VAL:HA	19	1.14
(1,854)	1:101:A:ILE:HG13	1:70:A:VAL:HG21	8	1.14
(1,854)	1:101:A:ILE:HG13	1:70:A:VAL:HG21	12	1.14
(1,730)	1:33:A:ILE:HD13	1:45:A:VAL:HG12	9	1.14
(1,106)	1:29:A:VAL:HG12	1:113:A:GLU:H	18	1.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,84)	1:99:A:VAL:HG21	1:91:A:CYS:H	15	1.14
(1,38)	1:99:A:VAL:HG11	1:90:A:VAL:H	6	1.14
(1,38)	1:99:A:VAL:HG13	1:90:A:VAL:H	10	1.14
(1,2616)	1:50:A:THR:HG21	1:47:A:ALA:HB2	7	1.13
(1,2595)	1:110:A:LEU:HD23	1:66:A:VAL:HG11	14	1.13
(1,2420)	1:100:A:ILE:HD11	1:102:A:THR:H	9	1.13
(1,2144)	1:7:A:VAL:HG23	1:4:A:TYR:HD1	15	1.13
(1,1823)	1:45:A:VAL:HG12	1:41:A:LYS:HE2	16	1.13
(1,1788)	1:75:A:LYS:HE3	1:100:A:ILE:HG23	10	1.13
(1,1778)	1:112:A:LEU:HD23	1:18:A:ALA:HB2	17	1.13
(1,1776)	1:80:A:VAL:HG11	1:73:A:GLU:HG2	3	1.13
(1,1717)	1:99:A:VAL:HG22	1:99:A:VAL:HA	3	1.13
(1,1717)	1:99:A:VAL:HG21	1:99:A:VAL:HA	14	1.13
(1,827)	1:101:A:ILE:HG21	1:102:A:THR:HG22	11	1.13
(1,730)	1:33:A:ILE:HD11	1:45:A:VAL:HG12	1	1.13
(1,458)	1:74:A:CYS:HB2	1:77:A:CYS:H	18	1.13
(1,2563)	1:45:A:VAL:HA	1:63:A:LEU:HD21	12	1.12
(1,2443)	1:30:A:VAL:HG22	1:109:A:LEU:HA	11	1.12
(1,2144)	1:7:A:VAL:HG21	1:4:A:TYR:HD1	10	1.12
(1,2137)	1:70:A:VAL:HG21	1:88:A:TYR:HD2	5	1.12
(1,1988)	1:40:A:ASP:HB2	1:43:A:LEU:HB3	12	1.12
(1,1864)	1:9:A:SER:HB2	1:12:A:ALA:HB2	1	1.12
(1,1778)	1:112:A:LEU:HD23	1:18:A:ALA:HB3	9	1.12
(1,1776)	1:80:A:VAL:HG11	1:73:A:GLU:HG2	12	1.12
(1,1775)	1:100:A:ILE:HD13	1:102:A:THR:HB	20	1.12
(1,1538)	1:99:A:VAL:HG21	1:91:A:CYS:HA	17	1.12
(1,1418)	1:91:A:CYS:HB2	1:99:A:VAL:HG21	9	1.12
(1,1363)	1:23:A:ALA:HB1	1:114:A:MET:HG2	6	1.12
(1,1289)	1:57:A:VAL:HG22	1:15:A:GLU:HG3	10	1.12
(1,788)	1:65:A:ILE:HD12	1:45:A:VAL:HG21	13	1.12
(1,38)	1:99:A:VAL:HG13	1:90:A:VAL:H	14	1.12
(1,38)	1:99:A:VAL:HG12	1:90:A:VAL:H	16	1.12
(1,15)	1:7:A:VAL:HG11	1:47:A:ALA:H	20	1.12
(1,2672)	1:10:A:LEU:HD12	1:48:A:PHE:HD1	2	1.11
(1,2576)	1:66:A:VAL:HA	1:110:A:LEU:HD13	6	1.11
(1,2126)	1:7:A:VAL:HG11	1:44:A:PHE:HE1	8	1.11
(1,1887)	1:82:A:LYS:HD3	1:71:A:GLU:HB3	8	1.11
(1,1732)	1:72:A:LEU:HD13	1:89:A:GLY:HA3	4	1.11
(1,1717)	1:99:A:VAL:HG21	1:99:A:VAL:HA	11	1.11
(1,1363)	1:23:A:ALA:HB3	1:114:A:MET:HG2	4	1.11
(1,1265)	1:102:A:THR:HG23	1:73:A:GLU:HG2	16	1.11
(1,857)	1:109:A:LEU:HD21	1:112:A:LEU:HD11	19	1.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,774)	1:66:A:VAL:HG23	1:32:A:GLY:HA3	14	1.11
(1,2654)	1:6:A:VAL:HA	1:107:A:MET:HE1	17	1.1
(1,2621)	1:18:A:ALA:HB3	1:21:A:ASN:HB2	7	1.1
(1,2576)	1:66:A:VAL:HA	1:110:A:LEU:HD11	18	1.1
(1,2426)	1:25:A:LYS:HD3	1:115:A:LEU:H	6	1.1
(1,2177)	1:6:A:VAL:HG13	1:44:A:PHE:HD2	15	1.1
(1,2170)	1:92:A:GLU:HG3	1:81:A:PHE:HD1	15	1.1
(1,2127)	1:7:A:VAL:HG12	1:4:A:TYR:HD1	11	1.1
(1,2019)	1:14:A:CYS:HB2	1:11:A:ILE:HG22	11	1.1
(1,1988)	1:40:A:ASP:HB2	1:43:A:LEU:HB3	7	1.1
(1,1840)	1:75:A:LYS:HG3	1:100:A:ILE:HG13	6	1.1
(1,1779)	1:31:A:VAL:HG11	1:33:A:ILE:HG12	3	1.1
(1,1743)	1:90:A:VAL:HG21	1:99:A:VAL:HG23	1	1.1
(1,1717)	1:99:A:VAL:HG23	1:99:A:VAL:HA	5	1.1
(1,1717)	1:99:A:VAL:HG23	1:99:A:VAL:HA	9	1.1
(1,1538)	1:99:A:VAL:HG23	1:91:A:CYS:HA	12	1.1
(1,1514)	1:43:A:LEU:HD23	1:42:A:SER:HB2	6	1.1
(1,1363)	1:23:A:ALA:HB1	1:114:A:MET:HG2	3	1.1
(1,1363)	1:23:A:ALA:HB3	1:114:A:MET:HG2	8	1.1
(1,1289)	1:57:A:VAL:HG22	1:15:A:GLU:HG3	18	1.1
(1,943)	1:6:A:VAL:HG12	1:107:A:MET:HG2	12	1.1
(1,881)	1:93:A:LYS:HB3	1:93:A:LYS:HE2	6	1.1
(1,827)	1:101:A:ILE:HG22	1:102:A:THR:HG23	13	1.1
(1,804)	1:66:A:VAL:HG13	1:32:A:GLY:HA3	4	1.1
(1,330)	1:68:A:GLU:HG2	1:33:A:ILE:H	9	1.1
(1,2177)	1:6:A:VAL:HG11	1:44:A:PHE:HD1	18	1.09
(1,2127)	1:7:A:VAL:HG13	1:4:A:TYR:HD1	8	1.09
(1,2126)	1:7:A:VAL:HG12	1:44:A:PHE:HE2	15	1.09
(1,2047)	1:33:A:ILE:HG21	1:37:A:SER:HA	10	1.09
(1,1988)	1:40:A:ASP:HB2	1:43:A:LEU:HB3	20	1.09
(1,1907)	1:25:A:LYS:HB2	1:57:A:VAL:HG11	18	1.09
(1,1857)	1:75:A:LYS:HG2	1:98:A:ASN:HB2	13	1.09
(1,1823)	1:45:A:VAL:HG12	1:41:A:LYS:HE2	11	1.09
(1,1737)	1:33:A:ILE:HG13	1:39:A:MET:HE1	10	1.09
(1,1732)	1:72:A:LEU:HD13	1:89:A:GLY:HA3	15	1.09
(1,1723)	1:45:A:VAL:HG11	1:63:A:LEU:HD22	7	1.09
(1,1717)	1:99:A:VAL:HG22	1:99:A:VAL:HA	6	1.09
(1,1717)	1:99:A:VAL:HG21	1:99:A:VAL:HA	8	1.09
(1,1717)	1:99:A:VAL:HG22	1:99:A:VAL:HA	12	1.09
(1,1717)	1:99:A:VAL:HG23	1:99:A:VAL:HA	16	1.09
(1,1363)	1:23:A:ALA:HB2	1:114:A:MET:HG2	10	1.09
(1,943)	1:6:A:VAL:HG13	1:107:A:MET:HG2	15	1.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,84)	1:99:A:VAL:HG22	1:91:A:CYS:H	2	1.09
(1,84)	1:99:A:VAL:HG23	1:91:A:CYS:H	19	1.09
(1,70)	1:112:A:LEU:HD22	1:17:A:HIS:H	8	1.09
(1,2621)	1:38:A:ALA:HB1	1:105:A:ASN:HB2	14	1.08
(1,2590)	1:33:A:ILE:HD13	1:39:A:MET:HG2	1	1.08
(1,2563)	1:45:A:VAL:HA	1:63:A:LEU:HD21	18	1.08
(1,1887)	1:82:A:LYS:HD3	1:71:A:GLU:HB3	20	1.08
(1,1823)	1:45:A:VAL:HG13	1:41:A:LYS:HE2	10	1.08
(1,1723)	1:45:A:VAL:HG13	1:63:A:LEU:HD23	4	1.08
(1,1717)	1:99:A:VAL:HG22	1:99:A:VAL:HA	7	1.08
(1,1717)	1:99:A:VAL:HG23	1:99:A:VAL:HA	15	1.08
(1,1514)	1:43:A:LEU:HD23	1:42:A:SER:HB2	12	1.08
(1,1418)	1:91:A:CYS:HB2	1:99:A:VAL:HG21	3	1.08
(1,1418)	1:91:A:CYS:HB2	1:99:A:VAL:HG23	13	1.08
(1,1363)	1:23:A:ALA:HB1	1:114:A:MET:HG2	16	1.08
(1,1265)	1:102:A:THR:HG23	1:73:A:GLU:HG2	6	1.08
(1,851)	1:101:A:ILE:HD13	1:105:A:ASN:HB3	19	1.08
(1,788)	1:65:A:ILE:HD11	1:45:A:VAL:HG23	4	1.08
(1,788)	1:65:A:ILE:HD12	1:45:A:VAL:HG21	15	1.08
(1,330)	1:68:A:GLU:HG2	1:33:A:ILE:H	20	1.08
(1,2654)	1:6:A:VAL:HA	1:107:A:MET:HE1	19	1.07
(1,2638)	1:107:A:MET:HA	1:107:A:MET:HE1	5	1.07
(1,2621)	1:38:A:ALA:HB1	1:105:A:ASN:HB2	16	1.07
(1,2588)	1:30:A:VAL:HG22	1:30:A:VAL:HA	9	1.07
(1,2420)	1:100:A:ILE:HD13	1:102:A:THR:H	13	1.07
(1,1988)	1:40:A:ASP:HB2	1:43:A:LEU:HB3	16	1.07
(1,1805)	1:10:A:LEU:HD12	1:63:A:LEU:HD22	17	1.07
(1,1803)	1:10:A:LEU:HD12	1:109:A:LEU:HB2	16	1.07
(1,1778)	1:112:A:LEU:HD22	1:18:A:ALA:HB1	16	1.07
(1,1717)	1:99:A:VAL:HG22	1:99:A:VAL:HA	17	1.07
(1,1517)	1:7:A:VAL:HG11	1:4:A:TYR:HA	19	1.07
(1,1421)	1:51:A:PHE:HB2	1:7:A:VAL:HG22	6	1.07
(1,1421)	1:51:A:PHE:HB2	1:7:A:VAL:HG23	12	1.07
(1,1418)	1:91:A:CYS:HB2	1:99:A:VAL:HG22	2	1.07
(1,1019)	1:102:A:THR:HG22	1:100:A:ILE:HG12	4	1.07
(1,854)	1:101:A:ILE:HG13	1:70:A:VAL:HG23	10	1.07
(1,788)	1:65:A:ILE:HD11	1:45:A:VAL:HG21	16	1.07
(1,84)	1:99:A:VAL:HG22	1:91:A:CYS:H	8	1.07
(1,44)	1:99:A:VAL:HG13	1:73:A:GLU:H	19	1.07
(1,38)	1:99:A:VAL:HG12	1:90:A:VAL:H	2	1.07
(1,2590)	1:33:A:ILE:HD11	1:39:A:MET:HG2	7	1.06
(1,2588)	1:30:A:VAL:HG21	1:30:A:VAL:HA	17	1.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2420)	1:100:A:ILE:HD12	1:102:A:THR:H	18	1.06
(1,2152)	1:99:A:VAL:HG21	1:81:A:PHE:HZ	10	1.06
(1,2152)	1:99:A:VAL:HG23	1:81:A:PHE:HZ	14	1.06
(1,2134)	1:72:A:LEU:HD21	1:81:A:PHE:HE1	16	1.06
(1,2127)	1:7:A:VAL:HG12	1:4:A:TYR:HD2	5	1.06
(1,1857)	1:75:A:LYS:HG2	1:98:A:ASN:HB2	4	1.06
(1,1803)	1:10:A:LEU:HD12	1:109:A:LEU:HB2	10	1.06
(1,1782)	1:109:A:LEU:HD23	1:107:A:MET:HE1	11	1.06
(1,1717)	1:99:A:VAL:HG21	1:99:A:VAL:HA	2	1.06
(1,1717)	1:99:A:VAL:HG23	1:99:A:VAL:HA	4	1.06
(1,1717)	1:99:A:VAL:HG21	1:99:A:VAL:HA	13	1.06
(1,1717)	1:99:A:VAL:HG22	1:99:A:VAL:HA	20	1.06
(1,1695)	1:64:A:ASP:HB2	1:30:A:VAL:HA	19	1.06
(1,1538)	1:99:A:VAL:HG21	1:91:A:CYS:HA	5	1.06
(1,1482)	1:7:A:VAL:HG23	1:48:A:PHE:HA	17	1.06
(1,1363)	1:23:A:ALA:HB3	1:114:A:MET:HG2	19	1.06
(1,1265)	1:102:A:THR:HG23	1:73:A:GLU:HG2	10	1.06
(1,1019)	1:102:A:THR:HG21	1:100:A:ILE:HG12	7	1.06
(1,1019)	1:102:A:THR:HG23	1:100:A:ILE:HG12	9	1.06
(1,1019)	1:102:A:THR:HG23	1:100:A:ILE:HG12	12	1.06
(1,854)	1:101:A:ILE:HG13	1:70:A:VAL:HG23	17	1.06
(1,788)	1:65:A:ILE:HD11	1:45:A:VAL:HG23	12	1.06
(1,742)	1:72:A:LEU:HD11	1:99:A:VAL:HG12	2	1.06
(1,742)	1:72:A:LEU:HD11	1:99:A:VAL:HG11	20	1.06
(1,40)	1:99:A:VAL:HG13	1:89:A:GLY:H	14	1.06
(1,2654)	1:6:A:VAL:HA	1:107:A:MET:HE1	7	1.05
(1,2588)	1:30:A:VAL:HG21	1:30:A:VAL:HA	18	1.05
(1,2576)	1:66:A:VAL:HA	1:110:A:LEU:HD12	5	1.05
(1,2563)	1:45:A:VAL:HA	1:63:A:LEU:HD22	11	1.05
(1,2177)	1:6:A:VAL:HG12	1:44:A:PHE:HD2	3	1.05
(1,2127)	1:7:A:VAL:HG12	1:4:A:TYR:HD1	3	1.05
(1,2124)	1:11:A:ILE:HD12	1:48:A:PHE:HD2	19	1.05
(1,1994)	1:3:A:GLU:HG2	1:40:A:ASP:HB2	4	1.05
(1,1947)	1:19:A:LYS:HB3	1:16:A:GLU:HB2	8	1.05
(1,1805)	1:10:A:LEU:HD12	1:63:A:LEU:HD21	18	1.05
(1,1803)	1:10:A:LEU:HD13	1:109:A:LEU:HB2	11	1.05
(1,1779)	1:31:A:VAL:HG13	1:33:A:ILE:HG12	15	1.05
(1,1732)	1:72:A:LEU:HD11	1:89:A:GLY:HA3	20	1.05
(1,1723)	1:45:A:VAL:HG12	1:63:A:LEU:HD21	18	1.05
(1,1695)	1:64:A:ASP:HB2	1:30:A:VAL:HA	4	1.05
(1,1421)	1:51:A:PHE:HB2	1:7:A:VAL:HG21	18	1.05
(1,1418)	1:91:A:CYS:HB2	1:99:A:VAL:HG21	10	1.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,943)	1:6:A:VAL:HG13	1:107:A:MET:HG2	13	1.05
(1,904)	1:31:A:VAL:HG11	1:10:A:LEU:HD12	19	1.05
(1,788)	1:65:A:ILE:HD11	1:45:A:VAL:HG23	18	1.05
(1,774)	1:66:A:VAL:HG22	1:32:A:GLY:HA3	8	1.05
(1,38)	1:99:A:VAL:HG13	1:90:A:VAL:H	8	1.05
(1,2643)	1:39:A:MET:HE1	1:106:A:GLU:HG2	19	1.04
(1,2588)	1:30:A:VAL:HG22	1:30:A:VAL:HA	10	1.04
(1,2144)	1:7:A:VAL:HG23	1:4:A:TYR:HD2	2	1.04
(1,1824)	1:25:A:LYS:HG3	1:56:A:LEU:HD13	13	1.04
(1,1800)	1:115:A:LEU:HD13	1:25:A:LYS:HG2	11	1.04
(1,1782)	1:109:A:LEU:HD23	1:107:A:MET:HE3	5	1.04
(1,1778)	1:112:A:LEU:HD21	1:18:A:ALA:HB1	5	1.04
(1,1738)	1:65:A:ILE:HG23	1:63:A:LEU:HD13	16	1.04
(1,1732)	1:72:A:LEU:HD12	1:89:A:GLY:HA3	3	1.04
(1,1732)	1:72:A:LEU:HD11	1:89:A:GLY:HA3	11	1.04
(1,1723)	1:45:A:VAL:HG11	1:63:A:LEU:HD23	15	1.04
(1,1717)	1:99:A:VAL:HG23	1:99:A:VAL:HA	18	1.04
(1,1538)	1:99:A:VAL:HG23	1:91:A:CYS:HA	13	1.04
(1,1517)	1:7:A:VAL:HG12	1:4:A:TYR:HA	9	1.04
(1,774)	1:66:A:VAL:HG21	1:32:A:GLY:HA3	17	1.04
(1,742)	1:72:A:LEU:HD13	1:99:A:VAL:HG12	9	1.04
(1,84)	1:99:A:VAL:HG21	1:91:A:CYS:H	3	1.04
(1,44)	1:99:A:VAL:HG13	1:73:A:GLU:H	13	1.04
(1,40)	1:99:A:VAL:HG12	1:89:A:GLY:H	2	1.04
(1,2638)	1:107:A:MET:HA	1:107:A:MET:HE3	15	1.03
(1,2588)	1:31:A:VAL:HG21	1:30:A:VAL:HA	4	1.03
(1,2588)	1:30:A:VAL:HG21	1:30:A:VAL:HA	5	1.03
(1,2588)	1:30:A:VAL:HG22	1:30:A:VAL:HA	7	1.03
(1,2588)	1:30:A:VAL:HG22	1:30:A:VAL:HA	14	1.03
(1,2563)	1:45:A:VAL:HA	1:63:A:LEU:HD22	7	1.03
(1,2420)	1:100:A:ILE:HD11	1:102:A:THR:H	17	1.03
(1,1887)	1:82:A:LYS:HD3	1:71:A:GLU:HB3	10	1.03
(1,1779)	1:31:A:VAL:HG12	1:33:A:ILE:HG12	7	1.03
(1,1778)	1:112:A:LEU:HD22	1:18:A:ALA:HB1	3	1.03
(1,1723)	1:45:A:VAL:HG12	1:63:A:LEU:HD22	13	1.03
(1,1717)	1:99:A:VAL:HG21	1:99:A:VAL:HA	1	1.03
(1,1717)	1:99:A:VAL:HG22	1:99:A:VAL:HA	10	1.03
(1,1538)	1:99:A:VAL:HG21	1:91:A:CYS:HA	15	1.03
(1,1443)	1:30:A:VAL:HG12	1:28:A:ARG:HD2	8	1.03
(1,1363)	1:23:A:ALA:HB3	1:114:A:MET:HG2	9	1.03
(1,914)	1:72:A:LEU:HD21	1:70:A:VAL:HG12	8	1.03
(1,40)	1:99:A:VAL:HG13	1:89:A:GLY:H	8	1.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2672)	1:70:A:VAL:HG11	1:88:A:TYR:HD2	19	1.02
(1,2597)	1:72:A:LEU:HB2	1:80:A:VAL:HG11	5	1.02
(1,2588)	1:30:A:VAL:HG23	1:30:A:VAL:HA	2	1.02
(1,2443)	1:30:A:VAL:HG22	1:109:A:LEU:HA	10	1.02
(1,2420)	1:100:A:ILE:HD11	1:102:A:THR:H	5	1.02
(1,2127)	1:7:A:VAL:HG13	1:4:A:TYR:HD2	14	1.02
(1,1864)	1:9:A:SER:HB2	1:12:A:ALA:HB2	11	1.02
(1,1743)	1:90:A:VAL:HG22	1:99:A:VAL:HG21	6	1.02
(1,1738)	1:65:A:ILE:HG22	1:63:A:LEU:HD12	12	1.02
(1,1538)	1:99:A:VAL:HG22	1:91:A:CYS:HA	8	1.02
(1,1517)	1:7:A:VAL:HG13	1:4:A:TYR:HA	2	1.02
(1,1265)	1:102:A:THR:HG21	1:73:A:GLU:HG2	8	1.02
(1,1019)	1:102:A:THR:HG22	1:100:A:ILE:HG12	14	1.02
(1,943)	1:6:A:VAL:HG11	1:107:A:MET:HG2	20	1.02
(1,822)	1:80:A:VAL:HG11	1:102:A:THR:HG22	13	1.02
(1,805)	1:7:A:VAL:HG21	1:48:A:PHE:HB3	7	1.02
(1,788)	1:65:A:ILE:HD11	1:45:A:VAL:HG21	3	1.02
(1,742)	1:72:A:LEU:HD11	1:99:A:VAL:HG11	7	1.02
(1,330)	1:68:A:GLU:HG2	1:33:A:ILE:H	10	1.02
(1,2654)	1:6:A:VAL:HA	1:107:A:MET:HE2	1	1.01
(1,2588)	1:30:A:VAL:HG22	1:30:A:VAL:HA	8	1.01
(1,2588)	1:30:A:VAL:HG22	1:30:A:VAL:HA	11	1.01
(1,2588)	1:30:A:VAL:HG23	1:30:A:VAL:HA	12	1.01
(1,2588)	1:30:A:VAL:HG22	1:30:A:VAL:HA	15	1.01
(1,2177)	1:6:A:VAL:HG12	1:44:A:PHE:HD2	11	1.01
(1,2158)	1:29:A:VAL:HG11	1:48:A:PHE:HZ	6	1.01
(1,2047)	1:33:A:ILE:HG21	1:37:A:SER:HA	6	1.01
(1,1938)	1:71:A:GLU:HG2	1:103:A:GLN:HG2	8	1.01
(1,1814)	1:107:A:MET:HE1	1:10:A:LEU:HD22	9	1.01
(1,1805)	1:10:A:LEU:HD13	1:63:A:LEU:HD22	6	1.01
(1,1805)	1:10:A:LEU:HD11	1:63:A:LEU:HD22	9	1.01
(1,1778)	1:112:A:LEU:HD23	1:18:A:ALA:HB3	8	1.01
(1,1739)	1:33:A:ILE:HG21	1:65:A:ILE:HG21	9	1.01
(1,1695)	1:64:A:ASP:HB2	1:30:A:VAL:HA	7	1.01
(1,1418)	1:91:A:CYS:HB2	1:99:A:VAL:HG21	16	1.01
(1,943)	1:6:A:VAL:HG12	1:107:A:MET:HG2	14	1.01
(1,881)	1:93:A:LYS:HB3	1:93:A:LYS:HE2	1	1.01
(1,881)	1:93:A:LYS:HB3	1:93:A:LYS:HE2	4	1.01
(1,881)	1:93:A:LYS:HB3	1:93:A:LYS:HE2	16	1.01
(1,854)	1:101:A:ILE:HG13	1:70:A:VAL:HG22	19	1.01
(1,458)	1:74:A:CYS:HB2	1:77:A:CYS:H	19	1.01
(1,2654)	1:6:A:VAL:HA	1:107:A:MET:HE3	15	1.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2621)	1:38:A:ALA:HB3	1:105:A:ASN:HB2	17	1.0
(1,2576)	1:66:A:VAL:HA	1:110:A:LEU:HD12	8	1.0
(1,2563)	1:45:A:VAL:HA	1:63:A:LEU:HD21	1	1.0
(1,2426)	1:25:A:LYS:HD3	1:115:A:LEU:H	19	1.0
(1,2420)	1:100:A:ILE:HD11	1:102:A:THR:H	10	1.0
(1,2206)	1:83:A:PRO:HB2	1:81:A:PHE:HD2	20	1.0
(1,2079)	1:71:A:GLU:HB2	1:103:A:GLN:HA	16	1.0
(1,2023)	1:7:A:VAL:HA	1:11:A:ILE:HD12	7	1.0
(1,1887)	1:82:A:LYS:HD3	1:71:A:GLU:HB3	18	1.0
(1,1870)	1:20:A:LYS:HG2	1:16:A:GLU:HG3	16	1.0
(1,1840)	1:75:A:LYS:HG3	1:100:A:ILE:HG13	19	1.0
(1,1803)	1:10:A:LEU:HD12	1:109:A:LEU:HB2	12	1.0
(1,1753)	1:65:A:ILE:HD11	1:41:A:LYS:HD3	9	1.0
(1,1517)	1:7:A:VAL:HG13	1:4:A:TYR:HA	16	1.0
(1,1363)	1:23:A:ALA:HB2	1:114:A:MET:HG2	1	1.0
(1,1265)	1:102:A:THR:HG22	1:73:A:GLU:HG2	20	1.0
(1,881)	1:93:A:LYS:HB3	1:93:A:LYS:HE2	3	1.0
(1,881)	1:93:A:LYS:HB3	1:93:A:LYS:HE2	9	1.0
(1,851)	1:101:A:ILE:HD13	1:105:A:ASN:HB3	17	1.0
(1,813)	1:29:A:VAL:HG23	1:10:A:LEU:HD12	18	1.0
(1,805)	1:7:A:VAL:HG23	1:48:A:PHE:HB3	17	1.0
(1,788)	1:65:A:ILE:HD13	1:45:A:VAL:HG23	2	1.0
(1,788)	1:65:A:ILE:HD11	1:45:A:VAL:HG21	17	1.0
(1,84)	1:99:A:VAL:HG23	1:91:A:CYS:H	14	1.0
(1,40)	1:99:A:VAL:HG13	1:89:A:GLY:H	13	1.0
(1,15)	1:7:A:VAL:HG12	1:47:A:ALA:H	18	1.0
(1,2622)	1:38:A:ALA:HB3	1:1:A:MET:HB2	19	0.99
(1,2588)	1:30:A:VAL:HG22	1:30:A:VAL:HA	19	0.99
(1,2563)	1:45:A:VAL:HA	1:63:A:LEU:HD23	8	0.99
(1,2563)	1:45:A:VAL:HA	1:63:A:LEU:HD22	20	0.99
(1,2177)	1:6:A:VAL:HG12	1:44:A:PHE:HD1	9	0.99
(1,2137)	1:70:A:VAL:HG22	1:88:A:TYR:HD2	2	0.99
(1,2127)	1:7:A:VAL:HG11	1:4:A:TYR:HD2	19	0.99
(1,2047)	1:33:A:ILE:HG22	1:37:A:SER:HA	9	0.99
(1,1994)	1:3:A:GLU:HG2	1:40:A:ASP:HB2	20	0.99
(1,1857)	1:75:A:LYS:HG2	1:98:A:ASN:HB2	9	0.99
(1,1751)	1:65:A:ILE:HD11	1:33:A:ILE:HG21	9	0.99
(1,1738)	1:65:A:ILE:HG21	1:63:A:LEU:HD12	14	0.99
(1,1538)	1:99:A:VAL:HG23	1:91:A:CYS:HA	19	0.99
(1,1265)	1:102:A:THR:HG23	1:73:A:GLU:HG2	4	0.99
(1,881)	1:93:A:LYS:HB3	1:93:A:LYS:HE2	5	0.99
(1,862)	1:109:A:LEU:HD22	1:13:A:LEU:HD23	20	0.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,854)	1:101:A:ILE:HG13	1:70:A:VAL:HG22	16	0.99
(1,822)	1:80:A:VAL:HG13	1:102:A:THR:HG22	17	0.99
(1,805)	1:7:A:VAL:HG21	1:48:A:PHE:HB3	5	0.99
(1,788)	1:65:A:ILE:HD13	1:45:A:VAL:HG23	11	0.99
(1,774)	1:66:A:VAL:HG22	1:32:A:GLY:HA3	12	0.99
(1,458)	1:74:A:CYS:HB2	1:77:A:CYS:H	8	0.99
(1,330)	1:68:A:GLU:HG2	1:33:A:ILE:H	6	0.99
(1,2606)	1:57:A:VAL:HG13	1:26:A:ILE:HA	11	0.98
(1,2590)	1:33:A:ILE:HD11	1:39:A:MET:HG2	5	0.98
(1,2588)	1:31:A:VAL:HG23	1:30:A:VAL:HA	1	0.98
(1,2588)	1:30:A:VAL:HG22	1:30:A:VAL:HA	6	0.98
(1,2588)	1:30:A:VAL:HG23	1:30:A:VAL:HA	13	0.98
(1,2588)	1:30:A:VAL:HG23	1:30:A:VAL:HA	20	0.98
(1,2153)	1:99:A:VAL:HG21	1:81:A:PHE:HE2	10	0.98
(1,2127)	1:7:A:VAL:HG12	1:4:A:TYR:HD1	9	0.98
(1,1864)	1:9:A:SER:HB2	1:12:A:ALA:HB1	8	0.98
(1,1864)	1:9:A:SER:HB2	1:12:A:ALA:HB2	12	0.98
(1,1857)	1:75:A:LYS:HG2	1:98:A:ASN:HB2	7	0.98
(1,1854)	1:75:A:LYS:HG2	1:100:A:ILE:HG13	14	0.98
(1,1823)	1:45:A:VAL:HG12	1:41:A:LYS:HE2	2	0.98
(1,1363)	1:23:A:ALA:HB3	1:114:A:MET:HG2	7	0.98
(1,1363)	1:23:A:ALA:HB2	1:114:A:MET:HG2	20	0.98
(1,881)	1:93:A:LYS:HB3	1:93:A:LYS:HE2	15	0.98
(1,804)	1:66:A:VAL:HG11	1:32:A:GLY:HA3	3	0.98
(1,804)	1:66:A:VAL:HG12	1:32:A:GLY:HA3	15	0.98
(1,788)	1:65:A:ILE:HD11	1:45:A:VAL:HG23	5	0.98
(1,742)	1:72:A:LEU:HD12	1:99:A:VAL:HG13	8	0.98
(1,458)	1:74:A:CYS:HB2	1:77:A:CYS:H	4	0.98
(1,148)	1:6:A:VAL:HG13	1:9:A:SER:H	5	0.98
(1,38)	1:99:A:VAL:HG11	1:90:A:VAL:H	20	0.98
(1,2576)	1:66:A:VAL:HA	1:110:A:LEU:HD11	12	0.97
(1,2576)	1:66:A:VAL:HA	1:110:A:LEU:HD13	14	0.97
(1,2420)	1:100:A:ILE:HD13	1:102:A:THR:H	2	0.97
(1,2206)	1:83:A:PRO:HB2	1:81:A:PHE:HD2	17	0.97
(1,2189)	1:92:A:GLU:HG2	1:81:A:PHE:HD2	10	0.97
(1,1823)	1:45:A:VAL:HG12	1:41:A:LYS:HE2	12	0.97
(1,1782)	1:109:A:LEU:HD22	1:107:A:MET:HE1	8	0.97
(1,1779)	1:31:A:VAL:HG13	1:33:A:ILE:HG12	16	0.97
(1,1517)	1:7:A:VAL:HG13	1:4:A:TYR:HA	1	0.97
(1,1517)	1:7:A:VAL:HG13	1:4:A:TYR:HA	12	0.97
(1,1482)	1:7:A:VAL:HG21	1:48:A:PHE:HA	7	0.97
(1,881)	1:93:A:LYS:HB3	1:93:A:LYS:HE2	13	0.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,854)	1:101:A:ILE:HG13	1:70:A:VAL:HG22	3	0.97
(1,805)	1:7:A:VAL:HG23	1:48:A:PHE:HB3	15	0.97
(1,788)	1:65:A:ILE:HD12	1:45:A:VAL:HG23	6	0.97
(1,2657)	1:20:A:LYS:HE2	1:20:A:LYS:HA	20	0.96
(1,2512)	1:56:A:LEU:HD23	1:56:A:LEU:HB3	14	0.96
(1,2180)	1:61:A:ALA:HB3	1:48:A:PHE:HD1	19	0.96
(1,2158)	1:29:A:VAL:HG11	1:48:A:PHE:HZ	10	0.96
(1,2158)	1:29:A:VAL:HG13	1:48:A:PHE:HZ	17	0.96
(1,2158)	1:29:A:VAL:HG12	1:48:A:PHE:HZ	19	0.96
(1,2144)	1:7:A:VAL:HG22	1:4:A:TYR:HD1	4	0.96
(1,2144)	1:7:A:VAL:HG22	1:4:A:TYR:HD1	6	0.96
(1,2063)	1:33:A:ILE:HA	1:107:A:MET:HG3	13	0.96
(1,1803)	1:10:A:LEU:HD11	1:109:A:LEU:HB2	5	0.96
(1,1738)	1:65:A:ILE:HG23	1:63:A:LEU:HD13	17	0.96
(1,1737)	1:33:A:ILE:HG13	1:39:A:MET:HE2	4	0.96
(1,1517)	1:7:A:VAL:HG11	1:4:A:TYR:HA	6	0.96
(1,1517)	1:7:A:VAL:HG11	1:4:A:TYR:HA	13	0.96
(1,1482)	1:7:A:VAL:HG21	1:48:A:PHE:HA	10	0.96
(1,1420)	1:25:A:LYS:HE3	1:25:A:LYS:HB3	3	0.96
(1,1418)	1:91:A:CYS:HB2	1:99:A:VAL:HG21	6	0.96
(1,1289)	1:57:A:VAL:HG22	1:15:A:GLU:HG3	8	0.96
(1,1265)	1:102:A:THR:HG21	1:73:A:GLU:HG2	12	0.96
(1,881)	1:93:A:LYS:HB3	1:93:A:LYS:HE2	2	0.96
(1,40)	1:99:A:VAL:HG11	1:89:A:GLY:H	11	0.96
(1,38)	1:99:A:VAL:HG11	1:90:A:VAL:H	11	0.96
(1,15)	1:7:A:VAL:HG11	1:47:A:ALA:H	6	0.96
(1,15)	1:7:A:VAL:HG13	1:47:A:ALA:H	12	0.96
(1,2672)	1:70:A:VAL:HG11	1:88:A:TYR:HD1	17	0.95
(1,2638)	1:107:A:MET:HA	1:107:A:MET:HE3	6	0.95
(1,2622)	1:38:A:ALA:HB3	1:1:A:MET:HB2	16	0.95
(1,2618)	1:6:A:VAL:HG21	1:2:A:HIS:HB2	12	0.95
(1,2597)	1:72:A:LEU:HB2	1:99:A:VAL:HG21	4	0.95
(1,2588)	1:31:A:VAL:HG22	1:30:A:VAL:HA	3	0.95
(1,2563)	1:45:A:VAL:HA	1:63:A:LEU:HD22	16	0.95
(1,2512)	1:10:A:LEU:HD12	1:10:A:LEU:HB3	9	0.95
(1,2158)	1:29:A:VAL:HG11	1:48:A:PHE:HZ	12	0.95
(1,2144)	1:7:A:VAL:HG21	1:4:A:TYR:HD1	9	0.95
(1,2127)	1:7:A:VAL:HG11	1:4:A:TYR:HD1	10	0.95
(1,1994)	1:3:A:GLU:HG2	1:40:A:ASP:HB2	16	0.95
(1,1870)	1:20:A:LYS:HG2	1:16:A:GLU:HG3	19	0.95
(1,1814)	1:107:A:MET:HE3	1:10:A:LEU:HD21	2	0.95
(1,1814)	1:107:A:MET:HE3	1:10:A:LEU:HD21	10	0.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1779)	1:31:A:VAL:HG11	1:33:A:ILE:HG12	19	0.95
(1,1738)	1:65:A:ILE:HG23	1:63:A:LEU:HD11	15	0.95
(1,1363)	1:23:A:ALA:HB2	1:114:A:MET:HG2	13	0.95
(1,1363)	1:23:A:ALA:HB3	1:114:A:MET:HG2	15	0.95
(1,1301)	1:1:A:MET:HE2	1:1:A:MET:HB2	5	0.95
(1,914)	1:72:A:LEU:HD21	1:70:A:VAL:HG13	12	0.95
(1,770)	1:72:A:LEU:HD12	1:70:A:VAL:HG23	11	0.95
(1,730)	1:33:A:ILE:HD12	1:45:A:VAL:HG11	6	0.95
(1,730)	1:33:A:ILE:HD13	1:45:A:VAL:HG11	18	0.95
(1,458)	1:74:A:CYS:HB2	1:77:A:CYS:H	6	0.95
(1,148)	1:6:A:VAL:HG13	1:9:A:SER:H	7	0.95
(1,84)	1:99:A:VAL:HG22	1:91:A:CYS:H	11	0.95
(1,55)	1:80:A:VAL:HG12	1:80:A:VAL:H	1	0.95
(1,40)	1:99:A:VAL:HG12	1:89:A:GLY:H	9	0.95
(1,15)	1:7:A:VAL:HG13	1:47:A:ALA:H	8	0.95
(1,2633)	1:115:A:LEU:HD11	1:27:A:GLU:HB3	16	0.94
(1,2606)	1:57:A:VAL:HG13	1:26:A:ILE:HA	12	0.94
(1,2590)	1:33:A:ILE:HD13	1:39:A:MET:HG2	17	0.94
(1,2512)	1:56:A:LEU:HD22	1:56:A:LEU:HB3	17	0.94
(1,2204)	1:83:A:PRO:HB3	1:88:A:TYR:HE1	1	0.94
(1,2204)	1:83:A:PRO:HB3	1:88:A:TYR:HE1	12	0.94
(1,2163)	1:45:A:VAL:HG23	1:44:A:PHE:HD2	18	0.94
(1,2127)	1:7:A:VAL:HG13	1:4:A:TYR:HD2	16	0.94
(1,2079)	1:71:A:GLU:HB2	1:103:A:GLN:HA	6	0.94
(1,1907)	1:25:A:LYS:HB2	1:57:A:VAL:HG11	13	0.94
(1,1857)	1:75:A:LYS:HG2	1:98:A:ASN:HB2	3	0.94
(1,1840)	1:75:A:LYS:HG3	1:100:A:ILE:HG13	18	0.94
(1,1824)	1:25:A:LYS:HG3	1:56:A:LEU:HD12	17	0.94
(1,1803)	1:10:A:LEU:HD12	1:109:A:LEU:HB2	1	0.94
(1,1779)	1:31:A:VAL:HG13	1:33:A:ILE:HG12	4	0.94
(1,1779)	1:31:A:VAL:HG12	1:33:A:ILE:HG12	5	0.94
(1,1776)	1:80:A:VAL:HG12	1:73:A:GLU:HG2	18	0.94
(1,1752)	1:90:A:VAL:HG13	1:97:A:LYS:HD2	12	0.94
(1,1743)	1:90:A:VAL:HG23	1:99:A:VAL:HG23	13	0.94
(1,1695)	1:64:A:ASP:HB2	1:30:A:VAL:HA	3	0.94
(1,1538)	1:99:A:VAL:HG21	1:91:A:CYS:HA	9	0.94
(1,1265)	1:102:A:THR:HG22	1:73:A:GLU:HG2	15	0.94
(1,148)	1:6:A:VAL:HG13	1:9:A:SER:H	16	0.94
(1,84)	1:99:A:VAL:HG21	1:91:A:CYS:H	5	0.94
(1,44)	1:99:A:VAL:HG13	1:73:A:GLU:H	2	0.94
(1,38)	1:99:A:VAL:HG13	1:90:A:VAL:H	13	0.94
(1,2672)	1:70:A:VAL:HG12	1:88:A:TYR:HD2	9	0.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2638)	1:107:A:MET:HA	1:107:A:MET:HE2	1	0.93
(1,2612)	1:59:A:LYS:HE2	1:56:A:LEU:HD11	16	0.93
(1,2606)	1:57:A:VAL:HG12	1:26:A:ILE:HA	18	0.93
(1,2597)	1:72:A:LEU:HB2	1:99:A:VAL:HG22	2	0.93
(1,2563)	1:45:A:VAL:HA	1:63:A:LEU:HD23	4	0.93
(1,2512)	1:56:A:LEU:HD21	1:56:A:LEU:HB3	4	0.93
(1,2512)	1:56:A:LEU:HD23	1:56:A:LEU:HB3	11	0.93
(1,2512)	1:56:A:LEU:HD22	1:56:A:LEU:HB3	16	0.93
(1,2158)	1:29:A:VAL:HG13	1:48:A:PHE:HZ	16	0.93
(1,2153)	1:99:A:VAL:HG21	1:81:A:PHE:HE1	16	0.93
(1,2134)	1:72:A:LEU:HD21	1:81:A:PHE:HE2	10	0.93
(1,2127)	1:7:A:VAL:HG11	1:4:A:TYR:HD1	15	0.93
(1,1738)	1:65:A:ILE:HG22	1:63:A:LEU:HD11	13	0.93
(1,1723)	1:45:A:VAL:HG12	1:63:A:LEU:HD21	19	0.93
(1,1695)	1:64:A:ASP:HB2	1:30:A:VAL:HA	5	0.93
(1,1482)	1:7:A:VAL:HG21	1:48:A:PHE:HA	9	0.93
(1,1019)	1:102:A:THR:HG23	1:100:A:ILE:HG12	13	0.93
(1,943)	1:6:A:VAL:HG13	1:107:A:MET:HG2	16	0.93
(1,881)	1:93:A:LYS:HB3	1:93:A:LYS:HE2	19	0.93
(1,862)	1:109:A:LEU:HD21	1:13:A:LEU:HD23	9	0.93
(1,854)	1:101:A:ILE:HG13	1:70:A:VAL:HG22	9	0.93
(1,804)	1:66:A:VAL:HG13	1:32:A:GLY:HA3	2	0.93
(1,804)	1:66:A:VAL:HG11	1:32:A:GLY:HA3	13	0.93
(1,330)	1:68:A:GLU:HG2	1:33:A:ILE:H	15	0.93
(1,44)	1:99:A:VAL:HG11	1:73:A:GLU:H	17	0.93
(1,38)	1:99:A:VAL:HG11	1:90:A:VAL:H	3	0.93
(1,2588)	1:31:A:VAL:HG22	1:30:A:VAL:HA	16	0.92
(1,2512)	1:56:A:LEU:HD22	1:56:A:LEU:HB3	2	0.92
(1,2512)	1:56:A:LEU:HD22	1:56:A:LEU:HB3	5	0.92
(1,2144)	1:7:A:VAL:HG23	1:4:A:TYR:HD2	16	0.92
(1,2127)	1:7:A:VAL:HG13	1:4:A:TYR:HD2	2	0.92
(1,2069)	1:112:A:LEU:HD22	1:29:A:VAL:HA	4	0.92
(1,1907)	1:25:A:LYS:HB2	1:57:A:VAL:HG13	7	0.92
(1,1857)	1:75:A:LYS:HG2	1:98:A:ASN:HB2	6	0.92
(1,1805)	1:10:A:LEU:HD13	1:63:A:LEU:HD23	4	0.92
(1,1805)	1:10:A:LEU:HD12	1:63:A:LEU:HD21	14	0.92
(1,1738)	1:65:A:ILE:HG22	1:63:A:LEU:HD11	5	0.92
(1,1738)	1:65:A:ILE:HG23	1:63:A:LEU:HD11	8	0.92
(1,1738)	1:65:A:ILE:HG22	1:63:A:LEU:HD13	18	0.92
(1,1732)	1:72:A:LEU:HD11	1:89:A:GLY:HA3	1	0.92
(1,1538)	1:99:A:VAL:HG21	1:91:A:CYS:HA	16	0.92
(1,1466)	1:14:A:CYS:HB2	1:11:A:ILE:HA	10	0.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1363)	1:23:A:ALA:HB3	1:114:A:MET:HG2	14	0.92
(1,1276)	1:19:A:LYS:HB2	1:19:A:LYS:HE3	18	0.92
(1,1265)	1:102:A:THR:HG22	1:73:A:GLU:HG2	3	0.92
(1,937)	1:102:A:THR:HG23	1:73:A:GLU:HA	13	0.92
(1,881)	1:93:A:LYS:HB3	1:93:A:LYS:HE2	8	0.92
(1,881)	1:93:A:LYS:HB3	1:93:A:LYS:HE2	14	0.92
(1,881)	1:93:A:LYS:HB3	1:93:A:LYS:HE2	17	0.92
(1,804)	1:66:A:VAL:HG11	1:32:A:GLY:HA3	5	0.92
(1,788)	1:65:A:ILE:HD12	1:45:A:VAL:HG23	8	0.92
(1,774)	1:66:A:VAL:HG21	1:32:A:GLY:HA3	1	0.92
(1,774)	1:66:A:VAL:HG22	1:32:A:GLY:HA3	20	0.92
(1,730)	1:33:A:ILE:HD11	1:45:A:VAL:HG12	3	0.92
(1,101)	1:57:A:VAL:HG11	1:15:A:GLU:H	17	0.92
(1,2638)	1:107:A:MET:HA	1:107:A:MET:HE3	7	0.91
(1,2618)	1:6:A:VAL:HG23	1:2:A:HIS:HB2	10	0.91
(1,2597)	1:72:A:LEU:HB2	1:99:A:VAL:HG22	11	0.91
(1,2512)	1:56:A:LEU:HD21	1:56:A:LEU:HB3	6	0.91
(1,2180)	1:61:A:ALA:HB2	1:48:A:PHE:HD2	13	0.91
(1,2144)	1:7:A:VAL:HG21	1:4:A:TYR:HD1	7	0.91
(1,2144)	1:7:A:VAL:HG21	1:4:A:TYR:HD2	18	0.91
(1,2089)	1:79:A:HIS:HA	1:80:A:VAL:HG23	12	0.91
(1,2063)	1:33:A:ILE:HA	1:107:A:MET:HG3	20	0.91
(1,2047)	1:33:A:ILE:HG23	1:37:A:SER:HA	19	0.91
(1,2023)	1:7:A:VAL:HA	1:11:A:ILE:HD11	16	0.91
(1,1907)	1:25:A:LYS:HB2	1:57:A:VAL:HG11	2	0.91
(1,1857)	1:75:A:LYS:HG2	1:98:A:ASN:HB2	8	0.91
(1,1739)	1:33:A:ILE:HG22	1:65:A:ILE:HG22	8	0.91
(1,1723)	1:45:A:VAL:HG11	1:63:A:LEU:HD23	2	0.91
(1,1538)	1:99:A:VAL:HG22	1:91:A:CYS:HA	11	0.91
(1,1517)	1:7:A:VAL:HG12	1:4:A:TYR:HA	11	0.91
(1,1517)	1:7:A:VAL:HG13	1:4:A:TYR:HA	14	0.91
(1,1517)	1:7:A:VAL:HG11	1:4:A:TYR:HA	20	0.91
(1,1420)	1:25:A:LYS:HE3	1:25:A:LYS:HB3	14	0.91
(1,1418)	1:91:A:CYS:HB2	1:99:A:VAL:HG21	4	0.91
(1,1363)	1:23:A:ALA:HB2	1:114:A:MET:HG2	18	0.91
(1,1356)	1:107:A:MET:HG2	1:107:A:MET:HE3	8	0.91
(1,1276)	1:19:A:LYS:HB2	1:19:A:LYS:HE3	16	0.91
(1,1211)	1:75:A:LYS:HB3	1:98:A:ASN:HB2	6	0.91
(1,1019)	1:102:A:THR:HG22	1:100:A:ILE:HG12	11	0.91
(1,943)	1:6:A:VAL:HG11	1:107:A:MET:HG2	7	0.91
(1,881)	1:93:A:LYS:HB3	1:93:A:LYS:HE2	20	0.91
(1,823)	1:30:A:VAL:HG12	1:111:A:SER:HB2	8	0.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,805)	1:7:A:VAL:HG21	1:48:A:PHE:HB3	10	0.91
(1,805)	1:7:A:VAL:HG22	1:48:A:PHE:HB3	13	0.91
(1,805)	1:7:A:VAL:HG23	1:48:A:PHE:HB3	14	0.91
(1,746)	1:72:A:LEU:HD11	1:83:A:PRO:HB2	13	0.91
(1,742)	1:72:A:LEU:HD13	1:99:A:VAL:HG13	15	0.91
(1,458)	1:74:A:CYS:HB2	1:77:A:CYS:H	12	0.91
(1,458)	1:74:A:CYS:HB2	1:77:A:CYS:H	13	0.91
(1,330)	1:68:A:GLU:HG2	1:33:A:ILE:H	4	0.91
(1,101)	1:57:A:VAL:HG11	1:15:A:GLU:H	7	0.91
(1,44)	1:99:A:VAL:HG13	1:73:A:GLU:H	9	0.91
(1,2633)	1:115:A:LEU:HD12	1:27:A:GLU:HB3	17	0.9
(1,2606)	1:57:A:VAL:HG11	1:26:A:ILE:HA	10	0.9
(1,2563)	1:45:A:VAL:HA	1:63:A:LEU:HD22	13	0.9
(1,2555)	1:25:A:LYS:HE3	1:56:A:LEU:HD13	20	0.9
(1,2512)	1:56:A:LEU:HD21	1:56:A:LEU:HB3	12	0.9
(1,2512)	1:56:A:LEU:HD22	1:56:A:LEU:HB3	20	0.9
(1,2177)	1:6:A:VAL:HG12	1:44:A:PHE:HD1	2	0.9
(1,1857)	1:75:A:LYS:HG2	1:98:A:ASN:HB2	5	0.9
(1,1840)	1:75:A:LYS:HG3	1:100:A:ILE:HG13	7	0.9
(1,1805)	1:10:A:LEU:HD12	1:63:A:LEU:HD21	1	0.9
(1,1779)	1:31:A:VAL:HG12	1:33:A:ILE:HG12	2	0.9
(1,1779)	1:31:A:VAL:HG12	1:33:A:ILE:HG12	6	0.9
(1,1738)	1:65:A:ILE:HG22	1:63:A:LEU:HD12	1	0.9
(1,1695)	1:64:A:ASP:HB2	1:30:A:VAL:HA	14	0.9
(1,1482)	1:7:A:VAL:HG23	1:48:A:PHE:HA	14	0.9
(1,1420)	1:25:A:LYS:HE3	1:25:A:LYS:HB3	6	0.9
(1,1420)	1:25:A:LYS:HE3	1:25:A:LYS:HB3	15	0.9
(1,1276)	1:19:A:LYS:HB2	1:19:A:LYS:HE2	7	0.9
(1,1265)	1:102:A:THR:HG22	1:73:A:GLU:HG2	9	0.9
(1,943)	1:6:A:VAL:HG13	1:107:A:MET:HG2	19	0.9
(1,862)	1:109:A:LEU:HD23	1:13:A:LEU:HD22	3	0.9
(1,862)	1:109:A:LEU:HD23	1:13:A:LEU:HD23	4	0.9
(1,805)	1:7:A:VAL:HG21	1:48:A:PHE:HB3	1	0.9
(1,195)	1:12:A:ALA:HB1	1:15:A:GLU:H	11	0.9
(1,148)	1:6:A:VAL:HG13	1:9:A:SER:H	18	0.9
(1,34)	1:33:A:ILE:HG23	1:39:A:MET:H	5	0.9
(1,15)	1:7:A:VAL:HG12	1:47:A:ALA:H	4	0.9
(1,15)	1:7:A:VAL:HG13	1:47:A:ALA:H	16	0.9
(1,2671)	1:115:A:LEU:HD13	1:24:A:HIS:HD2	11	0.89
(1,2657)	1:20:A:LYS:HE2	1:20:A:LYS:HA	5	0.89
(1,2597)	1:72:A:LEU:HB2	1:99:A:VAL:HG23	12	0.89
(1,2590)	1:33:A:ILE:HD12	1:39:A:MET:HG2	11	0.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2590)	1:33:A:ILE:HD13	1:39:A:MET:HG2	15	0.89
(1,2512)	1:56:A:LEU:HD21	1:56:A:LEU:HB3	1	0.89
(1,2512)	1:56:A:LEU:HD21	1:56:A:LEU:HB3	13	0.89
(1,2202)	1:83:A:PRO:HB3	1:88:A:TYR:HD1	20	0.89
(1,2177)	1:6:A:VAL:HG11	1:44:A:PHE:HD1	5	0.89
(1,2177)	1:6:A:VAL:HG12	1:44:A:PHE:HD1	19	0.89
(1,2163)	1:45:A:VAL:HG23	1:44:A:PHE:HD1	11	0.89
(1,2132)	1:72:A:LEU:HB3	1:81:A:PHE:HD1	14	0.89
(1,2023)	1:7:A:VAL:HA	1:11:A:ILE:HD12	11	0.89
(1,1870)	1:20:A:LYS:HG2	1:16:A:GLU:HG3	14	0.89
(1,1840)	1:75:A:LYS:HG3	1:100:A:ILE:HG13	16	0.89
(1,1823)	1:45:A:VAL:HG11	1:41:A:LYS:HE2	9	0.89
(1,1792)	1:11:A:ILE:HG22	1:52:A:ARG:HA	9	0.89
(1,1748)	1:33:A:ILE:HG22	1:107:A:MET:HG3	20	0.89
(1,1738)	1:65:A:ILE:HG22	1:63:A:LEU:HD13	9	0.89
(1,1738)	1:65:A:ILE:HG23	1:63:A:LEU:HD13	10	0.89
(1,1737)	1:33:A:ILE:HG13	1:39:A:MET:HE2	19	0.89
(1,1723)	1:45:A:VAL:HG11	1:63:A:LEU:HD21	1	0.89
(1,1723)	1:45:A:VAL:HG11	1:63:A:LEU:HD22	16	0.89
(1,1723)	1:45:A:VAL:HG12	1:63:A:LEU:HD22	20	0.89
(1,1514)	1:43:A:LEU:HD22	1:42:A:SER:HB2	13	0.89
(1,1420)	1:25:A:LYS:HE3	1:25:A:LYS:HB3	10	0.89
(1,1420)	1:25:A:LYS:HE3	1:25:A:LYS:HB3	19	0.89
(1,1269)	1:80:A:VAL:HG22	1:73:A:GLU:HG2	14	0.89
(1,1265)	1:102:A:THR:HG23	1:73:A:GLU:HG2	7	0.89
(1,1265)	1:102:A:THR:HG22	1:73:A:GLU:HG2	13	0.89
(1,943)	1:6:A:VAL:HG11	1:107:A:MET:HG2	5	0.89
(1,881)	1:93:A:LYS:HB3	1:93:A:LYS:HE2	11	0.89
(1,862)	1:109:A:LEU:HD21	1:13:A:LEU:HD23	13	0.89
(1,805)	1:7:A:VAL:HG21	1:48:A:PHE:HB3	9	0.89
(1,805)	1:7:A:VAL:HG22	1:48:A:PHE:HB3	19	0.89
(1,742)	1:72:A:LEU:HD11	1:99:A:VAL:HG13	14	0.89
(1,725)	1:33:A:ILE:HD11	1:33:A:ILE:HA	14	0.89
(1,458)	1:74:A:CYS:HB2	1:77:A:CYS:H	16	0.89
(1,148)	1:6:A:VAL:HG11	1:9:A:SER:H	19	0.89
(1,70)	1:112:A:LEU:HD21	1:17:A:HIS:H	6	0.89
(1,44)	1:99:A:VAL:HG12	1:73:A:GLU:H	5	0.89
(1,2672)	1:70:A:VAL:HG11	1:88:A:TYR:HD1	1	0.88
(1,2657)	1:20:A:LYS:HE2	1:20:A:LYS:HA	11	0.88
(1,2657)	1:20:A:LYS:HE2	1:20:A:LYS:HA	19	0.88
(1,2638)	1:107:A:MET:HA	1:39:A:MET:HE2	19	0.88
(1,2638)	1:107:A:MET:HA	1:107:A:MET:HE1	20	0.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2606)	1:57:A:VAL:HG13	1:26:A:ILE:HA	5	0.88
(1,2512)	1:10:A:LEU:HD11	1:10:A:LEU:HB3	7	0.88
(1,2204)	1:83:A:PRO:HB3	1:88:A:TYR:HE2	15	0.88
(1,2204)	1:83:A:PRO:HB3	1:88:A:TYR:HE2	19	0.88
(1,2180)	1:61:A:ALA:HB3	1:48:A:PHE:HD2	9	0.88
(1,2163)	1:45:A:VAL:HG21	1:44:A:PHE:HD2	13	0.88
(1,2047)	1:33:A:ILE:HG21	1:37:A:SER:HA	12	0.88
(1,1889)	1:82:A:LYS:HD2	1:71:A:GLU:HG3	10	0.88
(1,1842)	1:18:A:ALA:HB3	1:21:A:ASN:HB3	11	0.88
(1,1829)	1:26:A:ILE:HD13	1:23:A:ALA:HB1	15	0.88
(1,1805)	1:10:A:LEU:HD13	1:63:A:LEU:HD23	20	0.88
(1,1779)	1:31:A:VAL:HG13	1:33:A:ILE:HG12	10	0.88
(1,1778)	1:112:A:LEU:HD21	1:18:A:ALA:HB2	7	0.88
(1,1753)	1:65:A:ILE:HD11	1:41:A:LYS:HD3	8	0.88
(1,1751)	1:65:A:ILE:HD13	1:33:A:ILE:HG21	19	0.88
(1,1738)	1:65:A:ILE:HG21	1:63:A:LEU:HD11	19	0.88
(1,1708)	1:107:A:MET:HA	1:33:A:ILE:HD12	19	0.88
(1,1517)	1:7:A:VAL:HG13	1:4:A:TYR:HA	8	0.88
(1,1517)	1:7:A:VAL:HG12	1:4:A:TYR:HA	17	0.88
(1,1420)	1:25:A:LYS:HE3	1:25:A:LYS:HB3	20	0.88
(1,1276)	1:19:A:LYS:HB2	1:19:A:LYS:HE3	1	0.88
(1,1276)	1:19:A:LYS:HB2	1:19:A:LYS:HE3	10	0.88
(1,1276)	1:19:A:LYS:HB2	1:19:A:LYS:HE3	14	0.88
(1,1276)	1:19:A:LYS:HB2	1:19:A:LYS:HE3	15	0.88
(1,943)	1:6:A:VAL:HG11	1:107:A:MET:HG2	4	0.88
(1,914)	1:72:A:LEU:HD21	1:70:A:VAL:HG11	3	0.88
(1,881)	1:93:A:LYS:HB3	1:93:A:LYS:HE2	7	0.88
(1,881)	1:93:A:LYS:HB3	1:93:A:LYS:HE2	10	0.88
(1,725)	1:33:A:ILE:HD12	1:33:A:ILE:HA	19	0.88
(1,725)	1:33:A:ILE:HD11	1:33:A:ILE:HA	20	0.88
(1,55)	1:80:A:VAL:HG13	1:80:A:VAL:H	9	0.88
(1,2654)	1:6:A:VAL:HA	1:107:A:MET:HE1	20	0.87
(1,2638)	1:107:A:MET:HA	1:39:A:MET:HE1	11	0.87
(1,2633)	1:115:A:LEU:HD11	1:27:A:GLU:HB3	9	0.87
(1,2606)	1:57:A:VAL:HG13	1:26:A:ILE:HA	2	0.87
(1,2583)	1:100:A:ILE:HA	1:100:A:ILE:HD11	17	0.87
(1,2512)	1:10:A:LEU:HD13	1:10:A:LEU:HB3	3	0.87
(1,2512)	1:56:A:LEU:HD22	1:56:A:LEU:HB3	10	0.87
(1,2144)	1:7:A:VAL:HG22	1:4:A:TYR:HD1	13	0.87
(1,2127)	1:7:A:VAL:HG13	1:4:A:TYR:HD2	1	0.87
(1,2127)	1:7:A:VAL:HG11	1:4:A:TYR:HD1	13	0.87
(1,2123)	1:11:A:ILE:HD12	1:48:A:PHE:HE2	19	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2091)	1:65:A:ILE:HA	1:31:A:VAL:HG12	8	0.87
(1,2091)	1:65:A:ILE:HA	1:31:A:VAL:HG12	11	0.87
(1,2088)	1:105:A:ASN:HA	1:36:A:ARG:HB3	16	0.87
(1,2073)	1:27:A:GLU:HA	1:25:A:LYS:HE3	7	0.87
(1,2047)	1:33:A:ILE:HG21	1:37:A:SER:HA	4	0.87
(1,1870)	1:20:A:LYS:HG2	1:16:A:GLU:HG3	3	0.87
(1,1864)	1:9:A:SER:HB2	1:12:A:ALA:HB2	16	0.87
(1,1814)	1:107:A:MET:HE3	1:10:A:LEU:HD23	4	0.87
(1,1782)	1:109:A:LEU:HD22	1:107:A:MET:HE2	10	0.87
(1,1779)	1:31:A:VAL:HG11	1:33:A:ILE:HG12	11	0.87
(1,1776)	1:80:A:VAL:HG12	1:73:A:GLU:HG2	17	0.87
(1,1737)	1:33:A:ILE:HG13	1:39:A:MET:HE1	2	0.87
(1,1695)	1:64:A:ASP:HB2	1:30:A:VAL:HA	10	0.87
(1,1628)	1:61:A:ALA:HB2	1:27:A:GLU:HA	8	0.87
(1,1565)	1:100:A:ILE:HD11	1:102:A:THR:HA	15	0.87
(1,1565)	1:100:A:ILE:HD13	1:102:A:THR:HA	20	0.87
(1,1517)	1:7:A:VAL:HG12	1:4:A:TYR:HA	18	0.87
(1,1482)	1:7:A:VAL:HG21	1:48:A:PHE:HA	5	0.87
(1,1420)	1:25:A:LYS:HE3	1:25:A:LYS:HB3	11	0.87
(1,1356)	1:107:A:MET:HG2	1:107:A:MET:HE3	1	0.87
(1,1356)	1:107:A:MET:HG2	1:107:A:MET:HE2	13	0.87
(1,1265)	1:102:A:THR:HG23	1:73:A:GLU:HG2	14	0.87
(1,1019)	1:102:A:THR:HG22	1:100:A:ILE:HG12	10	0.87
(1,962)	1:33:A:ILE:HD13	1:41:A:LYS:HG3	5	0.87
(1,914)	1:72:A:LEU:HD21	1:70:A:VAL:HG11	17	0.87
(1,910)	1:109:A:LEU:HD12	1:13:A:LEU:HD13	6	0.87
(1,823)	1:30:A:VAL:HG12	1:111:A:SER:HB2	5	0.87
(1,823)	1:30:A:VAL:HG12	1:111:A:SER:HB2	17	0.87
(1,725)	1:33:A:ILE:HD13	1:33:A:ILE:HA	1	0.87
(1,725)	1:33:A:ILE:HD12	1:33:A:ILE:HA	11	0.87
(1,330)	1:68:A:GLU:HG2	1:33:A:ILE:H	18	0.87
(1,148)	1:6:A:VAL:HG13	1:9:A:SER:H	8	0.87
(1,84)	1:99:A:VAL:HG21	1:91:A:CYS:H	9	0.87
(1,55)	1:80:A:VAL:HG13	1:80:A:VAL:H	4	0.87
(1,55)	1:80:A:VAL:HG13	1:80:A:VAL:H	12	0.87
(1,55)	1:80:A:VAL:HG11	1:80:A:VAL:H	19	0.87
(1,2657)	1:20:A:LYS:HE2	1:20:A:LYS:HA	7	0.86
(1,2583)	1:100:A:ILE:HA	1:100:A:ILE:HD12	11	0.86
(1,2512)	1:56:A:LEU:HD21	1:56:A:LEU:HB3	15	0.86
(1,1938)	1:71:A:GLU:HG2	1:103:A:GLN:HG2	3	0.86
(1,1907)	1:25:A:LYS:HB2	1:57:A:VAL:HG13	19	0.86
(1,1778)	1:112:A:LEU:HD21	1:18:A:ALA:HB2	20	0.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1738)	1:65:A:ILE:HG21	1:63:A:LEU:HD11	4	0.86
(1,1695)	1:64:A:ASP:HB2	1:30:A:VAL:HA	12	0.86
(1,1606)	1:10:A:LEU:HD23	1:10:A:LEU:HA	4	0.86
(1,1606)	1:10:A:LEU:HD22	1:10:A:LEU:HA	14	0.86
(1,1517)	1:7:A:VAL:HG13	1:4:A:TYR:HA	7	0.86
(1,1517)	1:7:A:VAL:HG11	1:4:A:TYR:HA	10	0.86
(1,1482)	1:7:A:VAL:HG23	1:48:A:PHE:HA	15	0.86
(1,1421)	1:51:A:PHE:HB2	1:7:A:VAL:HG22	20	0.86
(1,1276)	1:19:A:LYS:HB2	1:19:A:LYS:HE3	9	0.86
(1,943)	1:6:A:VAL:HG13	1:107:A:MET:HG2	6	0.86
(1,823)	1:30:A:VAL:HG12	1:111:A:SER:HB2	2	0.86
(1,760)	1:110:A:LEU:HD12	1:110:A:LEU:HA	6	0.86
(1,760)	1:110:A:LEU:HD11	1:110:A:LEU:HA	14	0.86
(1,725)	1:33:A:ILE:HD11	1:33:A:ILE:HA	6	0.86
(1,330)	1:68:A:GLU:HG2	1:33:A:ILE:H	2	0.86
(1,148)	1:6:A:VAL:HG12	1:9:A:SER:H	4	0.86
(1,100)	1:57:A:VAL:HG13	1:57:A:VAL:H	19	0.86
(1,55)	1:80:A:VAL:HG13	1:80:A:VAL:H	2	0.86
(1,7)	1:72:A:LEU:HD11	1:73:A:GLU:H	10	0.86
(1,2657)	1:20:A:LYS:HE2	1:20:A:LYS:HA	14	0.85
(1,2657)	1:20:A:LYS:HE2	1:20:A:LYS:HA	18	0.85
(1,2638)	1:107:A:MET:HA	1:107:A:MET:HE2	17	0.85
(1,2633)	1:115:A:LEU:HD12	1:27:A:GLU:HB3	4	0.85
(1,2621)	1:38:A:ALA:HB3	1:105:A:ASN:HB2	10	0.85
(1,2583)	1:100:A:ILE:HA	1:100:A:ILE:HD13	13	0.85
(1,2563)	1:45:A:VAL:HA	1:63:A:LEU:HD21	5	0.85
(1,2563)	1:45:A:VAL:HA	1:63:A:LEU:HD23	14	0.85
(1,2563)	1:45:A:VAL:HA	1:63:A:LEU:HD23	15	0.85
(1,2512)	1:56:A:LEU:HD23	1:56:A:LEU:HB3	19	0.85
(1,2091)	1:65:A:ILE:HA	1:31:A:VAL:HG13	17	0.85
(1,2091)	1:65:A:ILE:HA	1:31:A:VAL:HG11	20	0.85
(1,2023)	1:7:A:VAL:HA	1:11:A:ILE:HD12	12	0.85
(1,1962)	1:97:A:LYS:HB2	1:90:A:VAL:HG13	12	0.85
(1,1907)	1:25:A:LYS:HB2	1:57:A:VAL:HG11	16	0.85
(1,1870)	1:20:A:LYS:HG2	1:16:A:GLU:HG3	18	0.85
(1,1840)	1:75:A:LYS:HG3	1:100:A:ILE:HG13	11	0.85
(1,1823)	1:45:A:VAL:HG11	1:41:A:LYS:HE2	6	0.85
(1,1782)	1:109:A:LEU:HD23	1:107:A:MET:HE3	16	0.85
(1,1746)	1:90:A:VAL:HG23	1:87:A:ASP:HB3	8	0.85
(1,1695)	1:64:A:ASP:HB2	1:30:A:VAL:HA	15	0.85
(1,1606)	1:10:A:LEU:HD21	1:10:A:LEU:HA	10	0.85
(1,1538)	1:99:A:VAL:HG21	1:91:A:CYS:HA	4	0.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1514)	1:43:A:LEU:HD22	1:42:A:SER:HB3	1	0.85
(1,1276)	1:19:A:LYS:HB2	1:19:A:LYS:HE3	8	0.85
(1,1140)	1:59:A:LYS:HD2	1:59:A:LYS:HA	13	0.85
(1,943)	1:6:A:VAL:HG13	1:107:A:MET:HG2	17	0.85
(1,914)	1:72:A:LEU:HD21	1:70:A:VAL:HG11	9	0.85
(1,804)	1:66:A:VAL:HG13	1:32:A:GLY:HA3	19	0.85
(1,742)	1:72:A:LEU:HD13	1:99:A:VAL:HG11	18	0.85
(1,725)	1:33:A:ILE:HD11	1:33:A:ILE:HA	7	0.85
(1,725)	1:33:A:ILE:HD13	1:33:A:ILE:HA	16	0.85
(1,458)	1:74:A:CYS:HB2	1:77:A:CYS:H	10	0.85
(1,330)	1:68:A:GLU:HG2	1:33:A:ILE:H	1	0.85
(1,253)	1:68:A:GLU:HG3	1:69:A:LYS:H	14	0.85
(1,197)	1:12:A:ALA:HB2	1:16:A:GLU:H	15	0.85
(1,148)	1:6:A:VAL:HG11	1:9:A:SER:H	10	0.85
(1,136)	1:102:A:THR:HG22	1:100:A:ILE:H	20	0.85
(1,120)	1:13:A:LEU:HD13	1:13:A:LEU:H	8	0.85
(1,70)	1:112:A:LEU:HD22	1:17:A:HIS:H	9	0.85
(1,15)	1:7:A:VAL:HG12	1:47:A:ALA:H	3	0.85
(1,7)	1:72:A:LEU:HD11	1:73:A:GLU:H	7	0.85
(1,2657)	1:20:A:LYS:HE2	1:20:A:LYS:HA	12	0.84
(1,2657)	1:20:A:LYS:HE2	1:20:A:LYS:HA	17	0.84
(1,2618)	1:6:A:VAL:HG22	1:2:A:HIS:HB2	20	0.84
(1,2091)	1:65:A:ILE:HA	1:31:A:VAL:HG12	9	0.84
(1,2016)	1:93:A:LYS:HD2	1:79:A:HIS:HB2	9	0.84
(1,1960)	1:113:A:GLU:HG3	1:27:A:GLU:HB3	2	0.84
(1,1870)	1:20:A:LYS:HG2	1:16:A:GLU:HG3	5	0.84
(1,1870)	1:20:A:LYS:HG2	1:16:A:GLU:HG3	11	0.84
(1,1842)	1:18:A:ALA:HB3	1:21:A:ASN:HB3	10	0.84
(1,1831)	1:58:A:CYS:HB2	1:61:A:ALA:HB1	1	0.84
(1,1829)	1:26:A:ILE:HD12	1:23:A:ALA:HB1	2	0.84
(1,1824)	1:25:A:LYS:HG3	1:56:A:LEU:HD12	9	0.84
(1,1739)	1:33:A:ILE:HG23	1:65:A:ILE:HG22	7	0.84
(1,1738)	1:65:A:ILE:HG23	1:63:A:LEU:HD13	7	0.84
(1,1645)	1:72:A:LEU:HD12	1:88:A:TYR:HA	13	0.84
(1,1628)	1:61:A:ALA:HB3	1:27:A:GLU:HA	12	0.84
(1,1538)	1:99:A:VAL:HG22	1:91:A:CYS:HA	2	0.84
(1,1538)	1:99:A:VAL:HG21	1:91:A:CYS:HA	3	0.84
(1,1391)	1:58:A:CYS:HB3	1:55:A:SER:HB2	8	0.84
(1,1276)	1:19:A:LYS:HB2	1:19:A:LYS:HE3	2	0.84
(1,1276)	1:19:A:LYS:HB2	1:19:A:LYS:HE2	20	0.84
(1,1140)	1:59:A:LYS:HD2	1:59:A:LYS:HA	4	0.84
(1,914)	1:72:A:LEU:HD22	1:70:A:VAL:HG13	11	0.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,862)	1:109:A:LEU:HD21	1:13:A:LEU:HD23	2	0.84
(1,805)	1:7:A:VAL:HG23	1:48:A:PHE:HB3	2	0.84
(1,804)	1:66:A:VAL:HG12	1:32:A:GLY:HA3	16	0.84
(1,770)	1:72:A:LEU:HD12	1:70:A:VAL:HG21	6	0.84
(1,760)	1:110:A:LEU:HD11	1:110:A:LEU:HA	9	0.84
(1,745)	1:72:A:LEU:HD11	1:72:A:LEU:HA	1	0.84
(1,745)	1:72:A:LEU:HD12	1:72:A:LEU:HA	4	0.84
(1,745)	1:72:A:LEU:HD11	1:72:A:LEU:HA	10	0.84
(1,745)	1:72:A:LEU:HD12	1:72:A:LEU:HA	17	0.84
(1,725)	1:33:A:ILE:HD13	1:33:A:ILE:HA	3	0.84
(1,725)	1:33:A:ILE:HD13	1:33:A:ILE:HA	4	0.84
(1,458)	1:74:A:CYS:HB2	1:77:A:CYS:H	1	0.84
(1,458)	1:74:A:CYS:HB2	1:77:A:CYS:H	2	0.84
(1,458)	1:74:A:CYS:HB2	1:77:A:CYS:H	15	0.84
(1,253)	1:68:A:GLU:HG3	1:69:A:LYS:H	18	0.84
(1,195)	1:12:A:ALA:HB2	1:15:A:GLU:H	9	0.84
(1,176)	1:18:A:ALA:HB2	1:16:A:GLU:H	18	0.84
(1,100)	1:57:A:VAL:HG11	1:57:A:VAL:H	10	0.84
(1,100)	1:57:A:VAL:HG13	1:57:A:VAL:H	20	0.84
(1,70)	1:112:A:LEU:HD21	1:17:A:HIS:H	16	0.84
(1,44)	1:99:A:VAL:HG12	1:73:A:GLU:H	16	0.84
(1,2657)	1:20:A:LYS:HE2	1:20:A:LYS:HA	13	0.83
(1,2651)	1:7:A:VAL:HA	1:48:A:PHE:HA	14	0.83
(1,2612)	1:59:A:LYS:HE2	1:56:A:LEU:HD13	20	0.83
(1,2606)	1:57:A:VAL:HG12	1:26:A:ILE:HA	4	0.83
(1,2606)	1:57:A:VAL:HG13	1:26:A:ILE:HA	6	0.83
(1,2563)	1:45:A:VAL:HA	1:63:A:LEU:HD21	3	0.83
(1,2563)	1:45:A:VAL:HA	1:63:A:LEU:HD23	6	0.83
(1,2512)	1:56:A:LEU:HD22	1:56:A:LEU:HB3	8	0.83
(1,2204)	1:83:A:PRO:HB3	1:88:A:TYR:HE1	4	0.83
(1,2204)	1:83:A:PRO:HB3	1:88:A:TYR:HE1	10	0.83
(1,2134)	1:72:A:LEU:HD21	1:81:A:PHE:HE1	20	0.83
(1,2084)	1:58:A:CYS:HA	1:26:A:ILE:HG23	11	0.83
(1,2023)	1:7:A:VAL:HA	1:11:A:ILE:HD12	10	0.83
(1,2016)	1:93:A:LYS:HD2	1:79:A:HIS:HB2	1	0.83
(1,1732)	1:72:A:LEU:HD11	1:89:A:GLY:HA3	9	0.83
(1,1723)	1:45:A:VAL:HG13	1:63:A:LEU:HD21	12	0.83
(1,1517)	1:7:A:VAL:HG11	1:4:A:TYR:HA	15	0.83
(1,1514)	1:43:A:LEU:HD22	1:42:A:SER:HB3	20	0.83
(1,1482)	1:7:A:VAL:HG22	1:48:A:PHE:HA	13	0.83
(1,943)	1:6:A:VAL:HG12	1:107:A:MET:HG2	2	0.83
(1,851)	1:101:A:ILE:HD11	1:105:A:ASN:HB3	1	0.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,823)	1:30:A:VAL:HG12	1:111:A:SER:HB2	11	0.83
(1,804)	1:66:A:VAL:HG11	1:32:A:GLY:HA3	7	0.83
(1,760)	1:110:A:LEU:HD12	1:110:A:LEU:HA	18	0.83
(1,725)	1:33:A:ILE:HD13	1:33:A:ILE:HA	15	0.83
(1,299)	1:39:A:MET:HE1	1:6:A:VAL:H	12	0.83
(1,253)	1:68:A:GLU:HG3	1:69:A:LYS:H	12	0.83
(1,253)	1:68:A:GLU:HG3	1:69:A:LYS:H	16	0.83
(1,176)	1:18:A:ALA:HB2	1:16:A:GLU:H	6	0.83
(1,148)	1:6:A:VAL:HG11	1:9:A:SER:H	2	0.83
(1,148)	1:6:A:VAL:HG11	1:9:A:SER:H	3	0.83
(1,144)	1:47:A:ALA:HB1	1:50:A:THR:H	9	0.83
(1,84)	1:99:A:VAL:HG21	1:91:A:CYS:H	6	0.83
(1,55)	1:80:A:VAL:HG11	1:80:A:VAL:H	5	0.83
(1,55)	1:80:A:VAL:HG12	1:80:A:VAL:H	7	0.83
(1,55)	1:80:A:VAL:HG12	1:80:A:VAL:H	8	0.83
(1,55)	1:80:A:VAL:HG13	1:80:A:VAL:H	11	0.83
(1,55)	1:80:A:VAL:HG13	1:80:A:VAL:H	16	0.83
(1,44)	1:99:A:VAL:HG11	1:73:A:GLU:H	11	0.83
(1,15)	1:7:A:VAL:HG12	1:47:A:ALA:H	11	0.83
(1,15)	1:7:A:VAL:HG11	1:47:A:ALA:H	13	0.83
(1,2678)	1:107:A:MET:HE1	1:44:A:PHE:HZ	17	0.82
(1,2672)	1:10:A:LEU:HD12	1:48:A:PHE:HD1	13	0.82
(1,2657)	1:20:A:LYS:HE2	1:20:A:LYS:HA	3	0.82
(1,2638)	1:107:A:MET:HA	1:107:A:MET:HE2	8	0.82
(1,2618)	1:6:A:VAL:HG22	1:2:A:HIS:HB2	8	0.82
(1,2606)	1:57:A:VAL:HG13	1:26:A:ILE:HA	20	0.82
(1,2583)	1:100:A:ILE:HA	1:100:A:ILE:HD13	7	0.82
(1,2225)	1:36:A:ARG:HD2	1:88:A:TYR:HD1	5	0.82
(1,2170)	1:92:A:GLU:HG3	1:81:A:PHE:HD1	6	0.82
(1,2163)	1:45:A:VAL:HG23	1:44:A:PHE:HD2	1	0.82
(1,2163)	1:45:A:VAL:HG23	1:44:A:PHE:HD2	4	0.82
(1,2144)	1:7:A:VAL:HG21	1:4:A:TYR:HD2	1	0.82
(1,2127)	1:7:A:VAL:HG11	1:4:A:TYR:HD1	6	0.82
(1,2125)	1:11:A:ILE:HD12	1:48:A:PHE:HZ	19	0.82
(1,2100)	1:97:A:LYS:HA	1:97:A:LYS:HE3	2	0.82
(1,2023)	1:7:A:VAL:HA	1:11:A:ILE:HD11	2	0.82
(1,2023)	1:7:A:VAL:HA	1:11:A:ILE:HD12	3	0.82
(1,2023)	1:7:A:VAL:HA	1:11:A:ILE:HD11	14	0.82
(1,2023)	1:7:A:VAL:HA	1:11:A:ILE:HD13	18	0.82
(1,1812)	1:50:A:THR:HG22	1:47:A:ALA:HA	12	0.82
(1,1792)	1:11:A:ILE:HG23	1:52:A:ARG:HA	20	0.82
(1,1776)	1:80:A:VAL:HG12	1:73:A:GLU:HG2	15	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1761)	1:110:A:LEU:HD23	1:108:A:ARG:HD2	19	0.82
(1,1751)	1:65:A:ILE:HD12	1:33:A:ILE:HG23	20	0.82
(1,1746)	1:90:A:VAL:HG21	1:87:A:ASP:HB3	6	0.82
(1,1695)	1:64:A:ASP:HB2	1:30:A:VAL:HA	16	0.82
(1,1606)	1:10:A:LEU:HD21	1:10:A:LEU:HA	2	0.82
(1,1606)	1:10:A:LEU:HD22	1:10:A:LEU:HA	20	0.82
(1,1517)	1:7:A:VAL:HG12	1:4:A:TYR:HA	3	0.82
(1,1514)	1:43:A:LEU:HD23	1:42:A:SER:HB2	4	0.82
(1,1418)	1:91:A:CYS:HB2	1:99:A:VAL:HG23	1	0.82
(1,1145)	1:41:A:LYS:HD2	1:33:A:ILE:HG22	11	0.82
(1,1140)	1:59:A:LYS:HD2	1:59:A:LYS:HA	10	0.82
(1,929)	1:100:A:ILE:HG22	1:100:A:ILE:HG13	13	0.82
(1,929)	1:100:A:ILE:HG21	1:100:A:ILE:HG13	19	0.82
(1,822)	1:80:A:VAL:HG11	1:102:A:THR:HG22	3	0.82
(1,813)	1:29:A:VAL:HG23	1:10:A:LEU:HD12	3	0.82
(1,760)	1:110:A:LEU:HD12	1:110:A:LEU:HA	12	0.82
(1,760)	1:110:A:LEU:HD11	1:110:A:LEU:HA	20	0.82
(1,725)	1:33:A:ILE:HD11	1:33:A:ILE:HA	5	0.82
(1,725)	1:33:A:ILE:HD11	1:33:A:ILE:HA	8	0.82
(1,725)	1:33:A:ILE:HD13	1:33:A:ILE:HA	10	0.82
(1,725)	1:33:A:ILE:HD13	1:33:A:ILE:HA	13	0.82
(1,458)	1:74:A:CYS:HB2	1:77:A:CYS:H	11	0.82
(1,195)	1:12:A:ALA:HB1	1:15:A:GLU:H	3	0.82
(1,148)	1:6:A:VAL:HG13	1:9:A:SER:H	11	0.82
(1,100)	1:57:A:VAL:HG13	1:57:A:VAL:H	11	0.82
(1,72)	1:31:A:VAL:HG13	1:108:A:ARG:H	19	0.82
(1,55)	1:80:A:VAL:HG13	1:80:A:VAL:H	6	0.82
(1,55)	1:80:A:VAL:HG13	1:80:A:VAL:H	15	0.82
(1,15)	1:7:A:VAL:HG11	1:47:A:ALA:H	19	0.82
(1,2672)	1:70:A:VAL:HG11	1:88:A:TYR:HD2	15	0.81
(1,2657)	1:20:A:LYS:HE2	1:20:A:LYS:HA	6	0.81
(1,2657)	1:20:A:LYS:HE2	1:20:A:LYS:HA	8	0.81
(1,2657)	1:20:A:LYS:HE2	1:20:A:LYS:HA	16	0.81
(1,2652)	1:45:A:VAL:HA	1:47:A:ALA:HB2	19	0.81
(1,2606)	1:57:A:VAL:HG13	1:26:A:ILE:HA	14	0.81
(1,2606)	1:57:A:VAL:HG11	1:26:A:ILE:HA	15	0.81
(1,2204)	1:83:A:PRO:HB3	1:88:A:TYR:HE2	16	0.81
(1,2127)	1:7:A:VAL:HG12	1:4:A:TYR:HD1	4	0.81
(1,2127)	1:7:A:VAL:HG12	1:4:A:TYR:HD2	18	0.81
(1,2047)	1:33:A:ILE:HG22	1:37:A:SER:HA	1	0.81
(1,1829)	1:26:A:ILE:HD12	1:23:A:ALA:HB3	11	0.81
(1,1751)	1:65:A:ILE:HD13	1:33:A:ILE:HG23	18	0.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1739)	1:33:A:ILE:HG23	1:65:A:ILE:HG21	18	0.81
(1,1723)	1:45:A:VAL:HG11	1:63:A:LEU:HD23	14	0.81
(1,1708)	1:107:A:MET:HA	1:33:A:ILE:HD11	7	0.81
(1,1695)	1:64:A:ASP:HB2	1:30:A:VAL:HA	2	0.81
(1,1606)	1:10:A:LEU:HD22	1:10:A:LEU:HA	9	0.81
(1,1466)	1:14:A:CYS:HB2	1:11:A:ILE:HA	11	0.81
(1,1324)	1:106:A:GLU:HG2	1:105:A:ASN:HB2	5	0.81
(1,1269)	1:80:A:VAL:HG21	1:73:A:GLU:HG2	10	0.81
(1,1140)	1:59:A:LYS:HD2	1:59:A:LYS:HA	17	0.81
(1,1020)	1:85:A:ALA:HB2	1:86:A:LEU:HA	9	0.81
(1,937)	1:102:A:THR:HG21	1:73:A:GLU:HA	10	0.81
(1,914)	1:72:A:LEU:HD22	1:70:A:VAL:HG11	6	0.81
(1,805)	1:7:A:VAL:HG22	1:48:A:PHE:HB3	4	0.81
(1,804)	1:66:A:VAL:HG12	1:32:A:GLY:HA3	9	0.81
(1,804)	1:66:A:VAL:HG12	1:32:A:GLY:HA3	14	0.81
(1,760)	1:110:A:LEU:HD11	1:110:A:LEU:HA	2	0.81
(1,745)	1:72:A:LEU:HD11	1:72:A:LEU:HA	19	0.81
(1,725)	1:33:A:ILE:HD12	1:33:A:ILE:HA	12	0.81
(1,253)	1:68:A:GLU:HG3	1:69:A:LYS:H	5	0.81
(1,253)	1:68:A:GLU:HG3	1:69:A:LYS:H	7	0.81
(1,195)	1:12:A:ALA:HB3	1:15:A:GLU:H	19	0.81
(1,123)	1:13:A:LEU:HD11	1:14:A:CYS:H	13	0.81
(1,120)	1:13:A:LEU:HD12	1:13:A:LEU:H	10	0.81
(1,110)	1:43:A:LEU:HD23	1:44:A:PHE:H	19	0.81
(1,110)	1:43:A:LEU:HD22	1:44:A:PHE:H	20	0.81
(1,100)	1:57:A:VAL:HG13	1:57:A:VAL:H	6	0.81
(1,100)	1:57:A:VAL:HG13	1:57:A:VAL:H	7	0.81
(1,100)	1:57:A:VAL:HG12	1:57:A:VAL:H	9	0.81
(1,100)	1:57:A:VAL:HG11	1:57:A:VAL:H	13	0.81
(1,55)	1:80:A:VAL:HG12	1:80:A:VAL:H	10	0.81
(1,40)	1:99:A:VAL:HG11	1:89:A:GLY:H	20	0.81
(1,38)	1:99:A:VAL:HG12	1:90:A:VAL:H	9	0.81
(1,2657)	1:20:A:LYS:HE2	1:20:A:LYS:HA	9	0.8
(1,2622)	1:38:A:ALA:HB3	1:1:A:MET:HB2	14	0.8
(1,2597)	1:72:A:LEU:HB2	1:99:A:VAL:HG23	1	0.8
(1,2597)	1:72:A:LEU:HB2	1:99:A:VAL:HG21	17	0.8
(1,2583)	1:100:A:ILE:HA	1:100:A:ILE:HD11	8	0.8
(1,2563)	1:45:A:VAL:HA	1:63:A:LEU:HD23	17	0.8
(1,2512)	1:10:A:LEU:HD13	1:10:A:LEU:HB3	18	0.8
(1,2463)	1:56:A:LEU:HD23	1:56:A:LEU:HD12	6	0.8
(1,2438)	1:65:A:ILE:HD13	1:41:A:LYS:HD2	8	0.8
(1,2177)	1:6:A:VAL:HG11	1:44:A:PHE:HD1	6	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2163)	1:45:A:VAL:HG23	1:44:A:PHE:HD2	2	0.8
(1,2100)	1:97:A:LYS:HA	1:97:A:LYS:HE3	6	0.8
(1,2089)	1:79:A:HIS:HA	1:80:A:VAL:HG23	2	0.8
(1,2047)	1:33:A:ILE:HG21	1:37:A:SER:HA	3	0.8
(1,2047)	1:33:A:ILE:HG21	1:37:A:SER:HA	7	0.8
(1,2023)	1:7:A:VAL:HA	1:11:A:ILE:HD13	13	0.8
(1,1907)	1:25:A:LYS:HB2	1:57:A:VAL:HG13	8	0.8
(1,1870)	1:20:A:LYS:HG2	1:16:A:GLU:HG3	12	0.8
(1,1870)	1:20:A:LYS:HG2	1:16:A:GLU:HG3	20	0.8
(1,1857)	1:75:A:LYS:HG2	1:98:A:ASN:HB2	12	0.8
(1,1831)	1:58:A:CYS:HB2	1:61:A:ALA:HB2	2	0.8
(1,1805)	1:10:A:LEU:HD13	1:63:A:LEU:HD22	11	0.8
(1,1793)	1:15:A:GLU:HG2	1:11:A:ILE:HG23	10	0.8
(1,1708)	1:107:A:MET:HA	1:33:A:ILE:HD13	15	0.8
(1,1695)	1:64:A:ASP:HB2	1:30:A:VAL:HA	17	0.8
(1,1628)	1:61:A:ALA:HB2	1:27:A:GLU:HA	20	0.8
(1,1517)	1:7:A:VAL:HG12	1:4:A:TYR:HA	4	0.8
(1,1482)	1:7:A:VAL:HG23	1:48:A:PHE:HA	2	0.8
(1,1276)	1:19:A:LYS:HB2	1:19:A:LYS:HE3	19	0.8
(1,1006)	1:100:A:ILE:HD13	1:75:A:LYS:HG3	10	0.8
(1,929)	1:100:A:ILE:HG21	1:100:A:ILE:HG13	7	0.8
(1,929)	1:100:A:ILE:HG21	1:100:A:ILE:HG13	8	0.8
(1,865)	1:26:A:ILE:HD13	1:114:A:MET:HE3	14	0.8
(1,851)	1:101:A:ILE:HD11	1:105:A:ASN:HB3	5	0.8
(1,760)	1:110:A:LEU:HD11	1:110:A:LEU:HA	7	0.8
(1,760)	1:110:A:LEU:HD11	1:110:A:LEU:HA	15	0.8
(1,745)	1:72:A:LEU:HD11	1:72:A:LEU:HA	6	0.8
(1,745)	1:72:A:LEU:HD11	1:72:A:LEU:HA	11	0.8
(1,725)	1:33:A:ILE:HD13	1:33:A:ILE:HA	17	0.8
(1,458)	1:74:A:CYS:HB2	1:77:A:CYS:H	3	0.8
(1,330)	1:68:A:GLU:HG2	1:33:A:ILE:H	3	0.8
(1,330)	1:68:A:GLU:HG2	1:33:A:ILE:H	13	0.8
(1,300)	1:107:A:MET:HE3	1:108:A:ARG:H	5	0.8
(1,253)	1:68:A:GLU:HG3	1:69:A:LYS:H	15	0.8
(1,197)	1:12:A:ALA:HB1	1:16:A:GLU:H	11	0.8
(1,176)	1:18:A:ALA:HB1	1:16:A:GLU:H	7	0.8
(1,176)	1:18:A:ALA:HB2	1:16:A:GLU:H	9	0.8
(1,176)	1:18:A:ALA:HB1	1:16:A:GLU:H	11	0.8
(1,123)	1:13:A:LEU:HD12	1:14:A:CYS:H	2	0.8
(1,110)	1:43:A:LEU:HD21	1:44:A:PHE:H	11	0.8
(1,100)	1:57:A:VAL:HG12	1:57:A:VAL:H	4	0.8
(1,100)	1:57:A:VAL:HG13	1:57:A:VAL:H	8	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,100)	1:57:A:VAL:HG13	1:57:A:VAL:H	17	0.8
(1,55)	1:80:A:VAL:HG11	1:80:A:VAL:H	3	0.8
(1,55)	1:80:A:VAL:HG11	1:80:A:VAL:H	13	0.8
(1,55)	1:80:A:VAL:HG11	1:80:A:VAL:H	18	0.8
(1,53)	1:66:A:VAL:HG12	1:33:A:ILE:H	18	0.8
(1,44)	1:99:A:VAL:HG13	1:73:A:GLU:H	1	0.8
(1,44)	1:99:A:VAL:HG13	1:73:A:GLU:H	4	0.8
(1,38)	1:99:A:VAL:HG13	1:90:A:VAL:H	15	0.8
(1,2672)	1:70:A:VAL:HG11	1:88:A:TYR:HD1	6	0.79
(1,2638)	1:107:A:MET:HA	1:107:A:MET:HE2	18	0.79
(1,2618)	1:6:A:VAL:HG23	1:2:A:HIS:HB2	17	0.79
(1,2606)	1:57:A:VAL:HG13	1:26:A:ILE:HA	19	0.79
(1,2463)	1:43:A:LEU:HD21	1:43:A:LEU:HD12	20	0.79
(1,2127)	1:7:A:VAL:HG13	1:4:A:TYR:HD1	7	0.79
(1,2105)	1:64:A:ASP:HA	1:62:A:ILE:HG21	19	0.79
(1,2088)	1:105:A:ASN:HA	1:36:A:ARG:HB3	1	0.79
(1,2088)	1:105:A:ASN:HA	1:36:A:ARG:HB3	8	0.79
(1,2069)	1:112:A:LEU:HD23	1:29:A:VAL:HA	18	0.79
(1,2047)	1:33:A:ILE:HG23	1:37:A:SER:HA	16	0.79
(1,1994)	1:3:A:GLU:HG2	1:40:A:ASP:HB2	14	0.79
(1,1870)	1:20:A:LYS:HG2	1:16:A:GLU:HG3	4	0.79
(1,1824)	1:25:A:LYS:HG3	1:56:A:LEU:HD11	16	0.79
(1,1814)	1:107:A:MET:HE2	1:10:A:LEU:HD22	12	0.79
(1,1776)	1:80:A:VAL:HG12	1:73:A:GLU:HG2	6	0.79
(1,1739)	1:33:A:ILE:HG23	1:65:A:ILE:HG21	1	0.79
(1,1739)	1:33:A:ILE:HG23	1:65:A:ILE:HG22	3	0.79
(1,1708)	1:107:A:MET:HA	1:33:A:ILE:HD12	2	0.79
(1,1695)	1:64:A:ASP:HB2	1:30:A:VAL:HA	6	0.79
(1,1606)	1:10:A:LEU:HD22	1:10:A:LEU:HA	17	0.79
(1,1363)	1:23:A:ALA:HB3	1:114:A:MET:HG2	17	0.79
(1,1276)	1:19:A:LYS:HB2	1:19:A:LYS:HE2	11	0.79
(1,1276)	1:19:A:LYS:HB2	1:19:A:LYS:HE3	17	0.79
(1,1019)	1:102:A:THR:HG23	1:100:A:ILE:HG12	3	0.79
(1,929)	1:100:A:ILE:HG22	1:100:A:ILE:HG13	3	0.79
(1,929)	1:100:A:ILE:HG22	1:100:A:ILE:HG13	4	0.79
(1,914)	1:72:A:LEU:HD22	1:70:A:VAL:HG11	14	0.79
(1,823)	1:30:A:VAL:HG11	1:111:A:SER:HB2	15	0.79
(1,760)	1:110:A:LEU:HD13	1:110:A:LEU:HA	8	0.79
(1,745)	1:72:A:LEU:HD13	1:72:A:LEU:HA	9	0.79
(1,745)	1:72:A:LEU:HD12	1:72:A:LEU:HA	16	0.79
(1,745)	1:72:A:LEU:HD13	1:72:A:LEU:HA	18	0.79
(1,330)	1:68:A:GLU:HG2	1:33:A:ILE:H	17	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,253)	1:68:A:GLU:HG3	1:69:A:LYS:H	1	0.79
(1,253)	1:68:A:GLU:HG3	1:69:A:LYS:H	9	0.79
(1,195)	1:12:A:ALA:HB3	1:15:A:GLU:H	17	0.79
(1,176)	1:18:A:ALA:HB2	1:16:A:GLU:H	5	0.79
(1,148)	1:6:A:VAL:HG12	1:9:A:SER:H	15	0.79
(1,110)	1:43:A:LEU:HD21	1:44:A:PHE:H	9	0.79
(1,100)	1:57:A:VAL:HG11	1:57:A:VAL:H	2	0.79
(1,100)	1:57:A:VAL:HG12	1:57:A:VAL:H	3	0.79
(1,100)	1:57:A:VAL:HG11	1:57:A:VAL:H	5	0.79
(1,84)	1:99:A:VAL:HG21	1:91:A:CYS:H	10	0.79
(1,84)	1:99:A:VAL:HG21	1:91:A:CYS:H	16	0.79
(1,70)	1:112:A:LEU:HD22	1:17:A:HIS:H	17	0.79
(1,55)	1:80:A:VAL:HG12	1:80:A:VAL:H	14	0.79
(1,55)	1:80:A:VAL:HG13	1:80:A:VAL:H	20	0.79
(1,44)	1:99:A:VAL:HG11	1:73:A:GLU:H	6	0.79
(1,44)	1:99:A:VAL:HG13	1:73:A:GLU:H	8	0.79
(1,34)	1:33:A:ILE:HG23	1:39:A:MET:H	6	0.79
(1,15)	1:7:A:VAL:HG12	1:47:A:ALA:H	9	0.79
(1,2672)	1:70:A:VAL:HG11	1:88:A:TYR:HD2	3	0.78
(1,2657)	1:20:A:LYS:HE2	1:20:A:LYS:HA	10	0.78
(1,2654)	1:6:A:VAL:HA	1:107:A:MET:HE1	13	0.78
(1,2651)	1:45:A:VAL:HA	1:48:A:PHE:HA	11	0.78
(1,2638)	1:107:A:MET:HA	1:39:A:MET:HE1	2	0.78
(1,2638)	1:107:A:MET:HA	1:107:A:MET:HE1	3	0.78
(1,2638)	1:107:A:MET:HA	1:39:A:MET:HE3	13	0.78
(1,2633)	1:115:A:LEU:HD13	1:27:A:GLU:HB3	6	0.78
(1,2597)	1:72:A:LEU:HB2	1:99:A:VAL:HG21	20	0.78
(1,2583)	1:100:A:ILE:HA	1:100:A:ILE:HD11	5	0.78
(1,2583)	1:100:A:ILE:HA	1:100:A:ILE:HD12	12	0.78
(1,2463)	1:56:A:LEU:HD22	1:56:A:LEU:HD11	5	0.78
(1,2180)	1:61:A:ALA:HB3	1:48:A:PHE:HD2	17	0.78
(1,2163)	1:45:A:VAL:HG21	1:44:A:PHE:HD1	15	0.78
(1,2163)	1:45:A:VAL:HG23	1:44:A:PHE:HD2	20	0.78
(1,2047)	1:33:A:ILE:HG21	1:37:A:SER:HA	20	0.78
(1,2023)	1:7:A:VAL:HA	1:11:A:ILE:HD13	5	0.78
(1,1870)	1:20:A:LYS:HG2	1:16:A:GLU:HG3	6	0.78
(1,1870)	1:20:A:LYS:HG2	1:16:A:GLU:HG3	9	0.78
(1,1840)	1:75:A:LYS:HG3	1:100:A:ILE:HG13	2	0.78
(1,1831)	1:58:A:CYS:HB2	1:61:A:ALA:HB3	18	0.78
(1,1825)	1:62:A:ILE:HG22	1:62:A:ILE:HG13	15	0.78
(1,1823)	1:45:A:VAL:HG13	1:41:A:LYS:HE2	14	0.78
(1,1782)	1:109:A:LEU:HD22	1:107:A:MET:HE1	1	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1739)	1:33:A:ILE:HG22	1:65:A:ILE:HG21	12	0.78
(1,1732)	1:72:A:LEU:HD13	1:89:A:GLY:HA3	8	0.78
(1,1420)	1:25:A:LYS:HE3	1:25:A:LYS:HB3	18	0.78
(1,1356)	1:107:A:MET:HG2	1:107:A:MET:HE2	20	0.78
(1,1324)	1:106:A:GLU:HG2	1:105:A:ASN:HB2	17	0.78
(1,943)	1:6:A:VAL:HG13	1:107:A:MET:HG2	10	0.78
(1,937)	1:102:A:THR:HG23	1:73:A:GLU:HA	3	0.78
(1,937)	1:102:A:THR:HG23	1:73:A:GLU:HA	17	0.78
(1,897)	1:29:A:VAL:HG11	1:112:A:LEU:HD23	3	0.78
(1,897)	1:29:A:VAL:HG13	1:112:A:LEU:HD21	4	0.78
(1,862)	1:109:A:LEU:HD21	1:13:A:LEU:HD23	8	0.78
(1,862)	1:109:A:LEU:HD23	1:13:A:LEU:HD23	11	0.78
(1,823)	1:30:A:VAL:HG13	1:111:A:SER:HB2	18	0.78
(1,770)	1:72:A:LEU:HD12	1:70:A:VAL:HG23	1	0.78
(1,760)	1:110:A:LEU:HD13	1:110:A:LEU:HA	11	0.78
(1,745)	1:72:A:LEU:HD12	1:72:A:LEU:HA	12	0.78
(1,745)	1:72:A:LEU:HD13	1:72:A:LEU:HA	15	0.78
(1,725)	1:33:A:ILE:HD12	1:33:A:ILE:HA	2	0.78
(1,458)	1:74:A:CYS:HB2	1:77:A:CYS:H	5	0.78
(1,351)	1:103:A:GLN:HG2	1:103:A:GLN:H	8	0.78
(1,253)	1:68:A:GLU:HG3	1:69:A:LYS:H	6	0.78
(1,148)	1:6:A:VAL:HG11	1:9:A:SER:H	9	0.78
(1,120)	1:13:A:LEU:HD11	1:13:A:LEU:H	2	0.78
(1,120)	1:13:A:LEU:HD12	1:13:A:LEU:H	12	0.78
(1,120)	1:13:A:LEU:HD13	1:13:A:LEU:H	14	0.78
(1,110)	1:43:A:LEU:HD23	1:44:A:PHE:H	5	0.78
(1,100)	1:57:A:VAL:HG11	1:57:A:VAL:H	15	0.78
(1,100)	1:57:A:VAL:HG12	1:57:A:VAL:H	18	0.78
(1,88)	1:26:A:ILE:HD12	1:15:A:GLU:H	4	0.78
(1,84)	1:99:A:VAL:HG23	1:91:A:CYS:H	13	0.78
(1,44)	1:99:A:VAL:HG12	1:73:A:GLU:H	12	0.78
(1,44)	1:99:A:VAL:HG11	1:73:A:GLU:H	18	0.78
(1,38)	1:99:A:VAL:HG12	1:90:A:VAL:H	19	0.78
(1,15)	1:7:A:VAL:HG13	1:47:A:ALA:H	1	0.78
(1,2669)	1:31:A:VAL:HG23	1:44:A:PHE:HD2	7	0.77
(1,2654)	1:6:A:VAL:HA	1:107:A:MET:HE1	6	0.77
(1,2651)	1:7:A:VAL:HA	1:48:A:PHE:HA	7	0.77
(1,2638)	1:107:A:MET:HA	1:39:A:MET:HE2	9	0.77
(1,2618)	1:6:A:VAL:HG23	1:2:A:HIS:HB2	1	0.77
(1,2597)	1:72:A:LEU:HB2	1:99:A:VAL:HG21	9	0.77
(1,2105)	1:64:A:ASP:HA	1:62:A:ILE:HG23	8	0.77
(1,2084)	1:58:A:CYS:HA	1:26:A:ILE:HG22	19	0.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2023)	1:7:A:VAL:HA	1:11:A:ILE:HD12	6	0.77
(1,1994)	1:3:A:GLU:HG2	1:40:A:ASP:HB2	12	0.77
(1,1907)	1:25:A:LYS:HB2	1:57:A:VAL:HG11	11	0.77
(1,1907)	1:25:A:LYS:HB2	1:57:A:VAL:HG12	20	0.77
(1,1857)	1:75:A:LYS:HG2	1:98:A:ASN:HB2	20	0.77
(1,1793)	1:15:A:GLU:HG2	1:11:A:ILE:HG23	11	0.77
(1,1788)	1:75:A:LYS:HE3	1:100:A:ILE:HG23	17	0.77
(1,1778)	1:112:A:LEU:HD23	1:18:A:ALA:HB2	1	0.77
(1,1753)	1:65:A:ILE:HD13	1:41:A:LYS:HD3	16	0.77
(1,1751)	1:65:A:ILE:HD11	1:33:A:ILE:HG23	1	0.77
(1,1748)	1:33:A:ILE:HG22	1:107:A:MET:HG3	13	0.77
(1,1746)	1:90:A:VAL:HG21	1:87:A:ASP:HB3	5	0.77
(1,1732)	1:72:A:LEU:HD11	1:89:A:GLY:HA3	19	0.77
(1,1615)	1:10:A:LEU:HA	1:107:A:MET:HE1	18	0.77
(1,1606)	1:10:A:LEU:HD23	1:10:A:LEU:HA	11	0.77
(1,1289)	1:57:A:VAL:HG22	1:15:A:GLU:HG3	11	0.77
(1,1276)	1:19:A:LYS:HB2	1:19:A:LYS:HE3	6	0.77
(1,1024)	1:57:A:VAL:HG11	1:18:A:ALA:HB3	14	0.77
(1,1024)	1:57:A:VAL:HG12	1:18:A:ALA:HB2	15	0.77
(1,1020)	1:85:A:ALA:HB1	1:86:A:LEU:HA	15	0.77
(1,998)	1:65:A:ILE:HG12	1:63:A:LEU:HD21	18	0.77
(1,943)	1:6:A:VAL:HG12	1:107:A:MET:HG2	11	0.77
(1,921)	1:45:A:VAL:HG23	1:45:A:VAL:HA	16	0.77
(1,869)	1:26:A:ILE:HD13	1:61:A:ALA:HB3	3	0.77
(1,822)	1:80:A:VAL:HG13	1:102:A:THR:HG21	11	0.77
(1,760)	1:110:A:LEU:HD11	1:110:A:LEU:HA	13	0.77
(1,760)	1:110:A:LEU:HD11	1:110:A:LEU:HA	17	0.77
(1,760)	1:110:A:LEU:HD12	1:110:A:LEU:HA	19	0.77
(1,745)	1:72:A:LEU:HD12	1:72:A:LEU:HA	3	0.77
(1,745)	1:72:A:LEU:HD11	1:72:A:LEU:HA	7	0.77
(1,745)	1:72:A:LEU:HD11	1:72:A:LEU:HA	20	0.77
(1,725)	1:33:A:ILE:HD12	1:33:A:ILE:HA	18	0.77
(1,351)	1:103:A:GLN:HG3	1:103:A:GLN:H	15	0.77
(1,253)	1:68:A:GLU:HG3	1:69:A:LYS:H	4	0.77
(1,253)	1:68:A:GLU:HG3	1:69:A:LYS:H	11	0.77
(1,176)	1:18:A:ALA:HB1	1:16:A:GLU:H	10	0.77
(1,148)	1:6:A:VAL:HG12	1:9:A:SER:H	1	0.77
(1,148)	1:6:A:VAL:HG11	1:9:A:SER:H	13	0.77
(1,136)	1:102:A:THR:HG22	1:100:A:ILE:H	19	0.77
(1,123)	1:13:A:LEU:HD12	1:14:A:CYS:H	17	0.77
(1,100)	1:57:A:VAL:HG13	1:57:A:VAL:H	16	0.77
(1,70)	1:112:A:LEU:HD21	1:17:A:HIS:H	4	0.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,27)	1:90:A:VAL:HG23	1:89:A:GLY:H	7	0.77
(1,15)	1:7:A:VAL:HG13	1:47:A:ALA:H	2	0.77
(1,2652)	1:45:A:VAL:HA	1:47:A:ALA:HB1	7	0.76
(1,2651)	1:45:A:VAL:HA	1:48:A:PHE:HA	9	0.76
(1,2633)	1:115:A:LEU:HD11	1:27:A:GLU:HB3	3	0.76
(1,2612)	1:59:A:LYS:HE2	1:56:A:LEU:HD12	7	0.76
(1,2612)	1:25:A:LYS:HE3	1:56:A:LEU:HD13	14	0.76
(1,2583)	1:100:A:ILE:HA	1:100:A:ILE:HD13	6	0.76
(1,2463)	1:56:A:LEU:HD23	1:56:A:LEU:HD13	4	0.76
(1,2463)	1:43:A:LEU:HD22	1:43:A:LEU:HD12	14	0.76
(1,2202)	1:83:A:PRO:HB3	1:88:A:TYR:HD2	19	0.76
(1,2144)	1:7:A:VAL:HG22	1:4:A:TYR:HD1	20	0.76
(1,2127)	1:7:A:VAL:HG11	1:4:A:TYR:HD1	20	0.76
(1,2023)	1:7:A:VAL:HA	1:11:A:ILE:HD12	19	0.76
(1,1854)	1:75:A:LYS:HG2	1:100:A:ILE:HG13	6	0.76
(1,1825)	1:62:A:ILE:HG22	1:62:A:ILE:HG13	4	0.76
(1,1806)	1:10:A:LEU:HD11	1:7:A:VAL:HA	8	0.76
(1,1761)	1:110:A:LEU:HD22	1:108:A:ARG:HD2	6	0.76
(1,1738)	1:65:A:ILE:HG23	1:63:A:LEU:HD12	20	0.76
(1,1737)	1:33:A:ILE:HG13	1:39:A:MET:HE2	16	0.76
(1,1606)	1:10:A:LEU:HD23	1:10:A:LEU:HA	6	0.76
(1,1597)	1:109:A:LEU:HD12	1:109:A:LEU:HA	4	0.76
(1,1597)	1:109:A:LEU:HD12	1:109:A:LEU:HA	20	0.76
(1,1538)	1:99:A:VAL:HG21	1:91:A:CYS:HA	6	0.76
(1,1356)	1:107:A:MET:HG2	1:107:A:MET:HE3	18	0.76
(1,1269)	1:80:A:VAL:HG21	1:73:A:GLU:HG2	20	0.76
(1,1265)	1:102:A:THR:HG21	1:73:A:GLU:HG2	11	0.76
(1,1204)	1:75:A:LYS:HB3	1:98:A:ASN:HB3	19	0.76
(1,1020)	1:85:A:ALA:HB1	1:86:A:LEU:HA	10	0.76
(1,929)	1:100:A:ILE:HG22	1:100:A:ILE:HG13	9	0.76
(1,921)	1:45:A:VAL:HG21	1:45:A:VAL:HA	1	0.76
(1,921)	1:45:A:VAL:HG23	1:45:A:VAL:HA	20	0.76
(1,862)	1:109:A:LEU:HD23	1:13:A:LEU:HD21	1	0.76
(1,804)	1:66:A:VAL:HG11	1:32:A:GLY:HA3	11	0.76
(1,804)	1:66:A:VAL:HG12	1:32:A:GLY:HA3	18	0.76
(1,725)	1:33:A:ILE:HD11	1:33:A:ILE:HA	9	0.76
(1,330)	1:68:A:GLU:HG2	1:33:A:ILE:H	11	0.76
(1,330)	1:68:A:GLU:HG2	1:33:A:ILE:H	14	0.76
(1,253)	1:68:A:GLU:HG3	1:69:A:LYS:H	20	0.76
(1,195)	1:12:A:ALA:HB1	1:15:A:GLU:H	1	0.76
(1,148)	1:6:A:VAL:HG11	1:9:A:SER:H	14	0.76
(1,144)	1:47:A:ALA:HB1	1:50:A:THR:H	16	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,144)	1:47:A:ALA:HB1	1:50:A:THR:H	20	0.76
(1,120)	1:13:A:LEU:HD11	1:13:A:LEU:H	17	0.76
(1,110)	1:43:A:LEU:HD23	1:44:A:PHE:H	12	0.76
(1,50)	1:7:A:VAL:HG21	1:8:A:SER:H	3	0.76
(1,7)	1:72:A:LEU:HD12	1:73:A:GLU:H	17	0.76
(1,2678)	1:107:A:MET:HE3	1:44:A:PHE:HZ	11	0.75
(1,2669)	1:31:A:VAL:HG21	1:44:A:PHE:HD2	16	0.75
(1,2654)	1:6:A:VAL:HA	1:107:A:MET:HE2	11	0.75
(1,2654)	1:6:A:VAL:HA	1:107:A:MET:HE1	14	0.75
(1,2652)	1:45:A:VAL:HA	1:47:A:ALA:HB2	4	0.75
