



Full wwPDB NMR Structure Validation Report ⓘ

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PDB ID : 2N0M / pdb_00002n0m
BMRB ID : 18636
Title : The solution structure of the soluble form of the Lipid-modified Azurin from *Neisseria gonorrhoeae*
Authors : Pauleta, S.R.; Matzapetakis, M.F.; Nobrega, C.F.; Carreira, C.; Saraiva, I.H.
Deposited on : 2015-03-10

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

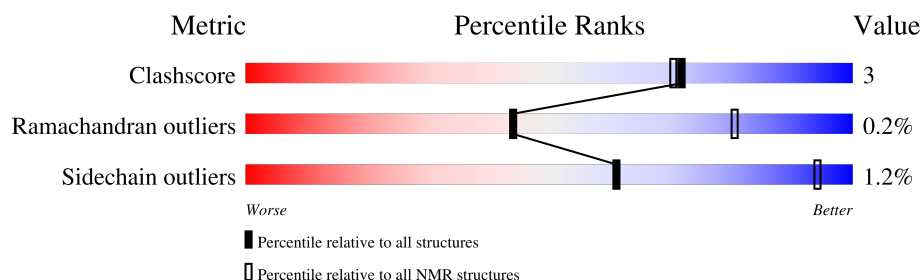
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 93%.

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	130	

2 Ensemble composition and analysis

This entry contains 10 models. Model 6 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:6-A:75, A:81-A:130 (120)	0.55	6

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

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

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

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1885 atoms, of which 932 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Lipid modified azurin protein.

Mol	Chain	Residues	Atoms						Trace
1	A	130	Total	C	H	N	O	S	0
			1884	589	932	162	194	7	

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	-	expression tag	UNP Q5F809
A	2	THR	-	expression tag	UNP Q5F809

- Molecule 2 is COPPER (I) ION (CCD ID: CU1) (formula: Cu).

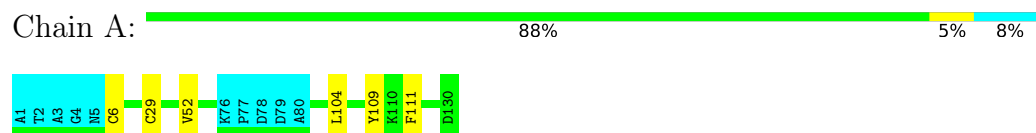
Mol	Chain	Residues	Atoms	
2	A	1	Total	Cu
			1	1

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Lipid modified azurin protein

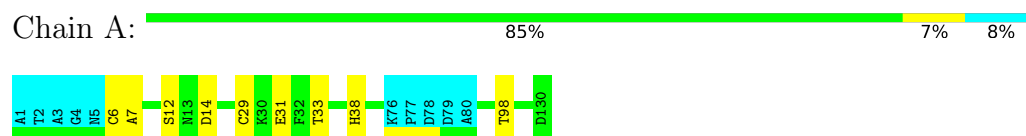


4.2 Scores per residue for each member of the ensemble

Colouring as in section [4.1](#) above.

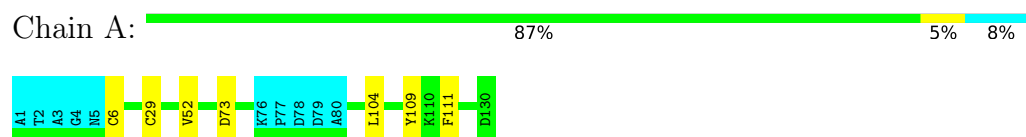
4.2.1 Score per residue for model 1

- Molecule 1: Lipid modified azurin protein



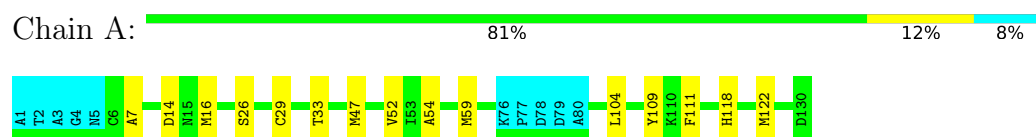
4.2.2 Score per residue for model 2

- Molecule 1: Lipid modified azurin protein



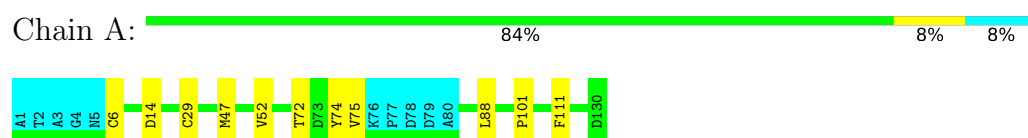
4.2.3 Score per residue for model 3

- Molecule 1: Lipid modified azurin protein



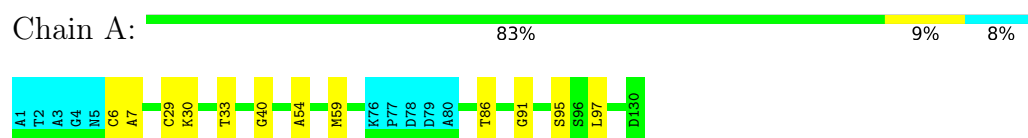
4.2.4 Score per residue for model 4

- Molecule 1: Lipid modified azurin protein



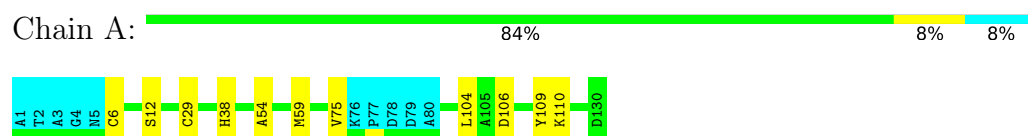
4.2.5 Score per residue for model 5

- Molecule 1: Lipid modified azurin protein



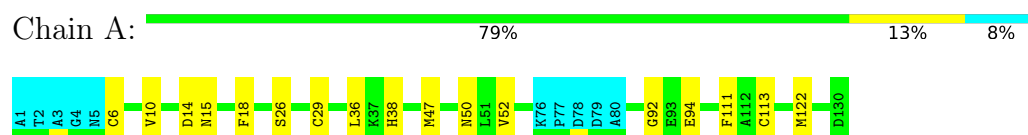
4.2.6 Score per residue for model 6 (medoid)

- Molecule 1: Lipid modified azurin protein



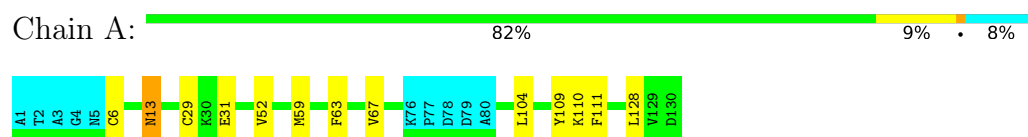
4.2.7 Score per residue for model 7

- Molecule 1: Lipid modified azurin protein



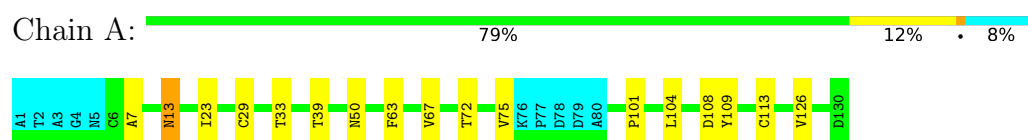
4.2.8 Score per residue for model 8

- Molecule 1: Lipid modified azurin protein



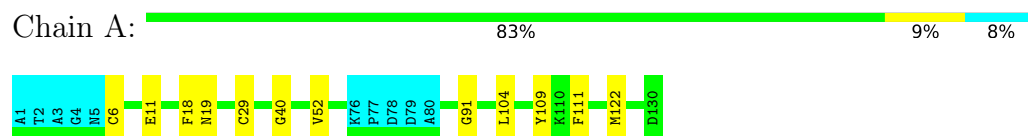
4.2.9 Score per residue for model 9

- Molecule 1: Lipid modified azurin protein



4.2.10 Score per residue for model 10

- Molecule 1: Lipid modified azurin protein



5 Refinement protocol and experimental data overview

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

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

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

Software name	Classification	Version
CNS	structure calculation	1.21
CNS	refinement	1.21

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	1503
Number of shifts mapped to atoms	1503
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	93%

6 Model quality

6.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CU1

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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	886	871	871	6±2
All	All	8870	8710	8710	60

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 3.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:6:CYS:SG	1:A:29:CYS:SG	0.80	2.79	7	6
1:A:6:CYS:HG	1:A:29:CYS:HG	0.80	1.08	7	3
1:A:59:MET:SD	1:A:110:LYS:HB2	0.67	2.29	8	1
1:A:50:ASN:O	1:A:113:CYS:HA	0.64	1.92	7	2
1:A:14:ASP:HA	1:A:47:MET:SD	0.63	2.33	7	3
1:A:54:ALA:HB3	1:A:59:MET:SD	0.62	2.34	6	3
1:A:52:VAL:O	1:A:111:PHE:HA	0.54	2.03	4	6
1:A:26:SER:HB3	1:A:29:CYS:SG	0.52	2.45	3	1
1:A:104:LEU:HA	1:A:109:TYR:CE1	0.51	2.41	3	5
1:A:29:CYS:O	1:A:101:PRO:HG2	0.51	2.04	9	2
1:A:30:LYS:HD2	1:A:30:LYS:N	0.51	2.21	5	1
1:A:72:THR:O	1:A:75:VAL:HG22	0.47	2.10	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:13:ASN:HD22	1:A:13:ASN:C	0.47	2.18	8	1
1:A:40:GLY:O	1:A:91:GLY:HA2	0.47	2.09	5	2
1:A:38:HIS:O	1:A:92:GLY:HA2	0.46	2.09	7	1
1:A:7:ALA:HA	1:A:33:THR:O	0.46	2.11	3	4
1:A:10:VAL:O	1:A:36:LEU:HA	0.44	2.12	7	1
1:A:18:PHE:CE2	1:A:122:MET:HB3	0.43	2.48	10	2
1:A:74:TYR:CD2	1:A:88:LEU:HD11	0.43	2.49	4	1
1:A:12:SER:O	1:A:38:HIS:HA	0.42	2.14	1	2
1:A:23:ILE:O	1:A:126:VAL:HA	0.42	2.14	9	1
1:A:104:LEU:HA	1:A:109:TYR:CZ	0.42	2.50	9	1
1:A:86:THR:HB	1:A:95:SER:OG	0.42	2.14	5	1
1:A:63:PHE:O	1:A:67:VAL:HG23	0.42	2.14	8	2
1:A:11:GLU:HB3	1:A:19:ASN:ND2	0.42	2.30	10	1
1:A:13:ASN:HA	1:A:39:THR:O	0.41	2.15	9	1
1:A:97:LEU:HD12	1:A:97:LEU:C	0.40	2.41	5	1
1:A:16:MET:HB3	1:A:122:MET:HE2	0.40	1.91	3	1
1:A:118:HIS:CG	1:A:122:MET:HE1	0.40	2.52	3	1
1:A:13:ASN:C	1:A:13:ASN:HD22	0.40	2.24	9	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	119/130 (92%)	113±1 (95±1%)	5±1 (5±1%)	0±0 (0±0%)	44	80
All	All	1190/1300 (92%)	1134 (95%)	54 (5%)	2 (0%)	44	80

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	73	ASP	1
1	A	106	ASP	1

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	95/101 (94%)	94±1 (99±1%)	1±1 (1±1%)	61	94
All	All	950/1010 (94%)	939 (99%)	11 (1%)	61	94

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	31	GLU	2
1	A	13	ASN	2
1	A	14	ASP	1
1	A	98	THR	1
1	A	110	LYS	1
1	A	15	ASN	1
1	A	94	GLU	1
1	A	128	LEU	1
1	A	108	ASP	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [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 [i](#)

The completeness of assignment taking into account all chemical shift lists is 93% for the well-defined parts and 93% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list*

7.1.1 Bookkeeping [i](#)

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	1503
Number of shifts mapped to atoms	1503
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	5

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	130	0.06 ± 0.19	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	117	0.04 ± 0.17	None needed (< 0.5 ppm)
$^{13}\text{C}'$	130	0.22 ± 0.16	None needed (< 0.5 ppm)
^{15}N	123	0.69 ± 0.67	None needed (imprecise)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 93%, i.e. 1408 atoms were assigned a chemical shift out of a possible 1509. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	601/606 (99%)	246/249 (99%)	240/240 (100%)	115/117 (98%)
Sidechain	729/803 (91%)	481/524 (92%)	240/257 (93%)	8/22 (36%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	78/100 (78%)	41/49 (84%)	30/43 (70%)	7/8 (88%)
Overall	1408/1509 (93%)	768/822 (93%)	510/540 (94%)	130/147 (88%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 93%, i.e. 1502 atoms were assigned a chemical shift out of a possible 1613. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	647/655 (99%)	264/269 (98%)	260/260 (100%)	123/126 (98%)
Sidechain	777/858 (91%)	512/559 (92%)	256/275 (93%)	9/24 (38%)
Aromatic	78/100 (78%)	41/49 (84%)	30/43 (70%)	7/8 (88%)
Overall	1502/1613 (93%)	817/877 (93%)	546/578 (94%)	139/158 (88%)

7.1.4 Statistically unusual chemical shifts [i](#)

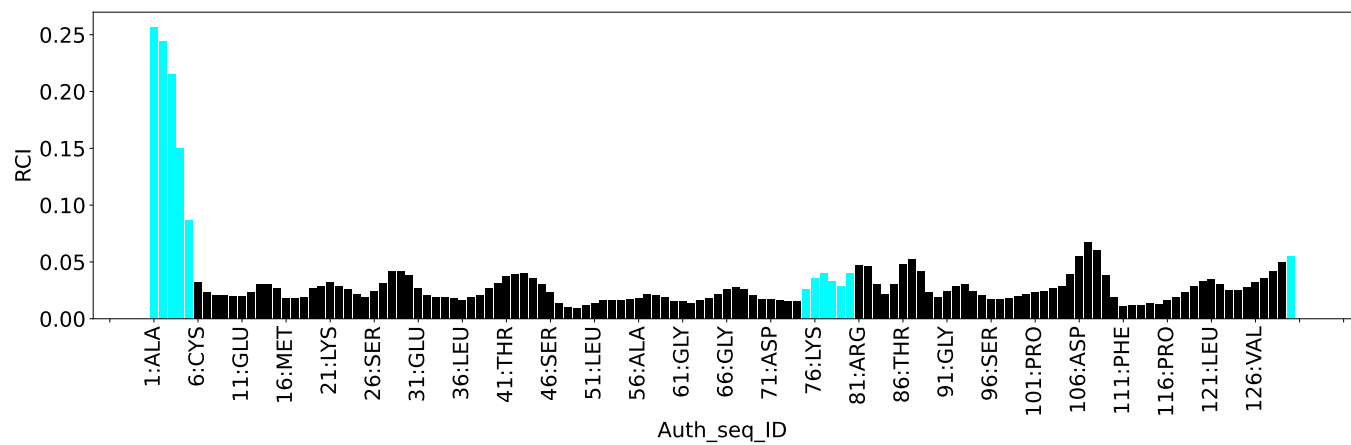
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	114	THR	HG1	5.05	0.08 – 2.19	18.5
1	A	116	PRO	HD3	0.64	1.76 – 5.48	-8.0
1	A	55	LYS	HD2	0.31	0.58 – 2.64	-6.3
1	A	116	PRO	HD2	1.87	1.93 – 5.38	-5.2
1	A	70	ALA	HA	2.07	2.13 – 6.34	-5.1

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	3266
Intra-residue ($ i-j =0$)	970
Sequential ($ i-j =1$)	691
Medium range ($ i-j >1$ and $ i-j <5$)	354
Long range ($ i-j \geq 5$)	1250
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	1
Total dihedral-angle restraints	129
Number of unmapped restraints	0
Number of restraints per residue	25.9
Number of long range restraints per residue ¹	9.5

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)	33.3	0.2
0.2-0.5 (Medium)	79.4	0.5
>0.5 (Large)	130.3	4.38

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)	2.0	3.35
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

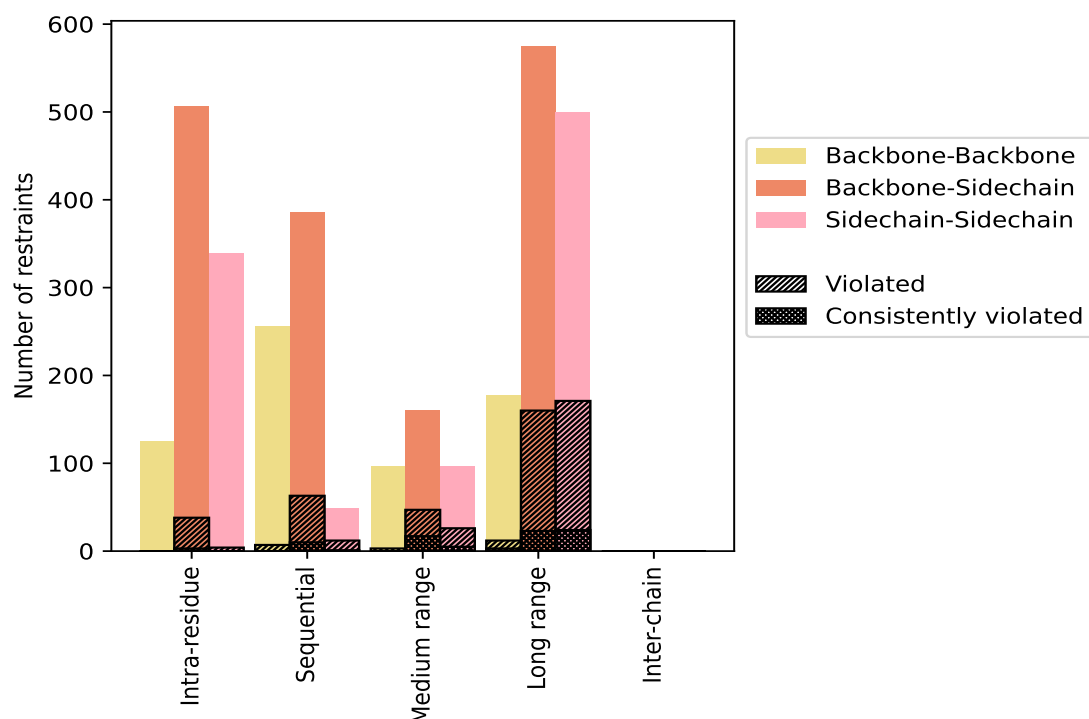
9.1 Summary of distance violations ⓘ

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)	970	29.7	42	4.3	1.3	3	0.3	0.1
Backbone-Backbone	125	3.8	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	506	15.5	38	7.5	1.2	3	0.6	0.1
Sidechain-Sidechain	339	10.4	4	1.2	0.1	0	0.0	0.0
Sequential (i-j =1)	691	21.2	82	11.9	2.5	11	1.6	0.3
Backbone-Backbone	256	7.8	7	2.7	0.2	0	0.0	0.0
Backbone-Sidechain	386	11.8	63	16.3	1.9	10	2.6	0.3
Sidechain-Sidechain	49	1.5	12	24.5	0.4	1	2.0	0.0
Medium range (i-j >1 & i-j <5)	354	10.8	76	21.5	2.3	22	6.2	0.7
Backbone-Backbone	97	3.0	3	3.1	0.1	0	0.0	0.0
Backbone-Sidechain	160	4.9	47	29.4	1.4	17	10.6	0.5
Sidechain-Sidechain	97	3.0	26	26.8	0.8	5	5.2	0.2
Long range (i-j ≥5)	1250	38.3	342	27.4	10.5	49	3.9	1.5
Backbone-Backbone	177	5.4	12	6.8	0.4	3	1.7	0.1
Backbone-Sidechain	575	17.6	160	27.8	4.9	23	4.0	0.7
Sidechain-Sidechain	498	15.2	170	34.1	5.2	23	4.6	0.7
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	1	0.0	1	100.0	0.0	1	100.0	0.0
Total	3266	100.0	543	16.6	16.6	86	2.6	2.6
Backbone-Backbone	655	20.1	22	3.4	0.7	3	0.5	0.1
Backbone-Sidechain	1627	49.8	308	18.9	9.4	53	3.3	1.6
Sidechain-Sidechain	984	30.1	213	21.6	6.5	30	3.0	0.9

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 disulfide bonds are counted in their appropriate category on the x-axis

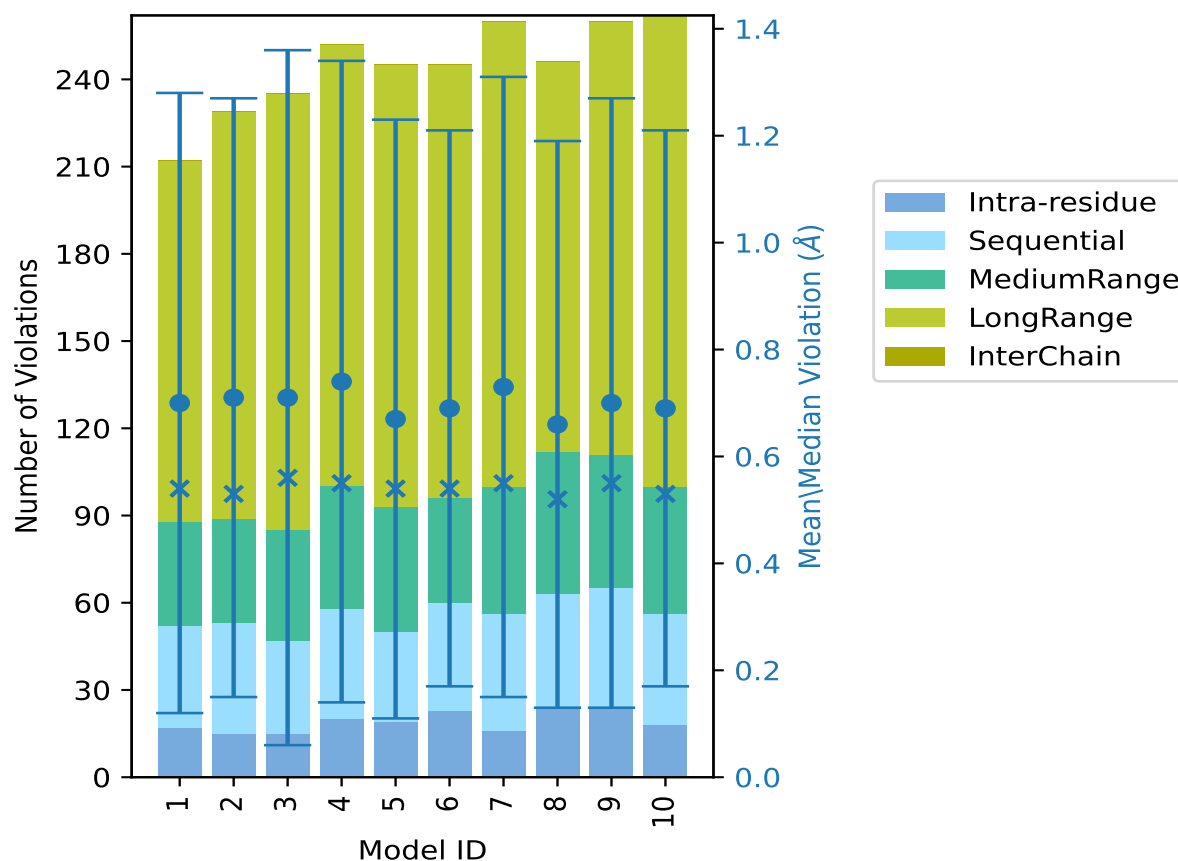
9.2 Distance violation statistics for each model [i](#)

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	17	35	36	124	0	212	0.7	3.03	0.58	0.54
2	15	38	36	140	0	229	0.71	3.7	0.56	0.53
3	15	32	38	150	0	235	0.71	4.38	0.65	0.56
4	20	38	42	152	0	252	0.74	3.14	0.6	0.55
5	19	31	43	152	0	245	0.67	3.32	0.56	0.54
6	23	37	36	149	0	245	0.69	3.11	0.52	0.54
7	16	40	44	160	0	260	0.73	3.01	0.58	0.55
8	24	39	49	134	0	246	0.66	3.14	0.53	0.52
9	24	41	46	149	0	260	0.7	3.83	0.57	0.55
10	18	38	44	162	0	262	0.69	3.23	0.52	0.53

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

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



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

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

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 2723(IR:928, SQ:609, MR:278, LR:908, 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	%
13	22	16	107	0	158	1	10.0
5	11	7	45	0	68	2	20.0
4	4	5	28	0	41	3	30.0

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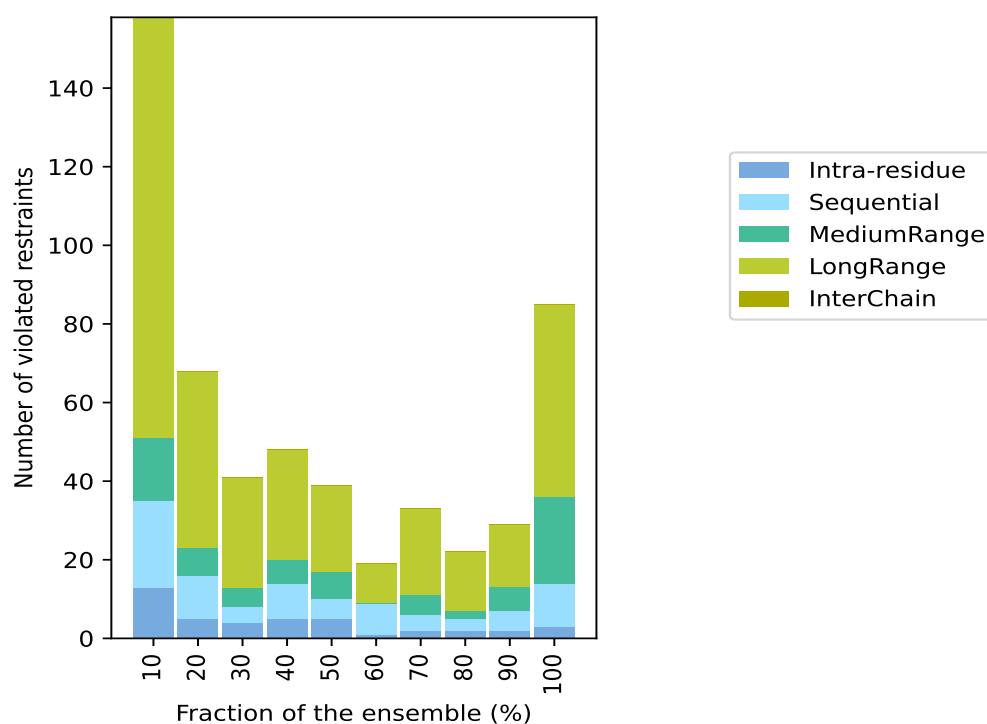
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
5	9	6	28	0	48	4	40.0
5	5	7	22	0	39	5	50.0
1	8	0	10	0	19	6	60.0
2	4	5	22	0	33	7	70.0
2	3	2	15	0	22	8	80.0
2	5	6	16	0	29	9	90.0
3	11	22	49	0	85	10	100.0