(1,2651)	1:45:A:VAL:HA	1:48:A:PHE:HA	10	0.75
(1,2618)	1:6:A:VAL:HG22	1:2:A:HIS:HB2	18	0.75
(1,2583)	1:100:A:ILE:HA	1:100:A:ILE:HD13	4	0.75
(1,2463)	1:43:A:LEU:HD21	1:43:A:LEU:HD13	16	0.75
(1,2463)	1:43:A:LEU:HD22	1:43:A:LEU:HD11	18	0.75
(1,2180)	1:61:A:ALA:HB3	1:48:A:PHE:HD2	10	0.75
(1,2170)	1:92:A:GLU:HG3	1:81:A:PHE:HD1	10	0.75
(1,2089)	1:79:A:HIS:HA	1:80:A:VAL:HG21	5	0.75
(1,2084)	1:58:A:CYS:HA	1:26:A:ILE:HG23	10	0.75
(1,2047)	1:33:A:ILE:HG23	1:37:A:SER:HA	2	0.75
(1,2047)	1:33:A:ILE:HG22	1:37:A:SER:HA	15	0.75
(1,1939)	1:39:A:MET:HE2	1:39:A:MET:HA	5	0.75
(1,1907)	1:25:A:LYS:HB2	1:57:A:VAL:HG11	10	0.75
(1,1907)	1:25:A:LYS:HB2	1:57:A:VAL:HG12	12	0.75
(1,1870)	1:20:A:LYS:HG2	1:16:A:GLU:HG3	15	0.75
(1,1842)	1:18:A:ALA:HB1	1:21:A:ASN:HB3	9	0.75
(1,1823)	1:45:A:VAL:HG12	1:41:A:LYS:HE2	1	0.75
(1,1753)	1:65:A:ILE:HD11	1:41:A:LYS:HD3	2	0.75
(1,1753)	1:65:A:ILE:HD12	1:41:A:LYS:HD3	12	0.75
(1,1751)	1:65:A:ILE:HD13	1:33:A:ILE:HG22	8	0.75
(1,1746)	1:90:A:VAL:HG22	1:87:A:ASP:HB3	9	0.75
(1,1739)	1:33:A:ILE:HG22	1:65:A:ILE:HG23	14	0.75
(1,1606)	1:10:A:LEU:HD23	1:10:A:LEU:HA	5	0.75
(1,1606)	1:10:A:LEU:HD22	1:10:A:LEU:HA	12	0.75
(1,1606)	1:10:A:LEU:HD21	1:10:A:LEU:HA	15	0.75
(1,1538)	1:99:A:VAL:HG21	1:91:A:CYS:HA	10	0.75
(1,1391)	1:58:A:CYS:HB3	1:55:A:SER:HB3	3	0.75
(1,1269)	1:80:A:VAL:HG21	1:73:A:GLU:HG2	7	0.75
(1,929)	1:100:A:ILE:HG23	1:100:A:ILE:HG13	11	0.75
(1,929)	1:100:A:ILE:HG23	1:100:A:ILE:HG13	16	0.75
(1,770)	1:72:A:LEU:HD13	1:70:A:VAL:HG21	17	0.75
(1,760)	1:110:A:LEU:HD13	1:110:A:LEU:HA	3	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,458)	1:74:A:CYS:HB2	1:77:A:CYS:H	9	0.75
(1,351)	1:103:A:GLN:HG2	1:103:A:GLN:H	3	0.75
(1,330)	1:68:A:GLU:HG2	1:33:A:ILE:H	16	0.75
(1,253)	1:68:A:GLU:HG3	1:69:A:LYS:H	8	0.75
(1,253)	1:68:A:GLU:HG3	1:69:A:LYS:H	13	0.75
(1,195)	1:12:A:ALA:HB3	1:15:A:GLU:H	7	0.75
(1,148)	1:6:A:VAL:HG12	1:9:A:SER:H	20	0.75
(1,123)	1:13:A:LEU:HD12	1:14:A:CYS:H	6	0.75
(1,123)	1:13:A:LEU:HD13	1:14:A:CYS:H	16	0.75
(1,123)	1:13:A:LEU:HD11	1:14:A:CYS:H	20	0.75
(1,110)	1:43:A:LEU:HD22	1:44:A:PHE:H	2	0.75
(1,100)	1:57:A:VAL:HG12	1:57:A:VAL:H	1	0.75
(1,100)	1:57:A:VAL:HG13	1:57:A:VAL:H	14	0.75
(1,55)	1:80:A:VAL:HG12	1:80:A:VAL:H	17	0.75
(1,50)	1:7:A:VAL:HG23	1:8:A:SER:H	9	0.75
(1,7)	1:72:A:LEU:HD11	1:73:A:GLU:H	14	0.75
(1,2660)	1:69:A:LYS:HA	1:69:A:LYS:HE3	7	0.74
(1,2657)	1:20:A:LYS:HE2	1:20:A:LYS:HA	15	0.74
(1,2651)	1:7:A:VAL:HA	1:48:A:PHE:HA	15	0.74
(1,2633)	1:115:A:LEU:HD13	1:27:A:GLU:HB3	7	0.74
(1,2612)	1:25:A:LYS:HE3	1:56:A:LEU:HD12	10	0.74
(1,2606)	1:57:A:VAL:HG13	1:26:A:ILE:HA	17	0.74
(1,2583)	1:100:A:ILE:HA	1:100:A:ILE:HD11	10	0.74
(1,2463)	1:56:A:LEU:HD23	1:56:A:LEU:HD12	9	0.74
(1,2463)	1:43:A:LEU:HD22	1:43:A:LEU:HD12	11	0.74
(1,2457)	1:43:A:LEU:HD21	1:43:A:LEU:HD23	14	0.74
(1,2457)	1:56:A:LEU:HD22	1:56:A:LEU:HD21	17	0.74
(1,2202)	1:83:A:PRO:HB3	1:88:A:TYR:HD2	16	0.74
(1,2177)	1:6:A:VAL:HG13	1:44:A:PHE:HD2	10	0.74
(1,2091)	1:65:A:ILE:HA	1:31:A:VAL:HG11	10	0.74
(1,2089)	1:79:A:HIS:HA	1:80:A:VAL:HG22	19	0.74
(1,2079)	1:71:A:GLU:HB2	1:103:A:GLN:HA	13	0.74
(1,2069)	1:112:A:LEU:HD21	1:29:A:VAL:HA	19	0.74
(1,1829)	1:26:A:ILE:HD13	1:23:A:ALA:HB1	9	0.74
(1,1825)	1:62:A:ILE:HG22	1:62:A:ILE:HG13	5	0.74
(1,1823)	1:45:A:VAL:HG13	1:41:A:LYS:HE2	19	0.74
(1,1803)	1:10:A:LEU:HD13	1:109:A:LEU:HB2	8	0.74
(1,1780)	1:112:A:LEU:HD21	1:17:A:HIS:HA	8	0.74
(1,1778)	1:112:A:LEU:HD22	1:18:A:ALA:HB2	13	0.74
(1,1739)	1:33:A:ILE:HG21	1:65:A:ILE:HG21	2	0.74
(1,1739)	1:33:A:ILE:HG22	1:65:A:ILE:HG22	6	0.74
(1,1723)	1:45:A:VAL:HG12	1:63:A:LEU:HD23	17	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1708)	1:107:A:MET:HA	1:33:A:ILE:HD13	3	0.74
(1,1606)	1:10:A:LEU:HD21	1:10:A:LEU:HA	3	0.74
(1,1597)	1:109:A:LEU:HD13	1:109:A:LEU:HA	7	0.74
(1,1265)	1:102:A:THR:HG22	1:73:A:GLU:HG2	17	0.74
(1,1254)	1:20:A:LYS:HB2	1:20:A:LYS:HE3	13	0.74
(1,1254)	1:20:A:LYS:HB2	1:20:A:LYS:HE3	20	0.74
(1,910)	1:109:A:LEU:HD11	1:13:A:LEU:HD12	13	0.74
(1,770)	1:72:A:LEU:HD13	1:70:A:VAL:HG21	12	0.74
(1,760)	1:110:A:LEU:HD11	1:110:A:LEU:HA	5	0.74
(1,760)	1:110:A:LEU:HD12	1:110:A:LEU:HA	16	0.74
(1,746)	1:72:A:LEU:HD12	1:83:A:PRO:HB2	9	0.74
(1,745)	1:72:A:LEU:HD12	1:72:A:LEU:HA	5	0.74
(1,330)	1:68:A:GLU:HG2	1:33:A:ILE:H	8	0.74
(1,253)	1:68:A:GLU:HG3	1:69:A:LYS:H	10	0.74
(1,176)	1:18:A:ALA:HB2	1:16:A:GLU:H	14	0.74
(1,176)	1:18:A:ALA:HB2	1:16:A:GLU:H	16	0.74
(1,176)	1:18:A:ALA:HB3	1:16:A:GLU:H	19	0.74
(1,120)	1:13:A:LEU:HD13	1:13:A:LEU:H	7	0.74
(1,110)	1:43:A:LEU:HD22	1:44:A:PHE:H	1	0.74
(1,110)	1:43:A:LEU:HD23	1:44:A:PHE:H	18	0.74
(1,84)	1:99:A:VAL:HG23	1:91:A:CYS:H	12	0.74
(1,7)	1:72:A:LEU:HD11	1:73:A:GLU:H	6	0.74
(1,7)	1:72:A:LEU:HD11	1:73:A:GLU:H	11	0.74
(1,2679)	1:7:A:VAL:HB	1:44:A:PHE:HD1	19	0.73
(1,2670)	1:11:A:ILE:HG23	1:51:A:PHE:HD2	19	0.73
(1,2651)	1:7:A:VAL:HA	1:48:A:PHE:HA	13	0.73
(1,2651)	1:7:A:VAL:HA	1:48:A:PHE:HA	16	0.73
(1,2651)	1:7:A:VAL:HA	1:48:A:PHE:HA	19	0.73
(1,2457)	1:43:A:LEU:HD22	1:43:A:LEU:HD21	16	0.73
(1,2206)	1:83:A:PRO:HB2	1:81:A:PHE:HD1	7	0.73
(1,2177)	1:6:A:VAL:HG11	1:44:A:PHE:HD1	1	0.73
(1,2177)	1:6:A:VAL:HG11	1:44:A:PHE:HD1	4	0.73
(1,2091)	1:65:A:ILE:HA	1:31:A:VAL:HG11	4	0.73
(1,2091)	1:65:A:ILE:HA	1:31:A:VAL:HG11	12	0.73
(1,2089)	1:79:A:HIS:HA	1:80:A:VAL:HG23	18	0.73
(1,2056)	1:15:A:GLU:HG2	1:12:A:ALA:HA	9	0.73
(1,1857)	1:75:A:LYS:HG2	1:98:A:ASN:HB2	16	0.73
(1,1825)	1:62:A:ILE:HG21	1:62:A:ILE:HG13	7	0.73
(1,1825)	1:62:A:ILE:HG22	1:62:A:ILE:HG13	12	0.73
(1,1825)	1:62:A:ILE:HG21	1:62:A:ILE:HG13	13	0.73
(1,1775)	1:100:A:ILE:HD13	1:102:A:THR:HB	1	0.73
(1,1738)	1:65:A:ILE:HG23	1:63:A:LEU:HD11	3	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1732)	1:72:A:LEU:HD12	1:89:A:GLY:HA3	16	0.73
(1,1695)	1:64:A:ASP:HB2	1:30:A:VAL:HA	13	0.73
(1,1628)	1:61:A:ALA:HB3	1:27:A:GLU:HA	2	0.73
(1,1606)	1:10:A:LEU:HD23	1:10:A:LEU:HA	13	0.73
(1,1597)	1:109:A:LEU:HD12	1:109:A:LEU:HA	12	0.73
(1,1538)	1:99:A:VAL:HG23	1:91:A:CYS:HA	1	0.73
(1,1482)	1:7:A:VAL:HG23	1:48:A:PHE:HA	16	0.73
(1,1356)	1:107:A:MET:HG2	1:107:A:MET:HE2	3	0.73
(1,1018)	1:100:A:ILE:HG22	1:100:A:ILE:HG12	15	0.73
(1,996)	1:26:A:ILE:HG12	1:57:A:VAL:HG11	4	0.73
(1,962)	1:33:A:ILE:HD12	1:41:A:LYS:HG3	6	0.73
(1,929)	1:100:A:ILE:HG22	1:100:A:ILE:HG13	12	0.73
(1,929)	1:100:A:ILE:HG23	1:100:A:ILE:HG13	17	0.73
(1,929)	1:100:A:ILE:HG21	1:100:A:ILE:HG13	18	0.73
(1,923)	1:57:A:VAL:HG23	1:56:A:LEU:HB2	6	0.73
(1,921)	1:45:A:VAL:HG21	1:45:A:VAL:HA	6	0.73
(1,921)	1:45:A:VAL:HG22	1:45:A:VAL:HA	12	0.73
(1,921)	1:45:A:VAL:HG23	1:45:A:VAL:HA	15	0.73
(1,910)	1:109:A:LEU:HD11	1:13:A:LEU:HD11	16	0.73
(1,828)	1:101:A:ILE:HG22	1:101:A:ILE:HG13	8	0.73
(1,805)	1:7:A:VAL:HG23	1:48:A:PHE:HB3	12	0.73
(1,760)	1:110:A:LEU:HD11	1:110:A:LEU:HA	10	0.73
(1,195)	1:12:A:ALA:HB1	1:15:A:GLU:H	10	0.73
(1,195)	1:12:A:ALA:HB3	1:15:A:GLU:H	18	0.73
(1,176)	1:18:A:ALA:HB1	1:16:A:GLU:H	12	0.73
(1,123)	1:13:A:LEU:HD13	1:14:A:CYS:H	4	0.73
(1,123)	1:13:A:LEU:HD12	1:14:A:CYS:H	5	0.73
(1,123)	1:13:A:LEU:HD12	1:14:A:CYS:H	18	0.73
(1,120)	1:13:A:LEU:HD11	1:13:A:LEU:H	11	0.73
(1,100)	1:57:A:VAL:HG12	1:57:A:VAL:H	12	0.73
(1,7)	1:72:A:LEU:HD11	1:73:A:GLU:H	1	0.73
(1,2678)	1:107:A:MET:HE1	1:44:A:PHE:HZ	6	0.72
(1,2618)	1:6:A:VAL:HG23	1:2:A:HIS:HB2	19	0.72
(1,2586)	1:31:A:VAL:HA	1:31:A:VAL:HG21	12	0.72
(1,2583)	1:100:A:ILE:HA	1:100:A:ILE:HD12	18	0.72
(1,2463)	1:56:A:LEU:HD23	1:56:A:LEU:HD13	2	0.72
(1,2463)	1:56:A:LEU:HD23	1:56:A:LEU:HD13	3	0.72
(1,2463)	1:56:A:LEU:HD21	1:56:A:LEU:HD12	7	0.72
(1,2463)	1:56:A:LEU:HD23	1:56:A:LEU:HD13	12	0.72
(1,2457)	1:43:A:LEU:HD22	1:43:A:LEU:HD21	2	0.72
(1,2457)	1:10:A:LEU:HD11	1:10:A:LEU:HD13	3	0.72
(1,2457)	1:43:A:LEU:HD22	1:43:A:LEU:HD21	6	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2457)	1:10:A:LEU:HD12	1:10:A:LEU:HD11	7	0.72
(1,2457)	1:10:A:LEU:HD12	1:10:A:LEU:HD13	13	0.72
(1,2457)	1:10:A:LEU:HD12	1:10:A:LEU:HD13	19	0.72
(1,2163)	1:45:A:VAL:HG21	1:44:A:PHE:HD2	16	0.72
(1,2091)	1:65:A:ILE:HA	1:31:A:VAL:HG12	1	0.72
(1,2091)	1:65:A:ILE:HA	1:31:A:VAL:HG13	2	0.72
(1,2089)	1:79:A:HIS:HA	1:80:A:VAL:HG23	13	0.72
(1,2089)	1:79:A:HIS:HA	1:80:A:VAL:HG23	20	0.72
(1,1992)	1:20:A:LYS:HE2	1:20:A:LYS:HA	20	0.72
(1,1939)	1:39:A:MET:HE1	1:39:A:MET:HA	6	0.72
(1,1888)	1:85:A:ALA:HB3	1:86:A:LEU:HG	2	0.72
(1,1870)	1:20:A:LYS:HG2	1:16:A:GLU:HG3	1	0.72
(1,1857)	1:75:A:LYS:HG2	1:98:A:ASN:HB2	11	0.72
(1,1840)	1:75:A:LYS:HG3	1:100:A:ILE:HG13	8	0.72
(1,1825)	1:62:A:ILE:HG23	1:62:A:ILE:HG13	14	0.72
(1,1753)	1:65:A:ILE:HD12	1:41:A:LYS:HD3	11	0.72
(1,1739)	1:33:A:ILE:HG22	1:65:A:ILE:HG21	17	0.72
(1,1606)	1:10:A:LEU:HD23	1:10:A:LEU:HA	7	0.72
(1,1597)	1:109:A:LEU:HD11	1:109:A:LEU:HA	6	0.72
(1,1597)	1:109:A:LEU:HD13	1:109:A:LEU:HA	13	0.72
(1,1597)	1:109:A:LEU:HD11	1:109:A:LEU:HA	15	0.72
(1,1517)	1:7:A:VAL:HG12	1:4:A:TYR:HA	5	0.72
(1,1514)	1:43:A:LEU:HD21	1:42:A:SER:HB2	3	0.72
(1,1514)	1:43:A:LEU:HD23	1:42:A:SER:HB3	5	0.72
(1,1391)	1:58:A:CYS:HB3	1:55:A:SER:HB3	20	0.72
(1,1254)	1:20:A:LYS:HB3	1:20:A:LYS:HE2	17	0.72
(1,1211)	1:75:A:LYS:HB3	1:98:A:ASN:HB2	19	0.72
(1,962)	1:33:A:ILE:HD12	1:41:A:LYS:HG3	16	0.72
(1,929)	1:100:A:ILE:HG22	1:100:A:ILE:HG13	2	0.72
(1,929)	1:100:A:ILE:HG23	1:100:A:ILE:HG13	6	0.72
(1,921)	1:45:A:VAL:HG22	1:45:A:VAL:HA	2	0.72
(1,921)	1:45:A:VAL:HG22	1:45:A:VAL:HA	5	0.72
(1,921)	1:45:A:VAL:HG22	1:45:A:VAL:HA	9	0.72
(1,921)	1:45:A:VAL:HG22	1:45:A:VAL:HA	18	0.72
(1,805)	1:7:A:VAL:HG23	1:48:A:PHE:HB3	3	0.72
(1,760)	1:110:A:LEU:HD11	1:110:A:LEU:HA	4	0.72
(1,745)	1:72:A:LEU:HD12	1:72:A:LEU:HA	8	0.72
(1,745)	1:72:A:LEU:HD11	1:72:A:LEU:HA	14	0.72
(1,300)	1:107:A:MET:HE1	1:108:A:ARG:H	19	0.72
(1,253)	1:68:A:GLU:HG3	1:69:A:LYS:H	3	0.72
(1,148)	1:6:A:VAL:HG11	1:9:A:SER:H	12	0.72
(1,144)	1:47:A:ALA:HB3	1:50:A:THR:H	13	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,130)	1:10:A:LEU:HD21	1:10:A:LEU:H	17	0.72
(1,126)	1:45:A:VAL:HG22	1:47:A:ALA:H	8	0.72
(1,70)	1:112:A:LEU:HD23	1:17:A:HIS:H	12	0.72
(1,50)	1:7:A:VAL:HG22	1:8:A:SER:H	15	0.72
(1,34)	1:33:A:ILE:HG22	1:39:A:MET:H	9	0.72
(1,7)	1:72:A:LEU:HD12	1:73:A:GLU:H	16	0.72
(1,2671)	1:115:A:LEU:HD12	1:24:A:HIS:HD2	5	0.71
(1,2669)	1:31:A:VAL:HG23	1:44:A:PHE:HD1	14	0.71
(1,2660)	1:69:A:LYS:HA	1:69:A:LYS:HE3	14	0.71
(1,2654)	1:6:A:VAL:HA	1:107:A:MET:HE1	12	0.71
(1,2650)	1:66:A:VAL:HG13	1:32:A:GLY:HA3	4	0.71
(1,2645)	1:33:A:ILE:HG23	1:39:A:MET:HG3	6	0.71
(1,2606)	1:57:A:VAL:HG12	1:26:A:ILE:HA	1	0.71
(1,2583)	1:100:A:ILE:HA	1:100:A:ILE:HD12	3	0.71
(1,2583)	1:100:A:ILE:HA	1:100:A:ILE:HD12	19	0.71
(1,2563)	1:45:A:VAL:HA	1:63:A:LEU:HD23	10	0.71
(1,2555)	1:25:A:LYS:HE3	1:56:A:LEU:HD13	14	0.71
(1,2463)	1:56:A:LEU:HD23	1:56:A:LEU:HD12	17	0.71
(1,2457)	1:43:A:LEU:HD22	1:43:A:LEU:HD23	1	0.71
(1,2457)	1:43:A:LEU:HD21	1:43:A:LEU:HD23	9	0.71
(1,2457)	1:43:A:LEU:HD22	1:43:A:LEU:HD21	11	0.71
(1,2457)	1:56:A:LEU:HD22	1:56:A:LEU:HD23	15	0.71
(1,2457)	1:43:A:LEU:HD22	1:43:A:LEU:HD21	20	0.71
(1,2204)	1:83:A:PRO:HB3	1:88:A:TYR:HE1	8	0.71
(1,2180)	1:61:A:ALA:HB2	1:48:A:PHE:HD2	16	0.71
(1,2134)	1:72:A:LEU:HD21	1:81:A:PHE:HE2	6	0.71
(1,2091)	1:65:A:ILE:HA	1:31:A:VAL:HG13	3	0.71
(1,2079)	1:71:A:GLU:HB2	1:103:A:GLN:HA	1	0.71
(1,2063)	1:33:A:ILE:HA	1:107:A:MET:HG3	1	0.71
(1,1986)	1:82:A:LYS:HE3	1:71:A:GLU:HB3	13	0.71
(1,1842)	1:18:A:ALA:HB3	1:21:A:ASN:HB3	13	0.71
(1,1831)	1:58:A:CYS:HB2	1:61:A:ALA:HB1	6	0.71
(1,1831)	1:58:A:CYS:HB2	1:61:A:ALA:HB2	14	0.71
(1,1825)	1:62:A:ILE:HG21	1:62:A:ILE:HG13	8	0.71
(1,1825)	1:62:A:ILE:HG22	1:62:A:ILE:HG13	10	0.71
(1,1825)	1:62:A:ILE:HG22	1:62:A:ILE:HG13	17	0.71
(1,1825)	1:62:A:ILE:HG23	1:62:A:ILE:HG13	19	0.71
(1,1823)	1:45:A:VAL:HG12	1:41:A:LYS:HE2	4	0.71
(1,1812)	1:50:A:THR:HG22	1:47:A:ALA:HA	19	0.71
(1,1803)	1:10:A:LEU:HD11	1:109:A:LEU:HB2	15	0.71
(1,1778)	1:112:A:LEU:HD23	1:18:A:ALA:HB1	2	0.71
(1,1739)	1:33:A:ILE:HG22	1:65:A:ILE:HG21	10	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1738)	1:65:A:ILE:HG21	1:63:A:LEU:HD11	11	0.71
(1,1697)	1:112:A:LEU:HD22	1:112:A:LEU:HA	13	0.71
(1,1695)	1:64:A:ASP:HB2	1:30:A:VAL:HA	11	0.71
(1,1606)	1:10:A:LEU:HD21	1:10:A:LEU:HA	1	0.71
(1,1606)	1:10:A:LEU:HD21	1:10:A:LEU:HA	16	0.71
(1,1606)	1:10:A:LEU:HD23	1:10:A:LEU:HA	19	0.71
(1,1391)	1:58:A:CYS:HB3	1:55:A:SER:HB3	5	0.71
(1,1391)	1:58:A:CYS:HB3	1:55:A:SER:HB3	12	0.71
(1,1385)	1:48:A:PHE:HB3	1:63:A:LEU:HD11	3	0.71
(1,1324)	1:106:A:GLU:HG2	1:105:A:ASN:HB2	12	0.71
(1,1248)	1:13:A:LEU:HD11	1:13:A:LEU:HB3	11	0.71
(1,1024)	1:57:A:VAL:HG13	1:18:A:ALA:HB1	3	0.71
(1,929)	1:100:A:ILE:HG23	1:100:A:ILE:HG13	10	0.71
(1,921)	1:45:A:VAL:HG23	1:45:A:VAL:HA	14	0.71
(1,898)	1:29:A:VAL:HG13	1:112:A:LEU:HA	8	0.71
(1,813)	1:29:A:VAL:HG22	1:10:A:LEU:HD11	15	0.71
(1,804)	1:66:A:VAL:HG13	1:32:A:GLY:HA3	6	0.71
(1,772)	1:66:A:VAL:HG21	1:64:A:ASP:HB2	1	0.71
(1,760)	1:110:A:LEU:HD11	1:110:A:LEU:HA	1	0.71
(1,742)	1:72:A:LEU:HD12	1:99:A:VAL:HG11	3	0.71
(1,253)	1:68:A:GLU:HG3	1:69:A:LYS:H	17	0.71
(1,130)	1:10:A:LEU:HD22	1:10:A:LEU:H	5	0.71
(1,123)	1:13:A:LEU:HD11	1:14:A:CYS:H	11	0.71
(1,120)	1:13:A:LEU:HD12	1:13:A:LEU:H	1	0.71
(1,120)	1:13:A:LEU:HD13	1:13:A:LEU:H	3	0.71
(1,120)	1:13:A:LEU:HD12	1:13:A:LEU:H	4	0.71
(1,118)	1:13:A:LEU:HD12	1:16:A:GLU:H	17	0.71
(1,101)	1:57:A:VAL:HG12	1:15:A:GLU:H	13	0.71
(1,50)	1:7:A:VAL:HG21	1:8:A:SER:H	8	0.71
(1,40)	1:99:A:VAL:HG11	1:89:A:GLY:H	3	0.71
(1,38)	1:99:A:VAL:HG11	1:90:A:VAL:H	7	0.71
(1,15)	1:7:A:VAL:HG13	1:47:A:ALA:H	14	0.71
(1,15)	1:7:A:VAL:HG11	1:47:A:ALA:H	15	0.71
(1,2672)	1:70:A:VAL:HG11	1:88:A:TYR:HD2	16	0.7
(1,2669)	1:31:A:VAL:HG22	1:44:A:PHE:HD2	19	0.7
(1,2665)	1:97:A:LYS:HA	1:90:A:VAL:HB	12	0.7
(1,2651)	1:45:A:VAL:HA	1:48:A:PHE:HA	2	0.7
(1,2651)	1:45:A:VAL:HA	1:48:A:PHE:HA	20	0.7
(1,2633)	1:115:A:LEU:HD12	1:27:A:GLU:HB3	11	0.7
(1,2618)	1:6:A:VAL:HG22	1:2:A:HIS:HB2	14	0.7
(1,2612)	1:25:A:LYS:HE2	1:56:A:LEU:HD12	17	0.7
(1,2463)	1:43:A:LEU:HD22	1:43:A:LEU:HD13	10	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2457)	1:10:A:LEU:HD12	1:10:A:LEU:HD13	5	0.7
(1,2457)	1:43:A:LEU:HD21	1:43:A:LEU:HD23	8	0.7
(1,2457)	1:56:A:LEU:HD22	1:56:A:LEU:HD23	10	0.7
(1,2457)	1:56:A:LEU:HD22	1:56:A:LEU:HD23	12	0.7
(1,2457)	1:10:A:LEU:HD12	1:10:A:LEU:HD13	18	0.7
(1,2438)	1:65:A:ILE:HD11	1:41:A:LYS:HD2	9	0.7
(1,2204)	1:83:A:PRO:HB3	1:88:A:TYR:HE1	7	0.7
(1,2180)	1:61:A:ALA:HB1	1:48:A:PHE:HD1	12	0.7
(1,2163)	1:45:A:VAL:HG21	1:44:A:PHE:HD2	17	0.7
(1,2033)	1:59:A:LYS:HB2	1:53:A:GLU:HA	11	0.7
(1,2023)	1:7:A:VAL:HA	1:11:A:ILE:HD11	15	0.7
(1,2016)	1:93:A:LYS:HD2	1:79:A:HIS:HB2	12	0.7
(1,1907)	1:25:A:LYS:HB2	1:57:A:VAL:HG12	17	0.7
(1,1870)	1:20:A:LYS:HG2	1:16:A:GLU:HG3	13	0.7
(1,1831)	1:58:A:CYS:HB2	1:61:A:ALA:HB2	15	0.7
(1,1829)	1:26:A:ILE:HD12	1:23:A:ALA:HB1	14	0.7
(1,1825)	1:62:A:ILE:HG21	1:62:A:ILE:HG13	6	0.7
(1,1825)	1:62:A:ILE:HG21	1:62:A:ILE:HG13	11	0.7
(1,1825)	1:62:A:ILE:HG21	1:62:A:ILE:HG13	16	0.7
(1,1746)	1:90:A:VAL:HG21	1:87:A:ASP:HB3	14	0.7
(1,1688)	1:97:A:LYS:HA	1:99:A:VAL:HG23	17	0.7
(1,1597)	1:109:A:LEU:HD11	1:109:A:LEU:HA	3	0.7
(1,1597)	1:109:A:LEU:HD13	1:109:A:LEU:HA	16	0.7
(1,1482)	1:7:A:VAL:HG21	1:48:A:PHE:HA	1	0.7
(1,1482)	1:7:A:VAL:HG23	1:48:A:PHE:HA	3	0.7
(1,1254)	1:20:A:LYS:HB2	1:20:A:LYS:HE3	9	0.7
(1,1020)	1:85:A:ALA:HB2	1:86:A:LEU:HA	7	0.7
(1,1018)	1:100:A:ILE:HG22	1:100:A:ILE:HG12	20	0.7
(1,962)	1:33:A:ILE:HD13	1:41:A:LYS:HG3	11	0.7
(1,937)	1:102:A:THR:HG21	1:73:A:GLU:HA	15	0.7
(1,923)	1:57:A:VAL:HG23	1:56:A:LEU:HB2	10	0.7
(1,921)	1:45:A:VAL:HG23	1:45:A:VAL:HA	7	0.7
(1,921)	1:45:A:VAL:HG23	1:45:A:VAL:HA	17	0.7
(1,887)	1:57:A:VAL:HG13	1:18:A:ALA:HA	3	0.7
(1,887)	1:57:A:VAL:HG12	1:18:A:ALA:HA	15	0.7
(1,875)	1:86:A:LEU:HD23	1:85:A:ALA:HA	16	0.7
(1,822)	1:80:A:VAL:HG11	1:102:A:THR:HG23	7	0.7
(1,809)	1:110:A:LEU:HD13	1:66:A:VAL:HG11	4	0.7
(1,750)	1:72:A:LEU:HD23	1:99:A:VAL:HG12	5	0.7
(1,195)	1:12:A:ALA:HB2	1:15:A:GLU:H	6	0.7
(1,176)	1:18:A:ALA:HB2	1:16:A:GLU:H	2	0.7
(1,176)	1:18:A:ALA:HB1	1:16:A:GLU:H	13	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,148)	1:6:A:VAL:HG11	1:9:A:SER:H	17	0.7
(1,144)	1:47:A:ALA:HB1	1:50:A:THR:H	6	0.7
(1,130)	1:10:A:LEU:HD21	1:10:A:LEU:H	18	0.7
(1,120)	1:13:A:LEU:HD12	1:13:A:LEU:H	9	0.7
(1,120)	1:13:A:LEU:HD11	1:13:A:LEU:H	19	0.7
(1,110)	1:43:A:LEU:HD22	1:44:A:PHE:H	7	0.7
(1,103)	1:43:A:LEU:HD22	1:46:A:SER:H	15	0.7
(1,88)	1:26:A:ILE:HD13	1:15:A:GLU:H	11	0.7
(1,50)	1:7:A:VAL:HG22	1:8:A:SER:H	14	0.7
(1,50)	1:7:A:VAL:HG22	1:8:A:SER:H	17	0.7
(1,50)	1:7:A:VAL:HG23	1:8:A:SER:H	19	0.7
(1,38)	1:99:A:VAL:HG12	1:90:A:VAL:H	17	0.7
(1,7)	1:72:A:LEU:HD12	1:73:A:GLU:H	4	0.7
(1,2678)	1:107:A:MET:HE2	1:44:A:PHE:HZ	5	0.69
(1,2672)	1:70:A:VAL:HG13	1:88:A:TYR:HD1	11	0.69
(1,2652)	1:45:A:VAL:HA	1:47:A:ALA:HB1	1	0.69
(1,2651)	1:7:A:VAL:HA	1:48:A:PHE:HA	18	0.69
(1,2613)	1:56:A:LEU:HD12	1:56:A:LEU:HD11	5	0.69
(1,2612)	1:59:A:LYS:HE2	1:56:A:LEU:HD12	9	0.69
(1,2606)	1:57:A:VAL:HG11	1:26:A:ILE:HA	13	0.69
(1,2583)	1:100:A:ILE:HA	1:100:A:ILE:HD13	2	0.69
(1,2583)	1:100:A:ILE:HA	1:100:A:ILE:HD12	14	0.69
(1,2555)	1:25:A:LYS:HE3	1:56:A:LEU:HD12	10	0.69
(1,2463)	1:43:A:LEU:HD23	1:43:A:LEU:HD13	13	0.69
(1,2457)	1:10:A:LEU:HD11	1:10:A:LEU:HD13	4	0.69
(1,2209)	1:1:A:MET:HG2	1:2:A:HIS:HD2	11	0.69
(1,2204)	1:83:A:PRO:HB3	1:88:A:TYR:HE2	14	0.69
(1,2202)	1:83:A:PRO:HB3	1:88:A:TYR:HD1	7	0.69
(1,2202)	1:83:A:PRO:HB3	1:88:A:TYR:HD1	10	0.69
(1,2202)	1:83:A:PRO:HB3	1:88:A:TYR:HD2	15	0.69
(1,2177)	1:6:A:VAL:HG12	1:44:A:PHE:HD2	14	0.69
(1,2163)	1:45:A:VAL:HG23	1:44:A:PHE:HD2	12	0.69
(1,2158)	1:29:A:VAL:HG12	1:48:A:PHE:HZ	7	0.69
(1,2133)	1:65:A:ILE:HG21	1:44:A:PHE:HD2	18	0.69
(1,2091)	1:65:A:ILE:HA	1:31:A:VAL:HG12	18	0.69
(1,2089)	1:79:A:HIS:HA	1:80:A:VAL:HG21	9	0.69
(1,2079)	1:71:A:GLU:HB2	1:103:A:GLN:HA	20	0.69
(1,2069)	1:112:A:LEU:HD23	1:29:A:VAL:HA	1	0.69
(1,1907)	1:25:A:LYS:HB2	1:57:A:VAL:HG12	1	0.69
(1,1825)	1:62:A:ILE:HG21	1:62:A:ILE:HG13	9	0.69
(1,1825)	1:62:A:ILE:HG23	1:62:A:ILE:HG13	20	0.69
(1,1820)	1:10:A:LEU:HD22	1:6:A:VAL:HG12	9	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1805)	1:10:A:LEU:HD11	1:63:A:LEU:HD22	10	0.69
(1,1751)	1:65:A:ILE:HD13	1:33:A:ILE:HG23	3	0.69
(1,1751)	1:65:A:ILE:HD13	1:33:A:ILE:HG22	17	0.69
(1,1615)	1:10:A:LEU:HA	1:107:A:MET:HE3	3	0.69
(1,1606)	1:10:A:LEU:HD21	1:10:A:LEU:HA	18	0.69
(1,1499)	1:6:A:VAL:HG21	1:3:A:GLU:HA	2	0.69
(1,1328)	1:103:A:GLN:HG3	1:103:A:GLN:HA	11	0.69
(1,1248)	1:13:A:LEU:HD12	1:13:A:LEU:HB3	14	0.69
(1,996)	1:26:A:ILE:HG12	1:57:A:VAL:HG12	3	0.69
(1,929)	1:100:A:ILE:HG21	1:100:A:ILE:HG13	14	0.69
(1,921)	1:45:A:VAL:HG23	1:45:A:VAL:HA	4	0.69
(1,921)	1:45:A:VAL:HG22	1:45:A:VAL:HA	13	0.69
(1,921)	1:45:A:VAL:HG21	1:45:A:VAL:HA	19	0.69
(1,862)	1:109:A:LEU:HD21	1:13:A:LEU:HD21	5	0.69
(1,805)	1:7:A:VAL:HG23	1:48:A:PHE:HB3	16	0.69
(1,195)	1:12:A:ALA:HB2	1:15:A:GLU:H	13	0.69
(1,144)	1:47:A:ALA:HB2	1:50:A:THR:H	10	0.69
(1,144)	1:47:A:ALA:HB3	1:50:A:THR:H	11	0.69
(1,130)	1:10:A:LEU:HD22	1:10:A:LEU:H	15	0.69
(1,123)	1:13:A:LEU:HD13	1:14:A:CYS:H	14	0.69
(1,110)	1:43:A:LEU:HD23	1:44:A:PHE:H	6	0.69
(1,110)	1:43:A:LEU:HD22	1:44:A:PHE:H	15	0.69
(1,103)	1:43:A:LEU:HD22	1:46:A:SER:H	7	0.69
(1,101)	1:57:A:VAL:HG11	1:15:A:GLU:H	14	0.69
(1,53)	1:66:A:VAL:HG13	1:33:A:ILE:H	2	0.69
(1,2679)	1:7:A:VAL:HB	1:48:A:PHE:HD1	1	0.68
(1,2660)	1:69:A:LYS:HA	1:69:A:LYS:HE3	15	0.68
(1,2651)	1:7:A:VAL:HA	1:48:A:PHE:HA	4	0.68
(1,2621)	1:38:A:ALA:HB3	1:105:A:ASN:HB2	13	0.68
(1,2606)	1:57:A:VAL:HG12	1:26:A:ILE:HA	3	0.68
(1,2605)	1:86:A:LEU:HD12	1:86:A:LEU:HD11	4	0.68
(1,2605)	1:115:A:LEU:HD12	1:115:A:LEU:HD13	13	0.68
(1,2463)	1:56:A:LEU:HD23	1:56:A:LEU:HD13	1	0.68
(1,2454)	1:62:A:ILE:HG21	1:62:A:ILE:HG13	16	0.68
(1,2433)	1:63:A:LEU:HD23	1:31:A:VAL:HG22	14	0.68
(1,2433)	1:63:A:LEU:HD23	1:31:A:VAL:HG22	17	0.68
(1,2163)	1:45:A:VAL:HG23	1:44:A:PHE:HD2	9	0.68
(1,2163)	1:45:A:VAL:HG21	1:44:A:PHE:HD1	10	0.68
(1,2160)	1:80:A:VAL:HG21	1:81:A:PHE:HD2	7	0.68
(1,2160)	1:80:A:VAL:HG22	1:81:A:PHE:HD2	9	0.68
(1,2156)	1:93:A:LYS:HB3	1:79:A:HIS:HD2	20	0.68
(1,2133)	1:65:A:ILE:HG22	1:44:A:PHE:HD2	7	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2133)	1:65:A:ILE:HG23	1:44:A:PHE:HD1	14	0.68
(1,2091)	1:65:A:ILE:HA	1:31:A:VAL:HG11	16	0.68
(1,2084)	1:58:A:CYS:HA	1:26:A:ILE:HG23	7	0.68
(1,2070)	1:109:A:LEU:HD23	1:29:A:VAL:HA	6	0.68
(1,2047)	1:33:A:ILE:HG21	1:37:A:SER:HA	8	0.68
(1,2047)	1:33:A:ILE:HG23	1:37:A:SER:HA	14	0.68
(1,2035)	1:42:A:SER:HB2	1:45:A:VAL:HG21	10	0.68
(1,1939)	1:39:A:MET:HE2	1:39:A:MET:HA	15	0.68
(1,1831)	1:58:A:CYS:HB2	1:61:A:ALA:HB1	7	0.68
(1,1831)	1:58:A:CYS:HB2	1:61:A:ALA:HB3	9	0.68
(1,1831)	1:58:A:CYS:HB2	1:61:A:ALA:HB2	11	0.68
(1,1831)	1:58:A:CYS:HB2	1:61:A:ALA:HB2	20	0.68
(1,1825)	1:62:A:ILE:HG21	1:62:A:ILE:HG13	1	0.68
(1,1806)	1:10:A:LEU:HD13	1:7:A:VAL:HA	1	0.68
(1,1803)	1:10:A:LEU:HD13	1:109:A:LEU:HB2	9	0.68
(1,1793)	1:15:A:GLU:HG2	1:11:A:ILE:HG21	9	0.68
(1,1777)	1:112:A:LEU:HD22	1:109:A:LEU:HD13	17	0.68
(1,1753)	1:65:A:ILE:HD11	1:41:A:LYS:HD3	13	0.68
(1,1723)	1:45:A:VAL:HG12	1:63:A:LEU:HD23	10	0.68
(1,1708)	1:107:A:MET:HA	1:33:A:ILE:HD11	5	0.68
(1,1628)	1:61:A:ALA:HB2	1:27:A:GLU:HA	18	0.68
(1,1606)	1:10:A:LEU:HD22	1:10:A:LEU:HA	8	0.68
(1,1597)	1:109:A:LEU:HD11	1:109:A:LEU:HA	11	0.68
(1,1254)	1:20:A:LYS:HB3	1:20:A:LYS:HE2	6	0.68
(1,1248)	1:13:A:LEU:HD11	1:13:A:LEU:HB3	2	0.68
(1,1159)	1:108:A:ARG:HB2	1:110:A:LEU:HD22	6	0.68
(1,1020)	1:85:A:ALA:HB2	1:86:A:LEU:HA	19	0.68
(1,1018)	1:100:A:ILE:HG22	1:100:A:ILE:HG12	1	0.68
(1,996)	1:26:A:ILE:HG12	1:57:A:VAL:HG13	5	0.68
(1,923)	1:57:A:VAL:HG21	1:56:A:LEU:HB2	8	0.68
(1,921)	1:45:A:VAL:HG21	1:45:A:VAL:HA	10	0.68
(1,828)	1:101:A:ILE:HG22	1:101:A:ILE:HG13	18	0.68
(1,805)	1:7:A:VAL:HG21	1:48:A:PHE:HB3	11	0.68
(1,330)	1:68:A:GLU:HG2	1:33:A:ILE:H	12	0.68
(1,253)	1:68:A:GLU:HG3	1:69:A:LYS:H	19	0.68
(1,195)	1:12:A:ALA:HB1	1:15:A:GLU:H	20	0.68
(1,176)	1:18:A:ALA:HB1	1:16:A:GLU:H	4	0.68
(1,176)	1:18:A:ALA:HB1	1:16:A:GLU:H	20	0.68
(1,144)	1:47:A:ALA:HB2	1:50:A:THR:H	7	0.68
(1,144)	1:47:A:ALA:HB3	1:50:A:THR:H	15	0.68
(1,130)	1:10:A:LEU:HD22	1:10:A:LEU:H	19	0.68
(1,110)	1:43:A:LEU:HD21	1:44:A:PHE:H	3	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,110)	1:43:A:LEU:HD22	1:44:A:PHE:H	13	0.68
(1,88)	1:26:A:ILE:HD11	1:15:A:GLU:H	19	0.68
(1,74)	1:99:A:VAL:HG21	1:73:A:GLU:H	2	0.68
(1,40)	1:99:A:VAL:HG11	1:89:A:GLY:H	18	0.68
(1,23)	1:110:A:LEU:HD12	1:111:A:SER:H	17	0.68
(1,2672)	1:70:A:VAL:HG12	1:88:A:TYR:HD1	7	0.67
(1,2669)	1:31:A:VAL:HG23	1:44:A:PHE:HD2	9	0.67
(1,2660)	1:69:A:LYS:HA	1:69:A:LYS:HE3	6	0.67
(1,2651)	1:7:A:VAL:HA	1:48:A:PHE:HA	8	0.67
(1,2651)	1:45:A:VAL:HA	1:48:A:PHE:HA	17	0.67
(1,2638)	1:107:A:MET:HA	1:39:A:MET:HE2	16	0.67
(1,2613)	1:56:A:LEU:HD12	1:56:A:LEU:HD11	3	0.67
(1,2613)	1:56:A:LEU:HD11	1:56:A:LEU:HD13	13	0.67
(1,2606)	1:57:A:VAL:HG12	1:26:A:ILE:HA	7	0.67
(1,2606)	1:57:A:VAL:HG13	1:26:A:ILE:HA	16	0.67
(1,2605)	1:86:A:LEU:HD11	1:86:A:LEU:HD13	7	0.67
(1,2605)	1:86:A:LEU:HD12	1:86:A:LEU:HD13	8	0.67
(1,2605)	1:115:A:LEU:HD12	1:115:A:LEU:HD13	12	0.67
(1,2605)	1:115:A:LEU:HD12	1:115:A:LEU:HD13	18	0.67
(1,2605)	1:115:A:LEU:HD11	1:115:A:LEU:HD13	20	0.67
(1,2583)	1:100:A:ILE:HA	1:100:A:ILE:HD13	9	0.67
(1,2465)	1:31:A:VAL:HG11	1:10:A:LEU:HD23	19	0.67
(1,2463)	1:56:A:LEU:HD21	1:56:A:LEU:HD12	8	0.67
(1,2463)	1:43:A:LEU:HD21	1:43:A:LEU:HD12	15	0.67
(1,2202)	1:83:A:PRO:HB3	1:88:A:TYR:HD1	4	0.67
(1,2202)	1:83:A:PRO:HB3	1:88:A:TYR:HD2	9	0.67
(1,2177)	1:6:A:VAL:HG13	1:44:A:PHE:HD1	20	0.67
(1,2160)	1:80:A:VAL:HG21	1:81:A:PHE:HD1	20	0.67
(1,2158)	1:29:A:VAL:HG13	1:48:A:PHE:HZ	5	0.67
(1,2133)	1:65:A:ILE:HG21	1:44:A:PHE:HD2	5	0.67
(1,2091)	1:65:A:ILE:HA	1:31:A:VAL:HG13	7	0.67
(1,2069)	1:112:A:LEU:HD21	1:29:A:VAL:HA	7	0.67
(1,1939)	1:39:A:MET:HE3	1:39:A:MET:HA	17	0.67
(1,1870)	1:20:A:LYS:HG2	1:16:A:GLU:HG3	10	0.67
(1,1825)	1:62:A:ILE:HG23	1:62:A:ILE:HG13	3	0.67
(1,1825)	1:62:A:ILE:HG23	1:62:A:ILE:HG13	18	0.67
(1,1814)	1:107:A:MET:HE3	1:10:A:LEU:HD23	11	0.67
(1,1803)	1:10:A:LEU:HD13	1:109:A:LEU:HB2	4	0.67
(1,1791)	1:62:A:ILE:HG23	1:64:A:ASP:HB3	8	0.67
(1,1777)	1:112:A:LEU:HD22	1:109:A:LEU:HD11	1	0.67
(1,1777)	1:112:A:LEU:HD21	1:109:A:LEU:HD12	18	0.67
(1,1752)	1:90:A:VAL:HG11	1:97:A:LYS:HD2	1	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1739)	1:33:A:ILE:HG21	1:65:A:ILE:HG23	19	0.67
(1,1739)	1:33:A:ILE:HG23	1:65:A:ILE:HG22	20	0.67
(1,1738)	1:65:A:ILE:HG23	1:63:A:LEU:HD13	6	0.67
(1,1723)	1:45:A:VAL:HG12	1:63:A:LEU:HD21	5	0.67
(1,1597)	1:109:A:LEU:HD13	1:109:A:LEU:HA	2	0.67
(1,1597)	1:109:A:LEU:HD11	1:109:A:LEU:HA	5	0.67
(1,1597)	1:109:A:LEU:HD11	1:109:A:LEU:HA	8	0.67
(1,1597)	1:109:A:LEU:HD11	1:109:A:LEU:HA	9	0.67
(1,1514)	1:43:A:LEU:HD21	1:42:A:SER:HB2	14	0.67
(1,1514)	1:43:A:LEU:HD22	1:42:A:SER:HB3	15	0.67
(1,1499)	1:6:A:VAL:HG22	1:3:A:GLU:HA	7	0.67
(1,1385)	1:48:A:PHE:HB3	1:63:A:LEU:HD13	19	0.67
(1,1384)	1:93:A:LYS:HE2	1:93:A:LYS:HA	12	0.67
(1,1328)	1:103:A:GLN:HG3	1:103:A:GLN:HA	16	0.67
(1,1276)	1:19:A:LYS:HB2	1:19:A:LYS:HE2	5	0.67
(1,1254)	1:20:A:LYS:HB2	1:20:A:LYS:HE3	14	0.67
(1,1248)	1:13:A:LEU:HD13	1:13:A:LEU:HB3	8	0.67
(1,1181)	1:68:A:GLU:HG3	1:66:A:VAL:HG11	5	0.67
(1,1020)	1:85:A:ALA:HB3	1:86:A:LEU:HA	18	0.67
(1,929)	1:100:A:ILE:HG23	1:100:A:ILE:HG13	5	0.67
(1,923)	1:57:A:VAL:HG23	1:56:A:LEU:HB2	9	0.67
(1,921)	1:45:A:VAL:HG21	1:45:A:VAL:HA	3	0.67
(1,887)	1:57:A:VAL:HG11	1:18:A:ALA:HA	14	0.67
(1,881)	1:93:A:LYS:HB3	1:93:A:LYS:HE2	12	0.67
(1,875)	1:86:A:LEU:HD21	1:85:A:ALA:HA	1	0.67
(1,770)	1:72:A:LEU:HD13	1:70:A:VAL:HG21	19	0.67
(1,745)	1:72:A:LEU:HD11	1:72:A:LEU:HA	2	0.67
(1,458)	1:74:A:CYS:HB2	1:77:A:CYS:H	14	0.67
(1,195)	1:12:A:ALA:HB2	1:15:A:GLU:H	14	0.67
(1,144)	1:47:A:ALA:HB1	1:50:A:THR:H	18	0.67
(1,130)	1:10:A:LEU:HD21	1:10:A:LEU:H	3	0.67
(1,130)	1:10:A:LEU:HD21	1:10:A:LEU:H	4	0.67
(1,123)	1:13:A:LEU:HD11	1:14:A:CYS:H	8	0.67
(1,120)	1:13:A:LEU:HD11	1:13:A:LEU:H	5	0.67
(1,110)	1:43:A:LEU:HD21	1:44:A:PHE:H	8	0.67
(1,110)	1:43:A:LEU:HD23	1:44:A:PHE:H	10	0.67
(1,70)	1:112:A:LEU:HD23	1:17:A:HIS:H	7	0.67
(1,50)	1:7:A:VAL:HG23	1:8:A:SER:H	18	0.67
(1,40)	1:99:A:VAL:HG12	1:89:A:GLY:H	19	0.67
(1,7)	1:72:A:LEU:HD13	1:73:A:GLU:H	15	0.67
(1,7)	1:72:A:LEU:HD11	1:73:A:GLU:H	19	0.67
(1,7)	1:72:A:LEU:HD11	1:73:A:GLU:H	20	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2645)	1:33:A:ILE:HG22	1:39:A:MET:HG3	3	0.66
(1,2645)	1:33:A:ILE:HG22	1:39:A:MET:HG3	18	0.66
(1,2633)	1:115:A:LEU:HD11	1:27:A:GLU:HB3	5	0.66
(1,2633)	1:115:A:LEU:HD23	1:27:A:GLU:HB3	15	0.66
(1,2618)	1:6:A:VAL:HG22	1:2:A:HIS:HB2	9	0.66
(1,2613)	1:56:A:LEU:HD12	1:56:A:LEU:HD11	6	0.66
(1,2613)	1:43:A:LEU:HD11	1:43:A:LEU:HD13	7	0.66
(1,2613)	1:43:A:LEU:HD12	1:43:A:LEU:HD13	8	0.66
(1,2613)	1:56:A:LEU:HD12	1:56:A:LEU:HD11	9	0.66
(1,2613)	1:56:A:LEU:HD12	1:56:A:LEU:HD11	11	0.66
(1,2613)	1:56:A:LEU:HD11	1:56:A:LEU:HD13	19	0.66
(1,2605)	1:115:A:LEU:HD12	1:115:A:LEU:HD13	1	0.66
(1,2605)	1:86:A:LEU:HD11	1:86:A:LEU:HD13	2	0.66
(1,2605)	1:86:A:LEU:HD12	1:86:A:LEU:HD13	3	0.66
(1,2605)	1:86:A:LEU:HD11	1:86:A:LEU:HD13	17	0.66
(1,2586)	1:31:A:VAL:HA	1:31:A:VAL:HG22	10	0.66
(1,2586)	1:31:A:VAL:HA	1:31:A:VAL:HG21	14	0.66
(1,2583)	1:100:A:ILE:HA	1:100:A:ILE:HD13	16	0.66
(1,2433)	1:63:A:LEU:HD23	1:31:A:VAL:HG21	18	0.66
(1,2180)	1:61:A:ALA:HB2	1:48:A:PHE:HD2	14	0.66
(1,2163)	1:45:A:VAL:HG22	1:44:A:PHE:HD2	7	0.66
(1,2089)	1:79:A:HIS:HA	1:80:A:VAL:HG22	11	0.66
(1,2079)	1:71:A:GLU:HB2	1:103:A:GLN:HA	11	0.66
(1,2056)	1:15:A:GLU:HG2	1:12:A:ALA:HA	11	0.66
(1,2056)	1:15:A:GLU:HG2	1:12:A:ALA:HA	19	0.66
(1,2023)	1:7:A:VAL:HA	1:11:A:ILE:HD12	17	0.66
(1,1992)	1:20:A:LYS:HE2	1:20:A:LYS:HA	5	0.66
(1,1975)	1:12:A:ALA:HB2	1:15:A:GLU:HB2	9	0.66
(1,1907)	1:25:A:LYS:HB2	1:57:A:VAL:HG11	6	0.66
(1,1870)	1:20:A:LYS:HG2	1:16:A:GLU:HG3	2	0.66
(1,1840)	1:75:A:LYS:HG3	1:100:A:ILE:HG13	3	0.66
(1,1829)	1:26:A:ILE:HD12	1:23:A:ALA:HB3	18	0.66
(1,1823)	1:45:A:VAL:HG13	1:41:A:LYS:HE2	15	0.66
(1,1812)	1:50:A:THR:HG21	1:47:A:ALA:HA	6	0.66
(1,1805)	1:10:A:LEU:HD12	1:63:A:LEU:HD21	12	0.66
(1,1803)	1:10:A:LEU:HD11	1:109:A:LEU:HB2	2	0.66
(1,1793)	1:15:A:GLU:HG2	1:11:A:ILE:HG21	1	0.66
(1,1772)	1:64:A:ASP:HB3	1:30:A:VAL:HG12	1	0.66
(1,1772)	1:64:A:ASP:HB3	1:30:A:VAL:HG13	8	0.66
(1,1753)	1:65:A:ILE:HD11	1:41:A:LYS:HD3	7	0.66
(1,1751)	1:65:A:ILE:HD13	1:33:A:ILE:HG22	14	0.66
(1,1739)	1:33:A:ILE:HG23	1:65:A:ILE:HG22	15	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1708)	1:107:A:MET:HA	1:33:A:ILE:HD11	8	0.66
(1,1697)	1:112:A:LEU:HD22	1:112:A:LEU:HA	3	0.66
(1,1597)	1:109:A:LEU:HD13	1:109:A:LEU:HA	10	0.66
(1,1597)	1:109:A:LEU:HD13	1:109:A:LEU:HA	17	0.66
(1,1597)	1:109:A:LEU:HD11	1:109:A:LEU:HA	19	0.66
(1,1514)	1:43:A:LEU:HD23	1:42:A:SER:HB3	19	0.66
(1,1367)	1:26:A:ILE:HD12	1:14:A:CYS:HB3	10	0.66
(1,1254)	1:20:A:LYS:HB2	1:20:A:LYS:HE3	7	0.66
(1,1248)	1:13:A:LEU:HD12	1:13:A:LEU:HB3	9	0.66
(1,996)	1:26:A:ILE:HG12	1:57:A:VAL:HG13	12	0.66
(1,937)	1:102:A:THR:HG22	1:73:A:GLU:HA	11	0.66
(1,910)	1:109:A:LEU:HD13	1:13:A:LEU:HD13	18	0.66
(1,910)	1:109:A:LEU:HD12	1:13:A:LEU:HD13	19	0.66
(1,904)	1:31:A:VAL:HG13	1:10:A:LEU:HD12	18	0.66
(1,865)	1:26:A:ILE:HD12	1:114:A:MET:HE1	15	0.66
(1,828)	1:101:A:ILE:HG21	1:101:A:ILE:HG13	13	0.66
(1,828)	1:101:A:ILE:HG23	1:101:A:ILE:HG13	15	0.66
(1,746)	1:72:A:LEU:HD13	1:83:A:PRO:HB2	10	0.66
(1,330)	1:68:A:GLU:HG2	1:33:A:ILE:H	19	0.66
(1,299)	1:39:A:MET:HE2	1:6:A:VAL:H	14	0.66
(1,197)	1:12:A:ALA:HB3	1:16:A:GLU:H	7	0.66
(1,195)	1:12:A:ALA:HB1	1:15:A:GLU:H	12	0.66
(1,195)	1:12:A:ALA:HB1	1:15:A:GLU:H	16	0.66
(1,144)	1:47:A:ALA:HB2	1:50:A:THR:H	3	0.66
(1,144)	1:47:A:ALA:HB1	1:50:A:THR:H	8	0.66
(1,144)	1:47:A:ALA:HB1	1:50:A:THR:H	19	0.66
(1,136)	1:102:A:THR:HG22	1:100:A:ILE:H	8	0.66
(1,130)	1:10:A:LEU:HD21	1:10:A:LEU:H	8	0.66
(1,123)	1:13:A:LEU:HD13	1:14:A:CYS:H	1	0.66
(1,123)	1:13:A:LEU:HD13	1:14:A:CYS:H	10	0.66
(1,123)	1:13:A:LEU:HD12	1:14:A:CYS:H	15	0.66
(1,120)	1:13:A:LEU:HD11	1:13:A:LEU:H	15	0.66
(1,120)	1:13:A:LEU:HD13	1:13:A:LEU:H	20	0.66
(1,110)	1:43:A:LEU:HD21	1:44:A:PHE:H	14	0.66
(1,34)	1:33:A:ILE:HG21	1:39:A:MET:H	4	0.66
(1,27)	1:90:A:VAL:HG23	1:89:A:GLY:H	1	0.66
(1,7)	1:72:A:LEU:HD13	1:73:A:GLU:H	9	0.66
(1,7)	1:72:A:LEU:HD12	1:73:A:GLU:H	12	0.66
(1,2669)	1:31:A:VAL:HG23	1:44:A:PHE:HD1	15	0.65
(1,2652)	1:45:A:VAL:HA	1:47:A:ALA:HB1	15	0.65
(1,2639)	1:39:A:MET:HE2	1:39:A:MET:HE1	8	0.65
(1,2639)	1:107:A:MET:HE2	1:107:A:MET:HE3	14	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2639)	1:114:A:MET:HE2	1:114:A:MET:HE1	15	0.65
(1,2613)	1:43:A:LEU:HD11	1:43:A:LEU:HD13	1	0.65
(1,2613)	1:56:A:LEU:HD12	1:56:A:LEU:HD13	4	0.65
(1,2613)	1:56:A:LEU:HD12	1:56:A:LEU:HD13	12	0.65
(1,2613)	1:56:A:LEU:HD12	1:56:A:LEU:HD11	17	0.65
(1,2613)	1:56:A:LEU:HD11	1:56:A:LEU:HD13	18	0.65
(1,2613)	1:56:A:LEU:HD12	1:56:A:LEU:HD11	20	0.65
(1,2605)	1:86:A:LEU:HD11	1:86:A:LEU:HD13	6	0.65
(1,2605)	1:86:A:LEU:HD12	1:86:A:LEU:HD11	9	0.65
(1,2605)	1:115:A:LEU:HD12	1:115:A:LEU:HD11	11	0.65
(1,2605)	1:86:A:LEU:HD12	1:86:A:LEU:HD13	14	0.65
(1,2605)	1:115:A:LEU:HD12	1:115:A:LEU:HD11	15	0.65
(1,2605)	1:86:A:LEU:HD12	1:86:A:LEU:HD11	19	0.65
(1,2586)	1:31:A:VAL:HA	1:31:A:VAL:HG22	9	0.65
(1,2206)	1:83:A:PRO:HB2	1:81:A:PHE:HD1	1	0.65
(1,2180)	1:61:A:ALA:HB1	1:48:A:PHE:HD2	4	0.65
(1,2163)	1:45:A:VAL:HG23	1:44:A:PHE:HD2	6	0.65
(1,2163)	1:45:A:VAL:HG23	1:44:A:PHE:HD1	14	0.65
(1,2163)	1:45:A:VAL:HG22	1:44:A:PHE:HD2	19	0.65
(1,2134)	1:72:A:LEU:HD21	1:81:A:PHE:HE1	18	0.65
(1,2132)	1:72:A:LEU:HB3	1:81:A:PHE:HD2	7	0.65
(1,2091)	1:65:A:ILE:HA	1:31:A:VAL:HG12	14	0.65
(1,2089)	1:79:A:HIS:HA	1:80:A:VAL:HG22	3	0.65
(1,2035)	1:42:A:SER:HB2	1:45:A:VAL:HG22	19	0.65
(1,2023)	1:7:A:VAL:HA	1:11:A:ILE:HD12	4	0.65
(1,2023)	1:7:A:VAL:HA	1:11:A:ILE:HD11	20	0.65
(1,1992)	1:20:A:LYS:HE2	1:20:A:LYS:HA	11	0.65
(1,1992)	1:20:A:LYS:HE2	1:20:A:LYS:HA	19	0.65
(1,1941)	1:107:A:MET:HE3	1:10:A:LEU:HB3	18	0.65
(1,1939)	1:39:A:MET:HE2	1:39:A:MET:HA	11	0.65
(1,1857)	1:75:A:LYS:HG2	1:98:A:ASN:HB2	2	0.65
(1,1825)	1:62:A:ILE:HG21	1:62:A:ILE:HG13	2	0.65
(1,1812)	1:50:A:THR:HG22	1:47:A:ALA:HA	8	0.65
(1,1778)	1:112:A:LEU:HD23	1:18:A:ALA:HB3	18	0.65
(1,1775)	1:100:A:ILE:HD11	1:102:A:THR:HB	15	0.65
(1,1753)	1:65:A:ILE:HD13	1:41:A:LYS:HD3	14	0.65
(1,1753)	1:65:A:ILE:HD13	1:41:A:LYS:HD3	17	0.65
(1,1753)	1:65:A:ILE:HD13	1:41:A:LYS:HD3	18	0.65
(1,1737)	1:33:A:ILE:HG13	1:39:A:MET:HE3	12	0.65
(1,1735)	1:72:A:LEU:HD21	1:88:A:TYR:HB3	5	0.65
(1,1708)	1:107:A:MET:HA	1:33:A:ILE:HD11	6	0.65
(1,1697)	1:112:A:LEU:HD23	1:112:A:LEU:HA	1	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1697)	1:112:A:LEU:HD23	1:112:A:LEU:HA	8	0.65
(1,1597)	1:109:A:LEU:HD11	1:109:A:LEU:HA	1	0.65
(1,1302)	1:1:A:MET:HE1	1:1:A:MET:HA	13	0.65
(1,1248)	1:13:A:LEU:HD13	1:13:A:LEU:HB3	7	0.65
(1,1248)	1:13:A:LEU:HD12	1:13:A:LEU:HB3	10	0.65
(1,1248)	1:13:A:LEU:HD11	1:13:A:LEU:HB3	12	0.65
(1,1248)	1:13:A:LEU:HD11	1:13:A:LEU:HB3	17	0.65
(1,921)	1:45:A:VAL:HG23	1:45:A:VAL:HA	8	0.65
(1,921)	1:45:A:VAL:HG21	1:45:A:VAL:HA	11	0.65
(1,828)	1:101:A:ILE:HG23	1:101:A:ILE:HG13	10	0.65
(1,828)	1:101:A:ILE:HG21	1:101:A:ILE:HG13	16	0.65
(1,805)	1:7:A:VAL:HG21	1:48:A:PHE:HB3	18	0.65
(1,770)	1:72:A:LEU:HD11	1:70:A:VAL:HG21	5	0.65
(1,420)	1:19:A:LYS:HE2	1:19:A:LYS:H	4	0.65
(1,300)	1:107:A:MET:HE2	1:108:A:ARG:H	10	0.65
(1,197)	1:12:A:ALA:HB1	1:16:A:GLU:H	16	0.65
(1,195)	1:12:A:ALA:HB1	1:15:A:GLU:H	4	0.65
(1,176)	1:18:A:ALA:HB1	1:16:A:GLU:H	15	0.65
(1,130)	1:10:A:LEU:HD21	1:10:A:LEU:H	11	0.65
(1,123)	1:13:A:LEU:HD11	1:14:A:CYS:H	3	0.65
(1,110)	1:43:A:LEU:HD23	1:44:A:PHE:H	17	0.65
(1,66)	1:100:A:ILE:HD11	1:100:A:ILE:H	3	0.65
(1,50)	1:7:A:VAL:HG21	1:8:A:SER:H	2	0.65
(1,50)	1:7:A:VAL:HG22	1:8:A:SER:H	5	0.65
(1,50)	1:7:A:VAL:HG23	1:8:A:SER:H	6	0.65
(1,50)	1:7:A:VAL:HG21	1:8:A:SER:H	12	0.65
(1,50)	1:7:A:VAL:HG23	1:8:A:SER:H	13	0.65
(1,44)	1:99:A:VAL:HG11	1:73:A:GLU:H	7	0.65
(1,37)	1:99:A:VAL:HG11	1:99:A:VAL:H	5	0.65
(1,15)	1:7:A:VAL:HG12	1:47:A:ALA:H	5	0.65
(1,2676)	1:47:A:ALA:HB2	1:44:A:PHE:HD1	9	0.64
(1,2676)	1:47:A:ALA:HB1	1:44:A:PHE:HD2	14	0.64
(1,2642)	1:114:A:MET:HE2	1:114:A:MET:HE3	14	0.64
(1,2639)	1:114:A:MET:HE2	1:114:A:MET:HE1	2	0.64
(1,2639)	1:114:A:MET:HE2	1:114:A:MET:HE3	4	0.64
(1,2639)	1:114:A:MET:HE2	1:114:A:MET:HE3	7	0.64
(1,2639)	1:107:A:MET:HE1	1:107:A:MET:HE3	10	0.64
(1,2639)	1:39:A:MET:HE1	1:39:A:MET:HE3	11	0.64
(1,2639)	1:107:A:MET:HE2	1:107:A:MET:HE1	12	0.64
(1,2639)	1:114:A:MET:HE1	1:114:A:MET:HE3	13	0.64
(1,2639)	1:107:A:MET:HE1	1:107:A:MET:HE3	18	0.64
(1,2639)	1:107:A:MET:HE2	1:107:A:MET:HE1	19	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2613)	1:56:A:LEU:HD12	1:56:A:LEU:HD11	2	0.64
(1,2613)	1:43:A:LEU:HD12	1:43:A:LEU:HD13	10	0.64
(1,2613)	1:56:A:LEU:HD12	1:56:A:LEU:HD13	14	0.64
(1,2613)	1:43:A:LEU:HD12	1:43:A:LEU:HD11	15	0.64
(1,2613)	1:43:A:LEU:HD12	1:43:A:LEU:HD13	16	0.64
(1,2605)	1:115:A:LEU:HD11	1:115:A:LEU:HD13	5	0.64
(1,2605)	1:86:A:LEU:HD12	1:86:A:LEU:HD11	10	0.64
(1,2605)	1:86:A:LEU:HD12	1:86:A:LEU:HD13	16	0.64
(1,2586)	1:31:A:VAL:HA	1:31:A:VAL:HG22	7	0.64
(1,2426)	1:97:A:LYS:HD3	1:97:A:LYS:H	3	0.64
(1,2160)	1:80:A:VAL:HG22	1:81:A:PHE:HD1	8	0.64
(1,2133)	1:65:A:ILE:HG21	1:44:A:PHE:HD2	1	0.64
(1,2105)	1:64:A:ASP:HA	1:62:A:ILE:HG23	12	0.64
(1,2100)	1:97:A:LYS:HA	1:97:A:LYS:HE3	19	0.64
(1,2089)	1:79:A:HIS:HA	1:80:A:VAL:HG22	10	0.64
(1,2047)	1:33:A:ILE:HG22	1:37:A:SER:HA	5	0.64
(1,2023)	1:7:A:VAL:HA	1:11:A:ILE:HD12	1	0.64
(1,1842)	1:18:A:ALA:HB3	1:21:A:ASN:HB3	16	0.64
(1,1746)	1:90:A:VAL:HG21	1:87:A:ASP:HB3	2	0.64
(1,1746)	1:90:A:VAL:HG23	1:87:A:ASP:HB3	13	0.64
(1,1739)	1:33:A:ILE:HG23	1:65:A:ILE:HG23	11	0.64
(1,1732)	1:72:A:LEU:HD11	1:89:A:GLY:HA3	6	0.64
(1,1697)	1:112:A:LEU:HD22	1:112:A:LEU:HA	6	0.64
(1,1697)	1:112:A:LEU:HD21	1:112:A:LEU:HA	7	0.64
(1,1697)	1:112:A:LEU:HD21	1:112:A:LEU:HA	12	0.64
(1,1628)	1:61:A:ALA:HB1	1:27:A:GLU:HA	14	0.64
(1,1597)	1:109:A:LEU:HD11	1:109:A:LEU:HA	14	0.64
(1,1597)	1:109:A:LEU:HD12	1:109:A:LEU:HA	18	0.64
(1,1514)	1:43:A:LEU:HD21	1:42:A:SER:HB2	8	0.64
(1,1514)	1:43:A:LEU:HD21	1:42:A:SER:HB3	9	0.64
(1,1514)	1:43:A:LEU:HD22	1:42:A:SER:HB2	16	0.64
(1,1363)	1:23:A:ALA:HB2	1:114:A:MET:HG2	2	0.64
(1,1248)	1:13:A:LEU:HD12	1:13:A:LEU:HB3	16	0.64
(1,1248)	1:13:A:LEU:HD13	1:13:A:LEU:HB3	20	0.64
(1,1020)	1:85:A:ALA:HB2	1:86:A:LEU:HA	1	0.64
(1,1020)	1:85:A:ALA:HB1	1:86:A:LEU:HA	3	0.64
(1,1020)	1:85:A:ALA:HB1	1:86:A:LEU:HA	5	0.64
(1,1020)	1:85:A:ALA:HB1	1:86:A:LEU:HA	20	0.64
(1,996)	1:26:A:ILE:HG12	1:57:A:VAL:HG12	10	0.64
(1,937)	1:102:A:THR:HG21	1:73:A:GLU:HA	5	0.64
(1,923)	1:57:A:VAL:HG23	1:56:A:LEU:HB2	13	0.64
(1,923)	1:57:A:VAL:HG21	1:56:A:LEU:HB2	19	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,828)	1:101:A:ILE:HG22	1:101:A:ILE:HG13	3	0.64
(1,828)	1:101:A:ILE:HG22	1:101:A:ILE:HG13	6	0.64
(1,828)	1:101:A:ILE:HG22	1:101:A:ILE:HG13	9	0.64
(1,809)	1:110:A:LEU:HD13	1:66:A:VAL:HG13	15	0.64
(1,809)	1:110:A:LEU:HD12	1:66:A:VAL:HG11	19	0.64
(1,770)	1:72:A:LEU:HD13	1:70:A:VAL:HG21	4	0.64
(1,195)	1:12:A:ALA:HB3	1:15:A:GLU:H	2	0.64
(1,195)	1:12:A:ALA:HB3	1:15:A:GLU:H	8	0.64
(1,185)	1:38:A:ALA:HB2	1:39:A:MET:H	4	0.64
(1,176)	1:18:A:ALA:HB2	1:16:A:GLU:H	8	0.64
(1,144)	1:47:A:ALA:HB2	1:50:A:THR:H	17	0.64
(1,110)	1:43:A:LEU:HD23	1:44:A:PHE:H	4	0.64
(1,50)	1:7:A:VAL:HG22	1:8:A:SER:H	7	0.64
(1,40)	1:99:A:VAL:HG11	1:89:A:GLY:H	7	0.64
(1,34)	1:33:A:ILE:HG22	1:39:A:MET:H	7	0.64
(1,15)	1:7:A:VAL:HG12	1:47:A:ALA:H	17	0.64
(1,2693)	1:44:A:PHE:HD2	1:44:A:PHE:HZ	3	0.63
(1,2671)	1:115:A:LEU:HD12	1:24:A:HIS:HD2	7	0.63
(1,2670)	1:11:A:ILE:HG21	1:51:A:PHE:HD2	7	0.63
(1,2652)	1:45:A:VAL:HA	1:47:A:ALA:HB2	8	0.63
(1,2652)	1:45:A:VAL:HA	1:47:A:ALA:HB2	13	0.63
(1,2643)	1:39:A:MET:HE1	1:106:A:GLU:HG2	16	0.63
(1,2642)	1:39:A:MET:HE2	1:39:A:MET:HE1	1	0.63
(1,2639)	1:107:A:MET:HE2	1:107:A:MET:HE1	1	0.63
(1,2639)	1:114:A:MET:HE2	1:114:A:MET:HE1	3	0.63
(1,2639)	1:107:A:MET:HE2	1:107:A:MET:HE1	5	0.63
(1,2639)	1:107:A:MET:HE1	1:107:A:MET:HE3	9	0.63
(1,2639)	1:39:A:MET:HE2	1:39:A:MET:HE3	16	0.63
(1,2639)	1:107:A:MET:HE1	1:107:A:MET:HE3	20	0.63
(1,2606)	1:57:A:VAL:HG13	1:26:A:ILE:HA	8	0.63
(1,2597)	1:72:A:LEU:HB2	1:99:A:VAL:HG21	15	0.63
(1,2177)	1:6:A:VAL:HG11	1:44:A:PHE:HD1	8	0.63
(1,2089)	1:79:A:HIS:HA	1:80:A:VAL:HG23	7	0.63
(1,2089)	1:79:A:HIS:HA	1:80:A:VAL:HG21	16	0.63
(1,2063)	1:33:A:ILE:HA	1:107:A:MET:HG3	8	0.63
(1,2047)	1:33:A:ILE:HG21	1:37:A:SER:HA	18	0.63
(1,1987)	1:23:A:ALA:HB1	1:21:A:ASN:HB2	5	0.63
(1,1889)	1:82:A:LYS:HD3	1:71:A:GLU:HG3	19	0.63
(1,1857)	1:75:A:LYS:HG2	1:98:A:ASN:HB2	18	0.63
(1,1831)	1:58:A:CYS:HB2	1:61:A:ALA:HB2	8	0.63
(1,1824)	1:25:A:LYS:HG3	1:56:A:LEU:HD13	1	0.63
(1,1806)	1:10:A:LEU:HD11	1:7:A:VAL:HA	16	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1805)	1:10:A:LEU:HD13	1:63:A:LEU:HD23	16	0.63
(1,1800)	1:115:A:LEU:HD13	1:25:A:LYS:HG2	3	0.63
(1,1798)	1:62:A:ILE:HD13	1:28:A:ARG:HD3	8	0.63
(1,1753)	1:65:A:ILE:HD13	1:41:A:LYS:HD3	5	0.63
(1,1739)	1:33:A:ILE:HG22	1:65:A:ILE:HG23	4	0.63
(1,1732)	1:72:A:LEU:HD13	1:89:A:GLY:HA3	12	0.63
(1,1697)	1:112:A:LEU:HD23	1:112:A:LEU:HA	9	0.63
(1,1628)	1:61:A:ALA:HB1	1:27:A:GLU:HA	10	0.63
(1,1482)	1:7:A:VAL:HG23	1:48:A:PHE:HA	12	0.63
(1,1302)	1:1:A:MET:HE1	1:1:A:MET:HA	3	0.63
(1,1254)	1:20:A:LYS:HB2	1:20:A:LYS:HE3	8	0.63
(1,1019)	1:102:A:THR:HG23	1:100:A:ILE:HG12	17	0.63
(1,943)	1:6:A:VAL:HG12	1:107:A:MET:HG2	9	0.63
(1,937)	1:102:A:THR:HG21	1:73:A:GLU:HA	7	0.63
(1,937)	1:102:A:THR:HG23	1:73:A:GLU:HA	9	0.63
(1,923)	1:57:A:VAL:HG23	1:56:A:LEU:HB2	17	0.63
(1,828)	1:101:A:ILE:HG22	1:101:A:ILE:HG13	2	0.63
(1,828)	1:101:A:ILE:HG21	1:101:A:ILE:HG13	19	0.63
(1,770)	1:72:A:LEU:HD11	1:70:A:VAL:HG21	15	0.63
(1,130)	1:10:A:LEU:HD21	1:10:A:LEU:H	6	0.63
(1,130)	1:10:A:LEU:HD23	1:10:A:LEU:H	7	0.63
(1,126)	1:45:A:VAL:HG23	1:47:A:ALA:H	10	0.63
(1,123)	1:13:A:LEU:HD12	1:14:A:CYS:H	19	0.63
(1,120)	1:13:A:LEU:HD11	1:13:A:LEU:H	6	0.63
(1,120)	1:13:A:LEU:HD13	1:13:A:LEU:H	13	0.63
(1,103)	1:43:A:LEU:HD21	1:46:A:SER:H	11	0.63
(1,70)	1:112:A:LEU:HD23	1:17:A:HIS:H	5	0.63
(1,53)	1:66:A:VAL:HG12	1:33:A:ILE:H	9	0.63
(1,50)	1:7:A:VAL:HG22	1:8:A:SER:H	1	0.63
(1,50)	1:7:A:VAL:HG22	1:8:A:SER:H	10	0.63
(1,50)	1:7:A:VAL:HG21	1:8:A:SER:H	16	0.63
(1,50)	1:7:A:VAL:HG23	1:8:A:SER:H	20	0.63
(1,44)	1:99:A:VAL:HG11	1:73:A:GLU:H	20	0.63
(1,37)	1:99:A:VAL:HG12	1:99:A:VAL:H	1	0.63
(1,37)	1:99:A:VAL:HG12	1:99:A:VAL:H	8	0.63
(1,27)	1:90:A:VAL:HG23	1:89:A:GLY:H	15	0.63
(1,2679)	1:7:A:VAL:HB	1:44:A:PHE:HD2	11	0.62
(1,2669)	1:31:A:VAL:HG21	1:44:A:PHE:HD2	6	0.62
(1,2652)	1:45:A:VAL:HA	1:47:A:ALA:HB2	16	0.62
(1,2651)	1:45:A:VAL:HA	1:48:A:PHE:HA	12	0.62
(1,2645)	1:33:A:ILE:HG21	1:39:A:MET:HG3	5	0.62
(1,2642)	1:114:A:MET:HE2	1:114:A:MET:HE3	5	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2642)	1:39:A:MET:HE2	1:39:A:MET:HE3	6	0.62
(1,2642)	1:114:A:MET:HE2	1:114:A:MET:HE3	7	0.62
(1,2642)	1:39:A:MET:HE2	1:39:A:MET:HE1	8	0.62
(1,2642)	1:39:A:MET:HE2	1:39:A:MET:HE1	9	0.62
(1,2642)	1:39:A:MET:HE1	1:39:A:MET:HE3	10	0.62
(1,2642)	1:39:A:MET:HE1	1:39:A:MET:HE3	11	0.62
(1,2642)	1:114:A:MET:HE2	1:114:A:MET:HE1	12	0.62
(1,2642)	1:114:A:MET:HE2	1:114:A:MET:HE1	15	0.62
(1,2642)	1:114:A:MET:HE1	1:114:A:MET:HE3	18	0.62
(1,2642)	1:114:A:MET:HE2	1:114:A:MET:HE3	19	0.62
(1,2642)	1:114:A:MET:HE2	1:114:A:MET:HE3	20	0.62
(1,2638)	1:107:A:MET:HA	1:39:A:MET:HE2	4	0.62
(1,2597)	1:72:A:LEU:HB2	1:99:A:VAL:HG23	7	0.62
(1,2586)	1:31:A:VAL:HA	1:31:A:VAL:HG21	2	0.62
(1,2586)	1:31:A:VAL:HA	1:31:A:VAL:HG23	4	0.62
(1,2586)	1:31:A:VAL:HA	1:31:A:VAL:HG22	15	0.62
(1,2586)	1:31:A:VAL:HA	1:31:A:VAL:HG21	19	0.62
(1,2474)	1:18:A:ALA:HB2	1:19:A:LYS:HA	8	0.62
(1,2454)	1:62:A:ILE:HG23	1:28:A:ARG:HG3	2	0.62
(1,2433)	1:63:A:LEU:HD23	1:31:A:VAL:HG22	3	0.62
(1,2206)	1:83:A:PRO:HB2	1:81:A:PHE:HD1	10	0.62
(1,2163)	1:45:A:VAL:HG23	1:44:A:PHE:HD2	5	0.62
(1,2153)	1:99:A:VAL:HG22	1:81:A:PHE:HE1	18	0.62
(1,2088)	1:105:A:ASN:HA	1:36:A:ARG:HB3	11	0.62
(1,2069)	1:112:A:LEU:HD23	1:29:A:VAL:HA	9	0.62
(1,2069)	1:112:A:LEU:HD21	1:29:A:VAL:HA	11	0.62
(1,2069)	1:112:A:LEU:HD21	1:29:A:VAL:HA	12	0.62
(1,1992)	1:20:A:LYS:HE2	1:20:A:LYS:HA	7	0.62
(1,1992)	1:20:A:LYS:HE2	1:20:A:LYS:HA	14	0.62
(1,1992)	1:20:A:LYS:HE2	1:20:A:LYS:HA	18	0.62
(1,1946)	1:114:A:MET:HA	1:114:A:MET:HE1	2	0.62
(1,1939)	1:39:A:MET:HE1	1:39:A:MET:HA	8	0.62
(1,1857)	1:75:A:LYS:HG2	1:98:A:ASN:HB2	1	0.62
(1,1857)	1:75:A:LYS:HG2	1:98:A:ASN:HB2	19	0.62
(1,1831)	1:58:A:CYS:HB2	1:61:A:ALA:HB3	5	0.62
(1,1803)	1:10:A:LEU:HD11	1:109:A:LEU:HB2	13	0.62
(1,1793)	1:15:A:GLU:HG2	1:11:A:ILE:HG23	17	0.62
(1,1793)	1:15:A:GLU:HG2	1:11:A:ILE:HG21	18	0.62
(1,1769)	1:66:A:VAL:HG11	1:68:A:GLU:HB2	3	0.62
(1,1753)	1:65:A:ILE:HD13	1:41:A:LYS:HD3	19	0.62
(1,1751)	1:65:A:ILE:HD12	1:33:A:ILE:HG22	12	0.62
(1,1739)	1:33:A:ILE:HG23	1:65:A:ILE:HG21	5	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1738)	1:65:A:ILE:HG22	1:63:A:LEU:HD13	2	0.62
(1,1723)	1:45:A:VAL:HG13	1:63:A:LEU:HD23	8	0.62
(1,1697)	1:112:A:LEU:HD22	1:112:A:LEU:HA	16	0.62
(1,1628)	1:61:A:ALA:HB2	1:27:A:GLU:HA	6	0.62
(1,1628)	1:61:A:ALA:HB3	1:27:A:GLU:HA	15	0.62
(1,1482)	1:7:A:VAL:HG22	1:48:A:PHE:HA	19	0.62
(1,1385)	1:48:A:PHE:HB3	1:63:A:LEU:HD12	6	0.62
(1,1254)	1:20:A:LYS:HB2	1:20:A:LYS:HE3	15	0.62
(1,1254)	1:20:A:LYS:HB2	1:20:A:LYS:HE3	16	0.62
(1,1254)	1:20:A:LYS:HB2	1:20:A:LYS:HE3	18	0.62
(1,1248)	1:13:A:LEU:HD13	1:13:A:LEU:HB3	3	0.62
(1,1248)	1:13:A:LEU:HD11	1:13:A:LEU:HB3	5	0.62
(1,1248)	1:13:A:LEU:HD11	1:13:A:LEU:HB3	6	0.62
(1,1248)	1:13:A:LEU:HD11	1:13:A:LEU:HB3	19	0.62
(1,996)	1:26:A:ILE:HG12	1:57:A:VAL:HG13	11	0.62
(1,923)	1:57:A:VAL:HG23	1:56:A:LEU:HB2	18	0.62
(1,875)	1:86:A:LEU:HD21	1:85:A:ALA:HA	19	0.62
(1,828)	1:101:A:ILE:HG23	1:101:A:ILE:HG13	1	0.62
(1,828)	1:101:A:ILE:HG22	1:101:A:ILE:HG13	5	0.62
(1,828)	1:101:A:ILE:HG21	1:101:A:ILE:HG13	7	0.62
(1,828)	1:101:A:ILE:HG23	1:101:A:ILE:HG13	11	0.62
(1,828)	1:101:A:ILE:HG23	1:101:A:ILE:HG13	20	0.62
(1,826)	1:101:A:ILE:HG21	1:103:A:GLN:HA	3	0.62
(1,809)	1:110:A:LEU:HD11	1:66:A:VAL:HG11	2	0.62
(1,809)	1:110:A:LEU:HD11	1:66:A:VAL:HG12	13	0.62
(1,804)	1:66:A:VAL:HG11	1:32:A:GLY:HA3	10	0.62
(1,804)	1:66:A:VAL:HG13	1:32:A:GLY:HA3	20	0.62
(1,770)	1:72:A:LEU:HD12	1:70:A:VAL:HG23	18	0.62
(1,420)	1:19:A:LYS:HE2	1:19:A:LYS:H	13	0.62
(1,253)	1:68:A:GLU:HG3	1:69:A:LYS:H	2	0.62
(1,239)	1:19:A:LYS:HD2	1:20:A:LYS:H	7	0.62
(1,208)	1:41:A:LYS:HG2	1:42:A:SER:H	20	0.62
(1,200)	1:12:A:ALA:HB1	1:11:A:ILE:H	19	0.62
(1,185)	1:38:A:ALA:HB2	1:39:A:MET:H	5	0.62
(1,176)	1:18:A:ALA:HB3	1:16:A:GLU:H	3	0.62
(1,144)	1:47:A:ALA:HB2	1:50:A:THR:H	1	0.62
(1,136)	1:102:A:THR:HG21	1:100:A:ILE:H	5	0.62
(1,136)	1:102:A:THR:HG21	1:100:A:ILE:H	16	0.62
(1,136)	1:102:A:THR:HG21	1:100:A:ILE:H	18	0.62
(1,130)	1:10:A:LEU:HD23	1:10:A:LEU:H	20	0.62
(1,120)	1:13:A:LEU:HD12	1:13:A:LEU:H	16	0.62
(1,116)	1:13:A:LEU:HD23	1:14:A:CYS:H	12	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,88)	1:26:A:ILE:HD13	1:15:A:GLU:H	10	0.62
(1,70)	1:112:A:LEU:HD23	1:17:A:HIS:H	19	0.62
(1,66)	1:100:A:ILE:HD11	1:100:A:ILE:H	11	0.62
(1,40)	1:99:A:VAL:HG13	1:89:A:GLY:H	15	0.62
(1,37)	1:99:A:VAL:HG11	1:99:A:VAL:H	2	0.62
(1,37)	1:99:A:VAL:HG13	1:99:A:VAL:H	17	0.62
(1,27)	1:90:A:VAL:HG23	1:89:A:GLY:H	19	0.62
(1,27)	1:90:A:VAL:HG22	1:89:A:GLY:H	20	0.62
(1,7)	1:72:A:LEU:HD13	1:73:A:GLU:H	13	0.62
(1,2676)	1:47:A:ALA:HB1	1:44:A:PHE:HD1	1	0.61
(1,2671)	1:115:A:LEU:HD12	1:24:A:HIS:HD2	9	0.61
(1,2651)	1:7:A:VAL:HA	1:48:A:PHE:HA	1	0.61
(1,2642)	1:114:A:MET:HE2	1:114:A:MET:HE1	2	0.61
(1,2642)	1:114:A:MET:HE2	1:114:A:MET:HE1	3	0.61
(1,2642)	1:114:A:MET:HE2	1:114:A:MET:HE3	4	0.61
(1,2642)	1:114:A:MET:HE1	1:114:A:MET:HE3	13	0.61
(1,2642)	1:39:A:MET:HE2	1:39:A:MET:HE3	16	0.61
(1,2639)	1:107:A:MET:HE2	1:107:A:MET:HE3	6	0.61
(1,2639)	1:114:A:MET:HE2	1:114:A:MET:HE3	17	0.61
(1,2597)	1:72:A:LEU:HB2	1:99:A:VAL:HG21	16	0.61
(1,2586)	1:31:A:VAL:HA	1:31:A:VAL:HG21	3	0.61
(1,2586)	1:31:A:VAL:HA	1:31:A:VAL:HG22	5	0.61
(1,2586)	1:31:A:VAL:HA	1:31:A:VAL:HG22	6	0.61
(1,2586)	1:31:A:VAL:HA	1:31:A:VAL:HG22	16	0.61
(1,2474)	1:18:A:ALA:HB1	1:19:A:LYS:HA	15	0.61
(1,2459)	1:86:A:LEU:HD11	1:86:A:LEU:HD13	7	0.61
(1,2459)	1:115:A:LEU:HD12	1:115:A:LEU:HD13	12	0.61
(1,2206)	1:83:A:PRO:HB2	1:81:A:PHE:HD2	8	0.61
(1,2204)	1:83:A:PRO:HB3	1:88:A:TYR:HE1	20	0.61
(1,2177)	1:6:A:VAL:HG11	1:44:A:PHE:HD1	13	0.61
(1,2133)	1:65:A:ILE:HG22	1:44:A:PHE:HD1	3	0.61
(1,2091)	1:65:A:ILE:HA	1:31:A:VAL:HG13	5	0.61
(1,2079)	1:71:A:GLU:HB2	1:103:A:GLN:HA	10	0.61
(1,2069)	1:112:A:LEU:HD22	1:29:A:VAL:HA	3	0.61
(1,2069)	1:112:A:LEU:HD22	1:29:A:VAL:HA	13	0.61
(1,2047)	1:33:A:ILE:HG23	1:37:A:SER:HA	13	0.61
(1,1993)	1:20:A:LYS:HG3	1:20:A:LYS:HE3	2	0.61
(1,1987)	1:23:A:ALA:HB3	1:21:A:ASN:HB2	13	0.61
(1,1984)	1:7:A:VAL:HG11	1:48:A:PHE:HB3	19	0.61
(1,1907)	1:25:A:LYS:HB2	1:57:A:VAL:HG13	9	0.61
(1,1907)	1:25:A:LYS:HB2	1:57:A:VAL:HG12	14	0.61
(1,1806)	1:10:A:LEU:HD12	1:7:A:VAL:HA	20	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1793)	1:15:A:GLU:HG2	1:11:A:ILE:HG23	2	0.61
(1,1761)	1:110:A:LEU:HD23	1:108:A:ARG:HD2	11	0.61
(1,1748)	1:33:A:ILE:HG22	1:107:A:MET:HG3	9	0.61
(1,1697)	1:112:A:LEU:HD21	1:112:A:LEU:HA	5	0.61
(1,1697)	1:112:A:LEU:HD23	1:112:A:LEU:HA	10	0.61
(1,1697)	1:112:A:LEU:HD23	1:112:A:LEU:HA	17	0.61
(1,1688)	1:97:A:LYS:HA	1:99:A:VAL:HG21	19	0.61
(1,1628)	1:61:A:ALA:HB1	1:27:A:GLU:HA	17	0.61
(1,1565)	1:100:A:ILE:HD13	1:102:A:THR:HA	1	0.61
(1,1482)	1:7:A:VAL:HG22	1:48:A:PHE:HA	4	0.61
(1,1452)	1:63:A:LEU:HD11	1:45:A:VAL:HA	3	0.61
(1,1420)	1:25:A:LYS:HE3	1:25:A:LYS:HB3	5	0.61
(1,1248)	1:13:A:LEU:HD12	1:13:A:LEU:HB3	4	0.61
(1,1006)	1:100:A:ILE:HD11	1:75:A:LYS:HG3	14	0.61
(1,948)	1:45:A:VAL:HG12	1:42:A:SER:HA	1	0.61
(1,923)	1:57:A:VAL:HG23	1:56:A:LEU:HB2	4	0.61
(1,910)	1:109:A:LEU:HD12	1:13:A:LEU:HD13	5	0.61
(1,898)	1:29:A:VAL:HG11	1:112:A:LEU:HA	2	0.61
(1,846)	1:31:A:VAL:HG11	1:10:A:LEU:HD23	19	0.61
(1,834)	1:72:A:LEU:HD23	1:101:A:ILE:HG22	15	0.61
(1,804)	1:66:A:VAL:HG12	1:32:A:GLY:HA3	12	0.61
(1,770)	1:72:A:LEU:HD11	1:70:A:VAL:HG21	3	0.61
(1,770)	1:72:A:LEU:HD11	1:70:A:VAL:HG23	9	0.61
(1,769)	1:72:A:LEU:HD21	1:70:A:VAL:HG22	1	0.61
(1,395)	1:87:A:ASP:HB3	1:87:A:ASP:H	20	0.61
(1,300)	1:107:A:MET:HE2	1:108:A:ARG:H	6	0.61
(1,213)	1:75:A:LYS:HD3	1:75:A:LYS:H	15	0.61
(1,148)	1:6:A:VAL:HG12	1:9:A:SER:H	6	0.61
(1,144)	1:47:A:ALA:HB3	1:50:A:THR:H	4	0.61
(1,144)	1:47:A:ALA:HB3	1:50:A:THR:H	14	0.61
(1,123)	1:13:A:LEU:HD11	1:14:A:CYS:H	7	0.61
(1,123)	1:13:A:LEU:HD13	1:14:A:CYS:H	9	0.61
(1,118)	1:13:A:LEU:HD11	1:16:A:GLU:H	8	0.61
(1,112)	1:10:A:LEU:HD13	1:11:A:ILE:H	15	0.61
(1,110)	1:43:A:LEU:HD22	1:44:A:PHE:H	16	0.61
(1,88)	1:26:A:ILE:HD13	1:15:A:GLU:H	9	0.61
(1,29)	1:70:A:VAL:HG22	1:72:A:LEU:H	13	0.61
(1,23)	1:110:A:LEU:HD12	1:111:A:SER:H	2	0.61
(1,23)	1:110:A:LEU:HD12	1:111:A:SER:H	5	0.61
(1,15)	1:7:A:VAL:HG13	1:47:A:ALA:H	7	0.61
(1,2618)	1:6:A:VAL:HG22	1:2:A:HIS:HB2	2	0.6
(1,2618)	1:6:A:VAL:HG21	1:2:A:HIS:HB2	3	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2597)	1:72:A:LEU:HB2	1:99:A:VAL:HG23	14	0.6
(1,2474)	1:18:A:ALA:HB1	1:19:A:LYS:HA	4	0.6
(1,2459)	1:86:A:LEU:HD12	1:86:A:LEU:HD13	3	0.6
(1,2459)	1:115:A:LEU:HD22	1:115:A:LEU:HD23	8	0.6
(1,2459)	1:115:A:LEU:HD22	1:115:A:LEU:HD23	13	0.6
(1,2459)	1:115:A:LEU:HD11	1:115:A:LEU:HD13	20	0.6
(1,2433)	1:63:A:LEU:HD21	1:31:A:VAL:HG21	15	0.6
(1,2177)	1:6:A:VAL:HG13	1:44:A:PHE:HD1	16	0.6
(1,2133)	1:65:A:ILE:HG22	1:44:A:PHE:HD2	8	0.6
(1,2091)	1:65:A:ILE:HA	1:31:A:VAL:HG13	6	0.6
(1,2089)	1:79:A:HIS:HA	1:80:A:VAL:HG23	14	0.6
(1,2084)	1:58:A:CYS:HA	1:26:A:ILE:HG22	6	0.6
(1,2084)	1:58:A:CYS:HA	1:26:A:ILE:HG21	18	0.6
(1,1992)	1:20:A:LYS:HE2	1:20:A:LYS:HA	12	0.6
(1,1992)	1:20:A:LYS:HE2	1:20:A:LYS:HA	17	0.6
(1,1975)	1:12:A:ALA:HB3	1:15:A:GLU:HB2	17	0.6
(1,1939)	1:39:A:MET:HE1	1:39:A:MET:HA	7	0.6
(1,1842)	1:18:A:ALA:HB3	1:21:A:ASN:HB3	1	0.6
(1,1840)	1:75:A:LYS:HG3	1:100:A:ILE:HG13	4	0.6
(1,1838)	1:75:A:LYS:HG3	1:98:A:ASN:HB3	10	0.6
(1,1769)	1:66:A:VAL:HG12	1:68:A:GLU:HB2	14	0.6
(1,1751)	1:65:A:ILE:HD13	1:33:A:ILE:HG23	15	0.6
(1,1748)	1:33:A:ILE:HG21	1:107:A:MET:HG3	1	0.6
(1,1727)	1:11:A:ILE:HD13	1:55:A:SER:HB3	17	0.6
(1,1697)	1:112:A:LEU:HD21	1:112:A:LEU:HA	11	0.6
(1,1697)	1:112:A:LEU:HD21	1:112:A:LEU:HA	19	0.6
(1,1601)	1:12:A:ALA:HB3	1:9:A:SER:HA	15	0.6
(1,1385)	1:48:A:PHE:HB3	1:63:A:LEU:HD12	5	0.6
(1,1367)	1:26:A:ILE:HD13	1:14:A:CYS:HB3	11	0.6
(1,1254)	1:20:A:LYS:HB2	1:20:A:LYS:HE3	4	0.6
(1,1254)	1:20:A:LYS:HB2	1:20:A:LYS:HE3	5	0.6
(1,1254)	1:20:A:LYS:HB2	1:20:A:LYS:HE3	19	0.6
(1,1248)	1:13:A:LEU:HD12	1:13:A:LEU:HB3	1	0.6
(1,1159)	1:108:A:ARG:HB2	1:110:A:LEU:HD22	7	0.6
(1,990)	1:59:A:LYS:HG3	1:59:A:LYS:HE3	19	0.6
(1,914)	1:72:A:LEU:HD23	1:70:A:VAL:HG11	7	0.6
(1,914)	1:72:A:LEU:HD23	1:70:A:VAL:HG13	20	0.6
(1,910)	1:109:A:LEU:HD13	1:13:A:LEU:HD11	4	0.6
(1,897)	1:29:A:VAL:HG11	1:112:A:LEU:HD23	7	0.6
(1,897)	1:29:A:VAL:HG11	1:112:A:LEU:HD23	19	0.6
(1,828)	1:101:A:ILE:HG21	1:101:A:ILE:HG13	14	0.6
(1,828)	1:101:A:ILE:HG23	1:101:A:ILE:HG13	17	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,805)	1:7:A:VAL:HG22	1:48:A:PHE:HB3	20	0.6
(1,804)	1:66:A:VAL:HG12	1:32:A:GLY:HA3	1	0.6
(1,804)	1:66:A:VAL:HG11	1:32:A:GLY:HA3	8	0.6
(1,770)	1:72:A:LEU:HD11	1:70:A:VAL:HG21	16	0.6
(1,208)	1:41:A:LYS:HG2	1:42:A:SER:H	10	0.6
(1,197)	1:12:A:ALA:HB1	1:16:A:GLU:H	10	0.6
(1,174)	1:100:A:ILE:HG12	1:101:A:ILE:H	12	0.6
(1,136)	1:102:A:THR:HG21	1:100:A:ILE:H	2	0.6
(1,130)	1:10:A:LEU:HD23	1:10:A:LEU:H	9	0.6
(1,126)	1:45:A:VAL:HG21	1:47:A:ALA:H	19	0.6
(1,74)	1:99:A:VAL:HG23	1:73:A:GLU:H	5	0.6
(1,66)	1:100:A:ILE:HD13	1:100:A:ILE:H	5	0.6
(1,66)	1:100:A:ILE:HD12	1:100:A:ILE:H	6	0.6
(1,53)	1:66:A:VAL:HG11	1:33:A:ILE:H	3	0.6
(1,44)	1:99:A:VAL:HG13	1:73:A:GLU:H	3	0.6
(1,37)	1:99:A:VAL:HG11	1:99:A:VAL:H	16	0.6
(1,37)	1:99:A:VAL:HG13	1:99:A:VAL:H	18	0.6
(1,7)	1:72:A:LEU:HD13	1:73:A:GLU:H	18	0.6
(1,2693)	1:48:A:PHE:HD1	1:44:A:PHE:HZ	1	0.59
(1,2693)	1:44:A:PHE:HD1	1:44:A:PHE:HZ	10	0.59
(1,2693)	1:44:A:PHE:HD2	1:44:A:PHE:HZ	14	0.59
(1,2657)	1:56:A:LEU:HA	1:25:A:LYS:HE3	4	0.59
(1,2650)	1:66:A:VAL:HG11	1:32:A:GLY:HA3	3	0.59
(1,2650)	1:66:A:VAL:HG12	1:32:A:GLY:HA3	15	0.59
(1,2645)	1:33:A:ILE:HG22	1:39:A:MET:HG3	9	0.59
(1,2642)	1:114:A:MET:HE2	1:114:A:MET:HE3	17	0.59
(1,2633)	1:115:A:LEU:HD13	1:27:A:GLU:HB3	8	0.59
(1,2594)	1:66:A:VAL:HG21	1:66:A:VAL:HG23	3	0.59
(1,2586)	1:31:A:VAL:HA	1:31:A:VAL:HG22	1	0.59
(1,2586)	1:31:A:VAL:HA	1:31:A:VAL:HG23	8	0.59
(1,2586)	1:31:A:VAL:HA	1:31:A:VAL:HG23	13	0.59
(1,2586)	1:31:A:VAL:HA	1:31:A:VAL:HG21	17	0.59
(1,2586)	1:31:A:VAL:HA	1:31:A:VAL:HG23	18	0.59
(1,2474)	1:18:A:ALA:HB1	1:19:A:LYS:HA	13	0.59
(1,2474)	1:18:A:ALA:HB1	1:19:A:LYS:HA	20	0.59
(1,2463)	1:43:A:LEU:HD22	1:43:A:LEU:HD11	19	0.59
(1,2459)	1:115:A:LEU:HD22	1:115:A:LEU:HD21	1	0.59
(1,2459)	1:86:A:LEU:HD11	1:86:A:LEU:HD13	2	0.59
(1,2459)	1:115:A:LEU:HD21	1:115:A:LEU:HD23	4	0.59
(1,2459)	1:115:A:LEU:HD12	1:115:A:LEU:HD11	11	0.59
(1,2459)	1:86:A:LEU:HD11	1:86:A:LEU:HD13	17	0.59
(1,2459)	1:86:A:LEU:HD12	1:86:A:LEU:HD11	19	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2170)	1:92:A:GLU:HG3	1:81:A:PHE:HD1	16	0.59
(1,2158)	1:29:A:VAL:HG13	1:48:A:PHE:HZ	18	0.59
(1,2133)	1:65:A:ILE:HG21	1:44:A:PHE:HD1	10	0.59
(1,2133)	1:65:A:ILE:HG21	1:44:A:PHE:HD2	17	0.59
(1,2133)	1:65:A:ILE:HG22	1:44:A:PHE:HD2	20	0.59
(1,2091)	1:65:A:ILE:HA	1:31:A:VAL:HG12	15	0.59
(1,2084)	1:58:A:CYS:HA	1:26:A:ILE:HG21	8	0.59
(1,2069)	1:112:A:LEU:HD21	1:29:A:VAL:HA	5	0.59
(1,2018)	1:90:A:VAL:HG11	1:95:A:HIS:HB3	17	0.59
(1,1992)	1:20:A:LYS:HE2	1:20:A:LYS:HA	13	0.59
(1,1982)	1:106:A:GLU:HG2	1:105:A:ASN:HB3	10	0.59
(1,1806)	1:10:A:LEU:HD13	1:7:A:VAL:HA	13	0.59
(1,1805)	1:10:A:LEU:HD12	1:63:A:LEU:HD21	5	0.59
(1,1794)	1:11:A:ILE:HG21	1:12:A:ALA:HB3	3	0.59
(1,1794)	1:11:A:ILE:HG21	1:12:A:ALA:HB1	14	0.59
(1,1782)	1:109:A:LEU:HD21	1:107:A:MET:HE3	3	0.59
(1,1778)	1:112:A:LEU:HD21	1:18:A:ALA:HB2	15	0.59
(1,1753)	1:65:A:ILE:HD12	1:41:A:LYS:HD3	20	0.59
(1,1751)	1:65:A:ILE:HD12	1:33:A:ILE:HG21	2	0.59
(1,1751)	1:65:A:ILE:HD13	1:33:A:ILE:HG22	10	0.59
(1,1732)	1:72:A:LEU:HD11	1:89:A:GLY:HA3	7	0.59
(1,1723)	1:45:A:VAL:HG13	1:63:A:LEU:HD21	3	0.59
(1,1697)	1:112:A:LEU:HD22	1:112:A:LEU:HA	4	0.59
(1,1514)	1:43:A:LEU:HD22	1:42:A:SER:HB2	7	0.59
(1,1499)	1:6:A:VAL:HG23	1:3:A:GLU:HA	1	0.59
(1,1430)	1:59:A:LYS:HG2	1:59:A:LYS:HE2	10	0.59
(1,1324)	1:106:A:GLU:HG2	1:105:A:ASN:HB2	10	0.59
(1,1302)	1:1:A:MET:HE1	1:1:A:MET:HA	1	0.59
(1,1254)	1:20:A:LYS:HB2	1:20:A:LYS:HE3	11	0.59
(1,1248)	1:13:A:LEU:HD13	1:13:A:LEU:HB3	13	0.59
(1,1020)	1:85:A:ALA:HB3	1:86:A:LEU:HA	16	0.59
(1,996)	1:26:A:ILE:HG12	1:57:A:VAL:HG13	16	0.59
(1,990)	1:59:A:LYS:HG3	1:59:A:LYS:HE3	6	0.59
(1,937)	1:102:A:THR:HG21	1:73:A:GLU:HA	16	0.59
(1,914)	1:72:A:LEU:HD23	1:70:A:VAL:HG13	2	0.59
(1,914)	1:72:A:LEU:HD23	1:70:A:VAL:HG12	10	0.59
(1,910)	1:109:A:LEU:HD11	1:13:A:LEU:HD13	2	0.59
(1,828)	1:101:A:ILE:HG21	1:101:A:ILE:HG13	4	0.59
(1,828)	1:101:A:ILE:HG22	1:101:A:ILE:HG13	12	0.59
(1,804)	1:66:A:VAL:HG11	1:32:A:GLY:HA3	17	0.59
(1,770)	1:72:A:LEU:HD13	1:70:A:VAL:HG22	8	0.59
(1,770)	1:72:A:LEU:HD13	1:70:A:VAL:HG21	20	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,769)	1:72:A:LEU:HD22	1:70:A:VAL:HG23	11	0.59
(1,458)	1:74:A:CYS:HB2	1:77:A:CYS:H	20	0.59
(1,213)	1:75:A:LYS:HD3	1:75:A:LYS:H	14	0.59
(1,208)	1:41:A:LYS:HG2	1:42:A:SER:H	14	0.59
(1,185)	1:38:A:ALA:HB2	1:39:A:MET:H	7	0.59
(1,185)	1:38:A:ALA:HB3	1:39:A:MET:H	9	0.59
(1,144)	1:47:A:ALA:HB2	1:50:A:THR:H	2	0.59
(1,136)	1:102:A:THR:HG21	1:100:A:ILE:H	6	0.59
(1,116)	1:13:A:LEU:HD21	1:14:A:CYS:H	5	0.59
(1,103)	1:43:A:LEU:HD22	1:46:A:SER:H	2	0.59
(1,101)	1:57:A:VAL:HG12	1:15:A:GLU:H	15	0.59
(1,70)	1:112:A:LEU:HD22	1:17:A:HIS:H	1	0.59
(1,66)	1:100:A:ILE:HD12	1:100:A:ILE:H	8	0.59
(1,23)	1:110:A:LEU:HD12	1:111:A:SER:H	4	0.59
(1,15)	1:7:A:VAL:HG11	1:47:A:ALA:H	10	0.59
(1,7)	1:72:A:LEU:HD12	1:73:A:GLU:H	8	0.59
(1,2693)	1:44:A:PHE:HD1	1:44:A:PHE:HZ	11	0.58
(1,2679)	1:7:A:VAL:HB	1:48:A:PHE:HD2	12	0.58
(1,2669)	1:31:A:VAL:HG22	1:44:A:PHE:HD2	17	0.58
(1,2669)	1:31:A:VAL:HG22	1:44:A:PHE:HD2	20	0.58
(1,2660)	1:69:A:LYS:HA	1:69:A:LYS:HE3	9	0.58
(1,2652)	1:45:A:VAL:HA	1:47:A:ALA:HB2	11	0.58
(1,2652)	1:45:A:VAL:HA	1:47:A:ALA:HB2	18	0.58
(1,2633)	1:115:A:LEU:HD11	1:27:A:GLU:HB3	12	0.58
(1,2621)	1:38:A:ALA:HB3	1:105:A:ASN:HB2	1	0.58
(1,2612)	1:59:A:LYS:HE2	1:56:A:LEU:HD11	5	0.58
(1,2612)	1:25:A:LYS:HE3	1:56:A:LEU:HD12	18	0.58
(1,2608)	1:115:A:LEU:HD22	1:27:A:GLU:HB2	13	0.58
(1,2597)	1:72:A:LEU:HB2	1:99:A:VAL:HG23	13	0.58
(1,2594)	1:66:A:VAL:HG22	1:66:A:VAL:HG23	6	0.58
(1,2474)	1:18:A:ALA:HB2	1:19:A:LYS:HA	5	0.58
(1,2459)	1:115:A:LEU:HD11	1:115:A:LEU:HD13	5	0.58
(1,2459)	1:86:A:LEU:HD11	1:86:A:LEU:HD13	6	0.58
(1,2459)	1:86:A:LEU:HD12	1:86:A:LEU:HD11	9	0.58
(1,2459)	1:86:A:LEU:HD12	1:86:A:LEU:HD11	10	0.58
(1,2459)	1:86:A:LEU:HD12	1:86:A:LEU:HD13	14	0.58
(1,2459)	1:115:A:LEU:HD12	1:115:A:LEU:HD11	15	0.58
(1,2459)	1:115:A:LEU:HD22	1:115:A:LEU:HD21	18	0.58
(1,2438)	1:65:A:ILE:HD13	1:41:A:LYS:HD2	18	0.58
(1,2204)	1:83:A:PRO:HB3	1:88:A:TYR:HE1	6	0.58
(1,2170)	1:92:A:GLU:HG3	1:81:A:PHE:HD1	5	0.58
(1,2160)	1:80:A:VAL:HG23	1:81:A:PHE:HD2	1	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2133)	1:65:A:ILE:HG21	1:44:A:PHE:HD2	2	0.58
(1,2133)	1:65:A:ILE:HG21	1:44:A:PHE:HD2	12	0.58
(1,2130)	1:72:A:LEU:HD12	1:81:A:PHE:HE1	14	0.58
(1,2089)	1:79:A:HIS:HA	1:80:A:VAL:HG22	1	0.58
(1,2089)	1:79:A:HIS:HA	1:80:A:VAL:HG23	4	0.58
(1,2084)	1:58:A:CYS:HA	1:26:A:ILE:HG22	4	0.58
(1,2079)	1:71:A:GLU:HB2	1:103:A:GLN:HA	9	0.58
(1,2069)	1:112:A:LEU:HD22	1:29:A:VAL:HA	16	0.58
(1,2056)	1:15:A:GLU:HG2	1:12:A:ALA:HA	10	0.58
(1,2056)	1:15:A:GLU:HG2	1:12:A:ALA:HA	17	0.58
(1,1992)	1:20:A:LYS:HE2	1:20:A:LYS:HA	3	0.58
(1,1992)	1:20:A:LYS:HE2	1:20:A:LYS:HA	6	0.58
(1,1992)	1:20:A:LYS:HE2	1:20:A:LYS:HA	8	0.58
(1,1987)	1:23:A:ALA:HB1	1:21:A:ASN:HB2	15	0.58
(1,1975)	1:12:A:ALA:HB1	1:15:A:GLU:HB2	11	0.58
(1,1939)	1:39:A:MET:HE2	1:39:A:MET:HA	3	0.58
(1,1842)	1:18:A:ALA:HB3	1:21:A:ASN:HB3	4	0.58
(1,1814)	1:107:A:MET:HE2	1:10:A:LEU:HD23	5	0.58
(1,1772)	1:64:A:ASP:HB3	1:30:A:VAL:HG12	9	0.58
(1,1772)	1:64:A:ASP:HB3	1:30:A:VAL:HG11	18	0.58
(1,1753)	1:65:A:ILE:HD13	1:41:A:LYS:HD3	3	0.58
(1,1746)	1:90:A:VAL:HG23	1:87:A:ASP:HB3	16	0.58
(1,1739)	1:33:A:ILE:HG21	1:65:A:ILE:HG21	13	0.58
(1,1723)	1:45:A:VAL:HG12	1:63:A:LEU:HD23	6	0.58
(1,1665)	1:24:A:HIS:HA	1:57:A:VAL:HG21	9	0.58
(1,1601)	1:12:A:ALA:HB3	1:9:A:SER:HA	13	0.58
(1,1601)	1:12:A:ALA:HB1	1:9:A:SER:HA	19	0.58
(1,1499)	1:6:A:VAL:HG22	1:3:A:GLU:HA	4	0.58
(1,1499)	1:6:A:VAL:HG21	1:3:A:GLU:HA	9	0.58
(1,1328)	1:103:A:GLN:HG3	1:103:A:GLN:HA	6	0.58
(1,1254)	1:20:A:LYS:HB2	1:20:A:LYS:HE3	3	0.58
(1,1026)	1:116:A:ALA:HB1	1:116:A:ALA:HB3	9	0.58
(1,990)	1:59:A:LYS:HG3	1:59:A:LYS:HE3	18	0.58
(1,963)	1:41:A:LYS:HG3	1:65:A:ILE:HD11	9	0.58
(1,937)	1:102:A:THR:HG21	1:73:A:GLU:HA	14	0.58
(1,923)	1:57:A:VAL:HG22	1:56:A:LEU:HB2	15	0.58
(1,862)	1:109:A:LEU:HD22	1:13:A:LEU:HD21	18	0.58
(1,809)	1:110:A:LEU:HD13	1:66:A:VAL:HG12	17	0.58
(1,809)	1:110:A:LEU:HD12	1:66:A:VAL:HG11	18	0.58
(1,239)	1:19:A:LYS:HD3	1:20:A:LYS:H	8	0.58
(1,200)	1:12:A:ALA:HB1	1:11:A:ILE:H	2	0.58
(1,197)	1:12:A:ALA:HB3	1:16:A:GLU:H	2	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,176)	1:18:A:ALA:HB1	1:16:A:GLU:H	1	0.58
(1,144)	1:47:A:ALA:HB2	1:50:A:THR:H	5	0.58
(1,126)	1:45:A:VAL:HG21	1:47:A:ALA:H	1	0.58
(1,123)	1:13:A:LEU:HD12	1:14:A:CYS:H	12	0.58
(1,118)	1:13:A:LEU:HD12	1:16:A:GLU:H	18	0.58
(1,70)	1:112:A:LEU:HD22	1:17:A:HIS:H	20	0.58
(1,66)	1:100:A:ILE:HD12	1:100:A:ILE:H	9	0.58
(1,66)	1:100:A:ILE:HD13	1:100:A:ILE:H	10	0.58
(1,66)	1:100:A:ILE:HD13	1:100:A:ILE:H	18	0.58
(1,2693)	1:44:A:PHE:HD1	1:44:A:PHE:HZ	4	0.57
(1,2652)	1:45:A:VAL:HA	1:47:A:ALA:HB3	10	0.57
(1,2594)	1:66:A:VAL:HG12	1:66:A:VAL:HG11	7	0.57
(1,2594)	1:66:A:VAL:HG12	1:66:A:VAL:HG11	11	0.57
(1,2594)	1:66:A:VAL:HG22	1:66:A:VAL:HG21	15	0.57
(1,2590)	1:33:A:ILE:HD12	1:39:A:MET:HG2	2	0.57
(1,2590)	1:33:A:ILE:HD13	1:39:A:MET:HG2	4	0.57
(1,2586)	1:31:A:VAL:HA	1:31:A:VAL:HG23	20	0.57
(1,2490)	1:82:A:LYS:HG2	1:82:A:LYS:HE2	8	0.57
(1,2474)	1:18:A:ALA:HB1	1:19:A:LYS:HA	17	0.57
(1,2459)	1:86:A:LEU:HD12	1:86:A:LEU:HD13	16	0.57
(1,2158)	1:29:A:VAL:HG11	1:48:A:PHE:HZ	13	0.57
(1,2158)	1:29:A:VAL:HG13	1:48:A:PHE:HZ	20	0.57
(1,2153)	1:99:A:VAL:HG21	1:81:A:PHE:HE2	5	0.57
(1,2105)	1:64:A:ASP:HA	1:62:A:ILE:HG22	9	0.57
(1,2084)	1:58:A:CYS:HA	1:26:A:ILE:HG21	5	0.57
(1,1992)	1:20:A:LYS:HE2	1:20:A:LYS:HA	16	0.57
(1,1939)	1:39:A:MET:HE2	1:39:A:MET:HA	2	0.57
(1,1939)	1:39:A:MET:HE3	1:39:A:MET:HA	4	0.57
(1,1939)	1:39:A:MET:HE2	1:39:A:MET:HA	18	0.57
(1,1831)	1:58:A:CYS:HB2	1:61:A:ALA:HB2	3	0.57
(1,1829)	1:26:A:ILE:HD13	1:23:A:ALA:HB3	20	0.57
(1,1824)	1:25:A:LYS:HG3	1:56:A:LEU:HD13	14	0.57
(1,1812)	1:50:A:THR:HG22	1:47:A:ALA:HA	3	0.57
(1,1812)	1:50:A:THR:HG22	1:47:A:ALA:HA	13	0.57
(1,1812)	1:50:A:THR:HG22	1:47:A:ALA:HA	16	0.57
(1,1800)	1:115:A:LEU:HD12	1:25:A:LYS:HG2	6	0.57
(1,1794)	1:11:A:ILE:HG23	1:12:A:ALA:HB2	2	0.57
(1,1794)	1:11:A:ILE:HG22	1:12:A:ALA:HB2	7	0.57
(1,1746)	1:90:A:VAL:HG22	1:87:A:ASP:HB3	18	0.57
(1,1452)	1:63:A:LEU:HD12	1:45:A:VAL:HA	9	0.57
(1,1391)	1:58:A:CYS:HB3	1:55:A:SER:HB3	18	0.57
(1,1302)	1:1:A:MET:HE1	1:1:A:MET:HA	7	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1302)	1:1:A:MET:HE2	1:1:A:MET:HA	18	0.57
(1,1254)	1:20:A:LYS:HB2	1:20:A:LYS:HE3	12	0.57
(1,1248)	1:13:A:LEU:HD11	1:13:A:LEU:HB3	18	0.57
(1,1026)	1:116:A:ALA:HB2	1:116:A:ALA:HB3	16	0.57
(1,1020)	1:85:A:ALA:HB3	1:86:A:LEU:HA	4	0.57
(1,996)	1:26:A:ILE:HG12	1:57:A:VAL:HG11	8	0.57
(1,990)	1:59:A:LYS:HG3	1:59:A:LYS:HE3	1	0.57
(1,990)	1:59:A:LYS:HG3	1:59:A:LYS:HE3	7	0.57
(1,923)	1:57:A:VAL:HG21	1:56:A:LEU:HB2	11	0.57
(1,889)	1:57:A:VAL:HG13	1:15:A:GLU:HG3	4	0.57
(1,889)	1:57:A:VAL:HG11	1:15:A:GLU:HG3	7	0.57
(1,875)	1:86:A:LEU:HD22	1:85:A:ALA:HA	15	0.57
(1,809)	1:110:A:LEU:HD13	1:66:A:VAL:HG12	20	0.57
(1,765)	1:90:A:VAL:HG22	1:90:A:VAL:HG21	11	0.57
(1,764)	1:70:A:VAL:HG22	1:70:A:VAL:HA	10	0.57
(1,746)	1:72:A:LEU:HD11	1:83:A:PRO:HB2	8	0.57
(1,746)	1:72:A:LEU:HD11	1:83:A:PRO:HB2	18	0.57
(1,330)	1:68:A:GLU:HG2	1:33:A:ILE:H	7	0.57
(1,182)	1:18:A:ALA:HB2	1:20:A:LYS:H	5	0.57
(1,130)	1:10:A:LEU:HD21	1:10:A:LEU:H	12	0.57
(1,126)	1:45:A:VAL:HG22	1:47:A:ALA:H	14	0.57
(1,126)	1:45:A:VAL:HG23	1:47:A:ALA:H	16	0.57
(1,103)	1:43:A:LEU:HD21	1:46:A:SER:H	9	0.57
(1,70)	1:112:A:LEU:HD23	1:17:A:HIS:H	11	0.57
(1,66)	1:100:A:ILE:HD12	1:100:A:ILE:H	2	0.57
(1,66)	1:100:A:ILE:HD11	1:100:A:ILE:H	19	0.57
(1,44)	1:99:A:VAL:HG11	1:73:A:GLU:H	14	0.57
(1,37)	1:99:A:VAL:HG12	1:99:A:VAL:H	14	0.57
(1,34)	1:33:A:ILE:HG22	1:39:A:MET:H	2	0.57
(1,23)	1:110:A:LEU:HD13	1:111:A:SER:H	19	0.57
(1,2693)	1:44:A:PHE:HD2	1:44:A:PHE:HZ	17	0.56
(1,2693)	1:48:A:PHE:HD1	1:44:A:PHE:HZ	20	0.56
(1,2679)	1:7:A:VAL:HB	1:48:A:PHE:HD1	4	0.56
(1,2679)	1:7:A:VAL:HB	1:48:A:PHE:HD1	18	0.56
(1,2660)	1:69:A:LYS:HA	1:69:A:LYS:HE3	10	0.56
(1,2652)	1:45:A:VAL:HA	1:47:A:ALA:HB1	14	0.56
(1,2652)	1:45:A:VAL:HA	1:47:A:ALA:HB3	17	0.56
(1,2652)	1:45:A:VAL:HA	1:47:A:ALA:HB2	20	0.56
(1,2620)	1:115:A:LEU:HD11	1:25:A:LYS:HG2	4	0.56
(1,2597)	1:72:A:LEU:HB2	1:99:A:VAL:HG21	3	0.56
(1,2597)	1:72:A:LEU:HB2	1:99:A:VAL:HG22	18	0.56
(1,2594)	1:66:A:VAL:HG12	1:66:A:VAL:HG13	1	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2594)	1:66:A:VAL:HG22	1:66:A:VAL:HG23	4	0.56
(1,2594)	1:90:A:VAL:HG12	1:90:A:VAL:HG11	8	0.56
(1,2594)	1:66:A:VAL:HG22	1:66:A:VAL:HG23	9	0.56
(1,2594)	1:66:A:VAL:HG12	1:66:A:VAL:HG13	13	0.56
(1,2594)	1:66:A:VAL:HG21	1:66:A:VAL:HG23	17	0.56
(1,2594)	1:66:A:VAL:HG22	1:66:A:VAL:HG21	19	0.56
(1,2474)	1:18:A:ALA:HB1	1:19:A:LYS:HA	1	0.56
(1,2202)	1:83:A:PRO:HB3	1:88:A:TYR:HD1	17	0.56
(1,2180)	1:61:A:ALA:HB1	1:48:A:PHE:HD2	1	0.56
(1,2158)	1:29:A:VAL:HG11	1:48:A:PHE:HZ	4	0.56
(1,2091)	1:65:A:ILE:HA	1:31:A:VAL:HG12	13	0.56
(1,2089)	1:79:A:HIS:HA	1:80:A:VAL:HG21	8	0.56
(1,2088)	1:105:A:ASN:HA	1:36:A:ARG:HB3	18	0.56
(1,2079)	1:71:A:GLU:HB2	1:103:A:GLN:HA	19	0.56
(1,1992)	1:20:A:LYS:HE2	1:20:A:LYS:HA	9	0.56
(1,1987)	1:23:A:ALA:HB2	1:21:A:ASN:HB2	12	0.56
(1,1975)	1:12:A:ALA:HB1	1:15:A:GLU:HB2	20	0.56
(1,1939)	1:39:A:MET:HE1	1:39:A:MET:HA	16	0.56
(1,1907)	1:25:A:LYS:HB2	1:57:A:VAL:HG11	15	0.56
(1,1842)	1:18:A:ALA:HB3	1:21:A:ASN:HB3	20	0.56
(1,1823)	1:45:A:VAL:HG11	1:41:A:LYS:HE2	20	0.56
(1,1814)	1:107:A:MET:HE2	1:10:A:LEU:HD22	14	0.56
(1,1794)	1:11:A:ILE:HG22	1:12:A:ALA:HB2	8	0.56
(1,1793)	1:15:A:GLU:HG2	1:11:A:ILE:HG21	13	0.56
(1,1751)	1:65:A:ILE:HD12	1:33:A:ILE:HG23	11	0.56
(1,1749)	1:65:A:ILE:HG13	1:63:A:LEU:HD23	18	0.56
(1,1708)	1:107:A:MET:HA	1:33:A:ILE:HD12	11	0.56
(1,1514)	1:43:A:LEU:HD23	1:42:A:SER:HB3	18	0.56
(1,1430)	1:59:A:LYS:HG2	1:59:A:LYS:HE2	4	0.56
(1,1391)	1:58:A:CYS:HB3	1:55:A:SER:HB3	15	0.56
(1,1302)	1:1:A:MET:HE2	1:1:A:MET:HA	4	0.56
(1,1248)	1:13:A:LEU:HD11	1:13:A:LEU:HB3	15	0.56
(1,1159)	1:108:A:ARG:HB2	1:110:A:LEU:HD23	18	0.56
(1,1145)	1:41:A:LYS:HD2	1:33:A:ILE:HG23	5	0.56
(1,1026)	1:116:A:ALA:HB2	1:116:A:ALA:HB3	11	0.56
(1,1026)	1:116:A:ALA:HB2	1:116:A:ALA:HB3	13	0.56
(1,1026)	1:116:A:ALA:HB2	1:116:A:ALA:HB1	14	0.56
(1,862)	1:109:A:LEU:HD21	1:13:A:LEU:HD23	12	0.56
(1,822)	1:80:A:VAL:HG13	1:102:A:THR:HG23	4	0.56
(1,765)	1:90:A:VAL:HG21	1:90:A:VAL:HG23	3	0.56
(1,765)	1:90:A:VAL:HG22	1:90:A:VAL:HG23	10	0.56
(1,420)	1:19:A:LYS:HE2	1:19:A:LYS:H	3	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,299)	1:39:A:MET:HE1	1:6:A:VAL:H	16	0.56
(1,200)	1:12:A:ALA:HB3	1:11:A:ILE:H	6	0.56
(1,195)	1:12:A:ALA:HB3	1:15:A:GLU:H	5	0.56
(1,185)	1:38:A:ALA:HB1	1:39:A:MET:H	11	0.56
(1,130)	1:10:A:LEU:HD23	1:10:A:LEU:H	10	0.56
(1,66)	1:100:A:ILE:HD11	1:100:A:ILE:H	12	0.56
(1,66)	1:100:A:ILE:HD11	1:100:A:ILE:H	14	0.56
(1,53)	1:66:A:VAL:HG13	1:33:A:ILE:H	6	0.56
(1,50)	1:7:A:VAL:HG23	1:8:A:SER:H	4	0.56
(1,38)	1:99:A:VAL:HG11	1:90:A:VAL:H	18	0.56
(1,37)	1:99:A:VAL:HG12	1:99:A:VAL:H	3	0.56
(1,37)	1:99:A:VAL:HG12	1:99:A:VAL:H	4	0.56
(1,37)	1:99:A:VAL:HG12	1:99:A:VAL:H	20	0.56
(1,27)	1:90:A:VAL:HG21	1:89:A:GLY:H	11	0.56
(1,23)	1:110:A:LEU:HD11	1:111:A:SER:H	8	0.56
(1,23)	1:110:A:LEU:HD11	1:111:A:SER:H	11	0.56
(1,13)	1:72:A:LEU:HD12	1:90:A:VAL:H	5	0.56
(1,2693)	1:44:A:PHE:HD2	1:44:A:PHE:HZ	5	0.55
(1,2676)	1:47:A:ALA:HB3	1:44:A:PHE:HD1	12	0.55
(1,2671)	1:115:A:LEU:HD13	1:24:A:HIS:HD2	12	0.55
(1,2659)	1:19:A:LYS:HG3	1:19:A:LYS:HA	8	0.55
(1,2652)	1:45:A:VAL:HA	1:47:A:ALA:HB3	2	0.55
(1,2651)	1:45:A:VAL:HA	1:48:A:PHE:HA	3	0.55
(1,2650)	1:66:A:VAL:HG13	1:32:A:GLY:HA3	2	0.55
(1,2650)	1:66:A:VAL:HG11	1:32:A:GLY:HA3	13	0.55
(1,2597)	1:72:A:LEU:HB2	1:99:A:VAL:HG21	10	0.55
(1,2594)	1:90:A:VAL:HG12	1:90:A:VAL:HG11	5	0.55
(1,2594)	1:90:A:VAL:HG12	1:90:A:VAL:HG13	10	0.55
(1,2594)	1:66:A:VAL:HG21	1:66:A:VAL:HG23	12	0.55
(1,2594)	1:90:A:VAL:HG12	1:90:A:VAL:HG11	16	0.55
(1,2594)	1:66:A:VAL:HG12	1:66:A:VAL:HG11	18	0.55
(1,2586)	1:31:A:VAL:HA	1:31:A:VAL:HG23	11	0.55
(1,2555)	1:115:A:LEU:HD12	1:25:A:LYS:HE2	7	0.55
(1,2490)	1:97:A:LYS:HG3	1:97:A:LYS:HE3	18	0.55
(1,2490)	1:82:A:LYS:HG2	1:82:A:LYS:HE2	20	0.55
(1,2474)	1:18:A:ALA:HB2	1:19:A:LYS:HA	9	0.55
(1,2474)	1:18:A:ALA:HB1	1:19:A:LYS:HA	12	0.55
(1,2445)	1:31:A:VAL:HG22	1:31:A:VAL:HG23	9	0.55
(1,2445)	1:80:A:VAL:HG11	1:80:A:VAL:HG13	10	0.55
(1,2445)	1:80:A:VAL:HG12	1:80:A:VAL:HG11	12	0.55
(1,2433)	1:63:A:LEU:HD21	1:31:A:VAL:HG23	10	0.55
(1,2433)	1:63:A:LEU:HD23	1:31:A:VAL:HG23	19	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2426)	1:97:A:LYS:HD3	1:97:A:LYS:H	17	0.55
(1,2260)	1:85:A:ALA:HA	1:88:A:TYR:HE2	6	0.55
(1,2206)	1:83:A:PRO:HB2	1:81:A:PHE:HD2	14	0.55
(1,2160)	1:80:A:VAL:HG21	1:81:A:PHE:HD2	4	0.55
(1,2160)	1:80:A:VAL:HG22	1:81:A:PHE:HD1	14	0.55
(1,2158)	1:29:A:VAL:HG11	1:48:A:PHE:HZ	11	0.55
(1,2070)	1:109:A:LEU:HD21	1:29:A:VAL:HA	18	0.55
(1,2063)	1:33:A:ILE:HA	1:107:A:MET:HG3	18	0.55
(1,2056)	1:15:A:GLU:HG2	1:12:A:ALA:HA	3	0.55
(1,2047)	1:33:A:ILE:HG22	1:37:A:SER:HA	11	0.55
(1,2035)	1:42:A:SER:HB2	1:45:A:VAL:HG23	1	0.55
(1,1939)	1:39:A:MET:HE1	1:39:A:MET:HA	19	0.55
(1,1887)	1:82:A:LYS:HD2	1:71:A:GLU:HB3	1	0.55
(1,1887)	1:82:A:LYS:HD2	1:71:A:GLU:HB3	11	0.55
(1,1840)	1:75:A:LYS:HG3	1:100:A:ILE:HG13	12	0.55
(1,1830)	1:112:A:LEU:HD11	1:112:A:LEU:HB3	1	0.55
(1,1829)	1:26:A:ILE:HD11	1:23:A:ALA:HB2	19	0.55
(1,1806)	1:10:A:LEU:HD11	1:7:A:VAL:HA	4	0.55
(1,1793)	1:15:A:GLU:HG2	1:11:A:ILE:HG21	12	0.55
(1,1793)	1:15:A:GLU:HG2	1:11:A:ILE:HG22	19	0.55
(1,1753)	1:65:A:ILE:HD13	1:41:A:LYS:HD3	15	0.55
(1,1697)	1:112:A:LEU:HD23	1:112:A:LEU:HA	2	0.55
(1,1697)	1:112:A:LEU:HD22	1:112:A:LEU:HA	14	0.55
(1,1697)	1:112:A:LEU:HD23	1:112:A:LEU:HA	18	0.55
(1,1697)	1:112:A:LEU:HD21	1:112:A:LEU:HA	20	0.55
(1,1677)	1:25:A:LYS:HA	1:57:A:VAL:HG21	2	0.55
(1,1601)	1:12:A:ALA:HB1	1:9:A:SER:HA	18	0.55
(1,1430)	1:59:A:LYS:HG2	1:59:A:LYS:HE2	17	0.55
(1,1254)	1:20:A:LYS:HB2	1:20:A:LYS:HE3	10	0.55
(1,1204)	1:75:A:LYS:HB3	1:98:A:ASN:HB3	6	0.55
(1,1026)	1:116:A:ALA:HB2	1:116:A:ALA:HB3	2	0.55
(1,1026)	1:116:A:ALA:HB1	1:116:A:ALA:HB3	5	0.55
(1,1026)	1:116:A:ALA:HB2	1:116:A:ALA:HB1	7	0.55
(1,1026)	1:116:A:ALA:HB1	1:116:A:ALA:HB3	15	0.55
(1,1026)	1:116:A:ALA:HB2	1:116:A:ALA:HB3	18	0.55
(1,1021)	1:85:A:ALA:HB2	1:85:A:ALA:HB1	16	0.55
(1,1020)	1:85:A:ALA:HB3	1:86:A:LEU:HA	13	0.55
(1,990)	1:59:A:LYS:HG3	1:59:A:LYS:HE3	5	0.55
(1,937)	1:102:A:THR:HG21	1:73:A:GLU:HA	6	0.55
(1,937)	1:102:A:THR:HG22	1:73:A:GLU:HA	8	0.55
(1,937)	1:102:A:THR:HG22	1:73:A:GLU:HA	12	0.55
(1,923)	1:57:A:VAL:HG22	1:56:A:LEU:HB2	5	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,923)	1:57:A:VAL:HG21	1:56:A:LEU:HB2	20	0.55
(1,811)	1:29:A:VAL:HG23	1:109:A:LEU:HD11	19	0.55
(1,809)	1:110:A:LEU:HD11	1:66:A:VAL:HG13	16	0.55
(1,765)	1:90:A:VAL:HG22	1:90:A:VAL:HG21	4	0.55
(1,765)	1:90:A:VAL:HG22	1:90:A:VAL:HG23	8	0.55
(1,765)	1:90:A:VAL:HG21	1:90:A:VAL:HG23	13	0.55
(1,300)	1:107:A:MET:HE2	1:108:A:ARG:H	1	0.55
(1,200)	1:12:A:ALA:HB2	1:11:A:ILE:H	4	0.55
(1,200)	1:12:A:ALA:HB1	1:11:A:ILE:H	7	0.55
(1,197)	1:12:A:ALA:HB1	1:16:A:GLU:H	3	0.55
(1,197)	1:12:A:ALA:HB2	1:16:A:GLU:H	9	0.55
(1,176)	1:18:A:ALA:HB1	1:16:A:GLU:H	17	0.55
(1,144)	1:47:A:ALA:HB2	1:50:A:THR:H	12	0.55
(1,126)	1:45:A:VAL:HG22	1:47:A:ALA:H	2	0.55
(1,118)	1:13:A:LEU:HD12	1:16:A:GLU:H	2	0.55
(1,116)	1:13:A:LEU:HD21	1:14:A:CYS:H	7	0.55
(1,116)	1:13:A:LEU:HD22	1:14:A:CYS:H	14	0.55
(1,116)	1:13:A:LEU:HD21	1:14:A:CYS:H	18	0.55
(1,113)	1:10:A:LEU:HD12	1:10:A:LEU:H	9	0.55
(1,103)	1:43:A:LEU:HD23	1:46:A:SER:H	10	0.55
(1,101)	1:57:A:VAL:HG13	1:15:A:GLU:H	3	0.55
(1,88)	1:26:A:ILE:HD11	1:15:A:GLU:H	8	0.55
(1,50)	1:7:A:VAL:HG22	1:8:A:SER:H	11	0.55
(1,44)	1:99:A:VAL:HG12	1:73:A:GLU:H	10	0.55
(1,37)	1:99:A:VAL:HG11	1:99:A:VAL:H	12	0.55
(1,37)	1:99:A:VAL:HG12	1:99:A:VAL:H	13	0.55
(1,37)	1:99:A:VAL:HG12	1:99:A:VAL:H	15	0.55
(1,34)	1:33:A:ILE:HG23	1:39:A:MET:H	8	0.55
(1,27)	1:90:A:VAL:HG21	1:89:A:GLY:H	2	0.55
(1,27)	1:90:A:VAL:HG22	1:89:A:GLY:H	9	0.55
(1,2693)	1:44:A:PHE:HD2	1:44:A:PHE:HZ	2	0.54
(1,2678)	1:39:A:MET:HE2	1:44:A:PHE:HZ	4	0.54
(1,2672)	1:70:A:VAL:HG13	1:88:A:TYR:HD1	10	0.54
(1,2670)	1:11:A:ILE:HG23	1:51:A:PHE:HD2	5	0.54
(1,2654)	1:6:A:VAL:HA	1:107:A:MET:HE2	5	0.54
(1,2654)	1:6:A:VAL:HA	1:107:A:MET:HE2	16	0.54
(1,2652)	1:45:A:VAL:HA	1:47:A:ALA:HB3	3	0.54
(1,2652)	1:45:A:VAL:HA	1:47:A:ALA:HB3	6	0.54
(1,2651)	1:7:A:VAL:HA	1:48:A:PHE:HA	6	0.54
(1,2643)	1:39:A:MET:HE2	1:106:A:GLU:HG2	14	0.54
(1,2606)	1:57:A:VAL:HG13	1:26:A:ILE:HA	9	0.54
(1,2594)	1:90:A:VAL:HG12	1:90:A:VAL:HG13	14	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2594)	1:90:A:VAL:HG12	1:90:A:VAL:HG11	20	0.54
(1,2474)	1:18:A:ALA:HB2	1:19:A:LYS:HA	2	0.54
(1,2464)	1:57:A:VAL:HG22	1:57:A:VAL:HG21	8	0.54
(1,2464)	1:45:A:VAL:HG22	1:45:A:VAL:HG23	11	0.54
(1,2464)	1:57:A:VAL:HG21	1:57:A:VAL:HG23	12	0.54
(1,2464)	1:45:A:VAL:HG22	1:45:A:VAL:HG21	16	0.54
(1,2464)	1:45:A:VAL:HG22	1:45:A:VAL:HG23	18	0.54
(1,2445)	1:80:A:VAL:HG11	1:80:A:VAL:HG13	1	0.54
(1,2445)	1:30:A:VAL:HG22	1:30:A:VAL:HG21	3	0.54
(1,2445)	1:30:A:VAL:HG22	1:30:A:VAL:HG21	8	0.54
(1,2445)	1:30:A:VAL:HG22	1:30:A:VAL:HG23	14	0.54
(1,2445)	1:80:A:VAL:HG12	1:80:A:VAL:HG11	16	0.54
(1,2206)	1:83:A:PRO:HB2	1:81:A:PHE:HD1	5	0.54
(1,2180)	1:61:A:ALA:HB1	1:48:A:PHE:HD1	6	0.54
(1,2172)	1:47:A:ALA:HB2	1:4:A:TYR:HD1	12	0.54
(1,2163)	1:45:A:VAL:HG21	1:44:A:PHE:HD1	3	0.54
(1,2133)	1:65:A:ILE:HG21	1:44:A:PHE:HD2	9	0.54
(1,2133)	1:65:A:ILE:HG21	1:44:A:PHE:HD2	13	0.54
(1,1992)	1:20:A:LYS:HE2	1:20:A:LYS:HA	10	0.54
(1,1987)	1:23:A:ALA:HB1	1:21:A:ASN:HB2	4	0.54
(1,1987)	1:23:A:ALA:HB1	1:21:A:ASN:HB2	14	0.54
(1,1939)	1:39:A:MET:HE3	1:39:A:MET:HA	10	0.54
(1,1888)	1:85:A:ALA:HB3	1:86:A:LEU:HG	6	0.54
(1,1840)	1:75:A:LYS:HG3	1:100:A:ILE:HG13	13	0.54
(1,1840)	1:75:A:LYS:HG3	1:100:A:ILE:HG13	20	0.54
(1,1751)	1:65:A:ILE:HD13	1:33:A:ILE:HG21	16	0.54
(1,1748)	1:33:A:ILE:HG23	1:107:A:MET:HG3	8	0.54
(1,1748)	1:33:A:ILE:HG23	1:107:A:MET:HG3	17	0.54
(1,1746)	1:90:A:VAL:HG22	1:87:A:ASP:HB3	4	0.54
(1,1739)	1:33:A:ILE:HG21	1:65:A:ILE:HG22	16	0.54
(1,1708)	1:107:A:MET:HA	1:33:A:ILE:HD13	1	0.54
(1,1688)	1:97:A:LYS:HA	1:99:A:VAL:HG21	1	0.54
(1,1601)	1:12:A:ALA:HB3	1:9:A:SER:HA	6	0.54
(1,1499)	1:6:A:VAL:HG21	1:3:A:GLU:HA	6	0.54
(1,1482)	1:7:A:VAL:HG21	1:48:A:PHE:HA	11	0.54
(1,1385)	1:48:A:PHE:HB3	1:63:A:LEU:HD13	8	0.54
(1,1302)	1:1:A:MET:HE3	1:1:A:MET:HA	15	0.54
(1,1145)	1:41:A:LYS:HD2	1:33:A:ILE:HG22	6	0.54
(1,1026)	1:116:A:ALA:HB2	1:116:A:ALA:HB3	1	0.54
(1,1026)	1:116:A:ALA:HB2	1:116:A:ALA:HB1	3	0.54
(1,1026)	1:116:A:ALA:HB1	1:116:A:ALA:HB3	6	0.54
(1,1026)	1:116:A:ALA:HB2	1:116:A:ALA:HB3	8	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1026)	1:116:A:ALA:HB1	1:116:A:ALA:HB3	10	0.54
(1,1026)	1:116:A:ALA:HB2	1:116:A:ALA:HB1	19	0.54
(1,1026)	1:116:A:ALA:HB1	1:116:A:ALA:HB3	20	0.54
(1,1021)	1:85:A:ALA:HB2	1:85:A:ALA:HB1	5	0.54
(1,1021)	1:85:A:ALA:HB1	1:85:A:ALA:HB3	12	0.54
(1,1021)	1:85:A:ALA:HB2	1:85:A:ALA:HB3	14	0.54
(1,1021)	1:85:A:ALA:HB2	1:85:A:ALA:HB3	17	0.54
(1,1021)	1:85:A:ALA:HB2	1:85:A:ALA:HB1	19	0.54
(1,976)	1:23:A:ALA:HB2	1:116:A:ALA:HA	17	0.54
(1,862)	1:109:A:LEU:HD21	1:13:A:LEU:HD21	7	0.54
(1,862)	1:109:A:LEU:HD21	1:13:A:LEU:HD23	10	0.54
(1,862)	1:109:A:LEU:HD21	1:13:A:LEU:HD22	16	0.54
(1,857)	1:109:A:LEU:HD23	1:112:A:LEU:HD12	6	0.54
(1,813)	1:29:A:VAL:HG21	1:10:A:LEU:HD13	7	0.54
(1,809)	1:110:A:LEU:HD12	1:66:A:VAL:HG13	3	0.54
(1,765)	1:90:A:VAL:HG22	1:90:A:VAL:HG21	5	0.54
(1,765)	1:90:A:VAL:HG22	1:90:A:VAL:HG23	14	0.54
(1,765)	1:90:A:VAL:HG22	1:90:A:VAL:HG21	15	0.54
(1,765)	1:90:A:VAL:HG22	1:90:A:VAL:HG23	16	0.54
(1,208)	1:41:A:LYS:HG2	1:42:A:SER:H	8	0.54
(1,200)	1:12:A:ALA:HB3	1:11:A:ILE:H	13	0.54
(1,197)	1:12:A:ALA:HB3	1:16:A:GLU:H	5	0.54
(1,197)	1:12:A:ALA:HB2	1:16:A:GLU:H	14	0.54
(1,162)	1:23:A:ALA:HB1	1:22:A:GLN:H	7	0.54
(1,146)	1:6:A:VAL:HG12	1:7:A:VAL:H	11	0.54
(1,136)	1:102:A:THR:HG23	1:100:A:ILE:H	1	0.54
(1,126)	1:45:A:VAL:HG23	1:47:A:ALA:H	3	0.54
(1,126)	1:45:A:VAL:HG21	1:47:A:ALA:H	6	0.54
(1,126)	1:45:A:VAL:HG22	1:47:A:ALA:H	12	0.54
(1,116)	1:13:A:LEU:HD21	1:14:A:CYS:H	1	0.54
(1,116)	1:13:A:LEU:HD23	1:14:A:CYS:H	2	0.54
(1,113)	1:10:A:LEU:HD13	1:10:A:LEU:H	17	0.54
(1,103)	1:43:A:LEU:HD23	1:46:A:SER:H	19	0.54
(1,88)	1:26:A:ILE:HD12	1:15:A:GLU:H	13	0.54
(1,70)	1:112:A:LEU:HD22	1:17:A:HIS:H	10	0.54
(1,66)	1:100:A:ILE:HD12	1:100:A:ILE:H	4	0.54
(1,53)	1:66:A:VAL:HG13	1:33:A:ILE:H	4	0.54
(1,53)	1:66:A:VAL:HG12	1:33:A:ILE:H	12	0.54
(1,53)	1:66:A:VAL:HG11	1:33:A:ILE:H	13	0.54
(1,37)	1:99:A:VAL:HG11	1:99:A:VAL:H	19	0.54
(1,27)	1:90:A:VAL:HG22	1:89:A:GLY:H	4	0.54
(1,27)	1:90:A:VAL:HG21	1:89:A:GLY:H	5	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,23)	1:110:A:LEU:HD12	1:111:A:SER:H	15	0.54
(1,7)	1:72:A:LEU:HD12	1:73:A:GLU:H	3	0.54
(1,7)	1:72:A:LEU:HD12	1:73:A:GLU:H	5	0.54
(1,2693)	1:44:A:PHE:HD1	1:44:A:PHE:HZ	16	0.53
(1,2679)	1:7:A:VAL:HB	1:44:A:PHE:HD1	5	0.53
(1,2676)	1:47:A:ALA:HB2	1:44:A:PHE:HD1	13	0.53
(1,2672)	1:70:A:VAL:HG13	1:88:A:TYR:HD1	20	0.53
(1,2670)	1:11:A:ILE:HG23	1:51:A:PHE:HD2	18	0.53
(1,2669)	1:31:A:VAL:HG22	1:44:A:PHE:HD2	2	0.53
(1,2669)	1:31:A:VAL:HG23	1:44:A:PHE:HD2	12	0.53
(1,2650)	1:66:A:VAL:HG11	1:32:A:GLY:HA3	5	0.53
(1,2618)	1:6:A:VAL:HG22	1:2:A:HIS:HB2	4	0.53
(1,2594)	1:66:A:VAL:HG22	1:66:A:VAL:HG23	2	0.53
(1,2590)	1:33:A:ILE:HD13	1:39:A:MET:HG2	10	0.53
(1,2555)	1:25:A:LYS:HE3	1:56:A:LEU:HD12	18	0.53
(1,2464)	1:45:A:VAL:HG21	1:45:A:VAL:HG23	1	0.53
(1,2464)	1:50:A:THR:HG21	1:50:A:THR:HG22	2	0.53
(1,2464)	1:50:A:THR:HG21	1:50:A:THR:HG22	3	0.53
(1,2464)	1:57:A:VAL:HG21	1:57:A:VAL:HG23	5	0.53
(1,2464)	1:50:A:THR:HG21	1:50:A:THR:HG23	6	0.53
(1,2464)	1:57:A:VAL:HG22	1:57:A:VAL:HG23	9	0.53
(1,2464)	1:45:A:VAL:HG21	1:45:A:VAL:HG23	13	0.53
(1,2464)	1:50:A:THR:HG22	1:50:A:THR:HG23	19	0.53
(1,2464)	1:57:A:VAL:HG21	1:57:A:VAL:HG23	20	0.53
(1,2445)	1:29:A:VAL:HG22	1:29:A:VAL:HG21	4	0.53
(1,2445)	1:30:A:VAL:HG22	1:30:A:VAL:HG23	7	0.53
(1,2445)	1:30:A:VAL:HG22	1:30:A:VAL:HG21	11	0.53
(1,2445)	1:30:A:VAL:HG22	1:30:A:VAL:HG21	19	0.53
(1,2426)	1:97:A:LYS:HD3	1:97:A:LYS:H	11	0.53
(1,2422)	1:47:A:ALA:HB2	1:7:A:VAL:H	7	0.53
(1,2246)	1:4:A:TYR:HA	1:4:A:TYR:HE2	5	0.53
(1,2206)	1:83:A:PRO:HB2	1:81:A:PHE:HD2	2	0.53
(1,2166)	1:50:A:THR:HG22	1:51:A:PHE:HE1	19	0.53
(1,2134)	1:72:A:LEU:HD23	1:81:A:PHE:HE2	19	0.53
(1,2133)	1:65:A:ILE:HG23	1:44:A:PHE:HD2	19	0.53
(1,2084)	1:58:A:CYS:HA	1:26:A:ILE:HG21	13	0.53
(1,2069)	1:112:A:LEU:HD22	1:29:A:VAL:HA	6	0.53
(1,2069)	1:112:A:LEU:HD23	1:29:A:VAL:HA	17	0.53
(1,2051)	1:114:A:MET:HE2	1:17:A:HIS:HA	4	0.53
(1,2016)	1:93:A:LYS:HD2	1:79:A:HIS:HB2	11	0.53
(1,2010)	1:114:A:MET:HE2	1:17:A:HIS:HB2	15	0.53
(1,1992)	1:20:A:LYS:HE2	1:20:A:LYS:HA	4	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1987)	1:23:A:ALA:HB3	1:21:A:ASN:HB2	11	0.53
(1,1854)	1:75:A:LYS:HG2	1:100:A:ILE:HG13	16	0.53
(1,1820)	1:10:A:LEU:HD23	1:6:A:VAL:HG11	4	0.53
(1,1812)	1:50:A:THR:HG23	1:47:A:ALA:HA	18	0.53
(1,1806)	1:10:A:LEU:HD13	1:7:A:VAL:HA	3	0.53
(1,1806)	1:10:A:LEU:HD11	1:7:A:VAL:HA	6	0.53
(1,1806)	1:10:A:LEU:HD13	1:7:A:VAL:HA	14	0.53
(1,1798)	1:62:A:ILE:HD11	1:28:A:ARG:HD3	20	0.53
(1,1795)	1:86:A:LEU:HD21	1:86:A:LEU:HD11	15	0.53
(1,1794)	1:11:A:ILE:HG21	1:12:A:ALA:HB3	1	0.53
(1,1774)	1:31:A:VAL:HG22	1:107:A:MET:HG2	19	0.53
(1,1697)	1:112:A:LEU:HD21	1:112:A:LEU:HA	15	0.53
(1,1687)	1:31:A:VAL:HA	1:110:A:LEU:HD13	19	0.53
(1,1628)	1:61:A:ALA:HB1	1:27:A:GLU:HA	19	0.53
(1,1385)	1:48:A:PHE:HB3	1:63:A:LEU:HD11	18	0.53
(1,1302)	1:1:A:MET:HE2	1:1:A:MET:HA	6	0.53
(1,1302)	1:1:A:MET:HE1	1:1:A:MET:HA	10	0.53
(1,1302)	1:1:A:MET:HE3	1:1:A:MET:HA	20	0.53
(1,1026)	1:116:A:ALA:HB1	1:116:A:ALA:HB3	4	0.53
(1,1026)	1:116:A:ALA:HB1	1:116:A:ALA:HB3	12	0.53
(1,1026)	1:116:A:ALA:HB2	1:116:A:ALA:HB1	17	0.53
(1,1021)	1:85:A:ALA:HB2	1:85:A:ALA:HB1	6	0.53
(1,1021)	1:85:A:ALA:HB2	1:85:A:ALA:HB3	11	0.53
(1,1021)	1:85:A:ALA:HB1	1:85:A:ALA:HB3	20	0.53
(1,1020)	1:85:A:ALA:HB3	1:86:A:LEU:HA	11	0.53
(1,962)	1:33:A:ILE:HD12	1:41:A:LYS:HG3	7	0.53
(1,937)	1:102:A:THR:HG21	1:73:A:GLU:HA	4	0.53
(1,937)	1:102:A:THR:HG22	1:73:A:GLU:HA	19	0.53
(1,912)	1:13:A:LEU:HD12	1:13:A:LEU:HD11	15	0.53
(1,904)	1:31:A:VAL:HG12	1:10:A:LEU:HD11	6	0.53
(1,904)	1:31:A:VAL:HG11	1:10:A:LEU:HD13	8	0.53
(1,898)	1:29:A:VAL:HG13	1:112:A:LEU:HA	13	0.53
(1,881)	1:93:A:LYS:HB3	1:93:A:LYS:HE2	18	0.53
(1,875)	1:86:A:LEU:HD23	1:85:A:ALA:HA	2	0.53
(1,874)	1:26:A:ILE:HG21	1:61:A:ALA:HB1	8	0.53
(1,849)	1:72:A:LEU:HD21	1:101:A:ILE:HG13	7	0.53
(1,765)	1:90:A:VAL:HG22	1:90:A:VAL:HG23	1	0.53
(1,765)	1:90:A:VAL:HG22	1:90:A:VAL:HG21	2	0.53
(1,765)	1:90:A:VAL:HG21	1:90:A:VAL:HG23	6	0.53
(1,765)	1:90:A:VAL:HG22	1:90:A:VAL:HG21	9	0.53
(1,765)	1:90:A:VAL:HG21	1:90:A:VAL:HG23	18	0.53
(1,765)	1:90:A:VAL:HG21	1:90:A:VAL:HG23	20	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,300)	1:107:A:MET:HE3	1:108:A:ARG:H	12	0.53
(1,208)	1:41:A:LYS:HG2	1:42:A:SER:H	12	0.53
(1,208)	1:41:A:LYS:HG2	1:42:A:SER:H	13	0.53
(1,200)	1:12:A:ALA:HB2	1:11:A:ILE:H	3	0.53
(1,197)	1:12:A:ALA:HB1	1:16:A:GLU:H	4	0.53
(1,146)	1:6:A:VAL:HG11	1:7:A:VAL:H	18	0.53
(1,116)	1:13:A:LEU:HD22	1:14:A:CYS:H	3	0.53
(1,66)	1:100:A:ILE:HD12	1:100:A:ILE:H	16	0.53
(1,66)	1:100:A:ILE:HD13	1:100:A:ILE:H	17	0.53
(1,27)	1:90:A:VAL:HG22	1:89:A:GLY:H	12	0.53
(1,18)	1:72:A:LEU:HD21	1:72:A:LEU:H	13	0.53
(1,13)	1:72:A:LEU:HD11	1:90:A:VAL:H	2	0.53
(1,2693)	1:48:A:PHE:HD1	1:44:A:PHE:HZ	9	0.52
(1,2693)	1:44:A:PHE:HD1	1:44:A:PHE:HZ	12	0.52
(1,2679)	1:7:A:VAL:HB	1:44:A:PHE:HD1	17	0.52
(1,2654)	1:6:A:VAL:HA	1:107:A:MET:HE3	9	0.52
(1,2652)	1:45:A:VAL:HA	1:47:A:ALA:HB2	9	0.52
(1,2622)	1:38:A:ALA:HB2	1:1:A:MET:HB2	13	0.52
(1,2618)	1:6:A:VAL:HG23	1:2:A:HIS:HB2	7	0.52
(1,2612)	1:59:A:LYS:HE2	1:56:A:LEU:HD13	2	0.52
(1,2571)	1:59:A:LYS:HD3	1:56:A:LEU:HA	7	0.52
(1,2464)	1:45:A:VAL:HG22	1:45:A:VAL:HG21	4	0.52
(1,2464)	1:57:A:VAL:HG22	1:57:A:VAL:HG23	10	0.52
(1,2464)	1:45:A:VAL:HG22	1:45:A:VAL:HG23	14	0.52
(1,2464)	1:50:A:THR:HG21	1:50:A:THR:HG22	15	0.52
(1,2464)	1:45:A:VAL:HG22	1:45:A:VAL:HG23	17	0.52
(1,2445)	1:31:A:VAL:HG22	1:31:A:VAL:HG23	2	0.52
(1,2445)	1:29:A:VAL:HG21	1:29:A:VAL:HG23	5	0.52
(1,2445)	1:80:A:VAL:HG12	1:80:A:VAL:HG13	6	0.52
(1,2445)	1:31:A:VAL:HG22	1:31:A:VAL:HG23	15	0.52
(1,2445)	1:30:A:VAL:HG22	1:30:A:VAL:HG23	20	0.52
(1,2438)	1:65:A:ILE:HD12	1:41:A:LYS:HD2	12	0.52
(1,2438)	1:65:A:ILE:HD13	1:41:A:LYS:HD2	16	0.52
(1,2433)	1:63:A:LEU:HD21	1:31:A:VAL:HG23	1	0.52
(1,2206)	1:83:A:PRO:HB2	1:81:A:PHE:HD2	12	0.52
(1,2204)	1:83:A:PRO:HB3	1:88:A:TYR:HE2	3	0.52
(1,2204)	1:83:A:PRO:HB3	1:88:A:TYR:HE2	9	0.52
(1,2177)	1:6:A:VAL:HG12	1:44:A:PHE:HD1	12	0.52
(1,2163)	1:45:A:VAL:HG23	1:44:A:PHE:HD2	8	0.52
(1,2130)	1:72:A:LEU:HD13	1:81:A:PHE:HE1	16	0.52
(1,2084)	1:58:A:CYS:HA	1:26:A:ILE:HG23	20	0.52
(1,2079)	1:71:A:GLU:HB2	1:103:A:GLN:HA	5	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2070)	1:109:A:LEU:HD21	1:29:A:VAL:HA	19	0.52
(1,2035)	1:42:A:SER:HB2	1:45:A:VAL:HG21	15	0.52
(1,2016)	1:93:A:LYS:HD2	1:79:A:HIS:HB2	8	0.52
(1,1950)	1:57:A:VAL:HG22	1:15:A:GLU:HB3	17	0.52
(1,1941)	1:107:A:MET:HE3	1:10:A:LEU:HB3	3	0.52
(1,1842)	1:18:A:ALA:HB2	1:21:A:ASN:HB3	3	0.52
(1,1823)	1:45:A:VAL:HG13	1:41:A:LYS:HE2	7	0.52
(1,1823)	1:45:A:VAL:HG11	1:41:A:LYS:HE2	13	0.52
(1,1803)	1:10:A:LEU:HD13	1:109:A:LEU:HB2	7	0.52
(1,1794)	1:11:A:ILE:HG22	1:12:A:ALA:HB2	5	0.52
(1,1794)	1:11:A:ILE:HG22	1:12:A:ALA:HB3	20	0.52
(1,1751)	1:65:A:ILE:HD11	1:33:A:ILE:HG23	7	0.52
(1,1499)	1:6:A:VAL:HG23	1:3:A:GLU:HA	3	0.52
(1,1499)	1:6:A:VAL:HG23	1:3:A:GLU:HA	10	0.52
(1,1302)	1:1:A:MET:HE3	1:1:A:MET:HA	14	0.52
(1,1263)	1:11:A:ILE:HD12	1:11:A:ILE:HB	2	0.52
(1,1263)	1:11:A:ILE:HD11	1:11:A:ILE:HB	5	0.52
(1,1263)	1:11:A:ILE:HD12	1:11:A:ILE:HB	15	0.52
(1,1021)	1:85:A:ALA:HB1	1:85:A:ALA:HB3	1	0.52
(1,1021)	1:85:A:ALA:HB1	1:85:A:ALA:HB3	2	0.52
(1,1021)	1:85:A:ALA:HB2	1:85:A:ALA:HB1	15	0.52
(1,1020)	1:85:A:ALA:HB3	1:86:A:LEU:HA	6	0.52
(1,1020)	1:85:A:ALA:HB1	1:86:A:LEU:HA	17	0.52
(1,990)	1:59:A:LYS:HG3	1:59:A:LYS:HE3	3	0.52
(1,990)	1:59:A:LYS:HG3	1:59:A:LYS:HE3	15	0.52
(1,990)	1:59:A:LYS:HG3	1:59:A:LYS:HE3	20	0.52
(1,937)	1:102:A:THR:HG21	1:73:A:GLU:HA	2	0.52
(1,914)	1:72:A:LEU:HD22	1:70:A:VAL:HG12	16	0.52
(1,912)	1:13:A:LEU:HD12	1:13:A:LEU:HD11	19	0.52
(1,904)	1:31:A:VAL:HG11	1:10:A:LEU:HD11	11	0.52
(1,897)	1:29:A:VAL:HG12	1:112:A:LEU:HD23	5	0.52
(1,770)	1:72:A:LEU:HD13	1:70:A:VAL:HG22	2	0.52
(1,765)	1:90:A:VAL:HG22	1:90:A:VAL:HG21	17	0.52
(1,371)	1:22:A:GLN:HG3	1:21:A:ASN:H	15	0.52
(1,208)	1:41:A:LYS:HG2	1:42:A:SER:H	4	0.52
(1,208)	1:41:A:LYS:HG2	1:42:A:SER:H	15	0.52
(1,200)	1:12:A:ALA:HB2	1:11:A:ILE:H	11	0.52
(1,197)	1:12:A:ALA:HB3	1:16:A:GLU:H	18	0.52
(1,195)	1:12:A:ALA:HB2	1:15:A:GLU:H	15	0.52
(1,146)	1:6:A:VAL:HG11	1:7:A:VAL:H	8	0.52
(1,130)	1:10:A:LEU:HD23	1:10:A:LEU:H	16	0.52
(1,126)	1:45:A:VAL:HG21	1:47:A:ALA:H	4	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,126)	1:45:A:VAL:HG22	1:47:A:ALA:H	20	0.52
(1,121)	1:70:A:VAL:HG13	1:71:A:GLU:H	18	0.52
(1,118)	1:13:A:LEU:HD13	1:16:A:GLU:H	4	0.52
(1,116)	1:13:A:LEU:HD23	1:14:A:CYS:H	19	0.52
(1,101)	1:57:A:VAL:HG11	1:15:A:GLU:H	20	0.52
(1,88)	1:26:A:ILE:HD12	1:15:A:GLU:H	12	0.52
(1,88)	1:26:A:ILE:HD12	1:15:A:GLU:H	18	0.52
(1,66)	1:100:A:ILE:HD11	1:100:A:ILE:H	7	0.52
(1,53)	1:66:A:VAL:HG11	1:33:A:ILE:H	11	0.52
(1,53)	1:66:A:VAL:HG12	1:33:A:ILE:H	14	0.52
(1,27)	1:90:A:VAL:HG22	1:89:A:GLY:H	10	0.52
(1,27)	1:90:A:VAL:HG22	1:89:A:GLY:H	17	0.52
(1,2693)	1:44:A:PHE:HD2	1:44:A:PHE:HZ	13	0.51
(1,2679)	1:7:A:VAL:HB	1:44:A:PHE:HD1	13	0.51
(1,2679)	1:7:A:VAL:HB	1:48:A:PHE:HD1	14	0.51
(1,2679)	1:7:A:VAL:HB	1:48:A:PHE:HD1	20	0.51
(1,2669)	1:31:A:VAL:HG23	1:44:A:PHE:HD2	5	0.51
(1,2654)	1:6:A:VAL:HA	1:107:A:MET:HE2	4	0.51
(1,2643)	1:107:A:MET:HE1	1:106:A:GLU:HG3	5	0.51
(1,2643)	1:107:A:MET:HE1	1:106:A:GLU:HG3	12	0.51
(1,2490)	1:82:A:LYS:HG2	1:82:A:LYS:HE2	10	0.51
(1,2475)	1:38:A:ALA:HB1	1:38:A:ALA:HB3	6	0.51
(1,2475)	1:18:A:ALA:HB1	1:18:A:ALA:HB3	20	0.51
(1,2474)	1:18:A:ALA:HB3	1:19:A:LYS:HA	3	0.51
(1,2474)	1:18:A:ALA:HB2	1:19:A:LYS:HA	14	0.51
(1,2464)	1:45:A:VAL:HG21	1:45:A:VAL:HG23	7	0.51
(1,2453)	1:62:A:ILE:HG22	1:62:A:ILE:HG23	8	0.51
(1,2445)	1:80:A:VAL:HG12	1:80:A:VAL:HG13	13	0.51
(1,2445)	1:31:A:VAL:HG22	1:31:A:VAL:HG23	18	0.51
(1,2438)	1:65:A:ILE:HD12	1:41:A:LYS:HD2	2	0.51
(1,2433)	1:63:A:LEU:HD23	1:31:A:VAL:HG21	13	0.51
(1,2426)	1:97:A:LYS:HD3	1:97:A:LYS:H	5	0.51
(1,2246)	1:4:A:TYR:HA	1:4:A:TYR:HE1	3	0.51
(1,2204)	1:83:A:PRO:HB3	1:88:A:TYR:HE2	18	0.51
(1,2105)	1:64:A:ASP:HA	1:62:A:ILE:HG21	5	0.51
(1,2089)	1:79:A:HIS:HA	1:80:A:VAL:HG21	6	0.51
(1,2089)	1:79:A:HIS:HA	1:80:A:VAL:HG23	15	0.51
(1,2064)	1:57:A:VAL:HA	1:25:A:LYS:HB2	7	0.51
(1,2056)	1:15:A:GLU:HG2	1:12:A:ALA:HA	7	0.51
(1,2024)	1:107:A:MET:HE2	1:7:A:VAL:HA	3	0.51
(1,1975)	1:12:A:ALA:HB1	1:15:A:GLU:HB2	1	0.51
(1,1975)	1:12:A:ALA:HB1	1:15:A:GLU:HB2	10	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1939)	1:39:A:MET:HE3	1:39:A:MET:HA	9	0.51
(1,1939)	1:39:A:MET:HE1	1:39:A:MET:HA	14	0.51
(1,1907)	1:25:A:LYS:HB2	1:57:A:VAL:HG12	4	0.51
(1,1907)	1:25:A:LYS:HB2	1:57:A:VAL:HG11	5	0.51
(1,1842)	1:18:A:ALA:HB3	1:21:A:ASN:HB3	15	0.51
(1,1798)	1:62:A:ILE:HD13	1:28:A:ARG:HD3	16	0.51
(1,1794)	1:11:A:ILE:HG21	1:12:A:ALA:HB2	18	0.51
(1,1793)	1:15:A:GLU:HG2	1:11:A:ILE:HG22	7	0.51
(1,1753)	1:65:A:ILE:HD13	1:41:A:LYS:HD3	4	0.51
(1,1753)	1:65:A:ILE:HD13	1:41:A:LYS:HD3	6	0.51
(1,1751)	1:65:A:ILE:HD11	1:33:A:ILE:HG21	13	0.51
(1,1732)	1:72:A:LEU:HD11	1:89:A:GLY:HA3	10	0.51
(1,1628)	1:61:A:ALA:HB1	1:27:A:GLU:HA	9	0.51
(1,1615)	1:10:A:LEU:HA	1:107:A:MET:HE2	19	0.51
(1,1601)	1:12:A:ALA:HB2	1:9:A:SER:HA	20	0.51
(1,1514)	1:43:A:LEU:HD21	1:42:A:SER:HB3	11	0.51
(1,1391)	1:58:A:CYS:HB3	1:55:A:SER:HB3	14	0.51
(1,1263)	1:11:A:ILE:HD13	1:11:A:ILE:HB	7	0.51
(1,1056)	1:69:A:LYS:HB3	1:69:A:LYS:HD3	20	0.51
(1,1021)	1:85:A:ALA:HB2	1:85:A:ALA:HB1	4	0.51
(1,1021)	1:85:A:ALA:HB1	1:85:A:ALA:HB3	8	0.51
(1,1021)	1:85:A:ALA:HB2	1:85:A:ALA:HB1	9	0.51
(1,1021)	1:85:A:ALA:HB1	1:85:A:ALA:HB3	10	0.51
(1,953)	1:65:A:ILE:HG22	1:33:A:ILE:HG12	5	0.51
(1,948)	1:45:A:VAL:HG13	1:42:A:SER:HA	19	0.51
(1,914)	1:72:A:LEU:HD21	1:70:A:VAL:HG11	5	0.51
(1,912)	1:13:A:LEU:HD12	1:13:A:LEU:HD11	3	0.51
(1,912)	1:13:A:LEU:HD12	1:13:A:LEU:HD13	6	0.51
(1,912)	1:13:A:LEU:HD12	1:13:A:LEU:HD11	17	0.51
(1,912)	1:13:A:LEU:HD12	1:13:A:LEU:HD13	18	0.51
(1,910)	1:109:A:LEU:HD12	1:13:A:LEU:HD12	3	0.51
(1,910)	1:109:A:LEU:HD12	1:13:A:LEU:HD12	8	0.51
(1,826)	1:101:A:ILE:HG21	1:103:A:GLN:HA	10	0.51
(1,809)	1:110:A:LEU:HD13	1:66:A:VAL:HG12	7	0.51
(1,809)	1:110:A:LEU:HD13	1:66:A:VAL:HG12	11	0.51
(1,765)	1:90:A:VAL:HG21	1:90:A:VAL:HG23	7	0.51
(1,764)	1:70:A:VAL:HG23	1:70:A:VAL:HA	8	0.51
(1,764)	1:70:A:VAL:HG22	1:70:A:VAL:HA	17	0.51
(1,764)	1:70:A:VAL:HG23	1:70:A:VAL:HA	18	0.51
(1,222)	1:101:A:ILE:HG12	1:101:A:ILE:H	14	0.51
(1,208)	1:41:A:LYS:HG2	1:42:A:SER:H	1	0.51
(1,208)	1:41:A:LYS:HG2	1:42:A:SER:H	2	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,208)	1:41:A:LYS:HG2	1:42:A:SER:H	9	0.51
(1,208)	1:41:A:LYS:HG2	1:42:A:SER:H	17	0.51
(1,200)	1:12:A:ALA:HB1	1:11:A:ILE:H	5	0.51
(1,200)	1:12:A:ALA:HB3	1:11:A:ILE:H	10	0.51
(1,130)	1:10:A:LEU:HD21	1:10:A:LEU:H	13	0.51
(1,116)	1:13:A:LEU:HD23	1:14:A:CYS:H	11	0.51
(1,116)	1:13:A:LEU:HD21	1:14:A:CYS:H	15	0.51
(1,101)	1:57:A:VAL:HG12	1:15:A:GLU:H	2	0.51
(1,101)	1:57:A:VAL:HG12	1:15:A:GLU:H	5	0.51
(1,101)	1:57:A:VAL:HG11	1:15:A:GLU:H	19	0.51
(1,53)	1:66:A:VAL:HG11	1:33:A:ILE:H	10	0.51
(1,53)	1:66:A:VAL:HG12	1:33:A:ILE:H	15	0.51
(1,40)	1:99:A:VAL:HG12	1:89:A:GLY:H	17	0.51
(1,37)	1:99:A:VAL:HG13	1:99:A:VAL:H	11	0.51
(1,34)	1:33:A:ILE:HG22	1:39:A:MET:H	11	0.51
(1,23)	1:110:A:LEU:HD12	1:111:A:SER:H	7	0.51
(1,2693)	1:48:A:PHE:HD2	1:44:A:PHE:HZ	7	0.5
(1,2676)	1:47:A:ALA:HB1	1:44:A:PHE:HD1	7	0.5
(1,2669)	1:31:A:VAL:HG22	1:44:A:PHE:HD2	13	0.5
(1,2618)	1:6:A:VAL:HG22	1:2:A:HIS:HB2	5	0.5
(1,2618)	1:6:A:VAL:HG21	1:2:A:HIS:HB2	13	0.5
(1,2592)	1:41:A:LYS:HD2	1:33:A:ILE:HG22	11	0.5
(1,2475)	1:38:A:ALA:HB2	1:38:A:ALA:HB1	10	0.5
(1,2475)	1:18:A:ALA:HB2	1:18:A:ALA:HB1	18	0.5
(1,2454)	1:62:A:ILE:HG21	1:28:A:ARG:HG3	14	0.5
(1,2453)	1:62:A:ILE:HG22	1:62:A:ILE:HG23	4	0.5
(1,2445)	1:31:A:VAL:HG21	1:31:A:VAL:HG23	17	0.5
(1,2426)	1:97:A:LYS:HD3	1:97:A:LYS:H	14	0.5
(1,2422)	1:47:A:ALA:HB1	1:7:A:VAL:H	19	0.5
(1,2210)	1:107:A:MET:HG2	1:44:A:PHE:HZ	19	0.5
(1,2206)	1:83:A:PRO:HB2	1:81:A:PHE:HD1	13	0.5
(1,2206)	1:83:A:PRO:HB2	1:81:A:PHE:HD1	19	0.5
(1,2171)	1:47:A:ALA:HB1	1:4:A:TYR:HE2	12	0.5
(1,2160)	1:80:A:VAL:HG23	1:81:A:PHE:HD1	16	0.5
(1,2158)	1:29:A:VAL:HG13	1:48:A:PHE:HZ	15	0.5
(1,2136)	1:70:A:VAL:HG22	1:88:A:TYR:HE2	5	0.5
(1,2134)	1:72:A:LEU:HD23	1:81:A:PHE:HE2	5	0.5
(1,2133)	1:65:A:ILE:HG22	1:44:A:PHE:HD2	6	0.5
(1,2077)	1:71:A:GLU:HA	1:82:A:LYS:HG2	7	0.5
(1,2035)	1:42:A:SER:HB2	1:45:A:VAL:HG23	9	0.5
(1,1993)	1:20:A:LYS:HG3	1:20:A:LYS:HE3	1	0.5
(1,1992)	1:20:A:LYS:HE2	1:20:A:LYS:HA	15	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1975)	1:12:A:ALA:HB1	1:15:A:GLU:HB2	3	0.5
(1,1975)	1:12:A:ALA:HB3	1:15:A:GLU:HB2	19	0.5
(1,1854)	1:75:A:LYS:HG2	1:100:A:ILE:HG13	19	0.5
(1,1840)	1:75:A:LYS:HG3	1:100:A:ILE:HG13	5	0.5
(1,1830)	1:112:A:LEU:HD12	1:112:A:LEU:HB3	3	0.5
(1,1830)	1:112:A:LEU:HD12	1:112:A:LEU:HB3	4	0.5
(1,1829)	1:26:A:ILE:HD12	1:23:A:ALA:HB3	1	0.5
(1,1806)	1:10:A:LEU:HD13	1:7:A:VAL:HA	10	0.5
(1,1806)	1:10:A:LEU:HD12	1:7:A:VAL:HA	19	0.5
(1,1795)	1:86:A:LEU:HD22	1:86:A:LEU:HD12	2	0.5
(1,1753)	1:65:A:ILE:HD13	1:41:A:LYS:HD3	10	0.5
(1,1734)	1:72:A:LEU:HD11	1:88:A:TYR:HB3	5	0.5
(1,1732)	1:72:A:LEU:HD13	1:89:A:GLY:HA3	18	0.5
(1,1525)	1:93:A:LYS:HD3	1:93:A:LYS:HA	12	0.5
(1,1430)	1:59:A:LYS:HG2	1:59:A:LYS:HE2	13	0.5
(1,1401)	1:41:A:LYS:HE3	1:33:A:ILE:HD13	11	0.5
(1,1269)	1:80:A:VAL:HG21	1:73:A:GLU:HG2	12	0.5
(1,1263)	1:11:A:ILE:HD13	1:11:A:ILE:HB	9	0.5
(1,1263)	1:11:A:ILE:HD11	1:11:A:ILE:HB	18	0.5
(1,1159)	1:108:A:ARG:HB2	1:110:A:LEU:HD23	15	0.5
(1,1056)	1:69:A:LYS:HB3	1:69:A:LYS:HD3	12	0.5
(1,1021)	1:85:A:ALA:HB1	1:85:A:ALA:HB3	3	0.5
(1,1021)	1:85:A:ALA:HB1	1:85:A:ALA:HB3	13	0.5
(1,1021)	1:85:A:ALA:HB2	1:85:A:ALA:HB1	18	0.5
(1,1020)	1:85:A:ALA:HB1	1:86:A:LEU:HA	8	0.5
(1,1010)	1:115:A:LEU:HB3	1:25:A:LYS:HB3	4	0.5
(1,990)	1:59:A:LYS:HG3	1:59:A:LYS:HE3	8	0.5
(1,937)	1:102:A:THR:HG22	1:73:A:GLU:HA	20	0.5
(1,923)	1:57:A:VAL:HG23	1:56:A:LEU:HB2	16	0.5
(1,912)	1:13:A:LEU:HD12	1:13:A:LEU:HD11	8	0.5
(1,912)	1:13:A:LEU:HD12	1:13:A:LEU:HD13	12	0.5
(1,897)	1:29:A:VAL:HG12	1:112:A:LEU:HD21	18	0.5
(1,889)	1:57:A:VAL:HG13	1:15:A:GLU:HG3	1	0.5
(1,765)	1:90:A:VAL:HG21	1:90:A:VAL:HG23	19	0.5
(1,764)	1:70:A:VAL:HG23	1:70:A:VAL:HA	5	0.5
(1,764)	1:70:A:VAL:HG23	1:70:A:VAL:HA	14	0.5
(1,764)	1:70:A:VAL:HG21	1:70:A:VAL:HA	16	0.5
(1,746)	1:72:A:LEU:HD12	1:83:A:PRO:HB2	14	0.5
(1,458)	1:74:A:CYS:HB2	1:77:A:CYS:H	7	0.5
(1,420)	1:19:A:LYS:HE2	1:19:A:LYS:H	12	0.5
(1,303)	1:107:A:MET:HE1	1:10:A:LEU:H	18	0.5
(1,300)	1:107:A:MET:HE3	1:108:A:ARG:H	14	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,300)	1:107:A:MET:HE1	1:108:A:ARG:H	20	0.5
(1,213)	1:75:A:LYS:HD3	1:75:A:LYS:H	12	0.5
(1,213)	1:75:A:LYS:HD3	1:75:A:LYS:H	18	0.5
(1,208)	1:41:A:LYS:HG2	1:42:A:SER:H	16	0.5
(1,136)	1:102:A:THR:HG23	1:100:A:ILE:H	9	0.5
(1,130)	1:10:A:LEU:HD23	1:10:A:LEU:H	14	0.5
(1,126)	1:45:A:VAL:HG22	1:47:A:ALA:H	18	0.5
(1,118)	1:13:A:LEU:HD13	1:16:A:GLU:H	16	0.5
(1,116)	1:13:A:LEU:HD21	1:14:A:CYS:H	6	0.5
(1,116)	1:13:A:LEU:HD23	1:14:A:CYS:H	13	0.5
(1,103)	1:43:A:LEU:HD22	1:46:A:SER:H	20	0.5
(1,74)	1:99:A:VAL:HG21	1:73:A:GLU:H	11	0.5
(1,44)	1:99:A:VAL:HG11	1:73:A:GLU:H	15	0.5
(1,2679)	1:7:A:VAL:HB	1:48:A:PHE:HD1	8	0.49
(1,2676)	1:47:A:ALA:HB3	1:44:A:PHE:HD2	10	0.49
(1,2676)	1:47:A:ALA:HB2	1:44:A:PHE:HD1	19	0.49
(1,2671)	1:115:A:LEU:HD12	1:24:A:HIS:HD2	8	0.49
(1,2660)	1:69:A:LYS:HA	1:69:A:LYS:HE3	8	0.49
(1,2621)	1:38:A:ALA:HB3	1:105:A:ASN:HB2	4	0.49
(1,2618)	1:6:A:VAL:HG22	1:2:A:HIS:HB2	15	0.49
(1,2516)	1:25:A:LYS:HD2	1:25:A:LYS:HD3	12	0.49
(1,2516)	1:25:A:LYS:HD2	1:25:A:LYS:HD3	13	0.49
(1,2516)	1:59:A:LYS:HD2	1:59:A:LYS:HD3	17	0.49
(1,2475)	1:18:A:ALA:HB2	1:18:A:ALA:HB3	3	0.49
(1,2475)	1:18:A:ALA:HB2	1:18:A:ALA:HB1	7	0.49
(1,2475)	1:18:A:ALA:HB2	1:18:A:ALA:HB1	8	0.49
(1,2475)	1:18:A:ALA:HB2	1:18:A:ALA:HB3	12	0.49
(1,2475)	1:18:A:ALA:HB2	1:18:A:ALA:HB1	14	0.49
(1,2475)	1:38:A:ALA:HB2	1:38:A:ALA:HB1	15	0.49
(1,2474)	1:18:A:ALA:HB2	1:19:A:LYS:HA	16	0.49
(1,2453)	1:62:A:ILE:HG22	1:62:A:ILE:HG21	1	0.49
(1,2453)	1:100:A:ILE:HG21	1:100:A:ILE:HG23	3	0.49
(1,2453)	1:62:A:ILE:HG22	1:62:A:ILE:HG21	5	0.49
(1,2453)	1:100:A:ILE:HG22	1:100:A:ILE:HG21	6	0.49
(1,2453)	1:100:A:ILE:HG22	1:100:A:ILE:HG23	13	0.49
(1,2453)	1:100:A:ILE:HG22	1:100:A:ILE:HG23	19	0.49
(1,2433)	1:63:A:LEU:HD21	1:31:A:VAL:HG21	5	0.49
(1,2426)	1:97:A:LYS:HD3	1:97:A:LYS:H	10	0.49
(1,2426)	1:97:A:LYS:HD3	1:97:A:LYS:H	18	0.49
(1,2262)	1:88:A:TYR:HA	1:88:A:TYR:HD2	15	0.49
(1,2255)	1:91:A:CYS:HA	1:81:A:PHE:HE1	17	0.49
(1,2206)	1:83:A:PRO:HB2	1:81:A:PHE:HD1	11	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2166)	1:50:A:THR:HG23	1:51:A:PHE:HE2	2	0.49
(1,2133)	1:65:A:ILE:HG23	1:44:A:PHE:HD1	11	0.49
(1,2052)	1:20:A:LYS:HG2	1:17:A:HIS:HA	8	0.49
(1,2016)	1:93:A:LYS:HD2	1:79:A:HIS:HB2	4	0.49
(1,1975)	1:12:A:ALA:HB3	1:15:A:GLU:HB2	7	0.49
(1,1960)	1:113:A:GLU:HG3	1:27:A:GLU:HB3	3	0.49
(1,1914)	1:68:A:GLU:HB2	1:34:A:GLY:HA3	15	0.49
(1,1888)	1:85:A:ALA:HB1	1:86:A:LEU:HG	20	0.49
(1,1842)	1:18:A:ALA:HB1	1:21:A:ASN:HB3	19	0.49
(1,1840)	1:75:A:LYS:HG3	1:100:A:ILE:HG13	9	0.49
(1,1812)	1:50:A:THR:HG22	1:47:A:ALA:HA	11	0.49
(1,1809)	1:70:A:VAL:HG11	1:35:A:GLU:HB3	20	0.49
(1,1800)	1:115:A:LEU:HD13	1:25:A:LYS:HG2	14	0.49
(1,1795)	1:86:A:LEU:HD23	1:86:A:LEU:HD13	3	0.49
(1,1795)	1:86:A:LEU:HD21	1:86:A:LEU:HD12	6	0.49
(1,1793)	1:15:A:GLU:HG2	1:11:A:ILE:HG23	4	0.49
(1,1780)	1:112:A:LEU:HD21	1:17:A:HIS:HA	3	0.49
(1,1778)	1:112:A:LEU:HD22	1:18:A:ALA:HB3	14	0.49
(1,1772)	1:64:A:ASP:HB3	1:30:A:VAL:HG11	20	0.49
(1,1737)	1:33:A:ILE:HG13	1:39:A:MET:HE3	14	0.49
(1,1708)	1:107:A:MET:HA	1:33:A:ILE:HD12	18	0.49
(1,1628)	1:61:A:ALA:HB2	1:27:A:GLU:HA	11	0.49
(1,1302)	1:1:A:MET:HE1	1:1:A:MET:HA	9	0.49
(1,1269)	1:80:A:VAL:HG23	1:73:A:GLU:HG2	1	0.49
(1,1269)	1:80:A:VAL:HG23	1:73:A:GLU:HG2	5	0.49
(1,1263)	1:11:A:ILE:HD11	1:11:A:ILE:HB	3	0.49
(1,1263)	1:11:A:ILE:HD12	1:11:A:ILE:HB	14	0.49
(1,1159)	1:108:A:ARG:HB2	1:110:A:LEU:HD23	19	0.49
(1,1056)	1:69:A:LYS:HB3	1:69:A:LYS:HD3	5	0.49
(1,1021)	1:85:A:ALA:HB2	1:85:A:ALA:HB1	7	0.49
(1,962)	1:33:A:ILE:HD11	1:41:A:LYS:HG3	13	0.49
(1,945)	1:109:A:LEU:HD22	1:109:A:LEU:HB2	14	0.49
(1,937)	1:102:A:THR:HG21	1:73:A:GLU:HA	18	0.49
(1,923)	1:57:A:VAL:HG21	1:56:A:LEU:HB2	14	0.49
(1,912)	1:13:A:LEU:HD11	1:13:A:LEU:HD13	5	0.49
(1,912)	1:13:A:LEU:HD12	1:13:A:LEU:HD13	10	0.49
(1,912)	1:13:A:LEU:HD12	1:13:A:LEU:HD13	16	0.49
(1,910)	1:109:A:LEU:HD13	1:13:A:LEU:HD12	20	0.49
(1,897)	1:29:A:VAL:HG13	1:112:A:LEU:HD22	1	0.49
(1,897)	1:29:A:VAL:HG13	1:112:A:LEU:HD23	11	0.49
(1,851)	1:101:A:ILE:HD13	1:105:A:ASN:HB3	20	0.49
(1,822)	1:80:A:VAL:HG12	1:102:A:THR:HG22	15	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,765)	1:90:A:VAL:HG22	1:90:A:VAL:HG21	12	0.49
(1,764)	1:70:A:VAL:HG21	1:70:A:VAL:HA	3	0.49
(1,764)	1:70:A:VAL:HG22	1:70:A:VAL:HA	7	0.49
(1,415)	1:20:A:LYS:HE3	1:20:A:LYS:H	2	0.49
(1,213)	1:75:A:LYS:HD3	1:75:A:LYS:H	20	0.49
(1,197)	1:12:A:ALA:HB2	1:16:A:GLU:H	6	0.49
(1,121)	1:70:A:VAL:HG12	1:71:A:GLU:H	15	0.49
(1,118)	1:13:A:LEU:HD11	1:16:A:GLU:H	13	0.49
(1,116)	1:13:A:LEU:HD23	1:14:A:CYS:H	9	0.49
(1,113)	1:10:A:LEU:HD11	1:10:A:LEU:H	5	0.49
(1,101)	1:57:A:VAL:HG13	1:15:A:GLU:H	1	0.49
(1,88)	1:26:A:ILE:HD11	1:15:A:GLU:H	6	0.49
(1,84)	1:99:A:VAL:HG21	1:91:A:CYS:H	4	0.49
(1,53)	1:66:A:VAL:HG11	1:33:A:ILE:H	5	0.49
(1,37)	1:99:A:VAL:HG11	1:99:A:VAL:H	9	0.49
(1,23)	1:110:A:LEU:HD12	1:111:A:SER:H	13	0.49
(1,23)	1:110:A:LEU:HD13	1:111:A:SER:H	16	0.49
(1,2645)	1:33:A:ILE:HG23	1:39:A:MET:HG3	8	0.48
(1,2612)	1:59:A:LYS:HE3	1:56:A:LEU:HD13	1	0.48
(1,2590)	1:33:A:ILE:HD11	1:39:A:MET:HG2	20	0.48
(1,2516)	1:25:A:LYS:HD2	1:25:A:LYS:HD3	3	0.48
(1,2516)	1:59:A:LYS:HD2	1:59:A:LYS:HD3	4	0.48
(1,2516)	1:25:A:LYS:HD2	1:25:A:LYS:HD3	6	0.48
(1,2516)	1:25:A:LYS:HD2	1:25:A:LYS:HD3	9	0.48
(1,2516)	1:59:A:LYS:HD2	1:59:A:LYS:HD3	15	0.48
(1,2516)	1:25:A:LYS:HD2	1:25:A:LYS:HD3	16	0.48
(1,2475)	1:18:A:ALA:HB2	1:18:A:ALA:HB1	1	0.48
(1,2475)	1:38:A:ALA:HB2	1:38:A:ALA:HB1	2	0.48
(1,2475)	1:38:A:ALA:HB2	1:38:A:ALA:HB3	13	0.48
(1,2475)	1:38:A:ALA:HB2	1:38:A:ALA:HB1	17	0.48
(1,2454)	1:62:A:ILE:HG21	1:28:A:ARG:HG3	3	0.48
(1,2454)	1:62:A:ILE:HG22	1:28:A:ARG:HG3	11	0.48
(1,2453)	1:62:A:ILE:HG22	1:62:A:ILE:HG23	2	0.48
(1,2453)	1:62:A:ILE:HG22	1:62:A:ILE:HG23	7	0.48
(1,2453)	1:100:A:ILE:HG21	1:100:A:ILE:HG23	9	0.48
(1,2453)	1:62:A:ILE:HG22	1:62:A:ILE:HG23	12	0.48
(1,2453)	1:62:A:ILE:HG22	1:62:A:ILE:HG21	14	0.48
(1,2453)	1:100:A:ILE:HG22	1:100:A:ILE:HG23	15	0.48
(1,2453)	1:62:A:ILE:HG22	1:62:A:ILE:HG21	16	0.48
(1,2453)	1:62:A:ILE:HG21	1:62:A:ILE:HG23	17	0.48
(1,2447)	1:101:A:ILE:HD12	1:101:A:ILE:HD13	3	0.48
(1,2422)	1:47:A:ALA:HB2	1:7:A:VAL:H	2	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2419)	1:69:A:LYS:HG3	1:69:A:LYS:H	10	0.48
(1,2246)	1:4:A:TYR:HA	1:4:A:TYR:HE1	11	0.48
(1,2206)	1:83:A:PRO:HB2	1:81:A:PHE:HD2	16	0.48
(1,2180)	1:61:A:ALA:HB3	1:48:A:PHE:HD2	8	0.48
(1,2160)	1:80:A:VAL:HG21	1:81:A:PHE:HD2	13	0.48
(1,2143)	1:7:A:VAL:HG21	1:51:A:PHE:HD1	5	0.48
(1,2016)	1:93:A:LYS:HD2	1:79:A:HIS:HB2	16	0.48
(1,1975)	1:12:A:ALA:HB1	1:15:A:GLU:HB2	16	0.48
(1,1975)	1:12:A:ALA:HB3	1:15:A:GLU:HB2	18	0.48
(1,1849)	1:38:A:ALA:HB1	1:1:A:MET:HE3	11	0.48
(1,1842)	1:18:A:ALA:HB1	1:21:A:ASN:HB3	6	0.48
(1,1830)	1:112:A:LEU:HD11	1:112:A:LEU:HB3	9	0.48
(1,1819)	1:7:A:VAL:HG13	1:47:A:ALA:HB1	8	0.48
(1,1814)	1:107:A:MET:HE2	1:10:A:LEU:HD21	16	0.48
(1,1812)	1:50:A:THR:HG22	1:47:A:ALA:HA	1	0.48
(1,1812)	1:50:A:THR:HG22	1:47:A:ALA:HA	14	0.48
(1,1795)	1:86:A:LEU:HD22	1:86:A:LEU:HD12	10	0.48
(1,1794)	1:11:A:ILE:HG22	1:12:A:ALA:HB1	6	0.48
(1,1794)	1:11:A:ILE:HG21	1:12:A:ALA:HB3	12	0.48
(1,1791)	1:62:A:ILE:HG22	1:64:A:ASP:HB3	20	0.48
(1,1769)	1:66:A:VAL:HG12	1:68:A:GLU:HB2	12	0.48
(1,1751)	1:65:A:ILE:HD13	1:33:A:ILE:HG23	5	0.48
(1,1751)	1:65:A:ILE:HD13	1:33:A:ILE:HG22	6	0.48
(1,1744)	1:90:A:VAL:HG11	1:90:A:VAL:HG23	5	0.48
(1,1744)	1:90:A:VAL:HG12	1:90:A:VAL:HG22	9	0.48
(1,1708)	1:107:A:MET:HA	1:33:A:ILE:HD13	16	0.48
(1,1628)	1:61:A:ALA:HB2	1:27:A:GLU:HA	7	0.48
(1,1601)	1:12:A:ALA:HB1	1:9:A:SER:HA	7	0.48
(1,1482)	1:7:A:VAL:HG22	1:48:A:PHE:HA	20	0.48
(1,1474)	1:41:A:LYS:HA	1:41:A:LYS:HE2	17	0.48
(1,1384)	1:93:A:LYS:HE2	1:93:A:LYS:HA	18	0.48
(1,1302)	1:1:A:MET:HE3	1:1:A:MET:HA	8	0.48
(1,1269)	1:80:A:VAL:HG22	1:73:A:GLU:HG2	2	0.48
(1,1269)	1:80:A:VAL:HG23	1:73:A:GLU:HG2	11	0.48
(1,1269)	1:80:A:VAL:HG21	1:73:A:GLU:HG2	19	0.48
(1,1263)	1:11:A:ILE:HD13	1:11:A:ILE:HB	4	0.48
(1,1263)	1:11:A:ILE:HD13	1:11:A:ILE:HB	11	0.48
(1,1263)	1:11:A:ILE:HD12	1:11:A:ILE:HB	12	0.48
(1,1263)	1:11:A:ILE:HD12	1:11:A:ILE:HB	13	0.48
(1,1140)	1:59:A:LYS:HD3	1:59:A:LYS:HA	1	0.48
(1,1140)	1:59:A:LYS:HD3	1:59:A:LYS:HA	11	0.48
(1,1093)	1:82:A:LYS:HD2	1:82:A:LYS:HA	13	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1056)	1:69:A:LYS:HB3	1:69:A:LYS:HD3	2	0.48
(1,1020)	1:85:A:ALA:HB3	1:86:A:LEU:HA	2	0.48
(1,996)	1:26:A:ILE:HG12	1:57:A:VAL:HG13	6	0.48
(1,996)	1:26:A:ILE:HG12	1:57:A:VAL:HG12	7	0.48
(1,990)	1:59:A:LYS:HG3	1:59:A:LYS:HE3	9	0.48
(1,962)	1:33:A:ILE:HD13	1:41:A:LYS:HG3	19	0.48
(1,953)	1:65:A:ILE:HG23	1:33:A:ILE:HG12	7	0.48
(1,912)	1:13:A:LEU:HD12	1:13:A:LEU:HD13	2	0.48
(1,912)	1:13:A:LEU:HD11	1:13:A:LEU:HD13	4	0.48
(1,912)	1:13:A:LEU:HD11	1:13:A:LEU:HD13	7	0.48
(1,912)	1:13:A:LEU:HD11	1:13:A:LEU:HD13	9	0.48
(1,912)	1:13:A:LEU:HD12	1:13:A:LEU:HD11	11	0.48
(1,912)	1:13:A:LEU:HD12	1:13:A:LEU:HD13	13	0.48
(1,912)	1:13:A:LEU:HD12	1:13:A:LEU:HD13	20	0.48
(1,910)	1:109:A:LEU:HD11	1:13:A:LEU:HD12	7	0.48
(1,910)	1:109:A:LEU:HD11	1:13:A:LEU:HD11	14	0.48
(1,889)	1:57:A:VAL:HG11	1:15:A:GLU:HG3	17	0.48
(1,874)	1:26:A:ILE:HG23	1:61:A:ALA:HB2	20	0.48
(1,764)	1:70:A:VAL:HG22	1:70:A:VAL:HA	12	0.48
(1,300)	1:107:A:MET:HE2	1:108:A:ARG:H	8	0.48
(1,300)	1:107:A:MET:HE2	1:108:A:ARG:H	9	0.48
(1,300)	1:107:A:MET:HE3	1:108:A:ARG:H	16	0.48
(1,208)	1:41:A:LYS:HG2	1:42:A:SER:H	18	0.48
(1,200)	1:12:A:ALA:HB1	1:11:A:ILE:H	18	0.48
(1,197)	1:12:A:ALA:HB3	1:16:A:GLU:H	17	0.48
(1,197)	1:12:A:ALA:HB1	1:16:A:GLU:H	20	0.48
(1,185)	1:38:A:ALA:HB2	1:39:A:MET:H	1	0.48
(1,162)	1:23:A:ALA:HB1	1:22:A:GLN:H	15	0.48
(1,138)	1:102:A:THR:HG22	1:103:A:GLN:H	11	0.48
(1,130)	1:10:A:LEU:HD22	1:10:A:LEU:H	1	0.48
(1,130)	1:10:A:LEU:HD23	1:10:A:LEU:H	2	0.48
(1,126)	1:45:A:VAL:HG22	1:47:A:ALA:H	5	0.48
(1,118)	1:13:A:LEU:HD13	1:16:A:GLU:H	1	0.48
(1,118)	1:13:A:LEU:HD12	1:16:A:GLU:H	6	0.48
(1,118)	1:13:A:LEU:HD11	1:16:A:GLU:H	20	0.48
(1,116)	1:13:A:LEU:HD22	1:14:A:CYS:H	16	0.48
(1,113)	1:10:A:LEU:HD11	1:10:A:LEU:H	14	0.48
(1,112)	1:10:A:LEU:HD12	1:11:A:ILE:H	3	0.48
(1,103)	1:43:A:LEU:HD23	1:46:A:SER:H	18	0.48
(1,37)	1:99:A:VAL:HG13	1:99:A:VAL:H	7	0.48
(1,27)	1:90:A:VAL:HG23	1:89:A:GLY:H	3	0.48
(1,27)	1:90:A:VAL:HG22	1:89:A:GLY:H	18	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2679)	1:7:A:VAL:HB	1:44:A:PHE:HD1	2	0.47
(1,2679)	1:7:A:VAL:HB	1:44:A:PHE:HD1	7	0.47
(1,2676)	1:47:A:ALA:HB3	1:44:A:PHE:HD2	3	0.47
(1,2669)	1:31:A:VAL:HG22	1:44:A:PHE:HD2	4	0.47
(1,2669)	1:31:A:VAL:HG21	1:44:A:PHE:HD1	10	0.47
(1,2654)	1:6:A:VAL:HA	1:107:A:MET:HE3	10	0.47
(1,2650)	1:66:A:VAL:HG13	1:32:A:GLY:HA3	19	0.47
(1,2643)	1:39:A:MET:HE3	1:106:A:GLU:HG2	11	0.47
(1,2597)	1:72:A:LEU:HB2	1:99:A:VAL:HG22	8	0.47
(1,2516)	1:25:A:LYS:HD2	1:25:A:LYS:HD3	1	0.47
(1,2516)	1:59:A:LYS:HD2	1:59:A:LYS:HD3	11	0.47
(1,2516)	1:25:A:LYS:HD2	1:25:A:LYS:HD3	19	0.47
(1,2475)	1:18:A:ALA:HB1	1:18:A:ALA:HB3	5	0.47
(1,2475)	1:18:A:ALA:HB1	1:18:A:ALA:HB3	16	0.47
(1,2474)	1:18:A:ALA:HB3	1:19:A:LYS:HA	19	0.47
(1,2453)	1:62:A:ILE:HG22	1:62:A:ILE:HG23	18	0.47
(1,2447)	1:100:A:ILE:HD12	1:100:A:ILE:HD11	5	0.47
(1,2447)	1:100:A:ILE:HD12	1:100:A:ILE:HD11	6	0.47
(1,2447)	1:100:A:ILE:HD11	1:100:A:ILE:HD13	7	0.47
(1,2447)	1:100:A:ILE:HD11	1:100:A:ILE:HD13	9	0.47
(1,2447)	1:100:A:ILE:HD11	1:100:A:ILE:HD13	19	0.47
(1,2438)	1:65:A:ILE:HD13	1:41:A:LYS:HD2	3	0.47
(1,2426)	1:97:A:LYS:HD3	1:97:A:LYS:H	15	0.47
(1,2422)	1:47:A:ALA:HB2	1:7:A:VAL:H	10	0.47
(1,2422)	1:47:A:ALA:HB3	1:7:A:VAL:H	13	0.47
(1,2172)	1:47:A:ALA:HB1	1:4:A:TYR:HD1	8	0.47
(1,2162)	1:43:A:LEU:HD13	1:4:A:TYR:HD2	20	0.47
(1,2160)	1:80:A:VAL:HG21	1:81:A:PHE:HD1	3	0.47
(1,2095)	1:25:A:LYS:HA	1:25:A:LYS:HD2	5	0.47
(1,2095)	1:25:A:LYS:HA	1:25:A:LYS:HD2	12	0.47
(1,2088)	1:105:A:ASN:HA	1:36:A:ARG:HB3	14	0.47
(1,2070)	1:109:A:LEU:HD21	1:29:A:VAL:HA	17	0.47
(1,2047)	1:33:A:ILE:HG21	1:37:A:SER:HA	17	0.47
(1,2016)	1:93:A:LYS:HD2	1:79:A:HIS:HB2	5	0.47
(1,1888)	1:85:A:ALA:HB1	1:86:A:LEU:HG	5	0.47
(1,1887)	1:82:A:LYS:HD2	1:71:A:GLU:HB3	4	0.47
(1,1857)	1:75:A:LYS:HG2	1:98:A:ASN:HB2	15	0.47
(1,1845)	1:38:A:ALA:HB1	1:39:A:MET:HA	4	0.47
(1,1830)	1:112:A:LEU:HD11	1:112:A:LEU:HB3	5	0.47
(1,1830)	1:112:A:LEU:HD11	1:112:A:LEU:HB3	18	0.47
(1,1820)	1:10:A:LEU:HD21	1:6:A:VAL:HG12	2	0.47
(1,1820)	1:10:A:LEU:HD23	1:6:A:VAL:HG12	11	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1812)	1:50:A:THR:HG21	1:47:A:ALA:HA	4	0.47
(1,1806)	1:10:A:LEU:HD13	1:7:A:VAL:HA	2	0.47
(1,1806)	1:10:A:LEU:HD12	1:7:A:VAL:HA	9	0.47
(1,1803)	1:10:A:LEU:HD11	1:109:A:LEU:HB2	3	0.47
(1,1803)	1:10:A:LEU:HD11	1:109:A:LEU:HB2	20	0.47
(1,1795)	1:86:A:LEU:HD21	1:86:A:LEU:HD13	13	0.47
(1,1793)	1:15:A:GLU:HG2	1:11:A:ILE:HG22	8	0.47
(1,1708)	1:107:A:MET:HA	1:33:A:ILE:HD11	20	0.47
(1,1576)	1:35:A:GLU:HG3	1:69:A:LYS:HA	3	0.47
(1,1452)	1:63:A:LEU:HD11	1:45:A:VAL:HA	19	0.47
(1,1263)	1:11:A:ILE:HD13	1:11:A:ILE:HB	1	0.47
(1,1263)	1:11:A:ILE:HD12	1:11:A:ILE:HB	6	0.47
(1,1263)	1:11:A:ILE:HD13	1:11:A:ILE:HB	17	0.47
(1,1263)	1:11:A:ILE:HD13	1:11:A:ILE:HB	20	0.47
(1,1211)	1:75:A:LYS:HB3	1:98:A:ASN:HB2	7	0.47
(1,1056)	1:69:A:LYS:HB3	1:69:A:LYS:HD3	19	0.47
(1,1020)	1:85:A:ALA:HB3	1:86:A:LEU:HA	14	0.47
(1,990)	1:59:A:LYS:HG3	1:59:A:LYS:HE3	2	0.47
(1,990)	1:59:A:LYS:HG3	1:59:A:LYS:HE3	14	0.47
(1,937)	1:102:A:THR:HG23	1:73:A:GLU:HA	1	0.47
(1,923)	1:57:A:VAL:HG21	1:56:A:LEU:HB2	7	0.47
(1,912)	1:13:A:LEU:HD12	1:13:A:LEU:HD11	14	0.47
(1,862)	1:109:A:LEU:HD23	1:13:A:LEU:HD21	15	0.47
(1,844)	1:112:A:LEU:HD22	1:114:A:MET:HE1	15	0.47
(1,809)	1:110:A:LEU:HD11	1:66:A:VAL:HG13	9	0.47
(1,809)	1:110:A:LEU:HD11	1:66:A:VAL:HG12	10	0.47
(1,764)	1:70:A:VAL:HG23	1:70:A:VAL:HA	1	0.47
(1,764)	1:70:A:VAL:HG21	1:70:A:VAL:HA	19	0.47
(1,764)	1:70:A:VAL:HG23	1:70:A:VAL:HA	20	0.47
(1,746)	1:72:A:LEU:HD11	1:83:A:PRO:HB2	16	0.47
(1,299)	1:39:A:MET:HE1	1:6:A:VAL:H	19	0.47
(1,222)	1:101:A:ILE:HG12	1:101:A:ILE:H	9	0.47
(1,208)	1:41:A:LYS:HG2	1:42:A:SER:H	3	0.47
(1,200)	1:12:A:ALA:HB3	1:11:A:ILE:H	9	0.47
(1,146)	1:6:A:VAL:HG12	1:7:A:VAL:H	9	0.47
(1,138)	1:102:A:THR:HG21	1:103:A:GLN:H	6	0.47
(1,131)	1:10:A:LEU:HD22	1:11:A:ILE:H	19	0.47
(1,126)	1:45:A:VAL:HG23	1:47:A:ALA:H	15	0.47
(1,126)	1:45:A:VAL:HG23	1:47:A:ALA:H	17	0.47
(1,116)	1:13:A:LEU:HD23	1:14:A:CYS:H	4	0.47
(1,113)	1:10:A:LEU:HD12	1:10:A:LEU:H	4	0.47
(1,70)	1:112:A:LEU:HD23	1:17:A:HIS:H	3	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,66)	1:100:A:ILE:HD12	1:100:A:ILE:H	13	0.47
(1,39)	1:90:A:VAL:HG12	1:90:A:VAL:H	1	0.47
(1,36)	1:99:A:VAL:HG11	1:100:A:ILE:H	1	0.47
(1,31)	1:33:A:ILE:HG21	1:33:A:ILE:H	3	0.47
(1,31)	1:33:A:ILE:HG23	1:33:A:ILE:H	9	0.47
(1,29)	1:70:A:VAL:HG22	1:72:A:LEU:H	6	0.47
(1,29)	1:70:A:VAL:HG21	1:72:A:LEU:H	11	0.47
(1,23)	1:110:A:LEU:HD13	1:111:A:SER:H	18	0.47
(1,2676)	1:47:A:ALA:HB3	1:44:A:PHE:HD1	2	0.46
(1,2676)	1:47:A:ALA:HB3	1:44:A:PHE:HD1	17	0.46
(1,2670)	1:11:A:ILE:HG22	1:51:A:PHE:HD2	1	0.46
(1,2670)	1:11:A:ILE:HG23	1:51:A:PHE:HD2	15	0.46
(1,2669)	1:31:A:VAL:HG22	1:44:A:PHE:HD1	11	0.46
(1,2651)	1:45:A:VAL:HA	1:48:A:PHE:HA	5	0.46
(1,2650)	1:66:A:VAL:HG12	1:32:A:GLY:HA3	16	0.46
(1,2622)	1:38:A:ALA:HB2	1:1:A:MET:HB2	15	0.46
(1,2601)	1:75:A:LYS:HG2	1:100:A:ILE:HD13	10	0.46
(1,2596)	1:110:A:LEU:HD21	1:66:A:VAL:HB	16	0.46
(1,2571)	1:59:A:LYS:HD3	1:56:A:LEU:HA	19	0.46
(1,2552)	1:41:A:LYS:HE2	1:41:A:LYS:HE3	20	0.46
(1,2516)	1:59:A:LYS:HD2	1:59:A:LYS:HD3	2	0.46
(1,2516)	1:59:A:LYS:HD2	1:59:A:LYS:HD3	5	0.46
(1,2516)	1:25:A:LYS:HD2	1:25:A:LYS:HD3	10	0.46
(1,2516)	1:25:A:LYS:HD2	1:25:A:LYS:HD3	18	0.46
(1,2516)	1:25:A:LYS:HD2	1:25:A:LYS:HD3	20	0.46
(1,2475)	1:18:A:ALA:HB1	1:18:A:ALA:HB3	9	0.46
(1,2475)	1:18:A:ALA:HB2	1:18:A:ALA:HB3	11	0.46
(1,2453)	1:100:A:ILE:HG22	1:100:A:ILE:HG21	10	0.46
(1,2453)	1:62:A:ILE:HG22	1:62:A:ILE:HG23	11	0.46
(1,2453)	1:100:A:ILE:HG22	1:100:A:ILE:HG23	20	0.46
(1,2447)	1:100:A:ILE:HD12	1:100:A:ILE:HD13	4	0.46
(1,2447)	1:101:A:ILE:HD12	1:101:A:ILE:HD13	10	0.46
(1,2447)	1:101:A:ILE:HD11	1:101:A:ILE:HD13	11	0.46
(1,2447)	1:101:A:ILE:HD12	1:101:A:ILE:HD11	12	0.46
(1,2447)	1:100:A:ILE:HD12	1:100:A:ILE:HD13	13	0.46
(1,2447)	1:101:A:ILE:HD12	1:101:A:ILE:HD13	14	0.46
(1,2447)	1:101:A:ILE:HD11	1:101:A:ILE:HD13	16	0.46
(1,2433)	1:63:A:LEU:HD21	1:31:A:VAL:HG21	4	0.46
(1,2427)	1:107:A:MET:HE2	1:107:A:MET:H	11	0.46
(1,2426)	1:97:A:LYS:HD3	1:97:A:LYS:H	12	0.46
(1,2426)	1:97:A:LYS:HD3	1:97:A:LYS:H	20	0.46
(1,2400)	1:96:A:SER:H	1:94:A:CYS:H	17	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2239)	1:41:A:LYS:HA	1:44:A:PHE:HD2	2	0.46
(1,2239)	1:41:A:LYS:HA	1:44:A:PHE:HD2	5	0.46
(1,2204)	1:83:A:PRO:HB3	1:88:A:TYR:HE1	13	0.46
(1,2152)	1:99:A:VAL:HG21	1:81:A:PHE:HZ	17	0.46
(1,2148)	1:80:A:VAL:HG13	1:81:A:PHE:HD1	8	0.46
(1,2133)	1:65:A:ILE:HG23	1:44:A:PHE:HD2	4	0.46
(1,2088)	1:105:A:ASN:HA	1:36:A:ARG:HB3	15	0.46
(1,2043)	1:56:A:LEU:HA	1:59:A:LYS:HB3	11	0.46
(1,1857)	1:75:A:LYS:HG2	1:98:A:ASN:HB2	14	0.46
(1,1842)	1:18:A:ALA:HB3	1:21:A:ASN:HB3	5	0.46
(1,1842)	1:18:A:ALA:HB3	1:21:A:ASN:HB3	12	0.46
(1,1830)	1:112:A:LEU:HD13	1:112:A:LEU:HB3	15	0.46
(1,1830)	1:112:A:LEU:HD11	1:112:A:LEU:HB3	17	0.46
(1,1830)	1:112:A:LEU:HD12	1:112:A:LEU:HB3	19	0.46
(1,1812)	1:50:A:THR:HG21	1:47:A:ALA:HA	2	0.46
(1,1803)	1:10:A:LEU:HD11	1:109:A:LEU:HB2	14	0.46
(1,1795)	1:86:A:LEU:HD23	1:86:A:LEU:HD11	1	0.46
(1,1769)	1:66:A:VAL:HG13	1:68:A:GLU:HB2	6	0.46
(1,1751)	1:65:A:ILE:HD13	1:33:A:ILE:HG22	4	0.46
(1,1499)	1:6:A:VAL:HG23	1:3:A:GLU:HA	17	0.46
(1,1445)	1:48:A:PHE:HB2	1:63:A:LEU:HD11	3	0.46
(1,1420)	1:25:A:LYS:HE2	1:25:A:LYS:HB3	9	0.46
(1,1269)	1:80:A:VAL:HG23	1:73:A:GLU:HG2	16	0.46
(1,1269)	1:80:A:VAL:HG21	1:73:A:GLU:HG2	17	0.46
(1,1263)	1:11:A:ILE:HD11	1:11:A:ILE:HB	8	0.46
(1,1263)	1:11:A:ILE:HD13	1:11:A:ILE:HB	10	0.46
(1,1140)	1:59:A:LYS:HD3	1:59:A:LYS:HA	18	0.46
(1,1093)	1:82:A:LYS:HD3	1:82:A:LYS:HA	8	0.46
(1,996)	1:26:A:ILE:HG12	1:57:A:VAL:HG11	1	0.46
(1,996)	1:26:A:ILE:HG12	1:57:A:VAL:HG13	13	0.46
(1,996)	1:26:A:ILE:HG12	1:57:A:VAL:HG13	19	0.46
(1,962)	1:33:A:ILE:HD11	1:41:A:LYS:HG3	4	0.46
(1,948)	1:45:A:VAL:HG12	1:42:A:SER:HA	11	0.46
(1,923)	1:57:A:VAL:HG21	1:56:A:LEU:HB2	1	0.46
(1,912)	1:13:A:LEU:HD11	1:13:A:LEU:HD13	1	0.46
(1,910)	1:109:A:LEU:HD12	1:13:A:LEU:HD11	9	0.46
(1,906)	1:13:A:LEU:HD22	1:13:A:LEU:HD21	10	0.46
(1,889)	1:57:A:VAL:HG12	1:15:A:GLU:HG3	13	0.46
(1,854)	1:101:A:ILE:HG13	1:70:A:VAL:HG23	15	0.46
(1,826)	1:101:A:ILE:HG21	1:103:A:GLN:HA	11	0.46
(1,825)	1:101:A:ILE:HG22	1:72:A:LEU:HA	15	0.46
(1,805)	1:7:A:VAL:HG23	1:48:A:PHE:HB3	8	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,771)	1:110:A:LEU:HD12	1:66:A:VAL:HG21	4	0.46
(1,769)	1:72:A:LEU:HD21	1:70:A:VAL:HG21	12	0.46
(1,764)	1:70:A:VAL:HG21	1:70:A:VAL:HA	11	0.46
(1,764)	1:70:A:VAL:HG22	1:70:A:VAL:HA	13	0.46
(1,750)	1:72:A:LEU:HD23	1:99:A:VAL:HG13	1	0.46
(1,208)	1:41:A:LYS:HG2	1:42:A:SER:H	6	0.46
(1,208)	1:41:A:LYS:HG2	1:42:A:SER:H	7	0.46
(1,200)	1:12:A:ALA:HB1	1:11:A:ILE:H	8	0.46
(1,200)	1:12:A:ALA:HB3	1:11:A:ILE:H	14	0.46
(1,196)	1:12:A:ALA:HB2	1:14:A:CYS:H	11	0.46
(1,146)	1:6:A:VAL:HG11	1:7:A:VAL:H	3	0.46
(1,146)	1:6:A:VAL:HG11	1:7:A:VAL:H	5	0.46
(1,146)	1:6:A:VAL:HG12	1:7:A:VAL:H	14	0.46
(1,121)	1:70:A:VAL:HG12	1:71:A:GLU:H	13	0.46
(1,88)	1:26:A:ILE:HD13	1:15:A:GLU:H	1	0.46
(1,75)	1:101:A:ILE:HG13	1:102:A:THR:H	17	0.46
(1,74)	1:99:A:VAL:HG22	1:73:A:GLU:H	12	0.46
(1,70)	1:112:A:LEU:HD21	1:17:A:HIS:H	18	0.46
(1,31)	1:33:A:ILE:HG22	1:33:A:ILE:H	7	0.46
(1,23)	1:110:A:LEU:HD12	1:111:A:SER:H	10	0.46
(1,2679)	1:7:A:VAL:HB	1:44:A:PHE:HD1	6	0.45
(1,2676)	1:47:A:ALA:HB2	1:44:A:PHE:HD1	4	0.45
(1,2672)	1:70:A:VAL:HG13	1:88:A:TYR:HD1	12	0.45
(1,2671)	1:115:A:LEU:HD12	1:24:A:HIS:HD2	1	0.45
(1,2669)	1:31:A:VAL:HG22	1:44:A:PHE:HD2	8	0.45
(1,2622)	1:38:A:ALA:HB2	1:1:A:MET:HB2	1	0.45
(1,2612)	1:25:A:LYS:HE3	1:56:A:LEU:HD11	11	0.45
(1,2571)	1:59:A:LYS:HD2	1:56:A:LEU:HA	4	0.45
(1,2571)	1:59:A:LYS:HD2	1:56:A:LEU:HA	10	0.45
(1,2552)	1:81:A:PHE:HB2	1:81:A:PHE:HB3	12	0.45
(1,2552)	1:81:A:PHE:HB2	1:81:A:PHE:HB3	13	0.45
(1,2552)	1:41:A:LYS:HE2	1:41:A:LYS:HE3	18	0.45
(1,2516)	1:19:A:LYS:HD2	1:19:A:LYS:HD3	7	0.45
(1,2516)	1:19:A:LYS:HD2	1:19:A:LYS:HD3	8	0.45
(1,2516)	1:25:A:LYS:HD2	1:25:A:LYS:HD3	14	0.45
(1,2475)	1:18:A:ALA:HB2	1:18:A:ALA:HB1	4	0.45
(1,2475)	1:18:A:ALA:HB1	1:18:A:ALA:HB3	19	0.45
(1,2447)	1:100:A:ILE:HD12	1:100:A:ILE:HD13	1	0.45
(1,2447)	1:101:A:ILE:HD12	1:101:A:ILE:HD11	2	0.45
(1,2447)	1:100:A:ILE:HD11	1:100:A:ILE:HD13	17	0.45
(1,2447)	1:101:A:ILE:HD12	1:101:A:ILE:HD13	18	0.45
(1,2426)	1:25:A:LYS:HD2	1:115:A:LEU:H	2	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2422)	1:47:A:ALA:HB3	1:7:A:VAL:H	4	0.45
(1,2206)	1:83:A:PRO:HB2	1:81:A:PHE:HD2	3	0.45
(1,2202)	1:83:A:PRO:HB3	1:88:A:TYR:HD2	3	0.45
(1,2160)	1:80:A:VAL:HG21	1:81:A:PHE:HD2	19	0.45
(1,2156)	1:93:A:LYS:HB3	1:79:A:HIS:HD2	10	0.45
(1,2143)	1:7:A:VAL:HG23	1:51:A:PHE:HD1	15	0.45
(1,2133)	1:65:A:ILE:HG22	1:44:A:PHE:HD2	16	0.45
(1,2105)	1:64:A:ASP:HA	1:62:A:ILE:HG22	20	0.45
(1,2084)	1:58:A:CYS:HA	1:26:A:ILE:HG23	12	0.45
(1,2079)	1:71:A:GLU:HB2	1:103:A:GLN:HA	2	0.45
(1,2056)	1:15:A:GLU:HG2	1:12:A:ALA:HA	1	0.45
(1,2024)	1:107:A:MET:HE3	1:7:A:VAL:HA	18	0.45
(1,2016)	1:93:A:LYS:HD2	1:79:A:HIS:HB2	18	0.45
(1,1987)	1:23:A:ALA:HB3	1:21:A:ASN:HB2	18	0.45
(1,1887)	1:82:A:LYS:HD2	1:71:A:GLU:HB3	15	0.45
(1,1845)	1:38:A:ALA:HB1	1:39:A:MET:HA	5	0.45
(1,1845)	1:38:A:ALA:HB1	1:39:A:MET:HA	7	0.45
(1,1830)	1:112:A:LEU:HD13	1:112:A:LEU:HB3	6	0.45
(1,1812)	1:50:A:THR:HG21	1:47:A:ALA:HA	17	0.45
(1,1806)	1:10:A:LEU:HD11	1:7:A:VAL:HA	11	0.45
(1,1806)	1:10:A:LEU:HD13	1:7:A:VAL:HA	12	0.45
(1,1803)	1:10:A:LEU:HD12	1:109:A:LEU:HB2	18	0.45
(1,1800)	1:115:A:LEU:HD13	1:25:A:LYS:HG2	10	0.45
(1,1795)	1:86:A:LEU:HD23	1:86:A:LEU:HD12	14	0.45
(1,1795)	1:86:A:LEU:HD23	1:86:A:LEU:HD11	19	0.45
(1,1794)	1:11:A:ILE:HG23	1:12:A:ALA:HB3	4	0.45
(1,1794)	1:11:A:ILE:HG22	1:12:A:ALA:HB1	15	0.45
(1,1794)	1:11:A:ILE:HG23	1:12:A:ALA:HB1	17	0.45
(1,1793)	1:15:A:GLU:HG2	1:11:A:ILE:HG21	3	0.45
(1,1744)	1:90:A:VAL:HG13	1:90:A:VAL:HG22	17	0.45
(1,1744)	1:90:A:VAL:HG12	1:90:A:VAL:HG22	20	0.45
(1,1698)	1:80:A:VAL:HG13	1:73:A:GLU:HA	20	0.45
(1,1677)	1:25:A:LYS:HA	1:57:A:VAL:HG23	7	0.45
(1,1514)	1:43:A:LEU:HD23	1:42:A:SER:HB3	10	0.45
(1,1474)	1:41:A:LYS:HA	1:41:A:LYS:HE2	9	0.45
(1,1420)	1:25:A:LYS:HE2	1:25:A:LYS:HB3	1	0.45
(1,1391)	1:58:A:CYS:HB3	1:55:A:SER:HB3	6	0.45
(1,1269)	1:80:A:VAL:HG22	1:73:A:GLU:HG2	9	0.45
(1,1056)	1:69:A:LYS:HB3	1:69:A:LYS:HD3	10	0.45
(1,1056)	1:69:A:LYS:HB3	1:69:A:LYS:HD3	11	0.45
(1,990)	1:59:A:LYS:HG3	1:59:A:LYS:HE3	12	0.45
(1,964)	1:41:A:LYS:HG3	1:41:A:LYS:HE3	2	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,964)	1:41:A:LYS:HG3	1:41:A:LYS:HE3	17	0.45
(1,906)	1:13:A:LEU:HD21	1:13:A:LEU:HD23	2	0.45
(1,906)	1:13:A:LEU:HD22	1:13:A:LEU:HD23	6	0.45
(1,906)	1:13:A:LEU:HD22	1:13:A:LEU:HD23	12	0.45
(1,898)	1:29:A:VAL:HG12	1:112:A:LEU:HA	9	0.45
(1,891)	1:62:A:ILE:HD11	1:62:A:ILE:HD13	4	0.45
(1,891)	1:62:A:ILE:HD11	1:62:A:ILE:HD13	5	0.45
(1,891)	1:62:A:ILE:HD12	1:62:A:ILE:HD11	10	0.45
(1,891)	1:62:A:ILE:HD12	1:62:A:ILE:HD13	13	0.45
(1,891)	1:62:A:ILE:HD12	1:62:A:ILE:HD13	17	0.45
(1,826)	1:101:A:ILE:HG22	1:103:A:GLN:HA	4	0.45
(1,764)	1:70:A:VAL:HG21	1:70:A:VAL:HA	2	0.45
(1,764)	1:70:A:VAL:HG22	1:70:A:VAL:HA	4	0.45
(1,764)	1:70:A:VAL:HG23	1:70:A:VAL:HA	9	0.45
(1,710)	1:72:A:LEU:HA	1:103:A:GLN:H	16	0.45
(1,415)	1:20:A:LYS:HE2	1:20:A:LYS:H	1	0.45
(1,371)	1:22:A:GLN:HG3	1:21:A:ASN:H	10	0.45
(1,330)	1:68:A:GLU:HG2	1:33:A:ILE:H	5	0.45
(1,239)	1:19:A:LYS:HD3	1:20:A:LYS:H	4	0.45
(1,222)	1:101:A:ILE:HG12	1:101:A:ILE:H	17	0.45
(1,222)	1:101:A:ILE:HG12	1:101:A:ILE:H	19	0.45
(1,213)	1:75:A:LYS:HD3	1:75:A:LYS:H	8	0.45
(1,213)	1:75:A:LYS:HD3	1:75:A:LYS:H	11	0.45
(1,208)	1:41:A:LYS:HG2	1:42:A:SER:H	11	0.45
(1,208)	1:41:A:LYS:HG2	1:42:A:SER:H	19	0.45
(1,197)	1:12:A:ALA:HB3	1:16:A:GLU:H	8	0.45
(1,146)	1:6:A:VAL:HG11	1:7:A:VAL:H	6	0.45
(1,146)	1:6:A:VAL:HG13	1:7:A:VAL:H	16	0.45
(1,138)	1:102:A:THR:HG23	1:103:A:GLN:H	3	0.45
(1,136)	1:102:A:THR:HG23	1:100:A:ILE:H	13	0.45
(1,75)	1:101:A:ILE:HG13	1:102:A:THR:H	8	0.45
(1,74)	1:99:A:VAL:HG21	1:73:A:GLU:H	14	0.45
(1,70)	1:112:A:LEU:HD21	1:17:A:HIS:H	2	0.45
(1,53)	1:66:A:VAL:HG11	1:33:A:ILE:H	17	0.45
(1,31)	1:33:A:ILE:HG22	1:33:A:ILE:H	5	0.45
(1,27)	1:90:A:VAL:HG23	1:89:A:GLY:H	16	0.45
(1,2678)	1:39:A:MET:HE3	1:44:A:PHE:HZ	14	0.44
(1,2671)	1:115:A:LEU:HD11	1:24:A:HIS:HD2	2	0.44