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

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

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

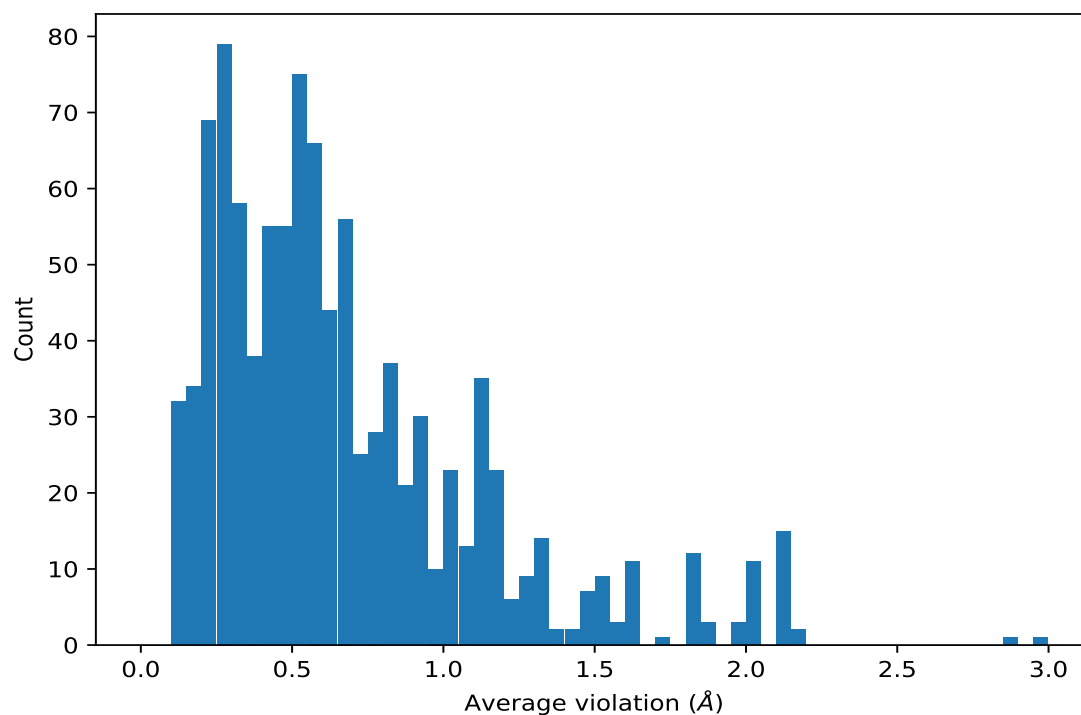


9.4 Most violated distance restraints in the ensemble [i](#)

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

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

in the ensemble



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,488)	1:114:A:THR:HG1	1:50:A:ASN:HA	10	2.95	0.34	3.11
(1,2590)	1:128:A:LEU:HB3	1:106:A:ASP:H	10	2.89	0.7	2.8
(1,2360)	1:76:A:LYS:HE2	1:79:A:ASP:H	10	2.18	1.22	2.24
(1,2360)	1:76:A:LYS:HE3	1:79:A:ASP:H	10	2.18	1.22	2.24
(1,1387)	1:101:A:PRO:HG2	1:25:A:VAL:HG21	10	2.14	0.27	2.1
(1,1387)	1:101:A:PRO:HG2	1:25:A:VAL:HG22	10	2.14	0.27	2.1
(1,1387)	1:101:A:PRO:HG2	1:25:A:VAL:HG23	10	2.14	0.27	2.1
(1,1701)	1:99:A:LEU:HD11	1:51:A:LEU:HD11	10	2.1	0.16	2.12
(1,1701)	1:99:A:LEU:HD11	1:51:A:LEU:HD12	10	2.1	0.16	2.12
(1,1701)	1:99:A:LEU:HD11	1:51:A:LEU:HD13	10	2.1	0.16	2.12
(1,1701)	1:99:A:LEU:HD12	1:51:A:LEU:HD11	10	2.1	0.16	2.12
(1,1701)	1:99:A:LEU:HD12	1:51:A:LEU:HD12	10	2.1	0.16	2.12
(1,1701)	1:99:A:LEU:HD12	1:51:A:LEU:HD13	10	2.1	0.16	2.12
(1,1701)	1:99:A:LEU:HD13	1:51:A:LEU:HD11	10	2.1	0.16	2.12
(1,1701)	1:99:A:LEU:HD13	1:51:A:LEU:HD12	10	2.1	0.16	2.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1701)	1:99:A:LEU:HD13	1:51:A:LEU:HD13	10	2.1	0.16	2.12
(1,1386)	1:101:A:PRO:HB2	1:25:A:VAL:HG21	10	2.05	0.34	2.17
(1,1386)	1:101:A:PRO:HB2	1:25:A:VAL:HG22	10	2.05	0.34	2.17
(1,1386)	1:101:A:PRO:HB2	1:25:A:VAL:HG23	10	2.05	0.34	2.17
(1,3149)	1:82:A:VAL:HG12	1:114:A:THR:HG23	10	2.04	0.34	2.08
(1,3149)	1:62:A:VAL:HG22	1:114:A:THR:HG21	10	2.04	0.34	2.08
(1,3149)	1:62:A:VAL:HG21	1:114:A:THR:HG23	10	2.04	0.34	2.08
(1,3149)	1:62:A:VAL:HG21	1:114:A:THR:HG21	10	2.04	0.34	2.08
(1,3149)	1:62:A:VAL:HG23	1:114:A:THR:HG22	10	2.04	0.34	2.08
(1,3149)	1:62:A:VAL:HG23	1:114:A:THR:HG23	10	2.04	0.34	2.08
(1,3149)	1:82:A:VAL:HG11	1:114:A:THR:HG23	10	2.04	0.34	2.08
(1,3149)	1:62:A:VAL:HG23	1:114:A:THR:HG21	10	2.04	0.34	2.08
(1,1037)	1:99:A:LEU:HD21	1:101:A:PRO:HG2	10	1.8	0.2	1.86
(1,1037)	1:99:A:LEU:HD22	1:101:A:PRO:HG2	10	1.8	0.2	1.86
(1,1037)	1:99:A:LEU:HD23	1:101:A:PRO:HG2	10	1.8	0.2	1.86
(1,55)	1:17:A:GLN:HG3	1:12:A:SER:HB3	10	1.73	0.46	1.62
(1,2396)	1:82:A:VAL:HG21	1:84:A:ALA:H	10	1.64	0.11	1.68
(1,2396)	1:82:A:VAL:HG22	1:84:A:ALA:H	10	1.64	0.11	1.68
(1,2396)	1:82:A:VAL:HG23	1:84:A:ALA:H	10	1.64	0.11	1.68
(1,58)	1:17:A:GLN:HG3	1:12:A:SER:HB2	10	1.6	0.54	1.6
(1,33)	1:10:A:VAL:HB	1:36:A:LEU:HD21	10	1.54	0.57	1.38
(1,33)	1:10:A:VAL:HB	1:36:A:LEU:HD22	10	1.54	0.57	1.38
(1,33)	1:10:A:VAL:HB	1:36:A:LEU:HD23	10	1.54	0.57	1.38
(1,1965)	1:29:A:CYS:H	1:25:A:VAL:HG21	10	1.5	0.08	1.5
(1,1965)	1:29:A:CYS:H	1:25:A:VAL:HG22	10	1.5	0.08	1.5
(1,1965)	1:29:A:CYS:H	1:25:A:VAL:HG23	10	1.5	0.08	1.5
(1,2211)	1:55:A:LYS:H	1:83:A:VAL:HB	10	1.47	0.29	1.44
(1,2411)	1:85:A:HIS:H	1:82:A:VAL:HG21	10	1.47	0.15	1.5
(1,2411)	1:85:A:HIS:H	1:82:A:VAL:HG22	10	1.47	0.15	1.5
(1,2411)	1:85:A:HIS:H	1:82:A:VAL:HG23	10	1.47	0.15	1.5
(1,1015)	1:99:A:LEU:HD21	1:101:A:PRO:HD2	10	1.46	0.25	1.5
(1,1015)	1:99:A:LEU:HD22	1:101:A:PRO:HD2	10	1.46	0.25	1.5
(1,1015)	1:99:A:LEU:HD23	1:101:A:PRO:HD2	10	1.46	0.25	1.5
(1,2121)	1:43:A:PRO:HG3	1:47:A:MET:H	10	1.4	0.15	1.38
(1,1669)	1:25:A:VAL:HG11	1:126:A:VAL:HG21	10	1.32	0.8	0.9
(1,1669)	1:25:A:VAL:HG11	1:126:A:VAL:HG22	10	1.32	0.8	0.9
(1,1669)	1:25:A:VAL:HG11	1:126:A:VAL:HG23	10	1.32	0.8	0.9
(1,1669)	1:25:A:VAL:HG12	1:126:A:VAL:HG21	10	1.32	0.8	0.9
(1,1669)	1:25:A:VAL:HG12	1:126:A:VAL:HG22	10	1.32	0.8	0.9
(1,1669)	1:25:A:VAL:HG12	1:126:A:VAL:HG23	10	1.32	0.8	0.9
(1,1669)	1:25:A:VAL:HG13	1:126:A:VAL:HG21	10	1.32	0.8	0.9
(1,1669)	1:25:A:VAL:HG13	1:126:A:VAL:HG22	10	1.32	0.8	0.9

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1669)	1:25:A:VAL:HG13	1:126:A:VAL:HG23	10	1.32	0.8	0.9
(1,823)	1:82:A:VAL:HG21	1:85:A:HIS:HB2	10	1.3	0.43	1.42
(1,823)	1:82:A:VAL:HG22	1:85:A:HIS:HB2	10	1.3	0.43	1.42
(1,823)	1:82:A:VAL:HG23	1:85:A:HIS:HB2	10	1.3	0.43	1.42
(1,766)	1:69:A:ALA:HA	1:77:A:PRO:HD2	10	1.29	0.66	1.1
(1,2060)	1:93:A:GLU:H	1:40:A:GLY:H	10	1.28	0.53	1.18
(1,1436)	1:47:A:MET:HE1	1:118:A:HIS:HB2	10	1.26	0.41	1.1
(1,1436)	1:47:A:MET:HE2	1:118:A:HIS:HB2	10	1.26	0.41	1.1
(1,1436)	1:47:A:MET:HE3	1:118:A:HIS:HB2	10	1.26	0.41	1.1
(1,3108)	1:128:A:LEU:HB3	1:105:A:ALA:HA	10	1.19	0.47	1.25
(1,1014)	1:101:A:PRO:HD2	1:25:A:VAL:HG21	10	1.18	0.11	1.21
(1,1014)	1:101:A:PRO:HD2	1:25:A:VAL:HG22	10	1.18	0.11	1.21
(1,1014)	1:101:A:PRO:HD2	1:25:A:VAL:HG23	10	1.18	0.11	1.21
(1,1526)	1:52:A:VAL:HG21	1:75:A:VAL:HG21	10	1.18	0.98	0.8
(1,1526)	1:52:A:VAL:HG21	1:75:A:VAL:HG22	10	1.18	0.98	0.8
(1,1526)	1:52:A:VAL:HG21	1:75:A:VAL:HG23	10	1.18	0.98	0.8
(1,1526)	1:52:A:VAL:HG22	1:75:A:VAL:HG21	10	1.18	0.98	0.8
(1,1526)	1:52:A:VAL:HG22	1:75:A:VAL:HG22	10	1.18	0.98	0.8
(1,1526)	1:52:A:VAL:HG22	1:75:A:VAL:HG23	10	1.18	0.98	0.8
(1,1526)	1:52:A:VAL:HG23	1:75:A:VAL:HG21	10	1.18	0.98	0.8
(1,1526)	1:52:A:VAL:HG23	1:75:A:VAL:HG22	10	1.18	0.98	0.8
(1,1526)	1:52:A:VAL:HG23	1:75:A:VAL:HG23	10	1.18	0.98	0.8
(1,2963)	1:109:A:TYR:HD1	1:128:A:LEU:HD11	10	1.17	0.3	1.21
(1,2963)	1:109:A:TYR:HD1	1:128:A:LEU:HD12	10	1.17	0.3	1.21
(1,2963)	1:109:A:TYR:HD1	1:128:A:LEU:HD13	10	1.17	0.3	1.21
(1,2963)	1:109:A:TYR:HD2	1:128:A:LEU:HD11	10	1.17	0.3	1.21
(1,2963)	1:109:A:TYR:HD2	1:128:A:LEU:HD12	10	1.17	0.3	1.21
(1,2963)	1:109:A:TYR:HD2	1:128:A:LEU:HD13	10	1.17	0.3	1.21
(1,1552)	1:109:A:TYR:HE1	1:83:A:VAL:HG11	10	1.09	0.38	1.12
(1,1552)	1:109:A:TYR:HE1	1:83:A:VAL:HG12	10	1.09	0.38	1.12
(1,1552)	1:109:A:TYR:HE1	1:83:A:VAL:HG13	10	1.09	0.38	1.12
(1,1552)	1:109:A:TYR:HE2	1:83:A:VAL:HG11	10	1.09	0.38	1.12
(1,1552)	1:109:A:TYR:HE2	1:83:A:VAL:HG12	10	1.09	0.38	1.12
(1,1552)	1:109:A:TYR:HE2	1:83:A:VAL:HG13	10	1.09	0.38	1.12
(1,3232)	1:112:A:ALA:H	1:126:A:VAL:HG13	10	1.03	0.13	1.06
(1,3232)	1:53:A:ILE:HG22	1:112:A:ALA:H	10	1.03	0.13	1.06
(1,3232)	1:53:A:ILE:HG21	1:112:A:ALA:H	10	1.03	0.13	1.06
(1,3232)	1:53:A:ILE:HG23	1:112:A:ALA:H	10	1.03	0.13	1.06
(1,3232)	1:112:A:ALA:H	1:126:A:VAL:HG11	10	1.03	0.13	1.06
(1,1035)	1:101:A:PRO:HG3	1:25:A:VAL:HG21	10	0.99	0.44	0.86
(1,1035)	1:101:A:PRO:HG3	1:25:A:VAL:HG22	10	0.99	0.44	0.86
(1,1035)	1:101:A:PRO:HG3	1:25:A:VAL:HG23	10	0.99	0.44	0.86

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2959)	1:104:A:LEU:HB2	1:109:A:TYR:HD1	10	0.98	0.1	0.97
(1,2959)	1:104:A:LEU:HB2	1:109:A:TYR:HD2	10	0.98	0.1	0.97
(1,1389)	1:27:A:LYS:HA	1:25:A:VAL:HG21	10	0.97	0.09	0.99
(1,1389)	1:27:A:LYS:HA	1:25:A:VAL:HG22	10	0.97	0.09	0.99
(1,1389)	1:27:A:LYS:HA	1:25:A:VAL:HG23	10	0.97	0.09	0.99
(1,882)	1:91:A:GLY:HA3	1:38:A:HIS:HB2	10	0.96	0.52	0.76
(1,1039)	1:99:A:LEU:HD21	1:101:A:PRO:HG3	10	0.95	0.34	0.91
(1,1039)	1:99:A:LEU:HD22	1:101:A:PRO:HG3	10	0.95	0.34	0.91
(1,1039)	1:99:A:LEU:HD23	1:101:A:PRO:HG3	10	0.95	0.34	0.91
(1,2880)	1:67:A:VAL:HG21	1:74:A:TYR:HD1	10	0.93	0.21	0.92
(1,2880)	1:67:A:VAL:HG21	1:74:A:TYR:HD2	10	0.93	0.21	0.92
(1,2880)	1:67:A:VAL:HG22	1:74:A:TYR:HD1	10	0.93	0.21	0.92
(1,2880)	1:67:A:VAL:HG22	1:74:A:TYR:HD2	10	0.93	0.21	0.92
(1,2880)	1:67:A:VAL:HG23	1:74:A:TYR:HD1	10	0.93	0.21	0.92
(1,2880)	1:67:A:VAL:HG23	1:74:A:TYR:HD2	10	0.93	0.21	0.92
(1,1753)	1:36:A:LEU:HD21	1:10:A:VAL:H	10	0.92	0.07	0.92
(1,1753)	1:36:A:LEU:HD22	1:10:A:VAL:H	10	0.92	0.07	0.92
(1,1753)	1:36:A:LEU:HD23	1:10:A:VAL:H	10	0.92	0.07	0.92
(1,2125)	1:47:A:MET:H	1:43:A:PRO:HD3	10	0.91	0.1	0.88
(1,493)	1:50:A:ASN:HA	1:36:A:LEU:HD11	10	0.86	0.22	0.78
(1,493)	1:50:A:ASN:HA	1:36:A:LEU:HD12	10	0.86	0.22	0.78
(1,493)	1:50:A:ASN:HA	1:36:A:LEU:HD13	10	0.86	0.22	0.78
(1,3165)	1:24:A:GLN:HB3	1:23:A:ILE:H	10	0.83	0.1	0.84
(2,1)	1:6:A:CYS:SG	1:29:A:CYS:SG	10	0.82	0.29	0.75
(1,1715)	1:59:A:MET:HE1	1:114:A:THR:HG1	10	0.82	0.27	0.72
(1,1715)	1:59:A:MET:HE2	1:114:A:THR:HG1	10	0.82	0.27	0.72
(1,1715)	1:59:A:MET:HE3	1:114:A:THR:HG1	10	0.82	0.27	0.72
(1,2884)	1:115:A:PHE:HB3	1:74:A:TYR:HD1	10	0.82	0.17	0.76
(1,2884)	1:115:A:PHE:HB3	1:74:A:TYR:HD2	10	0.82	0.17	0.76
(1,2652)	1:113:A:CYS:H	1:111:A:PHE:HB3	10	0.8	0.06	0.76
(1,3139)	1:51:A:LEU:HB2	1:86:A:THR:HG22	10	0.76	0.14	0.76
(1,3139)	1:51:A:LEU:HB2	1:86:A:THR:HG23	10	0.76	0.14	0.76
(1,3139)	1:51:A:LEU:HB2	1:86:A:THR:HG21	10	0.76	0.14	0.76
(1,2516)	1:97:A:LEU:H	1:36:A:LEU:HD11	10	0.75	0.13	0.74
(1,2516)	1:97:A:LEU:H	1:36:A:LEU:HD12	10	0.75	0.13	0.74
(1,2516)	1:97:A:LEU:H	1:36:A:LEU:HD13	10	0.75	0.13	0.74
(1,1428)	1:18:A:PHE:HD1	1:36:A:LEU:HD21	10	0.74	0.15	0.72
(1,1428)	1:18:A:PHE:HD1	1:36:A:LEU:HD22	10	0.74	0.15	0.72
(1,1428)	1:18:A:PHE:HD1	1:36:A:LEU:HD23	10	0.74	0.15	0.72
(1,1428)	1:18:A:PHE:HD2	1:36:A:LEU:HD21	10	0.74	0.15	0.72
(1,1428)	1:18:A:PHE:HD2	1:36:A:LEU:HD22	10	0.74	0.15	0.72
(1,1428)	1:18:A:PHE:HD2	1:36:A:LEU:HD23	10	0.74	0.15	0.72

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2966)	1:109:A:TYR:HE1	1:128:A:LEU:HD11	10	0.72	0.31	0.76
(1,2966)	1:109:A:TYR:HE1	1:128:A:LEU:HD12	10	0.72	0.31	0.76
(1,2966)	1:109:A:TYR:HE1	1:128:A:LEU:HD13	10	0.72	0.31	0.76
(1,2966)	1:109:A:TYR:HE2	1:128:A:LEU:HD11	10	0.72	0.31	0.76
(1,2966)	1:109:A:TYR:HE2	1:128:A:LEU:HD12	10	0.72	0.31	0.76
(1,2966)	1:109:A:TYR:HE2	1:128:A:LEU:HD13	10	0.72	0.31	0.76
(1,1686)	1:128:A:LEU:HD11	1:127:A:THR:HG21	10	0.68	0.08	0.68
(1,1686)	1:128:A:LEU:HD11	1:127:A:THR:HG22	10	0.68	0.08	0.68
(1,1686)	1:128:A:LEU:HD11	1:127:A:THR:HG23	10	0.68	0.08	0.68
(1,1686)	1:128:A:LEU:HD12	1:127:A:THR:HG21	10	0.68	0.08	0.68
(1,1686)	1:128:A:LEU:HD12	1:127:A:THR:HG22	10	0.68	0.08	0.68
(1,1686)	1:128:A:LEU:HD12	1:127:A:THR:HG23	10	0.68	0.08	0.68
(1,1686)	1:128:A:LEU:HD13	1:127:A:THR:HG21	10	0.68	0.08	0.68
(1,1686)	1:128:A:LEU:HD13	1:127:A:THR:HG22	10	0.68	0.08	0.68
(1,1686)	1:128:A:LEU:HD13	1:127:A:THR:HG23	10	0.68	0.08	0.68
(1,3220)	1:94:A:GLU:H	1:93:A:GLU:HB2	10	0.65	0.12	0.66
(1,3220)	1:94:A:GLU:H	1:93:A:GLU:HG2	10	0.65	0.12	0.66
(1,1980)	1:99:A:LEU:HB3	1:32:A:PHE:H	10	0.65	0.25	0.59
(1,2114)	1:46:A:SER:H	1:43:A:PRO:HD3	10	0.64	0.19	0.63
(1,2045)	1:94:A:GLU:HB2	1:38:A:HIS:H	10	0.6	0.47	0.42
(1,2032)	1:36:A:LEU:HD21	1:37:A:LYS:H	10	0.59	0.07	0.58
(1,2032)	1:36:A:LEU:HD22	1:37:A:LYS:H	10	0.59	0.07	0.58
(1,2032)	1:36:A:LEU:HD23	1:37:A:LYS:H	10	0.59	0.07	0.58
(1,1074)	1:107:A:GLY:HA2	1:109:A:TYR:HE1	10	0.59	0.19	0.57
(1,1074)	1:107:A:GLY:HA2	1:109:A:TYR:HE2	10	0.59	0.19	0.57
(1,1539)	1:82:A:VAL:H	1:82:A:VAL:HG11	10	0.55	0.05	0.54
(1,1539)	1:82:A:VAL:H	1:82:A:VAL:HG12	10	0.55	0.05	0.54
(1,1539)	1:82:A:VAL:H	1:82:A:VAL:HG13	10	0.55	0.05	0.54
(1,2659)	1:124:A:GLY:H	1:113:A:CYS:H	10	0.54	0.07	0.55
(1,1388)	1:101:A:PRO:HA	1:25:A:VAL:HG21	10	0.54	0.12	0.55
(1,1388)	1:101:A:PRO:HA	1:25:A:VAL:HG22	10	0.54	0.12	0.55
(1,1388)	1:101:A:PRO:HA	1:25:A:VAL:HG23	10	0.54	0.12	0.55
(1,2944)	1:107:A:GLY:HA3	1:109:A:TYR:HD1	10	0.52	0.24	0.42
(1,2944)	1:107:A:GLY:HA3	1:109:A:TYR:HD2	10	0.52	0.24	0.42
(1,1017)	1:101:A:PRO:HD3	1:25:A:VAL:HG21	10	0.51	0.18	0.6
(1,1017)	1:101:A:PRO:HD3	1:25:A:VAL:HG22	10	0.51	0.18	0.6
(1,1017)	1:101:A:PRO:HD3	1:25:A:VAL:HG23	10	0.51	0.18	0.6
(1,2117)	1:46:A:SER:H	1:43:A:PRO:HB3	10	0.5	0.13	0.5
(1,3177)	1:35:A:THR:HG23	1:35:A:THR:H	10	0.49	0.11	0.52
(1,3177)	1:35:A:THR:HG21	1:35:A:THR:H	10	0.49	0.11	0.52
(1,3177)	1:9:A:THR:HG21	1:35:A:THR:H	10	0.49	0.11	0.52
(1,3177)	1:9:A:THR:HG23	1:35:A:THR:H	10	0.49	0.11	0.52

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3177)	1:35:A:THR:HG22	1:35:A:THR:H	10	0.49	0.11	0.52
(1,1253)	1:124:A:GLY:HA2	1:111:A:PHE:HZ	10	0.49	0.11	0.5
(1,2478)	1:93:A:GLU:H	1:38:A:HIS:HB2	10	0.47	0.15	0.48
(1,1509)	1:62:A:VAL:HG21	1:114:A:THR:HG21	10	0.47	0.26	0.43
(1,1509)	1:62:A:VAL:HG21	1:114:A:THR:HG22	10	0.47	0.26	0.43
(1,1509)	1:62:A:VAL:HG21	1:114:A:THR:HG23	10	0.47	0.26	0.43
(1,1509)	1:62:A:VAL:HG22	1:114:A:THR:HG21	10	0.47	0.26	0.43
(1,1509)	1:62:A:VAL:HG22	1:114:A:THR:HG22	10	0.47	0.26	0.43
(1,1509)	1:62:A:VAL:HG22	1:114:A:THR:HG23	10	0.47	0.26	0.43
(1,1509)	1:62:A:VAL:HG23	1:114:A:THR:HG21	10	0.47	0.26	0.43
(1,1509)	1:62:A:VAL:HG23	1:114:A:THR:HG22	10	0.47	0.26	0.43
(1,1509)	1:62:A:VAL:HG23	1:114:A:THR:HG23	10	0.47	0.26	0.43
(1,426)	1:43:A:PRO:HG3	1:46:A:SER:H	10	0.46	0.11	0.45
(1,3014)	1:115:A:PHE:HE1	1:48:A:GLY:HA2	10	0.46	0.09	0.44
(1,3014)	1:115:A:PHE:HE2	1:48:A:GLY:HA2	10	0.46	0.09	0.44
(1,3134)	1:23:A:ILE:HG12	1:34:A:ILE:HG23	10	0.46	0.15	0.41
(1,3134)	1:23:A:ILE:HG12	1:34:A:ILE:HG22	10	0.46	0.15	0.41
(1,3134)	1:36:A:LEU:HB3	1:34:A:ILE:HG22	10	0.46	0.15	0.41
(1,2173)	1:51:A:LEU:H	1:36:A:LEU:HD11	10	0.45	0.13	0.44
(1,2173)	1:51:A:LEU:H	1:36:A:LEU:HD12	10	0.45	0.13	0.44
(1,2173)	1:51:A:LEU:H	1:36:A:LEU:HD13	10	0.45	0.13	0.44
(1,1392)	1:127:A:THR:H	1:25:A:VAL:HG11	10	0.45	0.11	0.47
(1,1392)	1:127:A:THR:H	1:25:A:VAL:HG12	10	0.45	0.11	0.47
(1,1392)	1:127:A:THR:H	1:25:A:VAL:HG13	10	0.45	0.11	0.47
(1,2264)	1:61:A:GLY:H	1:59:A:MET:HG2	10	0.45	0.25	0.37
(1,2264)	1:61:A:GLY:H	1:59:A:MET:HG3	10	0.45	0.25	0.37
(1,1613)	1:101:A:PRO:HA	1:99:A:LEU:HD21	10	0.41	0.18	0.39
(1,1613)	1:101:A:PRO:HA	1:99:A:LEU:HD22	10	0.41	0.18	0.39
(1,1613)	1:101:A:PRO:HA	1:99:A:LEU:HD23	10	0.41	0.18	0.39
(1,1393)	1:25:A:VAL:H	1:25:A:VAL:HG11	10	0.41	0.01	0.42
(1,1393)	1:25:A:VAL:H	1:25:A:VAL:HG12	10	0.41	0.01	0.42
(1,1393)	1:25:A:VAL:H	1:25:A:VAL:HG13	10	0.41	0.01	0.42
(1,2105)	1:43:A:PRO:HB3	1:45:A:ALA:H	10	0.41	0.17	0.36
(1,1897)	1:25:A:VAL:HG11	1:24:A:GLN:H	10	0.41	0.04	0.41
(1,1897)	1:25:A:VAL:HG12	1:24:A:GLN:H	10	0.41	0.04	0.41
(1,1897)	1:25:A:VAL:HG13	1:24:A:GLN:H	10	0.41	0.04	0.41
(1,830)	1:86:A:THR:HA	1:97:A:LEU:HB2	10	0.4	0.1	0.4
(1,178)	1:25:A:VAL:H	1:24:A:GLN:HG3	10	0.39	0.07	0.37
(1,952)	1:96:A:SER:HA	1:36:A:LEU:HB3	10	0.38	0.14	0.4
(1,1003)	1:100:A:ASP:HA	1:99:A:LEU:HD21	10	0.37	0.06	0.38
(1,1003)	1:100:A:ASP:HA	1:99:A:LEU:HD22	10	0.37	0.06	0.38
(1,1003)	1:100:A:ASP:HA	1:99:A:LEU:HD23	10	0.37	0.06	0.38

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1755)	1:86:A:THR:HG21	1:10:A:VAL:H	10	0.36	0.06	0.36
(1,1755)	1:86:A:THR:HG22	1:10:A:VAL:H	10	0.36	0.06	0.36
(1,1755)	1:86:A:THR:HG23	1:10:A:VAL:H	10	0.36	0.06	0.36
(1,2508)	1:85:A:HIS:H	1:97:A:LEU:H	10	0.36	0.14	0.3
(1,1930)	1:26:A:SER:H	1:25:A:VAL:HG21	10	0.3	0.03	0.31
(1,1930)	1:26:A:SER:H	1:25:A:VAL:HG22	10	0.3	0.03	0.31
(1,1930)	1:26:A:SER:H	1:25:A:VAL:HG23	10	0.3	0.03	0.31
(1,973)	1:98:A:THR:H	1:97:A:LEU:HB3	10	0.28	0.05	0.27
(1,2395)	1:83:A:VAL:HG21	1:84:A:ALA:H	10	0.24	0.06	0.23
(1,2395)	1:83:A:VAL:HG22	1:84:A:ALA:H	10	0.24	0.06	0.23
(1,2395)	1:83:A:VAL:HG23	1:84:A:ALA:H	10	0.24	0.06	0.23
(1,813)	1:85:A:HIS:HB3	1:86:A:THR:H	10	0.22	0.05	0.22
(1,3249)	1:128:A:LEU:HB2	1:129:A:VAL:H	10	0.21	0.08	0.19
(1,3249)	1:27:A:LYS:HG2	1:129:A:VAL:H	10	0.21	0.08	0.19
(1,21)	1:10:A:VAL:HB	1:9:A:THR:HA	10	0.2	0.03	0.2
(1,2568)	1:104:A:LEU:HB3	1:104:A:LEU:H	10	0.2	0.05	0.2
(1,2365)	1:79:A:ASP:H	1:75:A:VAL:HG11	9	2.11	0.74	1.76
(1,2365)	1:79:A:ASP:H	1:75:A:VAL:HG12	9	2.11	0.74	1.76
(1,2365)	1:79:A:ASP:H	1:75:A:VAL:HG13	9	2.11	0.74	1.76
(1,3261)	1:104:A:LEU:HB2	1:109:A:TYR:HE1	9	1.59	0.23	1.67
(1,3261)	1:109:A:TYR:HE2	1:55:A:LYS:HD3	9	1.59	0.23	1.67
(1,3261)	1:109:A:TYR:HE1	1:55:A:LYS:HD3	9	1.59	0.23	1.67
(1,2362)	1:79:A:ASP:H	1:76:A:LYS:HB2	9	1.35	0.87	1.01
(1,2303)	1:67:A:VAL:HG11	1:66:A:GLY:H	9	1.22	0.08	1.23
(1,2303)	1:67:A:VAL:HG12	1:66:A:GLY:H	9	1.22	0.08	1.23
(1,2303)	1:67:A:VAL:HG13	1:66:A:GLY:H	9	1.22	0.08	1.23
(1,3208)	1:76:A:LYS:HD3	1:79:A:ASP:H	9	1.16	0.55	1.07
(1,3208)	1:79:A:ASP:H	1:75:A:VAL:HB	9	1.16	0.55	1.07
(1,3208)	1:76:A:LYS:HD2	1:79:A:ASP:H	9	1.16	0.55	1.07
(1,1061)	1:105:A:ALA:HA	1:128:A:LEU:HD11	9	1.14	0.46	1.1
(1,1061)	1:105:A:ALA:HA	1:128:A:LEU:HD12	9	1.14	0.46	1.1
(1,1061)	1:105:A:ALA:HA	1:128:A:LEU:HD13	9	1.14	0.46	1.1
(1,551)	1:83:A:VAL:HG11	1:54:A:ALA:HA	9	1.13	0.17	1.15
(1,551)	1:83:A:VAL:HG12	1:54:A:ALA:HA	9	1.13	0.17	1.15
(1,551)	1:83:A:VAL:HG13	1:54:A:ALA:HA	9	1.13	0.17	1.15
(1,1797)	1:15:A:ASN:HB3	1:13:A:ASN:HD21	9	1.1	0.45	1.17
(1,2961)	1:83:A:VAL:HG11	1:109:A:TYR:HD1	9	1.1	0.16	1.16
(1,2961)	1:83:A:VAL:HG11	1:109:A:TYR:HD2	9	1.1	0.16	1.16
(1,2961)	1:83:A:VAL:HG12	1:109:A:TYR:HD1	9	1.1	0.16	1.16
(1,2961)	1:83:A:VAL:HG12	1:109:A:TYR:HD2	9	1.1	0.16	1.16
(1,2961)	1:83:A:VAL:HG13	1:109:A:TYR:HD1	9	1.1	0.16	1.16
(1,2961)	1:83:A:VAL:HG13	1:109:A:TYR:HD2	9	1.1	0.16	1.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1680)	1:27:A:LYS:HG2	1:128:A:LEU:HD21	9	1.1	0.63	0.86
(1,1680)	1:27:A:LYS:HG2	1:128:A:LEU:HD22	9	1.1	0.63	0.86
(1,1680)	1:27:A:LYS:HG2	1:128:A:LEU:HD23	9	1.1	0.63	0.86
(1,1680)	1:27:A:LYS:HG3	1:128:A:LEU:HD21	9	1.1	0.63	0.86
(1,1680)	1:27:A:LYS:HG3	1:128:A:LEU:HD22	9	1.1	0.63	0.86
(1,1680)	1:27:A:LYS:HG3	1:128:A:LEU:HD23	9	1.1	0.63	0.86
(1,580)	1:130:A:ASP:HA	1:128:A:LEU:HD21	9	0.89	0.66	0.84
(1,580)	1:130:A:ASP:HA	1:128:A:LEU:HD22	9	0.89	0.66	0.84
(1,580)	1:130:A:ASP:HA	1:128:A:LEU:HD23	9	0.89	0.66	0.84
(1,2214)	1:83:A:VAL:HG11	1:55:A:LYS:H	9	0.85	0.25	0.81
(1,2214)	1:83:A:VAL:HG12	1:55:A:LYS:H	9	0.85	0.25	0.81
(1,2214)	1:83:A:VAL:HG13	1:55:A:LYS:H	9	0.85	0.25	0.81
(1,1702)	1:83:A:VAL:HG21	1:99:A:LEU:HD11	9	0.83	0.41	0.64
(1,1702)	1:83:A:VAL:HG21	1:99:A:LEU:HD12	9	0.83	0.41	0.64
(1,1702)	1:83:A:VAL:HG21	1:99:A:LEU:HD13	9	0.83	0.41	0.64
(1,1702)	1:83:A:VAL:HG22	1:99:A:LEU:HD11	9	0.83	0.41	0.64
(1,1702)	1:83:A:VAL:HG22	1:99:A:LEU:HD12	9	0.83	0.41	0.64
(1,1702)	1:83:A:VAL:HG22	1:99:A:LEU:HD13	9	0.83	0.41	0.64
(1,1702)	1:83:A:VAL:HG23	1:99:A:LEU:HD11	9	0.83	0.41	0.64
(1,1702)	1:83:A:VAL:HG23	1:99:A:LEU:HD12	9	0.83	0.41	0.64
(1,1702)	1:83:A:VAL:HG23	1:99:A:LEU:HD13	9	0.83	0.41	0.64
(1,1303)	1:56:A:ALA:H	1:55:A:LYS:HD2	9	0.82	0.44	0.58
(1,1547)	1:83:A:VAL:HG21	1:84:A:ALA:HB1	9	0.79	0.03	0.79
(1,1547)	1:83:A:VAL:HG21	1:84:A:ALA:HB2	9	0.79	0.03	0.79
(1,1547)	1:83:A:VAL:HG21	1:84:A:ALA:HB3	9	0.79	0.03	0.79
(1,1547)	1:83:A:VAL:HG22	1:84:A:ALA:HB1	9	0.79	0.03	0.79
(1,1547)	1:83:A:VAL:HG22	1:84:A:ALA:HB2	9	0.79	0.03	0.79
(1,1547)	1:83:A:VAL:HG22	1:84:A:ALA:HB3	9	0.79	0.03	0.79
(1,1547)	1:83:A:VAL:HG23	1:84:A:ALA:HB1	9	0.79	0.03	0.79
(1,1547)	1:83:A:VAL:HG23	1:84:A:ALA:HB2	9	0.79	0.03	0.79
(1,1547)	1:83:A:VAL:HG23	1:84:A:ALA:HB3	9	0.79	0.03	0.79
(1,1506)	1:81:A:ARG:HB2	1:62:A:VAL:HG11	9	0.67	0.41	0.79
(1,1506)	1:81:A:ARG:HB2	1:62:A:VAL:HG12	9	0.67	0.41	0.79
(1,1506)	1:81:A:ARG:HB2	1:62:A:VAL:HG13	9	0.67	0.41	0.79
(1,1498)	1:62:A:VAL:HG11	1:54:A:ALA:H	9	0.65	0.2	0.7
(1,1498)	1:62:A:VAL:HG12	1:54:A:ALA:H	9	0.65	0.2	0.7
(1,1498)	1:62:A:VAL:HG13	1:54:A:ALA:H	9	0.65	0.2	0.7
(1,1064)	1:107:A:GLY:HA2	1:55:A:LYS:HD3	9	0.64	0.22	0.71
(1,2595)	1:74:A:TYR:HB3	1:50:A:ASN:HD21	9	0.64	0.31	0.59
(1,2304)	1:67:A:VAL:HG11	1:67:A:VAL:H	9	0.62	0.0	0.62
(1,2304)	1:67:A:VAL:HG12	1:67:A:VAL:H	9	0.62	0.0	0.62
(1,2304)	1:67:A:VAL:HG13	1:67:A:VAL:H	9	0.62	0.0	0.62