(1,2650)	1:66:A:VAL:HG11	1:32:A:GLY:HA3	7	0.44
(1,2618)	1:6:A:VAL:HG21	1:2:A:HIS:HB2	16	0.44
(1,2555)	1:115:A:LEU:HD11	1:25:A:LYS:HE2	17	0.44
(1,2552)	1:81:A:PHE:HB2	1:81:A:PHE:HB3	1	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2552)	1:41:A:LYS:HE2	1:41:A:LYS:HE3	7	0.44
(1,2474)	1:18:A:ALA:HB2	1:19:A:LYS:HA	6	0.44
(1,2454)	1:62:A:ILE:HG21	1:28:A:ARG:HG3	4	0.44
(1,2427)	1:107:A:MET:HE2	1:107:A:MET:H	2	0.44
(1,2427)	1:107:A:MET:HE3	1:107:A:MET:H	7	0.44
(1,2422)	1:47:A:ALA:HB2	1:7:A:VAL:H	3	0.44
(1,2419)	1:69:A:LYS:HG3	1:69:A:LYS:H	16	0.44
(1,2239)	1:41:A:LYS:HA	1:44:A:PHE:HD1	11	0.44
(1,2225)	1:36:A:ARG:HD2	1:88:A:TYR:HD1	8	0.44
(1,2180)	1:61:A:ALA:HB3	1:48:A:PHE:HD2	11	0.44
(1,2160)	1:80:A:VAL:HG21	1:81:A:PHE:HD2	10	0.44
(1,2157)	1:43:A:LEU:HD23	1:4:A:TYR:HE2	20	0.44
(1,2084)	1:58:A:CYS:HA	1:26:A:ILE:HG23	16	0.44
(1,2079)	1:71:A:GLU:HB2	1:103:A:GLN:HA	8	0.44
(1,2040)	1:90:A:VAL:HG23	1:92:A:GLU:HA	20	0.44
(1,2016)	1:93:A:LYS:HD2	1:79:A:HIS:HB2	19	0.44
(1,1987)	1:23:A:ALA:HB2	1:21:A:ASN:HB2	3	0.44
(1,1984)	1:7:A:VAL:HG12	1:48:A:PHE:HB3	4	0.44
(1,1975)	1:12:A:ALA:HB2	1:15:A:GLU:HB2	15	0.44
(1,1933)	1:38:A:ALA:HB3	1:1:A:MET:HB2	12	0.44
(1,1831)	1:58:A:CYS:HB2	1:61:A:ALA:HB2	16	0.44
(1,1829)	1:26:A:ILE:HD11	1:23:A:ALA:HB2	6	0.44
(1,1806)	1:10:A:LEU:HD12	1:7:A:VAL:HA	15	0.44
(1,1800)	1:115:A:LEU:HD12	1:25:A:LYS:HG2	15	0.44
(1,1800)	1:115:A:LEU:HD11	1:25:A:LYS:HG2	17	0.44
(1,1795)	1:86:A:LEU:HD21	1:86:A:LEU:HD13	4	0.44
(1,1795)	1:86:A:LEU:HD22	1:86:A:LEU:HD12	16	0.44
(1,1795)	1:86:A:LEU:HD23	1:86:A:LEU:HD11	20	0.44
(1,1794)	1:11:A:ILE:HG23	1:12:A:ALA:HB2	10	0.44
(1,1753)	1:65:A:ILE:HD11	1:41:A:LYS:HD3	1	0.44
(1,1748)	1:33:A:ILE:HG22	1:107:A:MET:HG3	18	0.44
(1,1744)	1:90:A:VAL:HG11	1:90:A:VAL:HG22	16	0.44
(1,1708)	1:107:A:MET:HA	1:33:A:ILE:HD11	14	0.44
(1,1482)	1:7:A:VAL:HG21	1:48:A:PHE:HA	18	0.44
(1,1420)	1:25:A:LYS:HE2	1:25:A:LYS:HB3	16	0.44
(1,1412)	1:20:A:LYS:HE2	1:16:A:GLU:HG3	1	0.44
(1,1391)	1:58:A:CYS:HB3	1:55:A:SER:HB3	2	0.44
(1,1093)	1:82:A:LYS:HD3	1:82:A:LYS:HA	20	0.44
(1,1056)	1:69:A:LYS:HB3	1:69:A:LYS:HD3	17	0.44
(1,1020)	1:85:A:ALA:HB2	1:86:A:LEU:HA	12	0.44
(1,1006)	1:100:A:ILE:HD11	1:75:A:LYS:HG3	6	0.44
(1,964)	1:41:A:LYS:HG3	1:41:A:LYS:HE3	15	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,948)	1:45:A:VAL:HG13	1:42:A:SER:HA	10	0.44
(1,910)	1:109:A:LEU:HD12	1:13:A:LEU:HD13	15	0.44
(1,906)	1:13:A:LEU:HD22	1:13:A:LEU:HD23	3	0.44
(1,905)	1:80:A:VAL:HG22	1:80:A:VAL:HG21	8	0.44
(1,905)	1:80:A:VAL:HG21	1:80:A:VAL:HG23	9	0.44
(1,905)	1:80:A:VAL:HG22	1:80:A:VAL:HG23	10	0.44
(1,905)	1:80:A:VAL:HG21	1:80:A:VAL:HG23	13	0.44
(1,905)	1:80:A:VAL:HG22	1:80:A:VAL:HG21	14	0.44
(1,905)	1:80:A:VAL:HG22	1:80:A:VAL:HG23	16	0.44
(1,905)	1:80:A:VAL:HG21	1:80:A:VAL:HG23	18	0.44
(1,905)	1:80:A:VAL:HG21	1:80:A:VAL:HG23	19	0.44
(1,897)	1:29:A:VAL:HG12	1:112:A:LEU:HD23	12	0.44
(1,891)	1:62:A:ILE:HD12	1:62:A:ILE:HD13	14	0.44
(1,891)	1:62:A:ILE:HD12	1:62:A:ILE:HD13	16	0.44
(1,891)	1:62:A:ILE:HD12	1:62:A:ILE:HD13	20	0.44
(1,805)	1:7:A:VAL:HG22	1:48:A:PHE:HB3	6	0.44
(1,771)	1:110:A:LEU:HD13	1:66:A:VAL:HG22	19	0.44
(1,764)	1:70:A:VAL:HG21	1:70:A:VAL:HA	15	0.44
(1,371)	1:22:A:GLN:HG3	1:21:A:ASN:H	13	0.44
(1,371)	1:22:A:GLN:HG3	1:21:A:ASN:H	14	0.44
(1,239)	1:19:A:LYS:HD2	1:20:A:LYS:H	15	0.44
(1,222)	1:101:A:ILE:HG12	1:101:A:ILE:H	11	0.44
(1,222)	1:101:A:ILE:HG12	1:101:A:ILE:H	13	0.44
(1,222)	1:101:A:ILE:HG12	1:101:A:ILE:H	16	0.44
(1,213)	1:75:A:LYS:HD3	1:75:A:LYS:H	1	0.44
(1,200)	1:12:A:ALA:HB3	1:11:A:ILE:H	15	0.44
(1,200)	1:12:A:ALA:HB2	1:11:A:ILE:H	17	0.44
(1,197)	1:12:A:ALA:HB1	1:16:A:GLU:H	1	0.44
(1,197)	1:12:A:ALA:HB1	1:16:A:GLU:H	12	0.44
(1,197)	1:12:A:ALA:HB3	1:16:A:GLU:H	19	0.44
(1,182)	1:18:A:ALA:HB2	1:20:A:LYS:H	14	0.44
(1,182)	1:18:A:ALA:HB1	1:20:A:LYS:H	17	0.44
(1,146)	1:6:A:VAL:HG11	1:7:A:VAL:H	4	0.44
(1,146)	1:6:A:VAL:HG13	1:7:A:VAL:H	17	0.44
(1,146)	1:6:A:VAL:HG13	1:7:A:VAL:H	20	0.44
(1,120)	1:13:A:LEU:HD11	1:13:A:LEU:H	18	0.44
(1,116)	1:13:A:LEU:HD22	1:14:A:CYS:H	17	0.44
(1,113)	1:10:A:LEU:HD11	1:10:A:LEU:H	12	0.44
(1,113)	1:10:A:LEU:HD12	1:10:A:LEU:H	16	0.44
(1,75)	1:101:A:ILE:HG13	1:102:A:THR:H	13	0.44
(1,74)	1:99:A:VAL:HG22	1:73:A:GLU:H	10	0.44
(1,39)	1:90:A:VAL:HG13	1:90:A:VAL:H	16	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,37)	1:99:A:VAL:HG13	1:99:A:VAL:H	6	0.44
(1,31)	1:33:A:ILE:HG23	1:33:A:ILE:H	2	0.44
(1,31)	1:33:A:ILE:HG21	1:33:A:ILE:H	4	0.44
(1,2672)	1:70:A:VAL:HG13	1:88:A:TYR:HD1	4	0.43
(1,2552)	1:81:A:PHE:HB2	1:81:A:PHE:HB3	3	0.43
(1,2552)	1:81:A:PHE:HB2	1:81:A:PHE:HB3	4	0.43
(1,2552)	1:41:A:LYS:HE2	1:41:A:LYS:HE3	6	0.43
(1,2552)	1:81:A:PHE:HB2	1:81:A:PHE:HB3	8	0.43
(1,2552)	1:81:A:PHE:HB2	1:81:A:PHE:HB3	10	0.43
(1,2552)	1:81:A:PHE:HB2	1:81:A:PHE:HB3	11	0.43
(1,2552)	1:41:A:LYS:HE2	1:41:A:LYS:HE3	14	0.43
(1,2552)	1:41:A:LYS:HE2	1:41:A:LYS:HE3	15	0.43
(1,2552)	1:81:A:PHE:HB2	1:81:A:PHE:HB3	16	0.43
(1,2552)	1:81:A:PHE:HB2	1:81:A:PHE:HB3	19	0.43
(1,2447)	1:100:A:ILE:HD12	1:100:A:ILE:HD11	8	0.43
(1,2447)	1:100:A:ILE:HD12	1:100:A:ILE:HD13	20	0.43
(1,2422)	1:47:A:ALA:HB3	1:7:A:VAL:H	15	0.43
(1,2419)	1:69:A:LYS:HG3	1:69:A:LYS:H	19	0.43
(1,2246)	1:4:A:TYR:HA	1:4:A:TYR:HE1	12	0.43
(1,2166)	1:50:A:THR:HG21	1:51:A:PHE:HE1	13	0.43
(1,2143)	1:7:A:VAL:HG23	1:51:A:PHE:HD1	3	0.43
(1,2143)	1:7:A:VAL:HG21	1:51:A:PHE:HD1	7	0.43
(1,2105)	1:64:A:ASP:HA	1:62:A:ILE:HG21	17	0.43
(1,2070)	1:109:A:LEU:HD22	1:29:A:VAL:HA	7	0.43
(1,2056)	1:15:A:GLU:HG2	1:12:A:ALA:HA	6	0.43
(1,1994)	1:3:A:GLU:HG2	1:40:A:ASP:HB2	13	0.43
(1,1987)	1:23:A:ALA:HB2	1:21:A:ASN:HB2	7	0.43
(1,1987)	1:23:A:ALA:HB1	1:21:A:ASN:HB2	8	0.43
(1,1984)	1:7:A:VAL:HG12	1:48:A:PHE:HB3	18	0.43
(1,1982)	1:106:A:GLU:HG2	1:105:A:ASN:HB3	2	0.43
(1,1931)	1:65:A:ILE:HD11	1:41:A:LYS:HB2	9	0.43
(1,1889)	1:82:A:LYS:HD3	1:71:A:GLU:HG3	8	0.43
(1,1887)	1:82:A:LYS:HD2	1:71:A:GLU:HB3	7	0.43
(1,1842)	1:18:A:ALA:HB1	1:21:A:ASN:HB3	18	0.43
(1,1805)	1:10:A:LEU:HD12	1:63:A:LEU:HD23	2	0.43
(1,1800)	1:115:A:LEU:HD12	1:25:A:LYS:HG2	18	0.43
(1,1800)	1:115:A:LEU:HD12	1:25:A:LYS:HG2	19	0.43
(1,1794)	1:11:A:ILE:HG23	1:12:A:ALA:HB3	11	0.43
(1,1794)	1:11:A:ILE:HG21	1:12:A:ALA:HB1	13	0.43
(1,1793)	1:15:A:GLU:HG2	1:11:A:ILE:HG21	14	0.43
(1,1793)	1:15:A:GLU:HG2	1:11:A:ILE:HG22	20	0.43
(1,1780)	1:112:A:LEU:HD21	1:17:A:HIS:HA	17	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1769)	1:66:A:VAL:HG13	1:68:A:GLU:HB2	2	0.43
(1,1748)	1:33:A:ILE:HG23	1:107:A:MET:HG3	12	0.43
(1,1618)	1:50:A:THR:HG21	1:51:A:PHE:HA	13	0.43
(1,1490)	1:6:A:VAL:HA	1:9:A:SER:HB3	5	0.43
(1,1420)	1:25:A:LYS:HE3	1:25:A:LYS:HB2	8	0.43
(1,1420)	1:25:A:LYS:HE2	1:25:A:LYS:HB3	17	0.43
(1,1311)	1:36:A:ARG:HB2	1:36:A:ARG:HD2	19	0.43
(1,1269)	1:80:A:VAL:HG21	1:73:A:GLU:HG2	4	0.43
(1,1269)	1:80:A:VAL:HG22	1:73:A:GLU:HG2	6	0.43
(1,1197)	1:80:A:VAL:HG12	1:71:A:GLU:HG3	20	0.43
(1,1143)	1:115:A:LEU:HD12	1:25:A:LYS:HD2	7	0.43
(1,1056)	1:69:A:LYS:HB3	1:69:A:LYS:HD2	4	0.43
(1,1056)	1:69:A:LYS:HB3	1:69:A:LYS:HD3	8	0.43
(1,1056)	1:69:A:LYS:HB3	1:69:A:LYS:HD3	18	0.43
(1,1024)	1:57:A:VAL:HG12	1:18:A:ALA:HB1	2	0.43
(1,1024)	1:57:A:VAL:HG11	1:18:A:ALA:HB2	20	0.43
(1,964)	1:41:A:LYS:HG3	1:41:A:LYS:HE3	11	0.43
(1,964)	1:41:A:LYS:HG3	1:41:A:LYS:HE3	20	0.43
(1,953)	1:65:A:ILE:HG21	1:33:A:ILE:HG12	14	0.43
(1,948)	1:45:A:VAL:HG13	1:42:A:SER:HA	7	0.43
(1,948)	1:45:A:VAL:HG13	1:42:A:SER:HA	17	0.43
(1,923)	1:57:A:VAL:HG23	1:56:A:LEU:HB2	3	0.43
(1,923)	1:57:A:VAL:HG21	1:56:A:LEU:HB2	12	0.43
(1,906)	1:13:A:LEU:HD22	1:13:A:LEU:HD21	1	0.43
(1,906)	1:13:A:LEU:HD21	1:13:A:LEU:HD23	4	0.43
(1,906)	1:13:A:LEU:HD21	1:13:A:LEU:HD23	14	0.43
(1,906)	1:13:A:LEU:HD22	1:13:A:LEU:HD23	15	0.43
(1,906)	1:13:A:LEU:HD22	1:13:A:LEU:HD23	16	0.43
(1,906)	1:13:A:LEU:HD22	1:13:A:LEU:HD21	18	0.43
(1,906)	1:13:A:LEU:HD21	1:13:A:LEU:HD23	20	0.43
(1,905)	1:80:A:VAL:HG22	1:80:A:VAL:HG21	1	0.43
(1,905)	1:80:A:VAL:HG22	1:80:A:VAL:HG23	2	0.43
(1,905)	1:80:A:VAL:HG22	1:80:A:VAL:HG23	3	0.43
(1,905)	1:80:A:VAL:HG21	1:80:A:VAL:HG23	7	0.43
(1,905)	1:80:A:VAL:HG22	1:80:A:VAL:HG23	11	0.43
(1,905)	1:80:A:VAL:HG21	1:80:A:VAL:HG23	15	0.43
(1,891)	1:62:A:ILE:HD11	1:62:A:ILE:HD13	1	0.43
(1,891)	1:62:A:ILE:HD11	1:62:A:ILE:HD13	6	0.43
(1,891)	1:62:A:ILE:HD12	1:62:A:ILE:HD13	18	0.43
(1,891)	1:62:A:ILE:HD12	1:62:A:ILE:HD11	19	0.43
(1,875)	1:86:A:LEU:HD21	1:85:A:ALA:HA	11	0.43
(1,875)	1:86:A:LEU:HD22	1:85:A:ALA:HA	12	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,834)	1:72:A:LEU:HD23	1:101:A:ILE:HG21	16	0.43
(1,821)	1:30:A:VAL:HG12	1:28:A:ARG:HG3	8	0.43
(1,781)	1:99:A:VAL:HG12	1:99:A:VAL:HG11	9	0.43
(1,763)	1:70:A:VAL:HG23	1:72:A:LEU:HG	13	0.43
(1,222)	1:101:A:ILE:HG12	1:101:A:ILE:H	6	0.43
(1,222)	1:101:A:ILE:HG12	1:101:A:ILE:H	15	0.43
(1,213)	1:75:A:LYS:HD3	1:75:A:LYS:H	13	0.43
(1,200)	1:12:A:ALA:HB2	1:11:A:ILE:H	16	0.43
(1,185)	1:38:A:ALA:HB1	1:39:A:MET:H	3	0.43
(1,182)	1:18:A:ALA:HB1	1:20:A:LYS:H	4	0.43
(1,182)	1:18:A:ALA:HB2	1:20:A:LYS:H	8	0.43
(1,146)	1:6:A:VAL:HG12	1:7:A:VAL:H	1	0.43
(1,146)	1:6:A:VAL:HG13	1:7:A:VAL:H	15	0.43
(1,135)	1:100:A:ILE:HG13	1:100:A:ILE:H	1	0.43
(1,126)	1:45:A:VAL:HG22	1:47:A:ALA:H	9	0.43
(1,121)	1:70:A:VAL:HG12	1:71:A:GLU:H	1	0.43
(1,121)	1:70:A:VAL:HG13	1:71:A:GLU:H	19	0.43
(1,113)	1:10:A:LEU:HD12	1:10:A:LEU:H	8	0.43
(1,113)	1:10:A:LEU:HD12	1:10:A:LEU:H	10	0.43
(1,113)	1:10:A:LEU:HD11	1:10:A:LEU:H	13	0.43
(1,113)	1:10:A:LEU:HD11	1:10:A:LEU:H	20	0.43
(1,103)	1:43:A:LEU:HD21	1:46:A:SER:H	14	0.43
(1,94)	1:93:A:LYS:HB3	1:94:A:CYS:H	18	0.43
(1,84)	1:99:A:VAL:HG23	1:91:A:CYS:H	1	0.43
(1,75)	1:101:A:ILE:HG13	1:102:A:THR:H	5	0.43
(1,75)	1:101:A:ILE:HG13	1:102:A:THR:H	18	0.43
(1,74)	1:99:A:VAL:HG22	1:73:A:GLU:H	9	0.43
(1,70)	1:112:A:LEU:HD21	1:17:A:HIS:H	13	0.43
(1,34)	1:33:A:ILE:HG22	1:39:A:MET:H	3	0.43
(1,31)	1:33:A:ILE:HG22	1:33:A:ILE:H	1	0.43
(1,31)	1:33:A:ILE:HG23	1:33:A:ILE:H	14	0.43
(1,31)	1:33:A:ILE:HG23	1:33:A:ILE:H	16	0.43
(1,2678)	1:39:A:MET:HE1	1:44:A:PHE:HZ	10	0.42
(1,2652)	1:45:A:VAL:HA	1:47:A:ALA:HB3	12	0.42
(1,2650)	1:66:A:VAL:HG12	1:32:A:GLY:HA3	9	0.42
(1,2650)	1:66:A:VAL:HG12	1:32:A:GLY:HA3	14	0.42
(1,2597)	1:72:A:LEU:HB2	1:99:A:VAL:HG21	6	0.42
(1,2590)	1:33:A:ILE:HD13	1:39:A:MET:HG2	13	0.42
(1,2552)	1:81:A:PHE:HB2	1:81:A:PHE:HB3	2	0.42
(1,2552)	1:81:A:PHE:HB2	1:81:A:PHE:HB3	5	0.42
(1,2552)	1:81:A:PHE:HB2	1:81:A:PHE:HB3	17	0.42
(1,2438)	1:65:A:ILE:HD13	1:41:A:LYS:HD2	5	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2426)	1:97:A:LYS:HD3	1:97:A:LYS:H	13	0.42
(1,2419)	1:69:A:LYS:HG3	1:69:A:LYS:H	3	0.42
(1,2419)	1:69:A:LYS:HG3	1:69:A:LYS:H	6	0.42
(1,2419)	1:69:A:LYS:HG3	1:69:A:LYS:H	8	0.42
(1,2262)	1:88:A:TYR:HA	1:88:A:TYR:HD1	1	0.42
(1,2246)	1:4:A:TYR:HA	1:4:A:TYR:HE1	9	0.42
(1,2246)	1:4:A:TYR:HA	1:4:A:TYR:HE1	15	0.42
(1,2239)	1:41:A:LYS:HA	1:44:A:PHE:HD2	9	0.42
(1,2172)	1:47:A:ALA:HB1	1:4:A:TYR:HD1	5	0.42
(1,2171)	1:47:A:ALA:HB1	1:4:A:TYR:HE1	11	0.42
(1,2143)	1:7:A:VAL:HG21	1:51:A:PHE:HD1	9	0.42
(1,2084)	1:58:A:CYS:HA	1:26:A:ILE:HG21	9	0.42
(1,2079)	1:71:A:GLU:HB2	1:103:A:GLN:HA	7	0.42
(1,2079)	1:71:A:GLU:HB2	1:103:A:GLN:HA	18	0.42
(1,2069)	1:112:A:LEU:HD23	1:29:A:VAL:HA	8	0.42
(1,2069)	1:112:A:LEU:HD23	1:29:A:VAL:HA	10	0.42
(1,2067)	1:10:A:LEU:HA	1:13:A:LEU:HG	16	0.42
(1,2058)	1:12:A:ALA:HB3	1:13:A:LEU:HA	17	0.42
(1,2056)	1:15:A:GLU:HG2	1:12:A:ALA:HA	18	0.42
(1,2035)	1:42:A:SER:HB2	1:45:A:VAL:HG23	2	0.42
(1,1962)	1:97:A:LYS:HB2	1:90:A:VAL:HG13	1	0.42
(1,1888)	1:85:A:ALA:HB3	1:86:A:LEU:HG	16	0.42
(1,1887)	1:82:A:LYS:HD2	1:71:A:GLU:HB3	3	0.42
(1,1845)	1:38:A:ALA:HB3	1:39:A:MET:HA	11	0.42
(1,1830)	1:112:A:LEU:HD13	1:112:A:LEU:HB3	8	0.42
(1,1830)	1:112:A:LEU:HD12	1:112:A:LEU:HB3	12	0.42
(1,1830)	1:112:A:LEU:HD11	1:112:A:LEU:HB3	20	0.42
(1,1820)	1:10:A:LEU:HD21	1:6:A:VAL:HG13	10	0.42
(1,1819)	1:7:A:VAL:HG12	1:47:A:ALA:HB2	3	0.42
(1,1806)	1:10:A:LEU:HD11	1:7:A:VAL:HA	7	0.42
(1,1793)	1:15:A:GLU:HG2	1:11:A:ILE:HG22	5	0.42
(1,1793)	1:15:A:GLU:HG2	1:11:A:ILE:HG22	6	0.42
(1,1793)	1:15:A:GLU:HG2	1:11:A:ILE:HG22	15	0.42
(1,1774)	1:31:A:VAL:HG22	1:107:A:MET:HG2	4	0.42
(1,1769)	1:66:A:VAL:HG11	1:68:A:GLU:HB3	7	0.42
(1,1744)	1:90:A:VAL:HG11	1:90:A:VAL:HG23	7	0.42
(1,1708)	1:107:A:MET:HA	1:33:A:ILE:HD12	12	0.42
(1,1688)	1:97:A:LYS:HA	1:99:A:VAL:HG21	18	0.42
(1,1545)	1:114:A:MET:HE2	1:18:A:ALA:HA	2	0.42
(1,1482)	1:7:A:VAL:HG23	1:48:A:PHE:HA	8	0.42
(1,1474)	1:41:A:LYS:HA	1:41:A:LYS:HE2	1	0.42
(1,1474)	1:41:A:LYS:HA	1:41:A:LYS:HE2	3	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1452)	1:63:A:LEU:HD13	1:45:A:VAL:HA	8	0.42
(1,1420)	1:25:A:LYS:HE3	1:25:A:LYS:HB2	4	0.42
(1,1420)	1:25:A:LYS:HE2	1:25:A:LYS:HB3	13	0.42
(1,1269)	1:80:A:VAL:HG21	1:73:A:GLU:HG2	3	0.42
(1,1263)	1:11:A:ILE:HD12	1:11:A:ILE:HB	16	0.42
(1,1249)	1:72:A:LEU:HD13	1:83:A:PRO:HG2	12	0.42
(1,1249)	1:72:A:LEU:HD13	1:83:A:PRO:HG2	20	0.42
(1,1056)	1:69:A:LYS:HB3	1:69:A:LYS:HD2	3	0.42
(1,998)	1:65:A:ILE:HG12	1:63:A:LEU:HD23	17	0.42
(1,996)	1:26:A:ILE:HG12	1:57:A:VAL:HG13	20	0.42
(1,964)	1:41:A:LYS:HG3	1:41:A:LYS:HE3	18	0.42
(1,964)	1:41:A:LYS:HG3	1:41:A:LYS:HE3	19	0.42
(1,963)	1:41:A:LYS:HG3	1:65:A:ILE:HD13	3	0.42
(1,948)	1:45:A:VAL:HG13	1:42:A:SER:HA	14	0.42
(1,948)	1:45:A:VAL:HG13	1:42:A:SER:HA	15	0.42
(1,945)	1:109:A:LEU:HD22	1:109:A:LEU:HB2	15	0.42
(1,923)	1:57:A:VAL:HG23	1:56:A:LEU:HB2	2	0.42
(1,906)	1:13:A:LEU:HD21	1:13:A:LEU:HD23	7	0.42
(1,906)	1:13:A:LEU:HD22	1:13:A:LEU:HD23	9	0.42
(1,906)	1:13:A:LEU:HD22	1:13:A:LEU:HD23	17	0.42
(1,906)	1:13:A:LEU:HD21	1:13:A:LEU:HD23	19	0.42
(1,905)	1:80:A:VAL:HG22	1:80:A:VAL:HG23	5	0.42
(1,905)	1:80:A:VAL:HG22	1:80:A:VAL:HG21	6	0.42
(1,905)	1:80:A:VAL:HG21	1:80:A:VAL:HG23	17	0.42
(1,891)	1:62:A:ILE:HD11	1:62:A:ILE:HD13	9	0.42
(1,891)	1:62:A:ILE:HD12	1:62:A:ILE:HD11	12	0.42
(1,891)	1:62:A:ILE:HD12	1:62:A:ILE:HD11	15	0.42
(1,846)	1:31:A:VAL:HG12	1:10:A:LEU:HD22	6	0.42
(1,781)	1:99:A:VAL:HG11	1:99:A:VAL:HG13	19	0.42
(1,781)	1:99:A:VAL:HG11	1:99:A:VAL:HG13	20	0.42
(1,770)	1:72:A:LEU:HD13	1:70:A:VAL:HG21	14	0.42
(1,689)	1:97:A:LYS:HA	1:99:A:VAL:H	17	0.42
(1,449)	1:79:A:HIS:HB2	1:79:A:HIS:H	17	0.42
(1,239)	1:19:A:LYS:HD2	1:20:A:LYS:H	10	0.42
(1,222)	1:101:A:ILE:HG12	1:101:A:ILE:H	7	0.42
(1,213)	1:75:A:LYS:HD3	1:75:A:LYS:H	2	0.42
(1,213)	1:75:A:LYS:HD3	1:75:A:LYS:H	3	0.42
(1,208)	1:41:A:LYS:HG2	1:42:A:SER:H	5	0.42
(1,200)	1:12:A:ALA:HB2	1:11:A:ILE:H	20	0.42
(1,197)	1:12:A:ALA:HB2	1:16:A:GLU:H	13	0.42
(1,182)	1:18:A:ALA:HB2	1:20:A:LYS:H	6	0.42
(1,182)	1:18:A:ALA:HB2	1:20:A:LYS:H	18	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,146)	1:6:A:VAL:HG13	1:7:A:VAL:H	10	0.42
(1,138)	1:102:A:THR:HG23	1:103:A:GLN:H	13	0.42
(1,136)	1:102:A:THR:HG21	1:100:A:ILE:H	7	0.42
(1,126)	1:45:A:VAL:HG23	1:47:A:ALA:H	7	0.42
(1,103)	1:43:A:LEU:HD22	1:46:A:SER:H	13	0.42
(1,101)	1:57:A:VAL:HG11	1:15:A:GLU:H	9	0.42
(1,75)	1:101:A:ILE:HG13	1:102:A:THR:H	6	0.42
(1,36)	1:99:A:VAL:HG11	1:100:A:ILE:H	8	0.42
(1,31)	1:33:A:ILE:HG21	1:33:A:ILE:H	6	0.42
(1,31)	1:33:A:ILE:HG21	1:33:A:ILE:H	10	0.42
(1,27)	1:90:A:VAL:HG21	1:89:A:GLY:H	14	0.42
(1,23)	1:110:A:LEU:HD11	1:111:A:SER:H	3	0.42
(1,2679)	1:7:A:VAL:HB	1:44:A:PHE:HD2	15	0.41
(1,2670)	1:11:A:ILE:HG21	1:51:A:PHE:HD2	2	0.41
(1,2661)	1:75:A:LYS:HA	1:75:A:LYS:HE3	10	0.41
(1,2647)	1:82:A:LYS:HE2	1:82:A:LYS:HB3	20	0.41
(1,2645)	1:33:A:ILE:HG23	1:39:A:MET:HG3	17	0.41
(1,2474)	1:18:A:ALA:HB1	1:19:A:LYS:HA	10	0.41
(1,2474)	1:18:A:ALA:HB1	1:19:A:LYS:HA	11	0.41
(1,2474)	1:18:A:ALA:HB2	1:19:A:LYS:HA	18	0.41
(1,2455)	1:57:A:VAL:HG12	1:57:A:VAL:HG11	7	0.41
(1,2455)	1:29:A:VAL:HG11	1:29:A:VAL:HG13	12	0.41
(1,2455)	1:57:A:VAL:HG12	1:57:A:VAL:HG11	13	0.41
(1,2455)	1:57:A:VAL:HG12	1:57:A:VAL:HG13	20	0.41
(1,2454)	1:62:A:ILE:HG21	1:28:A:ARG:HG3	18	0.41
(1,2447)	1:100:A:ILE:HD12	1:100:A:ILE:HD11	15	0.41
(1,2438)	1:65:A:ILE:HD12	1:41:A:LYS:HD2	11	0.41
(1,2270)	1:79:A:HIS:HD2	1:81:A:PHE:HD1	18	0.41
(1,2246)	1:4:A:TYR:HA	1:4:A:TYR:HE1	17	0.41
(1,2166)	1:50:A:THR:HG22	1:51:A:PHE:HE1	16	0.41
(1,2160)	1:80:A:VAL:HG23	1:81:A:PHE:HD2	5	0.41
(1,2158)	1:29:A:VAL:HG11	1:48:A:PHE:HZ	1	0.41
(1,2143)	1:7:A:VAL:HG23	1:51:A:PHE:HD1	17	0.41
(1,2095)	1:25:A:LYS:HA	1:25:A:LYS:HD2	8	0.41
(1,2088)	1:105:A:ASN:HA	1:36:A:ARG:HB3	3	0.41
(1,2079)	1:71:A:GLU:HB2	1:103:A:GLN:HA	17	0.41
(1,2070)	1:109:A:LEU:HD23	1:29:A:VAL:HA	12	0.41
(1,2061)	1:33:A:ILE:HA	1:65:A:ILE:HG21	19	0.41
(1,2056)	1:15:A:GLU:HG2	1:12:A:ALA:HA	8	0.41
(1,2056)	1:15:A:GLU:HG2	1:12:A:ALA:HA	20	0.41
(1,2051)	1:114:A:MET:HE2	1:17:A:HIS:HA	9	0.41
(1,2040)	1:90:A:VAL:HG21	1:92:A:GLU:HA	7	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2024)	1:107:A:MET:HE2	1:7:A:VAL:HA	12	0.41
(1,1987)	1:23:A:ALA:HB1	1:21:A:ASN:HB2	2	0.41
(1,1987)	1:23:A:ALA:HB1	1:21:A:ASN:HB2	9	0.41
(1,1975)	1:12:A:ALA:HB1	1:15:A:GLU:HB2	12	0.41
(1,1939)	1:39:A:MET:HE2	1:39:A:MET:HA	13	0.41
(1,1933)	1:38:A:ALA:HB3	1:1:A:MET:HB2	19	0.41
(1,1845)	1:38:A:ALA:HB3	1:39:A:MET:HA	9	0.41
(1,1830)	1:112:A:LEU:HD12	1:112:A:LEU:HB3	7	0.41
(1,1824)	1:25:A:LYS:HG3	1:56:A:LEU:HD11	5	0.41
(1,1812)	1:50:A:THR:HG21	1:47:A:ALA:HA	5	0.41
(1,1798)	1:62:A:ILE:HD13	1:28:A:ARG:HD3	5	0.41
(1,1793)	1:15:A:GLU:HG2	1:11:A:ILE:HG23	16	0.41
(1,1791)	1:62:A:ILE:HG22	1:64:A:ASP:HB3	9	0.41
(1,1771)	1:31:A:VAL:HG23	1:65:A:ILE:HB	17	0.41
(1,1761)	1:110:A:LEU:HD23	1:108:A:ARG:HD2	13	0.41
(1,1732)	1:72:A:LEU:HD11	1:89:A:GLY:HA3	14	0.41
(1,1708)	1:107:A:MET:HA	1:33:A:ILE:HD13	4	0.41
(1,1477)	1:45:A:VAL:HG13	1:41:A:LYS:HA	5	0.41
(1,1474)	1:41:A:LYS:HA	1:41:A:LYS:HE2	11	0.41
(1,1474)	1:41:A:LYS:HA	1:41:A:LYS:HE2	16	0.41
(1,1302)	1:1:A:MET:HE3	1:1:A:MET:HA	11	0.41
(1,1269)	1:80:A:VAL:HG22	1:73:A:GLU:HG2	18	0.41
(1,1263)	1:11:A:ILE:HD13	1:11:A:ILE:HB	19	0.41
(1,1197)	1:80:A:VAL:HG13	1:71:A:GLU:HG3	6	0.41
(1,1159)	1:108:A:ARG:HB2	1:110:A:LEU:HD23	13	0.41
(1,1145)	1:41:A:LYS:HD2	1:33:A:ILE:HG22	8	0.41
(1,1140)	1:59:A:LYS:HD3	1:59:A:LYS:HA	5	0.41
(1,1140)	1:59:A:LYS:HD3	1:59:A:LYS:HA	14	0.41
(1,1140)	1:59:A:LYS:HD3	1:59:A:LYS:HA	16	0.41
(1,1059)	1:12:A:ALA:HB2	1:12:A:ALA:HB1	8	0.41
(1,1059)	1:12:A:ALA:HB2	1:12:A:ALA:HB1	12	0.41
(1,1056)	1:69:A:LYS:HB3	1:69:A:LYS:HD2	16	0.41
(1,1010)	1:115:A:LEU:HB3	1:25:A:LYS:HB3	3	0.41
(1,998)	1:65:A:ILE:HG12	1:63:A:LEU:HD23	4	0.41
(1,963)	1:41:A:LYS:HG3	1:65:A:ILE:HD13	8	0.41
(1,953)	1:65:A:ILE:HG23	1:33:A:ILE:HG12	16	0.41
(1,948)	1:45:A:VAL:HG12	1:42:A:SER:HA	12	0.41
(1,945)	1:109:A:LEU:HD21	1:109:A:LEU:HB2	4	0.41
(1,945)	1:109:A:LEU:HD23	1:109:A:LEU:HB2	9	0.41
(1,945)	1:109:A:LEU:HD21	1:109:A:LEU:HB2	11	0.41
(1,907)	1:13:A:LEU:HD22	1:13:A:LEU:HD11	10	0.41
(1,906)	1:13:A:LEU:HD22	1:13:A:LEU:HD23	8	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,906)	1:13:A:LEU:HD22	1:13:A:LEU:HD21	13	0.41
(1,905)	1:80:A:VAL:HG21	1:80:A:VAL:HG23	4	0.41
(1,905)	1:80:A:VAL:HG22	1:80:A:VAL:HG23	12	0.41
(1,905)	1:80:A:VAL:HG22	1:80:A:VAL:HG23	20	0.41
(1,904)	1:31:A:VAL:HG12	1:10:A:LEU:HD11	3	0.41
(1,898)	1:29:A:VAL:HG13	1:112:A:LEU:HA	4	0.41
(1,898)	1:29:A:VAL:HG12	1:112:A:LEU:HA	16	0.41
(1,891)	1:62:A:ILE:HD12	1:62:A:ILE:HD11	2	0.41
(1,891)	1:62:A:ILE:HD12	1:62:A:ILE:HD13	7	0.41
(1,875)	1:86:A:LEU:HD23	1:85:A:ALA:HA	7	0.41
(1,874)	1:26:A:ILE:HG21	1:61:A:ALA:HB3	3	0.41
(1,864)	1:110:A:LEU:HD13	1:30:A:VAL:HG22	6	0.41
(1,849)	1:72:A:LEU:HD23	1:101:A:ILE:HG13	5	0.41
(1,826)	1:101:A:ILE:HG22	1:103:A:GLN:HA	7	0.41
(1,813)	1:29:A:VAL:HG23	1:10:A:LEU:HD13	4	0.41
(1,809)	1:110:A:LEU:HD13	1:66:A:VAL:HG11	14	0.41
(1,781)	1:99:A:VAL:HG11	1:99:A:VAL:HG13	6	0.41
(1,781)	1:99:A:VAL:HG12	1:99:A:VAL:HG13	11	0.41
(1,746)	1:72:A:LEU:HD12	1:83:A:PRO:HB2	15	0.41
(1,689)	1:97:A:LYS:HA	1:99:A:VAL:H	19	0.41
(1,371)	1:22:A:GLN:HG3	1:21:A:ASN:H	2	0.41
(1,300)	1:107:A:MET:HE1	1:108:A:ARG:H	13	0.41
(1,239)	1:19:A:LYS:HD2	1:20:A:LYS:H	11	0.41
(1,222)	1:101:A:ILE:HG12	1:101:A:ILE:H	4	0.41
(1,222)	1:101:A:ILE:HG12	1:101:A:ILE:H	5	0.41
(1,182)	1:18:A:ALA:HB1	1:20:A:LYS:H	13	0.41
(1,146)	1:6:A:VAL:HG12	1:7:A:VAL:H	7	0.41
(1,138)	1:102:A:THR:HG23	1:103:A:GLN:H	17	0.41
(1,116)	1:13:A:LEU:HD23	1:14:A:CYS:H	10	0.41
(1,116)	1:13:A:LEU:HD23	1:14:A:CYS:H	20	0.41
(1,113)	1:10:A:LEU:HD11	1:10:A:LEU:H	2	0.41
(1,103)	1:43:A:LEU:HD23	1:46:A:SER:H	17	0.41
(1,101)	1:57:A:VAL:HG13	1:15:A:GLU:H	4	0.41
(1,94)	1:93:A:LYS:HB3	1:94:A:CYS:H	12	0.41
(1,75)	1:101:A:ILE:HG13	1:102:A:THR:H	2	0.41
(1,75)	1:101:A:ILE:HG13	1:102:A:THR:H	12	0.41
(1,74)	1:99:A:VAL:HG23	1:73:A:GLU:H	4	0.41
(1,72)	1:31:A:VAL:HG11	1:108:A:ARG:H	18	0.41
(1,36)	1:99:A:VAL:HG13	1:100:A:ILE:H	16	0.41
(1,23)	1:110:A:LEU:HD13	1:111:A:SER:H	12	0.41
(1,2679)	1:7:A:VAL:HB	1:44:A:PHE:HD2	10	0.4
(1,2670)	1:11:A:ILE:HG22	1:51:A:PHE:HD2	17	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2661)	1:75:A:LYS:HA	1:75:A:LYS:HE3	17	0.4
(1,2638)	1:107:A:MET:HA	1:39:A:MET:HE1	10	0.4
(1,2612)	1:25:A:LYS:HE3	1:56:A:LEU:HD11	19	0.4
(1,2571)	1:59:A:LYS:HD2	1:56:A:LEU:HA	17	0.4
(1,2555)	1:115:A:LEU:HD13	1:25:A:LYS:HE3	5	0.4
(1,2555)	1:25:A:LYS:HE3	1:56:A:LEU:HD11	11	0.4
(1,2552)	1:81:A:PHE:HB2	1:81:A:PHE:HB3	9	0.4
(1,2455)	1:29:A:VAL:HG11	1:29:A:VAL:HG13	10	0.4
(1,2455)	1:29:A:VAL:HG12	1:29:A:VAL:HG13	15	0.4
(1,2455)	1:57:A:VAL:HG12	1:57:A:VAL:HG13	19	0.4
(1,2438)	1:65:A:ILE:HD13	1:41:A:LYS:HD2	17	0.4
(1,2433)	1:63:A:LEU:HD22	1:31:A:VAL:HG21	20	0.4
(1,2422)	1:47:A:ALA:HB2	1:7:A:VAL:H	17	0.4
(1,2422)	1:47:A:ALA:HB1	1:7:A:VAL:H	20	0.4
(1,2246)	1:4:A:TYR:HA	1:4:A:TYR:HE1	4	0.4
(1,2246)	1:4:A:TYR:HA	1:4:A:TYR:HE2	14	0.4
(1,2246)	1:4:A:TYR:HA	1:4:A:TYR:HE2	16	0.4
(1,2245)	1:14:A:CYS:HA	1:17:A:HIS:HD2	15	0.4
(1,2193)	1:25:A:LYS:HB3	1:24:A:HIS:HD2	5	0.4
(1,2160)	1:80:A:VAL:HG23	1:81:A:PHE:HD2	11	0.4
(1,2156)	1:93:A:LYS:HB3	1:79:A:HIS:HD2	7	0.4
(1,2095)	1:25:A:LYS:HA	1:25:A:LYS:HD2	4	0.4
(1,2084)	1:58:A:CYS:HA	1:26:A:ILE:HG21	17	0.4
(1,2079)	1:71:A:GLU:HB2	1:103:A:GLN:HA	4	0.4
(1,2079)	1:71:A:GLU:HB2	1:103:A:GLN:HA	14	0.4
(1,2070)	1:109:A:LEU:HD21	1:29:A:VAL:HA	1	0.4
(1,2058)	1:12:A:ALA:HB1	1:13:A:LEU:HA	8	0.4
(1,2030)	1:83:A:PRO:HD2	1:72:A:LEU:HD12	20	0.4
(1,1987)	1:23:A:ALA:HB3	1:21:A:ASN:HB2	16	0.4
(1,1975)	1:12:A:ALA:HB2	1:15:A:GLU:HB2	14	0.4
(1,1939)	1:39:A:MET:HE1	1:39:A:MET:HA	12	0.4
(1,1830)	1:112:A:LEU:HD12	1:112:A:LEU:HB3	11	0.4
(1,1819)	1:7:A:VAL:HG11	1:47:A:ALA:HB1	20	0.4
(1,1812)	1:50:A:THR:HG23	1:47:A:ALA:HA	20	0.4
(1,1795)	1:86:A:LEU:HD23	1:86:A:LEU:HD12	11	0.4
(1,1794)	1:11:A:ILE:HG22	1:12:A:ALA:HB2	19	0.4
(1,1782)	1:109:A:LEU:HD21	1:107:A:MET:HE2	15	0.4
(1,1744)	1:90:A:VAL:HG12	1:90:A:VAL:HG21	6	0.4
(1,1744)	1:90:A:VAL:HG13	1:90:A:VAL:HG22	18	0.4
(1,1601)	1:12:A:ALA:HB1	1:9:A:SER:HA	2	0.4
(1,1499)	1:6:A:VAL:HG22	1:3:A:GLU:HA	15	0.4
(1,1474)	1:41:A:LYS:HA	1:41:A:LYS:HE2	19	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1420)	1:25:A:LYS:HE3	1:25:A:LYS:HB2	12	0.4
(1,1385)	1:48:A:PHE:HB3	1:63:A:LEU:HD13	11	0.4
(1,1217)	1:72:A:LEU:HD12	1:99:A:VAL:HB	4	0.4
(1,1059)	1:12:A:ALA:HB2	1:12:A:ALA:HB1	5	0.4
(1,1059)	1:12:A:ALA:HB2	1:12:A:ALA:HB3	10	0.4
(1,1059)	1:12:A:ALA:HB2	1:12:A:ALA:HB3	11	0.4
(1,1059)	1:12:A:ALA:HB2	1:12:A:ALA:HB3	14	0.4
(1,1059)	1:12:A:ALA:HB2	1:12:A:ALA:HB1	15	0.4
(1,1056)	1:69:A:LYS:HB3	1:69:A:LYS:HD2	13	0.4
(1,1056)	1:69:A:LYS:HB3	1:69:A:LYS:HD3	14	0.4
(1,998)	1:65:A:ILE:HG12	1:63:A:LEU:HD21	5	0.4
(1,964)	1:41:A:LYS:HG3	1:41:A:LYS:HE3	1	0.4
(1,964)	1:41:A:LYS:HG3	1:41:A:LYS:HE3	13	0.4
(1,948)	1:45:A:VAL:HG12	1:42:A:SER:HA	3	0.4
(1,948)	1:45:A:VAL:HG11	1:42:A:SER:HA	13	0.4
(1,945)	1:109:A:LEU:HD22	1:109:A:LEU:HB2	2	0.4
(1,945)	1:109:A:LEU:HD22	1:109:A:LEU:HB2	3	0.4
(1,907)	1:13:A:LEU:HD21	1:13:A:LEU:HD11	12	0.4
(1,906)	1:13:A:LEU:HD22	1:13:A:LEU:HD23	5	0.4
(1,904)	1:31:A:VAL:HG12	1:10:A:LEU:HD12	17	0.4
(1,897)	1:29:A:VAL:HG13	1:112:A:LEU:HD21	13	0.4
(1,891)	1:62:A:ILE:HD11	1:62:A:ILE:HD13	3	0.4
(1,891)	1:62:A:ILE:HD12	1:62:A:ILE:HD11	8	0.4
(1,891)	1:62:A:ILE:HD12	1:62:A:ILE:HD11	11	0.4
(1,887)	1:57:A:VAL:HG11	1:18:A:ALA:HA	20	0.4
(1,875)	1:86:A:LEU:HD22	1:85:A:ALA:HA	4	0.4
(1,875)	1:86:A:LEU:HD22	1:85:A:ALA:HA	8	0.4
(1,875)	1:86:A:LEU:HD22	1:85:A:ALA:HA	17	0.4
(1,864)	1:110:A:LEU:HD12	1:30:A:VAL:HG21	5	0.4
(1,809)	1:110:A:LEU:HD13	1:66:A:VAL:HG13	1	0.4
(1,781)	1:99:A:VAL:HG12	1:99:A:VAL:HG13	2	0.4
(1,781)	1:99:A:VAL:HG12	1:99:A:VAL:HG11	5	0.4
(1,781)	1:99:A:VAL:HG12	1:99:A:VAL:HG11	7	0.4
(1,781)	1:99:A:VAL:HG12	1:99:A:VAL:HG13	13	0.4
(1,781)	1:99:A:VAL:HG12	1:99:A:VAL:HG11	15	0.4
(1,770)	1:72:A:LEU:HD12	1:70:A:VAL:HG21	10	0.4
(1,764)	1:70:A:VAL:HG22	1:70:A:VAL:HA	6	0.4
(1,449)	1:79:A:HIS:HB2	1:79:A:HIS:H	7	0.4
(1,371)	1:22:A:GLN:HG3	1:21:A:ASN:H	18	0.4
(1,300)	1:107:A:MET:HE1	1:108:A:ARG:H	4	0.4
(1,222)	1:101:A:ILE:HG12	1:101:A:ILE:H	18	0.4
(1,196)	1:12:A:ALA:HB3	1:14:A:CYS:H	9	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,182)	1:18:A:ALA:HB3	1:20:A:LYS:H	19	0.4
(1,174)	1:100:A:ILE:HG12	1:101:A:ILE:H	4	0.4
(1,162)	1:23:A:ALA:HB1	1:22:A:GLN:H	5	0.4
(1,146)	1:6:A:VAL:HG11	1:7:A:VAL:H	13	0.4
(1,146)	1:6:A:VAL:HG12	1:7:A:VAL:H	19	0.4
(1,138)	1:102:A:THR:HG21	1:103:A:GLN:H	16	0.4
(1,136)	1:102:A:THR:HG21	1:100:A:ILE:H	4	0.4
(1,121)	1:70:A:VAL:HG13	1:71:A:GLU:H	3	0.4
(1,118)	1:13:A:LEU:HD13	1:16:A:GLU:H	9	0.4
(1,116)	1:13:A:LEU:HD23	1:14:A:CYS:H	8	0.4
(1,112)	1:10:A:LEU:HD11	1:11:A:ILE:H	1	0.4
(1,112)	1:10:A:LEU:HD13	1:11:A:ILE:H	9	0.4
(1,101)	1:57:A:VAL:HG11	1:15:A:GLU:H	12	0.4
(1,75)	1:101:A:ILE:HG13	1:102:A:THR:H	16	0.4
(1,75)	1:101:A:ILE:HG13	1:102:A:THR:H	20	0.4
(1,74)	1:99:A:VAL:HG22	1:73:A:GLU:H	7	0.4
(1,37)	1:99:A:VAL:HG11	1:99:A:VAL:H	10	0.4
(1,36)	1:99:A:VAL:HG12	1:100:A:ILE:H	18	0.4
(1,31)	1:33:A:ILE:HG21	1:33:A:ILE:H	12	0.4
(1,23)	1:110:A:LEU:HD13	1:111:A:SER:H	6	0.4
(1,7)	1:72:A:LEU:HD11	1:73:A:GLU:H	2	0.4
(1,2693)	1:48:A:PHE:HD1	1:44:A:PHE:HZ	15	0.39
(1,2679)	1:7:A:VAL:HB	1:48:A:PHE:HD1	16	0.39
(1,2676)	1:47:A:ALA:HB3	1:44:A:PHE:HD1	5	0.39
(1,2671)	1:115:A:LEU:HD11	1:24:A:HIS:HD2	20	0.39
(1,2643)	1:39:A:MET:HE3	1:106:A:GLU:HG2	15	0.39
(1,2455)	1:29:A:VAL:HG12	1:29:A:VAL:HG11	3	0.39
(1,2455)	1:29:A:VAL:HG12	1:29:A:VAL:HG13	4	0.39
(1,2455)	1:57:A:VAL:HG12	1:57:A:VAL:HG11	9	0.39
(1,2455)	1:57:A:VAL:HG11	1:57:A:VAL:HG13	11	0.39
(1,2455)	1:57:A:VAL:HG12	1:57:A:VAL:HG11	14	0.39
(1,2454)	1:62:A:ILE:HG23	1:28:A:ARG:HG3	8	0.39
(1,2454)	1:62:A:ILE:HG23	1:28:A:ARG:HG3	13	0.39
(1,2444)	1:80:A:VAL:HG13	1:73:A:GLU:HA	20	0.39
(1,2433)	1:63:A:LEU:HD21	1:31:A:VAL:HG23	6	0.39
(1,2433)	1:63:A:LEU:HD22	1:31:A:VAL:HG22	7	0.39
(1,2427)	1:107:A:MET:HE1	1:107:A:MET:H	5	0.39
(1,2427)	1:107:A:MET:HE3	1:107:A:MET:H	15	0.39
(1,2419)	1:69:A:LYS:HG3	1:69:A:LYS:H	7	0.39
(1,2419)	1:69:A:LYS:HG3	1:69:A:LYS:H	15	0.39
(1,2262)	1:88:A:TYR:HA	1:88:A:TYR:HD2	19	0.39
(1,2204)	1:83:A:PRO:HB3	1:88:A:TYR:HE1	17	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2158)	1:29:A:VAL:HG11	1:48:A:PHE:HZ	9	0.39
(1,2079)	1:71:A:GLU:HB2	1:103:A:GLN:HA	12	0.39
(1,2024)	1:107:A:MET:HE3	1:7:A:VAL:HA	1	0.39
(1,2024)	1:107:A:MET:HE2	1:7:A:VAL:HA	14	0.39
(1,1987)	1:23:A:ALA:HB3	1:21:A:ASN:HB2	1	0.39
(1,1975)	1:12:A:ALA:HB2	1:15:A:GLU:HB2	6	0.39
(1,1931)	1:65:A:ILE:HD12	1:41:A:LYS:HB2	7	0.39
(1,1854)	1:75:A:LYS:HG2	1:100:A:ILE:HG13	7	0.39
(1,1842)	1:18:A:ALA:HB3	1:21:A:ASN:HB3	2	0.39
(1,1830)	1:112:A:LEU:HD13	1:112:A:LEU:HB3	2	0.39
(1,1819)	1:7:A:VAL:HG13	1:47:A:ALA:HB2	12	0.39
(1,1800)	1:115:A:LEU:HD13	1:25:A:LYS:HG2	16	0.39
(1,1795)	1:86:A:LEU:HD21	1:86:A:LEU:HD11	17	0.39
(1,1777)	1:112:A:LEU:HD22	1:109:A:LEU:HD12	20	0.39
(1,1774)	1:31:A:VAL:HG22	1:107:A:MET:HG2	2	0.39
(1,1749)	1:65:A:ILE:HG13	1:63:A:LEU:HD21	10	0.39
(1,1744)	1:90:A:VAL:HG11	1:90:A:VAL:HG21	10	0.39
(1,1744)	1:90:A:VAL:HG12	1:90:A:VAL:HG21	15	0.39
(1,1727)	1:11:A:ILE:HD13	1:55:A:SER:HB3	12	0.39
(1,1698)	1:80:A:VAL:HG12	1:73:A:GLU:HA	14	0.39
(1,1618)	1:50:A:THR:HG23	1:51:A:PHE:HA	6	0.39
(1,1601)	1:12:A:ALA:HB2	1:9:A:SER:HA	11	0.39
(1,1514)	1:43:A:LEU:HD23	1:42:A:SER:HB3	17	0.39
(1,1474)	1:41:A:LYS:HA	1:41:A:LYS:HE2	18	0.39
(1,1361)	1:26:A:ILE:HD11	1:114:A:MET:HG2	20	0.39
(1,1269)	1:80:A:VAL:HG22	1:73:A:GLU:HG2	8	0.39
(1,1211)	1:75:A:LYS:HB3	1:98:A:ASN:HB2	4	0.39
(1,1211)	1:75:A:LYS:HB3	1:98:A:ASN:HB2	16	0.39
(1,1140)	1:59:A:LYS:HD3	1:59:A:LYS:HA	3	0.39
(1,1059)	1:12:A:ALA:HB2	1:12:A:ALA:HB1	1	0.39
(1,1059)	1:12:A:ALA:HB2	1:12:A:ALA:HB1	4	0.39
(1,1059)	1:12:A:ALA:HB2	1:12:A:ALA:HB1	7	0.39
(1,1059)	1:12:A:ALA:HB2	1:12:A:ALA:HB1	17	0.39
(1,1059)	1:12:A:ALA:HB2	1:12:A:ALA:HB3	18	0.39
(1,1059)	1:12:A:ALA:HB2	1:12:A:ALA:HB3	20	0.39
(1,1056)	1:69:A:LYS:HB3	1:69:A:LYS:HD3	6	0.39
(1,1056)	1:69:A:LYS:HB3	1:69:A:LYS:HD3	7	0.39
(1,964)	1:41:A:LYS:HG3	1:41:A:LYS:HE3	4	0.39
(1,964)	1:41:A:LYS:HG3	1:41:A:LYS:HE3	14	0.39
(1,964)	1:41:A:LYS:HG3	1:41:A:LYS:HE3	16	0.39
(1,963)	1:41:A:LYS:HG3	1:65:A:ILE:HD11	13	0.39
(1,953)	1:65:A:ILE:HG22	1:33:A:ILE:HG12	12	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,953)	1:65:A:ILE:HG23	1:33:A:ILE:HG12	15	0.39
(1,948)	1:45:A:VAL:HG12	1:42:A:SER:HA	16	0.39
(1,945)	1:109:A:LEU:HD21	1:109:A:LEU:HB2	17	0.39
(1,944)	1:6:A:VAL:HG12	1:6:A:VAL:HG13	13	0.39
(1,911)	1:56:A:LEU:HD12	1:56:A:LEU:HA	9	0.39
(1,911)	1:56:A:LEU:HD13	1:56:A:LEU:HA	14	0.39
(1,907)	1:13:A:LEU:HD21	1:13:A:LEU:HD11	4	0.39
(1,907)	1:13:A:LEU:HD22	1:13:A:LEU:HD11	9	0.39
(1,906)	1:13:A:LEU:HD21	1:13:A:LEU:HD23	11	0.39
(1,898)	1:29:A:VAL:HG13	1:112:A:LEU:HA	1	0.39
(1,898)	1:29:A:VAL:HG12	1:112:A:LEU:HA	14	0.39
(1,897)	1:29:A:VAL:HG13	1:112:A:LEU:HD22	10	0.39
(1,889)	1:57:A:VAL:HG11	1:15:A:GLU:HG3	19	0.39
(1,886)	1:57:A:VAL:HG12	1:57:A:VAL:HG21	6	0.39
(1,886)	1:57:A:VAL:HG12	1:57:A:VAL:HG22	16	0.39
(1,875)	1:86:A:LEU:HD22	1:85:A:ALA:HA	6	0.39
(1,875)	1:86:A:LEU:HD23	1:85:A:ALA:HA	10	0.39
(1,869)	1:26:A:ILE:HD11	1:61:A:ALA:HB3	5	0.39
(1,864)	1:110:A:LEU:HD12	1:30:A:VAL:HG23	13	0.39
(1,826)	1:101:A:ILE:HG21	1:103:A:GLN:HA	9	0.39
(1,809)	1:110:A:LEU:HD11	1:66:A:VAL:HG13	12	0.39
(1,781)	1:99:A:VAL:HG12	1:99:A:VAL:HG13	1	0.39
(1,781)	1:99:A:VAL:HG12	1:99:A:VAL:HG13	3	0.39
(1,781)	1:99:A:VAL:HG11	1:99:A:VAL:HG13	4	0.39
(1,781)	1:99:A:VAL:HG11	1:99:A:VAL:HG13	8	0.39
(1,781)	1:99:A:VAL:HG12	1:99:A:VAL:HG13	10	0.39
(1,781)	1:99:A:VAL:HG11	1:99:A:VAL:HG13	12	0.39
(1,781)	1:99:A:VAL:HG11	1:99:A:VAL:HG13	17	0.39
(1,449)	1:79:A:HIS:HB2	1:79:A:HIS:H	20	0.39
(1,371)	1:22:A:GLN:HG3	1:21:A:ASN:H	20	0.39
(1,300)	1:107:A:MET:HE2	1:108:A:ARG:H	15	0.39
(1,239)	1:19:A:LYS:HD2	1:20:A:LYS:H	19	0.39
(1,222)	1:101:A:ILE:HG12	1:101:A:ILE:H	3	0.39
(1,222)	1:101:A:ILE:HG12	1:101:A:ILE:H	20	0.39
(1,213)	1:75:A:LYS:HD3	1:75:A:LYS:H	16	0.39
(1,213)	1:75:A:LYS:HD3	1:75:A:LYS:H	19	0.39
(1,196)	1:12:A:ALA:HB1	1:14:A:CYS:H	19	0.39
(1,182)	1:18:A:ALA:HB1	1:20:A:LYS:H	10	0.39
(1,162)	1:23:A:ALA:HB1	1:22:A:GLN:H	4	0.39
(1,146)	1:6:A:VAL:HG12	1:7:A:VAL:H	2	0.39
(1,118)	1:13:A:LEU:HD12	1:16:A:GLU:H	12	0.39
(1,112)	1:10:A:LEU:HD11	1:11:A:ILE:H	18	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,103)	1:43:A:LEU:HD21	1:46:A:SER:H	3	0.39
(1,103)	1:43:A:LEU:HD23	1:46:A:SER:H	4	0.39
(1,75)	1:101:A:ILE:HG13	1:102:A:THR:H	3	0.39
(1,75)	1:101:A:ILE:HG13	1:102:A:THR:H	9	0.39
(1,53)	1:66:A:VAL:HG13	1:33:A:ILE:H	19	0.39
(1,53)	1:66:A:VAL:HG13	1:33:A:ILE:H	20	0.39
(1,39)	1:90:A:VAL:HG12	1:90:A:VAL:H	11	0.39
(1,34)	1:33:A:ILE:HG21	1:39:A:MET:H	1	0.39
(1,31)	1:33:A:ILE:HG23	1:33:A:ILE:H	13	0.39
(1,31)	1:33:A:ILE:HG21	1:33:A:ILE:H	18	0.39
(1,2693)	1:48:A:PHE:HD1	1:44:A:PHE:HZ	18	0.38
(1,2678)	1:39:A:MET:HE1	1:44:A:PHE:HZ	2	0.38
(1,2671)	1:115:A:LEU:HD12	1:24:A:HIS:HD2	15	0.38
(1,2455)	1:29:A:VAL:HG12	1:29:A:VAL:HG13	2	0.38
(1,2455)	1:29:A:VAL:HG12	1:29:A:VAL:HG11	5	0.38
(1,2455)	1:29:A:VAL:HG12	1:29:A:VAL:HG11	8	0.38
(1,2455)	1:57:A:VAL:HG12	1:57:A:VAL:HG13	17	0.38
(1,2455)	1:29:A:VAL:HG11	1:29:A:VAL:HG13	18	0.38
(1,2454)	1:62:A:ILE:HG23	1:28:A:ARG:HG3	6	0.38
(1,2448)	1:26:A:ILE:HD11	1:26:A:ILE:HD13	6	0.38
(1,2427)	1:107:A:MET:HE1	1:107:A:MET:H	16	0.38
(1,2426)	1:97:A:LYS:HD3	1:97:A:LYS:H	1	0.38
(1,2426)	1:97:A:LYS:HD3	1:97:A:LYS:H	16	0.38
(1,2419)	1:69:A:LYS:HG3	1:69:A:LYS:H	4	0.38
(1,2246)	1:4:A:TYR:HA	1:4:A:TYR:HE1	7	0.38
(1,2239)	1:41:A:LYS:HA	1:44:A:PHE:HD2	13	0.38
(1,2239)	1:41:A:LYS:HA	1:44:A:PHE:HD2	18	0.38
(1,2202)	1:83:A:PRO:HB3	1:88:A:TYR:HD1	13	0.38
(1,2192)	1:92:A:GLU:HB2	1:95:A:HIS:HD2	10	0.38
(1,2183)	1:116:A:ALA:HB2	1:24:A:HIS:HD2	5	0.38
(1,2160)	1:80:A:VAL:HG21	1:81:A:PHE:HD1	17	0.38
(1,2148)	1:80:A:VAL:HG12	1:81:A:PHE:HD2	9	0.38
(1,2142)	1:7:A:VAL:HG23	1:48:A:PHE:HD1	10	0.38
(1,2069)	1:112:A:LEU:HD22	1:29:A:VAL:HA	14	0.38
(1,2060)	1:35:A:GLU:HA	1:33:A:ILE:HG21	8	0.38
(1,2056)	1:15:A:GLU:HG2	1:12:A:ALA:HA	13	0.38
(1,2035)	1:42:A:SER:HB2	1:45:A:VAL:HG23	20	0.38
(1,2023)	1:7:A:VAL:HA	1:11:A:ILE:HD13	8	0.38
(1,1994)	1:3:A:GLU:HG2	1:40:A:ASP:HB2	7	0.38
(1,1984)	1:7:A:VAL:HG11	1:48:A:PHE:HB3	13	0.38
(1,1975)	1:12:A:ALA:HB3	1:15:A:GLU:HB2	8	0.38
(1,1960)	1:113:A:GLU:HG3	1:27:A:GLU:HB3	12	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1960)	1:113:A:GLU:HG3	1:27:A:GLU:HB3	18	0.38
(1,1939)	1:39:A:MET:HE1	1:39:A:MET:HA	1	0.38
(1,1939)	1:39:A:MET:HE3	1:39:A:MET:HA	20	0.38
(1,1907)	1:25:A:LYS:HB2	1:57:A:VAL:HG11	3	0.38
(1,1854)	1:75:A:LYS:HG2	1:100:A:ILE:HG13	2	0.38
(1,1830)	1:112:A:LEU:HD11	1:112:A:LEU:HB3	10	0.38
(1,1830)	1:112:A:LEU:HD13	1:112:A:LEU:HB3	14	0.38
(1,1830)	1:112:A:LEU:HD12	1:112:A:LEU:HB3	16	0.38
(1,1824)	1:25:A:LYS:HG3	1:56:A:LEU:HD13	15	0.38
(1,1819)	1:7:A:VAL:HG11	1:47:A:ALA:HB1	6	0.38
(1,1819)	1:7:A:VAL:HG12	1:47:A:ALA:HB3	11	0.38
(1,1806)	1:10:A:LEU:HD11	1:7:A:VAL:HA	17	0.38
(1,1795)	1:86:A:LEU:HD22	1:86:A:LEU:HD13	9	0.38
(1,1780)	1:112:A:LEU:HD21	1:17:A:HIS:HA	9	0.38
(1,1744)	1:90:A:VAL:HG12	1:90:A:VAL:HG22	13	0.38
(1,1731)	1:72:A:LEU:HD12	1:91:A:CYS:HA	17	0.38
(1,1708)	1:107:A:MET:HA	1:33:A:ILE:HD11	9	0.38
(1,1618)	1:50:A:THR:HG22	1:51:A:PHE:HA	20	0.38
(1,1601)	1:12:A:ALA:HB2	1:9:A:SER:HA	4	0.38
(1,1474)	1:41:A:LYS:HA	1:41:A:LYS:HE2	8	0.38
(1,1385)	1:48:A:PHE:HB3	1:63:A:LEU:HD13	1	0.38
(1,1093)	1:82:A:LYS:HD3	1:82:A:LYS:HA	18	0.38
(1,1059)	1:12:A:ALA:HB2	1:12:A:ALA:HB1	2	0.38
(1,1059)	1:12:A:ALA:HB2	1:12:A:ALA:HB3	3	0.38
(1,1059)	1:12:A:ALA:HB2	1:12:A:ALA:HB1	6	0.38
(1,1059)	1:12:A:ALA:HB2	1:12:A:ALA:HB1	9	0.38
(1,1059)	1:12:A:ALA:HB2	1:12:A:ALA:HB1	19	0.38
(1,1056)	1:69:A:LYS:HB3	1:69:A:LYS:HD3	1	0.38
(1,1056)	1:69:A:LYS:HB3	1:69:A:LYS:HD3	9	0.38
(1,1010)	1:115:A:LEU:HB3	1:25:A:LYS:HB3	6	0.38
(1,998)	1:65:A:ILE:HG12	1:63:A:LEU:HD23	15	0.38
(1,964)	1:41:A:LYS:HG3	1:41:A:LYS:HE3	7	0.38
(1,948)	1:45:A:VAL:HG11	1:42:A:SER:HA	9	0.38
(1,944)	1:6:A:VAL:HG21	1:6:A:VAL:HG23	10	0.38
(1,944)	1:6:A:VAL:HG22	1:6:A:VAL:HG21	11	0.38
(1,944)	1:6:A:VAL:HG11	1:6:A:VAL:HG13	12	0.38
(1,933)	1:102:A:THR:HG21	1:100:A:ILE:HG13	1	0.38
(1,914)	1:72:A:LEU:HD22	1:70:A:VAL:HG13	4	0.38
(1,886)	1:57:A:VAL:HG12	1:57:A:VAL:HG22	2	0.38
(1,886)	1:57:A:VAL:HG11	1:57:A:VAL:HG22	20	0.38
(1,869)	1:26:A:ILE:HD13	1:61:A:ALA:HB2	8	0.38
(1,864)	1:110:A:LEU:HD13	1:30:A:VAL:HG22	19	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,826)	1:101:A:ILE:HG23	1:103:A:GLN:HA	16	0.38
(1,809)	1:110:A:LEU:HD12	1:66:A:VAL:HG12	8	0.38
(1,781)	1:99:A:VAL:HG11	1:99:A:VAL:HG13	14	0.38
(1,781)	1:99:A:VAL:HG11	1:99:A:VAL:HG13	16	0.38
(1,781)	1:99:A:VAL:HG11	1:99:A:VAL:HG13	18	0.38
(1,449)	1:79:A:HIS:HB2	1:79:A:HIS:H	10	0.38
(1,371)	1:22:A:GLN:HG3	1:21:A:ASN:H	9	0.38
(1,300)	1:107:A:MET:HE2	1:108:A:ARG:H	18	0.38
(1,239)	1:19:A:LYS:HD3	1:20:A:LYS:H	12	0.38
(1,222)	1:101:A:ILE:HG12	1:101:A:ILE:H	2	0.38
(1,222)	1:101:A:ILE:HG12	1:101:A:ILE:H	8	0.38
(1,213)	1:75:A:LYS:HD3	1:75:A:LYS:H	4	0.38
(1,213)	1:75:A:LYS:HD3	1:75:A:LYS:H	5	0.38
(1,182)	1:18:A:ALA:HB2	1:20:A:LYS:H	16	0.38
(1,182)	1:18:A:ALA:HB1	1:20:A:LYS:H	20	0.38
(1,141)	1:93:A:LYS:HD3	1:93:A:LYS:H	18	0.38
(1,134)	1:57:A:VAL:HG21	1:58:A:CYS:H	8	0.38
(1,126)	1:45:A:VAL:HG22	1:47:A:ALA:H	13	0.38
(1,112)	1:10:A:LEU:HD12	1:11:A:ILE:H	4	0.38
(1,105)	1:29:A:VAL:HG12	1:29:A:VAL:H	6	0.38
(1,105)	1:29:A:VAL:HG13	1:29:A:VAL:H	12	0.38
(1,105)	1:29:A:VAL:HG11	1:29:A:VAL:H	16	0.38
(1,105)	1:29:A:VAL:HG13	1:29:A:VAL:H	19	0.38
(1,96)	1:11:A:ILE:HG23	1:15:A:GLU:H	11	0.38
(1,75)	1:101:A:ILE:HG13	1:102:A:THR:H	7	0.38
(1,75)	1:101:A:ILE:HG13	1:102:A:THR:H	11	0.38
(1,75)	1:101:A:ILE:HG13	1:102:A:THR:H	19	0.38
(1,74)	1:99:A:VAL:HG23	1:73:A:GLU:H	3	0.38
(1,74)	1:99:A:VAL:HG22	1:73:A:GLU:H	17	0.38
(1,36)	1:99:A:VAL:HG11	1:100:A:ILE:H	15	0.38
(1,36)	1:99:A:VAL:HG11	1:100:A:ILE:H	17	0.38
(1,31)	1:33:A:ILE:HG21	1:33:A:ILE:H	8	0.38
(1,31)	1:33:A:ILE:HG22	1:33:A:ILE:H	11	0.38
(1,31)	1:33:A:ILE:HG21	1:33:A:ILE:H	17	0.38
(1,23)	1:110:A:LEU:HD12	1:111:A:SER:H	9	0.38
(1,2671)	1:115:A:LEU:HD11	1:24:A:HIS:HD2	18	0.37
(1,2652)	1:45:A:VAL:HA	1:47:A:ALA:HB3	5	0.37
(1,2650)	1:66:A:VAL:HG11	1:32:A:GLY:HA3	11	0.37
(1,2650)	1:66:A:VAL:HG12	1:32:A:GLY:HA3	18	0.37
(1,2645)	1:33:A:ILE:HG21	1:39:A:MET:HG3	15	0.37
(1,2638)	1:107:A:MET:HA	1:39:A:MET:HE3	14	0.37
(1,2618)	1:6:A:VAL:HG21	1:2:A:HIS:HB2	11	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2597)	1:72:A:LEU:HB2	1:99:A:VAL:HG23	19	0.37
(1,2576)	1:91:A:CYS:HA	1:72:A:LEU:HD23	13	0.37
(1,2474)	1:18:A:ALA:HB1	1:19:A:LYS:HA	7	0.37
(1,2454)	1:62:A:ILE:HG23	1:28:A:ARG:HG3	1	0.37
(1,2448)	1:26:A:ILE:HD12	1:26:A:ILE:HD11	5	0.37
(1,2448)	1:100:A:ILE:HD11	1:100:A:ILE:HD13	9	0.37
(1,2448)	1:101:A:ILE:HD12	1:101:A:ILE:HD13	10	0.37
(1,2448)	1:101:A:ILE:HD11	1:101:A:ILE:HD13	16	0.37
(1,2440)	1:30:A:VAL:HG12	1:30:A:VAL:HG11	2	0.37
(1,2440)	1:30:A:VAL:HG11	1:30:A:VAL:HG13	3	0.37
(1,2440)	1:90:A:VAL:HG11	1:90:A:VAL:HG13	19	0.37
(1,2438)	1:65:A:ILE:HD11	1:41:A:LYS:HD2	13	0.37
(1,2426)	1:97:A:LYS:HD3	1:97:A:LYS:H	7	0.37
(1,2422)	1:47:A:ALA:HB1	1:7:A:VAL:H	9	0.37
(1,2246)	1:4:A:TYR:HA	1:4:A:TYR:HE1	8	0.37
(1,2202)	1:83:A:PRO:HB3	1:88:A:TYR:HD1	12	0.37
(1,2192)	1:92:A:GLU:HB2	1:95:A:HIS:HD2	6	0.37
(1,2172)	1:47:A:ALA:HB3	1:4:A:TYR:HD2	14	0.37
(1,2158)	1:29:A:VAL:HG13	1:48:A:PHE:HZ	14	0.37
(1,2153)	1:99:A:VAL:HG22	1:81:A:PHE:HE1	2	0.37
(1,2153)	1:99:A:VAL:HG21	1:81:A:PHE:HE1	17	0.37
(1,2143)	1:7:A:VAL:HG21	1:51:A:PHE:HD1	10	0.37
(1,2142)	1:7:A:VAL:HG23	1:48:A:PHE:HD1	11	0.37
(1,2134)	1:72:A:LEU:HD21	1:81:A:PHE:HE2	15	0.37
(1,2105)	1:64:A:ASP:HA	1:62:A:ILE:HG22	2	0.37
(1,2089)	1:79:A:HIS:HA	1:80:A:VAL:HG22	17	0.37
(1,2063)	1:33:A:ILE:HA	1:107:A:MET:HG3	3	0.37
(1,2056)	1:15:A:GLU:HG2	1:12:A:ALA:HA	12	0.37
(1,2024)	1:107:A:MET:HE3	1:7:A:VAL:HA	4	0.37
(1,1984)	1:7:A:VAL:HG12	1:48:A:PHE:HB3	5	0.37
(1,1953)	1:68:A:GLU:HG2	1:32:A:GLY:HA3	15	0.37
(1,1944)	1:57:A:VAL:HB	1:26:A:ILE:HD13	11	0.37
(1,1933)	1:38:A:ALA:HB3	1:1:A:MET:HB2	16	0.37
(1,1914)	1:68:A:GLU:HB2	1:34:A:GLY:HA3	9	0.37
(1,1830)	1:112:A:LEU:HD13	1:112:A:LEU:HB3	13	0.37
(1,1798)	1:62:A:ILE:HD11	1:28:A:ARG:HD3	9	0.37
(1,1795)	1:86:A:LEU:HD23	1:86:A:LEU:HD12	5	0.37
(1,1795)	1:86:A:LEU:HD21	1:86:A:LEU:HD12	12	0.37
(1,1795)	1:86:A:LEU:HD22	1:86:A:LEU:HD12	18	0.37
(1,1794)	1:11:A:ILE:HG23	1:12:A:ALA:HB3	16	0.37
(1,1777)	1:112:A:LEU:HD23	1:109:A:LEU:HD13	14	0.37
(1,1744)	1:90:A:VAL:HG12	1:90:A:VAL:HG23	1	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1744)	1:90:A:VAL:HG13	1:90:A:VAL:HG22	4	0.37
(1,1744)	1:90:A:VAL:HG11	1:90:A:VAL:HG23	19	0.37
(1,1665)	1:24:A:HIS:HA	1:57:A:VAL:HG21	16	0.37
(1,1619)	1:85:A:ALA:HB2	1:85:A:ALA:HA	1	0.37
(1,1619)	1:85:A:ALA:HB2	1:85:A:ALA:HA	2	0.37
(1,1615)	1:10:A:LEU:HA	1:107:A:MET:HE1	15	0.37
(1,1499)	1:6:A:VAL:HG21	1:3:A:GLU:HA	14	0.37
(1,1499)	1:6:A:VAL:HG21	1:3:A:GLU:HA	19	0.37
(1,1420)	1:25:A:LYS:HE2	1:25:A:LYS:HB3	2	0.37
(1,1269)	1:80:A:VAL:HG21	1:73:A:GLU:HG2	13	0.37
(1,1211)	1:75:A:LYS:HB3	1:98:A:ASN:HB2	13	0.37
(1,1093)	1:82:A:LYS:HD3	1:82:A:LYS:HA	10	0.37
(1,1093)	1:82:A:LYS:HD3	1:82:A:LYS:HA	19	0.37
(1,1059)	1:12:A:ALA:HB1	1:12:A:ALA:HB3	13	0.37
(1,1059)	1:12:A:ALA:HB2	1:12:A:ALA:HB1	16	0.37
(1,1010)	1:115:A:LEU:HB3	1:25:A:LYS:HB3	18	0.37
(1,996)	1:26:A:ILE:HG12	1:57:A:VAL:HG12	9	0.37
(1,996)	1:26:A:ILE:HG12	1:57:A:VAL:HG13	15	0.37
(1,990)	1:59:A:LYS:HG3	1:59:A:LYS:HE3	16	0.37
(1,945)	1:109:A:LEU:HD23	1:109:A:LEU:HB2	12	0.37
(1,945)	1:109:A:LEU:HD22	1:109:A:LEU:HB2	16	0.37
(1,945)	1:109:A:LEU:HD21	1:109:A:LEU:HB2	18	0.37
(1,944)	1:6:A:VAL:HG11	1:6:A:VAL:HG13	1	0.37
(1,944)	1:6:A:VAL:HG12	1:6:A:VAL:HG11	5	0.37
(1,944)	1:6:A:VAL:HG21	1:6:A:VAL:HG23	7	0.37
(1,944)	1:6:A:VAL:HG11	1:6:A:VAL:HG13	8	0.37
(1,944)	1:6:A:VAL:HG22	1:6:A:VAL:HG21	9	0.37
(1,944)	1:6:A:VAL:HG22	1:6:A:VAL:HG23	15	0.37
(1,944)	1:6:A:VAL:HG22	1:6:A:VAL:HG23	18	0.37
(1,944)	1:6:A:VAL:HG22	1:6:A:VAL:HG21	20	0.37
(1,935)	1:102:A:THR:HG22	1:102:A:THR:HG23	5	0.37
(1,911)	1:56:A:LEU:HD12	1:56:A:LEU:HA	18	0.37
(1,907)	1:13:A:LEU:HD22	1:13:A:LEU:HD13	2	0.37
(1,898)	1:29:A:VAL:HG13	1:112:A:LEU:HA	10	0.37
(1,886)	1:57:A:VAL:HG13	1:57:A:VAL:HG22	18	0.37
(1,875)	1:86:A:LEU:HD22	1:85:A:ALA:HA	20	0.37
(1,874)	1:26:A:ILE:HG23	1:61:A:ALA:HB3	16	0.37
(1,849)	1:72:A:LEU:HD22	1:101:A:ILE:HG13	20	0.37
(1,803)	1:72:A:LEU:HD23	1:72:A:LEU:HB2	5	0.37
(1,754)	1:33:A:ILE:HG13	1:33:A:ILE:HG23	10	0.37
(1,750)	1:72:A:LEU:HD21	1:99:A:VAL:HG13	4	0.37
(1,750)	1:72:A:LEU:HD21	1:99:A:VAL:HG12	16	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,746)	1:72:A:LEU:HD12	1:83:A:PRO:HB2	2	0.37
(1,303)	1:107:A:MET:HE3	1:10:A:LEU:H	3	0.37
(1,239)	1:19:A:LYS:HD3	1:20:A:LYS:H	3	0.37
(1,239)	1:19:A:LYS:HD2	1:20:A:LYS:H	16	0.37
(1,222)	1:101:A:ILE:HG12	1:101:A:ILE:H	10	0.37
(1,196)	1:12:A:ALA:HB2	1:14:A:CYS:H	17	0.37
(1,182)	1:18:A:ALA:HB3	1:20:A:LYS:H	3	0.37
(1,182)	1:18:A:ALA:HB2	1:20:A:LYS:H	9	0.37
(1,138)	1:102:A:THR:HG21	1:103:A:GLN:H	15	0.37
(1,126)	1:45:A:VAL:HG21	1:47:A:ALA:H	11	0.37
(1,121)	1:70:A:VAL:HG13	1:71:A:GLU:H	14	0.37
(1,118)	1:13:A:LEU:HD12	1:16:A:GLU:H	19	0.37
(1,112)	1:10:A:LEU:HD12	1:11:A:ILE:H	10	0.37
(1,105)	1:29:A:VAL:HG11	1:29:A:VAL:H	18	0.37
(1,103)	1:43:A:LEU:HD23	1:46:A:SER:H	12	0.37
(1,96)	1:11:A:ILE:HG22	1:15:A:GLU:H	15	0.37
(1,83)	1:112:A:LEU:HD21	1:112:A:LEU:H	2	0.37
(1,53)	1:66:A:VAL:HG12	1:33:A:ILE:H	1	0.37
(1,53)	1:66:A:VAL:HG11	1:33:A:ILE:H	7	0.37
(1,39)	1:90:A:VAL:HG11	1:90:A:VAL:H	12	0.37
(1,36)	1:99:A:VAL:HG12	1:100:A:ILE:H	11	0.37
(1,36)	1:99:A:VAL:HG13	1:100:A:ILE:H	19	0.37
(1,2675)	1:10:A:LEU:HD21	1:48:A:PHE:HZ	7	0.36
(1,2673)	1:43:A:LEU:HD12	1:4:A:TYR:HE1	14	0.36
(1,2669)	1:31:A:VAL:HG23	1:44:A:PHE:HD1	3	0.36
(1,2622)	1:38:A:ALA:HB2	1:1:A:MET:HB2	10	0.36
(1,2612)	1:25:A:LYS:HE3	1:56:A:LEU:HD12	6	0.36
(1,2455)	1:57:A:VAL:HG11	1:57:A:VAL:HG13	1	0.36
(1,2455)	1:29:A:VAL:HG12	1:29:A:VAL:HG11	6	0.36
(1,2455)	1:29:A:VAL:HG11	1:29:A:VAL:HG13	16	0.36
(1,2454)	1:62:A:ILE:HG21	1:28:A:ARG:HG3	10	0.36
(1,2448)	1:26:A:ILE:HD11	1:26:A:ILE:HD13	2	0.36
(1,2448)	1:26:A:ILE:HD12	1:26:A:ILE:HD13	3	0.36
(1,2448)	1:100:A:ILE:HD12	1:100:A:ILE:HD13	4	0.36
(1,2448)	1:101:A:ILE:HD11	1:101:A:ILE:HD13	11	0.36
(1,2448)	1:26:A:ILE:HD11	1:26:A:ILE:HD13	13	0.36
(1,2448)	1:101:A:ILE:HD12	1:101:A:ILE:HD13	14	0.36
(1,2448)	1:101:A:ILE:HD12	1:101:A:ILE:HD13	18	0.36
(1,2448)	1:26:A:ILE:HD12	1:26:A:ILE:HD11	19	0.36
(1,2440)	1:66:A:VAL:HG12	1:66:A:VAL:HG11	7	0.36
(1,2440)	1:30:A:VAL:HG12	1:30:A:VAL:HG13	12	0.36
(1,2433)	1:63:A:LEU:HD21	1:31:A:VAL:HG22	12	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2426)	1:97:A:LYS:HD3	1:97:A:LYS:H	4	0.36
(1,2426)	1:97:A:LYS:HD3	1:97:A:LYS:H	9	0.36
(1,2276)	1:88:A:TYR:HE1	1:88:A:TYR:HD1	4	0.36
(1,2206)	1:83:A:PRO:HB2	1:81:A:PHE:HD1	4	0.36
(1,2134)	1:72:A:LEU:HD22	1:81:A:PHE:HE1	3	0.36
(1,2088)	1:105:A:ASN:HA	1:36:A:ARG:HB3	19	0.36
(1,2070)	1:109:A:LEU:HD22	1:29:A:VAL:HA	15	0.36
(1,2067)	1:10:A:LEU:HA	1:13:A:LEU:HG	2	0.36
(1,2067)	1:10:A:LEU:HA	1:13:A:LEU:HG	5	0.36
(1,2035)	1:42:A:SER:HB2	1:45:A:VAL:HG21	17	0.36
(1,2001)	1:59:A:LYS:HE2	1:56:A:LEU:HB2	16	0.36
(1,1984)	1:7:A:VAL:HG13	1:48:A:PHE:HB3	1	0.36
(1,1984)	1:7:A:VAL:HG11	1:48:A:PHE:HB3	20	0.36
(1,1975)	1:12:A:ALA:HB1	1:15:A:GLU:HB2	4	0.36
(1,1975)	1:12:A:ALA:HB2	1:15:A:GLU:HB2	13	0.36
(1,1888)	1:85:A:ALA:HB2	1:86:A:LEU:HG	7	0.36
(1,1887)	1:82:A:LYS:HD2	1:71:A:GLU:HB3	2	0.36
(1,1887)	1:82:A:LYS:HD2	1:71:A:GLU:HB3	17	0.36
(1,1819)	1:7:A:VAL:HG12	1:47:A:ALA:HB1	18	0.36
(1,1814)	1:107:A:MET:HE1	1:10:A:LEU:HD22	17	0.36
(1,1812)	1:50:A:THR:HG23	1:47:A:ALA:HA	10	0.36
(1,1806)	1:10:A:LEU:HD13	1:7:A:VAL:HA	5	0.36
(1,1805)	1:10:A:LEU:HD12	1:63:A:LEU:HD21	13	0.36
(1,1795)	1:86:A:LEU:HD22	1:86:A:LEU:HD12	7	0.36
(1,1769)	1:66:A:VAL:HG12	1:68:A:GLU:HB2	18	0.36
(1,1746)	1:90:A:VAL:HG23	1:87:A:ASP:HB3	3	0.36
(1,1744)	1:90:A:VAL:HG11	1:90:A:VAL:HG23	2	0.36
(1,1744)	1:90:A:VAL:HG13	1:90:A:VAL:HG21	3	0.36
(1,1735)	1:72:A:LEU:HD23	1:88:A:TYR:HB3	2	0.36
(1,1731)	1:72:A:LEU:HD12	1:91:A:CYS:HA	5	0.36
(1,1645)	1:72:A:LEU:HD11	1:88:A:TYR:HA	5	0.36
(1,1628)	1:61:A:ALA:HB3	1:27:A:GLU:HA	5	0.36
(1,1628)	1:61:A:ALA:HB3	1:27:A:GLU:HA	16	0.36
(1,1619)	1:85:A:ALA:HB1	1:85:A:ALA:HA	10	0.36
(1,1601)	1:12:A:ALA:HB3	1:9:A:SER:HA	14	0.36
(1,1499)	1:6:A:VAL:HG22	1:3:A:GLU:HA	20	0.36
(1,1474)	1:41:A:LYS:HA	1:41:A:LYS:HE2	2	0.36
(1,1474)	1:41:A:LYS:HA	1:41:A:LYS:HE2	10	0.36
(1,1474)	1:41:A:LYS:HA	1:41:A:LYS:HE2	14	0.36
(1,1391)	1:58:A:CYS:HB3	1:55:A:SER:HB3	16	0.36
(1,1140)	1:59:A:LYS:HD3	1:59:A:LYS:HA	9	0.36
(1,1010)	1:115:A:LEU:HB3	1:25:A:LYS:HB3	11	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,998)	1:65:A:ILE:HG12	1:63:A:LEU:HD21	3	0.36
(1,964)	1:41:A:LYS:HG3	1:41:A:LYS:HE3	3	0.36
(1,964)	1:41:A:LYS:HG3	1:41:A:LYS:HE3	5	0.36
(1,962)	1:33:A:ILE:HD12	1:41:A:LYS:HG3	8	0.36
(1,948)	1:45:A:VAL:HG12	1:42:A:SER:HA	2	0.36
(1,945)	1:109:A:LEU:HD21	1:109:A:LEU:HB2	1	0.36
(1,944)	1:6:A:VAL:HG22	1:6:A:VAL:HG21	3	0.36
(1,944)	1:6:A:VAL:HG12	1:6:A:VAL:HG11	14	0.36
(1,944)	1:6:A:VAL:HG21	1:6:A:VAL:HG23	19	0.36
(1,935)	1:102:A:THR:HG21	1:102:A:THR:HG23	11	0.36
(1,911)	1:56:A:LEU:HD13	1:56:A:LEU:HA	1	0.36
(1,898)	1:29:A:VAL:HG13	1:112:A:LEU:HA	11	0.36
(1,886)	1:57:A:VAL:HG12	1:57:A:VAL:HG22	11	0.36
(1,875)	1:86:A:LEU:HD21	1:85:A:ALA:HA	18	0.36
(1,874)	1:26:A:ILE:HG23	1:61:A:ALA:HB2	10	0.36
(1,854)	1:101:A:ILE:HG13	1:70:A:VAL:HG21	18	0.36
(1,844)	1:112:A:LEU:HD21	1:114:A:MET:HE3	14	0.36
(1,822)	1:80:A:VAL:HG13	1:102:A:THR:HG23	14	0.36
(1,803)	1:72:A:LEU:HD22	1:72:A:LEU:HB2	2	0.36
(1,803)	1:72:A:LEU:HD23	1:72:A:LEU:HB2	4	0.36
(1,803)	1:72:A:LEU:HD21	1:72:A:LEU:HB2	6	0.36
(1,754)	1:33:A:ILE:HG13	1:33:A:ILE:HG22	4	0.36
(1,239)	1:19:A:LYS:HD2	1:20:A:LYS:H	18	0.36
(1,182)	1:18:A:ALA:HB1	1:20:A:LYS:H	12	0.36
(1,118)	1:13:A:LEU:HD12	1:16:A:GLU:H	15	0.36
(1,112)	1:10:A:LEU:HD12	1:11:A:ILE:H	7	0.36
(1,112)	1:10:A:LEU:HD11	1:11:A:ILE:H	20	0.36
(1,105)	1:29:A:VAL:HG12	1:29:A:VAL:H	3	0.36
(1,105)	1:29:A:VAL:HG12	1:29:A:VAL:H	15	0.36
(1,88)	1:26:A:ILE:HD11	1:15:A:GLU:H	16	0.36
(1,83)	1:112:A:LEU:HD21	1:112:A:LEU:H	14	0.36
(1,75)	1:101:A:ILE:HG13	1:102:A:THR:H	10	0.36
(1,75)	1:101:A:ILE:HG13	1:102:A:THR:H	14	0.36
(1,74)	1:99:A:VAL:HG22	1:73:A:GLU:H	13	0.36
(1,74)	1:99:A:VAL:HG22	1:73:A:GLU:H	15	0.36
(1,74)	1:99:A:VAL:HG23	1:73:A:GLU:H	16	0.36
(1,53)	1:66:A:VAL:HG11	1:33:A:ILE:H	8	0.36
(1,36)	1:99:A:VAL:HG11	1:100:A:ILE:H	4	0.36
(1,36)	1:99:A:VAL:HG12	1:100:A:ILE:H	6	0.36
(1,36)	1:99:A:VAL:HG13	1:100:A:ILE:H	9	0.36
(1,36)	1:99:A:VAL:HG11	1:100:A:ILE:H	13	0.36
(1,34)	1:33:A:ILE:HG21	1:39:A:MET:H	15	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,34)	1:33:A:ILE:HG22	1:39:A:MET:H	18	0.36
(1,31)	1:33:A:ILE:HG23	1:33:A:ILE:H	19	0.36
(1,12)	1:72:A:LEU:HD13	1:72:A:LEU:H	11	0.36
(1,2676)	1:47:A:ALA:HB1	1:44:A:PHE:HD2	15	0.35
(1,2670)	1:11:A:ILE:HG22	1:51:A:PHE:HD2	10	0.35
(1,2670)	1:11:A:ILE:HG21	1:51:A:PHE:HD2	11	0.35
(1,2654)	1:6:A:VAL:HA	1:107:A:MET:HE2	2	0.35
(1,2555)	1:25:A:LYS:HE3	1:56:A:LEU:HD11	19	0.35
(1,2454)	1:62:A:ILE:HG23	1:28:A:ARG:HG3	12	0.35
(1,2448)	1:100:A:ILE:HD12	1:100:A:ILE:HD13	1	0.35
(1,2448)	1:26:A:ILE:HD12	1:26:A:ILE:HD11	7	0.35
(1,2448)	1:26:A:ILE:HD11	1:26:A:ILE:HD13	12	0.35
(1,2448)	1:100:A:ILE:HD11	1:100:A:ILE:HD13	17	0.35
(1,2440)	1:30:A:VAL:HG11	1:30:A:VAL:HG13	4	0.35
(1,2440)	1:30:A:VAL:HG12	1:30:A:VAL:HG11	6	0.35
(1,2440)	1:90:A:VAL:HG12	1:90:A:VAL:HG11	8	0.35
(1,2440)	1:30:A:VAL:HG12	1:30:A:VAL:HG13	9	0.35
(1,2440)	1:30:A:VAL:HG11	1:30:A:VAL:HG13	11	0.35
(1,2440)	1:30:A:VAL:HG12	1:30:A:VAL:HG13	13	0.35
(1,2440)	1:30:A:VAL:HG12	1:30:A:VAL:HG11	15	0.35
(1,2433)	1:63:A:LEU:HD22	1:31:A:VAL:HG21	9	0.35
(1,2426)	1:97:A:LYS:HD3	1:97:A:LYS:H	8	0.35
(1,2279)	1:4:A:TYR:HE1	1:4:A:TYR:HD1	12	0.35
(1,2276)	1:88:A:TYR:HE1	1:88:A:TYR:HD1	20	0.35
(1,2262)	1:88:A:TYR:HA	1:88:A:TYR:HD2	14	0.35
(1,2262)	1:88:A:TYR:HA	1:88:A:TYR:HD1	20	0.35
(1,2246)	1:4:A:TYR:HA	1:4:A:TYR:HE2	1	0.35
(1,2246)	1:4:A:TYR:HA	1:4:A:TYR:HE1	10	0.35
(1,2206)	1:83:A:PRO:HB2	1:81:A:PHE:HD1	6	0.35
(1,2171)	1:47:A:ALA:HB3	1:4:A:TYR:HE2	8	0.35
(1,2143)	1:7:A:VAL:HG22	1:51:A:PHE:HD1	4	0.35
(1,2084)	1:58:A:CYS:HA	1:26:A:ILE:HG22	2	0.35
(1,2079)	1:71:A:GLU:HB2	1:103:A:GLN:HA	15	0.35
(1,2069)	1:112:A:LEU:HD21	1:29:A:VAL:HA	20	0.35
(1,2060)	1:35:A:GLU:HA	1:33:A:ILE:HG21	17	0.35
(1,2035)	1:42:A:SER:HB2	1:45:A:VAL:HG23	18	0.35
(1,1984)	1:7:A:VAL:HG11	1:48:A:PHE:HB3	6	0.35
(1,1984)	1:7:A:VAL:HG12	1:48:A:PHE:HB3	11	0.35
(1,1930)	1:71:A:GLU:HB2	1:103:A:GLN:HB2	6	0.35
(1,1930)	1:71:A:GLU:HB2	1:103:A:GLN:HB2	16	0.35
(1,1889)	1:82:A:LYS:HD3	1:71:A:GLU:HG3	18	0.35
(1,1845)	1:38:A:ALA:HB2	1:39:A:MET:HA	1	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1831)	1:58:A:CYS:HB2	1:61:A:ALA:HB1	12	0.35
(1,1824)	1:25:A:LYS:HG3	1:56:A:LEU:HD12	10	0.35
(1,1769)	1:66:A:VAL:HG13	1:68:A:GLU:HB2	4	0.35
(1,1744)	1:90:A:VAL:HG11	1:90:A:VAL:HG22	12	0.35
(1,1698)	1:80:A:VAL:HG12	1:73:A:GLU:HA	7	0.35
(1,1687)	1:31:A:VAL:HA	1:110:A:LEU:HD12	10	0.35
(1,1619)	1:85:A:ALA:HB2	1:85:A:ALA:HA	19	0.35
(1,1615)	1:10:A:LEU:HA	1:107:A:MET:HE1	7	0.35
(1,1525)	1:93:A:LYS:HD3	1:93:A:LYS:HA	18	0.35
(1,1514)	1:43:A:LEU:HD22	1:42:A:SER:HB3	2	0.35
(1,1452)	1:63:A:LEU:HD12	1:45:A:VAL:HA	6	0.35
(1,1391)	1:58:A:CYS:HB3	1:55:A:SER:HB3	1	0.35
(1,1211)	1:75:A:LYS:HB3	1:98:A:ASN:HB2	18	0.35
(1,1081)	1:43:A:LEU:HG	1:43:A:LEU:HA	2	0.35
(1,996)	1:26:A:ILE:HG12	1:57:A:VAL:HG13	17	0.35
(1,964)	1:41:A:LYS:HG3	1:41:A:LYS:HE3	10	0.35
(1,948)	1:45:A:VAL:HG11	1:42:A:SER:HA	18	0.35
(1,948)	1:45:A:VAL:HG11	1:42:A:SER:HA	20	0.35
(1,945)	1:109:A:LEU:HD22	1:109:A:LEU:HB2	5	0.35
(1,945)	1:109:A:LEU:HD23	1:109:A:LEU:HB2	10	0.35
(1,944)	1:6:A:VAL:HG22	1:6:A:VAL:HG21	6	0.35
(1,944)	1:6:A:VAL:HG11	1:6:A:VAL:HG13	16	0.35
(1,944)	1:6:A:VAL:HG12	1:6:A:VAL:HG13	17	0.35
(1,935)	1:102:A:THR:HG21	1:102:A:THR:HG22	3	0.35
(1,935)	1:102:A:THR:HG21	1:102:A:THR:HG23	6	0.35
(1,935)	1:102:A:THR:HG21	1:102:A:THR:HG22	14	0.35
(1,935)	1:102:A:THR:HG21	1:102:A:THR:HG23	15	0.35
(1,935)	1:102:A:THR:HG22	1:102:A:THR:HG23	19	0.35
(1,911)	1:56:A:LEU:HD13	1:56:A:LEU:HA	15	0.35
(1,908)	1:56:A:LEU:HD11	1:57:A:VAL:HG22	13	0.35
(1,907)	1:13:A:LEU:HD22	1:13:A:LEU:HD11	1	0.35
(1,889)	1:57:A:VAL:HG12	1:15:A:GLU:HG3	15	0.35
(1,886)	1:57:A:VAL:HG13	1:57:A:VAL:HG21	4	0.35
(1,864)	1:110:A:LEU:HD12	1:30:A:VAL:HG22	4	0.35
(1,863)	1:72:A:LEU:HD12	1:99:A:VAL:HG22	13	0.35
(1,860)	1:109:A:LEU:HD23	1:31:A:VAL:HA	18	0.35
(1,849)	1:72:A:LEU:HD21	1:101:A:ILE:HG13	2	0.35
(1,834)	1:72:A:LEU:HD23	1:101:A:ILE:HG23	11	0.35
(1,834)	1:72:A:LEU:HD22	1:101:A:ILE:HG21	18	0.35
(1,821)	1:30:A:VAL:HG13	1:28:A:ARG:HG3	11	0.35
(1,803)	1:72:A:LEU:HD21	1:72:A:LEU:HB2	18	0.35
(1,771)	1:110:A:LEU:HD12	1:66:A:VAL:HG21	9	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,770)	1:72:A:LEU:HD12	1:70:A:VAL:HG23	7	0.35
(1,754)	1:33:A:ILE:HG13	1:33:A:ILE:HG23	6	0.35
(1,746)	1:72:A:LEU:HD11	1:83:A:PRO:HB2	4	0.35
(1,746)	1:72:A:LEU:HD12	1:83:A:PRO:HB2	20	0.35
(1,710)	1:72:A:LEU:HA	1:103:A:GLN:H	11	0.35
(1,363)	1:49:A:GLU:HG3	1:50:A:THR:H	13	0.35
(1,300)	1:107:A:MET:HE1	1:108:A:ARG:H	2	0.35
(1,299)	1:39:A:MET:HE3	1:6:A:VAL:H	4	0.35
(1,294)	1:117:A:GLU:HB3	1:117:A:GLU:H	12	0.35
(1,239)	1:19:A:LYS:HD2	1:20:A:LYS:H	6	0.35
(1,239)	1:19:A:LYS:HD2	1:20:A:LYS:H	20	0.35
(1,200)	1:12:A:ALA:HB2	1:11:A:ILE:H	1	0.35
(1,200)	1:12:A:ALA:HB2	1:11:A:ILE:H	12	0.35
(1,182)	1:18:A:ALA:HB1	1:20:A:LYS:H	1	0.35
(1,182)	1:18:A:ALA:HB2	1:20:A:LYS:H	2	0.35
(1,182)	1:18:A:ALA:HB1	1:20:A:LYS:H	15	0.35
(1,113)	1:10:A:LEU:HD13	1:10:A:LEU:H	19	0.35
(1,112)	1:10:A:LEU:HD11	1:11:A:ILE:H	14	0.35
(1,105)	1:29:A:VAL:HG13	1:29:A:VAL:H	9	0.35
(1,103)	1:43:A:LEU:HD21	1:46:A:SER:H	8	0.35
(1,88)	1:26:A:ILE:HD11	1:15:A:GLU:H	17	0.35
(1,88)	1:26:A:ILE:HD13	1:15:A:GLU:H	20	0.35
(1,83)	1:112:A:LEU:HD21	1:112:A:LEU:H	1	0.35
(1,75)	1:101:A:ILE:HG13	1:102:A:THR:H	1	0.35
(1,53)	1:66:A:VAL:HG12	1:33:A:ILE:H	16	0.35
(1,36)	1:99:A:VAL:HG13	1:100:A:ILE:H	5	0.35
(1,31)	1:33:A:ILE:HG22	1:33:A:ILE:H	15	0.35
(1,23)	1:110:A:LEU:HD12	1:111:A:SER:H	14	0.35
(1,2676)	1:47:A:ALA:HB2	1:44:A:PHE:HD2	11	0.34
(1,2671)	1:115:A:LEU:HD13	1:24:A:HIS:HD2	16	0.34
(1,2670)	1:11:A:ILE:HG21	1:51:A:PHE:HD2	6	0.34
(1,2670)	1:11:A:ILE:HG23	1:51:A:PHE:HD2	14	0.34
(1,2661)	1:75:A:LYS:HA	1:75:A:LYS:HE3	16	0.34
(1,2469)	1:6:A:VAL:HG13	1:39:A:MET:HE2	6	0.34
(1,2448)	1:100:A:ILE:HD12	1:100:A:ILE:HD13	20	0.34
(1,2440)	1:30:A:VAL:HG12	1:30:A:VAL:HG13	1	0.34
(1,2440)	1:30:A:VAL:HG11	1:30:A:VAL:HG13	5	0.34
(1,2440)	1:90:A:VAL:HG12	1:90:A:VAL:HG11	16	0.34
(1,2440)	1:30:A:VAL:HG11	1:30:A:VAL:HG13	17	0.34
(1,2440)	1:66:A:VAL:HG12	1:66:A:VAL:HG11	18	0.34
(1,2433)	1:63:A:LEU:HD23	1:31:A:VAL:HG23	2	0.34
(1,2422)	1:47:A:ALA:HB1	1:7:A:VAL:H	6	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2419)	1:69:A:LYS:HG3	1:69:A:LYS:H	12	0.34
(1,2276)	1:88:A:TYR:HE1	1:88:A:TYR:HD1	9	0.34
(1,2276)	1:88:A:TYR:HE2	1:88:A:TYR:HD2	13	0.34
(1,2239)	1:41:A:LYS:HA	1:44:A:PHE:HD2	4	0.34
(1,2209)	1:1:A:MET:HG3	1:2:A:HIS:HD2	12	0.34
(1,2204)	1:83:A:PRO:HB3	1:88:A:TYR:HE1	11	0.34
(1,2180)	1:61:A:ALA:HB2	1:48:A:PHE:HD2	3	0.34
(1,2170)	1:92:A:GLU:HG3	1:81:A:PHE:HD1	19	0.34
(1,2143)	1:7:A:VAL:HG23	1:51:A:PHE:HD1	8	0.34
(1,2142)	1:7:A:VAL:HG21	1:48:A:PHE:HD1	13	0.34
(1,2138)	1:65:A:ILE:HD11	1:44:A:PHE:HE2	18	0.34
(1,2134)	1:72:A:LEU:HD23	1:81:A:PHE:HE2	9	0.34
(1,2105)	1:64:A:ASP:HA	1:62:A:ILE:HG23	7	0.34
(1,2105)	1:64:A:ASP:HA	1:62:A:ILE:HG21	15	0.34
(1,2058)	1:12:A:ALA:HB2	1:13:A:LEU:HA	12	0.34
(1,2056)	1:15:A:GLU:HG2	1:12:A:ALA:HA	14	0.34
(1,2056)	1:15:A:GLU:HG2	1:12:A:ALA:HA	16	0.34
(1,1975)	1:12:A:ALA:HB3	1:15:A:GLU:HB2	2	0.34
(1,1887)	1:82:A:LYS:HD2	1:71:A:GLU:HB3	13	0.34
(1,1829)	1:26:A:ILE:HD12	1:23:A:ALA:HB1	4	0.34
(1,1812)	1:50:A:THR:HG22	1:47:A:ALA:HA	9	0.34
(1,1812)	1:50:A:THR:HG21	1:47:A:ALA:HA	15	0.34
(1,1795)	1:86:A:LEU:HD21	1:86:A:LEU:HD11	8	0.34
(1,1794)	1:11:A:ILE:HG21	1:12:A:ALA:HB1	9	0.34
(1,1780)	1:112:A:LEU:HD23	1:17:A:HIS:HA	6	0.34
(1,1777)	1:112:A:LEU:HD23	1:109:A:LEU:HD13	7	0.34
(1,1744)	1:90:A:VAL:HG11	1:90:A:VAL:HG21	14	0.34
(1,1687)	1:31:A:VAL:HA	1:110:A:LEU:HD12	2	0.34
(1,1665)	1:24:A:HIS:HA	1:57:A:VAL:HG23	15	0.34
(1,1628)	1:61:A:ALA:HB1	1:27:A:GLU:HA	13	0.34
(1,1619)	1:85:A:ALA:HB2	1:85:A:ALA:HA	13	0.34
(1,1619)	1:85:A:ALA:HB3	1:85:A:ALA:HA	16	0.34
(1,1619)	1:85:A:ALA:HB3	1:85:A:ALA:HA	17	0.34
(1,1619)	1:85:A:ALA:HB3	1:85:A:ALA:HA	18	0.34
(1,1601)	1:12:A:ALA:HB3	1:9:A:SER:HA	10	0.34
(1,1474)	1:41:A:LYS:HA	1:41:A:LYS:HE2	5	0.34
(1,1474)	1:41:A:LYS:HA	1:41:A:LYS:HE2	15	0.34
(1,1462)	1:11:A:ILE:HD12	1:52:A:ARG:HA	20	0.34
(1,1385)	1:48:A:PHE:HB3	1:63:A:LEU:HD11	20	0.34
(1,1361)	1:26:A:ILE:HD13	1:114:A:MET:HG2	13	0.34
(1,1140)	1:59:A:LYS:HD3	1:59:A:LYS:HA	6	0.34
(1,1140)	1:59:A:LYS:HD3	1:59:A:LYS:HA	15	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1056)	1:69:A:LYS:HB3	1:69:A:LYS:HD3	15	0.34
(1,1006)	1:100:A:ILE:HD13	1:75:A:LYS:HG3	17	0.34
(1,964)	1:41:A:LYS:HG3	1:41:A:LYS:HE3	12	0.34
(1,953)	1:65:A:ILE:HG21	1:33:A:ILE:HG12	4	0.34
(1,948)	1:45:A:VAL:HG12	1:42:A:SER:HA	4	0.34
(1,945)	1:109:A:LEU:HD22	1:109:A:LEU:HB2	13	0.34
(1,945)	1:109:A:LEU:HD21	1:109:A:LEU:HB2	19	0.34
(1,945)	1:109:A:LEU:HD21	1:109:A:LEU:HB2	20	0.34
(1,944)	1:6:A:VAL:HG12	1:6:A:VAL:HG13	2	0.34
(1,944)	1:6:A:VAL:HG12	1:6:A:VAL:HG13	4	0.34
(1,935)	1:102:A:THR:HG21	1:102:A:THR:HG23	2	0.34
(1,935)	1:102:A:THR:HG21	1:102:A:THR:HG22	4	0.34
(1,935)	1:102:A:THR:HG21	1:102:A:THR:HG22	9	0.34
(1,935)	1:102:A:THR:HG21	1:102:A:THR:HG22	16	0.34
(1,922)	1:45:A:VAL:HG21	1:45:A:VAL:HG11	13	0.34
(1,922)	1:45:A:VAL:HG22	1:45:A:VAL:HG12	15	0.34
(1,911)	1:56:A:LEU:HD13	1:56:A:LEU:HA	12	0.34
(1,910)	1:109:A:LEU:HD13	1:13:A:LEU:HD13	12	0.34
(1,907)	1:13:A:LEU:HD22	1:13:A:LEU:HD12	7	0.34
(1,907)	1:13:A:LEU:HD22	1:13:A:LEU:HD13	11	0.34
(1,907)	1:13:A:LEU:HD21	1:13:A:LEU:HD11	14	0.34
(1,897)	1:29:A:VAL:HG13	1:112:A:LEU:HD22	8	0.34
(1,886)	1:57:A:VAL:HG11	1:57:A:VAL:HG22	17	0.34
(1,844)	1:112:A:LEU:HD21	1:114:A:MET:HE3	19	0.34
(1,826)	1:101:A:ILE:HG21	1:103:A:GLN:HA	17	0.34
(1,818)	1:80:A:VAL:HG13	1:80:A:VAL:HG23	10	0.34
(1,803)	1:72:A:LEU:HD23	1:72:A:LEU:HB2	8	0.34
(1,803)	1:72:A:LEU:HD21	1:72:A:LEU:HB2	15	0.34
(1,754)	1:33:A:ILE:HG13	1:33:A:ILE:HG21	9	0.34
(1,754)	1:33:A:ILE:HG13	1:33:A:ILE:HG21	11	0.34
(1,750)	1:72:A:LEU:HD22	1:99:A:VAL:HG12	17	0.34
(1,746)	1:72:A:LEU:HD12	1:83:A:PRO:HB2	19	0.34
(1,448)	1:79:A:HIS:HB2	1:80:A:VAL:H	3	0.34
(1,371)	1:22:A:GLN:HG3	1:21:A:ASN:H	4	0.34
(1,371)	1:22:A:GLN:HG3	1:21:A:ASN:H	11	0.34
(1,182)	1:18:A:ALA:HB1	1:20:A:LYS:H	7	0.34
(1,174)	1:100:A:ILE:HG12	1:101:A:ILE:H	18	0.34
(1,121)	1:70:A:VAL:HG13	1:71:A:GLU:H	9	0.34
(1,88)	1:26:A:ILE:HD13	1:15:A:GLU:H	7	0.34
(1,83)	1:112:A:LEU:HD22	1:112:A:LEU:H	19	0.34
(1,77)	1:109:A:LEU:HD21	1:109:A:LEU:H	14	0.34
(1,75)	1:101:A:ILE:HG13	1:102:A:THR:H	15	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,74)	1:99:A:VAL:HG21	1:73:A:GLU:H	8	0.34
(1,36)	1:99:A:VAL:HG13	1:100:A:ILE:H	12	0.34
(1,31)	1:33:A:ILE:HG21	1:33:A:ILE:H	20	0.34
(1,23)	1:110:A:LEU:HD12	1:111:A:SER:H	1	0.34
(1,2671)	1:115:A:LEU:HD12	1:24:A:HIS:HD2	6	0.33
(1,2647)	1:82:A:LYS:HE2	1:82:A:LYS:HB3	10	0.33
(1,2469)	1:6:A:VAL:HG11	1:107:A:MET:HE1	14	0.33
(1,2454)	1:62:A:ILE:HG22	1:28:A:ARG:HG3	20	0.33
(1,2448)	1:100:A:ILE:HD12	1:100:A:ILE:HD11	8	0.33
(1,2444)	1:80:A:VAL:HG12	1:73:A:GLU:HA	14	0.33
(1,2440)	1:30:A:VAL:HG12	1:30:A:VAL:HG11	10	0.33
(1,2440)	1:90:A:VAL:HG12	1:90:A:VAL:HG13	14	0.33
(1,2440)	1:90:A:VAL:HG12	1:90:A:VAL:HG11	20	0.33
(1,2438)	1:65:A:ILE:HD13	1:41:A:LYS:HD2	6	0.33
(1,2422)	1:47:A:ALA:HB3	1:7:A:VAL:H	14	0.33
(1,2279)	1:4:A:TYR:HE2	1:4:A:TYR:HD2	3	0.33
(1,2276)	1:88:A:TYR:HE2	1:88:A:TYR:HD2	15	0.33
(1,2276)	1:88:A:TYR:HE1	1:88:A:TYR:HD1	16	0.33
(1,2276)	1:88:A:TYR:HE2	1:88:A:TYR:HD2	17	0.33
(1,2262)	1:88:A:TYR:HA	1:88:A:TYR:HD1	4	0.33
(1,2262)	1:88:A:TYR:HA	1:88:A:TYR:HD1	6	0.33
(1,2262)	1:88:A:TYR:HA	1:88:A:TYR:HD1	11	0.33
(1,2262)	1:88:A:TYR:HA	1:88:A:TYR:HD2	16	0.33
(1,2246)	1:4:A:TYR:HA	1:4:A:TYR:HE2	18	0.33
(1,2246)	1:4:A:TYR:HA	1:4:A:TYR:HE1	20	0.33
(1,2202)	1:83:A:PRO:HB3	1:88:A:TYR:HD1	8	0.33
(1,2180)	1:61:A:ALA:HB3	1:48:A:PHE:HD2	20	0.33
(1,2172)	1:47:A:ALA:HB1	1:4:A:TYR:HD2	19	0.33
(1,2171)	1:47:A:ALA:HB1	1:4:A:TYR:HE1	17	0.33
(1,2148)	1:80:A:VAL:HG12	1:81:A:PHE:HD2	6	0.33
(1,2148)	1:80:A:VAL:HG11	1:81:A:PHE:HD2	19	0.33
(1,2084)	1:58:A:CYS:HA	1:26:A:ILE:HG23	1	0.33
(1,2058)	1:12:A:ALA:HB2	1:13:A:LEU:HA	16	0.33
(1,2056)	1:15:A:GLU:HG2	1:12:A:ALA:HA	2	0.33
(1,2051)	1:114:A:MET:HE2	1:17:A:HIS:HA	15	0.33
(1,2024)	1:107:A:MET:HE1	1:7:A:VAL:HA	6	0.33
(1,2018)	1:90:A:VAL:HG13	1:95:A:HIS:HB3	20	0.33
(1,1887)	1:82:A:LYS:HD2	1:71:A:GLU:HB3	12	0.33
(1,1840)	1:75:A:LYS:HG3	1:100:A:ILE:HG13	15	0.33
(1,1829)	1:26:A:ILE:HD11	1:23:A:ALA:HB2	10	0.33
(1,1782)	1:109:A:LEU:HD23	1:107:A:MET:HE2	7	0.33
(1,1777)	1:112:A:LEU:HD23	1:109:A:LEU:HD11	3	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1744)	1:90:A:VAL:HG13	1:90:A:VAL:HG21	8	0.33
(1,1734)	1:72:A:LEU:HD13	1:88:A:TYR:HB3	2	0.33
(1,1707)	1:107:A:MET:HG3	1:107:A:MET:HA	18	0.33
(1,1619)	1:85:A:ALA:HB3	1:85:A:ALA:HA	4	0.33
(1,1619)	1:85:A:ALA:HB1	1:85:A:ALA:HA	15	0.33
(1,1615)	1:10:A:LEU:HA	1:107:A:MET:HE1	1	0.33
(1,1499)	1:6:A:VAL:HG22	1:3:A:GLU:HA	16	0.33
(1,1499)	1:6:A:VAL:HG22	1:3:A:GLU:HA	18	0.33
(1,1490)	1:6:A:VAL:HA	1:9:A:SER:HB3	18	0.33
(1,1477)	1:45:A:VAL:HG11	1:41:A:LYS:HA	18	0.33
(1,1448)	1:90:A:VAL:HG21	1:95:A:HIS:HB3	17	0.33
(1,1445)	1:48:A:PHE:HB2	1:63:A:LEU:HD13	8	0.33
(1,1361)	1:26:A:ILE:HD11	1:114:A:MET:HG2	7	0.33
(1,1159)	1:108:A:ARG:HB2	1:110:A:LEU:HD22	11	0.33
(1,1093)	1:82:A:LYS:HD2	1:82:A:LYS:HA	9	0.33
(1,1081)	1:43:A:LEU:HG	1:43:A:LEU:HA	7	0.33
(1,1006)	1:100:A:ILE:HD11	1:75:A:LYS:HG3	19	0.33
(1,998)	1:65:A:ILE:HG12	1:63:A:LEU:HD23	11	0.33
(1,964)	1:41:A:LYS:HG3	1:41:A:LYS:HE3	6	0.33
(1,964)	1:41:A:LYS:HG3	1:41:A:LYS:HE3	8	0.33
(1,953)	1:65:A:ILE:HG23	1:33:A:ILE:HG12	6	0.33
(1,953)	1:65:A:ILE:HG21	1:33:A:ILE:HG12	19	0.33
(1,952)	1:33:A:ILE:HG12	1:31:A:VAL:HG21	14	0.33
(1,945)	1:109:A:LEU:HD23	1:109:A:LEU:HB2	6	0.33
(1,945)	1:109:A:LEU:HD22	1:109:A:LEU:HB2	7	0.33
(1,935)	1:102:A:THR:HG22	1:102:A:THR:HG23	1	0.33
(1,935)	1:102:A:THR:HG21	1:102:A:THR:HG23	7	0.33
(1,935)	1:102:A:THR:HG21	1:102:A:THR:HG23	10	0.33
(1,910)	1:109:A:LEU:HD12	1:13:A:LEU:HD11	1	0.33
(1,907)	1:13:A:LEU:HD21	1:13:A:LEU:HD11	16	0.33
(1,874)	1:26:A:ILE:HG23	1:61:A:ALA:HB2	11	0.33
(1,834)	1:72:A:LEU:HD21	1:101:A:ILE:HG21	14	0.33
(1,803)	1:72:A:LEU:HD22	1:72:A:LEU:HB2	9	0.33
(1,773)	1:66:A:VAL:HG22	1:66:A:VAL:HG23	16	0.33
(1,754)	1:33:A:ILE:HG13	1:33:A:ILE:HG22	2	0.33
(1,754)	1:33:A:ILE:HG13	1:33:A:ILE:HG22	3	0.33
(1,750)	1:72:A:LEU:HD22	1:99:A:VAL:HG12	2	0.33
(1,750)	1:72:A:LEU:HD23	1:99:A:VAL:HG13	8	0.33
(1,710)	1:72:A:LEU:HA	1:103:A:GLN:H	6	0.33
(1,448)	1:79:A:HIS:HB2	1:80:A:VAL:H	8	0.33
(1,371)	1:22:A:GLN:HG3	1:21:A:ASN:H	17	0.33
(1,358)	1:22:A:GLN:HB2	1:23:A:ALA:H	2	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,300)	1:107:A:MET:HE1	1:108:A:ARG:H	11	0.33
(1,239)	1:19:A:LYS:HD2	1:20:A:LYS:H	2	0.33
(1,196)	1:12:A:ALA:HB3	1:14:A:CYS:H	10	0.33
(1,182)	1:18:A:ALA:HB1	1:20:A:LYS:H	11	0.33
(1,174)	1:100:A:ILE:HG12	1:101:A:ILE:H	6	0.33
(1,174)	1:100:A:ILE:HG12	1:101:A:ILE:H	8	0.33
(1,174)	1:100:A:ILE:HG12	1:101:A:ILE:H	16	0.33
(1,146)	1:6:A:VAL:HG12	1:7:A:VAL:H	12	0.33
(1,118)	1:13:A:LEU:HD11	1:16:A:GLU:H	7	0.33
(1,112)	1:10:A:LEU:HD11	1:11:A:ILE:H	12	0.33
(1,105)	1:29:A:VAL:HG12	1:29:A:VAL:H	1	0.33
(1,105)	1:29:A:VAL:HG11	1:29:A:VAL:H	8	0.33
(1,101)	1:57:A:VAL:HG13	1:15:A:GLU:H	10	0.33
(1,96)	1:11:A:ILE:HG23	1:15:A:GLU:H	10	0.33
(1,83)	1:112:A:LEU:HD23	1:112:A:LEU:H	6	0.33
(1,83)	1:112:A:LEU:HD23	1:112:A:LEU:H	16	0.33
(1,29)	1:70:A:VAL:HG22	1:72:A:LEU:H	12	0.33
(1,12)	1:72:A:LEU:HD11	1:72:A:LEU:H	12	0.33
(1,2665)	1:97:A:LYS:HA	1:90:A:VAL:HB	6	0.32
(1,2661)	1:75:A:LYS:HA	1:75:A:LYS:HE3	6	0.32
(1,2650)	1:66:A:VAL:HG13	1:32:A:GLY:HA3	6	0.32
(1,2621)	1:38:A:ALA:HB3	1:105:A:ASN:HB2	8	0.32
(1,2590)	1:33:A:ILE:HD13	1:39:A:MET:HG2	16	0.32
(1,2571)	1:59:A:LYS:HD3	1:56:A:LEU:HA	8	0.32
(1,2571)	1:59:A:LYS:HD2	1:56:A:LEU:HA	13	0.32
(1,2469)	1:6:A:VAL:HG13	1:39:A:MET:HE1	12	0.32
(1,2448)	1:100:A:ILE:HD12	1:100:A:ILE:HD11	15	0.32
(1,2435)	1:72:A:LEU:HD22	1:72:A:LEU:HD21	9	0.32
(1,2433)	1:63:A:LEU:HD21	1:31:A:VAL:HG22	16	0.32
(1,2422)	1:47:A:ALA:HB3	1:7:A:VAL:H	11	0.32
(1,2419)	1:69:A:LYS:HG3	1:69:A:LYS:H	14	0.32
(1,2419)	1:69:A:LYS:HG3	1:69:A:LYS:H	18	0.32
(1,2396)	1:101:A:ILE:H	1:100:A:ILE:H	2	0.32
(1,2378)	1:97:A:LYS:H	1:96:A:SER:H	3	0.32
(1,2378)	1:97:A:LYS:H	1:96:A:SER:H	14	0.32
(1,2378)	1:97:A:LYS:H	1:96:A:SER:H	15	0.32
(1,2276)	1:88:A:TYR:HE2	1:88:A:TYR:HD2	1	0.32
(1,2276)	1:88:A:TYR:HE2	1:88:A:TYR:HD2	3	0.32
(1,2276)	1:88:A:TYR:HE2	1:88:A:TYR:HD2	6	0.32
(1,2276)	1:88:A:TYR:HE1	1:88:A:TYR:HD1	7	0.32
(1,2276)	1:88:A:TYR:HE1	1:88:A:TYR:HD1	14	0.32
(1,2239)	1:41:A:LYS:HA	1:44:A:PHE:HD2	17	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2171)	1:47:A:ALA:HB1	1:4:A:TYR:HE1	5	0.32
(1,2165)	1:92:A:GLU:HG3	1:79:A:HIS:HD2	12	0.32
(1,2153)	1:99:A:VAL:HG22	1:81:A:PHE:HE2	11	0.32
(1,2078)	1:82:A:LYS:HD3	1:71:A:GLU:HA	10	0.32
(1,2067)	1:10:A:LEU:HA	1:13:A:LEU:HG	18	0.32
(1,1984)	1:7:A:VAL:HG13	1:48:A:PHE:HB3	8	0.32
(1,1944)	1:57:A:VAL:HB	1:26:A:ILE:HD13	4	0.32
(1,1854)	1:75:A:LYS:HG2	1:100:A:ILE:HG13	11	0.32
(1,1842)	1:18:A:ALA:HB3	1:21:A:ASN:HB3	17	0.32
(1,1829)	1:26:A:ILE:HD11	1:23:A:ALA:HB2	3	0.32
(1,1824)	1:25:A:LYS:HG3	1:56:A:LEU:HD12	18	0.32
(1,1798)	1:62:A:ILE:HD13	1:28:A:ARG:HD3	2	0.32
(1,1780)	1:112:A:LEU:HD22	1:17:A:HIS:HA	7	0.32
(1,1774)	1:31:A:VAL:HG23	1:107:A:MET:HG2	5	0.32
(1,1774)	1:31:A:VAL:HG23	1:107:A:MET:HG2	14	0.32
(1,1769)	1:66:A:VAL:HG11	1:68:A:GLU:HB2	13	0.32
(1,1708)	1:107:A:MET:HA	1:33:A:ILE:HD13	13	0.32
(1,1619)	1:85:A:ALA:HB3	1:85:A:ALA:HA	3	0.32
(1,1619)	1:85:A:ALA:HB2	1:85:A:ALA:HA	7	0.32
(1,1619)	1:85:A:ALA:HB2	1:85:A:ALA:HA	9	0.32
(1,1619)	1:85:A:ALA:HB3	1:85:A:ALA:HA	20	0.32
(1,1618)	1:50:A:THR:HG21	1:51:A:PHE:HA	3	0.32
(1,1618)	1:50:A:THR:HG21	1:51:A:PHE:HA	9	0.32
(1,1601)	1:12:A:ALA:HB2	1:9:A:SER:HA	1	0.32
(1,1561)	1:38:A:ALA:HB3	1:38:A:ALA:HA	13	0.32
(1,1554)	1:20:A:LYS:HE2	1:17:A:HIS:HA	1	0.32
(1,1554)	1:20:A:LYS:HE3	1:17:A:HIS:HA	2	0.32
(1,1477)	1:45:A:VAL:HG12	1:41:A:LYS:HA	2	0.32
(1,1474)	1:41:A:LYS:HA	1:41:A:LYS:HE2	4	0.32
(1,1452)	1:63:A:LEU:HD11	1:45:A:VAL:HA	18	0.32
(1,1445)	1:48:A:PHE:HB2	1:63:A:LEU:HD11	19	0.32
(1,1415)	1:20:A:LYS:HE2	1:20:A:LYS:HE3	12	0.32
(1,1388)	1:11:A:ILE:HD12	1:51:A:PHE:HB3	7	0.32
(1,1324)	1:106:A:GLU:HG3	1:105:A:ASN:HB2	7	0.32
(1,1081)	1:43:A:LEU:HG	1:43:A:LEU:HA	8	0.32
(1,996)	1:26:A:ILE:HG12	1:57:A:VAL:HG13	2	0.32
(1,963)	1:41:A:LYS:HG3	1:65:A:ILE:HD13	16	0.32
(1,945)	1:109:A:LEU:HD23	1:109:A:LEU:HB2	8	0.32
(1,935)	1:102:A:THR:HG21	1:102:A:THR:HG22	20	0.32
(1,922)	1:45:A:VAL:HG21	1:45:A:VAL:HG11	12	0.32
(1,922)	1:45:A:VAL:HG21	1:45:A:VAL:HG12	16	0.32
(1,907)	1:13:A:LEU:HD21	1:13:A:LEU:HD12	3	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,907)	1:13:A:LEU:HD23	1:13:A:LEU:HD13	5	0.32
(1,904)	1:31:A:VAL:HG13	1:10:A:LEU:HD12	1	0.32
(1,875)	1:86:A:LEU:HD22	1:85:A:ALA:HA	13	0.32
(1,869)	1:26:A:ILE:HD11	1:61:A:ALA:HB3	16	0.32
(1,864)	1:110:A:LEU:HD12	1:30:A:VAL:HG21	1	0.32
(1,854)	1:101:A:ILE:HG13	1:70:A:VAL:HG23	13	0.32
(1,849)	1:72:A:LEU:HD23	1:101:A:ILE:HG13	16	0.32
(1,832)	1:101:A:ILE:HG22	1:105:A:ASN:HB2	10	0.32
(1,826)	1:101:A:ILE:HG23	1:103:A:GLN:HA	14	0.32
(1,825)	1:101:A:ILE:HG23	1:72:A:LEU:HA	11	0.32
(1,803)	1:72:A:LEU:HD22	1:72:A:LEU:HB2	3	0.32
(1,803)	1:72:A:LEU:HD23	1:72:A:LEU:HB2	16	0.32
(1,773)	1:66:A:VAL:HG21	1:66:A:VAL:HG23	1	0.32
(1,773)	1:66:A:VAL:HG21	1:66:A:VAL:HG23	3	0.32
(1,773)	1:66:A:VAL:HG22	1:66:A:VAL:HG23	11	0.32
(1,773)	1:66:A:VAL:HG22	1:66:A:VAL:HG23	14	0.32
(1,754)	1:33:A:ILE:HG13	1:33:A:ILE:HG21	1	0.32
(1,754)	1:33:A:ILE:HG13	1:33:A:ILE:HG21	5	0.32
(1,420)	1:19:A:LYS:HE2	1:19:A:LYS:H	8	0.32
(1,371)	1:22:A:GLN:HG3	1:21:A:ASN:H	6	0.32
(1,300)	1:107:A:MET:HE3	1:108:A:ARG:H	17	0.32
(1,185)	1:38:A:ALA:HB2	1:39:A:MET:H	17	0.32
(1,162)	1:23:A:ALA:HB1	1:22:A:GLN:H	17	0.32
(1,138)	1:102:A:THR:HG21	1:103:A:GLN:H	7	0.32
(1,136)	1:102:A:THR:HG21	1:100:A:ILE:H	15	0.32
(1,135)	1:100:A:ILE:HG13	1:100:A:ILE:H	20	0.32
(1,121)	1:70:A:VAL:HG13	1:71:A:GLU:H	7	0.32
(1,121)	1:70:A:VAL:HG13	1:71:A:GLU:H	8	0.32
(1,121)	1:70:A:VAL:HG11	1:71:A:GLU:H	12	0.32
(1,118)	1:13:A:LEU:HD13	1:16:A:GLU:H	14	0.32
(1,113)	1:10:A:LEU:HD13	1:10:A:LEU:H	1	0.32
(1,113)	1:10:A:LEU:HD12	1:10:A:LEU:H	6	0.32
(1,113)	1:10:A:LEU:HD12	1:10:A:LEU:H	11	0.32
(1,112)	1:10:A:LEU:HD13	1:11:A:ILE:H	17	0.32
(1,105)	1:29:A:VAL:HG12	1:29:A:VAL:H	4	0.32
(1,105)	1:29:A:VAL:HG11	1:29:A:VAL:H	5	0.32
(1,105)	1:29:A:VAL:HG11	1:29:A:VAL:H	14	0.32
(1,83)	1:112:A:LEU:HD21	1:112:A:LEU:H	9	0.32
(1,75)	1:101:A:ILE:HG13	1:102:A:THR:H	4	0.32
(1,34)	1:33:A:ILE:HG22	1:39:A:MET:H	16	0.32
(1,2693)	1:48:A:PHE:HD2	1:44:A:PHE:HZ	6	0.31
(1,2692)	1:88:A:TYR:HE2	1:88:A:TYR:HD2	3	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2676)	1:47:A:ALA:HB2	1:44:A:PHE:HD1	16	0.31
(1,2669)	1:31:A:VAL:HG21	1:44:A:PHE:HD2	1	0.31
(1,2657)	1:20:A:LYS:HE3	1:20:A:LYS:HA	2	0.31
(1,2647)	1:59:A:LYS:HB3	1:25:A:LYS:HE3	8	0.31
(1,2622)	1:38:A:ALA:HB3	1:1:A:MET:HB2	8	0.31
(1,2590)	1:33:A:ILE:HD12	1:39:A:MET:HG2	19	0.31
(1,2555)	1:25:A:LYS:HE3	1:56:A:LEU:HD12	6	0.31
(1,2469)	1:6:A:VAL:HG12	1:39:A:MET:HE2	8	0.31
(1,2435)	1:72:A:LEU:HD21	1:72:A:LEU:HD23	1	0.31
(1,2435)	1:7:A:VAL:HG12	1:7:A:VAL:HG13	3	0.31
(1,2435)	1:7:A:VAL:HG12	1:7:A:VAL:HG11	5	0.31
(1,2435)	1:7:A:VAL:HG12	1:7:A:VAL:HG11	6	0.31
(1,2435)	1:72:A:LEU:HD22	1:72:A:LEU:HD23	8	0.31
(1,2435)	1:7:A:VAL:HG12	1:7:A:VAL:HG11	11	0.31
(1,2435)	1:72:A:LEU:HD21	1:72:A:LEU:HD23	13	0.31
(1,2435)	1:7:A:VAL:HG12	1:7:A:VAL:HG11	14	0.31
(1,2435)	1:7:A:VAL:HG11	1:7:A:VAL:HG13	15	0.31
(1,2435)	1:72:A:LEU:HD22	1:72:A:LEU:HD23	20	0.31
(1,2422)	1:47:A:ALA:HB1	1:7:A:VAL:H	16	0.31
(1,2419)	1:69:A:LYS:HG3	1:69:A:LYS:H	11	0.31
(1,2419)	1:69:A:LYS:HG3	1:69:A:LYS:H	17	0.31
(1,2279)	1:4:A:TYR:HE1	1:4:A:TYR:HD1	10	0.31
(1,2276)	1:88:A:TYR:HE2	1:88:A:TYR:HD2	10	0.31
(1,2276)	1:88:A:TYR:HE2	1:88:A:TYR:HD2	11	0.31
(1,2262)	1:88:A:TYR:HA	1:88:A:TYR:HD1	10	0.31
(1,2206)	1:83:A:PRO:HB2	1:81:A:PHE:HD1	15	0.31
(1,2202)	1:83:A:PRO:HB3	1:88:A:TYR:HD1	1	0.31
(1,2153)	1:99:A:VAL:HG21	1:81:A:PHE:HE2	6	0.31
(1,2153)	1:99:A:VAL:HG23	1:81:A:PHE:HE1	12	0.31
(1,2105)	1:64:A:ASP:HA	1:62:A:ILE:HG21	4	0.31
(1,2084)	1:58:A:CYS:HA	1:26:A:ILE:HG22	15	0.31
(1,2058)	1:12:A:ALA:HB1	1:13:A:LEU:HA	1	0.31
(1,2058)	1:12:A:ALA:HB3	1:13:A:LEU:HA	9	0.31
(1,2056)	1:15:A:GLU:HG2	1:12:A:ALA:HA	5	0.31
(1,2051)	1:114:A:MET:HE2	1:17:A:HIS:HA	1	0.31
(1,2051)	1:114:A:MET:HE1	1:17:A:HIS:HA	20	0.31
(1,2050)	1:17:A:HIS:HA	1:16:A:GLU:HB2	13	0.31
(1,2040)	1:90:A:VAL:HG23	1:92:A:GLU:HA	6	0.31
(1,1819)	1:7:A:VAL:HG12	1:47:A:ALA:HB3	4	0.31
(1,1780)	1:112:A:LEU:HD22	1:17:A:HIS:HA	12	0.31
(1,1780)	1:112:A:LEU:HD23	1:17:A:HIS:HA	20	0.31
(1,1769)	1:66:A:VAL:HG11	1:68:A:GLU:HB3	11	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1749)	1:65:A:ILE:HG13	1:63:A:LEU:HD23	5	0.31
(1,1749)	1:65:A:ILE:HG13	1:63:A:LEU:HD23	8	0.31
(1,1677)	1:25:A:LYS:HA	1:57:A:VAL:HG21	5	0.31
(1,1628)	1:61:A:ALA:HB3	1:27:A:GLU:HA	4	0.31
(1,1619)	1:85:A:ALA:HB1	1:85:A:ALA:HA	5	0.31
(1,1619)	1:85:A:ALA:HB3	1:85:A:ALA:HA	8	0.31
(1,1619)	1:85:A:ALA:HB2	1:85:A:ALA:HA	11	0.31
(1,1619)	1:85:A:ALA:HB2	1:85:A:ALA:HA	14	0.31
(1,1618)	1:50:A:THR:HG21	1:51:A:PHE:HA	11	0.31
(1,1618)	1:50:A:THR:HG21	1:51:A:PHE:HA	16	0.31
(1,1561)	1:38:A:ALA:HB1	1:38:A:ALA:HA	17	0.31
(1,1554)	1:20:A:LYS:HE3	1:17:A:HIS:HA	8	0.31
(1,1477)	1:45:A:VAL:HG12	1:41:A:LYS:HA	8	0.31
(1,1474)	1:41:A:LYS:HA	1:41:A:LYS:HE2	7	0.31
(1,1420)	1:25:A:LYS:HE2	1:25:A:LYS:HB3	7	0.31
(1,1415)	1:20:A:LYS:HE2	1:20:A:LYS:HE3	2	0.31
(1,1415)	1:20:A:LYS:HE2	1:20:A:LYS:HE3	19	0.31
(1,1249)	1:72:A:LEU:HD12	1:83:A:PRO:HG2	1	0.31
(1,1249)	1:72:A:LEU:HD12	1:83:A:PRO:HG2	6	0.31
(1,1159)	1:108:A:ARG:HB2	1:110:A:LEU:HD21	1	0.31
(1,1010)	1:115:A:LEU:HB3	1:25:A:LYS:HB3	17	0.31
(1,998)	1:65:A:ILE:HG12	1:63:A:LEU:HD23	10	0.31
(1,996)	1:26:A:ILE:HG12	1:57:A:VAL:HG12	18	0.31
(1,953)	1:65:A:ILE:HG21	1:33:A:ILE:HG12	11	0.31
(1,948)	1:45:A:VAL:HG12	1:42:A:SER:HA	8	0.31
(1,935)	1:102:A:THR:HG21	1:102:A:THR:HG22	8	0.31
(1,935)	1:102:A:THR:HG22	1:102:A:THR:HG23	13	0.31
(1,935)	1:102:A:THR:HG22	1:102:A:THR:HG23	17	0.31
(1,935)	1:102:A:THR:HG21	1:102:A:THR:HG22	18	0.31
(1,922)	1:45:A:VAL:HG21	1:45:A:VAL:HG13	10	0.31
(1,922)	1:45:A:VAL:HG22	1:45:A:VAL:HG13	19	0.31
(1,911)	1:56:A:LEU:HD13	1:56:A:LEU:HA	4	0.31
(1,911)	1:56:A:LEU:HD12	1:56:A:LEU:HA	8	0.31
(1,911)	1:56:A:LEU:HD12	1:56:A:LEU:HA	17	0.31
(1,910)	1:109:A:LEU:HD11	1:13:A:LEU:HD13	17	0.31
(1,907)	1:13:A:LEU:HD22	1:13:A:LEU:HD12	8	0.31
(1,898)	1:29:A:VAL:HG11	1:112:A:LEU:HA	20	0.31
(1,897)	1:29:A:VAL:HG12	1:112:A:LEU:HD21	16	0.31
(1,897)	1:29:A:VAL:HG11	1:112:A:LEU:HD22	20	0.31
(1,887)	1:57:A:VAL:HG12	1:18:A:ALA:HA	2	0.31
(1,886)	1:57:A:VAL:HG13	1:57:A:VAL:HG22	1	0.31
(1,886)	1:57:A:VAL:HG11	1:57:A:VAL:HG22	7	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,886)	1:57:A:VAL:HG12	1:57:A:VAL:HG21	15	0.31
(1,861)	1:109:A:LEU:HD21	1:112:A:LEU:HG	19	0.31
(1,832)	1:101:A:ILE:HG21	1:105:A:ASN:HB2	8	0.31
(1,832)	1:101:A:ILE:HG23	1:105:A:ASN:HB2	15	0.31
(1,826)	1:101:A:ILE:HG21	1:103:A:GLN:HA	15	0.31
(1,822)	1:80:A:VAL:HG11	1:102:A:THR:HG21	20	0.31
(1,821)	1:30:A:VAL:HG13	1:28:A:ARG:HG3	12	0.31
(1,803)	1:72:A:LEU:HD22	1:72:A:LEU:HB2	7	0.31
(1,803)	1:72:A:LEU:HD21	1:72:A:LEU:HB2	11	0.31
(1,787)	1:63:A:LEU:HD13	1:65:A:ILE:HD11	4	0.31
(1,773)	1:66:A:VAL:HG22	1:66:A:VAL:HG23	5	0.31
(1,773)	1:66:A:VAL:HG22	1:66:A:VAL:HG23	6	0.31
(1,773)	1:66:A:VAL:HG22	1:66:A:VAL:HG21	7	0.31
(1,773)	1:66:A:VAL:HG21	1:66:A:VAL:HG23	8	0.31
(1,773)	1:66:A:VAL:HG21	1:66:A:VAL:HG23	10	0.31
(1,771)	1:110:A:LEU:HD12	1:66:A:VAL:HG23	13	0.31
(1,754)	1:33:A:ILE:HG13	1:33:A:ILE:HG23	12	0.31
(1,750)	1:72:A:LEU:HD21	1:99:A:VAL:HG13	10	0.31
(1,750)	1:72:A:LEU:HD23	1:99:A:VAL:HG12	19	0.31
(1,746)	1:72:A:LEU:HD13	1:83:A:PRO:HB2	7	0.31
(1,239)	1:19:A:LYS:HD2	1:20:A:LYS:H	9	0.31
(1,239)	1:19:A:LYS:HD3	1:20:A:LYS:H	13	0.31
(1,239)	1:19:A:LYS:HD2	1:20:A:LYS:H	14	0.31
(1,196)	1:12:A:ALA:HB3	1:14:A:CYS:H	6	0.31
(1,162)	1:23:A:ALA:HB1	1:22:A:GLN:H	2	0.31
(1,162)	1:23:A:ALA:HB3	1:22:A:GLN:H	11	0.31
(1,138)	1:102:A:THR:HG22	1:103:A:GLN:H	8	0.31
(1,136)	1:102:A:THR:HG22	1:100:A:ILE:H	12	0.31
(1,134)	1:57:A:VAL:HG21	1:58:A:CYS:H	14	0.31
(1,134)	1:57:A:VAL:HG22	1:58:A:CYS:H	15	0.31
(1,131)	1:10:A:LEU:HD21	1:11:A:ILE:H	7	0.31
(1,121)	1:70:A:VAL:HG13	1:71:A:GLU:H	6	0.31
(1,121)	1:70:A:VAL:HG11	1:71:A:GLU:H	10	0.31
(1,118)	1:13:A:LEU:HD11	1:16:A:GLU:H	3	0.31
(1,118)	1:13:A:LEU:HD13	1:16:A:GLU:H	10	0.31
(1,118)	1:13:A:LEU:HD11	1:16:A:GLU:H	11	0.31
(1,112)	1:10:A:LEU:HD12	1:11:A:ILE:H	16	0.31
(1,105)	1:29:A:VAL:HG12	1:29:A:VAL:H	13	0.31
(1,103)	1:43:A:LEU:HD22	1:46:A:SER:H	16	0.31
(1,88)	1:26:A:ILE:HD11	1:15:A:GLU:H	5	0.31
(1,83)	1:112:A:LEU:HD22	1:112:A:LEU:H	12	0.31
(1,34)	1:33:A:ILE:HG23	1:39:A:MET:H	10	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,27)	1:90:A:VAL:HG23	1:89:A:GLY:H	8	0.31
(1,12)	1:72:A:LEU:HD13	1:72:A:LEU:H	3	0.31
(1,12)	1:72:A:LEU:HD12	1:72:A:LEU:H	19	0.31
(1,2692)	1:88:A:TYR:HE2	1:88:A:TYR:HD2	10	0.3
(1,2678)	1:39:A:MET:HE3	1:44:A:PHE:HZ	12	0.3
(1,2661)	1:75:A:LYS:HA	1:75:A:LYS:HE3	7	0.3
(1,2577)	1:54:A:GLU:HG2	1:54:A:GLU:HA	19	0.3
(1,2537)	1:115:A:LEU:HD11	1:27:A:GLU:HG2	1	0.3
(1,2496)	1:36:A:ARG:HG3	1:36:A:ARG:HG2	2	0.3
(1,2496)	1:36:A:ARG:HG3	1:36:A:ARG:HG2	3	0.3
(1,2496)	1:75:A:LYS:HD2	1:75:A:LYS:HD3	7	0.3
(1,2454)	1:62:A:ILE:HG21	1:28:A:ARG:HG3	15	0.3
(1,2435)	1:72:A:LEU:HD21	1:72:A:LEU:HD23	2	0.3
(1,2435)	1:7:A:VAL:HG12	1:7:A:VAL:HG11	4	0.3
(1,2435)	1:72:A:LEU:HD22	1:72:A:LEU:HD21	7	0.3
(1,2435)	1:7:A:VAL:HG11	1:7:A:VAL:HG13	19	0.3
(1,2419)	1:69:A:LYS:HG3	1:69:A:LYS:H	20	0.3
(1,2378)	1:97:A:LYS:H	1:96:A:SER:H	11	0.3
(1,2276)	1:88:A:TYR:HE2	1:88:A:TYR:HD2	2	0.3
(1,2276)	1:88:A:TYR:HE1	1:88:A:TYR:HD1	18	0.3
(1,2262)	1:88:A:TYR:HA	1:88:A:TYR:HD1	17	0.3
(1,2246)	1:4:A:TYR:HA	1:4:A:TYR:HE2	19	0.3
(1,2239)	1:41:A:LYS:HA	1:44:A:PHE:HD2	8	0.3
(1,2171)	1:47:A:ALA:HB1	1:4:A:TYR:HE2	3	0.3
(1,2171)	1:47:A:ALA:HB3	1:4:A:TYR:HE2	18	0.3
(1,2134)	1:72:A:LEU:HD23	1:81:A:PHE:HE1	8	0.3
(1,2130)	1:72:A:LEU:HD13	1:81:A:PHE:HE2	7	0.3
(1,2130)	1:72:A:LEU:HD11	1:81:A:PHE:HE1	8	0.3
(1,2105)	1:64:A:ASP:HA	1:62:A:ILE:HG21	14	0.3
(1,2105)	1:64:A:ASP:HA	1:62:A:ILE:HG22	16	0.3
(1,2084)	1:58:A:CYS:HA	1:26:A:ILE:HG21	14	0.3
(1,2067)	1:10:A:LEU:HA	1:13:A:LEU:HG	17	0.3
(1,2061)	1:33:A:ILE:HA	1:65:A:ILE:HG22	5	0.3
(1,2058)	1:12:A:ALA:HB1	1:13:A:LEU:HA	18	0.3
(1,2053)	1:17:A:HIS:HA	1:16:A:GLU:HG2	17	0.3
(1,2052)	1:20:A:LYS:HG2	1:17:A:HIS:HA	3	0.3
(1,2052)	1:20:A:LYS:HG2	1:17:A:HIS:HA	19	0.3
(1,2035)	1:42:A:SER:HB2	1:45:A:VAL:HG23	5	0.3
(1,2035)	1:42:A:SER:HB2	1:45:A:VAL:HG23	11	0.3
(1,2016)	1:93:A:LYS:HD2	1:79:A:HIS:HB2	15	0.3
(1,1987)	1:23:A:ALA:HB3	1:21:A:ASN:HB2	20	0.3
(1,1984)	1:7:A:VAL:HG13	1:48:A:PHE:HB3	12	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1944)	1:57:A:VAL:HB	1:26:A:ILE:HD12	12	0.3
(1,1829)	1:26:A:ILE:HD11	1:23:A:ALA:HB3	13	0.3
(1,1780)	1:112:A:LEU:HD23	1:17:A:HIS:HA	4	0.3
(1,1769)	1:66:A:VAL:HG11	1:68:A:GLU:HB2	8	0.3
(1,1769)	1:66:A:VAL:HG12	1:68:A:GLU:HB2	16	0.3
(1,1765)	1:72:A:LEU:HB2	1:99:A:VAL:HB	4	0.3
(1,1748)	1:33:A:ILE:HG23	1:107:A:MET:HG3	10	0.3
(1,1727)	1:11:A:ILE:HD11	1:55:A:SER:HB3	4	0.3
(1,1677)	1:25:A:LYS:HA	1:57:A:VAL:HG21	18	0.3
(1,1644)	1:88:A:TYR:HA	1:72:A:LEU:HD21	5	0.3
(1,1561)	1:38:A:ALA:HB2	1:38:A:ALA:HA	19	0.3
(1,1561)	1:38:A:ALA:HB3	1:38:A:ALA:HA	20	0.3
(1,1445)	1:48:A:PHE:HB2	1:63:A:LEU:HD12	6	0.3
(1,1415)	1:20:A:LYS:HE2	1:20:A:LYS:HE3	7	0.3
(1,1415)	1:20:A:LYS:HE2	1:20:A:LYS:HE3	9	0.3
(1,1415)	1:20:A:LYS:HE2	1:20:A:LYS:HE3	18	0.3
(1,1415)	1:20:A:LYS:HE2	1:20:A:LYS:HE3	20	0.3
(1,1392)	1:87:A:ASP:HB2	1:87:A:ASP:HA	20	0.3
(1,1385)	1:48:A:PHE:HB3	1:63:A:LEU:HD12	2	0.3
(1,1385)	1:48:A:PHE:HB3	1:63:A:LEU:HD12	9	0.3
(1,1361)	1:26:A:ILE:HD11	1:114:A:MET:HG2	1	0.3
(1,1361)	1:26:A:ILE:HD12	1:114:A:MET:HG2	8	0.3
(1,1324)	1:106:A:GLU:HG3	1:105:A:ASN:HB2	11	0.3
(1,1140)	1:59:A:LYS:HD3	1:59:A:LYS:HA	12	0.3
(1,1081)	1:43:A:LEU:HG	1:43:A:LEU:HA	4	0.3
(1,1055)	1:108:A:ARG:HG3	1:110:A:LEU:HD23	5	0.3
(1,964)	1:41:A:LYS:HG3	1:41:A:LYS:HE3	9	0.3
(1,963)	1:41:A:LYS:HG3	1:65:A:ILE:HD13	18	0.3
(1,953)	1:65:A:ILE:HG23	1:33:A:ILE:HG12	10	0.3
(1,950)	1:45:A:VAL:HG12	1:45:A:VAL:HG11	4	0.3
(1,935)	1:102:A:THR:HG21	1:102:A:THR:HG23	12	0.3
(1,922)	1:45:A:VAL:HG22	1:45:A:VAL:HG13	1	0.3
(1,922)	1:45:A:VAL:HG21	1:45:A:VAL:HG12	14	0.3
(1,911)	1:56:A:LEU:HD12	1:56:A:LEU:HA	6	0.3
(1,911)	1:56:A:LEU:HD11	1:56:A:LEU:HA	16	0.3
(1,911)	1:56:A:LEU:HD11	1:56:A:LEU:HA	19	0.3
(1,907)	1:13:A:LEU:HD21	1:13:A:LEU:HD12	13	0.3
(1,907)	1:13:A:LEU:HD22	1:13:A:LEU:HD13	19	0.3
(1,897)	1:29:A:VAL:HG12	1:112:A:LEU:HD22	9	0.3
(1,886)	1:57:A:VAL:HG11	1:57:A:VAL:HG22	3	0.3
(1,886)	1:57:A:VAL:HG13	1:57:A:VAL:HG22	10	0.3
(1,874)	1:26:A:ILE:HG23	1:61:A:ALA:HB2	12	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,864)	1:110:A:LEU:HD12	1:30:A:VAL:HG23	20	0.3
(1,860)	1:109:A:LEU:HD22	1:31:A:VAL:HA	8	0.3
(1,845)	1:31:A:VAL:HG12	1:31:A:VAL:HG13	5	0.3
(1,845)	1:31:A:VAL:HG11	1:31:A:VAL:HG13	9	0.3
(1,845)	1:31:A:VAL:HG12	1:31:A:VAL:HG13	15	0.3
(1,845)	1:31:A:VAL:HG11	1:31:A:VAL:HG13	17	0.3
(1,826)	1:101:A:ILE:HG23	1:103:A:GLN:HA	8	0.3
(1,822)	1:80:A:VAL:HG12	1:102:A:THR:HG22	9	0.3
(1,818)	1:80:A:VAL:HG11	1:80:A:VAL:HG23	6	0.3
(1,809)	1:110:A:LEU:HD11	1:66:A:VAL:HG12	5	0.3
(1,803)	1:72:A:LEU:HD21	1:72:A:LEU:HB2	10	0.3
(1,803)	1:72:A:LEU:HD23	1:72:A:LEU:HB2	12	0.3
(1,773)	1:66:A:VAL:HG22	1:66:A:VAL:HG23	4	0.3
(1,773)	1:66:A:VAL:HG21	1:66:A:VAL:HG23	13	0.3
(1,773)	1:66:A:VAL:HG22	1:66:A:VAL:HG21	15	0.3
(1,773)	1:66:A:VAL:HG21	1:66:A:VAL:HG23	18	0.3
(1,772)	1:66:A:VAL:HG21	1:64:A:ASP:HB2	18	0.3
(1,437)	1:24:A:HIS:HB3	1:25:A:LYS:H	13	0.3
(1,358)	1:22:A:GLN:HB2	1:23:A:ALA:H	1	0.3
(1,213)	1:75:A:LYS:HD3	1:75:A:LYS:H	6	0.3
(1,213)	1:75:A:LYS:HD3	1:75:A:LYS:H	10	0.3
(1,196)	1:12:A:ALA:HB2	1:14:A:CYS:H	1	0.3
(1,174)	1:100:A:ILE:HG12	1:101:A:ILE:H	2	0.3
(1,174)	1:100:A:ILE:HG12	1:101:A:ILE:H	10	0.3
(1,174)	1:100:A:ILE:HG12	1:101:A:ILE:H	13	0.3
(1,174)	1:100:A:ILE:HG12	1:101:A:ILE:H	14	0.3
(1,174)	1:100:A:ILE:HG12	1:101:A:ILE:H	19	0.3
(1,162)	1:23:A:ALA:HB1	1:22:A:GLN:H	8	0.3
(1,156)	1:23:A:ALA:HB1	1:21:A:ASN:H	5	0.3
(1,156)	1:23:A:ALA:HB1	1:21:A:ASN:H	7	0.3
(1,136)	1:102:A:THR:HG21	1:100:A:ILE:H	10	0.3
(1,136)	1:102:A:THR:HG21	1:100:A:ILE:H	14	0.3
(1,131)	1:10:A:LEU:HD21	1:11:A:ILE:H	11	0.3
(1,121)	1:70:A:VAL:HG13	1:71:A:GLU:H	16	0.3
(1,121)	1:70:A:VAL:HG12	1:71:A:GLU:H	20	0.3
(1,118)	1:13:A:LEU:HD12	1:16:A:GLU:H	5	0.3
(1,112)	1:10:A:LEU:HD11	1:11:A:ILE:H	5	0.3
(1,112)	1:10:A:LEU:HD11	1:11:A:ILE:H	13	0.3
(1,105)	1:29:A:VAL:HG11	1:29:A:VAL:H	17	0.3
(1,83)	1:112:A:LEU:HD22	1:112:A:LEU:H	11	0.3
(1,74)	1:99:A:VAL:HG23	1:73:A:GLU:H	20	0.3
(1,72)	1:31:A:VAL:HG11	1:108:A:ARG:H	7	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,72)	1:31:A:VAL:HG11	1:108:A:ARG:H	14	0.3
(1,71)	1:31:A:VAL:HG13	1:32:A:GLY:H	19	0.3
(1,36)	1:99:A:VAL:HG11	1:100:A:ILE:H	14	0.3
(1,29)	1:70:A:VAL:HG21	1:72:A:LEU:H	16	0.3
(1,23)	1:110:A:LEU:HD12	1:111:A:SER:H	20	0.3
(1,2692)	1:4:A:TYR:HE1	1:4:A:TYR:HD1	11	0.29
(1,2692)	1:4:A:TYR:HE1	1:4:A:TYR:HD1	13	0.29
(1,2678)	1:107:A:MET:HE1	1:44:A:PHE:HZ	7	0.29
(1,2496)	1:36:A:ARG:HG3	1:36:A:ARG:HG2	4	0.29
(1,2496)	1:36:A:ARG:HG3	1:36:A:ARG:HG2	8	0.29
(1,2496)	1:75:A:LYS:HD2	1:75:A:LYS:HD3	10	0.29
(1,2496)	1:36:A:ARG:HG3	1:36:A:ARG:HG2	11	0.29
(1,2496)	1:75:A:LYS:HD2	1:75:A:LYS:HD3	14	0.29
(1,2496)	1:36:A:ARG:HG3	1:36:A:ARG:HG2	18	0.29
(1,2469)	1:6:A:VAL:HG11	1:39:A:MET:HE2	7	0.29
(1,2469)	1:6:A:VAL:HG13	1:107:A:MET:HE3	15	0.29
(1,2469)	1:6:A:VAL:HG12	1:39:A:MET:HE1	17	0.29
(1,2444)	1:80:A:VAL:HG12	1:73:A:GLU:HA	7	0.29
(1,2442)	1:31:A:VAL:HG21	1:31:A:VAL:HG12	9	0.29
(1,2435)	1:7:A:VAL:HG12	1:7:A:VAL:HG11	10	0.29
(1,2435)	1:7:A:VAL:HG11	1:7:A:VAL:HG13	12	0.29
(1,2435)	1:7:A:VAL:HG12	1:7:A:VAL:HG13	17	0.29
(1,2419)	1:69:A:LYS:HG3	1:69:A:LYS:H	1	0.29
(1,2396)	1:101:A:ILE:H	1:100:A:ILE:H	4	0.29
(1,2378)	1:97:A:LYS:H	1:96:A:SER:H	10	0.29
(1,2294)	1:99:A:VAL:H	1:100:A:ILE:H	8	0.29
(1,2279)	1:4:A:TYR:HE1	1:4:A:TYR:HD1	11	0.29
(1,2279)	1:4:A:TYR:HE1	1:4:A:TYR:HD1	13	0.29
(1,2276)	1:88:A:TYR:HE1	1:88:A:TYR:HD1	8	0.29
(1,2276)	1:88:A:TYR:HE2	1:88:A:TYR:HD2	12	0.29
(1,2276)	1:88:A:TYR:HE1	1:88:A:TYR:HD1	19	0.29
(1,2246)	1:4:A:TYR:HA	1:4:A:TYR:HE1	13	0.29
(1,2239)	1:41:A:LYS:HA	1:44:A:PHE:HD2	7	0.29
(1,2231)	1:4:A:TYR:HB3	1:51:A:PHE:HD1	19	0.29
(1,2172)	1:47:A:ALA:HB2	1:4:A:TYR:HD1	17	0.29
(1,2166)	1:50:A:THR:HG22	1:51:A:PHE:HE1	10	0.29
(1,2157)	1:43:A:LEU:HD21	1:4:A:TYR:HE2	10	0.29
(1,2143)	1:7:A:VAL:HG22	1:51:A:PHE:HD1	6	0.29
(1,2142)	1:7:A:VAL:HG22	1:48:A:PHE:HD1	2	0.29
(1,2133)	1:65:A:ILE:HG22	1:44:A:PHE:HD1	15	0.29
(1,2105)	1:64:A:ASP:HA	1:62:A:ILE:HG23	1	0.29
(1,2069)	1:112:A:LEU:HD21	1:29:A:VAL:HA	15	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2058)	1:12:A:ALA:HB2	1:13:A:LEU:HA	15	0.29
(1,2058)	1:12:A:ALA:HB1	1:13:A:LEU:HA	19	0.29
(1,2058)	1:12:A:ALA:HB1	1:13:A:LEU:HA	20	0.29
(1,2041)	1:16:A:GLU:HA	1:17:A:HIS:HA	10	0.29
(1,2030)	1:83:A:PRO:HD2	1:72:A:LEU:HD11	16	0.29
(1,2024)	1:107:A:MET:HE3	1:7:A:VAL:HA	11	0.29
(1,2024)	1:107:A:MET:HE1	1:7:A:VAL:HA	17	0.29
(1,1987)	1:23:A:ALA:HB2	1:21:A:ASN:HB2	6	0.29
(1,1984)	1:7:A:VAL:HG13	1:48:A:PHE:HB3	2	0.29
(1,1984)	1:7:A:VAL:HG11	1:48:A:PHE:HB3	15	0.29
(1,1938)	1:71:A:GLU:HG2	1:103:A:GLN:HG2	15	0.29
(1,1847)	1:110:A:LEU:HD23	1:110:A:LEU:HB2	8	0.29
(1,1842)	1:18:A:ALA:HB3	1:21:A:ASN:HB3	7	0.29
(1,1842)	1:18:A:ALA:HB1	1:21:A:ASN:HB3	14	0.29
(1,1799)	1:29:A:VAL:HG12	1:109:A:LEU:HD13	17	0.29
(1,1749)	1:65:A:ILE:HG13	1:63:A:LEU:HD23	17	0.29
(1,1727)	1:11:A:ILE:HD12	1:55:A:SER:HB3	13	0.29
(1,1707)	1:107:A:MET:HG3	1:107:A:MET:HA	8	0.29
(1,1677)	1:25:A:LYS:HA	1:57:A:VAL:HG22	19	0.29
(1,1619)	1:85:A:ALA:HB2	1:85:A:ALA:HA	6	0.29
(1,1619)	1:85:A:ALA:HB1	1:85:A:ALA:HA	12	0.29
(1,1618)	1:50:A:THR:HG21	1:51:A:PHE:HA	1	0.29
(1,1618)	1:50:A:THR:HG21	1:51:A:PHE:HA	12	0.29
(1,1601)	1:12:A:ALA:HB1	1:9:A:SER:HA	5	0.29
(1,1576)	1:35:A:GLU:HG3	1:69:A:LYS:HA	5	0.29
(1,1561)	1:38:A:ALA:HB1	1:38:A:ALA:HA	15	0.29
(1,1547)	1:23:A:ALA:HB3	1:18:A:ALA:HA	11	0.29
(1,1507)	1:26:A:ILE:HD13	1:14:A:CYS:HA	18	0.29
(1,1499)	1:6:A:VAL:HG23	1:3:A:GLU:HA	13	0.29
(1,1474)	1:41:A:LYS:HA	1:41:A:LYS:HE2	13	0.29
(1,1452)	1:63:A:LEU:HD13	1:45:A:VAL:HA	11	0.29
(1,1415)	1:20:A:LYS:HE2	1:20:A:LYS:HE3	4	0.29
(1,1415)	1:20:A:LYS:HE2	1:20:A:LYS:HE3	5	0.29
(1,1415)	1:20:A:LYS:HE2	1:20:A:LYS:HE3	6	0.29
(1,1415)	1:20:A:LYS:HE2	1:20:A:LYS:HE3	8	0.29
(1,1415)	1:20:A:LYS:HE2	1:20:A:LYS:HE3	15	0.29
(1,1410)	1:84:A:ASN:HB3	1:84:A:ASN:HA	18	0.29
(1,1354)	1:1:A:MET:HG2	1:1:A:MET:HA	2	0.29
(1,1354)	1:1:A:MET:HG2	1:1:A:MET:HA	12	0.29
(1,1249)	1:72:A:LEU:HD11	1:83:A:PRO:HG2	8	0.29
(1,1217)	1:72:A:LEU:HD11	1:99:A:VAL:HB	1	0.29
(1,1145)	1:41:A:LYS:HD2	1:33:A:ILE:HG21	4	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1140)	1:59:A:LYS:HD3	1:59:A:LYS:HA	2	0.29
(1,1081)	1:43:A:LEU:HG	1:43:A:LEU:HA	10	0.29
(1,1081)	1:43:A:LEU:HG	1:43:A:LEU:HA	11	0.29
(1,1081)	1:43:A:LEU:HG	1:43:A:LEU:HA	13	0.29
(1,1081)	1:43:A:LEU:HG	1:43:A:LEU:HA	20	0.29
(1,950)	1:45:A:VAL:HG11	1:45:A:VAL:HG13	2	0.29
(1,950)	1:45:A:VAL:HG11	1:45:A:VAL:HG13	3	0.29
(1,950)	1:45:A:VAL:HG12	1:45:A:VAL:HG11	6	0.29
(1,950)	1:45:A:VAL:HG11	1:45:A:VAL:HG13	8	0.29
(1,950)	1:45:A:VAL:HG12	1:45:A:VAL:HG13	20	0.29
(1,948)	1:45:A:VAL:HG13	1:42:A:SER:HA	5	0.29
(1,940)	1:112:A:LEU:HD11	1:112:A:LEU:HA	13	0.29
(1,933)	1:102:A:THR:HG23	1:100:A:ILE:HG13	20	0.29
(1,911)	1:56:A:LEU:HD11	1:56:A:LEU:HA	5	0.29
(1,911)	1:56:A:LEU:HD12	1:56:A:LEU:HA	7	0.29
(1,911)	1:56:A:LEU:HD13	1:56:A:LEU:HA	13	0.29
(1,910)	1:109:A:LEU:HD12	1:13:A:LEU:HD12	11	0.29
(1,904)	1:31:A:VAL:HG12	1:10:A:LEU:HD11	10	0.29
(1,889)	1:57:A:VAL:HG11	1:15:A:GLU:HG3	14	0.29
(1,886)	1:57:A:VAL:HG11	1:57:A:VAL:HG22	9	0.29
(1,862)	1:109:A:LEU:HD22	1:13:A:LEU:HD21	6	0.29
(1,860)	1:109:A:LEU:HD23	1:31:A:VAL:HA	7	0.29
(1,858)	1:109:A:LEU:HD21	1:109:A:LEU:HD23	2	0.29
(1,858)	1:109:A:LEU:HD21	1:109:A:LEU:HD23	3	0.29
(1,858)	1:109:A:LEU:HD22	1:109:A:LEU:HD23	4	0.29
(1,845)	1:31:A:VAL:HG11	1:31:A:VAL:HG13	1	0.29
(1,845)	1:31:A:VAL:HG12	1:31:A:VAL:HG13	3	0.29
(1,845)	1:31:A:VAL:HG12	1:31:A:VAL:HG13	12	0.29
(1,845)	1:31:A:VAL:HG12	1:31:A:VAL:HG11	16	0.29
(1,845)	1:31:A:VAL:HG11	1:31:A:VAL:HG13	19	0.29
(1,831)	1:101:A:ILE:HG21	1:101:A:ILE:HG23	5	0.29
(1,831)	1:101:A:ILE:HG21	1:101:A:ILE:HG23	10	0.29
(1,773)	1:66:A:VAL:HG22	1:66:A:VAL:HG23	9	0.29
(1,773)	1:66:A:VAL:HG21	1:66:A:VAL:HG23	12	0.29
(1,773)	1:66:A:VAL:HG21	1:66:A:VAL:HG23	17	0.29
(1,773)	1:66:A:VAL:HG22	1:66:A:VAL:HG21	19	0.29
(1,754)	1:33:A:ILE:HG13	1:33:A:ILE:HG23	17	0.29
(1,754)	1:33:A:ILE:HG13	1:33:A:ILE:HG22	19	0.29
(1,448)	1:79:A:HIS:HB2	1:80:A:VAL:H	2	0.29
(1,371)	1:22:A:GLN:HG3	1:21:A:ASN:H	3	0.29
(1,358)	1:22:A:GLN:HB2	1:23:A:ALA:H	15	0.29
(1,300)	1:107:A:MET:HE1	1:108:A:ARG:H	3	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,299)	1:39:A:MET:HE2	1:6:A:VAL:H	10	0.29
(1,196)	1:12:A:ALA:HB3	1:14:A:CYS:H	13	0.29
(1,196)	1:12:A:ALA:HB3	1:14:A:CYS:H	15	0.29
(1,196)	1:12:A:ALA:HB1	1:14:A:CYS:H	18	0.29
(1,162)	1:23:A:ALA:HB2	1:22:A:GLN:H	12	0.29
(1,162)	1:23:A:ALA:HB3	1:22:A:GLN:H	18	0.29
(1,138)	1:102:A:THR:HG21	1:103:A:GLN:H	10	0.29
(1,136)	1:102:A:THR:HG23	1:100:A:ILE:H	3	0.29
(1,134)	1:57:A:VAL:HG21	1:58:A:CYS:H	12	0.29
(1,134)	1:57:A:VAL:HG21	1:58:A:CYS:H	20	0.29
(1,112)	1:10:A:LEU:HD11	1:11:A:ILE:H	2	0.29
(1,105)	1:29:A:VAL:HG12	1:29:A:VAL:H	10	0.29
(1,105)	1:29:A:VAL:HG12	1:29:A:VAL:H	11	0.29
(1,103)	1:43:A:LEU:HD23	1:46:A:SER:H	5	0.29
(1,95)	1:93:A:LYS:HB3	1:93:A:LYS:H	18	0.29
(1,83)	1:112:A:LEU:HD21	1:112:A:LEU:H	17	0.29
(1,71)	1:31:A:VAL:HG11	1:32:A:GLY:H	18	0.29
(1,70)	1:112:A:LEU:HD23	1:17:A:HIS:H	15	0.29
(1,36)	1:99:A:VAL:HG13	1:100:A:ILE:H	2	0.29
(1,36)	1:99:A:VAL:HG12	1:100:A:ILE:H	7	0.29
(1,29)	1:70:A:VAL:HG23	1:72:A:LEU:H	1	0.29
(1,12)	1:72:A:LEU:HD12	1:72:A:LEU:H	15	0.29
(1,2692)	1:4:A:TYR:HE2	1:4:A:TYR:HD2	4	0.28
(1,2692)	1:4:A:TYR:HE2	1:4:A:TYR:HD2	9	0.28
(1,2692)	1:88:A:TYR:HE2	1:88:A:TYR:HD2	12	0.28
(1,2507)	1:20:A:LYS:HD2	1:20:A:LYS:HD3	1	0.28
(1,2507)	1:82:A:LYS:HD2	1:82:A:LYS:HD3	4	0.28
(1,2507)	1:82:A:LYS:HD2	1:82:A:LYS:HD3	6	0.28
(1,2507)	1:82:A:LYS:HD2	1:82:A:LYS:HD3	7	0.28
(1,2507)	1:20:A:LYS:HD2	1:20:A:LYS:HD3	13	0.28
(1,2507)	1:82:A:LYS:HD2	1:82:A:LYS:HD3	15	0.28
(1,2507)	1:82:A:LYS:HD2	1:82:A:LYS:HD3	19	0.28
(1,2496)	1:75:A:LYS:HD2	1:75:A:LYS:HD3	5	0.28
(1,2496)	1:36:A:ARG:HG3	1:36:A:ARG:HG2	12	0.28
(1,2496)	1:36:A:ARG:HG3	1:36:A:ARG:HG2	19	0.28
(1,2496)	1:36:A:ARG:HG3	1:36:A:ARG:HG2	20	0.28
(1,2465)	1:10:A:LEU:HD21	1:7:A:VAL:HG21	6	0.28
(1,2442)	1:31:A:VAL:HG22	1:31:A:VAL:HG12	20	0.28
(1,2438)	1:65:A:ILE:HD13	1:41:A:LYS:HD2	19	0.28
(1,2435)	1:7:A:VAL:HG12	1:7:A:VAL:HG13	16	0.28
(1,2435)	1:72:A:LEU:HD22	1:72:A:LEU:HD21	18	0.28
(1,2422)	1:47:A:ALA:HB2	1:7:A:VAL:H	1	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2422)	1:47:A:ALA:HB2	1:7:A:VAL:H	5	0.28
(1,2294)	1:99:A:VAL:H	1:100:A:ILE:H	20	0.28
(1,2279)	1:4:A:TYR:HE2	1:4:A:TYR:HD2	4	0.28
(1,2279)	1:4:A:TYR:HE2	1:4:A:TYR:HD2	5	0.28
(1,2279)	1:4:A:TYR:HE2	1:4:A:TYR:HD2	9	0.28
(1,2279)	1:4:A:TYR:HE1	1:4:A:TYR:HD1	17	0.28
(1,2246)	1:4:A:TYR:HA	1:4:A:TYR:HE2	2	0.28
(1,2180)	1:61:A:ALA:HB3	1:48:A:PHE:HD2	18	0.28
(1,2166)	1:50:A:THR:HG23	1:51:A:PHE:HE1	6	0.28
(1,2160)	1:80:A:VAL:HG22	1:81:A:PHE:HD1	2	0.28
(1,2158)	1:29:A:VAL:HG12	1:48:A:PHE:HZ	2	0.28
(1,2148)	1:80:A:VAL:HG12	1:81:A:PHE:HD2	7	0.28
(1,2148)	1:80:A:VAL:HG12	1:81:A:PHE:HD2	15	0.28
(1,2142)	1:7:A:VAL:HG21	1:48:A:PHE:HD2	19	0.28
(1,2130)	1:72:A:LEU:HD12	1:81:A:PHE:HE2	19	0.28
(1,2121)	1:63:A:LEU:HD21	1:48:A:PHE:HD1	9	0.28
(1,2105)	1:64:A:ASP:HA	1:62:A:ILE:HG23	11	0.28
(1,2088)	1:105:A:ASN:HA	1:36:A:ARG:HB3	4	0.28
(1,2088)	1:105:A:ASN:HA	1:36:A:ARG:HB3	7	0.28
(1,2071)	1:26:A:ILE:HG22	1:29:A:VAL:HA	19	0.28
(1,2061)	1:33:A:ILE:HA	1:65:A:ILE:HG23	16	0.28
(1,2053)	1:17:A:HIS:HA	1:16:A:GLU:HG2	7	0.28
(1,2052)	1:20:A:LYS:HG2	1:17:A:HIS:HA	2	0.28
(1,2051)	1:114:A:MET:HE3	1:17:A:HIS:HA	13	0.28
(1,2041)	1:16:A:GLU:HA	1:17:A:HIS:HA	13	0.28
(1,2018)	1:90:A:VAL:HG12	1:95:A:HIS:HB3	7	0.28
(1,1984)	1:7:A:VAL:HG13	1:48:A:PHE:HB3	14	0.28
(1,1845)	1:38:A:ALA:HB3	1:39:A:MET:HA	3	0.28
(1,1845)	1:38:A:ALA:HB1	1:39:A:MET:HA	18	0.28
(1,1819)	1:7:A:VAL:HG13	1:47:A:ALA:HB1	16	0.28
(1,1798)	1:62:A:ILE:HD11	1:28:A:ARG:HD3	4	0.28
(1,1771)	1:31:A:VAL:HG22	1:65:A:ILE:HB	6	0.28
(1,1727)	1:11:A:ILE:HD13	1:55:A:SER:HB3	10	0.28
(1,1677)	1:25:A:LYS:HA	1:57:A:VAL:HG23	20	0.28
(1,1561)	1:38:A:ALA:HB1	1:38:A:ALA:HA	14	0.28
(1,1554)	1:20:A:LYS:HE3	1:17:A:HIS:HA	4	0.28
(1,1482)	1:7:A:VAL:HG22	1:48:A:PHE:HA	6	0.28
(1,1474)	1:41:A:LYS:HA	1:41:A:LYS:HE2	12	0.28
(1,1462)	1:11:A:ILE:HD13	1:52:A:ARG:HA	9	0.28
(1,1452)	1:63:A:LEU:HD11	1:45:A:VAL:HA	12	0.28
(1,1429)	1:59:A:LYS:HB2	1:59:A:LYS:HE3	11	0.28
(1,1415)	1:20:A:LYS:HE2	1:20:A:LYS:HE3	1	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1415)	1:20:A:LYS:HE2	1:20:A:LYS:HE3	10	0.28
(1,1415)	1:20:A:LYS:HE2	1:20:A:LYS:HE3	11	0.28
(1,1415)	1:20:A:LYS:HE2	1:20:A:LYS:HE3	14	0.28
(1,1415)	1:20:A:LYS:HE2	1:20:A:LYS:HE3	16	0.28
(1,1415)	1:20:A:LYS:HE2	1:20:A:LYS:HE3	17	0.28
(1,1303)	1:23:A:ALA:HB3	1:114:A:MET:HB2	3	0.28
(1,1269)	1:80:A:VAL:HG21	1:73:A:GLU:HG2	15	0.28
(1,1211)	1:75:A:LYS:HB3	1:98:A:ASN:HB2	8	0.28
(1,1145)	1:41:A:LYS:HD2	1:33:A:ILE:HG23	20	0.28
(1,1081)	1:43:A:LEU:HG	1:43:A:LEU:HA	14	0.28
(1,1081)	1:43:A:LEU:HG	1:43:A:LEU:HA	15	0.28
(1,1081)	1:43:A:LEU:HG	1:43:A:LEU:HA	17	0.28
(1,1024)	1:57:A:VAL:HG12	1:18:A:ALA:HB1	5	0.28
(1,998)	1:65:A:ILE:HG12	1:63:A:LEU:HD23	6	0.28
(1,980)	1:23:A:ALA:HB1	1:23:A:ALA:HB3	20	0.28
(1,963)	1:41:A:LYS:HG3	1:65:A:ILE:HD13	6	0.28
(1,962)	1:33:A:ILE:HD12	1:41:A:LYS:HG3	3	0.28
(1,953)	1:65:A:ILE:HG22	1:33:A:ILE:HG12	1	0.28
(1,953)	1:65:A:ILE:HG23	1:33:A:ILE:HG12	17	0.28
(1,950)	1:45:A:VAL:HG11	1:45:A:VAL:HG13	1	0.28
(1,950)	1:45:A:VAL:HG12	1:45:A:VAL:HG13	18	0.28
(1,950)	1:45:A:VAL:HG12	1:45:A:VAL:HG13	19	0.28
(1,922)	1:45:A:VAL:HG22	1:45:A:VAL:HG11	17	0.28
(1,911)	1:56:A:LEU:HD13	1:56:A:LEU:HA	20	0.28
(1,907)	1:13:A:LEU:HD22	1:13:A:LEU:HD13	6	0.28
(1,907)	1:13:A:LEU:HD23	1:13:A:LEU:HD13	18	0.28
(1,898)	1:29:A:VAL:HG12	1:112:A:LEU:HA	5	0.28
(1,897)	1:29:A:VAL:HG12	1:112:A:LEU:HD23	14	0.28
(1,886)	1:57:A:VAL:HG12	1:57:A:VAL:HG23	5	0.28
(1,864)	1:110:A:LEU:HD11	1:30:A:VAL:HG22	11	0.28
(1,864)	1:110:A:LEU:HD12	1:30:A:VAL:HG22	15	0.28
(1,864)	1:110:A:LEU:HD12	1:30:A:VAL:HG23	17	0.28
(1,858)	1:109:A:LEU:HD21	1:109:A:LEU:HD23	5	0.28
(1,858)	1:109:A:LEU:HD22	1:109:A:LEU:HD21	8	0.28
(1,858)	1:109:A:LEU:HD21	1:109:A:LEU:HD23	12	0.28
(1,858)	1:109:A:LEU:HD22	1:109:A:LEU:HD21	17	0.28
(1,849)	1:72:A:LEU:HD22	1:101:A:ILE:HG13	19	0.28
(1,845)	1:31:A:VAL:HG12	1:31:A:VAL:HG13	6	0.28
(1,845)	1:31:A:VAL:HG11	1:31:A:VAL:HG13	13	0.28
(1,845)	1:31:A:VAL:HG12	1:31:A:VAL:HG13	14	0.28
(1,845)	1:31:A:VAL:HG11	1:31:A:VAL:HG13	18	0.28
(1,844)	1:112:A:LEU:HD23	1:114:A:MET:HE1	17	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,831)	1:101:A:ILE:HG21	1:101:A:ILE:HG23	1	0.28
(1,831)	1:101:A:ILE:HG22	1:101:A:ILE:HG23	4	0.28
(1,831)	1:101:A:ILE:HG22	1:101:A:ILE:HG23	7	0.28
(1,831)	1:101:A:ILE:HG22	1:101:A:ILE:HG23	8	0.28
(1,831)	1:101:A:ILE:HG21	1:101:A:ILE:HG23	11	0.28
(1,831)	1:101:A:ILE:HG21	1:101:A:ILE:HG23	12	0.28
(1,831)	1:101:A:ILE:HG22	1:101:A:ILE:HG23	17	0.28
(1,831)	1:101:A:ILE:HG22	1:101:A:ILE:HG21	18	0.28
(1,831)	1:101:A:ILE:HG22	1:101:A:ILE:HG23	19	0.28
(1,831)	1:101:A:ILE:HG22	1:101:A:ILE:HG21	20	0.28
(1,826)	1:101:A:ILE:HG21	1:103:A:GLN:HA	5	0.28
(1,818)	1:80:A:VAL:HG12	1:80:A:VAL:HG23	3	0.28
(1,818)	1:80:A:VAL:HG11	1:80:A:VAL:HG23	8	0.28
(1,818)	1:80:A:VAL:HG11	1:80:A:VAL:HG22	15	0.28
(1,818)	1:80:A:VAL:HG12	1:80:A:VAL:HG23	19	0.28
(1,803)	1:72:A:LEU:HD23	1:72:A:LEU:HB2	1	0.28
(1,803)	1:72:A:LEU:HD23	1:72:A:LEU:HB2	19	0.28
(1,803)	1:72:A:LEU:HD21	1:72:A:LEU:HB2	20	0.28
(1,780)	1:99:A:VAL:HG11	1:99:A:VAL:HG21	20	0.28
(1,773)	1:66:A:VAL:HG22	1:66:A:VAL:HG21	20	0.28
(1,746)	1:72:A:LEU:HD13	1:83:A:PRO:HB2	3	0.28
(1,741)	1:72:A:LEU:HD12	1:72:A:LEU:HD11	7	0.28
(1,741)	1:72:A:LEU:HD11	1:72:A:LEU:HD13	16	0.28
(1,689)	1:97:A:LYS:HA	1:99:A:VAL:H	18	0.28
(1,449)	1:79:A:HIS:HB2	1:79:A:HIS:H	14	0.28
(1,448)	1:79:A:HIS:HB2	1:80:A:VAL:H	9	0.28
(1,448)	1:79:A:HIS:HB2	1:80:A:VAL:H	11	0.28
(1,438)	1:79:A:HIS:HB3	1:79:A:HIS:H	18	0.28
(1,437)	1:24:A:HIS:HB3	1:25:A:LYS:H	14	0.28
(1,358)	1:22:A:GLN:HB2	1:23:A:ALA:H	6	0.28
(1,358)	1:22:A:GLN:HB2	1:23:A:ALA:H	13	0.28
(1,358)	1:22:A:GLN:HB2	1:23:A:ALA:H	18	0.28
(1,358)	1:22:A:GLN:HB2	1:23:A:ALA:H	19	0.28
(1,239)	1:19:A:LYS:HD2	1:20:A:LYS:H	1	0.28
(1,239)	1:19:A:LYS:HD2	1:20:A:LYS:H	5	0.28
(1,225)	1:92:A:GLU:HG2	1:93:A:LYS:H	6	0.28
(1,222)	1:101:A:ILE:HG12	1:101:A:ILE:H	12	0.28
(1,196)	1:12:A:ALA:HB1	1:14:A:CYS:H	8	0.28
(1,174)	1:100:A:ILE:HG12	1:101:A:ILE:H	3	0.28
(1,162)	1:23:A:ALA:HB3	1:22:A:GLN:H	13	0.28
(1,156)	1:23:A:ALA:HB1	1:21:A:ASN:H	17	0.28
(1,142)	1:47:A:ALA:HB1	1:46:A:SER:H	7	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,142)	1:47:A:ALA:HB3	1:46:A:SER:H	17	0.28
(1,135)	1:100:A:ILE:HG13	1:100:A:ILE:H	15	0.28
(1,134)	1:57:A:VAL:HG22	1:58:A:CYS:H	5	0.28
(1,134)	1:57:A:VAL:HG23	1:58:A:CYS:H	9	0.28
(1,131)	1:10:A:LEU:HD22	1:11:A:ILE:H	15	0.28
(1,112)	1:10:A:LEU:HD12	1:11:A:ILE:H	11	0.28
(1,83)	1:112:A:LEU:HD22	1:112:A:LEU:H	15	0.28
(1,39)	1:90:A:VAL:HG13	1:90:A:VAL:H	18	0.28
(1,36)	1:99:A:VAL:HG13	1:100:A:ILE:H	20	0.28
(1,34)	1:33:A:ILE:HG23	1:39:A:MET:H	12	0.28
(1,12)	1:72:A:LEU:HD11	1:72:A:LEU:H	17	0.28
(1,2692)	1:4:A:TYR:HE1	1:4:A:TYR:HD1	14	0.27
(1,2692)	1:4:A:TYR:HE1	1:4:A:TYR:HD1	15	0.27
(1,2692)	1:4:A:TYR:HE1	1:4:A:TYR:HD1	17	0.27
(1,2692)	1:4:A:TYR:HE2	1:4:A:TYR:HD2	19	0.27
(1,2679)	1:7:A:VAL:HB	1:48:A:PHE:HD1	9	0.27
(1,2671)	1:115:A:LEU:HD11	1:24:A:HIS:HD2	4	0.27
(1,2661)	1:75:A:LYS:HA	1:75:A:LYS:HE3	20	0.27
(1,2653)	1:41:A:LYS:HD3	1:41:A:LYS:HA	1	0.27
(1,2618)	1:6:A:VAL:HG22	1:2:A:HIS:HB2	6	0.27
(1,2608)	1:115:A:LEU:HD23	1:27:A:GLU:HB2	10	0.27
(1,2507)	1:20:A:LYS:HD2	1:20:A:LYS:HD3	3	0.27
(1,2507)	1:82:A:LYS:HD2	1:82:A:LYS:HD3	5	0.27
(1,2507)	1:82:A:LYS:HD2	1:82:A:LYS:HD3	9	0.27
(1,2507)	1:20:A:LYS:HD2	1:20:A:LYS:HD3	10	0.27
(1,2507)	1:20:A:LYS:HD2	1:20:A:LYS:HD3	11	0.27
(1,2507)	1:82:A:LYS:HD2	1:82:A:LYS:HD3	12	0.27
(1,2507)	1:20:A:LYS:HD2	1:20:A:LYS:HD3	14	0.27
(1,2507)	1:20:A:LYS:HD2	1:20:A:LYS:HD3	16	0.27
(1,2507)	1:82:A:LYS:HD2	1:82:A:LYS:HD3	18	0.27
(1,2503)	1:36:A:ARG:HG3	1:36:A:ARG:HG2	3	0.27
(1,2503)	1:36:A:ARG:HG3	1:36:A:ARG:HG2	4	0.27
(1,2503)	1:69:A:LYS:HD2	1:69:A:LYS:HD3	7	0.27
(1,2503)	1:75:A:LYS:HD2	1:75:A:LYS:HD3	10	0.27
(1,2503)	1:36:A:ARG:HG3	1:36:A:ARG:HG2	11	0.27
(1,2496)	1:75:A:LYS:HD2	1:75:A:LYS:HD3	6	0.27
(1,2496)	1:36:A:ARG:HG3	1:36:A:ARG:HG2	9	0.27
(1,2496)	1:75:A:LYS:HD2	1:75:A:LYS:HD3	13	0.27
(1,2496)	1:36:A:ARG:HG3	1:36:A:ARG:HG2	15	0.27
(1,2465)	1:31:A:VAL:HG12	1:10:A:LEU:HD23	17	0.27
(1,2450)	1:99:A:VAL:HG21	1:99:A:VAL:HG23	9	0.27
(1,2450)	1:99:A:VAL:HG22	1:99:A:VAL:HG23	15	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2450)	1:30:A:VAL:HG22	1:30:A:VAL:HG21	16	0.27
(1,2450)	1:30:A:VAL:HG22	1:30:A:VAL:HG23	18	0.27
(1,2442)	1:31:A:VAL:HG21	1:31:A:VAL:HG12	15	0.27
(1,2396)	1:101:A:ILE:H	1:100:A:ILE:H	6	0.27
(1,2396)	1:101:A:ILE:H	1:100:A:ILE:H	8	0.27
(1,2378)	1:97:A:LYS:H	1:96:A:SER:H	12	0.27
(1,2378)	1:97:A:LYS:H	1:96:A:SER:H	17	0.27
(1,2378)	1:97:A:LYS:H	1:96:A:SER:H	18	0.27
(1,2294)	1:99:A:VAL:H	1:100:A:ILE:H	3	0.27
(1,2287)	1:80:A:VAL:H	1:81:A:PHE:H	16	0.27
(1,2279)	1:4:A:TYR:HE1	1:4:A:TYR:HD1	7	0.27
(1,2279)	1:4:A:TYR:HE1	1:4:A:TYR:HD1	14	0.27
(1,2279)	1:4:A:TYR:HE1	1:4:A:TYR:HD1	15	0.27
(1,2279)	1:4:A:TYR:HE2	1:4:A:TYR:HD2	16	0.27
(1,2279)	1:4:A:TYR:HE2	1:4:A:TYR:HD2	19	0.27
(1,2246)	1:4:A:TYR:HA	1:4:A:TYR:HE1	6	0.27
(1,2239)	1:41:A:LYS:HA	1:44:A:PHE:HD2	12	0.27
(1,2183)	1:116:A:ALA:HB3	1:24:A:HIS:HD2	7	0.27
(1,2183)	1:116:A:ALA:HB1	1:24:A:HIS:HD2	12	0.27
(1,2170)	1:92:A:GLU:HG3	1:81:A:PHE:HD1	20	0.27
(1,2153)	1:99:A:VAL:HG21	1:81:A:PHE:HE1	3	0.27
(1,2143)	1:7:A:VAL:HG22	1:51:A:PHE:HD1	19	0.27
(1,2143)	1:7:A:VAL:HG22	1:51:A:PHE:HD1	20	0.27
(1,2136)	1:70:A:VAL:HG23	1:88:A:TYR:HE2	2	0.27
(1,2061)	1:33:A:ILE:HA	1:65:A:ILE:HG23	15	0.27
(1,2052)	1:20:A:LYS:HG2	1:17:A:HIS:HA	7	0.27
(1,2052)	1:20:A:LYS:HG2	1:17:A:HIS:HA	17	0.27
(1,2050)	1:17:A:HIS:HA	1:16:A:GLU:HB2	14	0.27
(1,2050)	1:17:A:HIS:HA	1:16:A:GLU:HB2	19	0.27
(1,2041)	1:16:A:GLU:HA	1:17:A:HIS:HA	5	0.27
(1,2041)	1:16:A:GLU:HA	1:17:A:HIS:HA	20	0.27
(1,2024)	1:107:A:MET:HE2	1:7:A:VAL:HA	16	0.27
(1,1987)	1:23:A:ALA:HB2	1:21:A:ASN:HB2	10	0.27
(1,1982)	1:106:A:GLU:HG3	1:105:A:ASN:HB3	15	0.27
(1,1962)	1:97:A:LYS:HB2	1:90:A:VAL:HG13	6	0.27
(1,1931)	1:65:A:ILE:HD13	1:41:A:LYS:HB2	14	0.27
(1,1880)	1:36:A:ARG:HA	1:36:A:ARG:HG3	8	0.27
(1,1847)	1:110:A:LEU:HD22	1:110:A:LEU:HB2	3	0.27
(1,1847)	1:110:A:LEU:HD21	1:110:A:LEU:HB2	11	0.27
(1,1845)	1:38:A:ALA:HB2	1:39:A:MET:HA	17	0.27
(1,1842)	1:18:A:ALA:HB1	1:21:A:ASN:HB3	8	0.27
(1,1824)	1:25:A:LYS:HG3	1:56:A:LEU:HD13	12	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1798)	1:62:A:ILE:HD13	1:28:A:ARG:HD3	13	0.27
(1,1798)	1:62:A:ILE:HD13	1:28:A:ARG:HD3	19	0.27
(1,1780)	1:112:A:LEU:HD23	1:17:A:HIS:HA	16	0.27
(1,1771)	1:31:A:VAL:HG23	1:65:A:ILE:HB	8	0.27
(1,1769)	1:66:A:VAL:HG11	1:68:A:GLU:HB2	10	0.27
(1,1749)	1:65:A:ILE:HG13	1:63:A:LEU:HD21	6	0.27
(1,1744)	1:90:A:VAL:HG12	1:90:A:VAL:HG21	11	0.27
(1,1727)	1:11:A:ILE:HD11	1:55:A:SER:HB3	5	0.27
(1,1707)	1:107:A:MET:HG3	1:107:A:MET:HA	3	0.27
(1,1707)	1:107:A:MET:HG3	1:107:A:MET:HA	20	0.27
(1,1665)	1:24:A:HIS:HA	1:57:A:VAL:HG21	5	0.27
(1,1653)	1:106:A:GLU:HA	1:37:A:SER:HA	13	0.27
(1,1618)	1:50:A:THR:HG23	1:51:A:PHE:HA	5	0.27
(1,1576)	1:35:A:GLU:HG3	1:69:A:LYS:HA	2	0.27
(1,1576)	1:35:A:GLU:HG3	1:69:A:LYS:HA	20	0.27
(1,1561)	1:38:A:ALA:HB1	1:38:A:ALA:HA	1	0.27
(1,1561)	1:38:A:ALA:HB3	1:38:A:ALA:HA	7	0.27
(1,1507)	1:26:A:ILE:HD12	1:14:A:CYS:HA	15	0.27
(1,1499)	1:6:A:VAL:HG21	1:3:A:GLU:HA	11	0.27
(1,1477)	1:45:A:VAL:HG11	1:41:A:LYS:HA	13	0.27
(1,1474)	1:41:A:LYS:HA	1:41:A:LYS:HE2	20	0.27
(1,1411)	1:84:A:ASN:HB2	1:84:A:ASN:HB3	15	0.27
(1,1361)	1:26:A:ILE:HD13	1:114:A:MET:HG2	18	0.27
(1,1302)	1:1:A:MET:HE2	1:1:A:MET:HA	17	0.27
(1,1280)	1:39:A:MET:HB2	1:39:A:MET:HE2	13	0.27
(1,1197)	1:80:A:VAL:HG13	1:71:A:GLU:HG3	9	0.27
(1,1145)	1:41:A:LYS:HD2	1:33:A:ILE:HG21	9	0.27
(1,1081)	1:43:A:LEU:HG	1:43:A:LEU:HA	3	0.27
(1,1081)	1:43:A:LEU:HG	1:43:A:LEU:HA	16	0.27
(1,953)	1:65:A:ILE:HG23	1:33:A:ILE:HG12	3	0.27
(1,950)	1:45:A:VAL:HG12	1:45:A:VAL:HG13	10	0.27
(1,950)	1:45:A:VAL:HG12	1:45:A:VAL:HG11	11	0.27
(1,950)	1:45:A:VAL:HG12	1:45:A:VAL:HG13	13	0.27
(1,950)	1:45:A:VAL:HG12	1:45:A:VAL:HG11	17	0.27
(1,922)	1:45:A:VAL:HG22	1:45:A:VAL:HG11	3	0.27
(1,908)	1:56:A:LEU:HD13	1:57:A:VAL:HG21	17	0.27
(1,904)	1:31:A:VAL:HG12	1:10:A:LEU:HD13	7	0.27
(1,897)	1:29:A:VAL:HG11	1:112:A:LEU:HD23	15	0.27
(1,886)	1:57:A:VAL:HG12	1:57:A:VAL:HG22	8	0.27
(1,858)	1:109:A:LEU:HD21	1:109:A:LEU:HD23	7	0.27
(1,858)	1:109:A:LEU:HD22	1:109:A:LEU:HD23	16	0.27
(1,849)	1:72:A:LEU:HD22	1:101:A:ILE:HG13	8	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,845)	1:31:A:VAL:HG12	1:31:A:VAL:HG11	2	0.27
(1,845)	1:31:A:VAL:HG12	1:31:A:VAL:HG13	4	0.27
(1,845)	1:31:A:VAL:HG11	1:31:A:VAL:HG13	8	0.27
(1,845)	1:31:A:VAL:HG12	1:31:A:VAL:HG13	10	0.27
(1,845)	1:31:A:VAL:HG12	1:31:A:VAL:HG13	20	0.27
(1,831)	1:101:A:ILE:HG21	1:101:A:ILE:HG23	2	0.27
(1,831)	1:101:A:ILE:HG22	1:101:A:ILE:HG23	6	0.27
(1,831)	1:101:A:ILE:HG22	1:101:A:ILE:HG23	9	0.27
(1,831)	1:101:A:ILE:HG21	1:101:A:ILE:HG23	14	0.27
(1,831)	1:101:A:ILE:HG22	1:101:A:ILE:HG21	15	0.27
(1,825)	1:101:A:ILE:HG21	1:72:A:LEU:HA	16	0.27
(1,818)	1:80:A:VAL:HG13	1:80:A:VAL:HG21	1	0.27
(1,818)	1:80:A:VAL:HG13	1:80:A:VAL:HG21	18	0.27
(1,771)	1:110:A:LEU:HD12	1:66:A:VAL:HG23	15	0.27
(1,754)	1:33:A:ILE:HG13	1:33:A:ILE:HG23	7	0.27
(1,754)	1:33:A:ILE:HG13	1:33:A:ILE:HG23	8	0.27
(1,741)	1:72:A:LEU:HD12	1:72:A:LEU:HD13	14	0.27
(1,710)	1:72:A:LEU:HA	1:103:A:GLN:H	15	0.27
(1,690)	1:76:A:ASP:HA	1:77:A:CYS:H	13	0.27
(1,428)	1:59:A:LYS:HE2	1:59:A:LYS:H	12	0.27
(1,358)	1:22:A:GLN:HB2	1:23:A:ALA:H	4	0.27
(1,358)	1:22:A:GLN:HB2	1:23:A:ALA:H	5	0.27
(1,358)	1:22:A:GLN:HB2	1:23:A:ALA:H	8	0.27
(1,344)	1:113:A:GLU:HG3	1:113:A:GLU:H	1	0.27
(1,344)	1:113:A:GLU:HG3	1:113:A:GLU:H	2	0.27
(1,213)	1:75:A:LYS:HD3	1:75:A:LYS:H	7	0.27
(1,213)	1:75:A:LYS:HD3	1:75:A:LYS:H	9	0.27
(1,196)	1:12:A:ALA:HB2	1:14:A:CYS:H	16	0.27
(1,185)	1:38:A:ALA:HB1	1:39:A:MET:H	18	0.27
(1,174)	1:100:A:ILE:HG12	1:101:A:ILE:H	9	0.27
(1,162)	1:23:A:ALA:HB3	1:22:A:GLN:H	16	0.27
(1,134)	1:57:A:VAL:HG21	1:58:A:CYS:H	11	0.27
(1,121)	1:70:A:VAL:HG13	1:71:A:GLU:H	17	0.27
(1,112)	1:10:A:LEU:HD13	1:11:A:ILE:H	19	0.27
(1,105)	1:29:A:VAL:HG12	1:29:A:VAL:H	20	0.27
(1,82)	1:109:A:LEU:HD23	1:30:A:VAL:H	6	0.27
(1,72)	1:31:A:VAL:HG11	1:108:A:ARG:H	5	0.27
(1,36)	1:99:A:VAL:HG13	1:100:A:ILE:H	3	0.27
(1,2692)	1:4:A:TYR:HE2	1:4:A:TYR:HD2	1	0.26
(1,2692)	1:4:A:TYR:HE1	1:4:A:TYR:HD1	7	0.26
(1,2692)	1:4:A:TYR:HE2	1:4:A:TYR:HD2	16	0.26
(1,2692)	1:4:A:TYR:HE1	1:4:A:TYR:HD1	20	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2676)	1:47:A:ALA:HB2	1:44:A:PHE:HD1	20	0.26
(1,2670)	1:11:A:ILE:HG21	1:51:A:PHE:HD2	4	0.26
(1,2661)	1:75:A:LYS:HA	1:75:A:LYS:HE3	19	0.26
(1,2657)	1:20:A:LYS:HE2	1:20:A:LYS:HA	1	0.26
(1,2643)	1:39:A:MET:HE1	1:106:A:GLU:HG2	20	0.26
(1,2614)	1:70:A:VAL:HG12	1:70:A:VAL:HG13	11	0.26
(1,2614)	1:70:A:VAL:HG12	1:70:A:VAL:HG11	16	0.26
(1,2507)	1:20:A:LYS:HD2	1:20:A:LYS:HD3	8	0.26
(1,2507)	1:82:A:LYS:HD2	1:82:A:LYS:HD3	17	0.26
(1,2503)	1:75:A:LYS:HD2	1:75:A:LYS:HD3	5	0.26
(1,2503)	1:69:A:LYS:HD2	1:69:A:LYS:HD3	8	0.26
(1,2503)	1:69:A:LYS:HD2	1:69:A:LYS:HD3	14	0.26
(1,2503)	1:69:A:LYS:HD2	1:69:A:LYS:HD3	18	0.26
(1,2503)	1:36:A:ARG:HG3	1:36:A:ARG:HG2	20	0.26
(1,2496)	1:36:A:ARG:HG3	1:36:A:ARG:HG2	16	0.26
(1,2496)	1:36:A:ARG:HG3	1:36:A:ARG:HG2	17	0.26
(1,2469)	1:6:A:VAL:HG11	1:39:A:MET:HE2	16	0.26
(1,2469)	1:6:A:VAL:HG12	1:39:A:MET:HE1	18	0.26
(1,2450)	1:99:A:VAL:HG22	1:99:A:VAL:HG23	1	0.26
(1,2450)	1:99:A:VAL:HG22	1:99:A:VAL:HG23	2	0.26
(1,2450)	1:30:A:VAL:HG22	1:30:A:VAL:HG21	3	0.26
(1,2450)	1:99:A:VAL:HG22	1:99:A:VAL:HG21	6	0.26
(1,2450)	1:30:A:VAL:HG22	1:30:A:VAL:HG23	17	0.26
(1,2442)	1:31:A:VAL:HG21	1:31:A:VAL:HG11	1	0.26
(1,2442)	1:31:A:VAL:HG22	1:31:A:VAL:HG12	2	0.26
(1,2442)	1:31:A:VAL:HG22	1:31:A:VAL:HG12	17	0.26
(1,2422)	1:47:A:ALA:HB2	1:7:A:VAL:H	12	0.26
(1,2419)	1:69:A:LYS:HG3	1:69:A:LYS:H	5	0.26
(1,2419)	1:69:A:LYS:HG3	1:69:A:LYS:H	9	0.26
(1,2419)	1:69:A:LYS:HG3	1:69:A:LYS:H	13	0.26
(1,2287)	1:80:A:VAL:H	1:81:A:PHE:H	18	0.26
(1,2279)	1:4:A:TYR:HE2	1:4:A:TYR:HD2	1	0.26
(1,2279)	1:4:A:TYR:HE1	1:4:A:TYR:HD1	20	0.26
(1,2216)	1:81:A:PHE:HB3	1:79:A:HIS:HD2	18	0.26
(1,2199)	1:7:A:VAL:HB	1:4:A:TYR:HD1	12	0.26
(1,2148)	1:80:A:VAL:HG11	1:81:A:PHE:HD1	3	0.26
(1,2148)	1:80:A:VAL:HG11	1:81:A:PHE:HD2	13	0.26
(1,2148)	1:80:A:VAL:HG12	1:81:A:PHE:HD1	18	0.26
(1,2143)	1:7:A:VAL:HG23	1:51:A:PHE:HD1	14	0.26
(1,2130)	1:72:A:LEU:HD13	1:81:A:PHE:HE1	3	0.26
(1,2100)	1:97:A:LYS:HA	1:97:A:LYS:HE3	10	0.26
(1,2091)	1:65:A:ILE:HA	1:31:A:VAL:HG12	19	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2070)	1:109:A:LEU:HD22	1:29:A:VAL:HA	5	0.26
(1,2068)	1:30:A:VAL:HG12	1:29:A:VAL:HA	14	0.26
(1,2058)	1:12:A:ALA:HB2	1:13:A:LEU:HA	11	0.26
(1,2052)	1:20:A:LYS:HG2	1:17:A:HIS:HA	4	0.26
(1,2051)	1:114:A:MET:HE1	1:17:A:HIS:HA	18	0.26
(1,2050)	1:17:A:HIS:HA	1:16:A:GLU:HB2	1	0.26
(1,2050)	1:17:A:HIS:HA	1:16:A:GLU:HB2	5	0.26
(1,2050)	1:17:A:HIS:HA	1:16:A:GLU:HB2	8	0.26
(1,2050)	1:17:A:HIS:HA	1:16:A:GLU:HB2	16	0.26
(1,2041)	1:16:A:GLU:HA	1:17:A:HIS:HA	9	0.26
(1,2030)	1:83:A:PRO:HD2	1:72:A:LEU:HD13	5	0.26
(1,2024)	1:107:A:MET:HE3	1:7:A:VAL:HA	10	0.26
(1,2005)	1:59:A:LYS:HB3	1:59:A:LYS:HE2	11	0.26
(1,1986)	1:82:A:LYS:HE3	1:71:A:GLU:HB3	9	0.26
(1,1975)	1:12:A:ALA:HB3	1:15:A:GLU:HB2	5	0.26
(1,1962)	1:97:A:LYS:HB2	1:90:A:VAL:HG12	17	0.26
(1,1960)	1:113:A:GLU:HG3	1:27:A:GLU:HB3	16	0.26
(1,1949)	1:15:A:GLU:HB3	1:57:A:VAL:HG11	19	0.26
(1,1944)	1:57:A:VAL:HB	1:26:A:ILE:HD13	3	0.26
(1,1914)	1:68:A:GLU:HB2	1:34:A:GLY:HA3	4	0.26
(1,1847)	1:110:A:LEU:HD22	1:110:A:LEU:HB2	5	0.26
(1,1829)	1:26:A:ILE:HD13	1:23:A:ALA:HB2	12	0.26
(1,1824)	1:25:A:LYS:HG3	1:56:A:LEU:HD13	3	0.26
(1,1819)	1:7:A:VAL:HG12	1:47:A:ALA:HB1	9	0.26
(1,1769)	1:66:A:VAL:HG12	1:68:A:GLU:HB2	9	0.26
(1,1749)	1:65:A:ILE:HG13	1:63:A:LEU:HD22	1	0.26
(1,1749)	1:65:A:ILE:HG13	1:63:A:LEU:HD23	3	0.26
(1,1748)	1:33:A:ILE:HG22	1:107:A:MET:HG3	3	0.26
(1,1628)	1:61:A:ALA:HB3	1:27:A:GLU:HA	1	0.26
(1,1561)	1:38:A:ALA:HB3	1:38:A:ALA:HA	2	0.26
(1,1561)	1:38:A:ALA:HB3	1:38:A:ALA:HA	4	0.26
(1,1561)	1:38:A:ALA:HB3	1:38:A:ALA:HA	5	0.26
(1,1561)	1:38:A:ALA:HB1	1:38:A:ALA:HA	6	0.26
(1,1561)	1:38:A:ALA:HB1	1:38:A:ALA:HA	10	0.26
(1,1561)	1:38:A:ALA:HB1	1:38:A:ALA:HA	16	0.26
(1,1561)	1:38:A:ALA:HB3	1:38:A:ALA:HA	18	0.26
(1,1490)	1:6:A:VAL:HA	1:9:A:SER:HB3	15	0.26
(1,1452)	1:63:A:LEU:HD12	1:45:A:VAL:HA	16	0.26
(1,1415)	1:20:A:LYS:HE2	1:20:A:LYS:HE3	13	0.26
(1,1411)	1:84:A:ASN:HB2	1:84:A:ASN:HB3	9	0.26
(1,1385)	1:48:A:PHE:HB3	1:63:A:LEU:HD11	7	0.26
(1,1385)	1:48:A:PHE:HB3	1:63:A:LEU:HD11	10	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1301)	1:1:A:MET:HE2	1:1:A:MET:HB2	12	0.26
(1,1211)	1:75:A:LYS:HB3	1:98:A:ASN:HB2	5	0.26
(1,1211)	1:75:A:LYS:HB3	1:98:A:ASN:HB2	14	0.26
(1,1211)	1:75:A:LYS:HB3	1:98:A:ASN:HB2	20	0.26
(1,1197)	1:80:A:VAL:HG11	1:71:A:GLU:HG3	18	0.26
(1,1145)	1:41:A:LYS:HD2	1:33:A:ILE:HG21	2	0.26
(1,1053)	1:63:A:LEU:HD13	1:63:A:LEU:HB2	14	0.26
(1,998)	1:65:A:ILE:HG12	1:63:A:LEU:HD22	16	0.26
(1,980)	1:23:A:ALA:HB2	1:23:A:ALA:HB3	4	0.26
(1,980)	1:23:A:ALA:HB2	1:23:A:ALA:HB3	8	0.26
(1,980)	1:23:A:ALA:HB2	1:23:A:ALA:HB3	14	0.26
(1,980)	1:23:A:ALA:HB2	1:23:A:ALA:HB3	18	0.26
(1,963)	1:41:A:LYS:HG3	1:65:A:ILE:HD13	5	0.26
(1,953)	1:65:A:ILE:HG22	1:33:A:ILE:HG12	18	0.26
(1,950)	1:45:A:VAL:HG12	1:45:A:VAL:HG13	7	0.26
(1,950)	1:45:A:VAL:HG12	1:45:A:VAL:HG13	9	0.26
(1,950)	1:45:A:VAL:HG12	1:45:A:VAL:HG13	16	0.26
(1,940)	1:112:A:LEU:HD12	1:112:A:LEU:HA	14	0.26
(1,940)	1:112:A:LEU:HD13	1:112:A:LEU:HA	20	0.26
(1,922)	1:45:A:VAL:HG23	1:45:A:VAL:HG11	6	0.26
(1,922)	1:45:A:VAL:HG22	1:45:A:VAL:HG11	11	0.26
(1,922)	1:45:A:VAL:HG21	1:45:A:VAL:HG13	18	0.26
(1,911)	1:56:A:LEU:HD13	1:56:A:LEU:HA	2	0.26
(1,911)	1:56:A:LEU:HD13	1:56:A:LEU:HA	3	0.26
(1,911)	1:56:A:LEU:HD11	1:56:A:LEU:HA	11	0.26
(1,907)	1:13:A:LEU:HD22	1:13:A:LEU:HD12	20	0.26
(1,886)	1:57:A:VAL:HG12	1:57:A:VAL:HG21	13	0.26
(1,886)	1:57:A:VAL:HG11	1:57:A:VAL:HG23	14	0.26
(1,886)	1:57:A:VAL:HG11	1:57:A:VAL:HG23	19	0.26
(1,875)	1:86:A:LEU:HD22	1:85:A:ALA:HA	14	0.26
(1,874)	1:26:A:ILE:HG21	1:61:A:ALA:HB1	5	0.26
(1,860)	1:109:A:LEU:HD21	1:31:A:VAL:HA	15	0.26
(1,860)	1:109:A:LEU:HD23	1:31:A:VAL:HA	17	0.26
(1,858)	1:109:A:LEU:HD22	1:109:A:LEU:HD23	1	0.26
(1,858)	1:109:A:LEU:HD22	1:109:A:LEU:HD21	10	0.26
(1,858)	1:109:A:LEU:HD21	1:109:A:LEU:HD23	14	0.26
(1,858)	1:109:A:LEU:HD21	1:109:A:LEU:HD23	15	0.26
(1,858)	1:109:A:LEU:HD22	1:109:A:LEU:HD23	20	0.26
(1,845)	1:31:A:VAL:HG11	1:31:A:VAL:HG13	7	0.26
(1,845)	1:31:A:VAL:HG12	1:31:A:VAL:HG13	11	0.26
(1,842)	1:112:A:LEU:HD22	1:112:A:LEU:HD23	4	0.26
(1,842)	1:112:A:LEU:HD22	1:112:A:LEU:HD23	5	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,842)	1:112:A:LEU:HD22	1:112:A:LEU:HD21	8	0.26
(1,842)	1:112:A:LEU:HD21	1:112:A:LEU:HD23	14	0.26
(1,831)	1:101:A:ILE:HG22	1:101:A:ILE:HG21	13	0.26
(1,826)	1:101:A:ILE:HG23	1:103:A:GLN:HA	6	0.26
(1,826)	1:101:A:ILE:HG23	1:103:A:GLN:HA	12	0.26
(1,826)	1:101:A:ILE:HG22	1:103:A:GLN:HA	13	0.26
(1,818)	1:80:A:VAL:HG11	1:80:A:VAL:HG22	7	0.26
(1,773)	1:66:A:VAL:HG22	1:66:A:VAL:HG23	2	0.26
(1,754)	1:33:A:ILE:HG13	1:33:A:ILE:HG21	15	0.26
(1,754)	1:33:A:ILE:HG13	1:33:A:ILE:HG22	16	0.26
(1,750)	1:72:A:LEU:HD23	1:99:A:VAL:HG12	9	0.26
(1,741)	1:72:A:LEU:HD12	1:72:A:LEU:HD13	6	0.26
(1,741)	1:72:A:LEU:HD12	1:72:A:LEU:HD11	9	0.26
(1,741)	1:72:A:LEU:HD11	1:72:A:LEU:HD13	20	0.26
(1,448)	1:79:A:HIS:HB2	1:80:A:VAL:H	1	0.26
(1,448)	1:79:A:HIS:HB2	1:80:A:VAL:H	15	0.26
(1,448)	1:79:A:HIS:HB2	1:80:A:VAL:H	19	0.26
(1,437)	1:24:A:HIS:HB2	1:25:A:LYS:H	11	0.26
(1,358)	1:22:A:GLN:HB2	1:23:A:ALA:H	3	0.26
(1,358)	1:22:A:GLN:HB2	1:23:A:ALA:H	10	0.26
(1,358)	1:22:A:GLN:HB2	1:23:A:ALA:H	11	0.26
(1,358)	1:22:A:GLN:HB2	1:23:A:ALA:H	20	0.26
(1,213)	1:75:A:LYS:HD3	1:75:A:LYS:H	17	0.26
(1,196)	1:12:A:ALA:HB2	1:14:A:CYS:H	3	0.26
(1,196)	1:12:A:ALA:HB2	1:14:A:CYS:H	12	0.26
(1,174)	1:100:A:ILE:HG12	1:101:A:ILE:H	5	0.26
(1,162)	1:23:A:ALA:HB2	1:22:A:GLN:H	6	0.26
(1,142)	1:47:A:ALA:HB3	1:46:A:SER:H	3	0.26
(1,142)	1:47:A:ALA:HB2	1:46:A:SER:H	8	0.26
(1,142)	1:47:A:ALA:HB2	1:46:A:SER:H	11	0.26
(1,138)	1:102:A:THR:HG21	1:103:A:GLN:H	4	0.26
(1,134)	1:57:A:VAL:HG23	1:58:A:CYS:H	4	0.26
(1,134)	1:57:A:VAL:HG23	1:58:A:CYS:H	16	0.26
(1,134)	1:57:A:VAL:HG23	1:58:A:CYS:H	18	0.26
(1,131)	1:10:A:LEU:HD22	1:11:A:ILE:H	18	0.26
(1,105)	1:29:A:VAL:HG13	1:29:A:VAL:H	2	0.26
(1,105)	1:29:A:VAL:HG13	1:29:A:VAL:H	7	0.26
(1,103)	1:43:A:LEU:HD22	1:46:A:SER:H	1	0.26
(1,97)	1:11:A:ILE:HG22	1:12:A:ALA:H	8	0.26
(1,83)	1:112:A:LEU:HD21	1:112:A:LEU:H	10	0.26
(1,83)	1:112:A:LEU:HD23	1:112:A:LEU:H	20	0.26
(1,39)	1:90:A:VAL:HG13	1:90:A:VAL:H	4	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,39)	1:90:A:VAL:HG12	1:90:A:VAL:H	9	0.26
(1,39)	1:90:A:VAL:HG11	1:90:A:VAL:H	19	0.26
(1,12)	1:72:A:LEU:HD11	1:72:A:LEU:H	18	0.26
(1,2692)	1:4:A:TYR:HE2	1:4:A:TYR:HD2	2	0.25
(1,2670)	1:11:A:ILE:HG21	1:51:A:PHE:HD2	16	0.25
(1,2661)	1:75:A:LYS:HA	1:75:A:LYS:HE3	2	0.25
(1,2653)	1:41:A:LYS:HD3	1:41:A:LYS:HA	3	0.25
(1,2653)	1:41:A:LYS:HD3	1:41:A:LYS:HA	14	0.25
(1,2645)	1:33:A:ILE:HG21	1:39:A:MET:HG3	11	0.25
(1,2614)	1:10:A:LEU:HD11	1:10:A:LEU:HD13	1	0.25
(1,2614)	1:70:A:VAL:HG12	1:70:A:VAL:HG13	2	0.25
(1,2614)	1:70:A:VAL:HG12	1:70:A:VAL:HG11	6	0.25
(1,2614)	1:10:A:LEU:HD12	1:10:A:LEU:HD13	10	0.25
(1,2614)	1:70:A:VAL:HG11	1:70:A:VAL:HG13	12	0.25
(1,2614)	1:70:A:VAL:HG11	1:70:A:VAL:HG13	14	0.25
(1,2614)	1:70:A:VAL:HG11	1:70:A:VAL:HG13	17	0.25
(1,2614)	1:10:A:LEU:HD12	1:10:A:LEU:HD13	19	0.25
(1,2614)	1:10:A:LEU:HD12	1:10:A:LEU:HD11	20	0.25
(1,2537)	1:115:A:LEU:HD13	1:27:A:GLU:HG2	13	0.25
(1,2537)	1:115:A:LEU:HD12	1:27:A:GLU:HG2	20	0.25
(1,2507)	1:20:A:LYS:HD2	1:20:A:LYS:HD3	2	0.25
(1,2507)	1:82:A:LYS:HD2	1:82:A:LYS:HD3	20	0.25
(1,2503)	1:69:A:LYS:HD2	1:69:A:LYS:HD3	2	0.25
(1,2503)	1:36:A:ARG:HG3	1:36:A:ARG:HG2	12	0.25
(1,2503)	1:36:A:ARG:HG3	1:36:A:ARG:HG2	15	0.25
(1,2503)	1:69:A:LYS:HD2	1:69:A:LYS:HD3	19	0.25
(1,2450)	1:99:A:VAL:HG21	1:99:A:VAL:HG23	5	0.25
(1,2450)	1:30:A:VAL:HG22	1:30:A:VAL:HG23	7	0.25
(1,2450)	1:99:A:VAL:HG22	1:99:A:VAL:HG23	12	0.25
(1,2450)	1:30:A:VAL:HG22	1:30:A:VAL:HG23	14	0.25
(1,2442)	1:31:A:VAL:HG23	1:31:A:VAL:HG11	3	0.25
(1,2401)	1:90:A:VAL:H	1:91:A:CYS:H	2	0.25
(1,2396)	1:101:A:ILE:H	1:100:A:ILE:H	15	0.25
(1,2396)	1:101:A:ILE:H	1:100:A:ILE:H	19	0.25
(1,2380)	1:34:A:GLY:H	1:35:A:GLU:H	3	0.25
(1,2378)	1:97:A:LYS:H	1:96:A:SER:H	7	0.25
(1,2378)	1:97:A:LYS:H	1:96:A:SER:H	20	0.25
(1,2287)	1:80:A:VAL:H	1:81:A:PHE:H	8	0.25
(1,2279)	1:4:A:TYR:HE2	1:4:A:TYR:HD2	2	0.25
(1,2276)	1:88:A:TYR:HE2	1:88:A:TYR:HD2	5	0.25
(1,2262)	1:88:A:TYR:HA	1:88:A:TYR:HD1	13	0.25
(1,2229)	1:4:A:TYR:HB3	1:4:A:TYR:HE2	19	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2180)	1:61:A:ALA:HB1	1:48:A:PHE:HD1	7	0.25
(1,2160)	1:80:A:VAL:HG21	1:81:A:PHE:HD1	12	0.25
(1,2160)	1:80:A:VAL:HG22	1:81:A:PHE:HD1	18	0.25
(1,2142)	1:7:A:VAL:HG21	1:48:A:PHE:HD1	17	0.25
(1,2105)	1:64:A:ASP:HA	1:62:A:ILE:HG23	6	0.25
(1,2105)	1:64:A:ASP:HA	1:62:A:ILE:HG23	13	0.25
(1,2088)	1:105:A:ASN:HA	1:36:A:ARG:HB3	20	0.25
(1,2084)	1:58:A:CYS:HA	1:26:A:ILE:HG21	3	0.25
(1,2070)	1:109:A:LEU:HD22	1:29:A:VAL:HA	3	0.25
(1,2070)	1:109:A:LEU:HD21	1:29:A:VAL:HA	20	0.25
(1,2067)	1:10:A:LEU:HA	1:13:A:LEU:HG	13	0.25
(1,2041)	1:16:A:GLU:HA	1:17:A:HIS:HA	1	0.25
(1,2041)	1:16:A:GLU:HA	1:17:A:HIS:HA	7	0.25
(1,2030)	1:83:A:PRO:HD2	1:72:A:LEU:HD13	7	0.25
(1,1944)	1:57:A:VAL:HB	1:26:A:ILE:HD13	10	0.25
(1,1931)	1:65:A:ILE:HD11	1:41:A:LYS:HB2	13	0.25
(1,1897)	1:41:A:LYS:HD3	1:41:A:LYS:HA	1	0.25
(1,1847)	1:110:A:LEU:HD23	1:110:A:LEU:HB2	10	0.25
(1,1847)	1:110:A:LEU:HD21	1:110:A:LEU:HB2	17	0.25
(1,1820)	1:10:A:LEU:HD22	1:6:A:VAL:HG12	14	0.25
(1,1800)	1:115:A:LEU:HD11	1:25:A:LYS:HG2	20	0.25
(1,1798)	1:62:A:ILE:HD12	1:28:A:ARG:HD3	18	0.25
(1,1786)	1:26:A:ILE:HG23	1:114:A:MET:HE3	14	0.25
(1,1774)	1:31:A:VAL:HG23	1:107:A:MET:HG2	9	0.25
(1,1771)	1:31:A:VAL:HG21	1:65:A:ILE:HB	7	0.25
(1,1771)	1:31:A:VAL:HG23	1:65:A:ILE:HB	11	0.25
(1,1771)	1:31:A:VAL:HG22	1:65:A:ILE:HB	15	0.25
(1,1736)	1:65:A:ILE:HG21	1:41:A:LYS:HG3	5	0.25
(1,1708)	1:107:A:MET:HA	1:33:A:ILE:HD13	10	0.25
(1,1707)	1:107:A:MET:HG3	1:107:A:MET:HA	1	0.25
(1,1707)	1:107:A:MET:HG3	1:107:A:MET:HA	13	0.25
(1,1677)	1:25:A:LYS:HA	1:57:A:VAL:HG22	12	0.25
(1,1644)	1:88:A:TYR:HA	1:72:A:LEU:HD22	14	0.25
(1,1618)	1:50:A:THR:HG23	1:51:A:PHE:HA	4	0.25
(1,1618)	1:50:A:THR:HG21	1:51:A:PHE:HA	8	0.25
(1,1618)	1:50:A:THR:HG22	1:51:A:PHE:HA	18	0.25
(1,1570)	1:102:A:THR:HA	1:101:A:ILE:HG22	20	0.25
(1,1561)	1:38:A:ALA:HB2	1:38:A:ALA:HA	12	0.25
(1,1415)	1:20:A:LYS:HE2	1:20:A:LYS:HE3	3	0.25
(1,1411)	1:84:A:ASN:HB2	1:84:A:ASN:HB3	6	0.25
(1,1411)	1:84:A:ASN:HB2	1:84:A:ASN:HB3	11	0.25
(1,1411)	1:84:A:ASN:HB2	1:84:A:ASN:HB3	14	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1411)	1:84:A:ASN:HB2	1:84:A:ASN:HB3	19	0.25
(1,1411)	1:84:A:ASN:HB2	1:84:A:ASN:HB3	20	0.25
(1,1410)	1:84:A:ASN:HB2	1:84:A:ASN:HA	2	0.25
(1,1361)	1:26:A:ILE:HD13	1:114:A:MET:HG2	2	0.25
(1,1352)	1:22:A:GLN:HG2	1:22:A:GLN:HG3	2	0.25
(1,1301)	1:1:A:MET:HE3	1:1:A:MET:HB2	2	0.25
(1,1280)	1:39:A:MET:HB2	1:39:A:MET:HE2	12	0.25
(1,1140)	1:59:A:LYS:HD3	1:59:A:LYS:HA	8	0.25
(1,1081)	1:43:A:LEU:HG	1:43:A:LEU:HA	18	0.25
(1,1080)	1:36:A:ARG:HB3	1:36:A:ARG:HD2	19	0.25
(1,1053)	1:63:A:LEU:HD12	1:63:A:LEU:HB2	8	0.25
(1,1006)	1:100:A:ILE:HD11	1:75:A:LYS:HG3	18	0.25
(1,980)	1:23:A:ALA:HB2	1:23:A:ALA:HB1	7	0.25
(1,980)	1:23:A:ALA:HB1	1:23:A:ALA:HB3	10	0.25
(1,980)	1:23:A:ALA:HB1	1:23:A:ALA:HB3	12	0.25
(1,980)	1:23:A:ALA:HB1	1:23:A:ALA:HB3	19	0.25
(1,963)	1:41:A:LYS:HG3	1:65:A:ILE:HD13	19	0.25
(1,950)	1:45:A:VAL:HG12	1:45:A:VAL:HG11	5	0.25
(1,950)	1:45:A:VAL:HG12	1:45:A:VAL:HG13	12	0.25
(1,950)	1:45:A:VAL:HG12	1:45:A:VAL:HG13	14	0.25
(1,940)	1:112:A:LEU:HD11	1:112:A:LEU:HA	2	0.25
(1,940)	1:112:A:LEU:HD13	1:112:A:LEU:HA	11	0.25
(1,934)	1:102:A:THR:HG23	1:100:A:ILE:HB	20	0.25
(1,908)	1:56:A:LEU:HD13	1:57:A:VAL:HG23	8	0.25
(1,907)	1:13:A:LEU:HD23	1:13:A:LEU:HD13	15	0.25
(1,907)	1:13:A:LEU:HD21	1:13:A:LEU:HD13	17	0.25
(1,889)	1:57:A:VAL:HG11	1:15:A:GLU:HG3	20	0.25
(1,886)	1:57:A:VAL:HG11	1:57:A:VAL:HG23	12	0.25
(1,874)	1:26:A:ILE:HG23	1:61:A:ALA:HB3	7	0.25