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,646)	1:76:A:LYS:HB3	1:66:A:GLY:HA3	9	0.62	0.44	0.47
(1,639)	1:67:A:VAL:HG11	1:64:A:LYS:HA	9	0.61	0.24	0.66
(1,639)	1:67:A:VAL:HG12	1:64:A:LYS:HA	9	0.61	0.24	0.66
(1,639)	1:67:A:VAL:HG13	1:64:A:LYS:HA	9	0.61	0.24	0.66
(1,1514)	1:75:A:VAL:HB	1:69:A:ALA:HB1	9	0.61	0.12	0.59
(1,1514)	1:75:A:VAL:HB	1:69:A:ALA:HB2	9	0.61	0.12	0.59
(1,1514)	1:75:A:VAL:HB	1:69:A:ALA:HB3	9	0.61	0.12	0.59
(1,1461)	1:126:A:VAL:HG11	1:51:A:LEU:HD21	9	0.53	0.25	0.6
(1,1461)	1:126:A:VAL:HG11	1:51:A:LEU:HD22	9	0.53	0.25	0.6
(1,1461)	1:126:A:VAL:HG11	1:51:A:LEU:HD23	9	0.53	0.25	0.6
(1,1461)	1:126:A:VAL:HG12	1:51:A:LEU:HD21	9	0.53	0.25	0.6
(1,1461)	1:126:A:VAL:HG12	1:51:A:LEU:HD22	9	0.53	0.25	0.6
(1,1461)	1:126:A:VAL:HG12	1:51:A:LEU:HD23	9	0.53	0.25	0.6
(1,1461)	1:126:A:VAL:HG13	1:51:A:LEU:HD21	9	0.53	0.25	0.6
(1,1461)	1:126:A:VAL:HG13	1:51:A:LEU:HD22	9	0.53	0.25	0.6
(1,1461)	1:126:A:VAL:HG13	1:51:A:LEU:HD23	9	0.53	0.25	0.6
(1,678)	1:68:A:GLY:HA3	1:67:A:VAL:HG21	9	0.33	0.06	0.33
(1,678)	1:68:A:GLY:HA3	1:67:A:VAL:HG22	9	0.33	0.06	0.33
(1,678)	1:68:A:GLY:HA3	1:67:A:VAL:HG23	9	0.33	0.06	0.33
(1,1553)	1:83:A:VAL:HG11	1:83:A:VAL:H	9	0.32	0.01	0.31
(1,1553)	1:83:A:VAL:HG12	1:83:A:VAL:H	9	0.32	0.01	0.31
(1,1553)	1:83:A:VAL:HG13	1:83:A:VAL:H	9	0.32	0.01	0.31
(1,2925)	1:63:A:PHE:HD1	1:112:A:ALA:HB1	9	0.26	0.09	0.22
(1,2925)	1:63:A:PHE:HD1	1:112:A:ALA:HB2	9	0.26	0.09	0.22
(1,2925)	1:63:A:PHE:HD1	1:112:A:ALA:HB3	9	0.26	0.09	0.22
(1,2925)	1:63:A:PHE:HD2	1:112:A:ALA:HB1	9	0.26	0.09	0.22
(1,2925)	1:63:A:PHE:HD2	1:112:A:ALA:HB2	9	0.26	0.09	0.22
(1,2925)	1:63:A:PHE:HD2	1:112:A:ALA:HB3	9	0.26	0.09	0.22
(1,1426)	1:86:A:THR:HG21	1:36:A:LEU:HD11	9	0.24	0.06	0.24
(1,1426)	1:86:A:THR:HG21	1:36:A:LEU:HD12	9	0.24	0.06	0.24
(1,1426)	1:86:A:THR:HG21	1:36:A:LEU:HD13	9	0.24	0.06	0.24
(1,1426)	1:86:A:THR:HG22	1:36:A:LEU:HD11	9	0.24	0.06	0.24
(1,1426)	1:86:A:THR:HG22	1:36:A:LEU:HD12	9	0.24	0.06	0.24
(1,1426)	1:86:A:THR:HG22	1:36:A:LEU:HD13	9	0.24	0.06	0.24
(1,1426)	1:86:A:THR:HG23	1:36:A:LEU:HD11	9	0.24	0.06	0.24
(1,1426)	1:86:A:THR:HG23	1:36:A:LEU:HD12	9	0.24	0.06	0.24
(1,1426)	1:86:A:THR:HG23	1:36:A:LEU:HD13	9	0.24	0.06	0.24
(1,418)	1:43:A:PRO:HD3	1:42:A:GLN:HB2	9	0.22	0.06	0.19
(1,418)	1:43:A:PRO:HD3	1:42:A:GLN:HB3	9	0.22	0.06	0.19
(1,1684)	1:128:A:LEU:HD21	1:25:A:VAL:HG21	8	1.81	0.1	1.8
(1,1684)	1:128:A:LEU:HD21	1:25:A:VAL:HG22	8	1.81	0.1	1.8
(1,1684)	1:128:A:LEU:HD21	1:25:A:VAL:HG23	8	1.81	0.1	1.8

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1684)	1:128:A:LEU:HD22	1:25:A:VAL:HG21	8	1.81	0.1	1.8
(1,1684)	1:128:A:LEU:HD22	1:25:A:VAL:HG22	8	1.81	0.1	1.8
(1,1684)	1:128:A:LEU:HD22	1:25:A:VAL:HG23	8	1.81	0.1	1.8
(1,1684)	1:128:A:LEU:HD23	1:25:A:VAL:HG21	8	1.81	0.1	1.8
(1,1684)	1:128:A:LEU:HD23	1:25:A:VAL:HG22	8	1.81	0.1	1.8
(1,1684)	1:128:A:LEU:HD23	1:25:A:VAL:HG23	8	1.81	0.1	1.8
(1,1799)	1:13:A:ASN:HD21	1:17:A:GLN:HB3	8	1.63	0.48	1.74
(1,463)	1:88:A:LEU:HG	1:48:A:GLY:HA2	8	0.86	0.46	1.04
(1,643)	1:76:A:LYS:HD2	1:66:A:GLY:HA3	8	0.72	0.32	0.66
(1,643)	1:76:A:LYS:HD3	1:66:A:GLY:HA3	8	0.72	0.32	0.66
(1,2179)	1:51:A:LEU:H	1:95:A:SER:HB2	8	0.7	0.33	0.66
(1,1095)	1:110:A:LYS:HD3	1:109:A:TYR:HA	8	0.69	0.41	0.5
(1,2591)	1:106:A:ASP:H	1:128:A:LEU:HD11	8	0.63	0.3	0.68
(1,2591)	1:106:A:ASP:H	1:128:A:LEU:HD12	8	0.63	0.3	0.68
(1,2591)	1:106:A:ASP:H	1:128:A:LEU:HD13	8	0.63	0.3	0.68
(1,2676)	1:75:A:VAL:HG21	1:114:A:THR:H	8	0.55	0.24	0.56
(1,2676)	1:75:A:VAL:HG22	1:114:A:THR:H	8	0.55	0.24	0.56
(1,2676)	1:75:A:VAL:HG23	1:114:A:THR:H	8	0.55	0.24	0.56
(1,1525)	1:114:A:THR:HG21	1:75:A:VAL:HG21	8	0.54	0.26	0.56
(1,1525)	1:114:A:THR:HG21	1:75:A:VAL:HG22	8	0.54	0.26	0.56
(1,1525)	1:114:A:THR:HG21	1:75:A:VAL:HG23	8	0.54	0.26	0.56
(1,1525)	1:114:A:THR:HG22	1:75:A:VAL:HG21	8	0.54	0.26	0.56
(1,1525)	1:114:A:THR:HG22	1:75:A:VAL:HG22	8	0.54	0.26	0.56
(1,1525)	1:114:A:THR:HG22	1:75:A:VAL:HG23	8	0.54	0.26	0.56
(1,1525)	1:114:A:THR:HG23	1:75:A:VAL:HG21	8	0.54	0.26	0.56
(1,1525)	1:114:A:THR:HG23	1:75:A:VAL:HG22	8	0.54	0.26	0.56
(1,1525)	1:114:A:THR:HG23	1:75:A:VAL:HG23	8	0.54	0.26	0.56
(1,2469)	1:92:A:GLY:H	1:38:A:HIS:HB2	8	0.53	0.31	0.45
(1,3264)	1:111:A:PHE:HD2	1:20:A:THR:HG21	8	0.53	0.39	0.46
(1,3264)	1:111:A:PHE:HD2	1:36:A:LEU:HD22	8	0.53	0.39	0.46
(1,3264)	1:111:A:PHE:HD1	1:20:A:THR:HG23	8	0.53	0.39	0.46
(1,3264)	1:111:A:PHE:HD1	1:20:A:THR:HG21	8	0.53	0.39	0.46
(1,3264)	1:111:A:PHE:HD2	1:20:A:THR:HG22	8	0.53	0.39	0.46
(1,3264)	1:111:A:PHE:HD1	1:20:A:THR:HG22	8	0.53	0.39	0.46
(1,258)	1:6:A:CYS:HB2	1:32:A:PHE:HA	8	0.52	0.16	0.54
(1,2342)	1:75:A:VAL:HB	1:74:A:TYR:H	8	0.52	0.07	0.54
(1,2876)	1:38:A:HIS:HE1	1:13:A:ASN:HB2	8	0.48	0.14	0.46
(1,730)	1:75:A:VAL:HB	1:75:A:VAL:H	8	0.45	0.03	0.45
(1,2902)	1:49:A:HIS:HD2	1:90:A:GLY:HA3	8	0.35	0.15	0.36
(1,2200)	1:53:A:ILE:H	1:52:A:VAL:HG21	8	0.35	0.21	0.25
(1,2200)	1:53:A:ILE:H	1:52:A:VAL:HG22	8	0.35	0.21	0.25
(1,2200)	1:53:A:ILE:H	1:52:A:VAL:HG23	8	0.35	0.21	0.25

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3196)	1:59:A:MET:HG3	1:59:A:MET:H	8	0.32	0.03	0.33
(1,52)	1:49:A:HIS:HD2	1:12:A:SER:HB3	8	0.32	0.12	0.34
(1,2836)	1:18:A:PHE:HE1	1:36:A:LEU:HD21	8	0.28	0.09	0.29
(1,2836)	1:18:A:PHE:HE1	1:36:A:LEU:HD22	8	0.28	0.09	0.29
(1,2836)	1:18:A:PHE:HE1	1:36:A:LEU:HD23	8	0.28	0.09	0.29
(1,2836)	1:18:A:PHE:HE2	1:36:A:LEU:HD21	8	0.28	0.09	0.29
(1,2836)	1:18:A:PHE:HE2	1:36:A:LEU:HD22	8	0.28	0.09	0.29
(1,2836)	1:18:A:PHE:HE2	1:36:A:LEU:HD23	8	0.28	0.09	0.29
(1,1309)	1:114:A:THR:HG1	1:50:A:ASN:HB2	8	0.28	0.07	0.29
(1,487)	1:50:A:ASN:HD22	1:50:A:ASN:HA	8	0.16	0.01	0.16
(1,253)	1:98:A:THR:HB	1:31:A:GLU:HG2	7	1.44	0.35	1.38
(1,253)	1:98:A:THR:HB	1:31:A:GLU:HG3	7	1.44	0.35	1.38
(1,753)	1:76:A:LYS:HD2	1:77:A:PRO:HD3	7	1.3	0.19	1.32
(1,753)	1:76:A:LYS:HD3	1:77:A:PRO:HD3	7	1.3	0.19	1.32
(1,1671)	1:25:A:VAL:HB	1:126:A:VAL:HG11	7	1.24	0.21	1.36
(1,1671)	1:25:A:VAL:HB	1:126:A:VAL:HG12	7	1.24	0.21	1.36
(1,1671)	1:25:A:VAL:HB	1:126:A:VAL:HG13	7	1.24	0.21	1.36
(1,2209)	1:54:A:ALA:H	1:126:A:VAL:HG21	7	1.07	0.22	1.01
(1,2209)	1:54:A:ALA:H	1:126:A:VAL:HG22	7	1.07	0.22	1.01
(1,2209)	1:54:A:ALA:H	1:126:A:VAL:HG23	7	1.07	0.22	1.01
(1,3168)	1:24:A:GLN:H	1:34:A:ILE:HG12	7	1.04	0.22	1.11
(1,2413)	1:86:A:THR:H	1:52:A:VAL:HG21	7	0.92	0.32	1.1
(1,2413)	1:86:A:THR:H	1:52:A:VAL:HG22	7	0.92	0.32	1.1
(1,2413)	1:86:A:THR:H	1:52:A:VAL:HG23	7	0.92	0.32	1.1
(1,795)	1:82:A:VAL:HB	1:75:A:VAL:HG11	7	0.92	0.47	0.83
(1,795)	1:82:A:VAL:HB	1:75:A:VAL:HG12	7	0.92	0.47	0.83
(1,795)	1:82:A:VAL:HB	1:75:A:VAL:HG13	7	0.92	0.47	0.83
(1,1705)	1:99:A:LEU:HD11	1:31:A:GLU:HB2	7	0.87	0.3	0.81
(1,1705)	1:99:A:LEU:HD12	1:31:A:GLU:HB2	7	0.87	0.3	0.81
(1,1705)	1:99:A:LEU:HD13	1:31:A:GLU:HB2	7	0.87	0.3	0.81
(1,2623)	1:125:A:LYS:HD2	1:110:A:LYS:H	7	0.84	0.59	0.63
(1,2623)	1:125:A:LYS:HD3	1:110:A:LYS:H	7	0.84	0.59	0.63
(1,2529)	1:99:A:LEU:H	1:31:A:GLU:HB2	7	0.83	0.38	0.84
(1,2647)	1:112:A:ALA:H	1:126:A:VAL:HG21	7	0.79	0.12	0.76
(1,2647)	1:112:A:ALA:H	1:126:A:VAL:HG22	7	0.79	0.12	0.76
(1,2647)	1:112:A:ALA:H	1:126:A:VAL:HG23	7	0.79	0.12	0.76
(1,3166)	1:126:A:VAL:HG13	1:23:A:ILE:H	7	0.71	0.15	0.72
(1,3166)	1:126:A:VAL:HG12	1:23:A:ILE:H	7	0.71	0.15	0.72
(1,3166)	1:126:A:VAL:HG11	1:23:A:ILE:H	7	0.71	0.15	0.72
(1,1667)	1:53:A:ILE:HB	1:126:A:VAL:HG21	7	0.67	0.22	0.61
(1,1667)	1:53:A:ILE:HB	1:126:A:VAL:HG22	7	0.67	0.22	0.61
(1,1667)	1:53:A:ILE:HB	1:126:A:VAL:HG23	7	0.67	0.22	0.61

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1543)	1:85:A:HIS:HD2	1:82:A:VAL:HG21	7	0.62	0.35	0.64
(1,1543)	1:85:A:HIS:HD2	1:82:A:VAL:HG22	7	0.62	0.35	0.64
(1,1543)	1:85:A:HIS:HD2	1:82:A:VAL:HG23	7	0.62	0.35	0.64
(1,2542)	1:100:A:ASP:H	1:83:A:VAL:HA	7	0.61	0.39	0.47
(1,1016)	1:99:A:LEU:HD21	1:101:A:PRO:HD3	7	0.59	0.19	0.62
(1,1016)	1:99:A:LEU:HD22	1:101:A:PRO:HD3	7	0.59	0.19	0.62
(1,1016)	1:99:A:LEU:HD23	1:101:A:PRO:HD3	7	0.59	0.19	0.62
(1,741)	1:77:A:PRO:HA	1:75:A:VAL:HG11	7	0.56	0.13	0.54
(1,741)	1:77:A:PRO:HA	1:75:A:VAL:HG12	7	0.56	0.13	0.54
(1,741)	1:77:A:PRO:HA	1:75:A:VAL:HG13	7	0.56	0.13	0.54
(1,2302)	1:76:A:LYS:HB3	1:66:A:GLY:H	7	0.55	0.5	0.31
(1,2629)	1:125:A:LYS:HD2	1:111:A:PHE:H	7	0.55	0.59	0.29
(1,2629)	1:125:A:LYS:HD3	1:111:A:PHE:H	7	0.55	0.59	0.29
(1,1801)	1:13:A:ASN:HD22	1:17:A:GLN:HB3	7	0.54	0.16	0.45
(1,2840)	1:53:A:ILE:HD11	1:32:A:PHE:HD1	7	0.53	0.41	0.36
(1,2840)	1:53:A:ILE:HD11	1:32:A:PHE:HD2	7	0.53	0.41	0.36
(1,2840)	1:53:A:ILE:HD12	1:32:A:PHE:HD1	7	0.53	0.41	0.36
(1,2840)	1:53:A:ILE:HD12	1:32:A:PHE:HD2	7	0.53	0.41	0.36
(1,2840)	1:53:A:ILE:HD13	1:32:A:PHE:HD1	7	0.53	0.41	0.36
(1,2840)	1:53:A:ILE:HD13	1:32:A:PHE:HD2	7	0.53	0.41	0.36
(1,1879)	1:20:A:THR:H	1:19:A:ASN:HB3	7	0.52	0.19	0.62
(1,994)	1:83:A:VAL:HG21	1:99:A:LEU:HB3	7	0.52	0.23	0.46
(1,994)	1:83:A:VAL:HG22	1:99:A:LEU:HB3	7	0.52	0.23	0.46
(1,994)	1:83:A:VAL:HG23	1:99:A:LEU:HB3	7	0.52	0.23	0.46
(1,1653)	1:121:A:LEU:HA	1:121:A:LEU:HD21	7	0.51	0.05	0.5
(1,1653)	1:121:A:LEU:HA	1:121:A:LEU:HD22	7	0.51	0.05	0.5
(1,1653)	1:121:A:LEU:HA	1:121:A:LEU:HD23	7	0.51	0.05	0.5
(1,1609)	1:99:A:LEU:HD21	1:32:A:PHE:H	7	0.45	0.23	0.4
(1,1609)	1:99:A:LEU:HD22	1:32:A:PHE:H	7	0.45	0.23	0.4
(1,1609)	1:99:A:LEU:HD23	1:32:A:PHE:H	7	0.45	0.23	0.4
(1,2955)	1:55:A:LYS:HB3	1:109:A:TYR:HE1	7	0.43	0.14	0.39
(1,2955)	1:55:A:LYS:HB3	1:109:A:TYR:HE2	7	0.43	0.14	0.39
(1,1379)	1:53:A:ILE:HD11	1:23:A:ILE:HG21	7	0.38	0.09	0.37
(1,1379)	1:53:A:ILE:HD11	1:23:A:ILE:HG22	7	0.38	0.09	0.37
(1,1379)	1:53:A:ILE:HD11	1:23:A:ILE:HG23	7	0.38	0.09	0.37
(1,1379)	1:53:A:ILE:HD12	1:23:A:ILE:HG21	7	0.38	0.09	0.37
(1,1379)	1:53:A:ILE:HD12	1:23:A:ILE:HG22	7	0.38	0.09	0.37
(1,1379)	1:53:A:ILE:HD12	1:23:A:ILE:HG23	7	0.38	0.09	0.37
(1,1379)	1:53:A:ILE:HD13	1:23:A:ILE:HG21	7	0.38	0.09	0.37
(1,1379)	1:53:A:ILE:HD13	1:23:A:ILE:HG22	7	0.38	0.09	0.37
(1,1379)	1:53:A:ILE:HD13	1:23:A:ILE:HG23	7	0.38	0.09	0.37
(1,1249)	1:123:A:ASN:HB3	1:124:A:GLY:H	7	0.26	0.08	0.28

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1133)	1:111:A:PHE:HB2	1:126:A:VAL:HG21	7	0.25	0.1	0.23
(1,1133)	1:111:A:PHE:HB2	1:126:A:VAL:HG22	7	0.25	0.1	0.23
(1,1133)	1:111:A:PHE:HB2	1:126:A:VAL:HG23	7	0.25	0.1	0.23
(1,230)	1:29:A:CYS:HB2	1:25:A:VAL:HG21	7	0.24	0.09	0.23
(1,230)	1:29:A:CYS:HB2	1:25:A:VAL:HG22	7	0.24	0.09	0.23
(1,230)	1:29:A:CYS:HB2	1:25:A:VAL:HG23	7	0.24	0.09	0.23
(1,230)	1:29:A:CYS:HB3	1:25:A:VAL:HG21	7	0.24	0.09	0.23
(1,230)	1:29:A:CYS:HB3	1:25:A:VAL:HG22	7	0.24	0.09	0.23
(1,230)	1:29:A:CYS:HB3	1:25:A:VAL:HG23	7	0.24	0.09	0.23
(1,2293)	1:65:A:ASP:HB3	1:65:A:ASP:H	7	0.2	0.02	0.2
(1,3221)	1:94:A:GLU:HB3	1:95:A:SER:H	7	0.18	0.04	0.16
(1,3221)	1:94:A:GLU:HG2	1:95:A:SER:H	7	0.18	0.04	0.16
(1,496)	1:114:A:THR:HG1	1:50:A:ASN:HB3	7	0.17	0.07	0.16
(1,2812)	1:129:A:VAL:H	1:104:A:LEU:HD11	6	1.26	0.44	1.44
(1,2812)	1:129:A:VAL:H	1:104:A:LEU:HD12	6	1.26	0.44	1.44
(1,2812)	1:129:A:VAL:H	1:104:A:LEU:HD13	6	1.26	0.44	1.44
(1,3198)	1:64:A:LYS:HD3	1:61:A:GLY:H	6	0.75	0.55	0.5
(1,3198)	1:64:A:LYS:HD2	1:61:A:GLY:H	6	0.75	0.55	0.5
(1,3198)	1:81:A:ARG:HB3	1:61:A:GLY:H	6	0.75	0.55	0.5
(1,126)	1:21:A:LYS:HE2	1:21:A:LYS:HB2	6	0.73	0.14	0.81
(1,126)	1:21:A:LYS:HE3	1:21:A:LYS:HB2	6	0.73	0.14	0.81
(1,1978)	1:31:A:GLU:H	1:30:A:LYS:HD3	6	0.68	0.31	0.65
(1,1001)	1:100:A:ASP:HA	1:31:A:GLU:HB2	6	0.67	0.35	0.64
(1,2241)	1:57:A:GLU:HG3	1:58:A:ASP:H	6	0.54	0.29	0.41
(1,2611)	1:110:A:LYS:HG2	1:109:A:TYR:H	6	0.44	0.19	0.46
(1,1654)	1:122:A:MET:HG2	1:121:A:LEU:HD11	6	0.43	0.18	0.37
(1,1654)	1:122:A:MET:HG2	1:121:A:LEU:HD12	6	0.43	0.18	0.37
(1,1654)	1:122:A:MET:HG2	1:121:A:LEU:HD13	6	0.43	0.18	0.37
(1,1654)	1:122:A:MET:HG3	1:121:A:LEU:HD11	6	0.43	0.18	0.37
(1,1654)	1:122:A:MET:HG3	1:121:A:LEU:HD12	6	0.43	0.18	0.37
(1,1654)	1:122:A:MET:HG3	1:121:A:LEU:HD13	6	0.43	0.18	0.37
(1,46)	1:12:A:SER:HA	1:36:A:LEU:HD21	6	0.34	0.15	0.29
(1,46)	1:12:A:SER:HA	1:36:A:LEU:HD22	6	0.34	0.15	0.29
(1,46)	1:12:A:SER:HA	1:36:A:LEU:HD23	6	0.34	0.15	0.29
(1,1950)	1:27:A:LYS:HD2	1:28:A:ALA:H	6	0.34	0.12	0.4
(1,1950)	1:27:A:LYS:HD3	1:28:A:ALA:H	6	0.34	0.12	0.4
(1,2573)	1:105:A:ALA:H	1:128:A:LEU:HD11	6	0.32	0.19	0.29
(1,2573)	1:105:A:ALA:H	1:128:A:LEU:HD12	6	0.32	0.19	0.29
(1,2573)	1:105:A:ALA:H	1:128:A:LEU:HD13	6	0.32	0.19	0.29
(1,1698)	1:24:A:GLN:HG3	1:129:A:VAL:HG21	6	0.29	0.13	0.3
(1,1698)	1:24:A:GLN:HG3	1:129:A:VAL:HG22	6	0.29	0.13	0.3
(1,1698)	1:24:A:GLN:HG3	1:129:A:VAL:HG23	6	0.29	0.13	0.3

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,35)	1:11:A:GLU:HA	1:36:A:LEU:HD21	6	0.25	0.09	0.22
(1,35)	1:11:A:GLU:HA	1:36:A:LEU:HD22	6	0.25	0.09	0.22
(1,35)	1:11:A:GLU:HA	1:36:A:LEU:HD23	6	0.25	0.09	0.22
(1,228)	1:6:A:CYS:HB2	1:29:A:CYS:HB2	6	0.24	0.1	0.28
(1,228)	1:6:A:CYS:HB2	1:29:A:CYS:HB3	6	0.24	0.1	0.28
(1,3206)	1:78:A:ASP:HA	1:78:A:ASP:H	6	0.2	0.05	0.22
(1,1268)	1:127:A:THR:HB	1:24:A:GLN:HG3	6	0.19	0.05	0.17
(1,2889)	1:66:A:GLY:HA3	1:74:A:TYR:HD1	6	0.18	0.03	0.18
(1,2889)	1:66:A:GLY:HA3	1:74:A:TYR:HD2	6	0.18	0.03	0.18
(1,3226)	1:100:A:ASP:H	1:99:A:LEU:HB3	6	0.17	0.05	0.17
(1,3164)	1:17:A:GLN:H	1:17:A:GLN:HB2	6	0.14	0.03	0.14
(1,1929)	1:104:A:LEU:HD11	1:25:A:VAL:H	5	1.62	0.18	1.53
(1,1929)	1:104:A:LEU:HD12	1:25:A:VAL:H	5	1.62	0.18	1.53
(1,1929)	1:104:A:LEU:HD13	1:25:A:VAL:H	5	1.62	0.18	1.53
(1,1059)	1:104:A:LEU:HG	1:101:A:PRO:HA	5	1.18	0.21	1.24
(1,2556)	1:104:A:LEU:HG	1:103:A:LYS:H	5	1.15	0.14	1.05
(1,1619)	1:109:A:TYR:HE1	1:104:A:LEU:HD21	5	1.12	0.19	1.05
(1,1619)	1:109:A:TYR:HE1	1:104:A:LEU:HD22	5	1.12	0.19	1.05
(1,1619)	1:109:A:TYR:HE1	1:104:A:LEU:HD23	5	1.12	0.19	1.05
(1,1619)	1:109:A:TYR:HE2	1:104:A:LEU:HD21	5	1.12	0.19	1.05
(1,1619)	1:109:A:TYR:HE2	1:104:A:LEU:HD22	5	1.12	0.19	1.05
(1,1619)	1:109:A:TYR:HE2	1:104:A:LEU:HD23	5	1.12	0.19	1.05
(1,3132)	1:104:A:LEU:HD11	1:25:A:VAL:HG12	5	1.03	0.06	1.0
(1,3132)	1:104:A:LEU:HD13	1:25:A:VAL:HG12	5	1.03	0.06	1.0
(1,3132)	1:104:A:LEU:HD11	1:25:A:VAL:HG13	5	1.03	0.06	1.0
(1,3132)	1:104:A:LEU:HD12	1:25:A:VAL:HG12	5	1.03	0.06	1.0
(1,1549)	1:83:A:VAL:HG21	1:104:A:LEU:HD21	5	1.02	0.29	0.96
(1,1549)	1:83:A:VAL:HG21	1:104:A:LEU:HD22	5	1.02	0.29	0.96
(1,1549)	1:83:A:VAL:HG21	1:104:A:LEU:HD23	5	1.02	0.29	0.96
(1,1549)	1:83:A:VAL:HG22	1:104:A:LEU:HD21	5	1.02	0.29	0.96
(1,1549)	1:83:A:VAL:HG22	1:104:A:LEU:HD22	5	1.02	0.29	0.96
(1,1549)	1:83:A:VAL:HG22	1:104:A:LEU:HD23	5	1.02	0.29	0.96
(1,1549)	1:83:A:VAL:HG23	1:104:A:LEU:HD21	5	1.02	0.29	0.96
(1,1549)	1:83:A:VAL:HG23	1:104:A:LEU:HD22	5	1.02	0.29	0.96
(1,1549)	1:83:A:VAL:HG23	1:104:A:LEU:HD23	5	1.02	0.29	0.96
(1,2227)	1:110:A:LYS:HD3	1:56:A:ALA:H	5	0.97	0.62	1.29
(1,984)	1:98:A:THR:HB	1:31:A:GLU:HB2	5	0.94	0.27	0.82
(1,852)	1:88:A:LEU:HB3	1:73:A:ASP:H	5	0.89	0.51	0.68
(1,2569)	1:104:A:LEU:HG	1:104:A:LEU:H	5	0.85	0.11	0.81
(1,822)	1:85:A:HIS:HB3	1:52:A:VAL:HG21	5	0.73	0.19	0.67
(1,822)	1:85:A:HIS:HB3	1:52:A:VAL:HG22	5	0.73	0.19	0.67
(1,822)	1:85:A:HIS:HB3	1:52:A:VAL:HG23	5	0.73	0.19	0.67

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1497)	1:54:A:ALA:HB1	1:52:A:VAL:HG11	5	0.7	0.09	0.67
(1,1497)	1:54:A:ALA:HB1	1:52:A:VAL:HG12	5	0.7	0.09	0.67
(1,1497)	1:54:A:ALA:HB1	1:52:A:VAL:HG13	5	0.7	0.09	0.67
(1,1497)	1:54:A:ALA:HB2	1:52:A:VAL:HG11	5	0.7	0.09	0.67
(1,1497)	1:54:A:ALA:HB2	1:52:A:VAL:HG12	5	0.7	0.09	0.67
(1,1497)	1:54:A:ALA:HB2	1:52:A:VAL:HG13	5	0.7	0.09	0.67
(1,1497)	1:54:A:ALA:HB3	1:52:A:VAL:HG11	5	0.7	0.09	0.67
(1,1497)	1:54:A:ALA:HB3	1:52:A:VAL:HG12	5	0.7	0.09	0.67
(1,1497)	1:54:A:ALA:HB3	1:52:A:VAL:HG13	5	0.7	0.09	0.67
(1,211)	1:26:A:SER:HB3	1:25:A:VAL:HG21	5	0.67	0.41	0.99
(1,211)	1:26:A:SER:HB3	1:25:A:VAL:HG22	5	0.67	0.41	0.99
(1,211)	1:26:A:SER:HB3	1:25:A:VAL:HG23	5	0.67	0.41	0.99
(1,564)	1:55:A:LYS:HB2	1:58:A:ASP:H	5	0.62	0.13	0.63
(1,3143)	1:103:A:LYS:HB3	1:99:A:LEU:HD22	5	0.61	0.24	0.7
(1,3143)	1:103:A:LYS:HB2	1:99:A:LEU:HD23	5	0.61	0.24	0.7
(1,3143)	1:103:A:LYS:HB2	1:99:A:LEU:HD22	5	0.61	0.24	0.7
(1,3143)	1:103:A:LYS:HB2	1:99:A:LEU:HD21	5	0.61	0.24	0.7
(1,3143)	1:103:A:LYS:HB3	1:99:A:LEU:HD21	5	0.61	0.24	0.7
(1,1381)	1:104:A:LEU:HD11	1:25:A:VAL:HG21	5	0.58	0.16	0.47
(1,1381)	1:104:A:LEU:HD11	1:25:A:VAL:HG22	5	0.58	0.16	0.47
(1,1381)	1:104:A:LEU:HD11	1:25:A:VAL:HG23	5	0.58	0.16	0.47
(1,1381)	1:104:A:LEU:HD12	1:25:A:VAL:HG21	5	0.58	0.16	0.47
(1,1381)	1:104:A:LEU:HD12	1:25:A:VAL:HG22	5	0.58	0.16	0.47
(1,1381)	1:104:A:LEU:HD12	1:25:A:VAL:HG23	5	0.58	0.16	0.47
(1,1381)	1:104:A:LEU:HD13	1:25:A:VAL:HG21	5	0.58	0.16	0.47
(1,1381)	1:104:A:LEU:HD13	1:25:A:VAL:HG22	5	0.58	0.16	0.47
(1,1381)	1:104:A:LEU:HD13	1:25:A:VAL:HG23	5	0.58	0.16	0.47
(1,805)	1:85:A:HIS:HA	1:52:A:VAL:HG21	5	0.56	0.02	0.55
(1,805)	1:85:A:HIS:HA	1:52:A:VAL:HG22	5	0.56	0.02	0.55
(1,805)	1:85:A:HIS:HA	1:52:A:VAL:HG23	5	0.56	0.02	0.55
(1,3148)	1:104:A:LEU:HD22	1:126:A:VAL:HG22	5	0.54	0.11	0.55
(1,3148)	1:53:A:ILE:HD12	1:104:A:LEU:HD23	5	0.54	0.11	0.55
(1,3148)	1:53:A:ILE:HD11	1:104:A:LEU:HD21	5	0.54	0.11	0.55
(1,3148)	1:53:A:ILE:HD13	1:104:A:LEU:HD22	5	0.54	0.11	0.55
(1,3148)	1:53:A:ILE:HD11	1:104:A:LEU:HD22	5	0.54	0.11	0.55
(1,1627)	1:83:A:VAL:HG21	1:104:A:LEU:HD11	5	0.54	0.3	0.58
(1,1627)	1:83:A:VAL:HG21	1:104:A:LEU:HD12	5	0.54	0.3	0.58
(1,1627)	1:83:A:VAL:HG21	1:104:A:LEU:HD13	5	0.54	0.3	0.58
(1,1627)	1:83:A:VAL:HG22	1:104:A:LEU:HD11	5	0.54	0.3	0.58
(1,1627)	1:83:A:VAL:HG22	1:104:A:LEU:HD12	5	0.54	0.3	0.58
(1,1627)	1:83:A:VAL:HG22	1:104:A:LEU:HD13	5	0.54	0.3	0.58
(1,1627)	1:83:A:VAL:HG23	1:104:A:LEU:HD11	5	0.54	0.3	0.58

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1627)	1:83:A:VAL:HG23	1:104:A:LEU:HD12	5	0.54	0.3	0.58
(1,1627)	1:83:A:VAL:HG23	1:104:A:LEU:HD13	5	0.54	0.3	0.58
(1,2364)	1:82:A:VAL:HG11	1:79:A:ASP:H	5	0.49	0.45	0.24
(1,2364)	1:82:A:VAL:HG12	1:79:A:ASP:H	5	0.49	0.45	0.24
(1,2364)	1:82:A:VAL:HG13	1:79:A:ASP:H	5	0.49	0.45	0.24
(1,1533)	1:50:A:ASN:HD22	1:75:A:VAL:HG21	5	0.46	0.07	0.46
(1,1533)	1:50:A:ASN:HD22	1:75:A:VAL:HG22	5	0.46	0.07	0.46
(1,1533)	1:50:A:ASN:HD22	1:75:A:VAL:HG23	5	0.46	0.07	0.46
(1,1093)	1:56:A:ALA:HB1	1:108:A:ASP:HB2	5	0.42	0.18	0.42
(1,1093)	1:56:A:ALA:HB2	1:108:A:ASP:HB2	5	0.42	0.18	0.42
(1,1093)	1:56:A:ALA:HB3	1:108:A:ASP:HB2	5	0.42	0.18	0.42
(1,2081)	1:91:A:GLY:HA2	1:42:A:GLN:H	5	0.42	0.29	0.26
(1,233)	1:30:A:LYS:HA	1:30:A:LYS:HD3	5	0.4	0.09	0.35
(1,1063)	1:107:A:GLY:HA2	1:55:A:LYS:HD2	5	0.36	0.19	0.41
(1,1614)	1:32:A:PHE:HB2	1:99:A:LEU:HD21	5	0.35	0.16	0.34
(1,1614)	1:32:A:PHE:HB2	1:99:A:LEU:HD22	5	0.35	0.16	0.34
(1,1614)	1:32:A:PHE:HB2	1:99:A:LEU:HD23	5	0.35	0.16	0.34
(1,1618)	1:109:A:TYR:HD1	1:104:A:LEU:HD21	5	0.35	0.12	0.32
(1,1618)	1:109:A:TYR:HD1	1:104:A:LEU:HD22	5	0.35	0.12	0.32
(1,1618)	1:109:A:TYR:HD1	1:104:A:LEU:HD23	5	0.35	0.12	0.32
(1,1618)	1:109:A:TYR:HD2	1:104:A:LEU:HD21	5	0.35	0.12	0.32
(1,1618)	1:109:A:TYR:HD2	1:104:A:LEU:HD22	5	0.35	0.12	0.32
(1,1618)	1:109:A:TYR:HD2	1:104:A:LEU:HD23	5	0.35	0.12	0.32
(1,1042)	1:104:A:LEU:HA	1:104:A:LEU:HD21	5	0.3	0.01	0.3
(1,1042)	1:104:A:LEU:HA	1:104:A:LEU:HD22	5	0.3	0.01	0.3
(1,1042)	1:104:A:LEU:HA	1:104:A:LEU:HD23	5	0.3	0.01	0.3
(1,1780)	1:12:A:SER:H	1:36:A:LEU:HD21	5	0.28	0.14	0.26
(1,1780)	1:12:A:SER:H	1:36:A:LEU:HD22	5	0.28	0.14	0.26
(1,1780)	1:12:A:SER:H	1:36:A:LEU:HD23	5	0.28	0.14	0.26
(1,3048)	1:25:A:VAL:HB	1:23:A:ILE:HG21	5	0.27	0.11	0.22
(1,3048)	1:25:A:VAL:HB	1:23:A:ILE:HG22	5	0.27	0.11	0.22
(1,3048)	1:25:A:VAL:HB	1:23:A:ILE:HG23	5	0.27	0.11	0.22
(1,2728)	1:122:A:MET:H	1:118:A:HIS:HB2	5	0.23	0.09	0.23
(1,1420)	1:51:A:LEU:H	1:34:A:ILE:HG21	5	0.22	0.1	0.19
(1,1420)	1:51:A:LEU:H	1:34:A:ILE:HG22	5	0.22	0.1	0.19
(1,1420)	1:51:A:LEU:H	1:34:A:ILE:HG23	5	0.22	0.1	0.19
(1,248)	1:31:A:GLU:HB2	1:32:A:PHE:H	5	0.22	0.05	0.21
(1,1786)	1:38:A:HIS:HB3	1:13:A:ASN:H	5	0.2	0.07	0.19
(1,2710)	1:120:A:ALA:H	1:121:A:LEU:HD11	5	0.2	0.03	0.19
(1,2710)	1:120:A:ALA:H	1:121:A:LEU:HD12	5	0.2	0.03	0.19
(1,2710)	1:120:A:ALA:H	1:121:A:LEU:HD13	5	0.2	0.03	0.19
(1,1903)	1:24:A:GLN:HG2	1:24:A:GLN:H	5	0.2	0.06	0.19

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2496)	1:96:A:SER:H	1:36:A:LEU:HB3	5	0.19	0.06	0.16
(1,2950)	1:109:A:TYR:HE1	1:109:A:TYR:HB2	5	0.12	0.01	0.12
(1,2950)	1:109:A:TYR:HE2	1:109:A:TYR:HB2	5	0.12	0.01	0.12
(1,1281)	1:128:A:LEU:HB3	1:129:A:VAL:H	5	0.12	0.01	0.12
(1,3227)	1:104:A:LEU:HB3	1:102:A:ALA:H	4	1.96	1.03	2.51
(1,3227)	1:103:A:LYS:HG3	1:102:A:ALA:H	4	1.96	1.03	2.51
(1,3227)	1:103:A:LYS:HG2	1:102:A:ALA:H	4	1.96	1.03	2.51
(1,44)	1:39:A:THR:HG21	1:11:A:GLU:HG3	4	1.1	0.7	1.06
(1,44)	1:39:A:THR:HG22	1:11:A:GLU:HG3	4	1.1	0.7	1.06
(1,44)	1:39:A:THR:HG23	1:11:A:GLU:HG3	4	1.1	0.7	1.06
(1,82)	1:15:A:ASN:HB2	1:17:A:GLN:HB2	4	1.05	0.59	1.02
(1,2326)	1:88:A:LEU:HD11	1:73:A:ASP:H	4	1.03	0.43	0.86
(1,2326)	1:88:A:LEU:HD12	1:73:A:ASP:H	4	1.03	0.43	0.86
(1,2326)	1:88:A:LEU:HD13	1:73:A:ASP:H	4	1.03	0.43	0.86
(1,1870)	1:19:A:ASN:HD22	1:10:A:VAL:HA	4	0.93	0.12	0.94
(1,2061)	1:38:A:HIS:HA	1:40:A:GLY:H	4	0.93	0.18	1.02
(1,2987)	1:126:A:VAL:HG11	1:111:A:PHE:HD1	4	0.9	0.36	1.1
(1,2987)	1:126:A:VAL:HG11	1:111:A:PHE:HD2	4	0.9	0.36	1.1
(1,2987)	1:126:A:VAL:HG12	1:111:A:PHE:HD1	4	0.9	0.36	1.1
(1,2987)	1:126:A:VAL:HG12	1:111:A:PHE:HD2	4	0.9	0.36	1.1
(1,2987)	1:126:A:VAL:HG13	1:111:A:PHE:HD1	4	0.9	0.36	1.1
(1,2987)	1:126:A:VAL:HG13	1:111:A:PHE:HD2	4	0.9	0.36	1.1
(1,1682)	1:104:A:LEU:HG	1:128:A:LEU:HD21	4	0.88	0.21	0.98
(1,1682)	1:104:A:LEU:HG	1:128:A:LEU:HD22	4	0.88	0.21	0.98
(1,1682)	1:104:A:LEU:HG	1:128:A:LEU:HD23	4	0.88	0.21	0.98
(1,1067)	1:107:A:GLY:HA2	1:55:A:LYS:HG2	4	0.84	0.77	0.44
(1,1067)	1:107:A:GLY:HA2	1:55:A:LYS:HG3	4	0.84	0.77	0.44
(1,2062)	1:40:A:GLY:H	1:13:A:ASN:HA	4	0.84	0.1	0.84
(1,1132)	1:111:A:PHE:HB2	1:126:A:VAL:HG11	4	0.81	0.31	0.96
(1,1132)	1:111:A:PHE:HB2	1:126:A:VAL:HG12	4	0.81	0.31	0.96
(1,1132)	1:111:A:PHE:HB2	1:126:A:VAL:HG13	4	0.81	0.31	0.96
(1,2058)	1:40:A:GLY:H	1:39:A:THR:H	4	0.7	0.06	0.73
(1,1683)	1:104:A:LEU:HD11	1:128:A:LEU:HD21	4	0.66	0.22	0.66
(1,1683)	1:104:A:LEU:HD11	1:128:A:LEU:HD22	4	0.66	0.22	0.66
(1,1683)	1:104:A:LEU:HD11	1:128:A:LEU:HD23	4	0.66	0.22	0.66
(1,1683)	1:104:A:LEU:HD12	1:128:A:LEU:HD21	4	0.66	0.22	0.66
(1,1683)	1:104:A:LEU:HD12	1:128:A:LEU:HD22	4	0.66	0.22	0.66
(1,1683)	1:104:A:LEU:HD12	1:128:A:LEU:HD23	4	0.66	0.22	0.66
(1,1683)	1:104:A:LEU:HD13	1:128:A:LEU:HD21	4	0.66	0.22	0.66
(1,1683)	1:104:A:LEU:HD13	1:128:A:LEU:HD22	4	0.66	0.22	0.66
(1,1683)	1:104:A:LEU:HD13	1:128:A:LEU:HD23	4	0.66	0.22	0.66
(1,2696)	1:117:A:GLY:H	1:67:A:VAL:HG11	4	0.63	0.16	0.63

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2696)	1:117:A:GLY:H	1:67:A:VAL:HG12	4	0.63	0.16	0.63
(1,2696)	1:117:A:GLY:H	1:67:A:VAL:HG13	4	0.63	0.16	0.63
(1,1009)	1:101:A:PRO:HA	1:27:A:LYS:HA	4	0.62	0.17	0.66
(1,2832)	1:18:A:PHE:HE1	1:12:A:SER:HB2	4	0.58	0.15	0.62
(1,2832)	1:18:A:PHE:HE2	1:12:A:SER:HB2	4	0.58	0.15	0.62
(1,889)	1:92:A:GLY:HA2	1:93:A:GLU:HG3	4	0.56	0.15	0.59
(1,2528)	1:99:A:LEU:H	1:31:A:GLU:HG2	4	0.54	0.41	0.36
(1,2528)	1:99:A:LEU:H	1:31:A:GLU:HG3	4	0.54	0.41	0.36
(1,769)	1:77:A:PRO:HG2	1:72:A:THR:HG21	4	0.51	0.21	0.58
(1,769)	1:77:A:PRO:HG2	1:72:A:THR:HG22	4	0.51	0.21	0.58
(1,769)	1:77:A:PRO:HG2	1:72:A:THR:HG23	4	0.51	0.21	0.58
(1,2170)	1:88:A:LEU:HB3	1:50:A:ASN:HD22	4	0.51	0.26	0.5
(1,464)	1:88:A:LEU:HD11	1:48:A:GLY:HA2	4	0.49	0.1	0.47
(1,464)	1:88:A:LEU:HD12	1:48:A:GLY:HA2	4	0.49	0.1	0.47
(1,464)	1:88:A:LEU:HD13	1:48:A:GLY:HA2	4	0.49	0.1	0.47
(1,2068)	1:91:A:GLY:HA3	1:40:A:GLY:H	4	0.47	0.4	0.3
(1,2538)	1:100:A:ASP:H	1:83:A:VAL:HB	4	0.44	0.15	0.45
(1,387)	1:41:A:THR:HA	1:91:A:GLY:HA2	4	0.4	0.12	0.41
(1,1527)	1:82:A:VAL:HG11	1:75:A:VAL:HG21	4	0.4	0.28	0.32
(1,1527)	1:82:A:VAL:HG11	1:75:A:VAL:HG22	4	0.4	0.28	0.32
(1,1527)	1:82:A:VAL:HG11	1:75:A:VAL:HG23	4	0.4	0.28	0.32
(1,1527)	1:82:A:VAL:HG12	1:75:A:VAL:HG21	4	0.4	0.28	0.32
(1,1527)	1:82:A:VAL:HG12	1:75:A:VAL:HG22	4	0.4	0.28	0.32
(1,1527)	1:82:A:VAL:HG12	1:75:A:VAL:HG23	4	0.4	0.28	0.32
(1,1527)	1:82:A:VAL:HG13	1:75:A:VAL:HG21	4	0.4	0.28	0.32
(1,1527)	1:82:A:VAL:HG13	1:75:A:VAL:HG22	4	0.4	0.28	0.32
(1,1527)	1:82:A:VAL:HG13	1:75:A:VAL:HG23	4	0.4	0.28	0.32
(1,1628)	1:101:A:PRO:HB2	1:104:A:LEU:HD11	4	0.36	0.12	0.38
(1,1628)	1:101:A:PRO:HB2	1:104:A:LEU:HD12	4	0.36	0.12	0.38
(1,1628)	1:101:A:PRO:HB2	1:104:A:LEU:HD13	4	0.36	0.12	0.38
(1,3075)	1:55:A:LYS:HB2	1:54:A:ALA:HB3	4	0.36	0.12	0.37
(1,3075)	1:55:A:LYS:HB2	1:54:A:ALA:HB2	4	0.36	0.12	0.37
(1,3243)	1:123:A:ASN:HD21	1:120:A:ALA:HB1	4	0.35	0.15	0.3
(1,3243)	1:123:A:ASN:HD21	1:120:A:ALA:HB2	4	0.35	0.15	0.3
(1,2964)	1:109:A:TYR:HD1	1:128:A:LEU:HD21	4	0.34	0.09	0.35
(1,2964)	1:109:A:TYR:HD1	1:128:A:LEU:HD22	4	0.34	0.09	0.35
(1,2964)	1:109:A:TYR:HD1	1:128:A:LEU:HD23	4	0.34	0.09	0.35
(1,2964)	1:109:A:TYR:HD2	1:128:A:LEU:HD21	4	0.34	0.09	0.35
(1,2964)	1:109:A:TYR:HD2	1:128:A:LEU:HD22	4	0.34	0.09	0.35
(1,2964)	1:109:A:TYR:HD2	1:128:A:LEU:HD23	4	0.34	0.09	0.35
(1,2394)	1:84:A:ALA:H	1:104:A:LEU:HD21	4	0.33	0.1	0.3
(1,2394)	1:84:A:ALA:H	1:104:A:LEU:HD22	4	0.33	0.1	0.3

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2394)	1:84:A:ALA:H	1:104:A:LEU:HD23	4	0.33	0.1	0.3
(1,2945)	1:105:A:ALA:HA	1:109:A:TYR:HE1	4	0.32	0.12	0.38
(1,2945)	1:105:A:ALA:HA	1:109:A:TYR:HE2	4	0.32	0.12	0.38
(1,1301)	1:55:A:LYS:HA	1:55:A:LYS:HD2	4	0.29	0.05	0.28
(1,357)	1:37:A:LYS:HD2	1:35:A:THR:HG21	4	0.28	0.05	0.29
(1,357)	1:37:A:LYS:HD2	1:35:A:THR:HG22	4	0.28	0.05	0.29
(1,357)	1:37:A:LYS:HD2	1:35:A:THR:HG23	4	0.28	0.05	0.29
(1,357)	1:37:A:LYS:HD3	1:35:A:THR:HG21	4	0.28	0.05	0.29
(1,357)	1:37:A:LYS:HD3	1:35:A:THR:HG22	4	0.28	0.05	0.29
(1,357)	1:37:A:LYS:HD3	1:35:A:THR:HG23	4	0.28	0.05	0.29
(1,1535)	1:75:A:VAL:HG21	1:50:A:ASN:HD21	4	0.28	0.14	0.28
(1,1535)	1:75:A:VAL:HG22	1:50:A:ASN:HD21	4	0.28	0.14	0.28
(1,1535)	1:75:A:VAL:HG23	1:50:A:ASN:HD21	4	0.28	0.14	0.28
(1,3190)	1:51:A:LEU:H	1:36:A:LEU:HB3	4	0.27	0.14	0.25
(1,1986)	1:101:A:PRO:HD2	1:32:A:PHE:H	4	0.26	0.19	0.18
(1,2380)	1:82:A:VAL:H	1:79:A:ASP:HB2	4	0.26	0.08	0.26
(1,2380)	1:82:A:VAL:H	1:79:A:ASP:HB3	4	0.26	0.08	0.26
(1,1595)	1:53:A:ILE:HG12	1:97:A:LEU:HD11	4	0.23	0.13	0.2
(1,1595)	1:53:A:ILE:HG12	1:97:A:LEU:HD12	4	0.23	0.13	0.2
(1,1595)	1:53:A:ILE:HG12	1:97:A:LEU:HD13	4	0.23	0.13	0.2
(1,1127)	1:111:A:PHE:HA	1:126:A:VAL:HG21	4	0.22	0.09	0.22
(1,1127)	1:111:A:PHE:HA	1:126:A:VAL:HG22	4	0.22	0.09	0.22
(1,1127)	1:111:A:PHE:HA	1:126:A:VAL:HG23	4	0.22	0.09	0.22
(1,1304)	1:55:A:LYS:HD2	1:55:A:LYS:H	4	0.2	0.11	0.16
(1,1087)	1:108:A:ASP:H	1:108:A:ASP:HB3	4	0.2	0.05	0.22
(1,2624)	1:110:A:LYS:HG2	1:110:A:LYS:H	4	0.19	0.04	0.18
(1,581)	1:27:A:LYS:HB2	1:130:A:ASP:HA	4	0.18	0.04	0.16
(1,581)	1:27:A:LYS:HB3	1:130:A:ASP:HA	4	0.18	0.04	0.16
(1,1523)	1:72:A:THR:HG21	1:72:A:THR:HA	4	0.16	0.01	0.16
(1,1523)	1:72:A:THR:HG22	1:72:A:THR:HA	4	0.16	0.01	0.16
(1,1523)	1:72:A:THR:HG23	1:72:A:THR:HA	4	0.16	0.01	0.16
(1,1901)	1:23:A:ILE:HG13	1:24:A:GLN:H	4	0.15	0.05	0.12
(1,2400)	1:84:A:ALA:H	1:85:A:HIS:HB2	4	0.15	0.02	0.15
(1,2916)	1:122:A:MET:HE1	1:49:A:HIS:HE1	4	0.14	0.01	0.14
(1,2916)	1:122:A:MET:HE2	1:49:A:HIS:HE1	4	0.14	0.01	0.14
(1,2916)	1:122:A:MET:HE3	1:49:A:HIS:HE1	4	0.14	0.01	0.14
(1,1143)	1:111:A:PHE:HB3	1:112:A:ALA:H	4	0.13	0.01	0.14
(1,2817)	1:130:A:ASP:H	1:3:A:ALA:HB1	3	1.87	0.98	2.29
(1,2817)	1:130:A:ASP:H	1:3:A:ALA:HB2	3	1.87	0.98	2.29
(1,2817)	1:130:A:ASP:H	1:3:A:ALA:HB3	3	1.87	0.98	2.29
(1,185)	1:126:A:VAL:HG21	1:25:A:VAL:HA	3	1.62	0.13	1.6
(1,185)	1:126:A:VAL:HG22	1:25:A:VAL:HA	3	1.62	0.13	1.6

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,185)	1:126:A:VAL:HG23	1:25:A:VAL:HA	3	1.62	0.13	1.6
(1,1306)	1:25:A:VAL:HB	1:126:A:VAL:HG21	3	1.5	0.13	1.49
(1,1306)	1:25:A:VAL:HB	1:126:A:VAL:HG22	3	1.5	0.13	1.49
(1,1306)	1:25:A:VAL:HB	1:126:A:VAL:HG23	3	1.5	0.13	1.49
(1,1503)	1:81:A:ARG:HD2	1:62:A:VAL:HG11	3	1.15	0.65	0.82
(1,1503)	1:81:A:ARG:HD2	1:62:A:VAL:HG12	3	1.15	0.65	0.82
(1,1503)	1:81:A:ARG:HD2	1:62:A:VAL:HG13	3	1.15	0.65	0.82
(1,2627)	1:111:A:PHE:H	1:126:A:VAL:HG11	3	1.09	0.05	1.12
(1,2627)	1:111:A:PHE:H	1:126:A:VAL:HG12	3	1.09	0.05	1.12
(1,2627)	1:111:A:PHE:H	1:126:A:VAL:HG13	3	1.09	0.05	1.12
(1,2960)	1:109:A:TYR:HD1	1:127:A:THR:HG21	3	0.76	0.2	0.88
(1,2960)	1:109:A:TYR:HD1	1:127:A:THR:HG22	3	0.76	0.2	0.88
(1,2960)	1:109:A:TYR:HD1	1:127:A:THR:HG23	3	0.76	0.2	0.88
(1,2960)	1:109:A:TYR:HD2	1:127:A:THR:HG21	3	0.76	0.2	0.88
(1,2960)	1:109:A:TYR:HD2	1:127:A:THR:HG22	3	0.76	0.2	0.88
(1,2960)	1:109:A:TYR:HD2	1:127:A:THR:HG23	3	0.76	0.2	0.88
(1,1660)	1:25:A:VAL:H	1:126:A:VAL:HG21	3	0.72	0.1	0.75
(1,1660)	1:25:A:VAL:H	1:126:A:VAL:HG22	3	0.72	0.1	0.75
(1,1660)	1:25:A:VAL:H	1:126:A:VAL:HG23	3	0.72	0.1	0.75
(1,448)	1:43:A:PRO:HG3	1:46:A:SER:HB2	3	0.7	0.27	0.87
(1,448)	1:43:A:PRO:HG3	1:46:A:SER:HB3	3	0.7	0.27	0.87
(1,1079)	1:125:A:LYS:HE2	1:108:A:ASP:HA	3	0.65	0.44	0.65
(1,1079)	1:125:A:LYS:HE3	1:108:A:ASP:HA	3	0.65	0.44	0.65
(1,578)	1:56:A:ALA:HA	1:110:A:LYS:HD2	3	0.65	0.13	0.61
(1,1383)	1:128:A:LEU:HD11	1:25:A:VAL:HG21	3	0.63	0.69	0.18
(1,1383)	1:128:A:LEU:HD11	1:25:A:VAL:HG22	3	0.63	0.69	0.18
(1,1383)	1:128:A:LEU:HD11	1:25:A:VAL:HG23	3	0.63	0.69	0.18
(1,1383)	1:128:A:LEU:HD12	1:25:A:VAL:HG21	3	0.63	0.69	0.18
(1,1383)	1:128:A:LEU:HD12	1:25:A:VAL:HG22	3	0.63	0.69	0.18
(1,1383)	1:128:A:LEU:HD12	1:25:A:VAL:HG23	3	0.63	0.69	0.18
(1,1383)	1:128:A:LEU:HD13	1:25:A:VAL:HG21	3	0.63	0.69	0.18
(1,1383)	1:128:A:LEU:HD13	1:25:A:VAL:HG22	3	0.63	0.69	0.18
(1,1383)	1:128:A:LEU:HD13	1:25:A:VAL:HG23	3	0.63	0.69	0.18
(1,3167)	1:129:A:VAL:HG23	1:24:A:GLN:H	3	0.6	0.14	0.68
(1,3167)	1:129:A:VAL:HG22	1:24:A:GLN:H	3	0.6	0.14	0.68
(1,1659)	1:127:A:THR:H	1:126:A:VAL:HG21	3	0.57	0.03	0.56
(1,1659)	1:127:A:THR:H	1:126:A:VAL:HG22	3	0.57	0.03	0.56
(1,1659)	1:127:A:THR:H	1:126:A:VAL:HG23	3	0.57	0.03	0.56
(1,589)	1:57:A:GLU:HG3	1:57:A:GLU:H	3	0.53	0.02	0.55
(1,3262)	1:109:A:TYR:HE2	1:55:A:LYS:HD2	3	0.45	0.4	0.19
(1,3262)	1:109:A:TYR:HE1	1:104:A:LEU:HD12	3	0.45	0.4	0.19
(1,2745)	1:123:A:ASN:H	1:21:A:LYS:HG2	3	0.43	0.16	0.43