(1,862)	1:109:A:LEU:HD23	1:13:A:LEU:HD23	19	0.25
(1,858)	1:109:A:LEU:HD22	1:109:A:LEU:HD21	6	0.25
(1,858)	1:109:A:LEU:HD22	1:109:A:LEU:HD23	11	0.25
(1,858)	1:109:A:LEU:HD22	1:109:A:LEU:HD23	18	0.25
(1,842)	1:112:A:LEU:HD22	1:112:A:LEU:HD23	9	0.25
(1,842)	1:112:A:LEU:HD22	1:112:A:LEU:HD23	16	0.25
(1,834)	1:72:A:LEU:HD22	1:101:A:ILE:HG22	12	0.25
(1,831)	1:101:A:ILE:HG22	1:101:A:ILE:HG21	3	0.25
(1,831)	1:101:A:ILE:HG21	1:101:A:ILE:HG23	16	0.25
(1,818)	1:80:A:VAL:HG12	1:80:A:VAL:HG21	11	0.25
(1,803)	1:72:A:LEU:HD23	1:72:A:LEU:HB2	14	0.25
(1,771)	1:110:A:LEU:HD11	1:66:A:VAL:HG23	3	0.25
(1,769)	1:72:A:LEU:HD22	1:70:A:VAL:HG21	6	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,769)	1:72:A:LEU:HD22	1:70:A:VAL:HG22	14	0.25
(1,754)	1:33:A:ILE:HG13	1:33:A:ILE:HG22	13	0.25
(1,754)	1:33:A:ILE:HG13	1:33:A:ILE:HG22	20	0.25
(1,741)	1:72:A:LEU:HD11	1:72:A:LEU:HD13	2	0.25
(1,741)	1:72:A:LEU:HD12	1:72:A:LEU:HD13	3	0.25
(1,741)	1:72:A:LEU:HD12	1:72:A:LEU:HD11	4	0.25
(1,437)	1:24:A:HIS:HB3	1:25:A:LYS:H	9	0.25
(1,428)	1:59:A:LYS:HE2	1:59:A:LYS:H	16	0.25
(1,196)	1:12:A:ALA:HB3	1:14:A:CYS:H	14	0.25
(1,196)	1:12:A:ALA:HB2	1:14:A:CYS:H	20	0.25
(1,174)	1:100:A:ILE:HG12	1:101:A:ILE:H	7	0.25
(1,156)	1:23:A:ALA:HB3	1:21:A:ASN:H	11	0.25
(1,156)	1:23:A:ALA:HB2	1:21:A:ASN:H	12	0.25
(1,121)	1:70:A:VAL:HG11	1:71:A:GLU:H	2	0.25
(1,121)	1:70:A:VAL:HG11	1:71:A:GLU:H	11	0.25
(1,101)	1:57:A:VAL:HG12	1:15:A:GLU:H	16	0.25
(1,83)	1:112:A:LEU:HD22	1:112:A:LEU:H	5	0.25
(1,39)	1:90:A:VAL:HG11	1:90:A:VAL:H	7	0.25
(1,33)	1:33:A:ILE:HG21	1:37:A:SER:H	10	0.25
(1,2692)	1:88:A:TYR:HE2	1:88:A:TYR:HD2	5	0.24
(1,2692)	1:4:A:TYR:HE1	1:4:A:TYR:HD1	8	0.24
(1,2692)	1:4:A:TYR:HE2	1:4:A:TYR:HD2	18	0.24
(1,2614)	1:10:A:LEU:HD11	1:10:A:LEU:HD13	3	0.24
(1,2614)	1:10:A:LEU:HD12	1:10:A:LEU:HD11	7	0.24
(1,2614)	1:70:A:VAL:HG12	1:70:A:VAL:HG11	9	0.24
(1,2614)	1:10:A:LEU:HD12	1:10:A:LEU:HD13	13	0.24
(1,2614)	1:70:A:VAL:HG12	1:70:A:VAL:HG13	15	0.24
(1,2608)	1:115:A:LEU:HD21	1:27:A:GLU:HB2	14	0.24
(1,2592)	1:41:A:LYS:HD2	1:33:A:ILE:HG23	5	0.24
(1,2569)	1:92:A:GLU:HG2	1:92:A:GLU:HA	14	0.24
(1,2503)	1:75:A:LYS:HD2	1:75:A:LYS:HD3	6	0.24
(1,2503)	1:36:A:ARG:HG3	1:36:A:ARG:HG2	9	0.24
(1,2503)	1:75:A:LYS:HD2	1:75:A:LYS:HD3	13	0.24
(1,2503)	1:36:A:ARG:HG3	1:36:A:ARG:HG2	16	0.24
(1,2503)	1:36:A:ARG:HG3	1:36:A:ARG:HG2	17	0.24
(1,2496)	1:36:A:ARG:HG3	1:36:A:ARG:HG2	1	0.24
(1,2469)	1:6:A:VAL:HG12	1:39:A:MET:HE1	10	0.24
(1,2454)	1:62:A:ILE:HG22	1:28:A:ARG:HG3	9	0.24
(1,2451)	1:26:A:ILE:HD11	1:26:A:ILE:HD13	9	0.24
(1,2450)	1:99:A:VAL:HG21	1:99:A:VAL:HG23	4	0.24
(1,2450)	1:99:A:VAL:HG22	1:99:A:VAL:HG21	8	0.24
(1,2450)	1:30:A:VAL:HG22	1:30:A:VAL:HG21	11	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2450)	1:99:A:VAL:HG21	1:99:A:VAL:HG23	13	0.24
(1,2450)	1:30:A:VAL:HG22	1:30:A:VAL:HG21	19	0.24
(1,2442)	1:31:A:VAL:HG21	1:31:A:VAL:HG13	10	0.24
(1,2438)	1:65:A:ILE:HD13	1:41:A:LYS:HD2	4	0.24
(1,2427)	1:39:A:MET:HE2	1:107:A:MET:H	4	0.24
(1,2422)	1:47:A:ALA:HB1	1:7:A:VAL:H	18	0.24
(1,2396)	1:101:A:ILE:H	1:100:A:ILE:H	1	0.24
(1,2396)	1:101:A:ILE:H	1:100:A:ILE:H	5	0.24
(1,2396)	1:101:A:ILE:H	1:100:A:ILE:H	18	0.24
(1,2380)	1:34:A:GLY:H	1:35:A:GLU:H	20	0.24
(1,2378)	1:97:A:LYS:H	1:96:A:SER:H	13	0.24
(1,2298)	1:71:A:GLU:H	1:70:A:VAL:H	7	0.24
(1,2294)	1:99:A:VAL:H	1:100:A:ILE:H	1	0.24
(1,2294)	1:99:A:VAL:H	1:100:A:ILE:H	9	0.24
(1,2294)	1:99:A:VAL:H	1:100:A:ILE:H	13	0.24
(1,2287)	1:80:A:VAL:H	1:81:A:PHE:H	9	0.24
(1,2279)	1:4:A:TYR:HE1	1:4:A:TYR:HD1	8	0.24
(1,2279)	1:4:A:TYR:HE2	1:4:A:TYR:HD2	18	0.24
(1,2262)	1:88:A:TYR:HA	1:88:A:TYR:HD2	3	0.24
(1,2239)	1:41:A:LYS:HA	1:44:A:PHE:HD1	3	0.24
(1,2229)	1:4:A:TYR:HB3	1:4:A:TYR:HE2	16	0.24
(1,2229)	1:4:A:TYR:HB3	1:4:A:TYR:HE1	20	0.24
(1,2206)	1:83:A:PRO:HB2	1:81:A:PHE:HD2	18	0.24
(1,2202)	1:83:A:PRO:HB3	1:88:A:TYR:HD2	14	0.24
(1,2183)	1:116:A:ALA:HB3	1:24:A:HIS:HD2	16	0.24
(1,2166)	1:50:A:THR:HG23	1:51:A:PHE:HE1	17	0.24
(1,2160)	1:80:A:VAL:HG22	1:81:A:PHE:HD2	6	0.24
(1,2148)	1:80:A:VAL:HG12	1:81:A:PHE:HD2	10	0.24
(1,2143)	1:7:A:VAL:HG21	1:51:A:PHE:HD1	1	0.24
(1,2142)	1:7:A:VAL:HG23	1:48:A:PHE:HD2	7	0.24
(1,2132)	1:72:A:LEU:HB3	1:81:A:PHE:HD2	6	0.24
(1,2100)	1:97:A:LYS:HA	1:97:A:LYS:HE2	7	0.24
(1,2071)	1:26:A:ILE:HG23	1:29:A:VAL:HA	17	0.24
(1,2070)	1:109:A:LEU:HD23	1:29:A:VAL:HA	9	0.24
(1,2053)	1:17:A:HIS:HA	1:16:A:GLU:HG2	14	0.24
(1,2052)	1:20:A:LYS:HG2	1:17:A:HIS:HA	5	0.24
(1,2050)	1:17:A:HIS:HA	1:16:A:GLU:HB2	18	0.24
(1,2042)	1:16:A:GLU:HA	1:15:A:GLU:HB2	3	0.24
(1,2016)	1:93:A:LYS:HD2	1:79:A:HIS:HB2	6	0.24
(1,1987)	1:23:A:ALA:HB2	1:21:A:ASN:HB2	19	0.24
(1,1984)	1:7:A:VAL:HG12	1:48:A:PHE:HB3	3	0.24
(1,1984)	1:7:A:VAL:HG12	1:48:A:PHE:HB3	17	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1982)	1:106:A:GLU:HG3	1:105:A:ASN:HB3	18	0.24
(1,1944)	1:57:A:VAL:HB	1:26:A:ILE:HD11	16	0.24
(1,1905)	1:25:A:LYS:HD3	1:27:A:GLU:HG2	4	0.24
(1,1864)	1:9:A:SER:HB3	1:12:A:ALA:HB1	2	0.24
(1,1847)	1:110:A:LEU:HD22	1:110:A:LEU:HB2	15	0.24
(1,1847)	1:110:A:LEU:HD22	1:110:A:LEU:HB2	20	0.24
(1,1819)	1:7:A:VAL:HG13	1:47:A:ALA:HB2	2	0.24
(1,1800)	1:115:A:LEU:HD13	1:25:A:LYS:HG2	1	0.24
(1,1799)	1:29:A:VAL:HG11	1:109:A:LEU:HD13	3	0.24
(1,1799)	1:29:A:VAL:HG11	1:109:A:LEU:HD11	15	0.24
(1,1777)	1:112:A:LEU:HD21	1:109:A:LEU:HD11	6	0.24
(1,1774)	1:31:A:VAL:HG23	1:107:A:MET:HG2	12	0.24
(1,1771)	1:31:A:VAL:HG23	1:65:A:ILE:HB	20	0.24
(1,1760)	1:109:A:LEU:HD13	1:112:A:LEU:HG	17	0.24
(1,1748)	1:33:A:ILE:HG21	1:107:A:MET:HG3	14	0.24
(1,1708)	1:107:A:MET:HA	1:33:A:ILE:HD13	17	0.24
(1,1677)	1:25:A:LYS:HA	1:57:A:VAL:HG21	10	0.24
(1,1677)	1:25:A:LYS:HA	1:57:A:VAL:HG22	14	0.24
(1,1618)	1:50:A:THR:HG23	1:51:A:PHE:HA	15	0.24
(1,1601)	1:12:A:ALA:HB2	1:9:A:SER:HA	17	0.24
(1,1581)	1:35:A:GLU:HG3	1:35:A:GLU:HA	16	0.24
(1,1576)	1:35:A:GLU:HG3	1:69:A:LYS:HA	13	0.24
(1,1561)	1:38:A:ALA:HB2	1:38:A:ALA:HA	11	0.24
(1,1499)	1:6:A:VAL:HG22	1:3:A:GLU:HA	8	0.24
(1,1499)	1:6:A:VAL:HG21	1:3:A:GLU:HA	12	0.24
(1,1490)	1:6:A:VAL:HA	1:9:A:SER:HB3	4	0.24
(1,1490)	1:6:A:VAL:HA	1:9:A:SER:HB3	7	0.24
(1,1474)	1:41:A:LYS:HA	1:41:A:LYS:HE2	6	0.24
(1,1452)	1:63:A:LEU:HD11	1:45:A:VAL:HA	20	0.24
(1,1411)	1:84:A:ASN:HB2	1:84:A:ASN:HB3	4	0.24
(1,1411)	1:84:A:ASN:HB2	1:84:A:ASN:HB3	8	0.24
(1,1411)	1:84:A:ASN:HB2	1:84:A:ASN:HB3	13	0.24
(1,1411)	1:84:A:ASN:HB2	1:84:A:ASN:HB3	16	0.24
(1,1410)	1:84:A:ASN:HB3	1:84:A:ASN:HA	14	0.24
(1,1401)	1:41:A:LYS:HE3	1:33:A:ILE:HD12	16	0.24
(1,1391)	1:58:A:CYS:HB3	1:55:A:SER:HB3	7	0.24
(1,1385)	1:48:A:PHE:HB3	1:63:A:LEU:HD12	4	0.24
(1,1385)	1:48:A:PHE:HB3	1:63:A:LEU:HD11	14	0.24
(1,1384)	1:93:A:LYS:HE3	1:93:A:LYS:HA	19	0.24
(1,1324)	1:106:A:GLU:HG2	1:105:A:ASN:HB2	6	0.24
(1,1324)	1:106:A:GLU:HG2	1:105:A:ASN:HB2	9	0.24
(1,1303)	1:23:A:ALA:HB3	1:114:A:MET:HB2	12	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1299)	1:117:A:GLU:HB2	1:117:A:GLU:HG3	14	0.24
(1,1249)	1:72:A:LEU:HD13	1:83:A:PRO:HG2	2	0.24
(1,1211)	1:75:A:LYS:HB3	1:98:A:ASN:HB2	10	0.24
(1,1105)	1:69:A:LYS:HD3	1:69:A:LYS:HA	5	0.24
(1,1081)	1:43:A:LEU:HG	1:43:A:LEU:HA	6	0.24
(1,1024)	1:57:A:VAL:HG11	1:18:A:ALA:HB2	17	0.24
(1,998)	1:65:A:ILE:HG12	1:63:A:LEU:HD23	8	0.24
(1,980)	1:23:A:ALA:HB2	1:23:A:ALA:HB1	5	0.24
(1,980)	1:23:A:ALA:HB1	1:23:A:ALA:HB3	6	0.24
(1,980)	1:23:A:ALA:HB2	1:23:A:ALA:HB3	9	0.24
(1,980)	1:23:A:ALA:HB1	1:23:A:ALA:HB3	13	0.24
(1,980)	1:23:A:ALA:HB2	1:23:A:ALA:HB1	16	0.24
(1,963)	1:41:A:LYS:HG3	1:65:A:ILE:HD12	2	0.24
(1,963)	1:41:A:LYS:HG3	1:65:A:ILE:HD13	17	0.24
(1,953)	1:65:A:ILE:HG22	1:33:A:ILE:HG12	13	0.24
(1,950)	1:45:A:VAL:HG12	1:45:A:VAL:HG11	15	0.24
(1,922)	1:45:A:VAL:HG23	1:45:A:VAL:HG11	9	0.24
(1,911)	1:56:A:LEU:HD12	1:56:A:LEU:HA	10	0.24
(1,904)	1:31:A:VAL:HG13	1:10:A:LEU:HD13	20	0.24
(1,875)	1:86:A:LEU:HD22	1:85:A:ALA:HA	3	0.24
(1,875)	1:86:A:LEU:HD21	1:85:A:ALA:HA	5	0.24
(1,858)	1:109:A:LEU:HD22	1:109:A:LEU:HD23	13	0.24
(1,849)	1:72:A:LEU:HD23	1:101:A:ILE:HG13	6	0.24
(1,842)	1:112:A:LEU:HD22	1:112:A:LEU:HD21	2	0.24
(1,842)	1:112:A:LEU:HD21	1:112:A:LEU:HD23	10	0.24
(1,842)	1:112:A:LEU:HD21	1:112:A:LEU:HD23	15	0.24
(1,842)	1:112:A:LEU:HD21	1:112:A:LEU:HD23	17	0.24
(1,809)	1:110:A:LEU:HD12	1:66:A:VAL:HG11	6	0.24
(1,780)	1:99:A:VAL:HG12	1:99:A:VAL:HG22	14	0.24
(1,772)	1:66:A:VAL:HG22	1:64:A:ASP:HB2	8	0.24
(1,754)	1:33:A:ILE:HG13	1:33:A:ILE:HG22	18	0.24
(1,743)	1:72:A:LEU:HB3	1:72:A:LEU:HD11	13	0.24
(1,741)	1:72:A:LEU:HD11	1:72:A:LEU:HD13	5	0.24
(1,741)	1:72:A:LEU:HD11	1:72:A:LEU:HD13	8	0.24
(1,741)	1:72:A:LEU:HD12	1:72:A:LEU:HD11	10	0.24
(1,741)	1:72:A:LEU:HD12	1:72:A:LEU:HD11	12	0.24
(1,741)	1:72:A:LEU:HD11	1:72:A:LEU:HD13	13	0.24
(1,741)	1:72:A:LEU:HD12	1:72:A:LEU:HD13	18	0.24
(1,741)	1:72:A:LEU:HD12	1:72:A:LEU:HD13	19	0.24
(1,736)	1:11:A:ILE:HD11	1:11:A:ILE:HD13	16	0.24
(1,691)	1:97:A:LYS:HA	1:91:A:CYS:H	12	0.24
(1,437)	1:24:A:HIS:HB3	1:25:A:LYS:H	2	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,367)	1:54:A:GLU:HG2	1:55:A:SER:H	3	0.24
(1,299)	1:39:A:MET:HE1	1:6:A:VAL:H	13	0.24
(1,242)	1:19:A:LYS:HD3	1:19:A:LYS:H	8	0.24
(1,239)	1:19:A:LYS:HD2	1:20:A:LYS:H	17	0.24
(1,162)	1:23:A:ALA:HB1	1:22:A:GLN:H	9	0.24
(1,162)	1:23:A:ALA:HB1	1:22:A:GLN:H	14	0.24
(1,156)	1:23:A:ALA:HB1	1:21:A:ASN:H	4	0.24
(1,136)	1:102:A:THR:HG22	1:100:A:ILE:H	11	0.24
(1,134)	1:57:A:VAL:HG23	1:58:A:CYS:H	17	0.24
(1,112)	1:10:A:LEU:HD12	1:11:A:ILE:H	6	0.24
(1,101)	1:57:A:VAL:HG12	1:15:A:GLU:H	6	0.24
(1,83)	1:112:A:LEU:HD22	1:112:A:LEU:H	7	0.24
(1,39)	1:90:A:VAL:HG13	1:90:A:VAL:H	17	0.24
(1,33)	1:33:A:ILE:HG21	1:37:A:SER:H	17	0.24
(1,25)	1:90:A:VAL:HG22	1:91:A:CYS:H	5	0.24
(1,25)	1:90:A:VAL:HG21	1:91:A:CYS:H	19	0.24
(1,25)	1:90:A:VAL:HG23	1:91:A:CYS:H	20	0.24
(1,12)	1:72:A:LEU:HD11	1:72:A:LEU:H	8	0.24
(1,2678)	1:39:A:MET:HE2	1:44:A:PHE:HZ	16	0.23
(1,2671)	1:115:A:LEU:HD13	1:24:A:HIS:HD2	14	0.23
(1,2653)	1:41:A:LYS:HD3	1:41:A:LYS:HA	19	0.23
(1,2650)	1:66:A:VAL:HG11	1:32:A:GLY:HA3	10	0.23
(1,2650)	1:66:A:VAL:HG13	1:32:A:GLY:HA3	20	0.23
(1,2645)	1:33:A:ILE:HG21	1:39:A:MET:HG3	7	0.23
(1,2614)	1:10:A:LEU:HD11	1:10:A:LEU:HD13	8	0.23
(1,2592)	1:41:A:LYS:HD2	1:33:A:ILE:HG22	6	0.23
(1,2451)	1:26:A:ILE:HD12	1:26:A:ILE:HD13	1	0.23
(1,2451)	1:101:A:ILE:HD11	1:101:A:ILE:HD13	4	0.23
(1,2451)	1:26:A:ILE:HD12	1:26:A:ILE:HD11	5	0.23
(1,2451)	1:26:A:ILE:HD11	1:26:A:ILE:HD13	6	0.23
(1,2450)	1:99:A:VAL:HG21	1:99:A:VAL:HG23	20	0.23
(1,2442)	1:31:A:VAL:HG22	1:31:A:VAL:HG13	7	0.23
(1,2442)	1:31:A:VAL:HG23	1:31:A:VAL:HG13	14	0.23
(1,2442)	1:31:A:VAL:HG22	1:31:A:VAL:HG11	16	0.23
(1,2438)	1:65:A:ILE:HD13	1:41:A:LYS:HD2	10	0.23
(1,2427)	1:39:A:MET:HE2	1:107:A:MET:H	6	0.23
(1,2401)	1:90:A:VAL:H	1:91:A:CYS:H	5	0.23
(1,2397)	1:100:A:ILE:H	1:74:A:CYS:H	10	0.23
(1,2396)	1:101:A:ILE:H	1:100:A:ILE:H	13	0.23
(1,2378)	1:97:A:LYS:H	1:96:A:SER:H	9	0.23
(1,2378)	1:97:A:LYS:H	1:96:A:SER:H	19	0.23
(1,2294)	1:99:A:VAL:H	1:100:A:ILE:H	7	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2294)	1:99:A:VAL:H	1:100:A:ILE:H	14	0.23
(1,2287)	1:80:A:VAL:H	1:81:A:PHE:H	3	0.23
(1,2287)	1:80:A:VAL:H	1:81:A:PHE:H	6	0.23
(1,2287)	1:80:A:VAL:H	1:81:A:PHE:H	15	0.23
(1,2279)	1:4:A:TYR:HE2	1:4:A:TYR:HD2	6	0.23
(1,2229)	1:4:A:TYR:HB3	1:4:A:TYR:HE2	5	0.23
(1,2229)	1:4:A:TYR:HB3	1:4:A:TYR:HE1	13	0.23
(1,2183)	1:116:A:ALA:HB2	1:24:A:HIS:HD2	10	0.23
(1,2170)	1:92:A:GLU:HG3	1:81:A:PHE:HD1	9	0.23
(1,2153)	1:99:A:VAL:HG23	1:81:A:PHE:HE2	13	0.23
(1,2148)	1:80:A:VAL:HG12	1:81:A:PHE:HD1	14	0.23
(1,2148)	1:80:A:VAL:HG13	1:81:A:PHE:HD1	20	0.23
(1,2142)	1:7:A:VAL:HG22	1:48:A:PHE:HD2	12	0.23
(1,2132)	1:72:A:LEU:HB3	1:81:A:PHE:HD1	16	0.23
(1,2085)	1:58:A:CYS:HA	1:26:A:ILE:HD13	3	0.23
(1,2068)	1:30:A:VAL:HG11	1:29:A:VAL:HA	15	0.23
(1,2067)	1:10:A:LEU:HA	1:13:A:LEU:HG	6	0.23
(1,2060)	1:35:A:GLU:HA	1:33:A:ILE:HG22	11	0.23
(1,2053)	1:17:A:HIS:HA	1:16:A:GLU:HG2	11	0.23
(1,2053)	1:17:A:HIS:HA	1:16:A:GLU:HG2	16	0.23
(1,2052)	1:20:A:LYS:HG2	1:17:A:HIS:HA	1	0.23
(1,2052)	1:20:A:LYS:HG2	1:17:A:HIS:HA	16	0.23
(1,2050)	1:17:A:HIS:HA	1:16:A:GLU:HB2	6	0.23
(1,2050)	1:17:A:HIS:HA	1:16:A:GLU:HB2	20	0.23
(1,2042)	1:16:A:GLU:HA	1:15:A:GLU:HB2	9	0.23
(1,2041)	1:16:A:GLU:HA	1:17:A:HIS:HA	2	0.23
(1,2041)	1:16:A:GLU:HA	1:17:A:HIS:HA	6	0.23
(1,2041)	1:16:A:GLU:HA	1:17:A:HIS:HA	16	0.23
(1,1984)	1:7:A:VAL:HG11	1:48:A:PHE:HB3	10	0.23
(1,1944)	1:57:A:VAL:HB	1:26:A:ILE:HD11	5	0.23
(1,1897)	1:41:A:LYS:HD3	1:41:A:LYS:HA	14	0.23
(1,1888)	1:85:A:ALA:HB1	1:86:A:LEU:HG	3	0.23
(1,1888)	1:85:A:ALA:HB2	1:86:A:LEU:HG	9	0.23
(1,1864)	1:9:A:SER:HB2	1:12:A:ALA:HB3	6	0.23
(1,1864)	1:9:A:SER:HB2	1:12:A:ALA:HB3	15	0.23
(1,1847)	1:110:A:LEU:HD23	1:110:A:LEU:HB2	6	0.23
(1,1847)	1:110:A:LEU:HD22	1:110:A:LEU:HB2	12	0.23
(1,1820)	1:10:A:LEU:HD23	1:6:A:VAL:HG11	5	0.23
(1,1816)	1:102:A:THR:HG22	1:72:A:LEU:HD22	20	0.23
(1,1806)	1:10:A:LEU:HD13	1:7:A:VAL:HA	18	0.23
(1,1798)	1:62:A:ILE:HD13	1:28:A:ARG:HD3	12	0.23
(1,1777)	1:112:A:LEU:HD22	1:109:A:LEU:HD11	9	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1777)	1:112:A:LEU:HD23	1:109:A:LEU:HD11	15	0.23
(1,1749)	1:65:A:ILE:HG13	1:63:A:LEU:HD23	2	0.23
(1,1727)	1:11:A:ILE:HD12	1:55:A:SER:HB3	15	0.23
(1,1651)	1:61:A:ALA:HB1	1:58:A:CYS:HA	19	0.23
(1,1601)	1:12:A:ALA:HB2	1:9:A:SER:HA	3	0.23
(1,1601)	1:12:A:ALA:HB1	1:9:A:SER:HA	8	0.23
(1,1561)	1:38:A:ALA:HB2	1:38:A:ALA:HA	3	0.23
(1,1490)	1:6:A:VAL:HA	1:9:A:SER:HB3	6	0.23
(1,1477)	1:45:A:VAL:HG11	1:41:A:LYS:HA	9	0.23
(1,1452)	1:63:A:LEU:HD13	1:45:A:VAL:HA	5	0.23
(1,1445)	1:48:A:PHE:HB2	1:63:A:LEU:HD13	9	0.23
(1,1411)	1:84:A:ASN:HB2	1:84:A:ASN:HB3	1	0.23
(1,1411)	1:84:A:ASN:HB2	1:84:A:ASN:HB3	5	0.23
(1,1411)	1:84:A:ASN:HB2	1:84:A:ASN:HB3	7	0.23
(1,1411)	1:84:A:ASN:HB2	1:84:A:ASN:HB3	10	0.23
(1,1411)	1:84:A:ASN:HB2	1:84:A:ASN:HB3	12	0.23
(1,1411)	1:84:A:ASN:HB2	1:84:A:ASN:HB3	18	0.23
(1,1410)	1:84:A:ASN:HB3	1:84:A:ASN:HA	7	0.23
(1,1410)	1:84:A:ASN:HB3	1:84:A:ASN:HA	13	0.23
(1,1410)	1:84:A:ASN:HB3	1:84:A:ASN:HA	19	0.23
(1,1385)	1:48:A:PHE:HB3	1:63:A:LEU:HD13	15	0.23
(1,1384)	1:93:A:LYS:HE3	1:93:A:LYS:HA	1	0.23
(1,1352)	1:22:A:GLN:HG2	1:22:A:GLN:HG3	18	0.23
(1,1324)	1:106:A:GLU:HG3	1:105:A:ASN:HB2	13	0.23
(1,1299)	1:117:A:GLU:HB2	1:117:A:GLU:HG3	2	0.23
(1,1283)	1:15:A:GLU:HB3	1:12:A:ALA:HA	9	0.23
(1,1249)	1:72:A:LEU:HD12	1:83:A:PRO:HG2	11	0.23
(1,1053)	1:63:A:LEU:HD12	1:63:A:LEU:HB2	5	0.23
(1,1024)	1:57:A:VAL:HG12	1:18:A:ALA:HB1	16	0.23
(1,980)	1:23:A:ALA:HB2	1:23:A:ALA:HB1	3	0.23
(1,980)	1:23:A:ALA:HB2	1:23:A:ALA:HB3	11	0.23
(1,980)	1:23:A:ALA:HB1	1:23:A:ALA:HB3	17	0.23
(1,963)	1:41:A:LYS:HG3	1:65:A:ILE:HD11	7	0.23
(1,940)	1:112:A:LEU:HD11	1:112:A:LEU:HA	8	0.23
(1,922)	1:45:A:VAL:HG23	1:45:A:VAL:HG12	2	0.23
(1,922)	1:45:A:VAL:HG23	1:45:A:VAL:HG12	4	0.23
(1,922)	1:45:A:VAL:HG21	1:45:A:VAL:HG11	8	0.23
(1,922)	1:45:A:VAL:HG21	1:45:A:VAL:HG13	20	0.23
(1,908)	1:56:A:LEU:HD11	1:57:A:VAL:HG23	4	0.23
(1,889)	1:57:A:VAL:HG11	1:15:A:GLU:HG3	9	0.23
(1,858)	1:109:A:LEU:HD22	1:109:A:LEU:HD21	9	0.23
(1,849)	1:72:A:LEU:HD23	1:101:A:ILE:HG13	4	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,849)	1:72:A:LEU:HD21	1:101:A:ILE:HG13	14	0.23
(1,842)	1:112:A:LEU:HD21	1:112:A:LEU:HD23	6	0.23
(1,842)	1:112:A:LEU:HD22	1:112:A:LEU:HD23	7	0.23
(1,842)	1:112:A:LEU:HD21	1:112:A:LEU:HD23	12	0.23
(1,842)	1:112:A:LEU:HD22	1:112:A:LEU:HD21	19	0.23
(1,842)	1:112:A:LEU:HD22	1:112:A:LEU:HD23	20	0.23
(1,834)	1:72:A:LEU:HD23	1:101:A:ILE:HG22	6	0.23
(1,829)	1:101:A:ILE:HG23	1:105:A:ASN:HB3	19	0.23
(1,825)	1:101:A:ILE:HG22	1:72:A:LEU:HA	12	0.23
(1,821)	1:30:A:VAL:HG11	1:28:A:ARG:HG3	5	0.23
(1,818)	1:80:A:VAL:HG11	1:80:A:VAL:HG22	20	0.23
(1,803)	1:72:A:LEU:HD22	1:72:A:LEU:HB2	17	0.23
(1,793)	1:109:A:LEU:HD12	1:109:A:LEU:HD13	3	0.23
(1,780)	1:99:A:VAL:HG13	1:99:A:VAL:HG23	13	0.23
(1,771)	1:110:A:LEU:HD12	1:66:A:VAL:HG22	2	0.23
(1,754)	1:33:A:ILE:HG13	1:33:A:ILE:HG21	14	0.23
(1,741)	1:72:A:LEU:HD12	1:72:A:LEU:HD11	15	0.23
(1,741)	1:72:A:LEU:HD12	1:72:A:LEU:HD11	17	0.23
(1,736)	1:11:A:ILE:HD12	1:11:A:ILE:HD13	8	0.23
(1,736)	1:11:A:ILE:HD11	1:11:A:ILE:HD13	10	0.23
(1,736)	1:11:A:ILE:HD12	1:11:A:ILE:HD11	11	0.23
(1,457)	1:74:A:CYS:HB2	1:79:A:HIS:H	17	0.23
(1,358)	1:22:A:GLN:HB2	1:23:A:ALA:H	12	0.23
(1,174)	1:100:A:ILE:HG12	1:101:A:ILE:H	17	0.23
(1,162)	1:23:A:ALA:HB3	1:22:A:GLN:H	1	0.23
(1,162)	1:23:A:ALA:HB2	1:22:A:GLN:H	3	0.23
(1,162)	1:23:A:ALA:HB2	1:22:A:GLN:H	10	0.23
(1,134)	1:57:A:VAL:HG23	1:58:A:CYS:H	6	0.23
(1,131)	1:10:A:LEU:HD21	1:11:A:ILE:H	4	0.23
(1,131)	1:10:A:LEU:HD21	1:11:A:ILE:H	6	0.23
(1,121)	1:70:A:VAL:HG12	1:71:A:GLU:H	5	0.23
(1,88)	1:26:A:ILE:HD13	1:15:A:GLU:H	15	0.23
(1,83)	1:112:A:LEU:HD21	1:112:A:LEU:H	8	0.23
(1,83)	1:112:A:LEU:HD23	1:112:A:LEU:H	13	0.23
(1,71)	1:31:A:VAL:HG12	1:32:A:GLY:H	12	0.23
(1,25)	1:90:A:VAL:HG21	1:91:A:CYS:H	12	0.23
(1,2692)	1:4:A:TYR:HE2	1:4:A:TYR:HD2	6	0.22
(1,2671)	1:115:A:LEU:HD13	1:24:A:HIS:HD2	3	0.22
(1,2661)	1:75:A:LYS:HA	1:75:A:LYS:HE3	13	0.22
(1,2653)	1:41:A:LYS:HD3	1:41:A:LYS:HA	16	0.22
(1,2653)	1:41:A:LYS:HD3	1:41:A:LYS:HA	20	0.22
(1,2650)	1:66:A:VAL:HG12	1:32:A:GLY:HA3	1	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2650)	1:66:A:VAL:HG11	1:32:A:GLY:HA3	8	0.22
(1,2650)	1:66:A:VAL:HG12	1:32:A:GLY:HA3	12	0.22
(1,2622)	1:38:A:ALA:HB1	1:1:A:MET:HB2	18	0.22
(1,2614)	1:10:A:LEU:HD11	1:10:A:LEU:HD13	4	0.22
(1,2614)	1:10:A:LEU:HD12	1:10:A:LEU:HD13	5	0.22
(1,2614)	1:10:A:LEU:HD12	1:10:A:LEU:HD13	18	0.22
(1,2608)	1:115:A:LEU:HD22	1:27:A:GLU:HB2	18	0.22
(1,2608)	1:115:A:LEU:HD22	1:27:A:GLU:HB2	20	0.22
(1,2569)	1:92:A:GLU:HG2	1:92:A:GLU:HA	16	0.22
(1,2555)	1:115:A:LEU:HD13	1:25:A:LYS:HE2	16	0.22
(1,2541)	1:6:A:VAL:HB	1:39:A:MET:HE1	12	0.22
(1,2539)	1:106:A:GLU:HG2	1:106:A:GLU:HG3	4	0.22
(1,2451)	1:26:A:ILE:HD11	1:26:A:ILE:HD13	2	0.22
(1,2451)	1:26:A:ILE:HD12	1:26:A:ILE:HD13	3	0.22
(1,2451)	1:26:A:ILE:HD11	1:26:A:ILE:HD13	8	0.22
(1,2451)	1:101:A:ILE:HD12	1:101:A:ILE:HD13	10	0.22
(1,2451)	1:101:A:ILE:HD11	1:101:A:ILE:HD13	11	0.22
(1,2451)	1:101:A:ILE:HD12	1:101:A:ILE:HD13	14	0.22
(1,2451)	1:26:A:ILE:HD11	1:26:A:ILE:HD13	15	0.22
(1,2451)	1:101:A:ILE:HD11	1:101:A:ILE:HD13	16	0.22
(1,2451)	1:26:A:ILE:HD11	1:26:A:ILE:HD13	17	0.22
(1,2451)	1:101:A:ILE:HD12	1:101:A:ILE:HD13	18	0.22
(1,2451)	1:26:A:ILE:HD12	1:26:A:ILE:HD11	19	0.22
(1,2450)	1:99:A:VAL:HG21	1:99:A:VAL:HG23	10	0.22
(1,2436)	1:110:A:LEU:HD12	1:66:A:VAL:HG21	4	0.22
(1,2433)	1:63:A:LEU:HD23	1:31:A:VAL:HG21	8	0.22
(1,2397)	1:100:A:ILE:H	1:74:A:CYS:H	15	0.22
(1,2396)	1:101:A:ILE:H	1:100:A:ILE:H	10	0.22
(1,2378)	1:97:A:LYS:H	1:96:A:SER:H	4	0.22
(1,2378)	1:97:A:LYS:H	1:96:A:SER:H	16	0.22
(1,2294)	1:99:A:VAL:H	1:100:A:ILE:H	2	0.22
(1,2294)	1:99:A:VAL:H	1:100:A:ILE:H	16	0.22
(1,2294)	1:99:A:VAL:H	1:100:A:ILE:H	19	0.22
(1,2287)	1:80:A:VAL:H	1:81:A:PHE:H	12	0.22
(1,2229)	1:4:A:TYR:HB3	1:4:A:TYR:HE1	10	0.22
(1,2229)	1:4:A:TYR:HB3	1:4:A:TYR:HE1	12	0.22
(1,2229)	1:4:A:TYR:HB3	1:4:A:TYR:HE2	14	0.22
(1,2183)	1:116:A:ALA:HB2	1:24:A:HIS:HD2	3	0.22
(1,2183)	1:116:A:ALA:HB2	1:24:A:HIS:HD2	15	0.22
(1,2148)	1:80:A:VAL:HG13	1:81:A:PHE:HD1	16	0.22
(1,2143)	1:7:A:VAL:HG23	1:51:A:PHE:HD1	12	0.22
(1,2142)	1:7:A:VAL:HG23	1:48:A:PHE:HD1	5	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2134)	1:72:A:LEU:HD22	1:81:A:PHE:HE1	2	0.22
(1,2132)	1:72:A:LEU:HB3	1:81:A:PHE:HD1	20	0.22
(1,2067)	1:10:A:LEU:HA	1:13:A:LEU:HG	14	0.22
(1,2061)	1:33:A:ILE:HA	1:65:A:ILE:HG23	8	0.22
(1,2060)	1:35:A:GLU:HA	1:33:A:ILE:HG23	2	0.22
(1,2056)	1:15:A:GLU:HG2	1:12:A:ALA:HA	4	0.22
(1,2051)	1:114:A:MET:HE2	1:17:A:HIS:HA	8	0.22
(1,2042)	1:16:A:GLU:HA	1:15:A:GLU:HB2	17	0.22
(1,2041)	1:16:A:GLU:HA	1:17:A:HIS:HA	3	0.22
(1,2024)	1:107:A:MET:HE2	1:7:A:VAL:HA	20	0.22
(1,2016)	1:93:A:LYS:HD2	1:79:A:HIS:HB2	3	0.22
(1,1984)	1:7:A:VAL:HG13	1:48:A:PHE:HB3	7	0.22
(1,1984)	1:7:A:VAL:HG13	1:48:A:PHE:HB3	16	0.22
(1,1982)	1:106:A:GLU:HG3	1:105:A:ASN:HB3	16	0.22
(1,1968)	1:113:A:GLU:HG2	1:27:A:GLU:HB3	18	0.22
(1,1944)	1:57:A:VAL:HB	1:26:A:ILE:HD12	6	0.22
(1,1944)	1:57:A:VAL:HB	1:26:A:ILE:HD13	7	0.22
(1,1933)	1:38:A:ALA:HB3	1:1:A:MET:HB2	14	0.22
(1,1897)	1:41:A:LYS:HD3	1:41:A:LYS:HA	3	0.22
(1,1847)	1:110:A:LEU:HD23	1:110:A:LEU:HB2	2	0.22
(1,1847)	1:110:A:LEU:HD21	1:110:A:LEU:HB2	18	0.22
(1,1847)	1:110:A:LEU:HD21	1:110:A:LEU:HB2	19	0.22
(1,1820)	1:10:A:LEU:HD21	1:6:A:VAL:HG13	16	0.22
(1,1819)	1:7:A:VAL:HG13	1:47:A:ALA:HB2	7	0.22
(1,1799)	1:29:A:VAL:HG13	1:109:A:LEU:HD11	8	0.22
(1,1798)	1:62:A:ILE:HD11	1:28:A:ARG:HD3	7	0.22
(1,1788)	1:75:A:LYS:HE3	1:100:A:ILE:HG21	14	0.22
(1,1775)	1:100:A:ILE:HD12	1:102:A:THR:HB	8	0.22
(1,1774)	1:31:A:VAL:HG21	1:107:A:MET:HG2	10	0.22
(1,1774)	1:31:A:VAL:HG22	1:107:A:MET:HG2	11	0.22
(1,1769)	1:66:A:VAL:HG13	1:68:A:GLU:HB3	19	0.22
(1,1677)	1:25:A:LYS:HA	1:57:A:VAL:HG23	11	0.22
(1,1618)	1:50:A:THR:HG23	1:51:A:PHE:HA	2	0.22
(1,1618)	1:50:A:THR:HG22	1:51:A:PHE:HA	10	0.22
(1,1618)	1:50:A:THR:HG21	1:51:A:PHE:HA	14	0.22
(1,1581)	1:35:A:GLU:HG3	1:35:A:GLU:HA	2	0.22
(1,1581)	1:35:A:GLU:HG3	1:35:A:GLU:HA	10	0.22
(1,1570)	1:102:A:THR:HA	1:101:A:ILE:HG22	4	0.22
(1,1561)	1:38:A:ALA:HB1	1:38:A:ALA:HA	8	0.22
(1,1559)	1:12:A:ALA:HB2	1:12:A:ALA:HA	13	0.22
(1,1545)	1:114:A:MET:HE1	1:18:A:ALA:HA	14	0.22
(1,1507)	1:26:A:ILE:HD11	1:14:A:CYS:HA	11	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1477)	1:45:A:VAL:HG12	1:41:A:LYS:HA	16	0.22
(1,1411)	1:84:A:ASN:HB2	1:84:A:ASN:HB3	3	0.22
(1,1411)	1:84:A:ASN:HB2	1:84:A:ASN:HB3	17	0.22
(1,1410)	1:84:A:ASN:HB3	1:84:A:ASN:HA	10	0.22
(1,1352)	1:22:A:GLN:HG2	1:22:A:GLN:HG3	11	0.22
(1,1352)	1:22:A:GLN:HG2	1:22:A:GLN:HG3	14	0.22
(1,1352)	1:22:A:GLN:HG2	1:22:A:GLN:HG3	15	0.22
(1,1352)	1:22:A:GLN:HG2	1:22:A:GLN:HG3	16	0.22
(1,1299)	1:117:A:GLU:HB2	1:117:A:GLU:HG3	1	0.22
(1,1299)	1:117:A:GLU:HB2	1:117:A:GLU:HG3	17	0.22
(1,1273)	1:114:A:MET:HE3	1:112:A:LEU:HB3	8	0.22
(1,1197)	1:80:A:VAL:HG12	1:71:A:GLU:HG3	13	0.22
(1,1145)	1:41:A:LYS:HD2	1:33:A:ILE:HG21	12	0.22
(1,1081)	1:43:A:LEU:HG	1:43:A:LEU:HA	12	0.22
(1,1076)	1:36:A:ARG:HB3	1:70:A:VAL:HG13	2	0.22
(1,1053)	1:63:A:LEU:HD13	1:63:A:LEU:HB2	3	0.22
(1,1053)	1:63:A:LEU:HD13	1:63:A:LEU:HB2	13	0.22
(1,1024)	1:57:A:VAL:HG12	1:18:A:ALA:HB3	8	0.22
(1,1010)	1:115:A:LEU:HB3	1:25:A:LYS:HB3	14	0.22
(1,996)	1:26:A:ILE:HG12	1:57:A:VAL:HG13	14	0.22
(1,980)	1:23:A:ALA:HB1	1:23:A:ALA:HB3	1	0.22
(1,980)	1:23:A:ALA:HB2	1:23:A:ALA:HB3	15	0.22
(1,963)	1:41:A:LYS:HG3	1:65:A:ILE:HD12	12	0.22
(1,953)	1:65:A:ILE:HG23	1:33:A:ILE:HG12	8	0.22
(1,952)	1:33:A:ILE:HG12	1:31:A:VAL:HG21	1	0.22
(1,952)	1:33:A:ILE:HG12	1:31:A:VAL:HG22	20	0.22
(1,940)	1:112:A:LEU:HD12	1:112:A:LEU:HA	1	0.22
(1,940)	1:112:A:LEU:HD12	1:112:A:LEU:HA	5	0.22
(1,940)	1:112:A:LEU:HD12	1:112:A:LEU:HA	9	0.22
(1,922)	1:45:A:VAL:HG23	1:45:A:VAL:HG13	5	0.22
(1,922)	1:45:A:VAL:HG22	1:45:A:VAL:HG13	7	0.22
(1,887)	1:57:A:VAL:HG12	1:18:A:ALA:HA	5	0.22
(1,887)	1:57:A:VAL:HG12	1:18:A:ALA:HA	16	0.22
(1,874)	1:26:A:ILE:HG22	1:61:A:ALA:HB2	18	0.22
(1,858)	1:109:A:LEU:HD22	1:109:A:LEU:HD23	19	0.22
(1,842)	1:112:A:LEU:HD22	1:112:A:LEU:HD23	3	0.22
(1,842)	1:112:A:LEU:HD22	1:112:A:LEU:HD21	11	0.22
(1,825)	1:101:A:ILE:HG23	1:72:A:LEU:HA	10	0.22
(1,825)	1:101:A:ILE:HG21	1:72:A:LEU:HA	14	0.22
(1,821)	1:30:A:VAL:HG11	1:28:A:ARG:HG3	6	0.22
(1,818)	1:80:A:VAL:HG12	1:80:A:VAL:HG22	4	0.22
(1,818)	1:80:A:VAL:HG12	1:80:A:VAL:HG22	12	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,814)	1:31:A:VAL:HG23	1:63:A:LEU:HD12	19	0.22
(1,793)	1:109:A:LEU:HD12	1:109:A:LEU:HD13	10	0.22
(1,769)	1:72:A:LEU:HD21	1:70:A:VAL:HG21	5	0.22
(1,755)	1:65:A:ILE:HG21	1:41:A:LYS:HD2	5	0.22
(1,741)	1:72:A:LEU:HD12	1:72:A:LEU:HD13	1	0.22
(1,736)	1:11:A:ILE:HD12	1:11:A:ILE:HD11	1	0.22
(1,736)	1:11:A:ILE:HD11	1:11:A:ILE:HD13	6	0.22
(1,736)	1:11:A:ILE:HD12	1:11:A:ILE:HD13	14	0.22
(1,736)	1:11:A:ILE:HD12	1:11:A:ILE:HD13	15	0.22
(1,690)	1:76:A:ASP:HA	1:77:A:CYS:H	11	0.22
(1,448)	1:79:A:HIS:HB2	1:80:A:VAL:H	4	0.22
(1,448)	1:79:A:HIS:HB2	1:80:A:VAL:H	13	0.22
(1,371)	1:22:A:GLN:HG3	1:21:A:ASN:H	1	0.22
(1,358)	1:22:A:GLN:HB2	1:23:A:ALA:H	7	0.22
(1,358)	1:22:A:GLN:HB2	1:23:A:ALA:H	9	0.22
(1,344)	1:113:A:GLU:HG3	1:113:A:GLU:H	15	0.22
(1,196)	1:12:A:ALA:HB1	1:14:A:CYS:H	2	0.22
(1,196)	1:12:A:ALA:HB1	1:14:A:CYS:H	7	0.22
(1,156)	1:23:A:ALA:HB2	1:21:A:ASN:H	19	0.22
(1,141)	1:93:A:LYS:HD3	1:93:A:LYS:H	12	0.22
(1,134)	1:57:A:VAL:HG23	1:58:A:CYS:H	2	0.22
(1,134)	1:57:A:VAL:HG23	1:58:A:CYS:H	13	0.22
(1,107)	1:56:A:LEU:HD22	1:56:A:LEU:H	9	0.22
(1,107)	1:56:A:LEU:HD21	1:56:A:LEU:H	18	0.22
(1,103)	1:43:A:LEU:HD23	1:46:A:SER:H	6	0.22
(1,97)	1:11:A:ILE:HG21	1:12:A:ALA:H	3	0.22
(1,95)	1:93:A:LYS:HB3	1:93:A:LYS:H	12	0.22
(1,39)	1:90:A:VAL:HG12	1:90:A:VAL:H	3	0.22
(1,39)	1:90:A:VAL:HG13	1:90:A:VAL:H	5	0.22
(1,39)	1:90:A:VAL:HG11	1:90:A:VAL:H	14	0.22
(1,34)	1:33:A:ILE:HG22	1:39:A:MET:H	13	0.22
(1,29)	1:70:A:VAL:HG23	1:72:A:LEU:H	9	0.22
(1,12)	1:72:A:LEU:HD12	1:72:A:LEU:H	2	0.22
(1,2676)	1:47:A:ALA:HB2	1:44:A:PHE:HD1	18	0.21
(1,2671)	1:115:A:LEU:HD12	1:24:A:HIS:HD2	13	0.21
(1,2661)	1:75:A:LYS:HA	1:75:A:LYS:HE3	3	0.21
(1,2653)	1:41:A:LYS:HD3	1:41:A:LYS:HA	10	0.21
(1,2647)	1:59:A:LYS:HB3	1:25:A:LYS:HE3	19	0.21
(1,2645)	1:33:A:ILE:HG21	1:39:A:MET:HG3	1	0.21
(1,2569)	1:92:A:GLU:HG2	1:92:A:GLU:HA	7	0.21
(1,2569)	1:92:A:GLU:HG2	1:92:A:GLU:HA	17	0.21
(1,2539)	1:113:A:GLU:HG3	1:113:A:GLU:HG2	2	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2537)	1:115:A:LEU:HD13	1:27:A:GLU:HG2	18	0.21
(1,2503)	1:36:A:ARG:HG3	1:36:A:ARG:HG2	1	0.21
(1,2469)	1:6:A:VAL:HG11	1:107:A:MET:HE2	2	0.21
(1,2469)	1:6:A:VAL:HG12	1:107:A:MET:HE2	4	0.21
(1,2451)	1:26:A:ILE:HD12	1:26:A:ILE:HD11	7	0.21
(1,2451)	1:26:A:ILE:HD11	1:26:A:ILE:HD13	12	0.21
(1,2451)	1:26:A:ILE:HD11	1:26:A:ILE:HD13	13	0.21
(1,2451)	1:101:A:ILE:HD12	1:101:A:ILE:HD11	20	0.21
(1,2442)	1:31:A:VAL:HG21	1:31:A:VAL:HG12	8	0.21
(1,2438)	1:65:A:ILE:HD13	1:41:A:LYS:HD2	14	0.21
(1,2436)	1:110:A:LEU:HD13	1:66:A:VAL:HG22	19	0.21
(1,2397)	1:100:A:ILE:H	1:74:A:CYS:H	8	0.21
(1,2396)	1:101:A:ILE:H	1:100:A:ILE:H	16	0.21
(1,2396)	1:101:A:ILE:H	1:100:A:ILE:H	17	0.21
(1,2380)	1:34:A:GLY:H	1:35:A:GLU:H	7	0.21
(1,2380)	1:34:A:GLY:H	1:35:A:GLU:H	14	0.21
(1,2380)	1:34:A:GLY:H	1:35:A:GLU:H	15	0.21
(1,2380)	1:34:A:GLY:H	1:35:A:GLU:H	16	0.21
(1,2380)	1:34:A:GLY:H	1:35:A:GLU:H	18	0.21
(1,2378)	1:97:A:LYS:H	1:96:A:SER:H	5	0.21
(1,2378)	1:97:A:LYS:H	1:96:A:SER:H	6	0.21
(1,2378)	1:97:A:LYS:H	1:96:A:SER:H	8	0.21
(1,2298)	1:71:A:GLU:H	1:70:A:VAL:H	1	0.21
(1,2287)	1:80:A:VAL:H	1:81:A:PHE:H	11	0.21
(1,2287)	1:80:A:VAL:H	1:81:A:PHE:H	19	0.21
(1,2229)	1:4:A:TYR:HB3	1:4:A:TYR:HE2	1	0.21
(1,2229)	1:4:A:TYR:HB3	1:4:A:TYR:HE2	2	0.21
(1,2229)	1:4:A:TYR:HB3	1:4:A:TYR:HE1	15	0.21
(1,2171)	1:47:A:ALA:HB2	1:4:A:TYR:HE1	6	0.21
(1,2170)	1:92:A:GLU:HG3	1:81:A:PHE:HD2	7	0.21
(1,2166)	1:50:A:THR:HG22	1:51:A:PHE:HE1	20	0.21
(1,2158)	1:29:A:VAL:HG12	1:48:A:PHE:HZ	8	0.21
(1,2153)	1:99:A:VAL:HG21	1:81:A:PHE:HE2	9	0.21
(1,2132)	1:72:A:LEU:HB3	1:81:A:PHE:HD2	10	0.21
(1,2105)	1:64:A:ASP:HA	1:62:A:ILE:HG21	3	0.21
(1,2070)	1:109:A:LEU:HD21	1:29:A:VAL:HA	4	0.21
(1,2070)	1:109:A:LEU:HD22	1:29:A:VAL:HA	14	0.21
(1,2068)	1:30:A:VAL:HG13	1:29:A:VAL:HA	18	0.21
(1,2067)	1:10:A:LEU:HA	1:13:A:LEU:HG	8	0.21
(1,2061)	1:33:A:ILE:HA	1:65:A:ILE:HG22	1	0.21
(1,2058)	1:12:A:ALA:HB3	1:13:A:LEU:HA	6	0.21
(1,2058)	1:12:A:ALA:HB3	1:13:A:LEU:HA	10	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2051)	1:114:A:MET:HE1	1:17:A:HIS:HA	5	0.21
(1,2051)	1:114:A:MET:HE1	1:17:A:HIS:HA	12	0.21
(1,2050)	1:17:A:HIS:HA	1:16:A:GLU:HB2	10	0.21
(1,2041)	1:16:A:GLU:HA	1:17:A:HIS:HA	11	0.21
(1,2041)	1:16:A:GLU:HA	1:17:A:HIS:HA	17	0.21
(1,1953)	1:68:A:GLU:HG2	1:32:A:GLY:HA3	9	0.21
(1,1897)	1:41:A:LYS:HD3	1:41:A:LYS:HA	19	0.21
(1,1847)	1:110:A:LEU:HD23	1:110:A:LEU:HB2	1	0.21
(1,1847)	1:110:A:LEU:HD23	1:110:A:LEU:HB2	16	0.21
(1,1824)	1:25:A:LYS:HG3	1:56:A:LEU:HD12	8	0.21
(1,1820)	1:10:A:LEU:HD22	1:6:A:VAL:HG13	17	0.21
(1,1812)	1:50:A:THR:HG21	1:47:A:ALA:HA	7	0.21
(1,1771)	1:31:A:VAL:HG23	1:65:A:ILE:HB	16	0.21
(1,1749)	1:65:A:ILE:HG13	1:63:A:LEU:HD22	9	0.21
(1,1746)	1:90:A:VAL:HG22	1:87:A:ASP:HB3	15	0.21
(1,1677)	1:25:A:LYS:HA	1:57:A:VAL:HG23	15	0.21
(1,1601)	1:12:A:ALA:HB2	1:9:A:SER:HA	12	0.21
(1,1581)	1:35:A:GLU:HG3	1:35:A:GLU:HA	6	0.21
(1,1581)	1:35:A:GLU:HG3	1:35:A:GLU:HA	11	0.21
(1,1581)	1:35:A:GLU:HG3	1:35:A:GLU:HA	18	0.21
(1,1581)	1:35:A:GLU:HG3	1:35:A:GLU:HA	19	0.21
(1,1576)	1:35:A:GLU:HG3	1:69:A:LYS:HA	18	0.21
(1,1501)	1:3:A:GLU:HA	1:39:A:MET:HE1	12	0.21
(1,1499)	1:6:A:VAL:HG22	1:3:A:GLU:HA	5	0.21
(1,1477)	1:45:A:VAL:HG13	1:41:A:LYS:HA	17	0.21
(1,1452)	1:63:A:LEU:HD11	1:45:A:VAL:HA	1	0.21
(1,1411)	1:84:A:ASN:HB2	1:84:A:ASN:HB3	2	0.21
(1,1410)	1:84:A:ASN:HB3	1:84:A:ASN:HA	17	0.21
(1,1354)	1:1:A:MET:HG3	1:1:A:MET:HA	16	0.21
(1,1352)	1:22:A:GLN:HG2	1:22:A:GLN:HG3	4	0.21
(1,1352)	1:22:A:GLN:HG2	1:22:A:GLN:HG3	6	0.21
(1,1352)	1:22:A:GLN:HG2	1:22:A:GLN:HG3	7	0.21
(1,1352)	1:22:A:GLN:HG2	1:22:A:GLN:HG3	9	0.21
(1,1352)	1:22:A:GLN:HG2	1:22:A:GLN:HG3	17	0.21
(1,1303)	1:23:A:ALA:HB1	1:114:A:MET:HB2	1	0.21
(1,1299)	1:117:A:GLU:HB2	1:117:A:GLU:HG3	3	0.21
(1,1299)	1:117:A:GLU:HB2	1:117:A:GLU:HG3	10	0.21
(1,1283)	1:15:A:GLU:HB3	1:12:A:ALA:HA	11	0.21
(1,1280)	1:39:A:MET:HB2	1:39:A:MET:HE1	7	0.21
(1,1140)	1:59:A:LYS:HD3	1:59:A:LYS:HA	19	0.21
(1,1115)	1:70:A:VAL:HG22	1:83:A:PRO:HG3	13	0.21
(1,1081)	1:43:A:LEU:HG	1:43:A:LEU:HA	5	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1053)	1:63:A:LEU:HD12	1:63:A:LEU:HB2	9	0.21
(1,1053)	1:63:A:LEU:HD11	1:63:A:LEU:HB2	20	0.21
(1,1038)	1:20:A:LYS:HG3	1:20:A:LYS:HD2	7	0.21
(1,1010)	1:115:A:LEU:HB3	1:25:A:LYS:HB3	16	0.21
(1,998)	1:65:A:ILE:HG12	1:63:A:LEU:HD21	1	0.21
(1,980)	1:23:A:ALA:HB2	1:23:A:ALA:HB1	2	0.21
(1,962)	1:33:A:ILE:HD11	1:41:A:LYS:HG3	15	0.21
(1,953)	1:65:A:ILE:HG22	1:33:A:ILE:HG12	2	0.21
(1,940)	1:112:A:LEU:HD13	1:112:A:LEU:HA	12	0.21
(1,940)	1:112:A:LEU:HD13	1:112:A:LEU:HA	16	0.21
(1,908)	1:56:A:LEU:HD11	1:57:A:VAL:HG23	2	0.21
(1,908)	1:56:A:LEU:HD12	1:57:A:VAL:HG23	3	0.21
(1,904)	1:31:A:VAL:HG13	1:10:A:LEU:HD11	15	0.21
(1,846)	1:31:A:VAL:HG12	1:10:A:LEU:HD23	17	0.21
(1,842)	1:112:A:LEU:HD21	1:112:A:LEU:HD23	1	0.21
(1,842)	1:112:A:LEU:HD22	1:112:A:LEU:HD23	13	0.21
(1,842)	1:112:A:LEU:HD22	1:112:A:LEU:HD23	18	0.21
(1,826)	1:101:A:ILE:HG21	1:103:A:GLN:HA	2	0.21
(1,820)	1:30:A:VAL:HG11	1:64:A:ASP:HB2	7	0.21
(1,780)	1:99:A:VAL:HG12	1:99:A:VAL:HG21	1	0.21
(1,780)	1:99:A:VAL:HG12	1:99:A:VAL:HG23	8	0.21
(1,780)	1:99:A:VAL:HG13	1:99:A:VAL:HG21	18	0.21
(1,772)	1:66:A:VAL:HG22	1:64:A:ASP:HB2	20	0.21
(1,741)	1:72:A:LEU:HD12	1:72:A:LEU:HD11	11	0.21
(1,736)	1:11:A:ILE:HD12	1:11:A:ILE:HD11	2	0.21
(1,736)	1:11:A:ILE:HD12	1:11:A:ILE:HD13	3	0.21
(1,736)	1:11:A:ILE:HD12	1:11:A:ILE:HD11	9	0.21
(1,736)	1:11:A:ILE:HD11	1:11:A:ILE:HD13	13	0.21
(1,736)	1:11:A:ILE:HD12	1:11:A:ILE:HD11	17	0.21
(1,736)	1:11:A:ILE:HD12	1:11:A:ILE:HD11	18	0.21
(1,736)	1:11:A:ILE:HD12	1:11:A:ILE:HD11	20	0.21
(1,448)	1:79:A:HIS:HB2	1:80:A:VAL:H	5	0.21
(1,437)	1:24:A:HIS:HB3	1:25:A:LYS:H	20	0.21
(1,222)	1:101:A:ILE:HG12	1:101:A:ILE:H	1	0.21
(1,191)	1:93:A:LYS:HB2	1:94:A:CYS:H	9	0.21
(1,174)	1:100:A:ILE:HG12	1:101:A:ILE:H	11	0.21
(1,162)	1:23:A:ALA:HB3	1:22:A:GLN:H	20	0.21
(1,138)	1:102:A:THR:HG21	1:103:A:GLN:H	2	0.21
(1,138)	1:102:A:THR:HG23	1:103:A:GLN:H	9	0.21
(1,134)	1:57:A:VAL:HG23	1:58:A:CYS:H	3	0.21
(1,125)	1:43:A:LEU:HD13	1:43:A:LEU:H	7	0.21
(1,121)	1:70:A:VAL:HG11	1:71:A:GLU:H	4	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,113)	1:10:A:LEU:HD13	1:10:A:LEU:H	3	0.21
(1,108)	1:115:A:LEU:HD22	1:116:A:ALA:H	14	0.21
(1,107)	1:56:A:LEU:HD22	1:56:A:LEU:H	16	0.21
(1,97)	1:11:A:ILE:HG21	1:12:A:ALA:H	14	0.21
(1,83)	1:112:A:LEU:HD23	1:112:A:LEU:H	4	0.21
(1,74)	1:99:A:VAL:HG22	1:73:A:GLU:H	19	0.21
(1,71)	1:31:A:VAL:HG13	1:32:A:GLY:H	20	0.21
(1,39)	1:90:A:VAL:HG12	1:90:A:VAL:H	20	0.21
(1,36)	1:99:A:VAL:HG12	1:100:A:ILE:H	10	0.21
(1,29)	1:70:A:VAL:HG23	1:72:A:LEU:H	5	0.21
(1,29)	1:70:A:VAL:HG21	1:72:A:LEU:H	20	0.21
(1,12)	1:72:A:LEU:HD13	1:72:A:LEU:H	10	0.21
(1,2675)	1:10:A:LEU:HD22	1:48:A:PHE:HZ	13	0.2
(1,2673)	1:13:A:LEU:HD11	1:17:A:HIS:HD2	3	0.2
(1,2653)	1:41:A:LYS:HD3	1:41:A:LYS:HA	7	0.2
(1,2653)	1:41:A:LYS:HD3	1:41:A:LYS:HA	9	0.2
(1,2653)	1:41:A:LYS:HD3	1:41:A:LYS:HA	12	0.2
(1,2653)	1:41:A:LYS:HD3	1:41:A:LYS:HA	13	0.2
(1,2650)	1:66:A:VAL:HG11	1:32:A:GLY:HA3	17	0.2
(1,2612)	1:25:A:LYS:HE3	1:56:A:LEU:HD13	15	0.2
(1,2569)	1:92:A:GLU:HG2	1:92:A:GLU:HA	6	0.2
(1,2539)	1:113:A:GLU:HG3	1:113:A:GLU:HG2	5	0.2
(1,2539)	1:113:A:GLU:HG3	1:113:A:GLU:HG2	6	0.2
(1,2539)	1:113:A:GLU:HG3	1:113:A:GLU:HG2	9	0.2
(1,2537)	1:115:A:LEU:HD11	1:27:A:GLU:HG2	10	0.2
(1,2537)	1:115:A:LEU:HD21	1:27:A:GLU:HG2	14	0.2
(1,2442)	1:31:A:VAL:HG22	1:31:A:VAL:HG11	11	0.2
(1,2427)	1:107:A:MET:HE1	1:107:A:MET:H	3	0.2
(1,2396)	1:101:A:ILE:H	1:100:A:ILE:H	3	0.2
(1,2396)	1:101:A:ILE:H	1:100:A:ILE:H	9	0.2
(1,2396)	1:101:A:ILE:H	1:100:A:ILE:H	20	0.2
(1,2380)	1:34:A:GLY:H	1:35:A:GLU:H	5	0.2
(1,2380)	1:34:A:GLY:H	1:35:A:GLU:H	13	0.2
(1,2378)	1:97:A:LYS:H	1:96:A:SER:H	1	0.2
(1,2298)	1:71:A:GLU:H	1:70:A:VAL:H	9	0.2
(1,2298)	1:71:A:GLU:H	1:70:A:VAL:H	15	0.2
(1,2294)	1:99:A:VAL:H	1:100:A:ILE:H	4	0.2
(1,2294)	1:99:A:VAL:H	1:100:A:ILE:H	10	0.2
(1,2294)	1:99:A:VAL:H	1:100:A:ILE:H	12	0.2
(1,2287)	1:80:A:VAL:H	1:81:A:PHE:H	5	0.2
(1,2287)	1:80:A:VAL:H	1:81:A:PHE:H	7	0.2
(1,2287)	1:80:A:VAL:H	1:81:A:PHE:H	13	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2262)	1:88:A:TYR:HA	1:88:A:TYR:HD1	7	0.2
(1,2262)	1:88:A:TYR:HA	1:88:A:TYR:HD2	18	0.2
(1,2250)	1:4:A:TYR:HA	1:4:A:TYR:HD2	5	0.2
(1,2229)	1:4:A:TYR:HB3	1:4:A:TYR:HE1	3	0.2
(1,2202)	1:83:A:PRO:HB3	1:88:A:TYR:HD2	18	0.2
(1,2183)	1:116:A:ALA:HB1	1:24:A:HIS:HD2	2	0.2
(1,2172)	1:47:A:ALA:HB3	1:4:A:TYR:HD1	13	0.2
(1,2170)	1:92:A:GLU:HG3	1:81:A:PHE:HD2	2	0.2
(1,2166)	1:50:A:THR:HG22	1:51:A:PHE:HE1	14	0.2
(1,2160)	1:80:A:VAL:HG21	1:81:A:PHE:HD2	15	0.2
(1,2143)	1:7:A:VAL:HG23	1:51:A:PHE:HD1	2	0.2
(1,2143)	1:7:A:VAL:HG21	1:51:A:PHE:HD1	18	0.2
(1,2142)	1:7:A:VAL:HG22	1:48:A:PHE:HD1	9	0.2
(1,2121)	1:63:A:LEU:HD22	1:48:A:PHE:HD1	3	0.2
(1,2105)	1:64:A:ASP:HA	1:62:A:ILE:HG21	18	0.2
(1,2104)	1:82:A:LYS:HA	1:83:A:PRO:HG3	5	0.2
(1,2100)	1:97:A:LYS:HA	1:97:A:LYS:HE2	8	0.2
(1,2070)	1:109:A:LEU:HD23	1:29:A:VAL:HA	8	0.2
(1,2067)	1:10:A:LEU:HA	1:13:A:LEU:HG	7	0.2
(1,2061)	1:33:A:ILE:HA	1:65:A:ILE:HG23	3	0.2
(1,2061)	1:33:A:ILE:HA	1:65:A:ILE:HG23	7	0.2
(1,2061)	1:33:A:ILE:HA	1:65:A:ILE:HG21	11	0.2
(1,2061)	1:33:A:ILE:HA	1:65:A:ILE:HG21	14	0.2
(1,2050)	1:17:A:HIS:HA	1:16:A:GLU:HB2	4	0.2
(1,2050)	1:17:A:HIS:HA	1:16:A:GLU:HB2	7	0.2
(1,2050)	1:17:A:HIS:HA	1:16:A:GLU:HB2	11	0.2
(1,2050)	1:17:A:HIS:HA	1:16:A:GLU:HB2	17	0.2
(1,2042)	1:16:A:GLU:HA	1:15:A:GLU:HB2	10	0.2
(1,2041)	1:16:A:GLU:HA	1:17:A:HIS:HA	4	0.2
(1,2041)	1:16:A:GLU:HA	1:17:A:HIS:HA	18	0.2
(1,2030)	1:83:A:PRO:HD2	1:72:A:LEU:HD13	6	0.2
(1,2024)	1:107:A:MET:HE3	1:7:A:VAL:HA	2	0.2
(1,2010)	1:114:A:MET:HE1	1:17:A:HIS:HB2	14	0.2
(1,1897)	1:41:A:LYS:HD3	1:41:A:LYS:HA	16	0.2
(1,1889)	1:82:A:LYS:HD3	1:71:A:GLU:HG3	20	0.2
(1,1864)	1:9:A:SER:HB2	1:12:A:ALA:HB2	4	0.2
(1,1799)	1:29:A:VAL:HG12	1:109:A:LEU:HD12	12	0.2
(1,1780)	1:112:A:LEU:HD21	1:17:A:HIS:HA	1	0.2
(1,1769)	1:66:A:VAL:HG12	1:68:A:GLU:HB2	1	0.2
(1,1765)	1:72:A:LEU:HB2	1:99:A:VAL:HB	5	0.2
(1,1765)	1:72:A:LEU:HB2	1:99:A:VAL:HB	12	0.2
(1,1755)	1:65:A:ILE:HD11	1:45:A:VAL:HA	3	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1755)	1:65:A:ILE:HD11	1:45:A:VAL:HA	5	0.2
(1,1749)	1:65:A:ILE:HG13	1:63:A:LEU:HD21	4	0.2
(1,1748)	1:33:A:ILE:HG21	1:107:A:MET:HG3	11	0.2
(1,1618)	1:50:A:THR:HG23	1:51:A:PHE:HA	17	0.2
(1,1601)	1:12:A:ALA:HB3	1:9:A:SER:HA	9	0.2
(1,1581)	1:35:A:GLU:HG3	1:35:A:GLU:HA	4	0.2
(1,1581)	1:35:A:GLU:HG3	1:35:A:GLU:HA	8	0.2
(1,1581)	1:35:A:GLU:HG3	1:35:A:GLU:HA	14	0.2
(1,1581)	1:35:A:GLU:HG3	1:35:A:GLU:HA	20	0.2
(1,1561)	1:38:A:ALA:HB2	1:38:A:ALA:HA	9	0.2
(1,1554)	1:20:A:LYS:HE3	1:17:A:HIS:HA	7	0.2
(1,1554)	1:20:A:LYS:HE3	1:17:A:HIS:HA	16	0.2
(1,1477)	1:45:A:VAL:HG11	1:41:A:LYS:HA	6	0.2
(1,1452)	1:63:A:LEU:HD11	1:45:A:VAL:HA	17	0.2
(1,1410)	1:84:A:ASN:HB3	1:84:A:ASN:HA	3	0.2
(1,1410)	1:84:A:ASN:HB3	1:84:A:ASN:HA	5	0.2
(1,1410)	1:84:A:ASN:HB3	1:84:A:ASN:HA	8	0.2
(1,1410)	1:84:A:ASN:HB3	1:84:A:ASN:HA	9	0.2
(1,1384)	1:93:A:LYS:HE3	1:93:A:LYS:HA	8	0.2
(1,1361)	1:26:A:ILE:HD12	1:114:A:MET:HG2	19	0.2
(1,1352)	1:22:A:GLN:HG2	1:22:A:GLN:HG3	3	0.2
(1,1352)	1:22:A:GLN:HG2	1:22:A:GLN:HG3	12	0.2
(1,1352)	1:22:A:GLN:HG2	1:22:A:GLN:HG3	20	0.2
(1,1324)	1:106:A:GLU:HG3	1:105:A:ASN:HB2	1	0.2
(1,1324)	1:106:A:GLU:HG3	1:105:A:ASN:HB2	19	0.2
(1,1299)	1:117:A:GLU:HB2	1:117:A:GLU:HG3	15	0.2
(1,1280)	1:39:A:MET:HB2	1:39:A:MET:HE3	19	0.2
(1,1249)	1:72:A:LEU:HD13	1:83:A:PRO:HG2	4	0.2
(1,1217)	1:72:A:LEU:HD11	1:99:A:VAL:HB	11	0.2
(1,1211)	1:75:A:LYS:HB3	1:98:A:ASN:HB2	9	0.2
(1,1211)	1:75:A:LYS:HB3	1:98:A:ASN:HB2	11	0.2
(1,1145)	1:41:A:LYS:HD2	1:33:A:ILE:HG21	10	0.2
(1,1081)	1:43:A:LEU:HG	1:43:A:LEU:HA	9	0.2
(1,1053)	1:63:A:LEU:HD12	1:63:A:LEU:HB2	17	0.2
(1,1010)	1:115:A:LEU:HB3	1:25:A:LYS:HB3	15	0.2
(1,1010)	1:115:A:LEU:HB3	1:25:A:LYS:HB3	19	0.2
(1,962)	1:33:A:ILE:HD13	1:41:A:LYS:HG3	12	0.2
(1,908)	1:56:A:LEU:HD12	1:57:A:VAL:HG23	11	0.2
(1,887)	1:57:A:VAL:HG12	1:18:A:ALA:HA	8	0.2
(1,875)	1:86:A:LEU:HD23	1:85:A:ALA:HA	9	0.2
(1,849)	1:72:A:LEU:HD23	1:101:A:ILE:HG13	17	0.2
(1,844)	1:112:A:LEU:HD21	1:114:A:MET:HE1	11	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,832)	1:101:A:ILE:HG23	1:105:A:ASN:HB2	16	0.2
(1,818)	1:80:A:VAL:HG13	1:80:A:VAL:HG23	17	0.2
(1,813)	1:29:A:VAL:HG22	1:10:A:LEU:HD13	8	0.2
(1,793)	1:109:A:LEU:HD12	1:109:A:LEU:HD13	1	0.2
(1,793)	1:109:A:LEU:HD12	1:109:A:LEU:HD13	15	0.2
(1,769)	1:72:A:LEU:HD23	1:70:A:VAL:HG22	20	0.2
(1,767)	1:70:A:VAL:HG23	1:70:A:VAL:HG11	8	0.2
(1,767)	1:70:A:VAL:HG23	1:70:A:VAL:HG12	10	0.2
(1,767)	1:70:A:VAL:HG22	1:70:A:VAL:HG12	17	0.2
(1,759)	1:110:A:LEU:HD11	1:110:A:LEU:HD21	12	0.2
(1,758)	1:110:A:LEU:HD11	1:110:A:LEU:HD13	10	0.2
(1,758)	1:110:A:LEU:HD12	1:110:A:LEU:HD13	14	0.2
(1,750)	1:72:A:LEU:HD21	1:99:A:VAL:HG11	6	0.2
(1,744)	1:72:A:LEU:HD11	1:72:A:LEU:HD21	5	0.2
(1,736)	1:11:A:ILE:HD12	1:11:A:ILE:HD11	4	0.2
(1,736)	1:11:A:ILE:HD11	1:11:A:ILE:HD13	12	0.2
(1,736)	1:11:A:ILE:HD11	1:11:A:ILE:HD13	19	0.2
(1,457)	1:74:A:CYS:HB2	1:79:A:HIS:H	14	0.2
(1,437)	1:24:A:HIS:HB3	1:25:A:LYS:H	3	0.2
(1,437)	1:24:A:HIS:HB3	1:25:A:LYS:H	15	0.2
(1,415)	1:20:A:LYS:HE3	1:20:A:LYS:H	7	0.2
(1,371)	1:22:A:GLN:HG3	1:21:A:ASN:H	7	0.2
(1,371)	1:22:A:GLN:HG3	1:21:A:ASN:H	12	0.2
(1,358)	1:22:A:GLN:HB2	1:23:A:ALA:H	14	0.2
(1,248)	1:97:A:LYS:HB3	1:97:A:LYS:H	10	0.2
(1,134)	1:57:A:VAL:HG21	1:58:A:CYS:H	1	0.2
(1,125)	1:43:A:LEU:HD13	1:43:A:LEU:H	4	0.2
(1,125)	1:43:A:LEU:HD11	1:43:A:LEU:H	11	0.2
(1,107)	1:56:A:LEU:HD23	1:56:A:LEU:H	14	0.2
(1,101)	1:57:A:VAL:HG12	1:15:A:GLU:H	8	0.2
(1,96)	1:11:A:ILE:HG23	1:15:A:GLU:H	2	0.2
(1,71)	1:31:A:VAL:HG11	1:32:A:GLY:H	14	0.2
(1,45)	1:93:A:LYS:HG3	1:94:A:CYS:H	18	0.2
(1,42)	1:109:A:LEU:HD11	1:109:A:LEU:H	14	0.2
(1,39)	1:90:A:VAL:HG13	1:90:A:VAL:H	2	0.2
(1,39)	1:90:A:VAL:HG12	1:90:A:VAL:H	8	0.2
(1,33)	1:33:A:ILE:HG22	1:37:A:SER:H	1	0.2
(1,33)	1:33:A:ILE:HG23	1:37:A:SER:H	2	0.2
(1,33)	1:33:A:ILE:HG21	1:37:A:SER:H	8	0.2
(1,12)	1:72:A:LEU:HD13	1:72:A:LEU:H	16	0.2
(1,2676)	1:47:A:ALA:HB2	1:44:A:PHE:HD1	8	0.19
(1,2673)	1:13:A:LEU:HD13	1:17:A:HIS:HD2	16	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2671)	1:115:A:LEU:HD13	1:24:A:HIS:HD2	10	0.19
(1,2661)	1:75:A:LYS:HA	1:75:A:LYS:HE3	1	0.19
(1,2661)	1:75:A:LYS:HA	1:75:A:LYS:HE3	9	0.19
(1,2653)	1:41:A:LYS:HD3	1:41:A:LYS:HA	18	0.19
(1,2577)	1:54:A:GLU:HG2	1:54:A:GLU:HA	13	0.19
(1,2577)	1:54:A:GLU:HG2	1:54:A:GLU:HA	15	0.19
(1,2569)	1:92:A:GLU:HG2	1:92:A:GLU:HA	4	0.19
(1,2539)	1:113:A:GLU:HG3	1:113:A:GLU:HG2	10	0.19
(1,2539)	1:106:A:GLU:HG2	1:106:A:GLU:HG3	11	0.19
(1,2539)	1:113:A:GLU:HG3	1:113:A:GLU:HG2	14	0.19
(1,2539)	1:113:A:GLU:HG3	1:113:A:GLU:HG2	15	0.19
(1,2539)	1:113:A:GLU:HG3	1:113:A:GLU:HG2	16	0.19
(1,2539)	1:113:A:GLU:HG3	1:113:A:GLU:HG2	18	0.19
(1,2539)	1:113:A:GLU:HG3	1:113:A:GLU:HG2	19	0.19
(1,2469)	1:6:A:VAL:HG13	1:39:A:MET:HE2	9	0.19
(1,2442)	1:31:A:VAL:HG22	1:31:A:VAL:HG13	4	0.19
(1,2442)	1:31:A:VAL:HG23	1:31:A:VAL:HG12	19	0.19
(1,2438)	1:65:A:ILE:HD13	1:41:A:LYS:HD2	15	0.19
(1,2401)	1:90:A:VAL:H	1:91:A:CYS:H	6	0.19
(1,2397)	1:100:A:ILE:H	1:74:A:CYS:H	1	0.19
(1,2396)	1:101:A:ILE:H	1:100:A:ILE:H	7	0.19
(1,2396)	1:101:A:ILE:H	1:100:A:ILE:H	12	0.19
(1,2386)	1:101:A:ILE:H	1:102:A:THR:H	12	0.19
(1,2380)	1:34:A:GLY:H	1:35:A:GLU:H	1	0.19
(1,2380)	1:34:A:GLY:H	1:35:A:GLU:H	9	0.19
(1,2300)	1:39:A:MET:H	1:37:A:SER:H	8	0.19
(1,2298)	1:71:A:GLU:H	1:70:A:VAL:H	14	0.19
(1,2298)	1:71:A:GLU:H	1:70:A:VAL:H	20	0.19
(1,2287)	1:80:A:VAL:H	1:81:A:PHE:H	1	0.19
(1,2287)	1:80:A:VAL:H	1:81:A:PHE:H	2	0.19
(1,2262)	1:88:A:TYR:HA	1:88:A:TYR:HD1	12	0.19
(1,2239)	1:41:A:LYS:HA	1:44:A:PHE:HD1	14	0.19
(1,2229)	1:4:A:TYR:HB3	1:4:A:TYR:HE1	7	0.19
(1,2229)	1:4:A:TYR:HB3	1:4:A:TYR:HE1	11	0.19
(1,2202)	1:83:A:PRO:HB3	1:88:A:TYR:HD1	11	0.19
(1,2183)	1:116:A:ALA:HB3	1:24:A:HIS:HD2	4	0.19
(1,2183)	1:116:A:ALA:HB2	1:24:A:HIS:HD2	19	0.19
(1,2180)	1:61:A:ALA:HB2	1:48:A:PHE:HD2	15	0.19
(1,2158)	1:29:A:VAL:HG13	1:48:A:PHE:HZ	3	0.19
(1,2104)	1:82:A:LYS:HA	1:83:A:PRO:HG3	7	0.19
(1,2078)	1:82:A:LYS:HD2	1:71:A:GLU:HA	13	0.19
(1,2069)	1:112:A:LEU:HD23	1:29:A:VAL:HA	2	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2061)	1:33:A:ILE:HA	1:65:A:ILE:HG23	6	0.19
(1,2058)	1:12:A:ALA:HB3	1:13:A:LEU:HA	13	0.19
(1,2053)	1:17:A:HIS:HA	1:16:A:GLU:HG2	8	0.19
(1,2050)	1:17:A:HIS:HA	1:16:A:GLU:HB2	2	0.19
(1,2050)	1:17:A:HIS:HA	1:16:A:GLU:HB2	15	0.19
(1,2041)	1:16:A:GLU:HA	1:17:A:HIS:HA	15	0.19
(1,2041)	1:16:A:GLU:HA	1:17:A:HIS:HA	19	0.19
(1,2024)	1:107:A:MET:HE1	1:7:A:VAL:HA	9	0.19
(1,1984)	1:7:A:VAL:HG12	1:48:A:PHE:HB3	9	0.19
(1,1957)	1:71:A:GLU:HB3	1:103:A:GLN:HB2	6	0.19
(1,1944)	1:57:A:VAL:HB	1:26:A:ILE:HD13	17	0.19
(1,1944)	1:57:A:VAL:HB	1:26:A:ILE:HD13	19	0.19
(1,1914)	1:68:A:GLU:HB2	1:34:A:GLY:HA3	2	0.19
(1,1897)	1:41:A:LYS:HD3	1:41:A:LYS:HA	10	0.19
(1,1897)	1:41:A:LYS:HD3	1:41:A:LYS:HA	20	0.19
(1,1854)	1:75:A:LYS:HG2	1:100:A:ILE:HG13	4	0.19
(1,1854)	1:75:A:LYS:HG2	1:100:A:ILE:HG13	8	0.19
(1,1847)	1:110:A:LEU:HD21	1:110:A:LEU:HB2	7	0.19
(1,1847)	1:110:A:LEU:HD22	1:110:A:LEU:HB2	14	0.19
(1,1800)	1:115:A:LEU:HD12	1:25:A:LYS:HG2	9	0.19
(1,1731)	1:72:A:LEU:HD13	1:91:A:CYS:HA	18	0.19
(1,1687)	1:31:A:VAL:HA	1:110:A:LEU:HD12	4	0.19
(1,1687)	1:31:A:VAL:HA	1:110:A:LEU:HD13	6	0.19
(1,1665)	1:24:A:HIS:HA	1:57:A:VAL:HG21	17	0.19
(1,1581)	1:35:A:GLU:HG3	1:35:A:GLU:HA	5	0.19
(1,1581)	1:35:A:GLU:HG3	1:35:A:GLU:HA	13	0.19
(1,1581)	1:35:A:GLU:HG3	1:35:A:GLU:HA	15	0.19
(1,1581)	1:35:A:GLU:HG3	1:35:A:GLU:HA	17	0.19
(1,1559)	1:12:A:ALA:HB1	1:12:A:ALA:HA	3	0.19
(1,1554)	1:20:A:LYS:HE3	1:17:A:HIS:HA	19	0.19
(1,1507)	1:26:A:ILE:HD12	1:14:A:CYS:HA	10	0.19
(1,1501)	1:3:A:GLU:HA	1:39:A:MET:HE1	16	0.19
(1,1410)	1:84:A:ASN:HB3	1:84:A:ASN:HA	1	0.19
(1,1410)	1:84:A:ASN:HB3	1:84:A:ASN:HA	11	0.19
(1,1384)	1:93:A:LYS:HE3	1:93:A:LYS:HA	17	0.19
(1,1352)	1:22:A:GLN:HG2	1:22:A:GLN:HG3	5	0.19
(1,1352)	1:22:A:GLN:HG2	1:22:A:GLN:HG3	8	0.19
(1,1352)	1:22:A:GLN:HG2	1:22:A:GLN:HG3	10	0.19
(1,1352)	1:22:A:GLN:HG2	1:22:A:GLN:HG3	13	0.19
(1,1352)	1:22:A:GLN:HG2	1:22:A:GLN:HG3	19	0.19
(1,1299)	1:117:A:GLU:HB2	1:117:A:GLU:HG3	5	0.19
(1,1299)	1:117:A:GLU:HB2	1:117:A:GLU:HG3	6	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1299)	1:117:A:GLU:HB2	1:117:A:GLU:HG3	16	0.19
(1,1283)	1:15:A:GLU:HB3	1:12:A:ALA:HA	10	0.19
(1,1140)	1:59:A:LYS:HD3	1:59:A:LYS:HA	7	0.19
(1,1081)	1:43:A:LEU:HG	1:43:A:LEU:HA	1	0.19
(1,1081)	1:43:A:LEU:HG	1:43:A:LEU:HA	19	0.19
(1,1053)	1:63:A:LEU:HD12	1:63:A:LEU:HB2	4	0.19
(1,1053)	1:63:A:LEU:HD12	1:63:A:LEU:HB2	10	0.19
(1,1053)	1:63:A:LEU:HD11	1:63:A:LEU:HB2	16	0.19
(1,1038)	1:20:A:LYS:HG3	1:20:A:LYS:HD2	5	0.19
(1,998)	1:65:A:ILE:HG12	1:63:A:LEU:HD21	12	0.19
(1,953)	1:65:A:ILE:HG22	1:33:A:ILE:HG12	9	0.19
(1,940)	1:112:A:LEU:HD11	1:112:A:LEU:HA	3	0.19
(1,940)	1:112:A:LEU:HD13	1:112:A:LEU:HA	4	0.19
(1,940)	1:112:A:LEU:HD11	1:112:A:LEU:HA	15	0.19
(1,910)	1:109:A:LEU:HD11	1:13:A:LEU:HD11	10	0.19
(1,898)	1:29:A:VAL:HG11	1:112:A:LEU:HA	3	0.19
(1,897)	1:29:A:VAL:HG13	1:112:A:LEU:HD21	6	0.19
(1,853)	1:31:A:VAL:HG13	1:107:A:MET:HG2	14	0.19
(1,844)	1:112:A:LEU:HD23	1:114:A:MET:HE3	8	0.19
(1,826)	1:101:A:ILE:HG22	1:103:A:GLN:HA	1	0.19
(1,822)	1:80:A:VAL:HG13	1:102:A:THR:HG21	8	0.19
(1,818)	1:80:A:VAL:HG12	1:80:A:VAL:HG22	5	0.19
(1,793)	1:109:A:LEU:HD12	1:109:A:LEU:HD11	5	0.19
(1,793)	1:109:A:LEU:HD12	1:109:A:LEU:HD13	7	0.19
(1,793)	1:109:A:LEU:HD12	1:109:A:LEU:HD13	8	0.19
(1,793)	1:109:A:LEU:HD12	1:109:A:LEU:HD13	12	0.19
(1,793)	1:109:A:LEU:HD12	1:109:A:LEU:HD11	13	0.19
(1,787)	1:63:A:LEU:HD12	1:65:A:ILE:HD11	18	0.19
(1,780)	1:99:A:VAL:HG11	1:99:A:VAL:HG22	5	0.19
(1,762)	1:70:A:VAL:HG22	1:71:A:GLU:HA	13	0.19
(1,758)	1:110:A:LEU:HD12	1:110:A:LEU:HD11	6	0.19
(1,744)	1:72:A:LEU:HD12	1:72:A:LEU:HD21	4	0.19
(1,744)	1:72:A:LEU:HD11	1:72:A:LEU:HD21	6	0.19
(1,736)	1:11:A:ILE:HD11	1:11:A:ILE:HD13	7	0.19
(1,539)	1:19:A:LYS:HA	1:23:A:ALA:H	17	0.19
(1,437)	1:24:A:HIS:HB3	1:25:A:LYS:H	1	0.19
(1,437)	1:24:A:HIS:HB3	1:25:A:LYS:H	10	0.19
(1,415)	1:20:A:LYS:HE3	1:20:A:LYS:H	14	0.19
(1,371)	1:22:A:GLN:HG3	1:21:A:ASN:H	8	0.19
(1,344)	1:113:A:GLU:HG3	1:113:A:GLU:H	12	0.19
(1,301)	1:69:A:LYS:HB2	1:70:A:VAL:H	4	0.19
(1,301)	1:69:A:LYS:HB2	1:70:A:VAL:H	16	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,277)	1:54:A:GLU:HB3	1:54:A:GLU:H	1	0.19
(1,191)	1:93:A:LYS:HB2	1:94:A:CYS:H	6	0.19
(1,172)	1:18:A:ALA:HB1	1:23:A:ALA:H	9	0.19
(1,136)	1:102:A:THR:HG23	1:100:A:ILE:H	17	0.19
(1,134)	1:57:A:VAL:HG21	1:58:A:CYS:H	7	0.19
(1,97)	1:11:A:ILE:HG23	1:12:A:ALA:H	2	0.19
(1,97)	1:11:A:ILE:HG22	1:12:A:ALA:H	6	0.19
(1,97)	1:11:A:ILE:HG23	1:12:A:ALA:H	11	0.19
(1,88)	1:26:A:ILE:HD12	1:15:A:GLU:H	2	0.19
(1,74)	1:99:A:VAL:HG23	1:73:A:GLU:H	18	0.19
(1,72)	1:31:A:VAL:HG11	1:108:A:ARG:H	15	0.19
(1,39)	1:90:A:VAL:HG13	1:90:A:VAL:H	10	0.19
(1,39)	1:90:A:VAL:HG11	1:90:A:VAL:H	15	0.19
(1,34)	1:33:A:ILE:HG23	1:39:A:MET:H	17	0.19
(1,29)	1:70:A:VAL:HG21	1:72:A:LEU:H	2	0.19
(1,29)	1:70:A:VAL:HG23	1:72:A:LEU:H	7	0.19
(1,29)	1:70:A:VAL:HG23	1:72:A:LEU:H	18	0.19
(1,25)	1:90:A:VAL:HG22	1:91:A:CYS:H	2	0.19
(1,25)	1:90:A:VAL:HG22	1:91:A:CYS:H	15	0.19
(1,12)	1:72:A:LEU:HD13	1:72:A:LEU:H	7	0.19
(1,2675)	1:63:A:LEU:HG	1:48:A:PHE:HZ	12	0.18
(1,2661)	1:75:A:LYS:HA	1:75:A:LYS:HE3	5	0.18
(1,2655)	1:17:A:HIS:HB3	1:14:A:CYS:HA	7	0.18
(1,2653)	1:41:A:LYS:HD3	1:41:A:LYS:HA	4	0.18
(1,2577)	1:54:A:GLU:HG2	1:54:A:GLU:HA	5	0.18
(1,2577)	1:54:A:GLU:HG2	1:54:A:GLU:HA	7	0.18
(1,2577)	1:54:A:GLU:HG2	1:54:A:GLU:HA	9	0.18
(1,2569)	1:92:A:GLU:HG2	1:92:A:GLU:HA	19	0.18
(1,2569)	1:92:A:GLU:HG2	1:92:A:GLU:HA	20	0.18
(1,2555)	1:115:A:LEU:HD13	1:25:A:LYS:HE2	1	0.18
(1,2539)	1:113:A:GLU:HG3	1:113:A:GLU:HG2	1	0.18
(1,2539)	1:106:A:GLU:HG2	1:106:A:GLU:HG3	3	0.18
(1,2539)	1:106:A:GLU:HG2	1:106:A:GLU:HG3	7	0.18
(1,2539)	1:106:A:GLU:HG2	1:106:A:GLU:HG3	8	0.18
(1,2539)	1:113:A:GLU:HG3	1:113:A:GLU:HG2	12	0.18
(1,2539)	1:113:A:GLU:HG3	1:113:A:GLU:HG2	13	0.18
(1,2539)	1:113:A:GLU:HG3	1:113:A:GLU:HG2	17	0.18
(1,2454)	1:62:A:ILE:HG23	1:28:A:ARG:HG3	7	0.18
(1,2454)	1:62:A:ILE:HG21	1:28:A:ARG:HG3	17	0.18
(1,2438)	1:65:A:ILE:HD12	1:41:A:LYS:HD2	20	0.18
(1,2396)	1:101:A:ILE:H	1:100:A:ILE:H	14	0.18
(1,2386)	1:101:A:ILE:H	1:102:A:THR:H	1	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2386)	1:101:A:ILE:H	1:102:A:THR:H	8	0.18
(1,2378)	1:97:A:LYS:H	1:96:A:SER:H	2	0.18
(1,2294)	1:99:A:VAL:H	1:100:A:ILE:H	5	0.18
(1,2294)	1:99:A:VAL:H	1:100:A:ILE:H	11	0.18
(1,2294)	1:99:A:VAL:H	1:100:A:ILE:H	18	0.18
(1,2287)	1:80:A:VAL:H	1:81:A:PHE:H	4	0.18
(1,2287)	1:80:A:VAL:H	1:81:A:PHE:H	10	0.18
(1,2287)	1:80:A:VAL:H	1:81:A:PHE:H	17	0.18
(1,2239)	1:41:A:LYS:HA	1:44:A:PHE:HD1	10	0.18
(1,2229)	1:4:A:TYR:HB3	1:4:A:TYR:HE1	9	0.18
(1,2199)	1:7:A:VAL:HB	1:4:A:TYR:HD2	5	0.18
(1,2183)	1:116:A:ALA:HB3	1:24:A:HIS:HD2	13	0.18
(1,2180)	1:61:A:ALA:HB2	1:48:A:PHE:HD2	2	0.18
(1,2162)	1:43:A:LEU:HD12	1:4:A:TYR:HD2	8	0.18
(1,2143)	1:7:A:VAL:HG22	1:51:A:PHE:HD1	13	0.18
(1,2100)	1:97:A:LYS:HA	1:97:A:LYS:HE2	1	0.18
(1,2100)	1:97:A:LYS:HA	1:97:A:LYS:HE2	16	0.18
(1,2042)	1:16:A:GLU:HA	1:15:A:GLU:HB2	6	0.18
(1,2040)	1:90:A:VAL:HG21	1:92:A:GLU:HA	19	0.18
(1,2024)	1:107:A:MET:HE3	1:7:A:VAL:HA	8	0.18
(1,2016)	1:93:A:LYS:HD2	1:79:A:HIS:HB2	10	0.18
(1,2010)	1:114:A:MET:HE2	1:17:A:HIS:HB2	1	0.18
(1,2001)	1:59:A:LYS:HE3	1:56:A:LEU:HB2	1	0.18
(1,1967)	1:20:A:LYS:HD2	1:16:A:GLU:HG3	14	0.18
(1,1967)	1:20:A:LYS:HD2	1:16:A:GLU:HG3	15	0.18
(1,1949)	1:15:A:GLU:HB3	1:57:A:VAL:HG11	17	0.18
(1,1931)	1:65:A:ILE:HD12	1:41:A:LYS:HB2	20	0.18
(1,1914)	1:68:A:GLU:HB2	1:34:A:GLY:HA3	11	0.18
(1,1914)	1:68:A:GLU:HB2	1:34:A:GLY:HA3	20	0.18
(1,1897)	1:41:A:LYS:HD3	1:41:A:LYS:HA	7	0.18
(1,1897)	1:41:A:LYS:HD3	1:41:A:LYS:HA	13	0.18
(1,1847)	1:110:A:LEU:HD22	1:110:A:LEU:HB2	9	0.18
(1,1829)	1:26:A:ILE:HD12	1:23:A:ALA:HB3	16	0.18
(1,1774)	1:31:A:VAL:HG21	1:107:A:MET:HG2	16	0.18
(1,1727)	1:11:A:ILE:HD12	1:55:A:SER:HB3	14	0.18
(1,1722)	1:33:A:ILE:HD11	1:63:A:LEU:HD11	19	0.18
(1,1640)	1:72:A:LEU:HD23	1:101:A:ILE:HA	13	0.18
(1,1583)	1:35:A:GLU:HG2	1:35:A:GLU:HA	20	0.18
(1,1581)	1:35:A:GLU:HG3	1:35:A:GLU:HA	1	0.18
(1,1581)	1:35:A:GLU:HG3	1:35:A:GLU:HA	7	0.18
(1,1576)	1:35:A:GLU:HG3	1:69:A:LYS:HA	15	0.18
(1,1570)	1:102:A:THR:HA	1:101:A:ILE:HG23	18	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1559)	1:12:A:ALA:HB3	1:12:A:ALA:HA	4	0.18
(1,1559)	1:12:A:ALA:HB2	1:12:A:ALA:HA	10	0.18
(1,1558)	1:86:A:LEU:HD22	1:86:A:LEU:HA	13	0.18
(1,1491)	1:6:A:VAL:HG13	1:6:A:VAL:HA	1	0.18
(1,1477)	1:45:A:VAL:HG12	1:41:A:LYS:HA	3	0.18
(1,1477)	1:45:A:VAL:HG13	1:41:A:LYS:HA	15	0.18
(1,1410)	1:84:A:ASN:HB3	1:84:A:ASN:HA	12	0.18
(1,1410)	1:84:A:ASN:HB3	1:84:A:ASN:HA	16	0.18
(1,1374)	1:40:A:ASP:HB3	1:43:A:LEU:HD13	3	0.18
(1,1361)	1:26:A:ILE:HD13	1:114:A:MET:HG2	6	0.18
(1,1352)	1:22:A:GLN:HG2	1:22:A:GLN:HG3	1	0.18
(1,1324)	1:106:A:GLU:HG3	1:105:A:ASN:HB2	20	0.18
(1,1303)	1:23:A:ALA:HB3	1:114:A:MET:HB2	5	0.18
(1,1303)	1:23:A:ALA:HB2	1:114:A:MET:HB2	8	0.18
(1,1303)	1:23:A:ALA:HB1	1:114:A:MET:HB2	11	0.18
(1,1299)	1:117:A:GLU:HB2	1:117:A:GLU:HG3	7	0.18
(1,1299)	1:117:A:GLU:HB2	1:117:A:GLU:HG3	12	0.18
(1,1299)	1:117:A:GLU:HB2	1:117:A:GLU:HG3	13	0.18
(1,1299)	1:117:A:GLU:HB2	1:117:A:GLU:HG3	18	0.18
(1,1249)	1:72:A:LEU:HD13	1:83:A:PRO:HG2	17	0.18
(1,1217)	1:72:A:LEU:HD11	1:99:A:VAL:HB	7	0.18
(1,1140)	1:59:A:LYS:HD3	1:59:A:LYS:HA	20	0.18
(1,1115)	1:70:A:VAL:HG23	1:83:A:PRO:HG3	18	0.18
(1,1053)	1:63:A:LEU:HD11	1:63:A:LEU:HB2	18	0.18
(1,1038)	1:20:A:LYS:HG3	1:20:A:LYS:HD2	10	0.18
(1,962)	1:33:A:ILE:HD11	1:41:A:LYS:HG3	2	0.18
(1,962)	1:33:A:ILE:HD11	1:41:A:LYS:HG3	17	0.18
(1,952)	1:33:A:ILE:HG12	1:31:A:VAL:HG23	13	0.18
(1,952)	1:33:A:ILE:HG12	1:31:A:VAL:HG23	17	0.18
(1,940)	1:112:A:LEU:HD13	1:112:A:LEU:HA	7	0.18
(1,898)	1:29:A:VAL:HG12	1:112:A:LEU:HA	12	0.18
(1,864)	1:110:A:LEU:HD13	1:30:A:VAL:HG21	16	0.18
(1,860)	1:109:A:LEU:HD21	1:31:A:VAL:HA	6	0.18
(1,849)	1:72:A:LEU:HD22	1:101:A:ILE:HG13	9	0.18
(1,849)	1:72:A:LEU:HD22	1:101:A:ILE:HG13	10	0.18
(1,794)	1:109:A:LEU:HD11	1:109:A:LEU:HD23	4	0.18
(1,793)	1:109:A:LEU:HD12	1:109:A:LEU:HD13	11	0.18
(1,793)	1:109:A:LEU:HD11	1:109:A:LEU:HD13	16	0.18
(1,793)	1:109:A:LEU:HD11	1:109:A:LEU:HD13	19	0.18
(1,780)	1:99:A:VAL:HG11	1:99:A:VAL:HG21	3	0.18
(1,780)	1:99:A:VAL:HG13	1:99:A:VAL:HG21	15	0.18
(1,780)	1:99:A:VAL:HG13	1:99:A:VAL:HG23	17	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,771)	1:110:A:LEU:HD12	1:66:A:VAL:HG23	5	0.18
(1,771)	1:110:A:LEU:HD13	1:66:A:VAL:HG23	6	0.18
(1,750)	1:72:A:LEU:HD23	1:99:A:VAL:HG12	12	0.18
(1,744)	1:72:A:LEU:HD13	1:72:A:LEU:HD21	19	0.18
(1,437)	1:24:A:HIS:HB3	1:25:A:LYS:H	5	0.18
(1,371)	1:22:A:GLN:HG3	1:21:A:ASN:H	16	0.18
(1,358)	1:22:A:GLN:HB2	1:23:A:ALA:H	16	0.18
(1,353)	1:107:A:MET:HG3	1:108:A:ARG:H	18	0.18
(1,353)	1:107:A:MET:HG3	1:108:A:ARG:H	20	0.18
(1,310)	1:114:A:MET:HE2	1:18:A:ALA:H	15	0.18
(1,300)	1:107:A:MET:HE2	1:108:A:ARG:H	7	0.18
(1,277)	1:54:A:GLU:HB3	1:54:A:GLU:H	9	0.18
(1,277)	1:54:A:GLU:HB3	1:54:A:GLU:H	15	0.18
(1,248)	1:97:A:LYS:HB3	1:97:A:LYS:H	3	0.18
(1,196)	1:12:A:ALA:HB1	1:14:A:CYS:H	5	0.18
(1,172)	1:18:A:ALA:HB3	1:23:A:ALA:H	10	0.18
(1,142)	1:47:A:ALA:HB3	1:46:A:SER:H	12	0.18
(1,131)	1:10:A:LEU:HD23	1:11:A:ILE:H	3	0.18
(1,125)	1:43:A:LEU:HD11	1:43:A:LEU:H	15	0.18
(1,125)	1:43:A:LEU:HD11	1:43:A:LEU:H	17	0.18
(1,111)	1:10:A:LEU:HD11	1:13:A:LEU:H	20	0.18
(1,108)	1:115:A:LEU:HD23	1:116:A:ALA:H	13	0.18
(1,107)	1:56:A:LEU:HD22	1:56:A:LEU:H	10	0.18
(1,97)	1:11:A:ILE:HG21	1:12:A:ALA:H	12	0.18
(1,97)	1:11:A:ILE:HG21	1:12:A:ALA:H	18	0.18
(1,82)	1:109:A:LEU:HD21	1:30:A:VAL:H	18	0.18
(1,71)	1:31:A:VAL:HG13	1:32:A:GLY:H	1	0.18
(1,71)	1:31:A:VAL:HG11	1:32:A:GLY:H	9	0.18
(1,71)	1:31:A:VAL:HG13	1:32:A:GLY:H	13	0.18
(1,71)	1:31:A:VAL:HG11	1:32:A:GLY:H	17	0.18
(1,42)	1:109:A:LEU:HD12	1:109:A:LEU:H	19	0.18
(1,39)	1:90:A:VAL:HG13	1:90:A:VAL:H	13	0.18
(1,34)	1:33:A:ILE:HG21	1:39:A:MET:H	14	0.18
(1,33)	1:33:A:ILE:HG23	1:37:A:SER:H	9	0.18
(1,25)	1:90:A:VAL:HG22	1:91:A:CYS:H	3	0.18
(1,12)	1:72:A:LEU:HD12	1:72:A:LEU:H	20	0.18
(1,2679)	1:7:A:VAL:HB	1:48:A:PHE:HD1	3	0.17
(1,2675)	1:10:A:LEU:HD21	1:48:A:PHE:HZ	5	0.17
(1,2653)	1:41:A:LYS:HD3	1:41:A:LYS:HA	8	0.17
(1,2653)	1:41:A:LYS:HD3	1:41:A:LYS:HA	11	0.17
(1,2645)	1:33:A:ILE:HG22	1:39:A:MET:HG3	2	0.17
(1,2622)	1:38:A:ALA:HB2	1:1:A:MET:HB2	17	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2590)	1:33:A:ILE:HD11	1:39:A:MET:HG2	14	0.17
(1,2571)	1:59:A:LYS:HD3	1:56:A:LEU:HA	14	0.17
(1,2569)	1:92:A:GLU:HG2	1:92:A:GLU:HA	18	0.17
(1,2539)	1:106:A:GLU:HG2	1:106:A:GLU:HG3	20	0.17
(1,2518)	1:25:A:LYS:HD2	1:25:A:LYS:HE3	4	0.17
(1,2469)	1:6:A:VAL:HG13	1:39:A:MET:HE2	19	0.17
(1,2442)	1:31:A:VAL:HG22	1:31:A:VAL:HG11	13	0.17
(1,2442)	1:31:A:VAL:HG21	1:31:A:VAL:HG12	18	0.17
(1,2401)	1:90:A:VAL:H	1:91:A:CYS:H	13	0.17
(1,2401)	1:90:A:VAL:H	1:91:A:CYS:H	20	0.17
(1,2396)	1:101:A:ILE:H	1:100:A:ILE:H	11	0.17
(1,2380)	1:34:A:GLY:H	1:35:A:GLU:H	6	0.17
(1,2380)	1:34:A:GLY:H	1:35:A:GLU:H	8	0.17
(1,2298)	1:71:A:GLU:H	1:70:A:VAL:H	11	0.17
(1,2294)	1:99:A:VAL:H	1:100:A:ILE:H	6	0.17
(1,2294)	1:99:A:VAL:H	1:100:A:ILE:H	15	0.17
(1,2287)	1:80:A:VAL:H	1:81:A:PHE:H	14	0.17
(1,2229)	1:4:A:TYR:HB3	1:4:A:TYR:HE1	6	0.17
(1,2183)	1:116:A:ALA:HB1	1:24:A:HIS:HD2	8	0.17
(1,2183)	1:116:A:ALA:HB2	1:24:A:HIS:HD2	18	0.17
(1,2172)	1:47:A:ALA:HB3	1:4:A:TYR:HD1	11	0.17
(1,2167)	1:50:A:THR:HG22	1:4:A:TYR:HD1	13	0.17
(1,2148)	1:80:A:VAL:HG11	1:81:A:PHE:HD2	5	0.17
(1,2143)	1:7:A:VAL:HG21	1:51:A:PHE:HD1	11	0.17
(1,2143)	1:7:A:VAL:HG23	1:51:A:PHE:HD1	16	0.17
(1,2104)	1:82:A:LYS:HA	1:83:A:PRO:HG3	3	0.17
(1,2104)	1:82:A:LYS:HA	1:83:A:PRO:HG3	6	0.17
(1,2058)	1:12:A:ALA:HB2	1:13:A:LEU:HA	3	0.17
(1,2053)	1:17:A:HIS:HA	1:16:A:GLU:HG2	20	0.17
(1,2051)	1:114:A:MET:HE2	1:17:A:HIS:HA	7	0.17
(1,2042)	1:16:A:GLU:HA	1:15:A:GLU:HB2	7	0.17
(1,2042)	1:16:A:GLU:HA	1:15:A:GLU:HB2	13	0.17
(1,2041)	1:16:A:GLU:HA	1:17:A:HIS:HA	14	0.17
(1,2035)	1:42:A:SER:HB3	1:45:A:VAL:HG23	4	0.17
(1,2010)	1:114:A:MET:HE1	1:17:A:HIS:HB2	13	0.17
(1,1990)	1:17:A:HIS:HB3	1:14:A:CYS:HA	1	0.17
(1,1990)	1:17:A:HIS:HB3	1:14:A:CYS:HA	3	0.17
(1,1957)	1:71:A:GLU:HB3	1:103:A:GLN:HB2	16	0.17
(1,1949)	1:15:A:GLU:HB3	1:57:A:VAL:HG13	1	0.17
(1,1944)	1:57:A:VAL:HB	1:26:A:ILE:HD11	2	0.17
(1,1897)	1:41:A:LYS:HD3	1:41:A:LYS:HA	9	0.17
(1,1897)	1:41:A:LYS:HD3	1:41:A:LYS:HA	12	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1897)	1:41:A:LYS:HD3	1:41:A:LYS:HA	18	0.17
(1,1888)	1:85:A:ALA:HB3	1:86:A:LEU:HG	14	0.17
(1,1888)	1:85:A:ALA:HB2	1:86:A:LEU:HG	19	0.17
(1,1802)	1:29:A:VAL:HG23	1:29:A:VAL:HG13	3	0.17
(1,1802)	1:29:A:VAL:HG21	1:29:A:VAL:HG11	12	0.17
(1,1802)	1:29:A:VAL:HG23	1:29:A:VAL:HG11	20	0.17
(1,1799)	1:29:A:VAL:HG11	1:109:A:LEU:HD13	7	0.17
(1,1799)	1:29:A:VAL:HG12	1:109:A:LEU:HD13	16	0.17
(1,1792)	1:11:A:ILE:HG23	1:52:A:ARG:HA	3	0.17
(1,1787)	1:26:A:ILE:HG21	1:112:A:LEU:HA	2	0.17
(1,1771)	1:31:A:VAL:HG21	1:65:A:ILE:HB	3	0.17
(1,1755)	1:65:A:ILE:HD12	1:45:A:VAL:HA	6	0.17
(1,1749)	1:65:A:ILE:HG13	1:63:A:LEU:HD23	13	0.17
(1,1748)	1:33:A:ILE:HG23	1:107:A:MET:HG3	4	0.17
(1,1583)	1:35:A:GLU:HG2	1:35:A:GLU:HA	2	0.17
(1,1583)	1:35:A:GLU:HG2	1:35:A:GLU:HA	18	0.17
(1,1567)	1:102:A:THR:HG22	1:102:A:THR:HA	5	0.17
(1,1559)	1:12:A:ALA:HB2	1:12:A:ALA:HA	8	0.17
(1,1559)	1:12:A:ALA:HB2	1:12:A:ALA:HA	14	0.17
(1,1507)	1:26:A:ILE:HD13	1:14:A:CYS:HA	2	0.17
(1,1491)	1:6:A:VAL:HG13	1:6:A:VAL:HA	3	0.17
(1,1491)	1:6:A:VAL:HG13	1:6:A:VAL:HA	7	0.17
(1,1428)	1:56:A:LEU:HD22	1:59:A:LYS:HE3	17	0.17
(1,1410)	1:84:A:ASN:HB3	1:84:A:ASN:HA	4	0.17
(1,1401)	1:41:A:LYS:HE3	1:33:A:ILE:HD11	17	0.17
(1,1388)	1:11:A:ILE:HD12	1:51:A:PHE:HB3	8	0.17
(1,1385)	1:48:A:PHE:HB3	1:63:A:LEU:HD11	16	0.17
(1,1361)	1:26:A:ILE:HD12	1:114:A:MET:HG2	9	0.17
(1,1324)	1:106:A:GLU:HG3	1:105:A:ASN:HB2	14	0.17
(1,1303)	1:23:A:ALA:HB2	1:114:A:MET:HB2	7	0.17
(1,1299)	1:117:A:GLU:HB2	1:117:A:GLU:HG3	9	0.17
(1,1299)	1:117:A:GLU:HB2	1:117:A:GLU:HG3	19	0.17
(1,1283)	1:15:A:GLU:HB3	1:12:A:ALA:HA	15	0.17
(1,1280)	1:39:A:MET:HB2	1:39:A:MET:HE3	10	0.17
(1,1249)	1:72:A:LEU:HD12	1:83:A:PRO:HG2	7	0.17
(1,1204)	1:75:A:LYS:HB3	1:98:A:ASN:HB3	17	0.17
(1,1159)	1:108:A:ARG:HB2	1:110:A:LEU:HD21	3	0.17
(1,1145)	1:41:A:LYS:HD2	1:33:A:ILE:HG23	3	0.17
(1,1105)	1:69:A:LYS:HD3	1:69:A:LYS:HA	2	0.17
(1,1058)	1:11:A:ILE:HG23	1:11:A:ILE:HG12	15	0.17
(1,1053)	1:63:A:LEU:HD11	1:63:A:LEU:HB2	7	0.17
(1,1038)	1:20:A:LYS:HG3	1:20:A:LYS:HD2	6	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1038)	1:20:A:LYS:HG3	1:20:A:LYS:HD2	17	0.17
(1,1024)	1:57:A:VAL:HG11	1:18:A:ALA:HB2	7	0.17
(1,1010)	1:115:A:LEU:HB3	1:25:A:LYS:HB2	7	0.17
(1,1010)	1:115:A:LEU:HB3	1:25:A:LYS:HB3	12	0.17
(1,940)	1:112:A:LEU:HD13	1:112:A:LEU:HA	19	0.17
(1,908)	1:56:A:LEU:HD11	1:57:A:VAL:HG23	15	0.17
(1,897)	1:29:A:VAL:HG12	1:112:A:LEU:HD22	17	0.17
(1,889)	1:57:A:VAL:HG11	1:15:A:GLU:HG3	12	0.17
(1,849)	1:72:A:LEU:HD23	1:101:A:ILE:HG13	3	0.17
(1,826)	1:101:A:ILE:HG23	1:103:A:GLN:HA	18	0.17
(1,826)	1:101:A:ILE:HG22	1:103:A:GLN:HA	20	0.17
(1,825)	1:101:A:ILE:HG22	1:72:A:LEU:HA	5	0.17
(1,825)	1:101:A:ILE:HG22	1:72:A:LEU:HA	6	0.17
(1,821)	1:30:A:VAL:HG11	1:28:A:ARG:HG3	7	0.17
(1,818)	1:80:A:VAL:HG13	1:80:A:VAL:HG21	14	0.17
(1,793)	1:109:A:LEU:HD12	1:109:A:LEU:HD11	2	0.17
(1,793)	1:109:A:LEU:HD12	1:109:A:LEU:HD11	4	0.17
(1,793)	1:109:A:LEU:HD11	1:109:A:LEU:HD13	17	0.17
(1,793)	1:109:A:LEU:HD12	1:109:A:LEU:HD11	18	0.17
(1,793)	1:109:A:LEU:HD12	1:109:A:LEU:HD13	20	0.17
(1,780)	1:99:A:VAL:HG12	1:99:A:VAL:HG23	19	0.17
(1,767)	1:70:A:VAL:HG23	1:70:A:VAL:HG12	3	0.17
(1,767)	1:70:A:VAL:HG21	1:70:A:VAL:HG12	9	0.17
(1,758)	1:110:A:LEU:HD11	1:110:A:LEU:HD13	3	0.17
(1,758)	1:110:A:LEU:HD12	1:110:A:LEU:HD13	4	0.17
(1,758)	1:110:A:LEU:HD12	1:110:A:LEU:HD13	11	0.17
(1,758)	1:110:A:LEU:HD12	1:110:A:LEU:HD13	13	0.17
(1,758)	1:110:A:LEU:HD12	1:110:A:LEU:HD11	15	0.17
(1,758)	1:110:A:LEU:HD12	1:110:A:LEU:HD11	19	0.17
(1,744)	1:72:A:LEU:HD11	1:72:A:LEU:HD21	9	0.17
(1,736)	1:11:A:ILE:HD12	1:11:A:ILE:HD13	5	0.17
(1,457)	1:74:A:CYS:HB2	1:79:A:HIS:H	13	0.17
(1,438)	1:79:A:HIS:HB3	1:79:A:HIS:H	12	0.17
(1,437)	1:24:A:HIS:HB3	1:25:A:LYS:H	6	0.17
(1,437)	1:24:A:HIS:HB3	1:25:A:LYS:H	16	0.17
(1,396)	1:76:A:ASP:HB3	1:76:A:ASP:H	4	0.17
(1,277)	1:54:A:GLU:HB3	1:54:A:GLU:H	8	0.17
(1,248)	1:97:A:LYS:HB3	1:97:A:LYS:H	13	0.17
(1,234)	1:39:A:MET:HB3	1:39:A:MET:H	4	0.17
(1,234)	1:39:A:MET:HB3	1:39:A:MET:H	7	0.17
(1,191)	1:93:A:LYS:HB2	1:94:A:CYS:H	8	0.17
(1,138)	1:102:A:THR:HG22	1:103:A:GLN:H	20	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,125)	1:43:A:LEU:HD13	1:43:A:LEU:H	8	0.17
(1,97)	1:11:A:ILE:HG22	1:12:A:ALA:H	15	0.17
(1,88)	1:26:A:ILE:HD13	1:15:A:GLU:H	3	0.17
(1,72)	1:31:A:VAL:HG12	1:108:A:ARG:H	6	0.17
(1,71)	1:31:A:VAL:HG11	1:32:A:GLY:H	6	0.17
(1,70)	1:112:A:LEU:HD23	1:17:A:HIS:H	14	0.17
(1,25)	1:90:A:VAL:HG23	1:91:A:CYS:H	14	0.17
(1,12)	1:72:A:LEU:HD12	1:72:A:LEU:H	14	0.17
(1,2678)	1:107:A:MET:HE1	1:44:A:PHE:HZ	15	0.16
(1,2667)	1:7:A:VAL:HG12	1:48:A:PHE:HD2	19	0.16
(1,2653)	1:41:A:LYS:HD3	1:41:A:LYS:HA	6	0.16
(1,2653)	1:41:A:LYS:HD3	1:41:A:LYS:HA	15	0.16
(1,2653)	1:41:A:LYS:HD3	1:41:A:LYS:HA	17	0.16
(1,2647)	1:59:A:LYS:HB3	1:25:A:LYS:HE3	18	0.16
(1,2638)	1:107:A:MET:HA	1:39:A:MET:HE3	12	0.16
(1,2569)	1:92:A:GLU:HG2	1:92:A:GLU:HA	15	0.16
(1,2518)	1:25:A:LYS:HD2	1:25:A:LYS:HE3	2	0.16
(1,2469)	1:6:A:VAL:HG12	1:39:A:MET:HE1	5	0.16
(1,2422)	1:47:A:ALA:HB1	1:7:A:VAL:H	8	0.16
(1,2419)	1:69:A:LYS:HG3	1:69:A:LYS:H	2	0.16
(1,2401)	1:90:A:VAL:H	1:91:A:CYS:H	10	0.16
(1,2401)	1:90:A:VAL:H	1:91:A:CYS:H	14	0.16
(1,2397)	1:100:A:ILE:H	1:74:A:CYS:H	11	0.16
(1,2380)	1:34:A:GLY:H	1:35:A:GLU:H	2	0.16
(1,2380)	1:34:A:GLY:H	1:35:A:GLU:H	4	0.16
(1,2380)	1:34:A:GLY:H	1:35:A:GLU:H	10	0.16
(1,2380)	1:34:A:GLY:H	1:35:A:GLU:H	17	0.16
(1,2298)	1:71:A:GLU:H	1:70:A:VAL:H	12	0.16
(1,2298)	1:71:A:GLU:H	1:70:A:VAL:H	13	0.16
(1,2250)	1:4:A:TYR:HA	1:4:A:TYR:HD1	11	0.16
(1,2239)	1:41:A:LYS:HA	1:44:A:PHE:HD1	15	0.16
(1,2239)	1:41:A:LYS:HA	1:44:A:PHE:HD2	16	0.16
(1,2229)	1:4:A:TYR:HB3	1:4:A:TYR:HE1	4	0.16
(1,2229)	1:4:A:TYR:HB3	1:4:A:TYR:HE1	17	0.16
(1,2199)	1:7:A:VAL:HB	1:4:A:TYR:HD1	8	0.16
(1,2193)	1:25:A:LYS:HB3	1:24:A:HIS:HD2	9	0.16
(1,2172)	1:47:A:ALA:HB3	1:4:A:TYR:HD1	15	0.16
(1,2171)	1:47:A:ALA:HB2	1:4:A:TYR:HE2	14	0.16
(1,2157)	1:43:A:LEU:HD23	1:4:A:TYR:HE1	16	0.16
(1,2150)	1:31:A:VAL:HG12	1:44:A:PHE:HE2	7	0.16
(1,2148)	1:80:A:VAL:HG13	1:81:A:PHE:HD2	11	0.16
(1,2142)	1:7:A:VAL:HG21	1:48:A:PHE:HD1	4	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2121)	1:63:A:LEU:HD21	1:48:A:PHE:HD1	8	0.16
(1,2104)	1:82:A:LYS:HA	1:83:A:PRO:HG3	16	0.16
(1,2078)	1:82:A:LYS:HD3	1:71:A:GLU:HA	20	0.16
(1,2070)	1:109:A:LEU:HD23	1:29:A:VAL:HA	10	0.16
(1,2070)	1:109:A:LEU:HD22	1:29:A:VAL:HA	16	0.16
(1,2061)	1:33:A:ILE:HA	1:65:A:ILE:HG22	2	0.16
(1,2061)	1:33:A:ILE:HA	1:65:A:ILE:HG21	4	0.16
(1,2061)	1:33:A:ILE:HA	1:65:A:ILE:HG22	9	0.16
(1,2061)	1:33:A:ILE:HA	1:65:A:ILE:HG22	13	0.16
(1,2061)	1:33:A:ILE:HA	1:65:A:ILE:HG22	18	0.16
(1,2058)	1:12:A:ALA:HB1	1:13:A:LEU:HA	5	0.16
(1,2053)	1:17:A:HIS:HA	1:16:A:GLU:HG2	10	0.16
(1,2050)	1:17:A:HIS:HA	1:16:A:GLU:HB2	3	0.16
(1,2042)	1:16:A:GLU:HA	1:15:A:GLU:HB2	19	0.16
(1,1960)	1:113:A:GLU:HG3	1:27:A:GLU:HB3	11	0.16
(1,1931)	1:65:A:ILE:HD12	1:41:A:LYS:HB2	12	0.16
(1,1931)	1:65:A:ILE:HD13	1:41:A:LYS:HB2	16	0.16
(1,1931)	1:65:A:ILE:HD13	1:41:A:LYS:HB2	19	0.16
(1,1914)	1:68:A:GLU:HB2	1:34:A:GLY:HA3	8	0.16
(1,1887)	1:82:A:LYS:HD2	1:71:A:GLU:HB3	16	0.16
(1,1864)	1:9:A:SER:HB2	1:12:A:ALA:HB3	10	0.16
(1,1857)	1:75:A:LYS:HG2	1:98:A:ASN:HB2	17	0.16
(1,1854)	1:75:A:LYS:HG2	1:100:A:ILE:HG13	3	0.16
(1,1829)	1:26:A:ILE:HD12	1:23:A:ALA:HB1	5	0.16
(1,1829)	1:26:A:ILE:HD11	1:23:A:ALA:HB1	8	0.16
(1,1821)	1:109:A:LEU:HB2	1:112:A:LEU:HD11	14	0.16
(1,1802)	1:29:A:VAL:HG21	1:29:A:VAL:HG11	1	0.16
(1,1802)	1:29:A:VAL:HG23	1:29:A:VAL:HG13	5	0.16
(1,1802)	1:29:A:VAL:HG23	1:29:A:VAL:HG13	18	0.16
(1,1800)	1:115:A:LEU:HD12	1:25:A:LYS:HG2	7	0.16
(1,1798)	1:62:A:ILE:HD13	1:28:A:ARG:HD3	3	0.16
(1,1771)	1:31:A:VAL:HG22	1:65:A:ILE:HB	9	0.16
(1,1746)	1:90:A:VAL:HG23	1:87:A:ASP:HB3	1	0.16
(1,1746)	1:90:A:VAL:HG21	1:87:A:ASP:HB3	12	0.16
(1,1736)	1:65:A:ILE:HG22	1:41:A:LYS:HG3	3	0.16
(1,1583)	1:35:A:GLU:HG2	1:35:A:GLU:HA	6	0.16
(1,1583)	1:35:A:GLU:HG2	1:35:A:GLU:HA	10	0.16
(1,1583)	1:35:A:GLU:HG2	1:35:A:GLU:HA	15	0.16
(1,1581)	1:35:A:GLU:HG3	1:35:A:GLU:HA	3	0.16
(1,1576)	1:35:A:GLU:HG3	1:69:A:LYS:HA	11	0.16
(1,1570)	1:102:A:THR:HA	1:101:A:ILE:HG23	6	0.16
(1,1559)	1:12:A:ALA:HB3	1:12:A:ALA:HA	5	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1559)	1:12:A:ALA:HB1	1:12:A:ALA:HA	17	0.16
(1,1554)	1:20:A:LYS:HE3	1:17:A:HIS:HA	5	0.16
(1,1554)	1:20:A:LYS:HE3	1:17:A:HIS:HA	20	0.16
(1,1541)	1:19:A:LYS:HB3	1:19:A:LYS:HA	12	0.16
(1,1491)	1:6:A:VAL:HG11	1:6:A:VAL:HA	9	0.16
(1,1491)	1:6:A:VAL:HG11	1:6:A:VAL:HA	19	0.16
(1,1445)	1:48:A:PHE:HB2	1:63:A:LEU:HD12	20	0.16
(1,1428)	1:56:A:LEU:HD21	1:59:A:LYS:HE3	13	0.16
(1,1361)	1:26:A:ILE:HD12	1:114:A:MET:HG2	10	0.16
(1,1354)	1:1:A:MET:HG3	1:1:A:MET:HA	19	0.16
(1,1332)	1:16:A:GLU:HB3	1:16:A:GLU:HG2	1	0.16
(1,1332)	1:16:A:GLU:HB3	1:16:A:GLU:HG2	5	0.16
(1,1299)	1:117:A:GLU:HB2	1:117:A:GLU:HG3	4	0.16
(1,1299)	1:117:A:GLU:HB2	1:117:A:GLU:HG3	8	0.16
(1,1283)	1:15:A:GLU:HB3	1:12:A:ALA:HA	1	0.16
(1,1249)	1:72:A:LEU:HD11	1:83:A:PRO:HG2	5	0.16
(1,1217)	1:72:A:LEU:HD11	1:99:A:VAL:HB	6	0.16
(1,1217)	1:72:A:LEU:HD12	1:99:A:VAL:HB	12	0.16
(1,1159)	1:108:A:ARG:HB2	1:110:A:LEU:HD21	20	0.16
(1,1058)	1:11:A:ILE:HG21	1:11:A:ILE:HG12	6	0.16
(1,1058)	1:11:A:ILE:HG23	1:11:A:ILE:HG12	14	0.16
(1,1053)	1:63:A:LEU:HD13	1:63:A:LEU:HB2	19	0.16
(1,1038)	1:20:A:LYS:HG3	1:20:A:LYS:HD2	9	0.16
(1,1038)	1:20:A:LYS:HG3	1:20:A:LYS:HD2	14	0.16
(1,1038)	1:20:A:LYS:HG3	1:20:A:LYS:HD2	16	0.16
(1,1038)	1:20:A:LYS:HG3	1:20:A:LYS:HD2	18	0.16
(1,1038)	1:20:A:LYS:HG3	1:20:A:LYS:HD2	20	0.16
(1,1010)	1:115:A:LEU:HB3	1:25:A:LYS:HB3	10	0.16
(1,998)	1:65:A:ILE:HG12	1:63:A:LEU:HD22	9	0.16
(1,998)	1:65:A:ILE:HG12	1:63:A:LEU:HD22	13	0.16
(1,934)	1:102:A:THR:HG21	1:100:A:ILE:HB	1	0.16
(1,889)	1:57:A:VAL:HG12	1:15:A:GLU:HG3	2	0.16
(1,874)	1:26:A:ILE:HG22	1:61:A:ALA:HB3	6	0.16
(1,864)	1:110:A:LEU:HD12	1:30:A:VAL:HG22	7	0.16
(1,864)	1:110:A:LEU:HD11	1:30:A:VAL:HG22	8	0.16
(1,864)	1:110:A:LEU:HD12	1:30:A:VAL:HG21	9	0.16
(1,834)	1:72:A:LEU:HD22	1:101:A:ILE:HG21	1	0.16
(1,834)	1:72:A:LEU:HD22	1:101:A:ILE:HG23	10	0.16
(1,826)	1:101:A:ILE:HG23	1:103:A:GLN:HA	19	0.16
(1,818)	1:80:A:VAL:HG11	1:80:A:VAL:HG21	2	0.16
(1,818)	1:80:A:VAL:HG11	1:80:A:VAL:HG23	9	0.16
(1,793)	1:109:A:LEU:HD12	1:109:A:LEU:HD13	9	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,793)	1:109:A:LEU:HD11	1:109:A:LEU:HD13	14	0.16
(1,787)	1:63:A:LEU:HD11	1:65:A:ILE:HD11	17	0.16
(1,784)	1:65:A:ILE:HD12	1:65:A:ILE:HD13	13	0.16
(1,784)	1:65:A:ILE:HD12	1:65:A:ILE:HD11	14	0.16
(1,772)	1:66:A:VAL:HG22	1:64:A:ASP:HB2	9	0.16
(1,771)	1:110:A:LEU:HD12	1:66:A:VAL:HG21	20	0.16
(1,768)	1:70:A:VAL:HG22	1:70:A:VAL:HG21	1	0.16
(1,767)	1:70:A:VAL:HG22	1:70:A:VAL:HG11	14	0.16
(1,758)	1:110:A:LEU:HD12	1:110:A:LEU:HD11	2	0.16
(1,758)	1:110:A:LEU:HD12	1:110:A:LEU:HD13	9	0.16
(1,758)	1:110:A:LEU:HD12	1:110:A:LEU:HD11	12	0.16
(1,758)	1:110:A:LEU:HD11	1:110:A:LEU:HD13	16	0.16
(1,744)	1:72:A:LEU:HD12	1:72:A:LEU:HD22	11	0.16
(1,710)	1:72:A:LEU:HA	1:103:A:GLN:H	14	0.16
(1,448)	1:79:A:HIS:HB2	1:80:A:VAL:H	16	0.16
(1,353)	1:107:A:MET:HG3	1:108:A:ARG:H	8	0.16
(1,277)	1:54:A:GLU:HB3	1:54:A:GLU:H	4	0.16
(1,277)	1:54:A:GLU:HB3	1:54:A:GLU:H	6	0.16
(1,277)	1:54:A:GLU:HB3	1:54:A:GLU:H	12	0.16
(1,248)	1:97:A:LYS:HB3	1:97:A:LYS:H	14	0.16
(1,248)	1:97:A:LYS:HB3	1:97:A:LYS:H	15	0.16
(1,248)	1:97:A:LYS:HB3	1:97:A:LYS:H	18	0.16
(1,248)	1:97:A:LYS:HB3	1:97:A:LYS:H	20	0.16
(1,242)	1:19:A:LYS:HD2	1:19:A:LYS:H	7	0.16
(1,214)	1:36:A:ARG:HB3	1:36:A:ARG:H	8	0.16
(1,196)	1:12:A:ALA:HB2	1:14:A:CYS:H	4	0.16
(1,172)	1:18:A:ALA:HB3	1:23:A:ALA:H	16	0.16
(1,156)	1:23:A:ALA:HB1	1:21:A:ASN:H	15	0.16
(1,142)	1:47:A:ALA:HB3	1:46:A:SER:H	2	0.16
(1,142)	1:47:A:ALA:HB2	1:46:A:SER:H	9	0.16
(1,142)	1:47:A:ALA:HB2	1:46:A:SER:H	18	0.16
(1,142)	1:47:A:ALA:HB2	1:46:A:SER:H	19	0.16
(1,142)	1:47:A:ALA:HB2	1:46:A:SER:H	20	0.16
(1,138)	1:102:A:THR:HG22	1:103:A:GLN:H	12	0.16
(1,111)	1:10:A:LEU:HD13	1:13:A:LEU:H	15	0.16
(1,108)	1:115:A:LEU:HD22	1:116:A:ALA:H	7	0.16
(1,108)	1:115:A:LEU:HD21	1:116:A:ALA:H	19	0.16
(1,107)	1:56:A:LEU:HD22	1:56:A:LEU:H	3	0.16
(1,107)	1:56:A:LEU:HD21	1:56:A:LEU:H	6	0.16
(1,104)	1:43:A:LEU:HD23	1:43:A:LEU:H	12	0.16
(1,102)	1:86:A:LEU:HD11	1:86:A:LEU:H	2	0.16
(1,97)	1:11:A:ILE:HG22	1:12:A:ALA:H	5	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,97)	1:11:A:ILE:HG22	1:12:A:ALA:H	7	0.16
(1,97)	1:11:A:ILE:HG23	1:12:A:ALA:H	17	0.16
(1,83)	1:112:A:LEU:HD21	1:112:A:LEU:H	3	0.16
(1,77)	1:109:A:LEU:HD22	1:109:A:LEU:H	4	0.16
(1,71)	1:31:A:VAL:HG12	1:32:A:GLY:H	10	0.16
(1,29)	1:70:A:VAL:HG22	1:72:A:LEU:H	4	0.16
(1,29)	1:70:A:VAL:HG21	1:72:A:LEU:H	19	0.16
(1,25)	1:90:A:VAL:HG23	1:91:A:CYS:H	6	0.16
(1,25)	1:90:A:VAL:HG21	1:91:A:CYS:H	7	0.16
(1,25)	1:90:A:VAL:HG22	1:91:A:CYS:H	8	0.16
(1,25)	1:90:A:VAL:HG21	1:91:A:CYS:H	16	0.16
(1,12)	1:72:A:LEU:HD13	1:72:A:LEU:H	1	0.16
(1,12)	1:72:A:LEU:HD13	1:72:A:LEU:H	6	0.16
(1,2675)	1:10:A:LEU:HD23	1:48:A:PHE:HZ	15	0.15
(1,2670)	1:11:A:ILE:HG22	1:51:A:PHE:HD2	13	0.15
(1,2661)	1:75:A:LYS:HA	1:75:A:LYS:HE3	11	0.15
(1,2655)	1:17:A:HIS:HB3	1:14:A:CYS:HA	10	0.15
(1,2655)	1:17:A:HIS:HB3	1:14:A:CYS:HA	20	0.15
(1,2647)	1:82:A:LYS:HE2	1:82:A:LYS:HB2	6	0.15
(1,2647)	1:82:A:LYS:HE2	1:82:A:LYS:HB2	16	0.15
(1,2555)	1:25:A:LYS:HE3	1:56:A:LEU:HD13	15	0.15
(1,2518)	1:25:A:LYS:HD3	1:25:A:LYS:HE3	1	0.15
(1,2518)	1:19:A:LYS:HD2	1:19:A:LYS:HE3	8	0.15
(1,2518)	1:25:A:LYS:HD2	1:25:A:LYS:HE3	12	0.15
(1,2518)	1:25:A:LYS:HD2	1:25:A:LYS:HE2	13	0.15
(1,2487)	1:20:A:LYS:HG2	1:20:A:LYS:HD2	1	0.15
(1,2442)	1:31:A:VAL:HG23	1:31:A:VAL:HG13	12	0.15
(1,2427)	1:39:A:MET:HE2	1:107:A:MET:H	19	0.15
(1,2401)	1:90:A:VAL:H	1:91:A:CYS:H	12	0.15
(1,2380)	1:34:A:GLY:H	1:35:A:GLU:H	11	0.15
(1,2380)	1:34:A:GLY:H	1:35:A:GLU:H	12	0.15
(1,2379)	1:96:A:SER:H	1:91:A:CYS:H	14	0.15
(1,2369)	1:82:A:LYS:H	1:81:A:PHE:H	15	0.15
(1,2298)	1:71:A:GLU:H	1:70:A:VAL:H	18	0.15
(1,2206)	1:83:A:PRO:HB2	1:81:A:PHE:HD1	9	0.15
(1,2202)	1:83:A:PRO:HB3	1:88:A:TYR:HD2	2	0.15
(1,2199)	1:7:A:VAL:HB	1:4:A:TYR:HD1	17	0.15
(1,2172)	1:47:A:ALA:HB3	1:4:A:TYR:HD2	1	0.15
(1,2166)	1:50:A:THR:HG21	1:51:A:PHE:HE1	1	0.15
(1,2153)	1:99:A:VAL:HG21	1:81:A:PHE:HE2	4	0.15
(1,2153)	1:99:A:VAL:HG23	1:81:A:PHE:HE2	19	0.15
(1,2148)	1:80:A:VAL:HG13	1:81:A:PHE:HD2	4	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2134)	1:72:A:LEU:HD21	1:81:A:PHE:HE2	11	0.15
(1,2100)	1:97:A:LYS:HA	1:97:A:LYS:HE3	9	0.15
(1,2100)	1:97:A:LYS:HA	1:97:A:LYS:HE2	13	0.15
(1,2068)	1:30:A:VAL:HG11	1:29:A:VAL:HA	1	0.15
(1,2052)	1:20:A:LYS:HG2	1:17:A:HIS:HA	20	0.15
(1,2050)	1:17:A:HIS:HA	1:16:A:GLU:HB2	9	0.15
(1,2024)	1:107:A:MET:HE2	1:7:A:VAL:HA	13	0.15
(1,1990)	1:17:A:HIS:HB3	1:14:A:CYS:HA	7	0.15
(1,1968)	1:113:A:GLU:HG2	1:27:A:GLU:HB3	8	0.15
(1,1960)	1:113:A:GLU:HG3	1:27:A:GLU:HB3	15	0.15
(1,1959)	1:113:A:GLU:HG3	1:28:A:ARG:HB3	13	0.15
(1,1953)	1:68:A:GLU:HG2	1:32:A:GLY:HA3	20	0.15
(1,1950)	1:57:A:VAL:HG21	1:15:A:GLU:HB3	13	0.15
(1,1950)	1:57:A:VAL:HG23	1:15:A:GLU:HB3	19	0.15
(1,1949)	1:15:A:GLU:HB3	1:57:A:VAL:HG11	9	0.15
(1,1944)	1:57:A:VAL:HB	1:26:A:ILE:HD12	20	0.15
(1,1941)	1:107:A:MET:HE3	1:10:A:LEU:HB3	1	0.15
(1,1910)	1:41:A:LYS:HD2	1:33:A:ILE:HD13	11	0.15
(1,1897)	1:41:A:LYS:HD3	1:41:A:LYS:HA	4	0.15
(1,1897)	1:41:A:LYS:HD3	1:41:A:LYS:HA	8	0.15
(1,1897)	1:41:A:LYS:HD3	1:41:A:LYS:HA	11	0.15
(1,1847)	1:110:A:LEU:HD21	1:110:A:LEU:HB2	4	0.15
(1,1847)	1:110:A:LEU:HD21	1:110:A:LEU:HB2	13	0.15
(1,1840)	1:75:A:LYS:HG3	1:100:A:ILE:HG13	1	0.15
(1,1832)	1:61:A:ALA:HB2	1:61:A:ALA:HB3	1	0.15
(1,1832)	1:61:A:ALA:HB2	1:61:A:ALA:HB1	2	0.15
(1,1832)	1:61:A:ALA:HB2	1:61:A:ALA:HB1	16	0.15
(1,1819)	1:7:A:VAL:HG12	1:47:A:ALA:HB2	17	0.15
(1,1802)	1:29:A:VAL:HG23	1:29:A:VAL:HG12	9	0.15
(1,1802)	1:29:A:VAL:HG22	1:29:A:VAL:HG13	16	0.15
(1,1798)	1:62:A:ILE:HD11	1:28:A:ARG:HD3	17	0.15
(1,1796)	1:62:A:ILE:HD11	1:28:A:ARG:HA	20	0.15
(1,1777)	1:112:A:LEU:HD22	1:109:A:LEU:HD11	8	0.15
(1,1774)	1:31:A:VAL:HG23	1:107:A:MET:HG2	7	0.15
(1,1771)	1:31:A:VAL:HG21	1:65:A:ILE:HB	2	0.15
(1,1765)	1:72:A:LEU:HB2	1:99:A:VAL:HB	11	0.15
(1,1736)	1:65:A:ILE:HG22	1:41:A:LYS:HG3	6	0.15
(1,1735)	1:72:A:LEU:HD21	1:88:A:TYR:HB3	1	0.15
(1,1677)	1:25:A:LYS:HA	1:57:A:VAL:HG22	13	0.15
(1,1583)	1:35:A:GLU:HG2	1:35:A:GLU:HA	1	0.15
(1,1583)	1:35:A:GLU:HG2	1:35:A:GLU:HA	7	0.15
(1,1583)	1:35:A:GLU:HG2	1:35:A:GLU:HA	14	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1581)	1:35:A:GLU:HG3	1:35:A:GLU:HA	9	0.15
(1,1581)	1:35:A:GLU:HG3	1:35:A:GLU:HA	12	0.15
(1,1576)	1:35:A:GLU:HG3	1:69:A:LYS:HA	17	0.15
(1,1570)	1:102:A:THR:HA	1:101:A:ILE:HG22	1	0.15
(1,1559)	1:12:A:ALA:HB1	1:12:A:ALA:HA	6	0.15
(1,1559)	1:12:A:ALA:HB3	1:12:A:ALA:HA	19	0.15
(1,1554)	1:20:A:LYS:HE3	1:17:A:HIS:HA	3	0.15
(1,1554)	1:20:A:LYS:HE3	1:17:A:HIS:HA	13	0.15
(1,1554)	1:20:A:LYS:HE3	1:17:A:HIS:HA	17	0.15
(1,1534)	1:56:A:LEU:HB3	1:56:A:LEU:HA	13	0.15
(1,1477)	1:45:A:VAL:HG12	1:41:A:LYS:HA	12	0.15
(1,1384)	1:93:A:LYS:HE3	1:93:A:LYS:HA	2	0.15
(1,1384)	1:93:A:LYS:HE3	1:93:A:LYS:HA	11	0.15
(1,1384)	1:93:A:LYS:HE3	1:93:A:LYS:HA	16	0.15
(1,1332)	1:16:A:GLU:HB3	1:16:A:GLU:HG2	6	0.15
(1,1332)	1:16:A:GLU:HB3	1:16:A:GLU:HG2	13	0.15
(1,1303)	1:23:A:ALA:HB2	1:114:A:MET:HB2	4	0.15
(1,1299)	1:117:A:GLU:HB2	1:117:A:GLU:HG3	20	0.15
(1,1283)	1:15:A:GLU:HB3	1:12:A:ALA:HA	7	0.15
(1,1280)	1:39:A:MET:HB2	1:39:A:MET:HE1	1	0.15
(1,1280)	1:39:A:MET:HB2	1:39:A:MET:HE2	15	0.15
(1,1230)	1:54:A:GLU:HB3	1:54:A:GLU:HG2	1	0.15
(1,1230)	1:54:A:GLU:HB3	1:54:A:GLU:HG2	6	0.15
(1,1230)	1:54:A:GLU:HB3	1:54:A:GLU:HG2	9	0.15
(1,1211)	1:75:A:LYS:HB3	1:98:A:ASN:HB2	12	0.15
(1,1144)	1:59:A:LYS:HD3	1:56:A:LEU:HA	7	0.15
(1,1127)	1:10:A:LEU:HD11	1:10:A:LEU:HB3	14	0.15
(1,1058)	1:11:A:ILE:HG22	1:11:A:ILE:HG12	1	0.15
(1,1058)	1:11:A:ILE:HG21	1:11:A:ILE:HG12	4	0.15
(1,1058)	1:11:A:ILE:HG21	1:11:A:ILE:HG12	16	0.15
(1,1053)	1:63:A:LEU:HD11	1:63:A:LEU:HB2	6	0.15
(1,1038)	1:20:A:LYS:HG3	1:20:A:LYS:HD2	13	0.15
(1,953)	1:65:A:ILE:HG23	1:33:A:ILE:HG12	20	0.15
(1,948)	1:45:A:VAL:HG11	1:42:A:SER:HA	6	0.15
(1,893)	1:43:A:LEU:HD23	1:40:A:ASP:HB3	13	0.15
(1,887)	1:57:A:VAL:HG11	1:18:A:ALA:HA	9	0.15
(1,866)	1:26:A:ILE:HD11	1:18:A:ALA:HB2	19	0.15
(1,857)	1:109:A:LEU:HD22	1:112:A:LEU:HD11	7	0.15
(1,853)	1:31:A:VAL:HG11	1:107:A:MET:HG2	3	0.15
(1,844)	1:112:A:LEU:HD23	1:114:A:MET:HE3	1	0.15
(1,829)	1:101:A:ILE:HG21	1:105:A:ASN:HB3	5	0.15
(1,829)	1:101:A:ILE:HG22	1:105:A:ASN:HB3	7	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,829)	1:101:A:ILE:HG23	1:105:A:ASN:HB3	14	0.15
(1,787)	1:63:A:LEU:HD11	1:65:A:ILE:HD11	10	0.15
(1,784)	1:65:A:ILE:HD12	1:65:A:ILE:HD13	6	0.15
(1,784)	1:65:A:ILE:HD12	1:65:A:ILE:HD11	10	0.15
(1,784)	1:65:A:ILE:HD12	1:65:A:ILE:HD13	20	0.15
(1,780)	1:99:A:VAL:HG12	1:99:A:VAL:HG21	9	0.15
(1,771)	1:110:A:LEU:HD12	1:66:A:VAL:HG23	10	0.15
(1,768)	1:70:A:VAL:HG22	1:70:A:VAL:HG21	4	0.15
(1,768)	1:70:A:VAL:HG21	1:70:A:VAL:HG23	7	0.15
(1,768)	1:70:A:VAL:HG21	1:70:A:VAL:HG23	15	0.15
(1,759)	1:110:A:LEU:HD11	1:110:A:LEU:HD23	20	0.15
(1,758)	1:110:A:LEU:HD11	1:110:A:LEU:HD13	1	0.15
(1,758)	1:110:A:LEU:HD12	1:110:A:LEU:HD11	17	0.15
(1,755)	1:65:A:ILE:HG22	1:41:A:LYS:HD2	3	0.15
(1,752)	1:65:A:ILE:HG22	1:65:A:ILE:HG13	7	0.15
(1,752)	1:65:A:ILE:HG21	1:65:A:ILE:HG13	18	0.15
(1,750)	1:72:A:LEU:HD21	1:99:A:VAL:HG11	11	0.15
(1,710)	1:72:A:LEU:HA	1:103:A:GLN:H	20	0.15
(1,408)	1:76:A:ASP:HB2	1:77:A:CYS:H	1	0.15
(1,396)	1:76:A:ASP:HB3	1:76:A:ASP:H	3	0.15
(1,353)	1:107:A:MET:HG3	1:108:A:ARG:H	3	0.15
(1,344)	1:113:A:GLU:HG3	1:113:A:GLU:H	3	0.15
(1,277)	1:54:A:GLU:HB3	1:54:A:GLU:H	7	0.15
(1,277)	1:54:A:GLU:HB3	1:54:A:GLU:H	10	0.15
(1,277)	1:54:A:GLU:HB3	1:54:A:GLU:H	11	0.15
(1,277)	1:54:A:GLU:HB3	1:54:A:GLU:H	19	0.15
(1,248)	1:97:A:LYS:HB3	1:97:A:LYS:H	1	0.15
(1,214)	1:36:A:ARG:HB3	1:36:A:ARG:H	17	0.15
(1,214)	1:36:A:ARG:HB3	1:36:A:ARG:H	18	0.15
(1,191)	1:93:A:LYS:HB2	1:94:A:CYS:H	15	0.15
(1,156)	1:23:A:ALA:HB3	1:21:A:ASN:H	13	0.15
(1,142)	1:47:A:ALA:HB3	1:46:A:SER:H	6	0.15
(1,138)	1:102:A:THR:HG21	1:103:A:GLN:H	5	0.15
(1,138)	1:102:A:THR:HG22	1:103:A:GLN:H	19	0.15
(1,134)	1:57:A:VAL:HG23	1:58:A:CYS:H	10	0.15
(1,131)	1:10:A:LEU:HD21	1:11:A:ILE:H	8	0.15
(1,125)	1:43:A:LEU:HD13	1:43:A:LEU:H	6	0.15
(1,113)	1:10:A:LEU:HD11	1:10:A:LEU:H	7	0.15
(1,108)	1:115:A:LEU:HD21	1:116:A:ALA:H	1	0.15
(1,97)	1:11:A:ILE:HG21	1:12:A:ALA:H	1	0.15
(1,97)	1:11:A:ILE:HG22	1:12:A:ALA:H	20	0.15
(1,25)	1:90:A:VAL:HG23	1:91:A:CYS:H	17	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2676)	1:47:A:ALA:HB3	1:44:A:PHE:HD1	6	0.14
(1,2673)	1:13:A:LEU:HD12	1:17:A:HIS:HD2	17	0.14
(1,2673)	1:13:A:LEU:HD12	1:17:A:HIS:HD2	18	0.14
(1,2671)	1:115:A:LEU:HD11	1:24:A:HIS:HD2	17	0.14
(1,2660)	1:69:A:LYS:HA	1:69:A:LYS:HE2	2	0.14
(1,2653)	1:41:A:LYS:HD3	1:41:A:LYS:HA	2	0.14
(1,2643)	1:107:A:MET:HE1	1:106:A:GLU:HG3	10	0.14
(1,2600)	1:66:A:VAL:HG11	1:66:A:VAL:HG13	8	0.14
(1,2569)	1:92:A:GLU:HG2	1:92:A:GLU:HA	8	0.14
(1,2518)	1:19:A:LYS:HD3	1:19:A:LYS:HE2	9	0.14
(1,2518)	1:25:A:LYS:HD3	1:25:A:LYS:HE2	19	0.14
(1,2465)	1:31:A:VAL:HG11	1:10:A:LEU:HD23	1	0.14
(1,2442)	1:31:A:VAL:HG21	1:31:A:VAL:HG13	5	0.14
(1,2401)	1:90:A:VAL:H	1:91:A:CYS:H	3	0.14
(1,2401)	1:90:A:VAL:H	1:91:A:CYS:H	15	0.14
(1,2401)	1:90:A:VAL:H	1:91:A:CYS:H	17	0.14
(1,2397)	1:100:A:ILE:H	1:74:A:CYS:H	9	0.14
(1,2380)	1:34:A:GLY:H	1:35:A:GLU:H	19	0.14
(1,2369)	1:82:A:LYS:H	1:81:A:PHE:H	16	0.14
(1,2294)	1:99:A:VAL:H	1:100:A:ILE:H	17	0.14
(1,2287)	1:80:A:VAL:H	1:81:A:PHE:H	20	0.14
(1,2250)	1:4:A:TYR:HA	1:4:A:TYR:HD1	17	0.14
(1,2239)	1:41:A:LYS:HA	1:44:A:PHE:HD2	6	0.14
(1,2229)	1:4:A:TYR:HB3	1:4:A:TYR:HE1	8	0.14
(1,2183)	1:116:A:ALA:HB3	1:24:A:HIS:HD2	9	0.14
(1,2183)	1:116:A:ALA:HB2	1:24:A:HIS:HD2	14	0.14
(1,2179)	1:45:A:VAL:HG13	1:44:A:PHE:HE1	11	0.14
(1,2162)	1:43:A:LEU:HD11	1:4:A:TYR:HD2	10	0.14
(1,2148)	1:80:A:VAL:HG11	1:81:A:PHE:HD2	1	0.14
(1,2104)	1:82:A:LYS:HA	1:83:A:PRO:HG3	9	0.14
(1,2100)	1:97:A:LYS:HA	1:97:A:LYS:HE2	14	0.14
(1,2100)	1:97:A:LYS:HA	1:97:A:LYS:HE2	15	0.14
(1,2067)	1:10:A:LEU:HA	1:13:A:LEU:HG	4	0.14
(1,2060)	1:35:A:GLU:HA	1:33:A:ILE:HG23	13	0.14
(1,2058)	1:12:A:ALA:HB1	1:13:A:LEU:HA	7	0.14
(1,2051)	1:114:A:MET:HE1	1:17:A:HIS:HA	14	0.14
(1,2050)	1:17:A:HIS:HA	1:16:A:GLU:HB2	12	0.14
(1,2042)	1:16:A:GLU:HA	1:15:A:GLU:HB2	5	0.14
(1,2041)	1:16:A:GLU:HA	1:17:A:HIS:HA	12	0.14
(1,2040)	1:90:A:VAL:HG22	1:92:A:GLU:HA	2	0.14
(1,1990)	1:17:A:HIS:HB3	1:14:A:CYS:HA	17	0.14
(1,1950)	1:57:A:VAL:HG22	1:15:A:GLU:HB3	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1950)	1:57:A:VAL:HG23	1:15:A:GLU:HB3	14	0.14
(1,1949)	1:15:A:GLU:HB3	1:57:A:VAL:HG13	4	0.14
(1,1949)	1:15:A:GLU:HB3	1:57:A:VAL:HG11	7	0.14
(1,1897)	1:41:A:LYS:HD3	1:41:A:LYS:HA	6	0.14
(1,1885)	1:90:A:VAL:HG13	1:97:A:LYS:HG2	12	0.14
(1,1832)	1:61:A:ALA:HB2	1:61:A:ALA:HB1	5	0.14
(1,1832)	1:61:A:ALA:HB1	1:61:A:ALA:HB3	6	0.14
(1,1832)	1:61:A:ALA:HB2	1:61:A:ALA:HB3	12	0.14
(1,1832)	1:61:A:ALA:HB2	1:61:A:ALA:HB1	14	0.14
(1,1832)	1:61:A:ALA:HB2	1:61:A:ALA:HB3	18	0.14
(1,1832)	1:61:A:ALA:HB2	1:61:A:ALA:HB1	19	0.14
(1,1819)	1:7:A:VAL:HG13	1:47:A:ALA:HB2	1	0.14
(1,1814)	1:107:A:MET:HE1	1:10:A:LEU:HD23	6	0.14
(1,1802)	1:29:A:VAL:HG23	1:29:A:VAL:HG11	4	0.14
(1,1802)	1:29:A:VAL:HG22	1:29:A:VAL:HG11	6	0.14
(1,1802)	1:29:A:VAL:HG22	1:29:A:VAL:HG13	15	0.14
(1,1796)	1:62:A:ILE:HD13	1:28:A:ARG:HA	5	0.14
(1,1780)	1:112:A:LEU:HD22	1:17:A:HIS:HA	5	0.14
(1,1775)	1:100:A:ILE:HD12	1:102:A:THR:HB	19	0.14
(1,1771)	1:31:A:VAL:HG23	1:65:A:ILE:HB	4	0.14
(1,1771)	1:31:A:VAL:HG21	1:65:A:ILE:HB	12	0.14
(1,1769)	1:66:A:VAL:HG12	1:68:A:GLU:HB2	15	0.14
(1,1749)	1:65:A:ILE:HG13	1:63:A:LEU:HD23	12	0.14
(1,1746)	1:90:A:VAL:HG22	1:87:A:ASP:HB3	10	0.14
(1,1746)	1:90:A:VAL:HG22	1:87:A:ASP:HB3	11	0.14
(1,1736)	1:65:A:ILE:HG21	1:41:A:LYS:HG3	13	0.14
(1,1688)	1:97:A:LYS:HA	1:99:A:VAL:HG22	20	0.14
(1,1665)	1:24:A:HIS:HA	1:57:A:VAL:HG22	3	0.14
(1,1644)	1:88:A:TYR:HA	1:72:A:LEU:HD21	8	0.14
(1,1583)	1:35:A:GLU:HG2	1:35:A:GLU:HA	4	0.14
(1,1570)	1:102:A:THR:HA	1:101:A:ILE:HG21	9	0.14
(1,1559)	1:12:A:ALA:HB3	1:12:A:ALA:HA	2	0.14
(1,1559)	1:12:A:ALA:HB3	1:12:A:ALA:HA	11	0.14
(1,1528)	1:50:A:THR:HB	1:50:A:THR:HA	7	0.14
(1,1477)	1:45:A:VAL:HG12	1:41:A:LYS:HA	4	0.14
(1,1449)	1:26:A:ILE:HD11	1:14:A:CYS:HB2	18	0.14
(1,1410)	1:84:A:ASN:HB3	1:84:A:ASN:HA	15	0.14
(1,1388)	1:11:A:ILE:HD11	1:51:A:PHE:HB3	1	0.14
(1,1384)	1:93:A:LYS:HE3	1:93:A:LYS:HA	6	0.14
(1,1331)	1:16:A:GLU:HB2	1:16:A:GLU:HG3	16	0.14
(1,1314)	1:53:A:GLU:HB2	1:53:A:GLU:HG2	1	0.14
(1,1230)	1:54:A:GLU:HB3	1:54:A:GLU:HG2	4	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1159)	1:108:A:ARG:HB2	1:110:A:LEU:HD22	8	0.14
(1,1127)	1:10:A:LEU:HD11	1:10:A:LEU:HB3	20	0.14
(1,1058)	1:11:A:ILE:HG21	1:11:A:ILE:HG12	2	0.14
(1,1058)	1:11:A:ILE:HG22	1:11:A:ILE:HG12	10	0.14
(1,1058)	1:11:A:ILE:HG23	1:11:A:ILE:HG12	19	0.14
(1,1053)	1:63:A:LEU:HD11	1:63:A:LEU:HB2	2	0.14
(1,1053)	1:63:A:LEU:HD13	1:63:A:LEU:HB2	11	0.14
(1,1053)	1:63:A:LEU:HD13	1:63:A:LEU:HB2	12	0.14
(1,1053)	1:63:A:LEU:HD12	1:63:A:LEU:HB2	15	0.14
(1,1038)	1:20:A:LYS:HG3	1:20:A:LYS:HD2	4	0.14
(1,1038)	1:20:A:LYS:HG3	1:20:A:LYS:HD2	11	0.14
(1,1024)	1:57:A:VAL:HG13	1:18:A:ALA:HB3	18	0.14
(1,998)	1:65:A:ILE:HG12	1:63:A:LEU:HD23	14	0.14
(1,963)	1:41:A:LYS:HG3	1:65:A:ILE:HD13	14	0.14
(1,940)	1:112:A:LEU:HD13	1:112:A:LEU:HA	18	0.14
(1,898)	1:29:A:VAL:HG12	1:112:A:LEU:HA	17	0.14
(1,893)	1:43:A:LEU:HD23	1:40:A:ASP:HB3	1	0.14
(1,893)	1:43:A:LEU:HD22	1:40:A:ASP:HB3	14	0.14
(1,889)	1:57:A:VAL:HG12	1:15:A:GLU:HG3	5	0.14
(1,874)	1:26:A:ILE:HG22	1:61:A:ALA:HB2	4	0.14
(1,834)	1:72:A:LEU:HD21	1:101:A:ILE:HG21	7	0.14
(1,834)	1:72:A:LEU:HD22	1:101:A:ILE:HG22	9	0.14
(1,832)	1:101:A:ILE:HG23	1:105:A:ASN:HB2	2	0.14
(1,832)	1:101:A:ILE:HG22	1:105:A:ASN:HB2	18	0.14
(1,825)	1:101:A:ILE:HG21	1:72:A:LEU:HA	7	0.14
(1,818)	1:80:A:VAL:HG13	1:80:A:VAL:HG22	13	0.14
(1,784)	1:65:A:ILE:HD12	1:65:A:ILE:HD11	1	0.14
(1,784)	1:65:A:ILE:HD11	1:65:A:ILE:HD13	3	0.14
(1,784)	1:65:A:ILE:HD12	1:65:A:ILE:HD11	5	0.14
(1,784)	1:65:A:ILE:HD11	1:65:A:ILE:HD13	18	0.14
(1,780)	1:99:A:VAL:HG11	1:99:A:VAL:HG23	2	0.14
(1,780)	1:99:A:VAL:HG11	1:99:A:VAL:HG23	10	0.14
(1,780)	1:99:A:VAL:HG11	1:99:A:VAL:HG22	16	0.14
(1,776)	1:33:A:ILE:HG21	1:33:A:ILE:HG23	4	0.14
(1,776)	1:33:A:ILE:HG22	1:33:A:ILE:HG23	15	0.14
(1,768)	1:70:A:VAL:HG21	1:70:A:VAL:HG23	5	0.14
(1,768)	1:70:A:VAL:HG22	1:70:A:VAL:HG21	6	0.14
(1,768)	1:70:A:VAL:HG22	1:70:A:VAL:HG21	9	0.14
(1,768)	1:70:A:VAL:HG22	1:70:A:VAL:HG21	10	0.14
(1,768)	1:70:A:VAL:HG22	1:70:A:VAL:HG21	14	0.14
(1,768)	1:70:A:VAL:HG21	1:70:A:VAL:HG23	17	0.14
(1,767)	1:70:A:VAL:HG23	1:70:A:VAL:HG12	4	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,767)	1:70:A:VAL:HG23	1:70:A:VAL:HG13	11	0.14
(1,762)	1:70:A:VAL:HG23	1:71:A:GLU:HA	18	0.14
(1,759)	1:110:A:LEU:HD13	1:110:A:LEU:HD21	2	0.14
(1,759)	1:110:A:LEU:HD12	1:110:A:LEU:HD22	8	0.14
(1,758)	1:110:A:LEU:HD12	1:110:A:LEU:HD13	5	0.14
(1,758)	1:110:A:LEU:HD11	1:110:A:LEU:HD13	7	0.14
(1,758)	1:110:A:LEU:HD12	1:110:A:LEU:HD11	18	0.14
(1,758)	1:110:A:LEU:HD12	1:110:A:LEU:HD13	20	0.14
(1,457)	1:74:A:CYS:HB2	1:79:A:HIS:H	11	0.14
(1,437)	1:24:A:HIS:HB3	1:25:A:LYS:H	18	0.14
(1,437)	1:24:A:HIS:HB3	1:25:A:LYS:H	19	0.14
(1,428)	1:59:A:LYS:HE2	1:59:A:LYS:H	3	0.14
(1,407)	1:76:A:ASP:HB2	1:76:A:ASP:H	11	0.14
(1,407)	1:76:A:ASP:HB2	1:76:A:ASP:H	17	0.14
(1,367)	1:54:A:GLU:HG2	1:55:A:SER:H	10	0.14
(1,367)	1:54:A:GLU:HG2	1:55:A:SER:H	16	0.14
(1,348)	1:103:A:GLN:HG2	1:104:A:GLY:H	4	0.14
(1,301)	1:69:A:LYS:HB2	1:70:A:VAL:H	1	0.14
(1,301)	1:69:A:LYS:HB2	1:70:A:VAL:H	17	0.14
(1,277)	1:54:A:GLU:HB3	1:54:A:GLU:H	17	0.14
(1,248)	1:97:A:LYS:HB3	1:97:A:LYS:H	11	0.14
(1,248)	1:97:A:LYS:HB3	1:97:A:LYS:H	17	0.14
(1,248)	1:97:A:LYS:HB3	1:97:A:LYS:H	19	0.14
(1,234)	1:39:A:MET:HB3	1:39:A:MET:H	3	0.14
(1,234)	1:39:A:MET:HB3	1:39:A:MET:H	11	0.14
(1,203)	1:20:A:LYS:HG2	1:20:A:LYS:H	2	0.14
(1,172)	1:18:A:ALA:HB3	1:23:A:ALA:H	11	0.14
(1,138)	1:102:A:THR:HG21	1:103:A:GLN:H	18	0.14
(1,134)	1:57:A:VAL:HG21	1:58:A:CYS:H	19	0.14
(1,131)	1:10:A:LEU:HD23	1:11:A:ILE:H	10	0.14
(1,125)	1:43:A:LEU:HD13	1:43:A:LEU:H	3	0.14
(1,113)	1:10:A:LEU:HD12	1:10:A:LEU:H	15	0.14
(1,108)	1:115:A:LEU:HD21	1:116:A:ALA:H	10	0.14
(1,108)	1:115:A:LEU:HD21	1:116:A:ALA:H	15	0.14
(1,108)	1:115:A:LEU:HD23	1:116:A:ALA:H	18	0.14
(1,107)	1:56:A:LEU:HD21	1:56:A:LEU:H	5	0.14
(1,104)	1:43:A:LEU:HD22	1:43:A:LEU:H	1	0.14
(1,101)	1:57:A:VAL:HG13	1:15:A:GLU:H	18	0.14
(1,97)	1:11:A:ILE:HG23	1:12:A:ALA:H	16	0.14
(1,82)	1:109:A:LEU:HD22	1:30:A:VAL:H	15	0.14
(1,71)	1:31:A:VAL:HG12	1:32:A:GLY:H	3	0.14
(1,33)	1:33:A:ILE:HG21	1:37:A:SER:H	4	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,33)	1:33:A:ILE:HG22	1:37:A:SER:H	11	0.14
(1,29)	1:70:A:VAL:HG21	1:72:A:LEU:H	14	0.14
(1,25)	1:90:A:VAL:HG22	1:91:A:CYS:H	11	0.14
(1,18)	1:72:A:LEU:HD23	1:72:A:LEU:H	11	0.14
(1,2673)	1:13:A:LEU:HD12	1:17:A:HIS:HD2	6	0.13
(1,2608)	1:115:A:LEU:HD23	1:27:A:GLU:HB2	1	0.13
(1,2600)	1:30:A:VAL:HG12	1:30:A:VAL:HG11	2	0.13
(1,2600)	1:30:A:VAL:HG11	1:30:A:VAL:HG13	3	0.13
(1,2600)	1:66:A:VAL:HG11	1:66:A:VAL:HG13	14	0.13
(1,2600)	1:66:A:VAL:HG12	1:66:A:VAL:HG13	16	0.13
(1,2600)	1:66:A:VAL:HG12	1:66:A:VAL:HG13	19	0.13
(1,2600)	1:66:A:VAL:HG12	1:66:A:VAL:HG11	20	0.13
(1,2590)	1:33:A:ILE:HD12	1:39:A:MET:HG2	12	0.13
(1,2577)	1:54:A:GLU:HG2	1:54:A:GLU:HA	8	0.13
(1,2569)	1:92:A:GLU:HG2	1:92:A:GLU:HA	1	0.13
(1,2518)	1:25:A:LYS:HD3	1:25:A:LYS:HE2	5	0.13
(1,2421)	1:115:A:LEU:HD21	1:115:A:LEU:H	4	0.13
(1,2421)	1:115:A:LEU:HD21	1:115:A:LEU:H	8	0.13
(1,2401)	1:90:A:VAL:H	1:91:A:CYS:H	18	0.13
(1,2397)	1:100:A:ILE:H	1:74:A:CYS:H	4	0.13
(1,2397)	1:100:A:ILE:H	1:74:A:CYS:H	5	0.13
(1,2386)	1:101:A:ILE:H	1:102:A:THR:H	6	0.13
(1,2386)	1:101:A:ILE:H	1:102:A:THR:H	15	0.13
(1,2298)	1:71:A:GLU:H	1:70:A:VAL:H	8	0.13
(1,2298)	1:71:A:GLU:H	1:70:A:VAL:H	17	0.13
(1,2262)	1:88:A:TYR:HA	1:88:A:TYR:HD1	8	0.13
(1,2250)	1:4:A:TYR:HA	1:4:A:TYR:HD1	12	0.13
(1,2250)	1:4:A:TYR:HA	1:4:A:TYR:HD2	16	0.13
(1,2239)	1:41:A:LYS:HA	1:44:A:PHE:HD2	19	0.13
(1,2210)	1:107:A:MET:HG2	1:44:A:PHE:HZ	15	0.13
(1,2172)	1:47:A:ALA:HB1	1:4:A:TYR:HD2	18	0.13
(1,2157)	1:43:A:LEU:HD23	1:4:A:TYR:HE2	8	0.13
(1,2150)	1:31:A:VAL:HG12	1:44:A:PHE:HE2	6	0.13
(1,2104)	1:82:A:LYS:HA	1:83:A:PRO:HG3	4	0.13
(1,2104)	1:82:A:LYS:HA	1:83:A:PRO:HG3	17	0.13
(1,2100)	1:97:A:LYS:HA	1:97:A:LYS:HE2	4	0.13
(1,2088)	1:105:A:ASN:HA	1:36:A:ARG:HB3	12	0.13
(1,2079)	1:71:A:GLU:HB2	1:103:A:GLN:HA	3	0.13
(1,2068)	1:30:A:VAL:HG13	1:29:A:VAL:HA	6	0.13
(1,2058)	1:12:A:ALA:HB1	1:13:A:LEU:HA	2	0.13
(1,2052)	1:20:A:LYS:HG2	1:17:A:HIS:HA	18	0.13
(1,2051)	1:114:A:MET:HE1	1:17:A:HIS:HA	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2042)	1:16:A:GLU:HA	1:15:A:GLU:HB2	11	0.13
(1,2042)	1:16:A:GLU:HA	1:15:A:GLU:HB2	16	0.13
(1,2042)	1:16:A:GLU:HA	1:15:A:GLU:HB2	18	0.13
(1,2041)	1:16:A:GLU:HA	1:17:A:HIS:HA	8	0.13
(1,2034)	1:59:A:LYS:HB3	1:53:A:GLU:HA	20	0.13
(1,2001)	1:59:A:LYS:HE2	1:56:A:LEU:HB2	14	0.13
(1,1959)	1:113:A:GLU:HG3	1:28:A:ARG:HB3	2	0.13
(1,1949)	1:15:A:GLU:HB3	1:57:A:VAL:HG12	13	0.13
(1,1930)	1:71:A:GLU:HB2	1:103:A:GLN:HB2	11	0.13
(1,1914)	1:68:A:GLU:HB2	1:34:A:GLY:HA3	18	0.13
(1,1901)	1:57:A:VAL:HG21	1:56:A:LEU:HB3	8	0.13
(1,1897)	1:41:A:LYS:HD3	1:41:A:LYS:HA	15	0.13
(1,1897)	1:41:A:LYS:HD3	1:41:A:LYS:HA	17	0.13
(1,1854)	1:75:A:LYS:HG2	1:100:A:ILE:HG13	13	0.13
(1,1832)	1:61:A:ALA:HB1	1:61:A:ALA:HB3	4	0.13
(1,1832)	1:61:A:ALA:HB2	1:61:A:ALA:HB1	7	0.13
(1,1832)	1:61:A:ALA:HB2	1:61:A:ALA:HB1	9	0.13
(1,1832)	1:61:A:ALA:HB2	1:61:A:ALA:HB3	10	0.13
(1,1832)	1:61:A:ALA:HB2	1:61:A:ALA:HB1	15	0.13
(1,1832)	1:61:A:ALA:HB2	1:61:A:ALA:HB3	17	0.13
(1,1832)	1:61:A:ALA:HB1	1:61:A:ALA:HB3	20	0.13
(1,1802)	1:29:A:VAL:HG21	1:29:A:VAL:HG13	8	0.13
(1,1799)	1:29:A:VAL:HG12	1:109:A:LEU:HD12	18	0.13
(1,1796)	1:62:A:ILE:HD13	1:28:A:ARG:HA	13	0.13
(1,1789)	1:100:A:ILE:HD11	1:100:A:ILE:HG23	14	0.13
(1,1787)	1:26:A:ILE:HG21	1:112:A:LEU:HA	7	0.13
(1,1731)	1:72:A:LEU:HD12	1:91:A:CYS:HA	19	0.13
(1,1688)	1:97:A:LYS:HA	1:99:A:VAL:HG23	2	0.13
(1,1687)	1:31:A:VAL:HA	1:110:A:LEU:HD13	16	0.13
(1,1583)	1:35:A:GLU:HG2	1:35:A:GLU:HA	5	0.13
(1,1583)	1:35:A:GLU:HG2	1:35:A:GLU:HA	11	0.13
(1,1583)	1:35:A:GLU:HG2	1:35:A:GLU:HA	12	0.13
(1,1583)	1:35:A:GLU:HG2	1:35:A:GLU:HA	13	0.13
(1,1583)	1:35:A:GLU:HG2	1:35:A:GLU:HA	16	0.13
(1,1583)	1:35:A:GLU:HG2	1:35:A:GLU:HA	17	0.13
(1,1576)	1:35:A:GLU:HG3	1:69:A:LYS:HA	8	0.13
(1,1570)	1:102:A:THR:HA	1:101:A:ILE:HG21	2	0.13
(1,1570)	1:102:A:THR:HA	1:101:A:ILE:HG23	19	0.13
(1,1567)	1:102:A:THR:HG22	1:102:A:THR:HA	16	0.13
(1,1567)	1:102:A:THR:HG21	1:102:A:THR:HA	17	0.13
(1,1559)	1:12:A:ALA:HB1	1:12:A:ALA:HA	9	0.13
(1,1559)	1:12:A:ALA:HB3	1:12:A:ALA:HA	16	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1559)	1:12:A:ALA:HB2	1:12:A:ALA:HA	18	0.13
(1,1534)	1:56:A:LEU:HB3	1:56:A:LEU:HA	2	0.13
(1,1534)	1:56:A:LEU:HB3	1:56:A:LEU:HA	12	0.13
(1,1452)	1:63:A:LEU:HD11	1:45:A:VAL:HA	14	0.13
(1,1388)	1:11:A:ILE:HD12	1:51:A:PHE:HB3	5	0.13
(1,1385)	1:48:A:PHE:HB3	1:63:A:LEU:HD13	12	0.13
(1,1385)	1:48:A:PHE:HB3	1:63:A:LEU:HD11	17	0.13
(1,1384)	1:93:A:LYS:HE3	1:93:A:LYS:HA	15	0.13
(1,1361)	1:26:A:ILE:HD12	1:114:A:MET:HG2	15	0.13
(1,1332)	1:16:A:GLU:HB3	1:16:A:GLU:HG2	18	0.13
(1,1324)	1:106:A:GLU:HG2	1:105:A:ASN:HB2	2	0.13
(1,1283)	1:15:A:GLU:HB3	1:12:A:ALA:HA	14	0.13
(1,1280)	1:39:A:MET:HB2	1:39:A:MET:HE2	3	0.13
(1,1230)	1:54:A:GLU:HB3	1:54:A:GLU:HG2	3	0.13
(1,1230)	1:54:A:GLU:HB3	1:54:A:GLU:HG2	5	0.13
(1,1230)	1:54:A:GLU:HB3	1:54:A:GLU:HG2	8	0.13
(1,1230)	1:54:A:GLU:HB3	1:54:A:GLU:HG2	10	0.13
(1,1230)	1:54:A:GLU:HB3	1:54:A:GLU:HG2	13	0.13
(1,1230)	1:54:A:GLU:HB3	1:54:A:GLU:HG2	15	0.13
(1,1217)	1:72:A:LEU:HD12	1:99:A:VAL:HB	16	0.13
(1,1217)	1:72:A:LEU:HD12	1:99:A:VAL:HB	17	0.13
(1,1197)	1:80:A:VAL:HG11	1:71:A:GLU:HG3	17	0.13
(1,1058)	1:11:A:ILE:HG22	1:11:A:ILE:HG12	13	0.13
(1,1038)	1:20:A:LYS:HG3	1:20:A:LYS:HD2	3	0.13
(1,1038)	1:20:A:LYS:HG3	1:20:A:LYS:HD2	8	0.13
(1,1038)	1:20:A:LYS:HG3	1:20:A:LYS:HD2	12	0.13
(1,1038)	1:20:A:LYS:HG3	1:20:A:LYS:HD2	15	0.13
(1,1038)	1:20:A:LYS:HG3	1:20:A:LYS:HD2	19	0.13
(1,1024)	1:57:A:VAL:HG11	1:18:A:ALA:HB3	9	0.13
(1,1010)	1:115:A:LEU:HB3	1:25:A:LYS:HB3	1	0.13
(1,1010)	1:115:A:LEU:HB3	1:25:A:LYS:HB3	20	0.13
(1,962)	1:33:A:ILE:HD11	1:41:A:LYS:HG3	10	0.13
(1,952)	1:33:A:ILE:HG12	1:31:A:VAL:HG21	12	0.13
(1,940)	1:112:A:LEU:HD11	1:112:A:LEU:HA	6	0.13
(1,874)	1:26:A:ILE:HG21	1:61:A:ALA:HB3	13	0.13
(1,874)	1:26:A:ILE:HG21	1:61:A:ALA:HB1	17	0.13
(1,864)	1:110:A:LEU:HD12	1:30:A:VAL:HG22	14	0.13
(1,853)	1:31:A:VAL:HG11	1:107:A:MET:HG2	19	0.13
(1,849)	1:72:A:LEU:HD23	1:101:A:ILE:HG13	15	0.13
(1,844)	1:112:A:LEU:HD21	1:114:A:MET:HE2	3	0.13
(1,829)	1:101:A:ILE:HG21	1:105:A:ASN:HB3	11	0.13
(1,825)	1:101:A:ILE:HG22	1:72:A:LEU:HA	2	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,821)	1:30:A:VAL:HG12	1:28:A:ARG:HG3	3	0.13
(1,793)	1:109:A:LEU:HD11	1:109:A:LEU:HD13	6	0.13
(1,784)	1:65:A:ILE:HD11	1:65:A:ILE:HD13	4	0.13
(1,784)	1:65:A:ILE:HD12	1:65:A:ILE:HD13	7	0.13
(1,784)	1:65:A:ILE:HD11	1:65:A:ILE:HD13	12	0.13
(1,784)	1:65:A:ILE:HD11	1:65:A:ILE:HD13	19	0.13
(1,780)	1:99:A:VAL:HG13	1:99:A:VAL:HG23	11	0.13
(1,776)	1:33:A:ILE:HG21	1:33:A:ILE:HG23	2	0.13
(1,776)	1:33:A:ILE:HG22	1:33:A:ILE:HG21	3	0.13
(1,776)	1:33:A:ILE:HG22	1:33:A:ILE:HG23	5	0.13
(1,776)	1:33:A:ILE:HG22	1:33:A:ILE:HG21	6	0.13
(1,776)	1:33:A:ILE:HG22	1:33:A:ILE:HG23	7	0.13
(1,776)	1:33:A:ILE:HG21	1:33:A:ILE:HG23	8	0.13
(1,776)	1:33:A:ILE:HG21	1:33:A:ILE:HG23	9	0.13
(1,776)	1:33:A:ILE:HG22	1:33:A:ILE:HG23	11	0.13
(1,776)	1:33:A:ILE:HG22	1:33:A:ILE:HG21	12	0.13
(1,776)	1:33:A:ILE:HG22	1:33:A:ILE:HG23	14	0.13
(1,776)	1:33:A:ILE:HG21	1:33:A:ILE:HG23	16	0.13
(1,776)	1:33:A:ILE:HG21	1:33:A:ILE:HG23	17	0.13
(1,776)	1:33:A:ILE:HG21	1:33:A:ILE:HG23	18	0.13
(1,771)	1:110:A:LEU:HD12	1:66:A:VAL:HG23	14	0.13
(1,769)	1:72:A:LEU:HD23	1:70:A:VAL:HG23	18	0.13
(1,768)	1:70:A:VAL:HG22	1:70:A:VAL:HG21	2	0.13
(1,768)	1:70:A:VAL:HG22	1:70:A:VAL:HG21	8	0.13
(1,768)	1:70:A:VAL:HG22	1:70:A:VAL:HG23	11	0.13
(1,768)	1:70:A:VAL:HG22	1:70:A:VAL:HG23	13	0.13
(1,768)	1:70:A:VAL:HG22	1:70:A:VAL:HG21	18	0.13
(1,768)	1:70:A:VAL:HG21	1:70:A:VAL:HG23	19	0.13
(1,768)	1:70:A:VAL:HG22	1:70:A:VAL:HG21	20	0.13
(1,767)	1:70:A:VAL:HG21	1:70:A:VAL:HG11	1	0.13
(1,767)	1:70:A:VAL:HG22	1:70:A:VAL:HG12	7	0.13
(1,755)	1:65:A:ILE:HG22	1:41:A:LYS:HD2	6	0.13
(1,746)	1:72:A:LEU:HD11	1:83:A:PRO:HB2	17	0.13
(1,744)	1:72:A:LEU:HD12	1:72:A:LEU:HD23	10	0.13
(1,744)	1:72:A:LEU:HD11	1:72:A:LEU:HD22	15	0.13
(1,744)	1:72:A:LEU:HD13	1:72:A:LEU:HD23	20	0.13
(1,690)	1:76:A:ASP:HA	1:77:A:CYS:H	6	0.13
(1,457)	1:74:A:CYS:HB2	1:79:A:HIS:H	18	0.13
(1,437)	1:24:A:HIS:HB3	1:25:A:LYS:H	8	0.13
(1,437)	1:24:A:HIS:HB3	1:25:A:LYS:H	12	0.13
(1,437)	1:24:A:HIS:HB3	1:25:A:LYS:H	17	0.13
(1,428)	1:59:A:LYS:HE2	1:59:A:LYS:H	20	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,407)	1:76:A:ASP:HB2	1:76:A:ASP:H	7	0.13
(1,407)	1:76:A:ASP:HB2	1:76:A:ASP:H	9	0.13
(1,371)	1:22:A:GLN:HG3	1:21:A:ASN:H	5	0.13
(1,301)	1:69:A:LYS:HB2	1:70:A:VAL:H	15	0.13
(1,277)	1:54:A:GLU:HB3	1:54:A:GLU:H	2	0.13
(1,277)	1:54:A:GLU:HB3	1:54:A:GLU:H	14	0.13
(1,277)	1:54:A:GLU:HB3	1:54:A:GLU:H	16	0.13
(1,277)	1:54:A:GLU:HB3	1:54:A:GLU:H	20	0.13
(1,248)	1:97:A:LYS:HB3	1:97:A:LYS:H	2	0.13
(1,248)	1:97:A:LYS:HB3	1:97:A:LYS:H	7	0.13
(1,248)	1:97:A:LYS:HB3	1:97:A:LYS:H	16	0.13
(1,234)	1:39:A:MET:HB3	1:39:A:MET:H	18	0.13
(1,228)	1:86:A:LEU:HB2	1:87:A:ASP:H	2	0.13
(1,228)	1:86:A:LEU:HB2	1:87:A:ASP:H	16	0.13
(1,191)	1:93:A:LYS:HB2	1:94:A:CYS:H	10	0.13
(1,152)	1:45:A:VAL:HG12	1:44:A:PHE:H	2	0.13
(1,152)	1:45:A:VAL:HG12	1:44:A:PHE:H	8	0.13
(1,131)	1:10:A:LEU:HD23	1:11:A:ILE:H	9	0.13
(1,125)	1:43:A:LEU:HD13	1:43:A:LEU:H	18	0.13
(1,107)	1:56:A:LEU:HD21	1:56:A:LEU:H	4	0.13
(1,97)	1:11:A:ILE:HG23	1:12:A:ALA:H	10	0.13
(1,97)	1:11:A:ILE:HG21	1:12:A:ALA:H	13	0.13
(1,96)	1:11:A:ILE:HG21	1:15:A:GLU:H	18	0.13
(1,83)	1:112:A:LEU:HD22	1:112:A:LEU:H	18	0.13
(1,74)	1:99:A:VAL:HG23	1:73:A:GLU:H	6	0.13
(1,72)	1:31:A:VAL:HG13	1:108:A:ARG:H	1	0.13
(1,71)	1:31:A:VAL:HG12	1:32:A:GLY:H	16	0.13
(1,25)	1:90:A:VAL:HG21	1:91:A:CYS:H	1	0.13
(1,18)	1:72:A:LEU:HD21	1:72:A:LEU:H	2	0.13
(1,18)	1:72:A:LEU:HD22	1:72:A:LEU:H	18	0.13
(1,12)	1:72:A:LEU:HD13	1:72:A:LEU:H	5	0.13
(1,2661)	1:75:A:LYS:HA	1:75:A:LYS:HE3	4	0.12
(1,2655)	1:17:A:HIS:HB3	1:14:A:CYS:HA	4	0.12
(1,2647)	1:82:A:LYS:HE2	1:82:A:LYS:HB2	11	0.12
(1,2600)	1:66:A:VAL:HG12	1:66:A:VAL:HG11	7	0.12
(1,2600)	1:30:A:VAL:HG12	1:30:A:VAL:HG13	12	0.12
(1,2569)	1:92:A:GLU:HG2	1:92:A:GLU:HA	2	0.12
(1,2569)	1:92:A:GLU:HG2	1:92:A:GLU:HA	5	0.12
(1,2518)	1:19:A:LYS:HD2	1:19:A:LYS:HE3	3	0.12
(1,2518)	1:25:A:LYS:HD3	1:25:A:LYS:HE2	6	0.12
(1,2518)	1:25:A:LYS:HD3	1:25:A:LYS:HE2	10	0.12
(1,2518)	1:25:A:LYS:HD2	1:25:A:LYS:HE3	16	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2518)	1:19:A:LYS:HD2	1:19:A:LYS:HE3	17	0.12
(1,2518)	1:25:A:LYS:HD3	1:25:A:LYS:HE2	20	0.12
(1,2500)	1:97:A:LYS:HG2	1:97:A:LYS:HD2	3	0.12
(1,2487)	1:20:A:LYS:HG2	1:20:A:LYS:HD3	6	0.12
(1,2487)	1:20:A:LYS:HG2	1:20:A:LYS:HD3	7	0.12
(1,2487)	1:20:A:LYS:HG2	1:20:A:LYS:HD3	13	0.12
(1,2436)	1:110:A:LEU:HD12	1:66:A:VAL:HG21	9	0.12
(1,2417)	1:39:A:MET:H	1:40:A:ASP:H	13	0.12
(1,2417)	1:39:A:MET:H	1:40:A:ASP:H	20	0.12
(1,2401)	1:90:A:VAL:H	1:91:A:CYS:H	19	0.12
(1,2390)	1:79:A:HIS:H	1:77:A:CYS:H	20	0.12
(1,2386)	1:101:A:ILE:H	1:102:A:THR:H	3	0.12
(1,2369)	1:82:A:LYS:H	1:81:A:PHE:H	1	0.12
(1,2298)	1:71:A:GLU:H	1:70:A:VAL:H	3	0.12
(1,2298)	1:71:A:GLU:H	1:70:A:VAL:H	5	0.12
(1,2298)	1:71:A:GLU:H	1:70:A:VAL:H	10	0.12
(1,2250)	1:4:A:TYR:HA	1:4:A:TYR:HD1	3	0.12
(1,2225)	1:36:A:ARG:HD2	1:88:A:TYR:HD1	2	0.12
(1,2199)	1:7:A:VAL:HB	1:4:A:TYR:HD2	14	0.12
(1,2183)	1:116:A:ALA:HB3	1:24:A:HIS:HD2	1	0.12
(1,2183)	1:116:A:ALA:HB3	1:24:A:HIS:HD2	17	0.12
(1,2172)	1:47:A:ALA:HB1	1:4:A:TYR:HD2	16	0.12
(1,2166)	1:50:A:THR:HG21	1:51:A:PHE:HE1	4	0.12
(1,2148)	1:80:A:VAL:HG11	1:81:A:PHE:HD1	12	0.12
(1,2138)	1:65:A:ILE:HD13	1:44:A:PHE:HE1	11	0.12
(1,2138)	1:65:A:ILE:HD11	1:44:A:PHE:HE2	17	0.12
(1,2104)	1:82:A:LYS:HA	1:83:A:PRO:HG3	1	0.12
(1,2071)	1:26:A:ILE:HG23	1:29:A:VAL:HA	3	0.12
(1,2071)	1:26:A:ILE:HG22	1:29:A:VAL:HA	7	0.12
(1,2068)	1:30:A:VAL:HG12	1:29:A:VAL:HA	10	0.12
(1,2067)	1:10:A:LEU:HA	1:13:A:LEU:HG	9	0.12
(1,2061)	1:33:A:ILE:HA	1:65:A:ILE:HG22	12	0.12
(1,2061)	1:33:A:ILE:HA	1:65:A:ILE:HG23	17	0.12
(1,2058)	1:12:A:ALA:HB2	1:13:A:LEU:HA	4	0.12
(1,2053)	1:17:A:HIS:HA	1:16:A:GLU:HG2	18	0.12
(1,2049)	1:86:A:LEU:HA	1:85:A:ALA:HA	12	0.12
(1,1990)	1:17:A:HIS:HB3	1:14:A:CYS:HA	19	0.12
(1,1959)	1:113:A:GLU:HG3	1:28:A:ARG:HB3	9	0.12
(1,1944)	1:57:A:VAL:HB	1:26:A:ILE:HD13	8	0.12
(1,1944)	1:57:A:VAL:HB	1:26:A:ILE:HD12	13	0.12
(1,1936)	1:114:A:MET:HE2	1:114:A:MET:HB3	14	0.12
(1,1936)	1:114:A:MET:HE3	1:114:A:MET:HB3	15	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1897)	1:41:A:LYS:HD3	1:41:A:LYS:HA	2	0.12
(1,1880)	1:36:A:ARG:HA	1:36:A:ARG:HG3	2	0.12
(1,1832)	1:61:A:ALA:HB2	1:61:A:ALA:HB1	3	0.12
(1,1832)	1:61:A:ALA:HB1	1:61:A:ALA:HB3	8	0.12
(1,1819)	1:7:A:VAL:HG11	1:47:A:ALA:HB2	10	0.12
(1,1819)	1:7:A:VAL:HG11	1:47:A:ALA:HB3	13	0.12
(1,1819)	1:7:A:VAL:HG11	1:47:A:ALA:HB1	19	0.12
(1,1799)	1:29:A:VAL:HG13	1:109:A:LEU:HD13	1	0.12
(1,1796)	1:62:A:ILE:HD13	1:28:A:ARG:HA	8	0.12
(1,1787)	1:26:A:ILE:HG21	1:112:A:LEU:HA	16	0.12
(1,1786)	1:26:A:ILE:HG23	1:114:A:MET:HE1	15	0.12
(1,1774)	1:31:A:VAL:HG23	1:107:A:MET:HG2	15	0.12
(1,1771)	1:31:A:VAL:HG23	1:65:A:ILE:HB	18	0.12
(1,1765)	1:72:A:LEU:HB2	1:99:A:VAL:HB	1	0.12
(1,1727)	1:11:A:ILE:HD13	1:55:A:SER:HB3	1	0.12
(1,1727)	1:11:A:ILE:HD13	1:55:A:SER:HB3	2	0.12
(1,1725)	1:31:A:VAL:HG13	1:63:A:LEU:HD21	17	0.12
(1,1618)	1:50:A:THR:HG23	1:51:A:PHE:HA	7	0.12
(1,1583)	1:35:A:GLU:HG2	1:35:A:GLU:HA	3	0.12
(1,1583)	1:35:A:GLU:HG2	1:35:A:GLU:HA	19	0.12
(1,1576)	1:35:A:GLU:HG3	1:69:A:LYS:HA	12	0.12
(1,1576)	1:35:A:GLU:HG3	1:69:A:LYS:HA	14	0.12
(1,1567)	1:102:A:THR:HG22	1:102:A:THR:HA	2	0.12
(1,1567)	1:102:A:THR:HG23	1:102:A:THR:HA	20	0.12
(1,1548)	1:66:A:VAL:HG22	1:66:A:VAL:HA	16	0.12
(1,1548)	1:66:A:VAL:HG22	1:66:A:VAL:HA	18	0.12
(1,1541)	1:19:A:LYS:HB3	1:19:A:LYS:HA	6	0.12
(1,1534)	1:56:A:LEU:HB3	1:56:A:LEU:HA	9	0.12
(1,1534)	1:56:A:LEU:HB3	1:56:A:LEU:HA	14	0.12
(1,1534)	1:56:A:LEU:HB3	1:56:A:LEU:HA	16	0.12
(1,1534)	1:56:A:LEU:HB3	1:56:A:LEU:HA	17	0.12
(1,1507)	1:26:A:ILE:HD13	1:14:A:CYS:HA	14	0.12
(1,1477)	1:45:A:VAL:HG13	1:41:A:LYS:HA	7	0.12
(1,1428)	1:56:A:LEU:HD23	1:59:A:LYS:HE3	4	0.12
(1,1388)	1:11:A:ILE:HD12	1:51:A:PHE:HB3	4	0.12
(1,1384)	1:93:A:LYS:HE3	1:93:A:LYS:HA	3	0.12
(1,1384)	1:93:A:LYS:HE3	1:93:A:LYS:HA	20	0.12
(1,1374)	1:40:A:ASP:HB3	1:43:A:LEU:HD13	9	0.12
(1,1374)	1:40:A:ASP:HB3	1:43:A:LEU:HD11	17	0.12
(1,1331)	1:16:A:GLU:HB2	1:16:A:GLU:HG3	17	0.12
(1,1314)	1:53:A:GLU:HB2	1:53:A:GLU:HG2	2	0.12
(1,1314)	1:53:A:GLU:HB2	1:53:A:GLU:HG2	18	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1303)	1:23:A:ALA:HB3	1:114:A:MET:HB2	6	0.12
(1,1280)	1:39:A:MET:HB2	1:39:A:MET:HE3	17	0.12
(1,1279)	1:53:A:GLU:HB3	1:53:A:GLU:HG2	20	0.12
(1,1230)	1:54:A:GLU:HB3	1:54:A:GLU:HG2	2	0.12
(1,1230)	1:54:A:GLU:HB3	1:54:A:GLU:HG2	7	0.12
(1,1230)	1:54:A:GLU:HB3	1:54:A:GLU:HG2	18	0.12
(1,1230)	1:54:A:GLU:HB3	1:54:A:GLU:HG2	19	0.12
(1,1217)	1:72:A:LEU:HD11	1:99:A:VAL:HB	10	0.12
(1,1127)	1:10:A:LEU:HD11	1:10:A:LEU:HB3	4	0.12
(1,1127)	1:10:A:LEU:HD13	1:10:A:LEU:HB3	5	0.12
(1,1127)	1:10:A:LEU:HD12	1:10:A:LEU:HB3	10	0.12
(1,1058)	1:11:A:ILE:HG23	1:11:A:ILE:HG12	5	0.12
(1,1058)	1:11:A:ILE:HG22	1:11:A:ILE:HG12	17	0.12
(1,1024)	1:57:A:VAL:HG11	1:18:A:ALA:HB2	12	0.12
(1,1010)	1:115:A:LEU:HB3	1:25:A:LYS:HB3	8	0.12
(1,908)	1:56:A:LEU:HD11	1:57:A:VAL:HG22	14	0.12
(1,904)	1:31:A:VAL:HG11	1:10:A:LEU:HD13	13	0.12
(1,904)	1:31:A:VAL:HG12	1:10:A:LEU:HD13	16	0.12
(1,889)	1:57:A:VAL:HG12	1:15:A:GLU:HG3	16	0.12
(1,887)	1:57:A:VAL:HG12	1:18:A:ALA:HA	6	0.12
(1,887)	1:57:A:VAL:HG11	1:18:A:ALA:HA	12	0.12
(1,887)	1:57:A:VAL:HG11	1:18:A:ALA:HA	18	0.12
(1,874)	1:26:A:ILE:HG21	1:61:A:ALA:HB1	9	0.12
(1,864)	1:110:A:LEU:HD12	1:30:A:VAL:HG22	10	0.12
(1,864)	1:110:A:LEU:HD13	1:30:A:VAL:HG23	18	0.12
(1,862)	1:109:A:LEU:HD22	1:13:A:LEU:HD22	17	0.12
(1,834)	1:72:A:LEU:HD22	1:101:A:ILE:HG22	8	0.12
(1,833)	1:101:A:ILE:HG23	1:70:A:VAL:HG11	13	0.12
(1,832)	1:101:A:ILE:HG22	1:105:A:ASN:HB2	4	0.12
(1,784)	1:65:A:ILE:HD11	1:65:A:ILE:HD13	2	0.12
(1,784)	1:65:A:ILE:HD12	1:65:A:ILE:HD11	8	0.12
(1,784)	1:65:A:ILE:HD11	1:65:A:ILE:HD13	17	0.12
(1,780)	1:99:A:VAL:HG13	1:99:A:VAL:HG22	6	0.12
(1,776)	1:33:A:ILE:HG22	1:33:A:ILE:HG23	1	0.12
(1,776)	1:33:A:ILE:HG21	1:33:A:ILE:HG23	20	0.12
(1,771)	1:110:A:LEU:HD12	1:66:A:VAL:HG23	17	0.12
(1,769)	1:72:A:LEU:HD21	1:70:A:VAL:HG22	3	0.12
(1,769)	1:72:A:LEU:HD21	1:70:A:VAL:HG21	8	0.12
(1,768)	1:70:A:VAL:HG22	1:70:A:VAL:HG21	12	0.12
(1,768)	1:70:A:VAL:HG22	1:70:A:VAL:HG23	16	0.12
(1,767)	1:70:A:VAL:HG21	1:70:A:VAL:HG13	13	0.12
(1,758)	1:110:A:LEU:HD12	1:110:A:LEU:HD11	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,752)	1:65:A:ILE:HG21	1:65:A:ILE:HG13	2	0.12
(1,752)	1:65:A:ILE:HG22	1:65:A:ILE:HG13	6	0.12
(1,752)	1:65:A:ILE:HG21	1:65:A:ILE:HG13	9	0.12
(1,752)	1:65:A:ILE:HG21	1:65:A:ILE:HG13	13	0.12
(1,752)	1:65:A:ILE:HG23	1:65:A:ILE:HG13	20	0.12
(1,744)	1:72:A:LEU:HD11	1:72:A:LEU:HD22	2	0.12
(1,744)	1:72:A:LEU:HD12	1:72:A:LEU:HD21	16	0.12
(1,744)	1:72:A:LEU:HD13	1:72:A:LEU:HD21	17	0.12
(1,744)	1:72:A:LEU:HD12	1:72:A:LEU:HD23	18	0.12
(1,737)	1:7:A:VAL:HG12	1:7:A:VAL:HG13	9	0.12
(1,737)	1:7:A:VAL:HG11	1:7:A:VAL:HG13	13	0.12
(1,710)	1:72:A:LEU:HA	1:103:A:GLN:H	18	0.12
(1,690)	1:76:A:ASP:HA	1:77:A:CYS:H	9	0.12
(1,558)	1:12:A:ALA:HA	1:16:A:GLU:H	15	0.12
(1,476)	1:111:A:SER:HB3	1:112:A:LEU:H	2	0.12
(1,440)	1:79:A:HIS:HB3	1:80:A:VAL:H	17	0.12
(1,437)	1:24:A:HIS:HB3	1:25:A:LYS:H	4	0.12
(1,344)	1:113:A:GLU:HG3	1:113:A:GLU:H	5	0.12
(1,344)	1:113:A:GLU:HG3	1:113:A:GLU:H	9	0.12
(1,301)	1:69:A:LYS:HB2	1:70:A:VAL:H	7	0.12
(1,301)	1:69:A:LYS:HB2	1:70:A:VAL:H	10	0.12
(1,301)	1:69:A:LYS:HB2	1:70:A:VAL:H	18	0.12
(1,277)	1:54:A:GLU:HB3	1:54:A:GLU:H	5	0.12
(1,277)	1:54:A:GLU:HB3	1:54:A:GLU:H	18	0.12
(1,248)	1:97:A:LYS:HB3	1:97:A:LYS:H	12	0.12
(1,242)	1:19:A:LYS:HD2	1:19:A:LYS:H	11	0.12
(1,234)	1:39:A:MET:HB3	1:39:A:MET:H	1	0.12
(1,203)	1:20:A:LYS:HG2	1:20:A:LYS:H	7	0.12
(1,191)	1:93:A:LYS:HB2	1:94:A:CYS:H	1	0.12
(1,138)	1:102:A:THR:HG21	1:103:A:GLN:H	14	0.12
(1,125)	1:43:A:LEU:HD13	1:43:A:LEU:H	5	0.12
(1,125)	1:43:A:LEU:HD12	1:43:A:LEU:H	16	0.12
(1,111)	1:10:A:LEU:HD13	1:13:A:LEU:H	9	0.12
(1,107)	1:56:A:LEU:HD21	1:56:A:LEU:H	12	0.12
(1,97)	1:11:A:ILE:HG23	1:12:A:ALA:H	4	0.12
(1,97)	1:11:A:ILE:HG22	1:12:A:ALA:H	19	0.12
(1,96)	1:11:A:ILE:HG23	1:15:A:GLU:H	4	0.12
(1,82)	1:109:A:LEU:HD21	1:30:A:VAL:H	17	0.12
(1,77)	1:109:A:LEU:HD22	1:109:A:LEU:H	9	0.12
(1,74)	1:99:A:VAL:HG22	1:73:A:GLU:H	1	0.12
(1,71)	1:31:A:VAL:HG13	1:32:A:GLY:H	8	0.12
(1,71)	1:31:A:VAL:HG13	1:32:A:GLY:H	11	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,69)	1:93:A:LYS:HG2	1:93:A:LYS:H	6	0.12
(1,42)	1:109:A:LEU:HD12	1:109:A:LEU:H	1	0.12
(1,29)	1:70:A:VAL:HG22	1:72:A:LEU:H	8	0.12
(1,25)	1:90:A:VAL:HG23	1:91:A:CYS:H	4	0.12
(1,12)	1:72:A:LEU:HD12	1:72:A:LEU:H	9	0.12
(1,2666)	1:7:A:VAL:HG12	1:51:A:PHE:HE1	12	0.11
(1,2661)	1:75:A:LYS:HA	1:75:A:LYS:HE3	8	0.11
(1,2655)	1:17:A:HIS:HB3	1:14:A:CYS:HA	13	0.11
(1,2653)	1:41:A:LYS:HD3	1:41:A:LYS:HA	5	0.11
(1,2647)	1:82:A:LYS:HE2	1:82:A:LYS:HB2	14	0.11
(1,2620)	1:25:A:LYS:HG2	1:56:A:LEU:HD13	20	0.11
(1,2600)	1:30:A:VAL:HG12	1:30:A:VAL:HG11	6	0.11
(1,2600)	1:30:A:VAL:HG12	1:30:A:VAL:HG13	9	0.11
(1,2600)	1:30:A:VAL:HG11	1:30:A:VAL:HG13	11	0.11
(1,2600)	1:30:A:VAL:HG12	1:30:A:VAL:HG13	13	0.11
(1,2600)	1:30:A:VAL:HG12	1:30:A:VAL:HG11	15	0.11
(1,2577)	1:54:A:GLU:HG2	1:54:A:GLU:HA	1	0.11
(1,2577)	1:54:A:GLU:HG2	1:54:A:GLU:HA	18	0.11
(1,2569)	1:92:A:GLU:HG2	1:92:A:GLU:HA	13	0.11
(1,2518)	1:25:A:LYS:HD2	1:25:A:LYS:HE3	7	0.11
(1,2518)	1:25:A:LYS:HD3	1:25:A:LYS:HE2	15	0.11
(1,2513)	1:59:A:LYS:HD3	1:59:A:LYS:HB3	19	0.11
(1,2500)	1:19:A:LYS:HG2	1:19:A:LYS:HD2	4	0.11
(1,2458)	1:115:A:LEU:HD22	1:27:A:GLU:HG3	13	0.11
(1,2438)	1:65:A:ILE:HD11	1:41:A:LYS:HD2	7	0.11
(1,2417)	1:39:A:MET:H	1:40:A:ASP:H	6	0.11
(1,2417)	1:39:A:MET:H	1:40:A:ASP:H	8	0.11
(1,2413)	1:100:A:ILE:H	1:75:A:LYS:H	10	0.11
(1,2401)	1:90:A:VAL:H	1:91:A:CYS:H	11	0.11
(1,2397)	1:100:A:ILE:H	1:74:A:CYS:H	6	0.11
(1,2397)	1:100:A:ILE:H	1:74:A:CYS:H	14	0.11
(1,2386)	1:101:A:ILE:H	1:102:A:THR:H	14	0.11
(1,2386)	1:101:A:ILE:H	1:102:A:THR:H	20	0.11
(1,2369)	1:82:A:LYS:H	1:81:A:PHE:H	3	0.11
(1,2369)	1:82:A:LYS:H	1:81:A:PHE:H	18	0.11
(1,2311)	1:87:A:ASP:H	1:88:A:TYR:H	20	0.11
(1,2298)	1:71:A:GLU:H	1:70:A:VAL:H	4	0.11
(1,2298)	1:71:A:GLU:H	1:70:A:VAL:H	6	0.11
(1,2239)	1:41:A:LYS:HA	1:44:A:PHE:HD2	20	0.11
(1,2180)	1:61:A:ALA:HB2	1:48:A:PHE:HD2	5	0.11
(1,2166)	1:50:A:THR:HG21	1:51:A:PHE:HE1	7	0.11
(1,2138)	1:65:A:ILE:HD11	1:44:A:PHE:HE2	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2100)	1:97:A:LYS:HA	1:97:A:LYS:HE2	12	0.11
(1,2067)	1:10:A:LEU:HA	1:13:A:LEU:HG	20	0.11
(1,2058)	1:12:A:ALA:HB3	1:13:A:LEU:HA	14	0.11
(1,2053)	1:17:A:HIS:HA	1:16:A:GLU:HG2	9	0.11
(1,2040)	1:90:A:VAL:HG23	1:92:A:GLU:HA	10	0.11
(1,2039)	1:26:A:ILE:HG21	1:61:A:ALA:HA	5	0.11
(1,2039)	1:26:A:ILE:HG21	1:61:A:ALA:HA	8	0.11
(1,2030)	1:83:A:PRO:HD2	1:72:A:LEU:HD13	11	0.11
(1,2024)	1:107:A:MET:HE1	1:7:A:VAL:HA	7	0.11
(1,1990)	1:17:A:HIS:HB3	1:14:A:CYS:HA	10	0.11
(1,1990)	1:17:A:HIS:HB3	1:14:A:CYS:HA	20	0.11
(1,1982)	1:106:A:GLU:HG3	1:105:A:ASN:HB3	8	0.11
(1,1944)	1:57:A:VAL:HB	1:26:A:ILE:HD11	15	0.11
(1,1901)	1:57:A:VAL:HG23	1:56:A:LEU:HB3	10	0.11
(1,1887)	1:82:A:LYS:HD2	1:71:A:GLU:HB3	14	0.11
(1,1832)	1:61:A:ALA:HB2	1:61:A:ALA:HB1	13	0.11
(1,1802)	1:29:A:VAL:HG22	1:29:A:VAL:HG13	17	0.11
(1,1798)	1:62:A:ILE:HD13	1:28:A:ARG:HD3	15	0.11
(1,1787)	1:26:A:ILE:HG21	1:112:A:LEU:HA	12	0.11
(1,1782)	1:109:A:LEU:HD23	1:107:A:MET:HE1	18	0.11
(1,1777)	1:112:A:LEU:HD21	1:109:A:LEU:HD12	4	0.11
(1,1735)	1:72:A:LEU:HD21	1:88:A:TYR:HB3	12	0.11
(1,1735)	1:72:A:LEU:HD23	1:88:A:TYR:HB3	18	0.11
(1,1731)	1:72:A:LEU:HD11	1:91:A:CYS:HA	7	0.11
(1,1731)	1:72:A:LEU:HD13	1:91:A:CYS:HA	15	0.11
(1,1727)	1:11:A:ILE:HD11	1:55:A:SER:HB2	8	0.11
(1,1687)	1:31:A:VAL:HA	1:110:A:LEU:HD12	5	0.11
(1,1687)	1:31:A:VAL:HA	1:110:A:LEU:HD11	11	0.11
(1,1645)	1:72:A:LEU:HD13	1:88:A:TYR:HA	2	0.11
(1,1583)	1:35:A:GLU:HG2	1:35:A:GLU:HA	9	0.11
(1,1570)	1:102:A:THR:HA	1:101:A:ILE:HG21	5	0.11
(1,1559)	1:12:A:ALA:HB3	1:12:A:ALA:HA	7	0.11
(1,1559)	1:12:A:ALA:HB3	1:12:A:ALA:HA	12	0.11
(1,1559)	1:12:A:ALA:HB3	1:12:A:ALA:HA	20	0.11
(1,1558)	1:86:A:LEU:HD21	1:86:A:LEU:HA	5	0.11
(1,1541)	1:19:A:LYS:HB3	1:19:A:LYS:HA	3	0.11
(1,1541)	1:19:A:LYS:HB3	1:19:A:LYS:HA	13	0.11
(1,1541)	1:19:A:LYS:HB3	1:19:A:LYS:HA	16	0.11
(1,1541)	1:19:A:LYS:HB3	1:19:A:LYS:HA	18	0.11
(1,1534)	1:56:A:LEU:HB3	1:56:A:LEU:HA	7	0.11
(1,1528)	1:50:A:THR:HB	1:50:A:THR:HA	4	0.11
(1,1507)	1:26:A:ILE:HD12	1:14:A:CYS:HA	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1491)	1:6:A:VAL:HG11	1:6:A:VAL:HA	2	0.11
(1,1491)	1:6:A:VAL:HG13	1:6:A:VAL:HA	5	0.11
(1,1491)	1:6:A:VAL:HG13	1:6:A:VAL:HA	8	0.11
(1,1491)	1:6:A:VAL:HG11	1:6:A:VAL:HA	12	0.11
(1,1490)	1:6:A:VAL:HA	1:9:A:SER:HB3	17	0.11
(1,1471)	1:49:A:GLU:HG3	1:49:A:GLU:HA	13	0.11
(1,1452)	1:63:A:LEU:HD12	1:45:A:VAL:HA	7	0.11
(1,1442)	1:79:A:HIS:HB3	1:79:A:HIS:HB2	17	0.11
(1,1405)	1:3:A:GLU:HG3	1:3:A:GLU:HG2	6	0.11
(1,1405)	1:3:A:GLU:HG3	1:3:A:GLU:HG2	9	0.11
(1,1388)	1:11:A:ILE:HD11	1:51:A:PHE:HB3	2	0.11
(1,1332)	1:16:A:GLU:HB3	1:16:A:GLU:HG2	9	0.11
(1,1332)	1:16:A:GLU:HB3	1:16:A:GLU:HG2	15	0.11
(1,1332)	1:16:A:GLU:HB3	1:16:A:GLU:HG2	16	0.11
(1,1332)	1:16:A:GLU:HB3	1:16:A:GLU:HG2	19	0.11
(1,1331)	1:16:A:GLU:HB2	1:16:A:GLU:HG3	7	0.11
(1,1331)	1:16:A:GLU:HB2	1:16:A:GLU:HG3	10	0.11
(1,1331)	1:16:A:GLU:HB2	1:16:A:GLU:HG3	11	0.11
(1,1303)	1:23:A:ALA:HB1	1:114:A:MET:HB2	13	0.11
(1,1283)	1:15:A:GLU:HB3	1:12:A:ALA:HA	16	0.11
(1,1273)	1:114:A:MET:HE3	1:112:A:LEU:HB3	19	0.11
(1,1251)	1:75:A:LYS:HB3	1:75:A:LYS:HB2	4	0.11
(1,1230)	1:54:A:GLU:HB3	1:54:A:GLU:HG2	11	0.11
(1,1230)	1:54:A:GLU:HB3	1:54:A:GLU:HG2	12	0.11
(1,1211)	1:75:A:LYS:HB3	1:98:A:ASN:HB2	3	0.11
(1,1145)	1:41:A:LYS:HD2	1:33:A:ILE:HG22	17	0.11
(1,1127)	1:10:A:LEU:HD13	1:10:A:LEU:HB3	2	0.11
(1,1127)	1:10:A:LEU:HD11	1:10:A:LEU:HB3	13	0.11
(1,1127)	1:10:A:LEU:HD11	1:10:A:LEU:HB3	16	0.11
(1,1127)	1:10:A:LEU:HD11	1:10:A:LEU:HB3	17	0.11
(1,1097)	1:86:A:LEU:HD22	1:86:A:LEU:HG	15	0.11
(1,1058)	1:11:A:ILE:HG22	1:11:A:ILE:HG12	12	0.11
(1,1058)	1:11:A:ILE:HG23	1:11:A:ILE:HG12	18	0.11
(1,1010)	1:115:A:LEU:HB3	1:25:A:LYS:HB3	9	0.11
(1,940)	1:112:A:LEU:HD12	1:112:A:LEU:HA	10	0.11
(1,934)	1:102:A:THR:HG23	1:100:A:ILE:HB	8	0.11
(1,898)	1:29:A:VAL:HG13	1:112:A:LEU:HA	6	0.11
(1,879)	1:93:A:LYS:HB3	1:93:A:LYS:HD3	13	0.11
(1,869)	1:26:A:ILE:HD13	1:61:A:ALA:HB2	11	0.11
(1,864)	1:110:A:LEU:HD13	1:30:A:VAL:HG23	12	0.11
(1,849)	1:72:A:LEU:HD23	1:101:A:ILE:HG13	11	0.11
(1,834)	1:72:A:LEU:HD23	1:101:A:ILE:HG22	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,822)	1:80:A:VAL:HG11	1:102:A:THR:HG23	6	0.11
(1,794)	1:109:A:LEU:HD13	1:109:A:LEU:HD23	19	0.11
(1,787)	1:63:A:LEU:HD11	1:65:A:ILE:HD12	13	0.11
(1,787)	1:63:A:LEU:HD13	1:65:A:ILE:HD12	15	0.11
(1,784)	1:65:A:ILE:HD12	1:65:A:ILE:HD13	9	0.11
(1,784)	1:65:A:ILE:HD11	1:65:A:ILE:HD13	11	0.11
(1,784)	1:65:A:ILE:HD12	1:65:A:ILE:HD13	15	0.11
(1,776)	1:33:A:ILE:HG22	1:33:A:ILE:HG21	10	0.11
(1,776)	1:33:A:ILE:HG21	1:33:A:ILE:HG23	19	0.11
(1,771)	1:110:A:LEU:HD11	1:66:A:VAL:HG22	11	0.11
(1,769)	1:72:A:LEU:HD21	1:70:A:VAL:HG23	17	0.11
(1,768)	1:70:A:VAL:HG22	1:70:A:VAL:HG23	3	0.11
(1,767)	1:70:A:VAL:HG22	1:70:A:VAL:HG13	5	0.11
(1,767)	1:70:A:VAL:HG23	1:70:A:VAL:HG12	12	0.11
(1,767)	1:70:A:VAL:HG22	1:70:A:VAL:HG11	15	0.11
(1,759)	1:110:A:LEU:HD13	1:110:A:LEU:HD22	7	0.11
(1,759)	1:110:A:LEU:HD13	1:110:A:LEU:HD21	14	0.11
(1,752)	1:65:A:ILE:HG21	1:65:A:ILE:HG13	5	0.11
(1,752)	1:65:A:ILE:HG22	1:65:A:ILE:HG13	16	0.11
(1,752)	1:65:A:ILE:HG23	1:65:A:ILE:HG13	19	0.11
(1,746)	1:72:A:LEU:HD13	1:83:A:PRO:HB2	5	0.11
(1,746)	1:72:A:LEU:HD13	1:83:A:PRO:HB2	6	0.11
(1,690)	1:76:A:ASP:HA	1:77:A:CYS:H	7	0.11
(1,684)	1:98:A:ASN:HA	1:99:A:VAL:H	10	0.11
(1,560)	1:13:A:LEU:HA	1:17:A:HIS:H	15	0.11
(1,448)	1:79:A:HIS:HB2	1:80:A:VAL:H	6	0.11
(1,437)	1:24:A:HIS:HB3	1:25:A:LYS:H	7	0.11
(1,407)	1:76:A:ASP:HB2	1:76:A:ASP:H	2	0.11
(1,398)	1:15:A:GLU:HG2	1:15:A:GLU:H	2	0.11
(1,398)	1:15:A:GLU:HG2	1:15:A:GLU:H	11	0.11
(1,396)	1:76:A:ASP:HB3	1:76:A:ASP:H	12	0.11
(1,344)	1:113:A:GLU:HG3	1:113:A:GLU:H	4	0.11
(1,344)	1:113:A:GLU:HG3	1:113:A:GLU:H	7	0.11
(1,344)	1:113:A:GLU:HG3	1:113:A:GLU:H	14	0.11
(1,301)	1:69:A:LYS:HB2	1:70:A:VAL:H	11	0.11
(1,248)	1:97:A:LYS:HB3	1:97:A:LYS:H	5	0.11
(1,248)	1:97:A:LYS:HB3	1:97:A:LYS:H	6	0.11
(1,214)	1:36:A:ARG:HB3	1:36:A:ARG:H	2	0.11
(1,214)	1:36:A:ARG:HB3	1:36:A:ARG:H	7	0.11
(1,214)	1:36:A:ARG:HB3	1:36:A:ARG:H	15	0.11
(1,203)	1:20:A:LYS:HG2	1:20:A:LYS:H	4	0.11
(1,199)	1:12:A:ALA:HB2	1:12:A:ALA:H	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,191)	1:93:A:LYS:HB2	1:94:A:CYS:H	2	0.11
(1,191)	1:93:A:LYS:HB2	1:94:A:CYS:H	5	0.11
(1,156)	1:23:A:ALA:HB2	1:21:A:ASN:H	3	0.11
(1,156)	1:23:A:ALA:HB1	1:21:A:ASN:H	8	0.11
(1,152)	1:45:A:VAL:HG13	1:44:A:PHE:H	7	0.11
(1,152)	1:45:A:VAL:HG11	1:44:A:PHE:H	13	0.11
(1,152)	1:45:A:VAL:HG12	1:44:A:PHE:H	16	0.11
(1,142)	1:47:A:ALA:HB2	1:46:A:SER:H	4	0.11
(1,142)	1:47:A:ALA:HB2	1:46:A:SER:H	16	0.11
(1,138)	1:102:A:THR:HG23	1:103:A:GLN:H	1	0.11
(1,131)	1:10:A:LEU:HD23	1:11:A:ILE:H	16	0.11
(1,125)	1:43:A:LEU:HD11	1:43:A:LEU:H	12	0.11
(1,112)	1:10:A:LEU:HD12	1:11:A:ILE:H	8	0.11
(1,111)	1:10:A:LEU:HD11	1:13:A:LEU:H	12	0.11
(1,108)	1:115:A:LEU:HD23	1:116:A:ALA:H	6	0.11
(1,107)	1:56:A:LEU:HD22	1:56:A:LEU:H	20	0.11
(1,77)	1:109:A:LEU:HD22	1:109:A:LEU:H	12	0.11
(1,71)	1:31:A:VAL:HG11	1:32:A:GLY:H	5	0.11
(1,71)	1:31:A:VAL:HG11	1:32:A:GLY:H	7	0.11
(1,71)	1:31:A:VAL:HG11	1:32:A:GLY:H	15	0.11
(1,42)	1:109:A:LEU:HD13	1:109:A:LEU:H	4	0.11
(1,39)	1:90:A:VAL:HG11	1:90:A:VAL:H	6	0.11
(1,34)	1:33:A:ILE:HG22	1:39:A:MET:H	19	0.11
(1,33)	1:33:A:ILE:HG23	1:37:A:SER:H	19	0.11
(1,18)	1:72:A:LEU:HD22	1:72:A:LEU:H	12	0.11
(1,18)	1:72:A:LEU:HD23	1:72:A:LEU:H	15	0.11
(1,2673)	1:43:A:LEU:HD11	1:4:A:TYR:HE1	2	0.1
(1,2673)	1:13:A:LEU:HD11	1:17:A:HIS:HD2	11	0.1
(1,2622)	1:38:A:ALA:HB1	1:1:A:MET:HB2	3	0.1
(1,2620)	1:25:A:LYS:HG2	1:56:A:LEU:HD12	7	0.1
(1,2600)	1:30:A:VAL:HG11	1:30:A:VAL:HG13	4	0.1
(1,2513)	1:59:A:LYS:HD3	1:59:A:LYS:HB3	7	0.1
(1,2500)	1:97:A:LYS:HG2	1:97:A:LYS:HD2	13	0.1
(1,2487)	1:82:A:LYS:HG2	1:82:A:LYS:HD3	2	0.1
(1,2487)	1:20:A:LYS:HG2	1:20:A:LYS:HD3	9	0.1
(1,2454)	1:62:A:ILE:HG21	1:28:A:ARG:HG3	5	0.1
(1,2397)	1:100:A:ILE:H	1:74:A:CYS:H	2	0.1
(1,2397)	1:100:A:ILE:H	1:74:A:CYS:H	3	0.1
(1,2386)	1:101:A:ILE:H	1:102:A:THR:H	16	0.1
(1,2369)	1:82:A:LYS:H	1:81:A:PHE:H	4	0.1
(1,2298)	1:71:A:GLU:H	1:70:A:VAL:H	16	0.1
(1,2250)	1:4:A:TYR:HA	1:4:A:TYR:HD1	4	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2239)	1:41:A:LYS:HA	1:44:A:PHE:HD2	1	0.1
(1,2175)	1:6:A:VAL:HG12	1:44:A:PHE:HZ	9	0.1
(1,2172)	1:47:A:ALA:HB1	1:4:A:TYR:HD1	6	0.1
(1,2172)	1:47:A:ALA:HB2	1:4:A:TYR:HD1	10	0.1
(1,2167)	1:50:A:THR:HG22	1:4:A:TYR:HD2	19	0.1
(1,2138)	1:65:A:ILE:HD11	1:44:A:PHE:HE2	4	0.1
(1,2134)	1:72:A:LEU:HD23	1:81:A:PHE:HE1	12	0.1
(1,2130)	1:72:A:LEU:HD13	1:81:A:PHE:HE2	1	0.1
(1,2130)	1:72:A:LEU:HD13	1:81:A:PHE:HE2	5	0.1
(1,2104)	1:82:A:LYS:HA	1:83:A:PRO:HG3	2	0.1
(1,2104)	1:82:A:LYS:HA	1:83:A:PRO:HG3	20	0.1
(1,2068)	1:30:A:VAL:HG12	1:29:A:VAL:HA	19	0.1
(1,2017)	1:79:A:HIS:HB2	1:93:A:LYS:HB2	12	0.1
(1,1960)	1:113:A:GLU:HG3	1:27:A:GLU:HB3	5	0.1
(1,1832)	1:61:A:ALA:HB2	1:61:A:ALA:HB1	11	0.1
(1,1824)	1:25:A:LYS:HG3	1:56:A:LEU:HD11	19	0.1
(1,1777)	1:112:A:LEU:HD21	1:109:A:LEU:HD13	16	0.1
(1,1771)	1:31:A:VAL:HG22	1:65:A:ILE:HB	10	0.1
(1,1761)	1:110:A:LEU:HD23	1:108:A:ARG:HD2	7	0.1
(1,1749)	1:65:A:ILE:HG13	1:63:A:LEU:HD22	20	0.1
(1,1698)	1:80:A:VAL:HG11	1:73:A:GLU:HA	1	0.1
(1,1698)	1:80:A:VAL:HG13	1:73:A:GLU:HA	4	0.1
(1,1567)	1:102:A:THR:HG22	1:102:A:THR:HA	7	0.1
(1,1534)	1:56:A:LEU:HB3	1:56:A:LEU:HA	11	0.1
(1,1528)	1:50:A:THR:HB	1:50:A:THR:HA	19	0.1
(1,1477)	1:45:A:VAL:HG12	1:41:A:LYS:HA	11	0.1
(1,1384)	1:93:A:LYS:HE3	1:93:A:LYS:HA	5	0.1
(1,1361)	1:26:A:ILE:HD11	1:114:A:MET:HG2	4	0.1
(1,1361)	1:26:A:ILE:HD13	1:114:A:MET:HG2	5	0.1
(1,1361)	1:26:A:ILE:HD12	1:114:A:MET:HG2	17	0.1
(1,1332)	1:16:A:GLU:HB3	1:16:A:GLU:HG2	12	0.1
(1,1332)	1:16:A:GLU:HB3	1:16:A:GLU:HG2	17	0.1
(1,1251)	1:75:A:LYS:HB3	1:75:A:LYS:HB2	5	0.1
(1,1251)	1:75:A:LYS:HB3	1:75:A:LYS:HB2	18	0.1
(1,1249)	1:72:A:LEU:HD11	1:83:A:PRO:HG2	15	0.1
(1,1230)	1:54:A:GLU:HB3	1:54:A:GLU:HG2	16	0.1
(1,1230)	1:54:A:GLU:HB3	1:54:A:GLU:HG2	20	0.1
(1,1159)	1:108:A:ARG:HB2	1:110:A:LEU:HD21	9	0.1
(1,1145)	1:41:A:LYS:HD2	1:33:A:ILE:HG23	15	0.1
(1,1145)	1:41:A:LYS:HD2	1:33:A:ILE:HG21	19	0.1
(1,934)	1:102:A:THR:HG22	1:100:A:ILE:HB	2	0.1
(1,893)	1:43:A:LEU:HD22	1:40:A:ASP:HB3	19	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,857)	1:109:A:LEU:HD21	1:112:A:LEU:HD12	18	0.1
(1,821)	1:30:A:VAL:HG12	1:28:A:ARG:HG3	2	0.1
(1,780)	1:99:A:VAL:HG13	1:99:A:VAL:HG21	7	0.1
(1,776)	1:33:A:ILE:HG21	1:33:A:ILE:HG23	13	0.1
(1,771)	1:110:A:LEU:HD11	1:66:A:VAL:HG21	8	0.1
(1,752)	1:65:A:ILE:HG22	1:65:A:ILE:HG13	15	0.1
(1,746)	1:72:A:LEU:HD11	1:83:A:PRO:HB2	12	0.1
(1,744)	1:72:A:LEU:HD12	1:72:A:LEU:HD21	1	0.1
(1,737)	1:7:A:VAL:HG12	1:7:A:VAL:HG13	1	0.1
(1,737)	1:7:A:VAL:HG12	1:7:A:VAL:HG11	5	0.1
(1,737)	1:7:A:VAL:HG11	1:7:A:VAL:HG13	7	0.1
(1,737)	1:7:A:VAL:HG12	1:7:A:VAL:HG13	8	0.1
(1,737)	1:7:A:VAL:HG12	1:7:A:VAL:HG11	11	0.1
(1,737)	1:7:A:VAL:HG11	1:7:A:VAL:HG13	20	0.1
(1,727)	1:33:A:ILE:HD11	1:33:A:ILE:HD13	10	0.1
(1,415)	1:20:A:LYS:HE3	1:20:A:LYS:H	6	0.1
(1,408)	1:76:A:ASP:HB2	1:77:A:CYS:H	12	0.1
(1,407)	1:76:A:ASP:HB2	1:76:A:ASP:H	6	0.1
(1,398)	1:15:A:GLU:HG2	1:15:A:GLU:H	12	0.1
(1,358)	1:22:A:GLN:HB2	1:23:A:ALA:H	17	0.1
(1,277)	1:54:A:GLU:HB3	1:54:A:GLU:H	3	0.1
(1,203)	1:20:A:LYS:HG2	1:20:A:LYS:H	1	0.1
(1,191)	1:93:A:LYS:HB2	1:94:A:CYS:H	11	0.1
(1,191)	1:93:A:LYS:HB2	1:94:A:CYS:H	13	0.1
(1,191)	1:93:A:LYS:HB2	1:94:A:CYS:H	20	0.1
(1,152)	1:45:A:VAL:HG13	1:44:A:PHE:H	15	0.1
(1,142)	1:47:A:ALA:HB2	1:46:A:SER:H	13	0.1
(1,107)	1:56:A:LEU:HD23	1:56:A:LEU:H	19	0.1
(1,71)	1:31:A:VAL:HG12	1:32:A:GLY:H	4	0.1
(1,4)	1:33:A:ILE:HD13	1:33:A:ILE:H	20	0.1