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2745)	1:123:A:ASN:H	1:21:A:LYS:HG3	3	0.43	0.16	0.43
(1,204)	1:26:A:SER:HB3	1:25:A:VAL:HA	3	0.41	0.02	0.42
(1,2534)	1:100:A:ASP:H	1:83:A:VAL:HG21	3	0.39	0.11	0.44
(1,2534)	1:100:A:ASP:H	1:83:A:VAL:HG22	3	0.39	0.11	0.44
(1,2534)	1:100:A:ASP:H	1:83:A:VAL:HG23	3	0.39	0.11	0.44
(1,390)	1:41:A:THR:HB	1:91:A:GLY:HA2	3	0.38	0.1	0.45
(1,2074)	1:91:A:GLY:HA2	1:41:A:THR:H	3	0.38	0.04	0.36
(1,2540)	1:100:A:ASP:H	1:100:A:ASP:HB3	3	0.33	0.03	0.33
(1,156)	1:126:A:VAL:HG11	1:23:A:ILE:HB	3	0.32	0.21	0.25
(1,156)	1:126:A:VAL:HG12	1:23:A:ILE:HB	3	0.32	0.21	0.25
(1,156)	1:126:A:VAL:HG13	1:23:A:ILE:HB	3	0.32	0.21	0.25
(1,2077)	1:38:A:HIS:HE1	1:41:A:THR:H	3	0.3	0.01	0.3
(1,586)	1:27:A:LYS:HE2	1:130:A:ASP:HA	3	0.29	0.14	0.19
(1,586)	1:27:A:LYS:HE3	1:130:A:ASP:HA	3	0.29	0.14	0.19
(1,1532)	1:114:A:THR:HG1	1:75:A:VAL:HG21	3	0.27	0.11	0.31
(1,1532)	1:114:A:THR:HG1	1:75:A:VAL:HG22	3	0.27	0.11	0.31
(1,1532)	1:114:A:THR:HG1	1:75:A:VAL:HG23	3	0.27	0.11	0.31
(1,2138)	1:88:A:LEU:HD11	1:48:A:GLY:H	3	0.27	0.1	0.25
(1,2138)	1:88:A:LEU:HD12	1:48:A:GLY:H	3	0.27	0.1	0.25
(1,2138)	1:88:A:LEU:HD13	1:48:A:GLY:H	3	0.27	0.1	0.25
(1,711)	1:74:A:TYR:HB3	1:88:A:LEU:HD11	3	0.24	0.02	0.25
(1,711)	1:74:A:TYR:HB3	1:88:A:LEU:HD12	3	0.24	0.02	0.25
(1,711)	1:74:A:TYR:HB3	1:88:A:LEU:HD13	3	0.24	0.02	0.25
(1,2065)	1:40:A:GLY:H	1:38:A:HIS:HB2	3	0.24	0.01	0.25
(1,748)	1:77:A:PRO:HA	1:78:A:ASP:H	3	0.24	0.03	0.24
(1,2967)	1:109:A:TYR:HD1	1:126:A:VAL:HG21	3	0.24	0.04	0.22
(1,2967)	1:109:A:TYR:HD1	1:126:A:VAL:HG22	3	0.24	0.04	0.22
(1,2967)	1:109:A:TYR:HD1	1:126:A:VAL:HG23	3	0.24	0.04	0.22
(1,2967)	1:109:A:TYR:HD2	1:126:A:VAL:HG21	3	0.24	0.04	0.22
(1,2967)	1:109:A:TYR:HD2	1:126:A:VAL:HG22	3	0.24	0.04	0.22
(1,2967)	1:109:A:TYR:HD2	1:126:A:VAL:HG23	3	0.24	0.04	0.22
(1,2779)	1:126:A:VAL:HG11	1:126:A:VAL:H	3	0.23	0.01	0.23
(1,2779)	1:126:A:VAL:HG12	1:126:A:VAL:H	3	0.23	0.01	0.23
(1,2779)	1:126:A:VAL:HG13	1:126:A:VAL:H	3	0.23	0.01	0.23
(1,468)	1:88:A:LEU:HG	1:48:A:GLY:HA3	3	0.22	0.03	0.21
(1,2970)	1:109:A:TYR:HD1	1:53:A:ILE:HD11	3	0.19	0.06	0.21
(1,2970)	1:109:A:TYR:HD1	1:53:A:ILE:HD12	3	0.19	0.06	0.21
(1,2970)	1:109:A:TYR:HD1	1:53:A:ILE:HD13	3	0.19	0.06	0.21
(1,2970)	1:109:A:TYR:HD2	1:53:A:ILE:HD11	3	0.19	0.06	0.21
(1,2970)	1:109:A:TYR:HD2	1:53:A:ILE:HD12	3	0.19	0.06	0.21
(1,2970)	1:109:A:TYR:HD2	1:53:A:ILE:HD13	3	0.19	0.06	0.21
(1,2926)	1:63:A:PHE:HE1	1:59:A:MET:HB3	3	0.16	0.04	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2926)	1:63:A:PHE:HE2	1:59:A:MET:HB3	3	0.16	0.04	0.13
(1,61)	1:18:A:PHE:HD1	1:12:A:SER:HB2	3	0.15	0.04	0.14
(1,61)	1:18:A:PHE:HD2	1:12:A:SER:HB2	3	0.15	0.04	0.14
(1,2882)	1:74:A:TYR:HD1	1:88:A:LEU:HD11	3	0.15	0.04	0.13
(1,2882)	1:74:A:TYR:HD1	1:88:A:LEU:HD12	3	0.15	0.04	0.13
(1,2882)	1:74:A:TYR:HD1	1:88:A:LEU:HD13	3	0.15	0.04	0.13
(1,2882)	1:74:A:TYR:HD2	1:88:A:LEU:HD11	3	0.15	0.04	0.13
(1,2882)	1:74:A:TYR:HD2	1:88:A:LEU:HD12	3	0.15	0.04	0.13
(1,2882)	1:74:A:TYR:HD2	1:88:A:LEU:HD13	3	0.15	0.04	0.13
(1,175)	1:24:A:GLN:HG3	1:129:A:VAL:HG11	3	0.13	0.02	0.12
(1,175)	1:24:A:GLN:HG3	1:129:A:VAL:HG12	3	0.13	0.02	0.12
(1,175)	1:24:A:GLN:HG3	1:129:A:VAL:HG13	3	0.13	0.02	0.12
(1,1994)	1:6:A:CYS:HB2	1:33:A:THR:H	3	0.12	0.0	0.12
(1,619)	1:65:A:ASP:HB3	1:62:A:VAL:HA	3	0.12	0.02	0.11
(1,743)	1:77:A:PRO:HG3	1:77:A:PRO:HA	3	0.12	0.01	0.12
(1,2575)	1:105:A:ALA:H	1:104:A:LEU:HB3	3	0.12	0.01	0.12
(1,2168)	1:74:A:TYR:HB3	1:50:A:ASN:HD22	2	1.28	0.44	1.28
(1,2172)	1:50:A:ASN:HD22	1:88:A:LEU:HD21	2	1.12	0.88	1.12
(1,2172)	1:50:A:ASN:HD22	1:88:A:LEU:HD22	2	1.12	0.88	1.12
(1,2172)	1:50:A:ASN:HD22	1:88:A:LEU:HD23	2	1.12	0.88	1.12
(1,2274)	1:81:A:ARG:HB3	1:62:A:VAL:H	2	1.04	0.05	1.04
(1,2764)	1:124:A:GLY:H	1:110:A:LYS:HE2	2	0.94	0.5	0.94
(1,2764)	1:124:A:GLY:H	1:110:A:LYS:HE3	2	0.94	0.5	0.94
(1,2674)	1:52:A:VAL:HG21	1:114:A:THR:H	2	0.89	0.1	0.89
(1,2674)	1:52:A:VAL:HG22	1:114:A:THR:H	2	0.89	0.1	0.89
(1,2674)	1:52:A:VAL:HG23	1:114:A:THR:H	2	0.89	0.1	0.89
(1,1385)	1:128:A:LEU:HB2	1:25:A:VAL:HG21	2	0.86	0.66	0.86
(1,1385)	1:128:A:LEU:HB2	1:25:A:VAL:HG22	2	0.86	0.66	0.86
(1,1385)	1:128:A:LEU:HB2	1:25:A:VAL:HG23	2	0.86	0.66	0.86
(1,2626)	1:53:A:ILE:HG12	1:111:A:PHE:H	2	0.86	0.04	0.86
(1,2363)	1:79:A:ASP:H	1:76:A:LYS:HB3	2	0.84	0.15	0.84
(1,3147)	1:128:A:LEU:H	1:104:A:LEU:HD22	2	0.82	0.7	0.82
(1,3147)	1:128:A:LEU:H	1:104:A:LEU:HD23	2	0.82	0.7	0.82
(1,1231)	1:122:A:MET:HA	1:121:A:LEU:HD11	2	0.8	0.2	0.8
(1,1231)	1:122:A:MET:HA	1:121:A:LEU:HD12	2	0.8	0.2	0.8
(1,1231)	1:122:A:MET:HA	1:121:A:LEU:HD13	2	0.8	0.2	0.8
(1,3043)	1:19:A:ASN:HB3	1:11:A:GLU:HB3	2	0.76	0.07	0.76
(1,2356)	1:78:A:ASP:H	1:76:A:LYS:HD2	2	0.68	0.21	0.68
(1,2356)	1:78:A:ASP:H	1:76:A:LYS:HD3	2	0.68	0.21	0.68
(1,2491)	1:37:A:LYS:HD2	1:95:A:SER:H	2	0.65	0.01	0.65
(1,2491)	1:37:A:LYS:HD3	1:95:A:SER:H	2	0.65	0.01	0.65
(1,2985)	1:53:A:ILE:HG13	1:111:A:PHE:HD1	2	0.62	0.06	0.62

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2985)	1:53:A:ILE:HG13	1:111:A:PHE:HD2	2	0.62	0.06	0.62
(1,1555)	1:98:A:THR:H	1:84:A:ALA:HB1	2	0.61	0.4	0.61
(1,1555)	1:98:A:THR:H	1:84:A:ALA:HB2	2	0.61	0.4	0.61
(1,1555)	1:98:A:THR:H	1:84:A:ALA:HB3	2	0.61	0.4	0.61
(1,579)	1:56:A:ALA:HA	1:110:A:LYS:HD3	2	0.6	0.09	0.6
(1,45)	1:11:A:GLU:HG3	1:9:A:THR:HG21	2	0.58	0.12	0.58
(1,45)	1:11:A:GLU:HG3	1:9:A:THR:HG22	2	0.58	0.12	0.58
(1,45)	1:11:A:GLU:HG3	1:9:A:THR:HG23	2	0.58	0.12	0.58
(1,760)	1:76:A:LYS:HD2	1:77:A:PRO:HD2	2	0.58	0.18	0.58
(1,760)	1:76:A:LYS:HD3	1:77:A:PRO:HD2	2	0.58	0.18	0.58
(1,1156)	1:52:A:VAL:HG21	1:113:A:CYS:HA	2	0.58	0.03	0.58
(1,1156)	1:52:A:VAL:HG22	1:113:A:CYS:HA	2	0.58	0.03	0.58
(1,1156)	1:52:A:VAL:HG23	1:113:A:CYS:HA	2	0.58	0.03	0.58
(1,1467)	1:85:A:HIS:HB2	1:52:A:VAL:HG11	2	0.57	0.03	0.57
(1,1467)	1:85:A:HIS:HB2	1:52:A:VAL:HG12	2	0.57	0.03	0.57
(1,1467)	1:85:A:HIS:HB2	1:52:A:VAL:HG13	2	0.57	0.03	0.57
(1,255)	1:98:A:THR:HG21	1:31:A:GLU:HG2	2	0.57	0.11	0.57
(1,255)	1:98:A:THR:HG21	1:31:A:GLU:HG3	2	0.57	0.11	0.57
(1,255)	1:98:A:THR:HG22	1:31:A:GLU:HG2	2	0.57	0.11	0.57
(1,255)	1:98:A:THR:HG22	1:31:A:GLU:HG3	2	0.57	0.11	0.57
(1,255)	1:98:A:THR:HG23	1:31:A:GLU:HG2	2	0.57	0.11	0.57
(1,255)	1:98:A:THR:HG23	1:31:A:GLU:HG3	2	0.57	0.11	0.57
(1,3178)	1:37:A:LYS:HG2	1:36:A:LEU:H	2	0.57	0.06	0.57
(1,3178)	1:37:A:LYS:HG3	1:36:A:LEU:H	2	0.57	0.06	0.57
(1,2747)	1:123:A:ASN:H	1:121:A:LEU:HD11	2	0.57	0.16	0.57
(1,2747)	1:123:A:ASN:H	1:121:A:LEU:HD12	2	0.57	0.16	0.57
(1,2747)	1:123:A:ASN:H	1:121:A:LEU:HD13	2	0.57	0.16	0.57
(1,2808)	1:27:A:LYS:HE2	1:129:A:VAL:H	2	0.55	0.23	0.55
(1,2808)	1:27:A:LYS:HE3	1:129:A:VAL:H	2	0.55	0.23	0.55
(1,498)	1:50:A:ASN:HB2	1:51:A:LEU:H	2	0.52	0.03	0.52
(1,2712)	1:121:A:LEU:HB3	1:120:A:ALA:H	2	0.5	0.17	0.5
(1,2878)	1:38:A:HIS:HE1	1:47:A:MET:HG3	2	0.46	0.12	0.46
(1,1513)	1:76:A:LYS:HB3	1:69:A:ALA:HB1	2	0.46	0.3	0.46
(1,1513)	1:76:A:LYS:HB3	1:69:A:ALA:HB2	2	0.46	0.3	0.46
(1,1513)	1:76:A:LYS:HB3	1:69:A:ALA:HB3	2	0.46	0.3	0.46
(1,1031)	1:101:A:PRO:HG2	1:29:A:CYS:HB2	2	0.45	0.16	0.45
(1,1031)	1:101:A:PRO:HG2	1:29:A:CYS:HB3	2	0.45	0.16	0.45
(1,2759)	1:123:A:ASN:HD22	1:21:A:LYS:HG2	2	0.45	0.04	0.45
(1,2759)	1:123:A:ASN:HD22	1:21:A:LYS:HG3	2	0.45	0.04	0.45
(1,2631)	1:110:A:LYS:HE2	1:111:A:PHE:H	2	0.43	0.25	0.43
(1,2631)	1:110:A:LYS:HE3	1:111:A:PHE:H	2	0.43	0.25	0.43
(1,2749)	1:123:A:ASN:HD21	1:119:A:GLY:HA2	2	0.43	0.08	0.43

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2046)	1:37:A:LYS:HD2	1:38:A:HIS:H	2	0.42	0.16	0.42
(1,2046)	1:37:A:LYS:HD3	1:38:A:HIS:H	2	0.42	0.16	0.42
(1,1867)	1:19:A:ASN:HD22	1:11:A:GLU:HG2	2	0.4	0.0	0.4
(1,1668)	1:23:A:ILE:HG21	1:126:A:VAL:HG21	2	0.4	0.27	0.4
(1,1668)	1:23:A:ILE:HG21	1:126:A:VAL:HG22	2	0.4	0.27	0.4
(1,1668)	1:23:A:ILE:HG21	1:126:A:VAL:HG23	2	0.4	0.27	0.4
(1,1668)	1:23:A:ILE:HG22	1:126:A:VAL:HG21	2	0.4	0.27	0.4
(1,1668)	1:23:A:ILE:HG22	1:126:A:VAL:HG22	2	0.4	0.27	0.4
(1,1668)	1:23:A:ILE:HG22	1:126:A:VAL:HG23	2	0.4	0.27	0.4
(1,1668)	1:23:A:ILE:HG23	1:126:A:VAL:HG21	2	0.4	0.27	0.4
(1,1668)	1:23:A:ILE:HG23	1:126:A:VAL:HG22	2	0.4	0.27	0.4
(1,1668)	1:23:A:ILE:HG23	1:126:A:VAL:HG23	2	0.4	0.27	0.4
(1,1960)	1:101:A:PRO:HG2	1:29:A:CYS:H	2	0.4	0.02	0.4
(1,1100)	1:110:A:LYS:HA	1:126:A:VAL:HG11	2	0.39	0.12	0.39
(1,1100)	1:110:A:LYS:HA	1:126:A:VAL:HG12	2	0.39	0.12	0.39
(1,1100)	1:110:A:LYS:HA	1:126:A:VAL:HG13	2	0.39	0.12	0.39
(1,759)	1:77:A:PRO:HD2	1:69:A:ALA:HB1	2	0.38	0.03	0.38
(1,759)	1:77:A:PRO:HD2	1:69:A:ALA:HB2	2	0.38	0.03	0.38
(1,759)	1:77:A:PRO:HD2	1:69:A:ALA:HB3	2	0.38	0.03	0.38
(1,1293)	1:130:A:ASP:HB3	1:130:A:ASP:H	2	0.38	0.01	0.38
(1,2350)	1:76:A:LYS:H	1:65:A:ASP:HB2	2	0.37	0.04	0.37
(1,2368)	1:80:A:ALA:H	1:79:A:ASP:HA	2	0.37	0.22	0.37
(1,1961)	1:101:A:PRO:HB2	1:29:A:CYS:H	2	0.34	0.14	0.34
(1,1984)	1:100:A:ASP:HB2	1:32:A:PHE:H	2	0.33	0.06	0.33
(1,2078)	1:42:A:GLN:H	1:41:A:THR:H	2	0.33	0.02	0.33
(1,3246)	1:123:A:ASN:HD22	1:120:A:ALA:HB1	2	0.32	0.12	0.32
(1,3246)	1:123:A:ASN:HD22	1:120:A:ALA:HB2	2	0.32	0.12	0.32
(1,1706)	1:53:A:ILE:HB	1:99:A:LEU:HD11	2	0.32	0.06	0.32
(1,1706)	1:53:A:ILE:HB	1:99:A:LEU:HD12	2	0.32	0.06	0.32
(1,1706)	1:53:A:ILE:HB	1:99:A:LEU:HD13	2	0.32	0.06	0.32
(1,2216)	1:58:A:ASP:HB2	1:55:A:LYS:H	2	0.32	0.06	0.32
(1,2646)	1:112:A:ALA:H	1:52:A:VAL:HG21	2	0.31	0.08	0.31
(1,2646)	1:112:A:ALA:H	1:52:A:VAL:HG22	2	0.31	0.08	0.31
(1,2646)	1:112:A:ALA:H	1:52:A:VAL:HG23	2	0.31	0.08	0.31
(1,1320)	1:47:A:MET:HE1	1:118:A:HIS:HE1	2	0.3	0.2	0.3
(1,1320)	1:47:A:MET:HE2	1:118:A:HIS:HE1	2	0.3	0.2	0.3
(1,1320)	1:47:A:MET:HE3	1:118:A:HIS:HE1	2	0.3	0.2	0.3
(1,1125)	1:53:A:ILE:HG13	1:111:A:PHE:HA	2	0.26	0.03	0.26
(1,1341)	1:51:A:LEU:HG	1:10:A:VAL:HG21	2	0.26	0.09	0.26
(1,1341)	1:51:A:LEU:HG	1:10:A:VAL:HG22	2	0.26	0.09	0.26
(1,1341)	1:51:A:LEU:HG	1:10:A:VAL:HG23	2	0.26	0.09	0.26
(1,2572)	1:105:A:ALA:H	1:104:A:LEU:HD21	2	0.26	0.09	0.26

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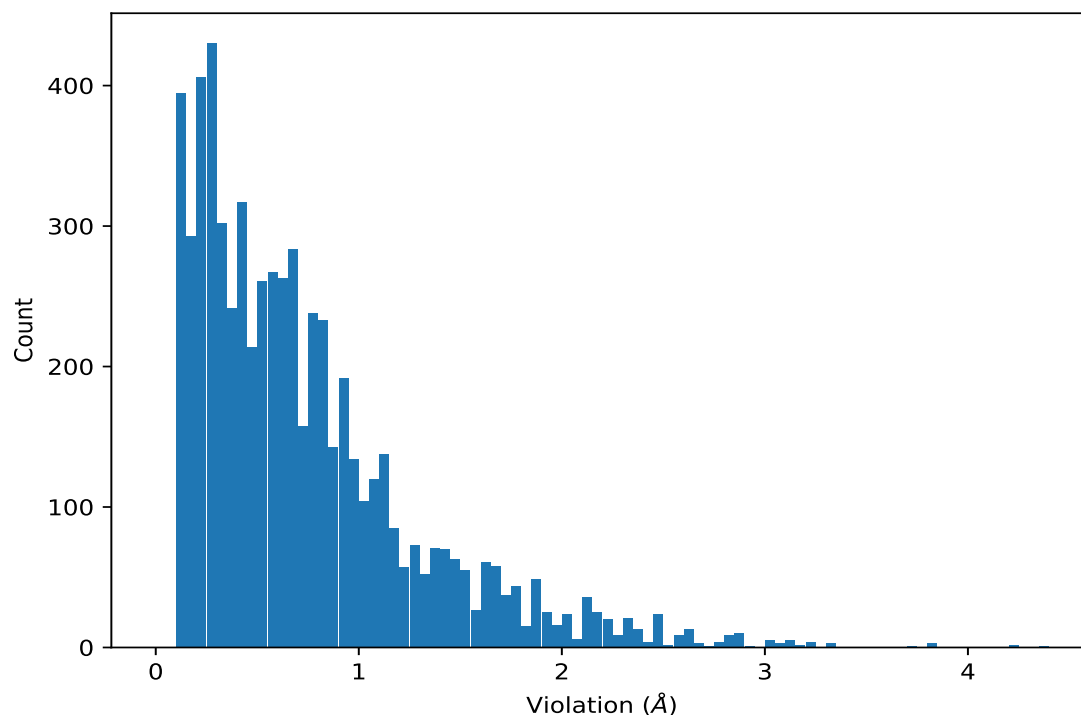
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2572)	1:105:A:ALA:H	1:104:A:LEU:HD22	2	0.26	0.09	0.26
(1,2572)	1:105:A:ALA:H	1:104:A:LEU:HD23	2	0.26	0.09	0.26
(1,3213)	1:89:A:ILE:H	1:49:A:HIS:HB3	2	0.26	0.02	0.26
(1,1550)	1:83:A:VAL:HG11	1:104:A:LEU:HD21	2	0.25	0.15	0.25
(1,1550)	1:83:A:VAL:HG11	1:104:A:LEU:HD22	2	0.25	0.15	0.25
(1,1550)	1:83:A:VAL:HG11	1:104:A:LEU:HD23	2	0.25	0.15	0.25
(1,1550)	1:83:A:VAL:HG12	1:104:A:LEU:HD21	2	0.25	0.15	0.25
(1,1550)	1:83:A:VAL:HG12	1:104:A:LEU:HD22	2	0.25	0.15	0.25
(1,1550)	1:83:A:VAL:HG12	1:104:A:LEU:HD23	2	0.25	0.15	0.25
(1,1550)	1:83:A:VAL:HG13	1:104:A:LEU:HD21	2	0.25	0.15	0.25
(1,1550)	1:83:A:VAL:HG13	1:104:A:LEU:HD22	2	0.25	0.15	0.25
(1,1550)	1:83:A:VAL:HG13	1:104:A:LEU:HD23	2	0.25	0.15	0.25
(1,1192)	1:116:A:PRO:HD2	1:74:A:TYR:HA	2	0.24	0.03	0.24
(1,2823)	1:52:A:VAL:HG11	1:114:A:THR:H	2	0.24	0.08	0.24
(1,2823)	1:52:A:VAL:HG12	1:114:A:THR:H	2	0.24	0.08	0.24
(1,2823)	1:52:A:VAL:HG13	1:114:A:THR:H	2	0.24	0.08	0.24
(1,1763)	1:11:A:GLU:HG3	1:11:A:GLU:H	2	0.24	0.0	0.24
(1,2962)	1:53:A:ILE:HG12	1:109:A:TYR:HD1	2	0.23	0.01	0.23
(1,2962)	1:53:A:ILE:HG12	1:109:A:TYR:HD2	2	0.23	0.01	0.23
(1,3263)	1:23:A:ILE:HG12	1:111:A:PHE:HD1	2	0.19	0.05	0.19
(1,1086)	1:108:A:ASP:HB2	1:56:A:ALA:H	2	0.18	0.04	0.18
(1,2651)	1:113:A:CYS:H	1:52:A:VAL:HG11	2	0.18	0.0	0.18
(1,2651)	1:113:A:CYS:H	1:52:A:VAL:HG12	2	0.18	0.0	0.18
(1,2651)	1:113:A:CYS:H	1:52:A:VAL:HG13	2	0.18	0.0	0.18
(1,2736)	1:123:A:ASN:H	1:18:A:PHE:HE1	2	0.18	0.0	0.18
(1,2736)	1:123:A:ASN:H	1:18:A:PHE:HE2	2	0.18	0.0	0.18
(1,1834)	1:17:A:GLN:HE21	1:17:A:GLN:HB2	2	0.16	0.04	0.16
(1,1689)	1:128:A:LEU:H	1:128:A:LEU:HD11	2	0.16	0.05	0.16
(1,1689)	1:128:A:LEU:H	1:128:A:LEU:HD12	2	0.16	0.05	0.16
(1,1689)	1:128:A:LEU:H	1:128:A:LEU:HD13	2	0.16	0.05	0.16
(1,2177)	1:50:A:ASN:HB3	1:51:A:LEU:H	2	0.15	0.01	0.15
(1,2291)	1:64:A:LYS:HG3	1:64:A:LYS:H	2	0.13	0.01	0.13
(1,1598)	1:53:A:ILE:HG12	1:97:A:LEU:HD21	2	0.12	0.01	0.12
(1,1598)	1:53:A:ILE:HG12	1:97:A:LEU:HD22	2	0.12	0.01	0.12
(1,1598)	1:53:A:ILE:HG12	1:97:A:LEU:HD23	2	0.12	0.01	0.12
(1,3192)	1:53:A:ILE:HD11	1:53:A:ILE:H	2	0.12	0.01	0.12
(1,3192)	1:53:A:ILE:HD12	1:53:A:ILE:H	2	0.12	0.01	0.12

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)
(1,2590)	1:128:A:LEU:HB3	1:106:A:ASP:H	3	4.38
(1,2360)	1:76:A:LYS:HE2	1:79:A:ASP:H	3	4.24
(1,2360)	1:76:A:LYS:HE3	1:79:A:ASP:H	3	4.24
(1,2365)	1:79:A:ASP:H	1:75:A:VAL:HG11	9	3.83
(1,2365)	1:79:A:ASP:H	1:75:A:VAL:HG12	9	3.83
(1,2365)	1:79:A:ASP:H	1:75:A:VAL:HG13	9	3.83
(1,2590)	1:128:A:LEU:HB3	1:106:A:ASP:H	2	3.7
(1,2590)	1:128:A:LEU:HB3	1:106:A:ASP:H	5	3.32
(1,2360)	1:76:A:LYS:HE2	1:79:A:ASP:H	5	3.32
(1,2360)	1:76:A:LYS:HE3	1:79:A:ASP:H	5	3.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,33)	1:10:A:VAL:HB	1:36:A:LEU:HD21	10	3.23
(1,33)	1:10:A:VAL:HB	1:36:A:LEU:HD22	10	3.23
(1,33)	1:10:A:VAL:HB	1:36:A:LEU:HD23	10	3.23
(1,2362)	1:79:A:ASP:H	1:76:A:LYS:HB2	9	3.2
(1,488)	1:114:A:THR:HG1	1:50:A:ASN:HA	3	3.17
(1,488)	1:114:A:THR:HG1	1:50:A:ASN:HA	10	3.16
(1,488)	1:114:A:THR:HG1	1:50:A:ASN:HA	4	3.14
(1,488)	1:114:A:THR:HG1	1:50:A:ASN:HA	8	3.14
(1,488)	1:114:A:THR:HG1	1:50:A:ASN:HA	2	3.11
(1,488)	1:114:A:THR:HG1	1:50:A:ASN:HA	6	3.11
(1,58)	1:17:A:GLN:HG3	1:12:A:SER:HB2	3	3.1
(1,2360)	1:76:A:LYS:HE2	1:79:A:ASP:H	9	3.08
(1,2360)	1:76:A:LYS:HE3	1:79:A:ASP:H	9	3.08
(1,488)	1:114:A:THR:HG1	1:50:A:ASN:HA	5	3.06
(1,488)	1:114:A:THR:HG1	1:50:A:ASN:HA	1	3.03
(1,2360)	1:76:A:LYS:HE2	1:79:A:ASP:H	7	3.01
(1,2360)	1:76:A:LYS:HE3	1:79:A:ASP:H	7	3.01
(1,2360)	1:76:A:LYS:HE2	1:79:A:ASP:H	1	3.0
(1,2360)	1:76:A:LYS:HE3	1:79:A:ASP:H	1	3.0
(1,2590)	1:128:A:LEU:HB3	1:106:A:ASP:H	7	2.94
(1,1526)	1:52:A:VAL:HG21	1:75:A:VAL:HG21	7	2.9
(1,1526)	1:52:A:VAL:HG21	1:75:A:VAL:HG22	7	2.9
(1,1526)	1:52:A:VAL:HG21	1:75:A:VAL:HG23	7	2.9
(1,1526)	1:52:A:VAL:HG22	1:75:A:VAL:HG21	7	2.9
(1,1526)	1:52:A:VAL:HG22	1:75:A:VAL:HG22	7	2.9
(1,1526)	1:52:A:VAL:HG22	1:75:A:VAL:HG23	7	2.9
(1,1526)	1:52:A:VAL:HG23	1:75:A:VAL:HG21	7	2.9
(1,1526)	1:52:A:VAL:HG23	1:75:A:VAL:HG22	7	2.9
(1,1526)	1:52:A:VAL:HG23	1:75:A:VAL:HG23	7	2.9
(1,2590)	1:128:A:LEU:HB3	1:106:A:ASP:H	1	2.85
(1,1680)	1:27:A:LYS:HG2	1:128:A:LEU:HD21	3	2.84
(1,1680)	1:27:A:LYS:HG2	1:128:A:LEU:HD22	3	2.84
(1,1680)	1:27:A:LYS:HG2	1:128:A:LEU:HD23	3	2.84
(1,1680)	1:27:A:LYS:HG3	1:128:A:LEU:HD21	3	2.84
(1,1680)	1:27:A:LYS:HG3	1:128:A:LEU:HD22	3	2.84
(1,1680)	1:27:A:LYS:HG3	1:128:A:LEU:HD23	3	2.84
(1,2365)	1:79:A:ASP:H	1:75:A:VAL:HG11	4	2.83
(1,2365)	1:79:A:ASP:H	1:75:A:VAL:HG12	4	2.83
(1,2365)	1:79:A:ASP:H	1:75:A:VAL:HG13	4	2.83
(1,2817)	1:130:A:ASP:H	1:3:A:ALA:HB1	1	2.8
(1,2817)	1:130:A:ASP:H	1:3:A:ALA:HB2	1	2.8
(1,2817)	1:130:A:ASP:H	1:3:A:ALA:HB3	1	2.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,55)	1:17:A:GLN:HG3	1:12:A:SER:HB3	3	2.8
(1,2590)	1:128:A:LEU:HB3	1:106:A:ASP:H	9	2.74
(1,1387)	1:101:A:PRO:HG2	1:25:A:VAL:HG21	7	2.68
(1,1387)	1:101:A:PRO:HG2	1:25:A:VAL:HG22	7	2.68
(1,1387)	1:101:A:PRO:HG2	1:25:A:VAL:HG23	7	2.68
(1,3227)	1:104:A:LEU:HB3	1:102:A:ALA:H	8	2.65
(1,580)	1:130:A:ASP:HA	1:128:A:LEU:HD21	3	2.63
(1,580)	1:130:A:ASP:HA	1:128:A:LEU:HD22	3	2.63
(1,580)	1:130:A:ASP:HA	1:128:A:LEU:HD23	3	2.63
(1,1669)	1:25:A:VAL:HG11	1:126:A:VAL:HG21	4	2.62
(1,1669)	1:25:A:VAL:HG11	1:126:A:VAL:HG22	4	2.62
(1,1669)	1:25:A:VAL:HG11	1:126:A:VAL:HG23	4	2.62
(1,1669)	1:25:A:VAL:HG12	1:126:A:VAL:HG21	4	2.62
(1,1669)	1:25:A:VAL:HG12	1:126:A:VAL:HG22	4	2.62
(1,1669)	1:25:A:VAL:HG12	1:126:A:VAL:HG23	4	2.62
(1,1669)	1:25:A:VAL:HG13	1:126:A:VAL:HG21	4	2.62
(1,1669)	1:25:A:VAL:HG13	1:126:A:VAL:HG22	4	2.62
(1,1669)	1:25:A:VAL:HG13	1:126:A:VAL:HG23	4	2.62
(1,1526)	1:52:A:VAL:HG21	1:75:A:VAL:HG21	8	2.59
(1,1526)	1:52:A:VAL:HG21	1:75:A:VAL:HG22	8	2.59
(1,1526)	1:52:A:VAL:HG21	1:75:A:VAL:HG23	8	2.59
(1,1526)	1:52:A:VAL:HG22	1:75:A:VAL:HG21	8	2.59
(1,1526)	1:52:A:VAL:HG22	1:75:A:VAL:HG22	8	2.59
(1,1526)	1:52:A:VAL:HG22	1:75:A:VAL:HG23	8	2.59
(1,1526)	1:52:A:VAL:HG23	1:75:A:VAL:HG21	8	2.59
(1,1526)	1:52:A:VAL:HG23	1:75:A:VAL:HG22	8	2.59
(1,1526)	1:52:A:VAL:HG23	1:75:A:VAL:HG23	8	2.59
(1,3227)	1:103:A:LYS:HG3	1:102:A:ALA:H	1	2.53
(1,2590)	1:128:A:LEU:HB3	1:106:A:ASP:H	4	2.52
(1,3227)	1:104:A:LEU:HB3	1:102:A:ALA:H	6	2.49
(1,3149)	1:62:A:VAL:HG23	1:114:A:THR:HG23	8	2.49
(1,1669)	1:25:A:VAL:HG11	1:126:A:VAL:HG21	2	2.49
(1,1669)	1:25:A:VAL:HG11	1:126:A:VAL:HG22	2	2.49
(1,1669)	1:25:A:VAL:HG11	1:126:A:VAL:HG23	2	2.49
(1,1669)	1:25:A:VAL:HG12	1:126:A:VAL:HG21	2	2.49
(1,1669)	1:25:A:VAL:HG12	1:126:A:VAL:HG22	2	2.49
(1,1669)	1:25:A:VAL:HG12	1:126:A:VAL:HG23	2	2.49
(1,1669)	1:25:A:VAL:HG13	1:126:A:VAL:HG21	2	2.49
(1,1669)	1:25:A:VAL:HG13	1:126:A:VAL:HG22	2	2.49
(1,1669)	1:25:A:VAL:HG13	1:126:A:VAL:HG23	2	2.49
(1,766)	1:69:A:ALA:HA	1:77:A:PRO:HD2	4	2.49
(1,1669)	1:25:A:VAL:HG11	1:126:A:VAL:HG21	8	2.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1669)	1:25:A:VAL:HG11	1:126:A:VAL:HG22	8	2.48
(1,1669)	1:25:A:VAL:HG11	1:126:A:VAL:HG23	8	2.48
(1,1669)	1:25:A:VAL:HG12	1:126:A:VAL:HG21	8	2.48
(1,1669)	1:25:A:VAL:HG12	1:126:A:VAL:HG22	8	2.48
(1,1669)	1:25:A:VAL:HG12	1:126:A:VAL:HG23	8	2.48
(1,1669)	1:25:A:VAL:HG13	1:126:A:VAL:HG21	8	2.48
(1,1669)	1:25:A:VAL:HG13	1:126:A:VAL:HG22	8	2.48
(1,1669)	1:25:A:VAL:HG13	1:126:A:VAL:HG23	8	2.48
(1,1387)	1:101:A:PRO:HG2	1:25:A:VAL:HG21	5	2.47
(1,1387)	1:101:A:PRO:HG2	1:25:A:VAL:HG22	5	2.47
(1,1387)	1:101:A:PRO:HG2	1:25:A:VAL:HG23	5	2.47
(1,1386)	1:101:A:PRO:HB2	1:25:A:VAL:HG21	3	2.42
(1,1386)	1:101:A:PRO:HB2	1:25:A:VAL:HG22	3	2.42
(1,1386)	1:101:A:PRO:HB2	1:25:A:VAL:HG23	3	2.42
(1,3149)	1:82:A:VAL:HG11	1:114:A:THR:HG23	7	2.41
(1,2365)	1:79:A:ASP:H	1:75:A:VAL:HG11	1	2.4
(1,2365)	1:79:A:ASP:H	1:75:A:VAL:HG12	1	2.4
(1,2365)	1:79:A:ASP:H	1:75:A:VAL:HG13	1	2.4
(1,1526)	1:52:A:VAL:HG21	1:75:A:VAL:HG21	4	2.4
(1,1526)	1:52:A:VAL:HG21	1:75:A:VAL:HG22	4	2.4
(1,1526)	1:52:A:VAL:HG21	1:75:A:VAL:HG23	4	2.4
(1,1526)	1:52:A:VAL:HG22	1:75:A:VAL:HG21	4	2.4
(1,1526)	1:52:A:VAL:HG22	1:75:A:VAL:HG22	4	2.4
(1,1526)	1:52:A:VAL:HG22	1:75:A:VAL:HG23	4	2.4
(1,1526)	1:52:A:VAL:HG23	1:75:A:VAL:HG21	4	2.4
(1,1526)	1:52:A:VAL:HG23	1:75:A:VAL:HG22	4	2.4
(1,1526)	1:52:A:VAL:HG23	1:75:A:VAL:HG23	4	2.4
(1,3149)	1:62:A:VAL:HG22	1:114:A:THR:HG21	10	2.37
(1,1701)	1:99:A:LEU:HD11	1:51:A:LEU:HD11	4	2.34
(1,1701)	1:99:A:LEU:HD11	1:51:A:LEU:HD12	4	2.34
(1,1701)	1:99:A:LEU:HD11	1:51:A:LEU:HD13	4	2.34
(1,1701)	1:99:A:LEU:HD12	1:51:A:LEU:HD11	4	2.34
(1,1701)	1:99:A:LEU:HD12	1:51:A:LEU:HD12	4	2.34
(1,1701)	1:99:A:LEU:HD12	1:51:A:LEU:HD13	4	2.34
(1,1701)	1:99:A:LEU:HD13	1:51:A:LEU:HD11	4	2.34
(1,1701)	1:99:A:LEU:HD13	1:51:A:LEU:HD12	4	2.34
(1,1701)	1:99:A:LEU:HD13	1:51:A:LEU:HD13	4	2.34
(1,1386)	1:101:A:PRO:HB2	1:25:A:VAL:HG21	2	2.34
(1,1386)	1:101:A:PRO:HB2	1:25:A:VAL:HG22	2	2.34
(1,1386)	1:101:A:PRO:HB2	1:25:A:VAL:HG23	2	2.34
(1,1701)	1:99:A:LEU:HD11	1:51:A:LEU:HD11	7	2.31
(1,1701)	1:99:A:LEU:HD11	1:51:A:LEU:HD12	7	2.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1701)	1:99:A:LEU:HD11	1:51:A:LEU:HD13	7	2.31
(1,1701)	1:99:A:LEU:HD12	1:51:A:LEU:HD11	7	2.31
(1,1701)	1:99:A:LEU:HD12	1:51:A:LEU:HD12	7	2.31
(1,1701)	1:99:A:LEU:HD12	1:51:A:LEU:HD13	7	2.31
(1,1701)	1:99:A:LEU:HD13	1:51:A:LEU:HD11	7	2.31
(1,1701)	1:99:A:LEU:HD13	1:51:A:LEU:HD12	7	2.31
(1,1701)	1:99:A:LEU:HD13	1:51:A:LEU:HD13	7	2.31
(1,488)	1:114:A:THR:HG1	1:50:A:ASN:HA	7	2.3
(1,3149)	1:82:A:VAL:HG12	1:114:A:THR:HG23	1	2.29
(1,2817)	1:130:A:ASP:H	1:3:A:ALA:HB1	9	2.29
(1,2817)	1:130:A:ASP:H	1:3:A:ALA:HB2	9	2.29
(1,2817)	1:130:A:ASP:H	1:3:A:ALA:HB3	9	2.29
(1,2590)	1:128:A:LEU:HB3	1:106:A:ASP:H	8	2.28
(1,1386)	1:101:A:PRO:HB2	1:25:A:VAL:HG21	4	2.28
(1,1386)	1:101:A:PRO:HB2	1:25:A:VAL:HG22	4	2.28
(1,1386)	1:101:A:PRO:HB2	1:25:A:VAL:HG23	4	2.28
(1,3149)	1:62:A:VAL:HG23	1:114:A:THR:HG22	5	2.24
(1,2623)	1:125:A:LYS:HD2	1:110:A:LYS:H	10	2.24
(1,2623)	1:125:A:LYS:HD3	1:110:A:LYS:H	10	2.24
(1,1386)	1:101:A:PRO:HB2	1:25:A:VAL:HG21	10	2.24
(1,1386)	1:101:A:PRO:HB2	1:25:A:VAL:HG22	10	2.24
(1,1386)	1:101:A:PRO:HB2	1:25:A:VAL:HG23	10	2.24
(1,488)	1:114:A:THR:HG1	1:50:A:ASN:HA	9	2.24
(1,55)	1:17:A:GLN:HG3	1:12:A:SER:HB3	4	2.24
(1,766)	1:69:A:ALA:HA	1:77:A:PRO:HD2	6	2.23
(1,2362)	1:79:A:ASP:H	1:76:A:LYS:HB2	5	2.22
(1,1436)	1:47:A:MET:HE1	1:118:A:HIS:HB2	4	2.22
(1,1436)	1:47:A:MET:HE2	1:118:A:HIS:HB2	4	2.22
(1,1436)	1:47:A:MET:HE3	1:118:A:HIS:HB2	4	2.22
(1,1387)	1:101:A:PRO:HG2	1:25:A:VAL:HG21	3	2.22
(1,1387)	1:101:A:PRO:HG2	1:25:A:VAL:HG22	3	2.22
(1,1387)	1:101:A:PRO:HG2	1:25:A:VAL:HG23	3	2.22
(1,1386)	1:101:A:PRO:HB2	1:25:A:VAL:HG21	6	2.21
(1,1386)	1:101:A:PRO:HB2	1:25:A:VAL:HG22	6	2.21
(1,1386)	1:101:A:PRO:HB2	1:25:A:VAL:HG23	6	2.21
(1,2590)	1:128:A:LEU:HB3	1:106:A:ASP:H	10	2.2
(1,2060)	1:93:A:GLU:H	1:40:A:GLY:H	2	2.18
(1,1701)	1:99:A:LEU:HD11	1:51:A:LEU:HD11	2	2.18
(1,1701)	1:99:A:LEU:HD11	1:51:A:LEU:HD12	2	2.18
(1,1701)	1:99:A:LEU:HD11	1:51:A:LEU:HD13	2	2.18
(1,1701)	1:99:A:LEU:HD12	1:51:A:LEU:HD11	2	2.18
(1,1701)	1:99:A:LEU:HD12	1:51:A:LEU:HD12	2	2.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1701)	1:99:A:LEU:HD12	1:51:A:LEU:HD13	2	2.18
(1,1701)	1:99:A:LEU:HD13	1:51:A:LEU:HD11	2	2.18
(1,1701)	1:99:A:LEU:HD13	1:51:A:LEU:HD12	2	2.18
(1,1701)	1:99:A:LEU:HD13	1:51:A:LEU:HD13	2	2.18
(1,1067)	1:107:A:GLY:HA2	1:55:A:LYS:HG2	4	2.17
(1,1067)	1:107:A:GLY:HA2	1:55:A:LYS:HG3	4	2.17
(1,1799)	1:13:A:ASN:HD21	1:17:A:GLN:HB3	7	2.16
(1,1701)	1:99:A:LEU:HD11	1:51:A:LEU:HD11	9	2.15
(1,1701)	1:99:A:LEU:HD11	1:51:A:LEU:HD12	9	2.15
(1,1701)	1:99:A:LEU:HD11	1:51:A:LEU:HD13	9	2.15
(1,1701)	1:99:A:LEU:HD12	1:51:A:LEU:HD11	9	2.15
(1,1701)	1:99:A:LEU:HD12	1:51:A:LEU:HD12	9	2.15
(1,1701)	1:99:A:LEU:HD12	1:51:A:LEU:HD13	9	2.15
(1,1701)	1:99:A:LEU:HD13	1:51:A:LEU:HD11	9	2.15
(1,1701)	1:99:A:LEU:HD13	1:51:A:LEU:HD12	9	2.15
(1,1701)	1:99:A:LEU:HD13	1:51:A:LEU:HD13	9	2.15
(1,1387)	1:101:A:PRO:HG2	1:25:A:VAL:HG21	2	2.15
(1,1387)	1:101:A:PRO:HG2	1:25:A:VAL:HG22	2	2.15
(1,1387)	1:101:A:PRO:HG2	1:25:A:VAL:HG23	2	2.15
(1,1037)	1:99:A:LEU:HD21	1:101:A:PRO:HG2	6	2.14
(1,1037)	1:99:A:LEU:HD22	1:101:A:PRO:HG2	6	2.14
(1,1037)	1:99:A:LEU:HD23	1:101:A:PRO:HG2	6	2.14
(1,1701)	1:99:A:LEU:HD11	1:51:A:LEU:HD11	1	2.13
(1,1701)	1:99:A:LEU:HD11	1:51:A:LEU:HD12	1	2.13
(1,1701)	1:99:A:LEU:HD11	1:51:A:LEU:HD13	1	2.13
(1,1701)	1:99:A:LEU:HD12	1:51:A:LEU:HD11	1	2.13
(1,1701)	1:99:A:LEU:HD12	1:51:A:LEU:HD12	1	2.13
(1,1701)	1:99:A:LEU:HD12	1:51:A:LEU:HD13	1	2.13
(1,1701)	1:99:A:LEU:HD13	1:51:A:LEU:HD11	1	2.13
(1,1701)	1:99:A:LEU:HD13	1:51:A:LEU:HD12	1	2.13
(1,1701)	1:99:A:LEU:HD13	1:51:A:LEU:HD13	1	2.13
(1,1386)	1:101:A:PRO:HB2	1:25:A:VAL:HG21	8	2.13
(1,1386)	1:101:A:PRO:HB2	1:25:A:VAL:HG22	8	2.13
(1,1386)	1:101:A:PRO:HB2	1:25:A:VAL:HG23	8	2.13
(1,44)	1:39:A:THR:HG21	1:11:A:GLU:HG3	6	2.13
(1,44)	1:39:A:THR:HG22	1:11:A:GLU:HG3	6	2.13
(1,44)	1:39:A:THR:HG23	1:11:A:GLU:HG3	6	2.13
(1,1701)	1:99:A:LEU:HD11	1:51:A:LEU:HD11	8	2.11
(1,1701)	1:99:A:LEU:HD11	1:51:A:LEU:HD12	8	2.11
(1,1701)	1:99:A:LEU:HD11	1:51:A:LEU:HD13	8	2.11
(1,1701)	1:99:A:LEU:HD12	1:51:A:LEU:HD11	8	2.11
(1,1701)	1:99:A:LEU:HD12	1:51:A:LEU:HD12	8	2.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1701)	1:99:A:LEU:HD12	1:51:A:LEU:HD13	8	2.11
(1,1701)	1:99:A:LEU:HD13	1:51:A:LEU:HD11	8	2.11
(1,1701)	1:99:A:LEU:HD13	1:51:A:LEU:HD12	8	2.11
(1,1701)	1:99:A:LEU:HD13	1:51:A:LEU:HD13	8	2.11
(1,1387)	1:101:A:PRO:HG2	1:25:A:VAL:HG21	6	2.11
(1,1387)	1:101:A:PRO:HG2	1:25:A:VAL:HG22	6	2.11
(1,1387)	1:101:A:PRO:HG2	1:25:A:VAL:HG23	6	2.11
(1,1387)	1:101:A:PRO:HG2	1:25:A:VAL:HG21	4	2.1
(1,1387)	1:101:A:PRO:HG2	1:25:A:VAL:HG22	4	2.1
(1,1387)	1:101:A:PRO:HG2	1:25:A:VAL:HG23	4	2.1
(1,1387)	1:101:A:PRO:HG2	1:25:A:VAL:HG21	10	2.1
(1,1387)	1:101:A:PRO:HG2	1:25:A:VAL:HG22	10	2.1
(1,1387)	1:101:A:PRO:HG2	1:25:A:VAL:HG23	10	2.1
(1,1386)	1:101:A:PRO:HB2	1:25:A:VAL:HG21	9	2.08
(1,1386)	1:101:A:PRO:HB2	1:25:A:VAL:HG22	9	2.08
(1,1386)	1:101:A:PRO:HB2	1:25:A:VAL:HG23	9	2.08
(1,1503)	1:81:A:ARG:HD2	1:62:A:VAL:HG11	1	2.06
(1,1503)	1:81:A:ARG:HD2	1:62:A:VAL:HG12	1	2.06
(1,1503)	1:81:A:ARG:HD2	1:62:A:VAL:HG13	1	2.06
(1,1701)	1:99:A:LEU:HD11	1:51:A:LEU:HD11	5	2.05
(1,1701)	1:99:A:LEU:HD11	1:51:A:LEU:HD12	5	2.05
(1,1701)	1:99:A:LEU:HD11	1:51:A:LEU:HD13	5	2.05
(1,1701)	1:99:A:LEU:HD12	1:51:A:LEU:HD11	5	2.05
(1,1701)	1:99:A:LEU:HD12	1:51:A:LEU:HD12	5	2.05
(1,1701)	1:99:A:LEU:HD12	1:51:A:LEU:HD13	5	2.05
(1,1701)	1:99:A:LEU:HD13	1:51:A:LEU:HD11	5	2.05
(1,1701)	1:99:A:LEU:HD13	1:51:A:LEU:HD12	5	2.05
(1,1701)	1:99:A:LEU:HD13	1:51:A:LEU:HD13	5	2.05
(1,2157)	1:50:A:ASN:H	1:88:A:LEU:HD21	7	2.03
(1,2157)	1:50:A:ASN:H	1:88:A:LEU:HD22	7	2.03
(1,2157)	1:50:A:ASN:H	1:88:A:LEU:HD23	7	2.03
(1,1701)	1:99:A:LEU:HD11	1:51:A:LEU:HD11	6	2.03
(1,1701)	1:99:A:LEU:HD11	1:51:A:LEU:HD12	6	2.03
(1,1701)	1:99:A:LEU:HD11	1:51:A:LEU:HD13	6	2.03
(1,1701)	1:99:A:LEU:HD12	1:51:A:LEU:HD11	6	2.03
(1,1701)	1:99:A:LEU:HD12	1:51:A:LEU:HD12	6	2.03
(1,1701)	1:99:A:LEU:HD12	1:51:A:LEU:HD13	6	2.03
(1,1701)	1:99:A:LEU:HD13	1:51:A:LEU:HD11	6	2.03
(1,1701)	1:99:A:LEU:HD13	1:51:A:LEU:HD12	6	2.03
(1,1701)	1:99:A:LEU:HD13	1:51:A:LEU:HD13	6	2.03
(1,2172)	1:50:A:ASN:HD22	1:88:A:LEU:HD21	7	2.0
(1,2172)	1:50:A:ASN:HD22	1:88:A:LEU:HD22	7	2.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2172)	1:50:A:ASN:HD22	1:88:A:LEU:HD23	7	2.0
(1,1684)	1:128:A:LEU:HD21	1:25:A:VAL:HG21	6	1.99
(1,1684)	1:128:A:LEU:HD21	1:25:A:VAL:HG22	6	1.99
(1,1684)	1:128:A:LEU:HD21	1:25:A:VAL:HG23	6	1.99
(1,1684)	1:128:A:LEU:HD22	1:25:A:VAL:HG21	6	1.99
(1,1684)	1:128:A:LEU:HD22	1:25:A:VAL:HG22	6	1.99
(1,1684)	1:128:A:LEU:HD22	1:25:A:VAL:HG23	6	1.99
(1,1684)	1:128:A:LEU:HD23	1:25:A:VAL:HG21	6	1.99
(1,1684)	1:128:A:LEU:HD23	1:25:A:VAL:HG22	6	1.99
(1,1684)	1:128:A:LEU:HD23	1:25:A:VAL:HG23	6	1.99
(1,1387)	1:101:A:PRO:HG2	1:25:A:VAL:HG21	9	1.99
(1,1387)	1:101:A:PRO:HG2	1:25:A:VAL:HG22	9	1.99
(1,1387)	1:101:A:PRO:HG2	1:25:A:VAL:HG23	9	1.99
(1,882)	1:91:A:GLY:HA3	1:38:A:HIS:HB2	5	1.98
(1,253)	1:98:A:THR:HB	1:31:A:GLU:HG2	4	1.98
(1,253)	1:98:A:THR:HB	1:31:A:GLU:HG3	4	1.98
(1,3208)	1:76:A:LYS:HD3	1:79:A:ASP:H	9	1.97
(1,2629)	1:125:A:LYS:HD2	1:111:A:PHE:H	10	1.95
(1,2629)	1:125:A:LYS:HD3	1:111:A:PHE:H	10	1.95
(1,2590)	1:128:A:LEU:HB3	1:106:A:ASP:H	6	1.95
(1,3108)	1:128:A:LEU:HB3	1:105:A:ALA:HA	3	1.94
(1,2211)	1:55:A:LYS:H	1:83:A:VAL:HB	6	1.94
(1,1035)	1:101:A:PRO:HG3	1:25:A:VAL:HG21	7	1.94
(1,1035)	1:101:A:PRO:HG3	1:25:A:VAL:HG22	7	1.94
(1,1035)	1:101:A:PRO:HG3	1:25:A:VAL:HG23	7	1.94
(1,3149)	1:62:A:VAL:HG21	1:114:A:THR:HG21	4	1.93
(1,1386)	1:101:A:PRO:HB2	1:25:A:VAL:HG21	1	1.93
(1,1386)	1:101:A:PRO:HB2	1:25:A:VAL:HG22	1	1.93
(1,1386)	1:101:A:PRO:HB2	1:25:A:VAL:HG23	1	1.93
(1,1701)	1:99:A:LEU:HD11	1:51:A:LEU:HD11	10	1.92
(1,1701)	1:99:A:LEU:HD11	1:51:A:LEU:HD12	10	1.92
(1,1701)	1:99:A:LEU:HD11	1:51:A:LEU:HD13	10	1.92
(1,1701)	1:99:A:LEU:HD12	1:51:A:LEU:HD11	10	1.92
(1,1701)	1:99:A:LEU:HD12	1:51:A:LEU:HD12	10	1.92
(1,1701)	1:99:A:LEU:HD12	1:51:A:LEU:HD13	10	1.92
(1,1701)	1:99:A:LEU:HD13	1:51:A:LEU:HD11	10	1.92
(1,1701)	1:99:A:LEU:HD13	1:51:A:LEU:HD12	10	1.92
(1,1701)	1:99:A:LEU:HD13	1:51:A:LEU:HD13	10	1.92
(1,1037)	1:99:A:LEU:HD21	1:101:A:PRO:HG2	2	1.92
(1,1037)	1:99:A:LEU:HD22	1:101:A:PRO:HG2	2	1.92
(1,1037)	1:99:A:LEU:HD23	1:101:A:PRO:HG2	2	1.92
(1,706)	1:88:A:LEU:HG	1:74:A:TYR:HA	7	1.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1037)	1:99:A:LEU:HD21	1:101:A:PRO:HG2	9	1.9
(1,1037)	1:99:A:LEU:HD22	1:101:A:PRO:HG2	9	1.9
(1,1037)	1:99:A:LEU:HD23	1:101:A:PRO:HG2	9	1.9
(1,1684)	1:128:A:LEU:HD21	1:25:A:VAL:HG21	1	1.89
(1,1684)	1:128:A:LEU:HD21	1:25:A:VAL:HG22	1	1.89
(1,1684)	1:128:A:LEU:HD21	1:25:A:VAL:HG23	1	1.89
(1,1684)	1:128:A:LEU:HD22	1:25:A:VAL:HG21	1	1.89
(1,1684)	1:128:A:LEU:HD22	1:25:A:VAL:HG22	1	1.89
(1,1684)	1:128:A:LEU:HD22	1:25:A:VAL:HG23	1	1.89
(1,1684)	1:128:A:LEU:HD23	1:25:A:VAL:HG21	1	1.89
(1,1684)	1:128:A:LEU:HD23	1:25:A:VAL:HG22	1	1.89
(1,1684)	1:128:A:LEU:HD23	1:25:A:VAL:HG23	1	1.89
(1,1015)	1:99:A:LEU:HD21	1:101:A:PRO:HD2	6	1.89
(1,1015)	1:99:A:LEU:HD22	1:101:A:PRO:HD2	6	1.89
(1,1015)	1:99:A:LEU:HD23	1:101:A:PRO:HD2	6	1.89
(1,3208)	1:79:A:ASP:H	1:75:A:VAL:HB	2	1.87
(1,3198)	1:64:A:LYS:HD3	1:61:A:GLY:H	4	1.87
(1,1684)	1:128:A:LEU:HD21	1:25:A:VAL:HG21	7	1.87
(1,1684)	1:128:A:LEU:HD21	1:25:A:VAL:HG22	7	1.87
(1,1684)	1:128:A:LEU:HD21	1:25:A:VAL:HG23	7	1.87
(1,1684)	1:128:A:LEU:HD22	1:25:A:VAL:HG21	7	1.87
(1,1684)	1:128:A:LEU:HD22	1:25:A:VAL:HG22	7	1.87
(1,1684)	1:128:A:LEU:HD22	1:25:A:VAL:HG23	7	1.87
(1,1684)	1:128:A:LEU:HD23	1:25:A:VAL:HG21	7	1.87
(1,1684)	1:128:A:LEU:HD23	1:25:A:VAL:HG22	7	1.87
(1,1684)	1:128:A:LEU:HD23	1:25:A:VAL:HG23	7	1.87
(1,55)	1:17:A:GLN:HG3	1:12:A:SER:HB3	7	1.87
(1,1799)	1:13:A:ASN:HD21	1:17:A:GLN:HB3	5	1.86
(1,1037)	1:99:A:LEU:HD21	1:101:A:PRO:HG2	3	1.86
(1,1037)	1:99:A:LEU:HD22	1:101:A:PRO:HG2	3	1.86
(1,1037)	1:99:A:LEU:HD23	1:101:A:PRO:HG2	3	1.86
(1,1037)	1:99:A:LEU:HD21	1:101:A:PRO:HG2	5	1.86
(1,1037)	1:99:A:LEU:HD22	1:101:A:PRO:HG2	5	1.86
(1,1037)	1:99:A:LEU:HD23	1:101:A:PRO:HG2	5	1.86
(1,2365)	1:79:A:ASP:H	1:75:A:VAL:HG11	7	1.85
(1,2365)	1:79:A:ASP:H	1:75:A:VAL:HG12	7	1.85
(1,2365)	1:79:A:ASP:H	1:75:A:VAL:HG13	7	1.85
(1,1684)	1:128:A:LEU:HD21	1:25:A:VAL:HG21	9	1.85