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

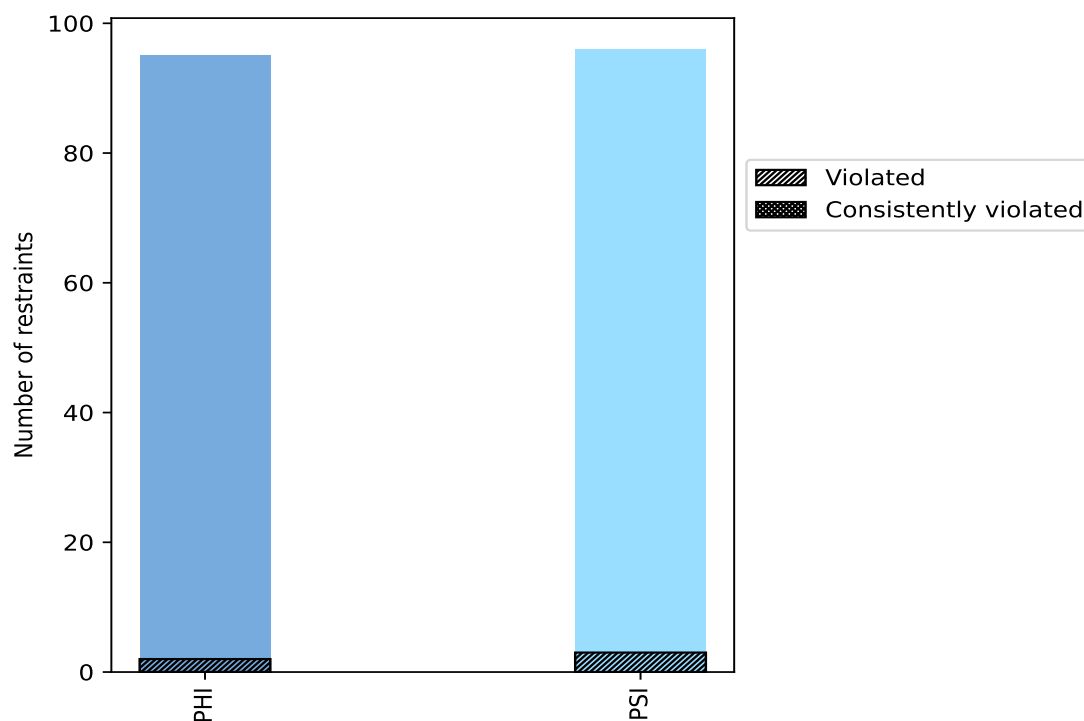
10.1 Summary of dihedral-angle violations [i](#)

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

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PHI	95	49.7	2	2.1	1.0	0	0.0	0.0
PSI	96	50.3	3	3.1	1.6	0	0.0	0.0
Total	191	100.0	5	2.6	2.6	0	0.0	0.0

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

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



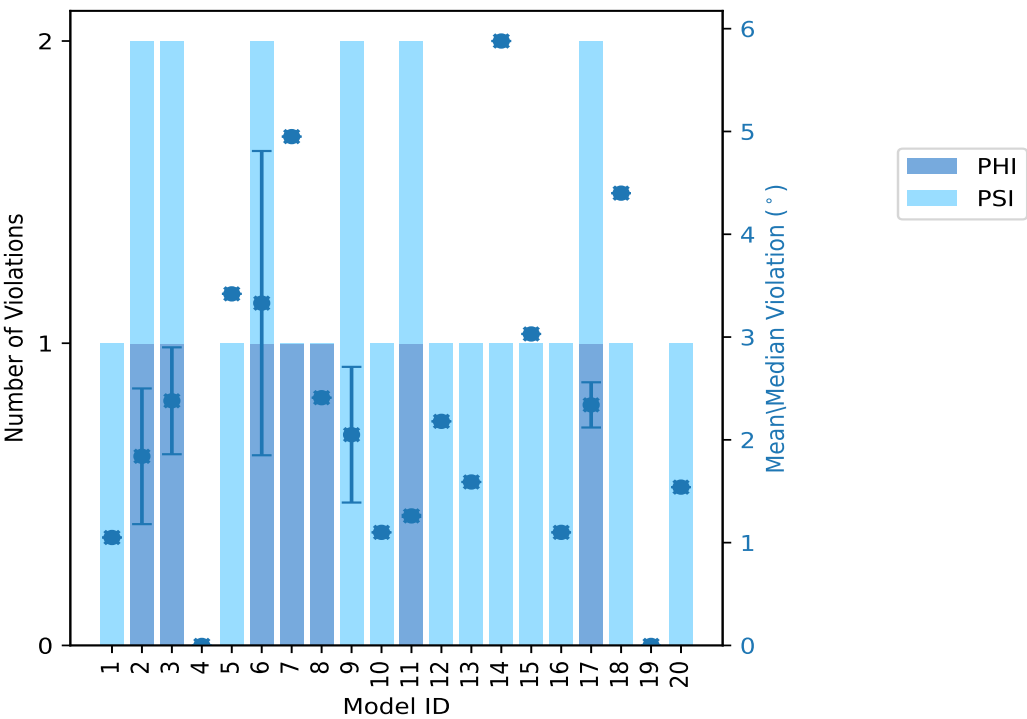
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	0	1	1	1.05	1.05	0.0	1.05
2	1	1	2	1.84	2.49	0.66	1.84
3	1	1	2	2.38	2.9	0.52	2.38
4	0	0	0	0.0	0.0	0.0	0.0
5	0	1	1	3.42	3.42	0.0	3.42
6	1	1	2	3.33	4.81	1.48	3.33
7	1	0	1	4.95	4.95	0.0	4.95
8	1	0	1	2.41	2.41	0.0	2.41
9	0	2	2	2.05	2.71	0.66	2.05
10	0	1	1	1.1	1.1	0.0	1.1
11	1	1	2	1.26	1.27	0.01	1.26
12	0	1	1	2.18	2.18	0.0	2.18
13	0	1	1	1.59	1.59	0.0	1.59
14	0	1	1	5.88	5.88	0.0	5.88
15	0	1	1	3.03	3.03	0.0	3.03
16	0	1	1	1.1	1.1	0.0	1.1
17	1	1	2	2.34	2.57	0.22	2.34
18	0	1	1	4.4	4.4	0.0	4.4
19	0	0	0	0.0	0.0	0.0	0.0
20	0	1	1	1.54	1.54	0.0	1.54

10.2.1 Bar graph : Dihedral violation statistics for each model ⓘ



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

10.3 Dihedral-angle violation statistics for the ensemble ⓘ

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

Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
1	2	3	1	5.0
0	0	0	2	10.0
0	0	0	3	15.0
0	0	0	4	20.0
0	0	0	5	25.0
1	0	1	6	30.0
0	0	0	7	35.0
0	0	0	8	40.0
0	0	0	9	45.0
0	0	0	10	50.0
0	0	0	11	55.0

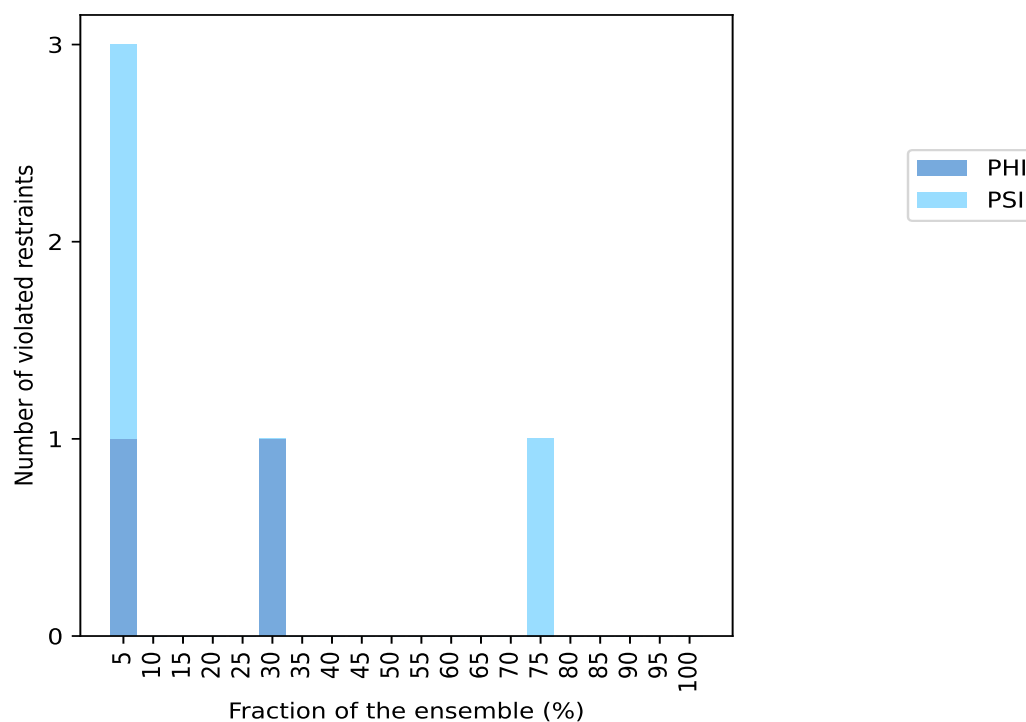
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Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
0	0	0	12	60.0
0	0	0	13	65.0
0	0	0	14	70.0
0	1	1	15	75.0
0	0	0	16	80.0
0	0	0	17	85.0
0	0	0	18	90.0
0	0	0	19	95.0
0	0	0	20	100.0

¹ Number of models with violations

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

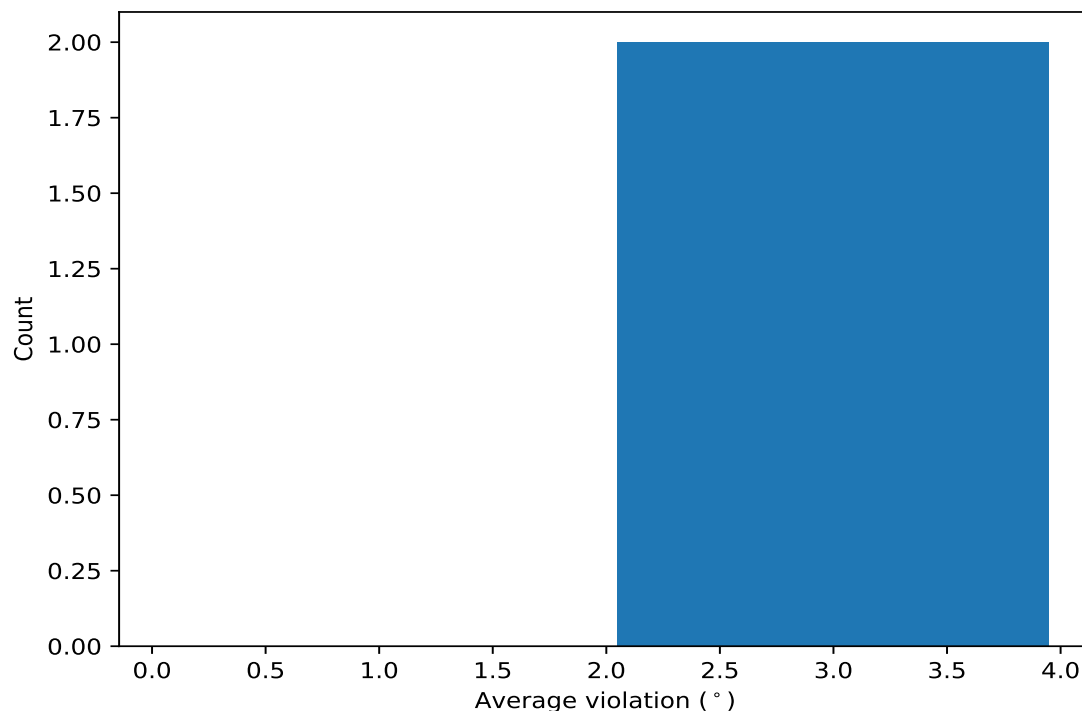


10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

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

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

in the ensemble



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

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

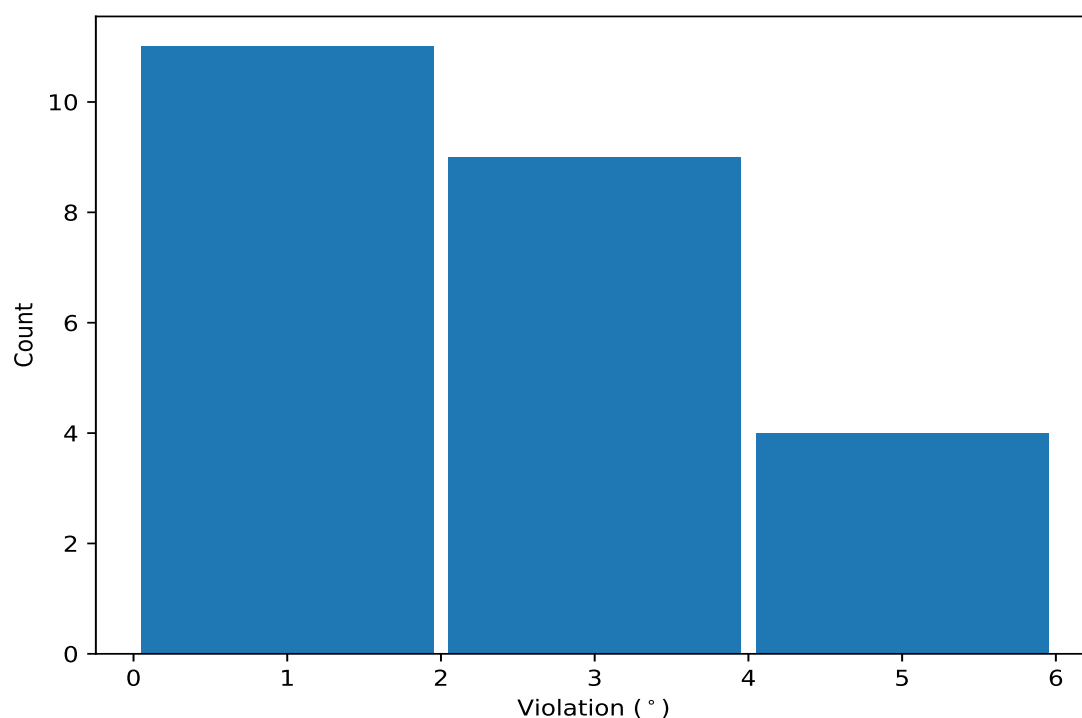
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,142)	1:79:A:HIS:N	1:79:A:HIS:CA	1:79:A:HIS:C	1:80:A:VAL:N	15	2.61	1.44	2.18
(1,143)	1:79:A:HIS:C	1:80:A:VAL:N	1:80:A:VAL:CA	1:80:A:VAL:C	6	2.59	1.15	2.45

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

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

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

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



10.5.2 Table: All violated dihedral-angle restraints ⓘ

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,142)	1:79:A:HIS:N	1:79:A:HIS:CA	1:79:A:HIS:C	1:80:A:VAL:N	14	5.88
(1,143)	1:79:A:HIS:C	1:80:A:VAL:N	1:80:A:VAL:CA	1:80:A:VAL:C	7	4.95
(1,142)	1:79:A:HIS:N	1:79:A:HIS:CA	1:79:A:HIS:C	1:80:A:VAL:N	6	4.81
(1,142)	1:79:A:HIS:N	1:79:A:HIS:CA	1:79:A:HIS:C	1:80:A:VAL:N	18	4.4
(1,142)	1:79:A:HIS:N	1:79:A:HIS:CA	1:79:A:HIS:C	1:80:A:VAL:N	5	3.42
(1,142)	1:79:A:HIS:N	1:79:A:HIS:CA	1:79:A:HIS:C	1:80:A:VAL:N	15	3.03
(1,142)	1:79:A:HIS:N	1:79:A:HIS:CA	1:79:A:HIS:C	1:80:A:VAL:N	3	2.9
(1,142)	1:79:A:HIS:N	1:79:A:HIS:CA	1:79:A:HIS:C	1:80:A:VAL:N	9	2.71
(1,143)	1:79:A:HIS:C	1:80:A:VAL:N	1:80:A:VAL:CA	1:80:A:VAL:C	17	2.57
(1,143)	1:79:A:HIS:C	1:80:A:VAL:N	1:80:A:VAL:CA	1:80:A:VAL:C	2	2.49
(1,143)	1:79:A:HIS:C	1:80:A:VAL:N	1:80:A:VAL:CA	1:80:A:VAL:C	8	2.41
(1,142)	1:79:A:HIS:N	1:79:A:HIS:CA	1:79:A:HIS:C	1:80:A:VAL:N	12	2.18
(1,142)	1:79:A:HIS:N	1:79:A:HIS:CA	1:79:A:HIS:C	1:80:A:VAL:N	17	2.12
(1,143)	1:79:A:HIS:C	1:80:A:VAL:N	1:80:A:VAL:CA	1:80:A:VAL:C	3	1.85
(1,137)	1:75:A:LYS:C	1:76:A:ASP:N	1:76:A:ASP:CA	1:76:A:ASP:C	6	1.85
(1,142)	1:79:A:HIS:N	1:79:A:HIS:CA	1:79:A:HIS:C	1:80:A:VAL:N	13	1.59
(1,142)	1:79:A:HIS:N	1:79:A:HIS:CA	1:79:A:HIS:C	1:80:A:VAL:N	20	1.54
(1,92)	1:51:A:PHE:N	1:51:A:PHE:CA	1:51:A:PHE:C	1:52:A:ARG:N	9	1.4
(1,142)	1:79:A:HIS:N	1:79:A:HIS:CA	1:79:A:HIS:C	1:80:A:VAL:N	11	1.27
(1,143)	1:79:A:HIS:C	1:80:A:VAL:N	1:80:A:VAL:CA	1:80:A:VAL:C	11	1.25
(1,136)	1:75:A:LYS:N	1:75:A:LYS:CA	1:75:A:LYS:C	1:76:A:ASP:N	2	1.18

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,142)	1:79:A:HIS:N	1:79:A:HIS:CA	1:79:A:HIS:C	1:80:A:VAL:N	10	1.1
(1,142)	1:79:A:HIS:N	1:79:A:HIS:CA	1:79:A:HIS:C	1:80:A:VAL:N	16	1.1
(1,142)	1:79:A:HIS:N	1:79:A:HIS:CA	1:79:A:HIS:C	1:80:A:VAL:N	1	1.05