(1,1684)	1:128:A:LEU:HD21	1:25:A:VAL:HG22	9	1.85
(1,1684)	1:128:A:LEU:HD21	1:25:A:VAL:HG23	9	1.85
(1,1684)	1:128:A:LEU:HD22	1:25:A:VAL:HG21	9	1.85
(1,1684)	1:128:A:LEU:HD22	1:25:A:VAL:HG22	9	1.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1684)	1:128:A:LEU:HD22	1:25:A:VAL:HG23	9	1.85
(1,1684)	1:128:A:LEU:HD23	1:25:A:VAL:HG21	9	1.85
(1,1684)	1:128:A:LEU:HD23	1:25:A:VAL:HG22	9	1.85
(1,1684)	1:128:A:LEU:HD23	1:25:A:VAL:HG23	9	1.85
(1,1037)	1:99:A:LEU:HD21	1:101:A:PRO:HG2	7	1.85
(1,1037)	1:99:A:LEU:HD22	1:101:A:PRO:HG2	7	1.85
(1,1037)	1:99:A:LEU:HD23	1:101:A:PRO:HG2	7	1.85
(1,2362)	1:79:A:ASP:H	1:76:A:LYS:HB2	1	1.84
(1,1929)	1:104:A:LEU:HD11	1:25:A:VAL:H	8	1.84
(1,1929)	1:104:A:LEU:HD12	1:25:A:VAL:H	8	1.84
(1,1929)	1:104:A:LEU:HD13	1:25:A:VAL:H	8	1.84
(1,3261)	1:104:A:LEU:HB2	1:109:A:TYR:HE1	8	1.83
(1,1436)	1:47:A:MET:HE1	1:118:A:HIS:HB2	7	1.83
(1,1436)	1:47:A:MET:HE2	1:118:A:HIS:HB2	7	1.83
(1,1436)	1:47:A:MET:HE3	1:118:A:HIS:HB2	7	1.83
(1,852)	1:88:A:LEU:HB3	1:73:A:ASP:H	10	1.83
(1,2211)	1:55:A:LYS:H	1:83:A:VAL:HB	7	1.82
(1,1929)	1:104:A:LEU:HD11	1:25:A:VAL:H	5	1.82
(1,1929)	1:104:A:LEU:HD12	1:25:A:VAL:H	5	1.82
(1,1929)	1:104:A:LEU:HD13	1:25:A:VAL:H	5	1.82
(1,646)	1:76:A:LYS:HB3	1:66:A:GLY:HA3	4	1.81
(1,766)	1:69:A:ALA:HA	1:77:A:PRO:HD2	5	1.8
(1,3108)	1:128:A:LEU:HB3	1:105:A:ALA:HA	2	1.79
(1,1387)	1:101:A:PRO:HG2	1:25:A:VAL:HG21	1	1.79
(1,1387)	1:101:A:PRO:HG2	1:25:A:VAL:HG22	1	1.79
(1,1387)	1:101:A:PRO:HG2	1:25:A:VAL:HG23	1	1.79
(1,185)	1:126:A:VAL:HG21	1:25:A:VAL:HA	2	1.79
(1,185)	1:126:A:VAL:HG22	1:25:A:VAL:HA	2	1.79
(1,185)	1:126:A:VAL:HG23	1:25:A:VAL:HA	2	1.79
(1,55)	1:17:A:GLN:HG3	1:12:A:SER:HB3	9	1.79
(1,3261)	1:109:A:TYR:HE1	1:55:A:LYS:HD3	5	1.78
(1,2396)	1:82:A:VAL:HG21	1:84:A:ALA:H	5	1.78
(1,2396)	1:82:A:VAL:HG22	1:84:A:ALA:H	5	1.78
(1,2396)	1:82:A:VAL:HG23	1:84:A:ALA:H	5	1.78
(1,2121)	1:43:A:PRO:HG3	1:47:A:MET:H	3	1.78
(1,1037)	1:99:A:LEU:HD21	1:101:A:PRO:HG2	10	1.78
(1,1037)	1:99:A:LEU:HD22	1:101:A:PRO:HG2	10	1.78
(1,1037)	1:99:A:LEU:HD23	1:101:A:PRO:HG2	10	1.78
(1,3261)	1:104:A:LEU:HB2	1:109:A:TYR:HE1	7	1.77
(1,3149)	1:62:A:VAL:HG23	1:114:A:THR:HG21	9	1.77
(1,1701)	1:99:A:LEU:HD11	1:51:A:LEU:HD11	3	1.77
(1,1701)	1:99:A:LEU:HD11	1:51:A:LEU:HD12	3	1.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1701)	1:99:A:LEU:HD11	1:51:A:LEU:HD13	3	1.77
(1,1701)	1:99:A:LEU:HD12	1:51:A:LEU:HD11	3	1.77
(1,1701)	1:99:A:LEU:HD12	1:51:A:LEU:HD12	3	1.77
(1,1701)	1:99:A:LEU:HD12	1:51:A:LEU:HD13	3	1.77
(1,1701)	1:99:A:LEU:HD13	1:51:A:LEU:HD11	3	1.77
(1,1701)	1:99:A:LEU:HD13	1:51:A:LEU:HD12	3	1.77
(1,1701)	1:99:A:LEU:HD13	1:51:A:LEU:HD13	3	1.77
(1,2365)	1:79:A:ASP:H	1:75:A:VAL:HG11	8	1.76
(1,2365)	1:79:A:ASP:H	1:75:A:VAL:HG12	8	1.76
(1,2365)	1:79:A:ASP:H	1:75:A:VAL:HG13	8	1.76
(1,2326)	1:88:A:LEU:HD11	1:73:A:ASP:H	2	1.76
(1,2326)	1:88:A:LEU:HD12	1:73:A:ASP:H	2	1.76
(1,2326)	1:88:A:LEU:HD13	1:73:A:ASP:H	2	1.76
(1,2302)	1:76:A:LYS:HB3	1:66:A:GLY:H	4	1.76
(1,1799)	1:13:A:ASN:HD21	1:17:A:GLN:HB3	4	1.76
(1,3149)	1:62:A:VAL:HG23	1:114:A:THR:HG23	6	1.75
(1,2060)	1:93:A:GLU:H	1:40:A:GLY:H	8	1.75
(1,1799)	1:13:A:ASN:HD21	1:17:A:GLN:HB3	6	1.75
(1,1387)	1:101:A:PRO:HG2	1:25:A:VAL:HG21	8	1.75
(1,1387)	1:101:A:PRO:HG2	1:25:A:VAL:HG22	8	1.75
(1,1387)	1:101:A:PRO:HG2	1:25:A:VAL:HG23	8	1.75
(1,1061)	1:105:A:ALA:HA	1:128:A:LEU:HD11	1	1.75
(1,1061)	1:105:A:ALA:HA	1:128:A:LEU:HD12	1	1.75
(1,1061)	1:105:A:ALA:HA	1:128:A:LEU:HD13	1	1.75
(1,3261)	1:109:A:TYR:HE1	1:55:A:LYS:HD3	9	1.74
(1,1797)	1:15:A:ASN:HB3	1:13:A:ASN:HD21	5	1.74
(1,1684)	1:128:A:LEU:HD21	1:25:A:VAL:HG21	5	1.74
(1,1684)	1:128:A:LEU:HD21	1:25:A:VAL:HG22	5	1.74
(1,1684)	1:128:A:LEU:HD21	1:25:A:VAL:HG23	5	1.74
(1,1684)	1:128:A:LEU:HD22	1:25:A:VAL:HG21	5	1.74
(1,1684)	1:128:A:LEU:HD22	1:25:A:VAL:HG22	5	1.74
(1,1684)	1:128:A:LEU:HD22	1:25:A:VAL:HG23	5	1.74
(1,1684)	1:128:A:LEU:HD23	1:25:A:VAL:HG21	5	1.74
(1,1684)	1:128:A:LEU:HD23	1:25:A:VAL:HG22	5	1.74
(1,1684)	1:128:A:LEU:HD23	1:25:A:VAL:HG23	5	1.74
(1,1037)	1:99:A:LEU:HD21	1:101:A:PRO:HG2	4	1.74
(1,1037)	1:99:A:LEU:HD22	1:101:A:PRO:HG2	4	1.74
(1,1037)	1:99:A:LEU:HD23	1:101:A:PRO:HG2	4	1.74
(1,253)	1:98:A:THR:HB	1:31:A:GLU:HG2	10	1.74
(1,253)	1:98:A:THR:HB	1:31:A:GLU:HG3	10	1.74
(1,2168)	1:74:A:TYR:HB3	1:50:A:ASN:HD22	9	1.73
(1,2060)	1:93:A:GLU:H	1:40:A:GLY:H	3	1.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2396)	1:82:A:VAL:HG21	1:84:A:ALA:H	6	1.72
(1,2396)	1:82:A:VAL:HG22	1:84:A:ALA:H	6	1.72
(1,2396)	1:82:A:VAL:HG23	1:84:A:ALA:H	6	1.72
(1,2396)	1:82:A:VAL:HG21	1:84:A:ALA:H	10	1.72
(1,2396)	1:82:A:VAL:HG22	1:84:A:ALA:H	10	1.72
(1,2396)	1:82:A:VAL:HG23	1:84:A:ALA:H	10	1.72
(1,2227)	1:110:A:LYS:HD3	1:56:A:ALA:H	3	1.72
(1,1799)	1:13:A:ASN:HD21	1:17:A:GLN:HB3	10	1.72
(1,1684)	1:128:A:LEU:HD21	1:25:A:VAL:HG21	4	1.72
(1,1684)	1:128:A:LEU:HD21	1:25:A:VAL:HG22	4	1.72
(1,1684)	1:128:A:LEU:HD21	1:25:A:VAL:HG23	4	1.72
(1,1684)	1:128:A:LEU:HD22	1:25:A:VAL:HG21	4	1.72
(1,1684)	1:128:A:LEU:HD22	1:25:A:VAL:HG22	4	1.72
(1,1684)	1:128:A:LEU:HD22	1:25:A:VAL:HG23	4	1.72
(1,1684)	1:128:A:LEU:HD23	1:25:A:VAL:HG21	4	1.72
(1,1684)	1:128:A:LEU:HD23	1:25:A:VAL:HG22	4	1.72
(1,1684)	1:128:A:LEU:HD23	1:25:A:VAL:HG23	4	1.72
(1,882)	1:91:A:GLY:HA3	1:38:A:HIS:HB2	7	1.71
(1,82)	1:15:A:ASN:HB2	1:17:A:GLN:HB2	1	1.71
(1,2411)	1:85:A:HIS:H	1:82:A:VAL:HG21	10	1.7
(1,2411)	1:85:A:HIS:H	1:82:A:VAL:HG22	10	1.7
(1,2411)	1:85:A:HIS:H	1:82:A:VAL:HG23	10	1.7
(1,2365)	1:79:A:ASP:H	1:75:A:VAL:HG11	3	1.7
(1,2365)	1:79:A:ASP:H	1:75:A:VAL:HG12	3	1.7
(1,2365)	1:79:A:ASP:H	1:75:A:VAL:HG13	3	1.7
(1,1799)	1:13:A:ASN:HD21	1:17:A:GLN:HB3	2	1.7
(1,1552)	1:109:A:TYR:HE1	1:83:A:VAL:HG11	7	1.7
(1,1552)	1:109:A:TYR:HE1	1:83:A:VAL:HG12	7	1.7
(1,1552)	1:109:A:TYR:HE1	1:83:A:VAL:HG13	7	1.7
(1,1552)	1:109:A:TYR:HE2	1:83:A:VAL:HG11	7	1.7
(1,1552)	1:109:A:TYR:HE2	1:83:A:VAL:HG12	7	1.7
(1,1552)	1:109:A:TYR:HE2	1:83:A:VAL:HG13	7	1.7
(1,1799)	1:13:A:ASN:HD21	1:17:A:GLN:HB3	1	1.69
(1,1684)	1:128:A:LEU:HD21	1:25:A:VAL:HG21	2	1.69
(1,1684)	1:128:A:LEU:HD21	1:25:A:VAL:HG22	2	1.69
(1,1684)	1:128:A:LEU:HD21	1:25:A:VAL:HG23	2	1.69
(1,1684)	1:128:A:LEU:HD22	1:25:A:VAL:HG21	2	1.69
(1,1684)	1:128:A:LEU:HD22	1:25:A:VAL:HG22	2	1.69
(1,1684)	1:128:A:LEU:HD22	1:25:A:VAL:HG23	2	1.69
(1,1684)	1:128:A:LEU:HD23	1:25:A:VAL:HG21	2	1.69
(1,1684)	1:128:A:LEU:HD23	1:25:A:VAL:HG22	2	1.69
(1,1684)	1:128:A:LEU:HD23	1:25:A:VAL:HG23	2	1.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1684)	1:128:A:LEU:HD21	1:25:A:VAL:HG21	10	1.69
(1,1684)	1:128:A:LEU:HD21	1:25:A:VAL:HG22	10	1.69
(1,1684)	1:128:A:LEU:HD21	1:25:A:VAL:HG23	10	1.69
(1,1684)	1:128:A:LEU:HD22	1:25:A:VAL:HG21	10	1.69
(1,1684)	1:128:A:LEU:HD22	1:25:A:VAL:HG22	10	1.69
(1,1684)	1:128:A:LEU:HD22	1:25:A:VAL:HG23	10	1.69
(1,1684)	1:128:A:LEU:HD23	1:25:A:VAL:HG21	10	1.69
(1,1684)	1:128:A:LEU:HD23	1:25:A:VAL:HG22	10	1.69
(1,1684)	1:128:A:LEU:HD23	1:25:A:VAL:HG23	10	1.69
(1,2396)	1:82:A:VAL:HG21	1:84:A:ALA:H	3	1.68
(1,2396)	1:82:A:VAL:HG22	1:84:A:ALA:H	3	1.68
(1,2396)	1:82:A:VAL:HG23	1:84:A:ALA:H	3	1.68
(1,2396)	1:82:A:VAL:HG21	1:84:A:ALA:H	4	1.68
(1,2396)	1:82:A:VAL:HG22	1:84:A:ALA:H	4	1.68
(1,2396)	1:82:A:VAL:HG23	1:84:A:ALA:H	4	1.68
(1,2396)	1:82:A:VAL:HG21	1:84:A:ALA:H	7	1.68
(1,2396)	1:82:A:VAL:HG22	1:84:A:ALA:H	7	1.68
(1,2396)	1:82:A:VAL:HG23	1:84:A:ALA:H	7	1.68
(1,1035)	1:101:A:PRO:HG3	1:25:A:VAL:HG21	5	1.68
(1,1035)	1:101:A:PRO:HG3	1:25:A:VAL:HG22	5	1.68
(1,1035)	1:101:A:PRO:HG3	1:25:A:VAL:HG23	5	1.68
(1,3261)	1:109:A:TYR:HE2	1:55:A:LYS:HD3	6	1.67
(1,1306)	1:25:A:VAL:HB	1:126:A:VAL:HG21	4	1.67
(1,1306)	1:25:A:VAL:HB	1:126:A:VAL:HG22	4	1.67
(1,1306)	1:25:A:VAL:HB	1:126:A:VAL:HG23	4	1.67
(1,2396)	1:82:A:VAL:HG21	1:84:A:ALA:H	2	1.66
(1,2396)	1:82:A:VAL:HG22	1:84:A:ALA:H	2	1.66
(1,2396)	1:82:A:VAL:HG23	1:84:A:ALA:H	2	1.66
(1,2211)	1:55:A:LYS:H	1:83:A:VAL:HB	5	1.66
(1,1015)	1:99:A:LEU:HD21	1:101:A:PRO:HD2	3	1.66
(1,1015)	1:99:A:LEU:HD22	1:101:A:PRO:HD2	3	1.66
(1,1015)	1:99:A:LEU:HD23	1:101:A:PRO:HD2	3	1.66
(1,823)	1:82:A:VAL:HG21	1:85:A:HIS:HB2	1	1.66
(1,823)	1:82:A:VAL:HG22	1:85:A:HIS:HB2	1	1.66
(1,823)	1:82:A:VAL:HG23	1:85:A:HIS:HB2	1	1.66
(1,1015)	1:99:A:LEU:HD21	1:101:A:PRO:HD2	2	1.65
(1,1015)	1:99:A:LEU:HD22	1:101:A:PRO:HD2	2	1.65
(1,1015)	1:99:A:LEU:HD23	1:101:A:PRO:HD2	2	1.65
(1,253)	1:98:A:THR:HB	1:31:A:GLU:HG2	3	1.65
(1,253)	1:98:A:THR:HB	1:31:A:GLU:HG3	3	1.65
(1,58)	1:17:A:GLN:HG3	1:12:A:SER:HB2	4	1.65
(1,58)	1:17:A:GLN:HG3	1:12:A:SER:HB2	9	1.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,55)	1:17:A:GLN:HG3	1:12:A:SER:HB3	6	1.65
(1,2211)	1:55:A:LYS:H	1:83:A:VAL:HB	4	1.64
(1,2060)	1:93:A:GLU:H	1:40:A:GLY:H	4	1.64
(1,1303)	1:56:A:ALA:H	1:55:A:LYS:HD2	2	1.64
(1,1037)	1:99:A:LEU:HD21	1:101:A:PRO:HG2	8	1.64
(1,1037)	1:99:A:LEU:HD22	1:101:A:PRO:HG2	8	1.64
(1,1037)	1:99:A:LEU:HD23	1:101:A:PRO:HG2	8	1.64
(1,58)	1:17:A:GLN:HG3	1:12:A:SER:HB2	8	1.64
(1,2365)	1:79:A:ASP:H	1:75:A:VAL:HG11	5	1.63
(1,2365)	1:79:A:ASP:H	1:75:A:VAL:HG12	5	1.63
(1,2365)	1:79:A:ASP:H	1:75:A:VAL:HG13	5	1.63
(1,1061)	1:105:A:ALA:HA	1:128:A:LEU:HD11	4	1.63
(1,1061)	1:105:A:ALA:HA	1:128:A:LEU:HD12	4	1.63
(1,1061)	1:105:A:ALA:HA	1:128:A:LEU:HD13	4	1.63
(1,1015)	1:99:A:LEU:HD21	1:101:A:PRO:HD2	9	1.63
(1,1015)	1:99:A:LEU:HD22	1:101:A:PRO:HD2	9	1.63
(1,1015)	1:99:A:LEU:HD23	1:101:A:PRO:HD2	9	1.63
(1,795)	1:82:A:VAL:HB	1:75:A:VAL:HG11	1	1.63
(1,795)	1:82:A:VAL:HB	1:75:A:VAL:HG12	1	1.63
(1,795)	1:82:A:VAL:HB	1:75:A:VAL:HG13	1	1.63
(1,3208)	1:76:A:LYS:HD2	1:79:A:ASP:H	4	1.62
(1,1965)	1:29:A:CYS:H	1:25:A:VAL:HG21	2	1.62
(1,1965)	1:29:A:CYS:H	1:25:A:VAL:HG22	2	1.62
(1,1965)	1:29:A:CYS:H	1:25:A:VAL:HG23	2	1.62
(1,2396)	1:82:A:VAL:HG21	1:84:A:ALA:H	1	1.61
(1,2396)	1:82:A:VAL:HG22	1:84:A:ALA:H	1	1.61
(1,2396)	1:82:A:VAL:HG23	1:84:A:ALA:H	1	1.61
(1,1965)	1:29:A:CYS:H	1:25:A:VAL:HG21	5	1.61
(1,1965)	1:29:A:CYS:H	1:25:A:VAL:HG22	5	1.61
(1,1965)	1:29:A:CYS:H	1:25:A:VAL:HG23	5	1.61
(1,1383)	1:128:A:LEU:HD11	1:25:A:VAL:HG21	8	1.61
(1,1383)	1:128:A:LEU:HD11	1:25:A:VAL:HG22	8	1.61
(1,1383)	1:128:A:LEU:HD11	1:25:A:VAL:HG23	8	1.61
(1,1383)	1:128:A:LEU:HD12	1:25:A:VAL:HG21	8	1.61
(1,1383)	1:128:A:LEU:HD12	1:25:A:VAL:HG22	8	1.61
(1,1383)	1:128:A:LEU:HD12	1:25:A:VAL:HG23	8	1.61
(1,1383)	1:128:A:LEU:HD13	1:25:A:VAL:HG21	8	1.61
(1,1383)	1:128:A:LEU:HD13	1:25:A:VAL:HG22	8	1.61
(1,1383)	1:128:A:LEU:HD13	1:25:A:VAL:HG23	8	1.61
(1,823)	1:82:A:VAL:HG21	1:85:A:HIS:HB2	3	1.61
(1,823)	1:82:A:VAL:HG22	1:85:A:HIS:HB2	3	1.61
(1,823)	1:82:A:VAL:HG23	1:85:A:HIS:HB2	3	1.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,823)	1:82:A:VAL:HG21	1:85:A:HIS:HB2	10	1.61
(1,823)	1:82:A:VAL:HG22	1:85:A:HIS:HB2	10	1.61
(1,823)	1:82:A:VAL:HG23	1:85:A:HIS:HB2	10	1.61
(1,58)	1:17:A:GLN:HG3	1:12:A:SER:HB2	7	1.61
(1,2365)	1:79:A:ASP:H	1:75:A:VAL:HG11	6	1.6
(1,2365)	1:79:A:ASP:H	1:75:A:VAL:HG12	6	1.6
(1,2365)	1:79:A:ASP:H	1:75:A:VAL:HG13	6	1.6
(1,1797)	1:15:A:ASN:HB3	1:13:A:ASN:HD21	10	1.6
(1,185)	1:126:A:VAL:HG21	1:25:A:VAL:HA	4	1.6
(1,185)	1:126:A:VAL:HG22	1:25:A:VAL:HA	4	1.6
(1,185)	1:126:A:VAL:HG23	1:25:A:VAL:HA	4	1.6
(1,55)	1:17:A:GLN:HG3	1:12:A:SER:HB3	5	1.6
(1,2411)	1:85:A:HIS:H	1:82:A:VAL:HG21	6	1.59
(1,2411)	1:85:A:HIS:H	1:82:A:VAL:HG22	6	1.59
(1,2411)	1:85:A:HIS:H	1:82:A:VAL:HG23	6	1.59
(1,3261)	1:104:A:LEU:HB2	1:109:A:TYR:HE1	1	1.58
(1,2411)	1:85:A:HIS:H	1:82:A:VAL:HG21	1	1.58
(1,2411)	1:85:A:HIS:H	1:82:A:VAL:HG22	1	1.58
(1,2411)	1:85:A:HIS:H	1:82:A:VAL:HG23	1	1.58
(1,1965)	1:29:A:CYS:H	1:25:A:VAL:HG21	10	1.58
(1,1965)	1:29:A:CYS:H	1:25:A:VAL:HG22	10	1.58
(1,1965)	1:29:A:CYS:H	1:25:A:VAL:HG23	10	1.58
(1,58)	1:17:A:GLN:HG3	1:12:A:SER:HB2	6	1.58
(1,2411)	1:85:A:HIS:H	1:82:A:VAL:HG21	4	1.57
(1,2411)	1:85:A:HIS:H	1:82:A:VAL:HG22	4	1.57
(1,2411)	1:85:A:HIS:H	1:82:A:VAL:HG23	4	1.57
(1,3149)	1:62:A:VAL:HG22	1:114:A:THR:HG21	2	1.56
(1,2045)	1:94:A:GLU:HB2	1:38:A:HIS:H	6	1.56
(1,1386)	1:101:A:PRO:HB2	1:25:A:VAL:HG21	7	1.56
(1,1386)	1:101:A:PRO:HB2	1:25:A:VAL:HG22	7	1.56
(1,1386)	1:101:A:PRO:HB2	1:25:A:VAL:HG23	7	1.56
(1,3149)	1:62:A:VAL:HG21	1:114:A:THR:HG23	3	1.55
(1,1039)	1:99:A:LEU:HD21	1:101:A:PRO:HG3	5	1.55
(1,1039)	1:99:A:LEU:HD22	1:101:A:PRO:HG3	5	1.55
(1,1039)	1:99:A:LEU:HD23	1:101:A:PRO:HG3	5	1.55
(1,795)	1:82:A:VAL:HB	1:75:A:VAL:HG11	4	1.55
(1,795)	1:82:A:VAL:HB	1:75:A:VAL:HG12	4	1.55
(1,795)	1:82:A:VAL:HB	1:75:A:VAL:HG13	4	1.55
(1,82)	1:15:A:ASN:HB2	1:17:A:GLN:HB2	4	1.55
(1,2411)	1:85:A:HIS:H	1:82:A:VAL:HG21	3	1.54
(1,2411)	1:85:A:HIS:H	1:82:A:VAL:HG22	3	1.54
(1,2411)	1:85:A:HIS:H	1:82:A:VAL:HG23	3	1.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,823)	1:82:A:VAL:HG21	1:85:A:HIS:HB2	6	1.54
(1,823)	1:82:A:VAL:HG22	1:85:A:HIS:HB2	6	1.54
(1,823)	1:82:A:VAL:HG23	1:85:A:HIS:HB2	6	1.54
(1,2396)	1:82:A:VAL:HG21	1:84:A:ALA:H	8	1.53
(1,2396)	1:82:A:VAL:HG22	1:84:A:ALA:H	8	1.53
(1,2396)	1:82:A:VAL:HG23	1:84:A:ALA:H	8	1.53
(1,1929)	1:104:A:LEU:HD11	1:25:A:VAL:H	6	1.53
(1,1929)	1:104:A:LEU:HD12	1:25:A:VAL:H	6	1.53
(1,1929)	1:104:A:LEU:HD13	1:25:A:VAL:H	6	1.53
(1,1929)	1:104:A:LEU:HD11	1:25:A:VAL:H	9	1.53
(1,1929)	1:104:A:LEU:HD12	1:25:A:VAL:H	9	1.53
(1,1929)	1:104:A:LEU:HD13	1:25:A:VAL:H	9	1.53
(1,3147)	1:128:A:LEU:H	1:104:A:LEU:HD23	3	1.52
(1,2812)	1:129:A:VAL:H	1:104:A:LEU:HD11	6	1.52
(1,2812)	1:129:A:VAL:H	1:104:A:LEU:HD12	6	1.52
(1,2812)	1:129:A:VAL:H	1:104:A:LEU:HD13	6	1.52
(1,2211)	1:55:A:LYS:H	1:83:A:VAL:HB	2	1.52
(1,1385)	1:128:A:LEU:HB2	1:25:A:VAL:HG21	3	1.52
(1,1385)	1:128:A:LEU:HB2	1:25:A:VAL:HG22	3	1.52
(1,1385)	1:128:A:LEU:HB2	1:25:A:VAL:HG23	3	1.52
(1,2812)	1:129:A:VAL:H	1:104:A:LEU:HD11	5	1.51
(1,2812)	1:129:A:VAL:H	1:104:A:LEU:HD12	5	1.51
(1,2812)	1:129:A:VAL:H	1:104:A:LEU:HD13	5	1.51
(1,1965)	1:29:A:CYS:H	1:25:A:VAL:HG21	4	1.51
(1,1965)	1:29:A:CYS:H	1:25:A:VAL:HG22	4	1.51
(1,1965)	1:29:A:CYS:H	1:25:A:VAL:HG23	4	1.51
(1,1965)	1:29:A:CYS:H	1:25:A:VAL:HG21	9	1.51
(1,1965)	1:29:A:CYS:H	1:25:A:VAL:HG22	9	1.51
(1,1965)	1:29:A:CYS:H	1:25:A:VAL:HG23	9	1.51
(1,1061)	1:105:A:ALA:HA	1:128:A:LEU:HD11	2	1.51
(1,1061)	1:105:A:ALA:HA	1:128:A:LEU:HD12	2	1.51
(1,1061)	1:105:A:ALA:HA	1:128:A:LEU:HD13	2	1.51
(1,1015)	1:99:A:LEU:HD21	1:101:A:PRO:HD2	4	1.51
(1,1015)	1:99:A:LEU:HD22	1:101:A:PRO:HD2	4	1.51
(1,1015)	1:99:A:LEU:HD23	1:101:A:PRO:HD2	4	1.51
(1,33)	1:10:A:VAL:HB	1:36:A:LEU:HD21	4	1.51
(1,33)	1:10:A:VAL:HB	1:36:A:LEU:HD22	4	1.51
(1,33)	1:10:A:VAL:HB	1:36:A:LEU:HD23	4	1.51
(1,2963)	1:109:A:TYR:HD1	1:128:A:LEU:HD11	1	1.5
(1,2963)	1:109:A:TYR:HD1	1:128:A:LEU:HD12	1	1.5
(1,2963)	1:109:A:TYR:HD1	1:128:A:LEU:HD13	1	1.5
(1,2963)	1:109:A:TYR:HD2	1:128:A:LEU:HD11	1	1.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2963)	1:109:A:TYR:HD2	1:128:A:LEU:HD12	1	1.5
(1,2963)	1:109:A:TYR:HD2	1:128:A:LEU:HD13	1	1.5
(1,1015)	1:99:A:LEU:HD21	1:101:A:PRO:HD2	10	1.5
(1,1015)	1:99:A:LEU:HD22	1:101:A:PRO:HD2	10	1.5
(1,1015)	1:99:A:LEU:HD23	1:101:A:PRO:HD2	10	1.5
(1,823)	1:82:A:VAL:HG21	1:85:A:HIS:HB2	4	1.5
(1,823)	1:82:A:VAL:HG22	1:85:A:HIS:HB2	4	1.5
(1,823)	1:82:A:VAL:HG23	1:85:A:HIS:HB2	4	1.5
(1,753)	1:76:A:LYS:HD2	1:77:A:PRO:HD3	6	1.5
(1,753)	1:76:A:LYS:HD3	1:77:A:PRO:HD3	6	1.5
(2,1)	1:6:A:CYS:SG	1:29:A:CYS:SG	9	1.49
(1,3261)	1:104:A:LEU:HB2	1:109:A:TYR:HE1	3	1.49
(1,2605)	1:108:A:ASP:H	1:55:A:LYS:HG2	4	1.49
(1,2605)	1:108:A:ASP:H	1:55:A:LYS:HG3	4	1.49
(1,2360)	1:76:A:LYS:HE2	1:79:A:ASP:H	4	1.49
(1,2360)	1:76:A:LYS:HE3	1:79:A:ASP:H	4	1.49
(1,1965)	1:29:A:CYS:H	1:25:A:VAL:HG21	7	1.49
(1,1965)	1:29:A:CYS:H	1:25:A:VAL:HG22	7	1.49
(1,1965)	1:29:A:CYS:H	1:25:A:VAL:HG23	7	1.49
(1,1797)	1:15:A:ASN:HB3	1:13:A:ASN:HD21	2	1.49
(1,1506)	1:81:A:ARG:HB2	1:62:A:VAL:HG11	4	1.49
(1,1506)	1:81:A:ARG:HB2	1:62:A:VAL:HG12	4	1.49
(1,1506)	1:81:A:ARG:HB2	1:62:A:VAL:HG13	4	1.49
(1,1306)	1:25:A:VAL:HB	1:126:A:VAL:HG21	2	1.49
(1,1306)	1:25:A:VAL:HB	1:126:A:VAL:HG22	2	1.49
(1,1306)	1:25:A:VAL:HB	1:126:A:VAL:HG23	2	1.49
(1,753)	1:76:A:LYS:HD2	1:77:A:PRO:HD3	7	1.49
(1,753)	1:76:A:LYS:HD3	1:77:A:PRO:HD3	7	1.49
(1,2179)	1:51:A:LEU:H	1:95:A:SER:HB2	8	1.48
(1,185)	1:126:A:VAL:HG21	1:25:A:VAL:HA	8	1.48
(1,185)	1:126:A:VAL:HG22	1:25:A:VAL:HA	8	1.48
(1,185)	1:126:A:VAL:HG23	1:25:A:VAL:HA	8	1.48
(1,2963)	1:109:A:TYR:HD1	1:128:A:LEU:HD11	9	1.47
(1,2963)	1:109:A:TYR:HD1	1:128:A:LEU:HD12	9	1.47
(1,2963)	1:109:A:TYR:HD1	1:128:A:LEU:HD13	9	1.47
(1,2963)	1:109:A:TYR:HD2	1:128:A:LEU:HD11	9	1.47
(1,2963)	1:109:A:TYR:HD2	1:128:A:LEU:HD12	9	1.47
(1,2963)	1:109:A:TYR:HD2	1:128:A:LEU:HD13	9	1.47
(1,1702)	1:83:A:VAL:HG21	1:99:A:LEU:HD11	10	1.47
(1,1702)	1:83:A:VAL:HG21	1:99:A:LEU:HD12	10	1.47
(1,1702)	1:83:A:VAL:HG21	1:99:A:LEU:HD13	10	1.47
(1,1702)	1:83:A:VAL:HG22	1:99:A:LEU:HD11	10	1.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1702)	1:83:A:VAL:HG22	1:99:A:LEU:HD12	10	1.47
(1,1702)	1:83:A:VAL:HG22	1:99:A:LEU:HD13	10	1.47
(1,1702)	1:83:A:VAL:HG23	1:99:A:LEU:HD11	10	1.47
(1,1702)	1:83:A:VAL:HG23	1:99:A:LEU:HD12	10	1.47
(1,1702)	1:83:A:VAL:HG23	1:99:A:LEU:HD13	10	1.47
(1,1619)	1:109:A:TYR:HE1	1:104:A:LEU:HD21	7	1.47
(1,1619)	1:109:A:TYR:HE1	1:104:A:LEU:HD22	7	1.47
(1,1619)	1:109:A:TYR:HE1	1:104:A:LEU:HD23	7	1.47
(1,1619)	1:109:A:TYR:HE2	1:104:A:LEU:HD21	7	1.47
(1,1619)	1:109:A:TYR:HE2	1:104:A:LEU:HD22	7	1.47
(1,1619)	1:109:A:TYR:HE2	1:104:A:LEU:HD23	7	1.47
(1,1059)	1:104:A:LEU:HG	1:101:A:PRO:HA	9	1.47
(1,55)	1:17:A:GLN:HG3	1:12:A:SER:HB3	8	1.47
(1,2121)	1:43:A:PRO:HG3	1:47:A:MET:H	1	1.46
(1,2121)	1:43:A:PRO:HG3	1:47:A:MET:H	7	1.46
(1,2121)	1:43:A:PRO:HG3	1:47:A:MET:H	8	1.46
(1,1965)	1:29:A:CYS:H	1:25:A:VAL:HG21	8	1.46
(1,1965)	1:29:A:CYS:H	1:25:A:VAL:HG22	8	1.46
(1,1965)	1:29:A:CYS:H	1:25:A:VAL:HG23	8	1.46
(1,1715)	1:59:A:MET:HE1	1:114:A:THR:HG1	7	1.46
(1,1715)	1:59:A:MET:HE2	1:114:A:THR:HG1	7	1.46
(1,1715)	1:59:A:MET:HE3	1:114:A:THR:HG1	7	1.46
(1,1702)	1:83:A:VAL:HG21	1:99:A:LEU:HD11	3	1.46
(1,1702)	1:83:A:VAL:HG21	1:99:A:LEU:HD12	3	1.46
(1,1702)	1:83:A:VAL:HG21	1:99:A:LEU:HD13	3	1.46
(1,1702)	1:83:A:VAL:HG22	1:99:A:LEU:HD11	3	1.46
(1,1702)	1:83:A:VAL:HG22	1:99:A:LEU:HD12	3	1.46
(1,1702)	1:83:A:VAL:HG22	1:99:A:LEU:HD13	3	1.46
(1,1702)	1:83:A:VAL:HG23	1:99:A:LEU:HD11	3	1.46
(1,1702)	1:83:A:VAL:HG23	1:99:A:LEU:HD12	3	1.46
(1,1702)	1:83:A:VAL:HG23	1:99:A:LEU:HD13	3	1.46
(1,3264)	1:111:A:PHE:HD2	1:36:A:LEU:HD22	2	1.45
(1,2812)	1:129:A:VAL:H	1:104:A:LEU:HD11	9	1.45
(1,2812)	1:129:A:VAL:H	1:104:A:LEU:HD12	9	1.45
(1,2812)	1:129:A:VAL:H	1:104:A:LEU:HD13	9	1.45
(1,2411)	1:85:A:HIS:H	1:82:A:VAL:HG21	2	1.45
(1,2411)	1:85:A:HIS:H	1:82:A:VAL:HG22	2	1.45
(1,2411)	1:85:A:HIS:H	1:82:A:VAL:HG23	2	1.45
(1,753)	1:76:A:LYS:HD2	1:77:A:PRO:HD3	10	1.45
(1,753)	1:76:A:LYS:HD3	1:77:A:PRO:HD3	10	1.45
(1,2764)	1:124:A:GLY:H	1:110:A:LYS:HE2	10	1.44
(1,2764)	1:124:A:GLY:H	1:110:A:LYS:HE3	10	1.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1671)	1:25:A:VAL:HB	1:126:A:VAL:HG11	1	1.44
(1,1671)	1:25:A:VAL:HB	1:126:A:VAL:HG12	1	1.44
(1,1671)	1:25:A:VAL:HB	1:126:A:VAL:HG13	1	1.44
(1,1552)	1:109:A:TYR:HE1	1:83:A:VAL:HG11	3	1.44
(1,1552)	1:109:A:TYR:HE1	1:83:A:VAL:HG12	3	1.44
(1,1552)	1:109:A:TYR:HE1	1:83:A:VAL:HG13	3	1.44
(1,1552)	1:109:A:TYR:HE2	1:83:A:VAL:HG11	3	1.44
(1,1552)	1:109:A:TYR:HE2	1:83:A:VAL:HG12	3	1.44
(1,1552)	1:109:A:TYR:HE2	1:83:A:VAL:HG13	3	1.44
(1,33)	1:10:A:VAL:HB	1:36:A:LEU:HD21	2	1.44
(1,33)	1:10:A:VAL:HB	1:36:A:LEU:HD22	2	1.44
(1,33)	1:10:A:VAL:HB	1:36:A:LEU:HD23	2	1.44
(1,2812)	1:129:A:VAL:H	1:104:A:LEU:HD11	8	1.43
(1,2812)	1:129:A:VAL:H	1:104:A:LEU:HD12	8	1.43
(1,2812)	1:129:A:VAL:H	1:104:A:LEU:HD13	8	1.43
(1,2209)	1:54:A:ALA:H	1:126:A:VAL:HG21	3	1.43
(1,2209)	1:54:A:ALA:H	1:126:A:VAL:HG22	3	1.43
(1,2209)	1:54:A:ALA:H	1:126:A:VAL:HG23	3	1.43
(1,1965)	1:29:A:CYS:H	1:25:A:VAL:HG21	6	1.43
(1,1965)	1:29:A:CYS:H	1:25:A:VAL:HG22	6	1.43
(1,1965)	1:29:A:CYS:H	1:25:A:VAL:HG23	6	1.43
(1,2963)	1:109:A:TYR:HD1	1:128:A:LEU:HD11	8	1.42
(1,2963)	1:109:A:TYR:HD1	1:128:A:LEU:HD12	8	1.42
(1,2963)	1:109:A:TYR:HD1	1:128:A:LEU:HD13	8	1.42
(1,2963)	1:109:A:TYR:HD2	1:128:A:LEU:HD11	8	1.42
(1,2963)	1:109:A:TYR:HD2	1:128:A:LEU:HD12	8	1.42
(1,2963)	1:109:A:TYR:HD2	1:128:A:LEU:HD13	8	1.42
(1,1039)	1:99:A:LEU:HD21	1:101:A:PRO:HG3	7	1.42
(1,1039)	1:99:A:LEU:HD22	1:101:A:PRO:HG3	7	1.42
(1,1039)	1:99:A:LEU:HD23	1:101:A:PRO:HG3	7	1.42
(1,33)	1:10:A:VAL:HB	1:36:A:LEU:HD21	3	1.42
(1,33)	1:10:A:VAL:HB	1:36:A:LEU:HD22	3	1.42
(1,33)	1:10:A:VAL:HB	1:36:A:LEU:HD23	3	1.42
(1,2963)	1:109:A:TYR:HD1	1:128:A:LEU:HD11	7	1.41
(1,2963)	1:109:A:TYR:HD1	1:128:A:LEU:HD12	7	1.41
(1,2963)	1:109:A:TYR:HD1	1:128:A:LEU:HD13	7	1.41
(1,2963)	1:109:A:TYR:HD2	1:128:A:LEU:HD11	7	1.41
(1,2963)	1:109:A:TYR:HD2	1:128:A:LEU:HD12	7	1.41
(1,2963)	1:109:A:TYR:HD2	1:128:A:LEU:HD13	7	1.41
(1,2911)	1:49:A:HIS:HE2	1:17:A:GLN:HG3	3	1.41
(1,2362)	1:79:A:ASP:H	1:76:A:LYS:HB2	7	1.41
(1,2121)	1:43:A:PRO:HG3	1:47:A:MET:H	6	1.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2045)	1:94:A:GLU:HB2	1:38:A:HIS:H	4	1.41
(1,1965)	1:29:A:CYS:H	1:25:A:VAL:HG21	1	1.41
(1,1965)	1:29:A:CYS:H	1:25:A:VAL:HG22	1	1.41
(1,1965)	1:29:A:CYS:H	1:25:A:VAL:HG23	1	1.41
(1,1549)	1:83:A:VAL:HG21	1:104:A:LEU:HD21	9	1.41
(1,1549)	1:83:A:VAL:HG21	1:104:A:LEU:HD22	9	1.41
(1,1549)	1:83:A:VAL:HG21	1:104:A:LEU:HD23	9	1.41
(1,1549)	1:83:A:VAL:HG22	1:104:A:LEU:HD21	9	1.41
(1,1549)	1:83:A:VAL:HG22	1:104:A:LEU:HD22	9	1.41
(1,1549)	1:83:A:VAL:HG22	1:104:A:LEU:HD23	9	1.41
(1,1549)	1:83:A:VAL:HG23	1:104:A:LEU:HD21	9	1.41
(1,1549)	1:83:A:VAL:HG23	1:104:A:LEU:HD22	9	1.41
(1,1549)	1:83:A:VAL:HG23	1:104:A:LEU:HD23	9	1.41
(1,55)	1:17:A:GLN:HG3	1:12:A:SER:HB3	10	1.41
(1,33)	1:10:A:VAL:HB	1:36:A:LEU:HD21	6	1.41
(1,33)	1:10:A:VAL:HB	1:36:A:LEU:HD22	6	1.41
(1,33)	1:10:A:VAL:HB	1:36:A:LEU:HD23	6	1.41
(1,2303)	1:67:A:VAL:HG11	1:66:A:GLY:H	10	1.4
(1,2303)	1:67:A:VAL:HG12	1:66:A:GLY:H	10	1.4
(1,2303)	1:67:A:VAL:HG13	1:66:A:GLY:H	10	1.4
(1,39)	1:19:A:ASN:HD22	1:11:A:GLU:HG3	8	1.4
(1,2365)	1:79:A:ASP:H	1:75:A:VAL:HG11	10	1.39
(1,2365)	1:79:A:ASP:H	1:75:A:VAL:HG12	10	1.39
(1,2365)	1:79:A:ASP:H	1:75:A:VAL:HG13	10	1.39
(1,2360)	1:76:A:LYS:HE2	1:79:A:ASP:H	2	1.39
(1,2360)	1:76:A:LYS:HE3	1:79:A:ASP:H	2	1.39
(1,1929)	1:104:A:LEU:HD11	1:25:A:VAL:H	7	1.39
(1,1929)	1:104:A:LEU:HD12	1:25:A:VAL:H	7	1.39
(1,1929)	1:104:A:LEU:HD13	1:25:A:VAL:H	7	1.39
(1,882)	1:91:A:GLY:HA3	1:38:A:HIS:HB2	10	1.39
(1,3168)	1:24:A:GLN:H	1:34:A:ILE:HG12	1	1.38
(1,2840)	1:53:A:ILE:HD11	1:32:A:PHE:HD1	9	1.38
(1,2840)	1:53:A:ILE:HD11	1:32:A:PHE:HD2	9	1.38
(1,2840)	1:53:A:ILE:HD12	1:32:A:PHE:HD1	9	1.38
(1,2840)	1:53:A:ILE:HD12	1:32:A:PHE:HD2	9	1.38
(1,2840)	1:53:A:ILE:HD13	1:32:A:PHE:HD1	9	1.38
(1,2840)	1:53:A:ILE:HD13	1:32:A:PHE:HD2	9	1.38
(1,2411)	1:85:A:HIS:H	1:82:A:VAL:HG21	7	1.38
(1,2411)	1:85:A:HIS:H	1:82:A:VAL:HG22	7	1.38
(1,2411)	1:85:A:HIS:H	1:82:A:VAL:HG23	7	1.38
(1,2411)	1:85:A:HIS:H	1:82:A:VAL:HG21	8	1.38
(1,2411)	1:85:A:HIS:H	1:82:A:VAL:HG22	8	1.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2411)	1:85:A:HIS:H	1:82:A:VAL:HG23	8	1.38
(1,1671)	1:25:A:VAL:HB	1:126:A:VAL:HG11	7	1.38
(1,1671)	1:25:A:VAL:HB	1:126:A:VAL:HG12	7	1.38
(1,1671)	1:25:A:VAL:HB	1:126:A:VAL:HG13	7	1.38
(1,253)	1:98:A:THR:HB	1:31:A:GLU:HG2	5	1.38
(1,253)	1:98:A:THR:HB	1:31:A:GLU:HG3	5	1.38
(1,2556)	1:104:A:LEU:HG	1:103:A:LYS:H	6	1.37
(1,2211)	1:55:A:LYS:H	1:83:A:VAL:HB	9	1.37
(1,1671)	1:25:A:VAL:HB	1:126:A:VAL:HG11	9	1.37
(1,1671)	1:25:A:VAL:HB	1:126:A:VAL:HG12	9	1.37
(1,1671)	1:25:A:VAL:HB	1:126:A:VAL:HG13	9	1.37
(1,1015)	1:99:A:LEU:HD21	1:101:A:PRO:HD2	8	1.37
(1,1015)	1:99:A:LEU:HD22	1:101:A:PRO:HD2	8	1.37
(1,1015)	1:99:A:LEU:HD23	1:101:A:PRO:HD2	8	1.37
(1,1014)	1:101:A:PRO:HD2	1:25:A:VAL:HG21	2	1.37
(1,1014)	1:101:A:PRO:HD2	1:25:A:VAL:HG22	2	1.37
(1,1014)	1:101:A:PRO:HD2	1:25:A:VAL:HG23	2	1.37
(1,253)	1:98:A:THR:HB	1:31:A:GLU:HG2	9	1.37
(1,253)	1:98:A:THR:HB	1:31:A:GLU:HG3	9	1.37
(1,3108)	1:128:A:LEU:HB3	1:105:A:ALA:HA	4	1.36
(1,3108)	1:128:A:LEU:HB3	1:105:A:ALA:HA	10	1.36
(1,2542)	1:100:A:ASP:H	1:83:A:VAL:HA	2	1.36
(1,2529)	1:99:A:LEU:H	1:31:A:GLU:HB2	9	1.36
(1,2396)	1:82:A:VAL:HG21	1:84:A:ALA:H	9	1.36
(1,2396)	1:82:A:VAL:HG22	1:84:A:ALA:H	9	1.36
(1,2396)	1:82:A:VAL:HG23	1:84:A:ALA:H	9	1.36
(1,2227)	1:110:A:LYS:HD3	1:56:A:ALA:H	2	1.36
(1,2121)	1:43:A:PRO:HG3	1:47:A:MET:H	10	1.36
(1,1671)	1:25:A:VAL:HB	1:126:A:VAL:HG11	6	1.36
(1,1671)	1:25:A:VAL:HB	1:126:A:VAL:HG12	6	1.36
(1,1671)	1:25:A:VAL:HB	1:126:A:VAL:HG13	6	1.36
(1,2812)	1:129:A:VAL:H	1:104:A:LEU:HD11	7	1.35
(1,2812)	1:129:A:VAL:H	1:104:A:LEU:HD12	7	1.35
(1,2812)	1:129:A:VAL:H	1:104:A:LEU:HD13	7	1.35
(1,2364)	1:82:A:VAL:HG11	1:79:A:ASP:H	9	1.35
(1,2364)	1:82:A:VAL:HG12	1:79:A:ASP:H	9	1.35
(1,2364)	1:82:A:VAL:HG13	1:79:A:ASP:H	9	1.35
(1,1965)	1:29:A:CYS:H	1:25:A:VAL:HG21	3	1.35
(1,1965)	1:29:A:CYS:H	1:25:A:VAL:HG22	3	1.35
(1,1965)	1:29:A:CYS:H	1:25:A:VAL:HG23	3	1.35
(1,1306)	1:25:A:VAL:HB	1:126:A:VAL:HG21	8	1.35
(1,1306)	1:25:A:VAL:HB	1:126:A:VAL:HG22	8	1.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1306)	1:25:A:VAL:HB	1:126:A:VAL:HG23	8	1.35
(1,33)	1:10:A:VAL:HB	1:36:A:LEU:HD21	5	1.35
(1,33)	1:10:A:VAL:HB	1:36:A:LEU:HD22	5	1.35
(1,33)	1:10:A:VAL:HB	1:36:A:LEU:HD23	5	1.35
(1,2961)	1:83:A:VAL:HG11	1:109:A:TYR:HD1	3	1.34
(1,2961)	1:83:A:VAL:HG11	1:109:A:TYR:HD2	3	1.34
(1,2961)	1:83:A:VAL:HG12	1:109:A:TYR:HD1	3	1.34
(1,2961)	1:83:A:VAL:HG12	1:109:A:TYR:HD2	3	1.34
(1,2961)	1:83:A:VAL:HG13	1:109:A:TYR:HD1	3	1.34
(1,2961)	1:83:A:VAL:HG13	1:109:A:TYR:HD2	3	1.34
(1,2121)	1:43:A:PRO:HG3	1:47:A:MET:H	4	1.34
(1,1705)	1:99:A:LEU:HD11	1:31:A:GLU:HB2	4	1.34
(1,1705)	1:99:A:LEU:HD12	1:31:A:GLU:HB2	4	1.34
(1,1705)	1:99:A:LEU:HD13	1:31:A:GLU:HB2	4	1.34
(1,823)	1:82:A:VAL:HG21	1:85:A:HIS:HB2	7	1.34
(1,823)	1:82:A:VAL:HG22	1:85:A:HIS:HB2	7	1.34
(1,823)	1:82:A:VAL:HG23	1:85:A:HIS:HB2	7	1.34
(1,823)	1:82:A:VAL:HG21	1:85:A:HIS:HB2	8	1.34
(1,823)	1:82:A:VAL:HG22	1:85:A:HIS:HB2	8	1.34
(1,823)	1:82:A:VAL:HG23	1:85:A:HIS:HB2	8	1.34
(1,551)	1:83:A:VAL:HG11	1:54:A:ALA:HA	7	1.34
(1,551)	1:83:A:VAL:HG12	1:54:A:ALA:HA	7	1.34
(1,551)	1:83:A:VAL:HG13	1:54:A:ALA:HA	7	1.34
(1,58)	1:17:A:GLN:HG3	1:12:A:SER:HB2	5	1.34
(1,33)	1:10:A:VAL:HB	1:36:A:LEU:HD21	8	1.34
(1,33)	1:10:A:VAL:HB	1:36:A:LEU:HD22	8	1.34
(1,33)	1:10:A:VAL:HB	1:36:A:LEU:HD23	8	1.34
(1,766)	1:69:A:ALA:HA	1:77:A:PRO:HD2	9	1.33
(1,463)	1:88:A:LEU:HG	1:48:A:GLY:HA2	4	1.33
(1,2529)	1:99:A:LEU:H	1:31:A:GLU:HB2	4	1.32
(1,2060)	1:93:A:GLU:H	1:40:A:GLY:H	10	1.32
(1,1797)	1:15:A:ASN:HB3	1:13:A:ASN:HD21	7	1.32
(1,1061)	1:105:A:ALA:HA	1:128:A:LEU:HD11	9	1.32
(1,1061)	1:105:A:ALA:HA	1:128:A:LEU:HD12	9	1.32
(1,1061)	1:105:A:ALA:HA	1:128:A:LEU:HD13	9	1.32
(1,1037)	1:99:A:LEU:HD21	1:101:A:PRO:HG2	1	1.32
(1,1037)	1:99:A:LEU:HD22	1:101:A:PRO:HG2	1	1.32
(1,1037)	1:99:A:LEU:HD23	1:101:A:PRO:HG2	1	1.32
(1,753)	1:76:A:LYS:HD2	1:77:A:PRO:HD3	8	1.32
(1,753)	1:76:A:LYS:HD3	1:77:A:PRO:HD3	8	1.32
(1,691)	1:88:A:LEU:HG	1:70:A:ALA:HA	7	1.32
(1,3108)	1:128:A:LEU:HB3	1:105:A:ALA:HA	5	1.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2211)	1:55:A:LYS:H	1:83:A:VAL:HB	3	1.31
(1,1881)	1:20:A:THR:H	1:10:A:VAL:HG11	10	1.31
(1,1881)	1:20:A:THR:H	1:10:A:VAL:HG12	10	1.31
(1,1881)	1:20:A:THR:H	1:10:A:VAL:HG13	10	1.31
(1,984)	1:98:A:THR:HB	1:31:A:GLU:HB2	9	1.31
(1,1386)	1:101:A:PRO:HB2	1:25:A:VAL:HG21	5	1.3
(1,1386)	1:101:A:PRO:HB2	1:25:A:VAL:HG22	5	1.3
(1,1386)	1:101:A:PRO:HB2	1:25:A:VAL:HG23	5	1.3
(1,493)	1:50:A:ASN:HA	1:36:A:LEU:HD11	9	1.3
(1,493)	1:50:A:ASN:HA	1:36:A:LEU:HD12	9	1.3
(1,493)	1:50:A:ASN:HA	1:36:A:LEU:HD13	9	1.3
(1,33)	1:10:A:VAL:HB	1:36:A:LEU:HD21	7	1.3
(1,33)	1:10:A:VAL:HB	1:36:A:LEU:HD22	7	1.3
(1,33)	1:10:A:VAL:HB	1:36:A:LEU:HD23	7	1.3
(1,2961)	1:83:A:VAL:HG11	1:109:A:TYR:HD1	2	1.29
(1,2961)	1:83:A:VAL:HG11	1:109:A:TYR:HD2	2	1.29
(1,2961)	1:83:A:VAL:HG12	1:109:A:TYR:HD1	2	1.29
(1,2961)	1:83:A:VAL:HG12	1:109:A:TYR:HD2	2	1.29
(1,2961)	1:83:A:VAL:HG13	1:109:A:TYR:HD1	2	1.29
(1,2961)	1:83:A:VAL:HG13	1:109:A:TYR:HD2	2	1.29
(1,2227)	1:110:A:LYS:HD3	1:56:A:ALA:H	10	1.29
(1,2211)	1:55:A:LYS:H	1:83:A:VAL:HB	8	1.29
(1,1167)	1:114:A:THR:HB	1:67:A:VAL:HG21	5	1.29
(1,1167)	1:114:A:THR:HB	1:67:A:VAL:HG22	5	1.29
(1,1167)	1:114:A:THR:HB	1:67:A:VAL:HG23	5	1.29
(1,1014)	1:101:A:PRO:HD2	1:25:A:VAL:HG21	3	1.29
(1,1014)	1:101:A:PRO:HD2	1:25:A:VAL:HG22	3	1.29
(1,1014)	1:101:A:PRO:HD2	1:25:A:VAL:HG23	3	1.29
(1,551)	1:83:A:VAL:HG11	1:54:A:ALA:HA	2	1.29
(1,551)	1:83:A:VAL:HG12	1:54:A:ALA:HA	2	1.29
(1,551)	1:83:A:VAL:HG13	1:54:A:ALA:HA	2	1.29
(1,3261)	1:109:A:TYR:HE2	1:55:A:LYS:HD3	2	1.28
(1,2303)	1:67:A:VAL:HG11	1:66:A:GLY:H	6	1.28
(1,2303)	1:67:A:VAL:HG12	1:66:A:GLY:H	6	1.28
(1,2303)	1:67:A:VAL:HG13	1:66:A:GLY:H	6	1.28
(1,2121)	1:43:A:PRO:HG3	1:47:A:MET:H	5	1.28
(1,551)	1:83:A:VAL:HG11	1:54:A:ALA:HA	3	1.28
(1,551)	1:83:A:VAL:HG12	1:54:A:ALA:HA	3	1.28
(1,551)	1:83:A:VAL:HG13	1:54:A:ALA:HA	3	1.28
(1,2556)	1:104:A:LEU:HG	1:103:A:LYS:H	7	1.27
(1,2411)	1:85:A:HIS:H	1:82:A:VAL:HG21	5	1.27
(1,2411)	1:85:A:HIS:H	1:82:A:VAL:HG22	5	1.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2411)	1:85:A:HIS:H	1:82:A:VAL:HG23	5	1.27
(1,2121)	1:43:A:PRO:HG3	1:47:A:MET:H	9	1.27
(1,1436)	1:47:A:MET:HE1	1:118:A:HIS:HB2	2	1.27
(1,1436)	1:47:A:MET:HE2	1:118:A:HIS:HB2	2	1.27
(1,1436)	1:47:A:MET:HE3	1:118:A:HIS:HB2	2	1.27
(1,1095)	1:110:A:LYS:HD3	1:109:A:TYR:HA	3	1.27
(1,1059)	1:104:A:LEU:HG	1:101:A:PRO:HA	6	1.27
(1,2880)	1:67:A:VAL:HG21	1:74:A:TYR:HD1	10	1.26
(1,2880)	1:67:A:VAL:HG21	1:74:A:TYR:HD2	10	1.26
(1,2880)	1:67:A:VAL:HG22	1:74:A:TYR:HD1	10	1.26
(1,2880)	1:67:A:VAL:HG22	1:74:A:TYR:HD2	10	1.26
(1,2880)	1:67:A:VAL:HG23	1:74:A:TYR:HD1	10	1.26
(1,2880)	1:67:A:VAL:HG23	1:74:A:TYR:HD2	10	1.26
(1,1671)	1:25:A:VAL:HB	1:126:A:VAL:HG11	10	1.26
(1,1671)	1:25:A:VAL:HB	1:126:A:VAL:HG12	10	1.26
(1,1671)	1:25:A:VAL:HB	1:126:A:VAL:HG13	10	1.26
(1,1552)	1:109:A:TYR:HE1	1:83:A:VAL:HG11	4	1.26
(1,1552)	1:109:A:TYR:HE1	1:83:A:VAL:HG12	4	1.26
(1,1552)	1:109:A:TYR:HE1	1:83:A:VAL:HG13	4	1.26
(1,1552)	1:109:A:TYR:HE2	1:83:A:VAL:HG11	4	1.26
(1,1552)	1:109:A:TYR:HE2	1:83:A:VAL:HG12	4	1.26
(1,1552)	1:109:A:TYR:HE2	1:83:A:VAL:HG13	4	1.26
(1,753)	1:76:A:LYS:HD2	1:77:A:PRO:HD3	2	1.26
(1,753)	1:76:A:LYS:HD3	1:77:A:PRO:HD3	2	1.26
(1,463)	1:88:A:LEU:HG	1:48:A:GLY:HA2	10	1.26
(1,2303)	1:67:A:VAL:HG11	1:66:A:GLY:H	8	1.25
(1,2303)	1:67:A:VAL:HG12	1:66:A:GLY:H	8	1.25
(1,2303)	1:67:A:VAL:HG13	1:66:A:GLY:H	8	1.25
(1,2214)	1:83:A:VAL:HG11	1:55:A:LYS:H	7	1.25
(1,2214)	1:83:A:VAL:HG12	1:55:A:LYS:H	7	1.25
(1,2214)	1:83:A:VAL:HG13	1:55:A:LYS:H	7	1.25
(1,2209)	1:54:A:ALA:H	1:126:A:VAL:HG21	10	1.25
(1,2209)	1:54:A:ALA:H	1:126:A:VAL:HG22	10	1.25
(1,2209)	1:54:A:ALA:H	1:126:A:VAL:HG23	10	1.25
(1,1095)	1:110:A:LYS:HD3	1:109:A:TYR:HA	2	1.25
(1,1014)	1:101:A:PRO:HD2	1:25:A:VAL:HG21	4	1.25
(1,1014)	1:101:A:PRO:HD2	1:25:A:VAL:HG22	4	1.25
(1,1014)	1:101:A:PRO:HD2	1:25:A:VAL:HG23	4	1.25
(1,493)	1:50:A:ASN:HA	1:36:A:LEU:HD11	7	1.25
(1,493)	1:50:A:ASN:HA	1:36:A:LEU:HD12	7	1.25
(1,493)	1:50:A:ASN:HA	1:36:A:LEU:HD13	7	1.25
(1,55)	1:17:A:GLN:HG3	1:12:A:SER:HB3	1	1.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,33)	1:10:A:VAL:HB	1:36:A:LEU:HD21	9	1.25
(1,33)	1:10:A:VAL:HB	1:36:A:LEU:HD22	9	1.25
(1,33)	1:10:A:VAL:HB	1:36:A:LEU:HD23	9	1.25
(1,2528)	1:99:A:LEU:H	1:31:A:GLU:HG2	4	1.24
(1,2528)	1:99:A:LEU:H	1:31:A:GLU:HG3	4	1.24
(1,2303)	1:67:A:VAL:HG11	1:66:A:GLY:H	4	1.24
(1,2303)	1:67:A:VAL:HG12	1:66:A:GLY:H	4	1.24
(1,2303)	1:67:A:VAL:HG13	1:66:A:GLY:H	4	1.24
(1,1059)	1:104:A:LEU:HG	1:101:A:PRO:HA	7	1.24
(1,463)	1:88:A:LEU:HG	1:48:A:GLY:HA2	9	1.24
(1,2963)	1:109:A:TYR:HD1	1:128:A:LEU:HD11	6	1.23
(1,2963)	1:109:A:TYR:HD1	1:128:A:LEU:HD12	6	1.23
(1,2963)	1:109:A:TYR:HD1	1:128:A:LEU:HD13	6	1.23
(1,2963)	1:109:A:TYR:HD2	1:128:A:LEU:HD11	6	1.23
(1,2963)	1:109:A:TYR:HD2	1:128:A:LEU:HD12	6	1.23
(1,2963)	1:109:A:TYR:HD2	1:128:A:LEU:HD13	6	1.23
(1,2303)	1:67:A:VAL:HG11	1:66:A:GLY:H	1	1.23
(1,2303)	1:67:A:VAL:HG12	1:66:A:GLY:H	1	1.23
(1,2303)	1:67:A:VAL:HG13	1:66:A:GLY:H	1	1.23
(1,1549)	1:83:A:VAL:HG21	1:104:A:LEU:HD21	5	1.23
(1,1549)	1:83:A:VAL:HG21	1:104:A:LEU:HD22	5	1.23
(1,1549)	1:83:A:VAL:HG21	1:104:A:LEU:HD23	5	1.23
(1,1549)	1:83:A:VAL:HG22	1:104:A:LEU:HD21	5	1.23
(1,1549)	1:83:A:VAL:HG22	1:104:A:LEU:HD22	5	1.23
(1,1549)	1:83:A:VAL:HG22	1:104:A:LEU:HD23	5	1.23
(1,1549)	1:83:A:VAL:HG23	1:104:A:LEU:HD21	5	1.23
(1,1549)	1:83:A:VAL:HG23	1:104:A:LEU:HD22	5	1.23
(1,1549)	1:83:A:VAL:HG23	1:104:A:LEU:HD23	5	1.23
(1,1014)	1:101:A:PRO:HD2	1:25:A:VAL:HG21	7	1.23
(1,1014)	1:101:A:PRO:HD2	1:25:A:VAL:HG22	7	1.23
(1,1014)	1:101:A:PRO:HD2	1:25:A:VAL:HG23	7	1.23
(1,58)	1:17:A:GLN:HG3	1:12:A:SER:HB2	10	1.23
(1,2211)	1:55:A:LYS:H	1:83:A:VAL:HB	10	1.22
(1,1543)	1:85:A:HIS:HD2	1:82:A:VAL:HG21	5	1.22
(1,1543)	1:85:A:HIS:HD2	1:82:A:VAL:HG22	5	1.22
(1,1543)	1:85:A:HIS:HD2	1:82:A:VAL:HG23	5	1.22
(1,1014)	1:101:A:PRO:HD2	1:25:A:VAL:HG21	10	1.22
(1,1014)	1:101:A:PRO:HD2	1:25:A:VAL:HG22	10	1.22
(1,1014)	1:101:A:PRO:HD2	1:25:A:VAL:HG23	10	1.22
(1,1001)	1:100:A:ASP:HA	1:31:A:GLU:HB2	4	1.22
(1,984)	1:98:A:THR:HB	1:31:A:GLU:HB2	4	1.22
(1,2411)	1:85:A:HIS:H	1:82:A:VAL:HG21	9	1.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2411)	1:85:A:HIS:H	1:82:A:VAL:HG22	9	1.21
(1,2411)	1:85:A:HIS:H	1:82:A:VAL:HG23	9	1.21
(1,2209)	1:54:A:ALA:H	1:126:A:VAL:HG21	7	1.21
(1,2209)	1:54:A:ALA:H	1:126:A:VAL:HG22	7	1.21
(1,2209)	1:54:A:ALA:H	1:126:A:VAL:HG23	7	1.21
(1,2121)	1:43:A:PRO:HG3	1:47:A:MET:H	2	1.21
(1,1552)	1:109:A:TYR:HE1	1:83:A:VAL:HG11	1	1.21
(1,1552)	1:109:A:TYR:HE1	1:83:A:VAL:HG12	1	1.21
(1,1552)	1:109:A:TYR:HE1	1:83:A:VAL:HG13	1	1.21
(1,1552)	1:109:A:TYR:HE2	1:83:A:VAL:HG11	1	1.21
(1,1552)	1:109:A:TYR:HE2	1:83:A:VAL:HG12	1	1.21
(1,1552)	1:109:A:TYR:HE2	1:83:A:VAL:HG13	1	1.21
(1,1014)	1:101:A:PRO:HD2	1:25:A:VAL:HG21	6	1.21
(1,1014)	1:101:A:PRO:HD2	1:25:A:VAL:HG22	6	1.21
(1,1014)	1:101:A:PRO:HD2	1:25:A:VAL:HG23	6	1.21
(1,823)	1:82:A:VAL:HG21	1:85:A:HIS:HB2	2	1.21
(1,823)	1:82:A:VAL:HG22	1:85:A:HIS:HB2	2	1.21
(1,823)	1:82:A:VAL:HG23	1:85:A:HIS:HB2	2	1.21
(1,3168)	1:24:A:GLN:H	1:34:A:ILE:HG12	3	1.2
(1,2963)	1:109:A:TYR:HD1	1:128:A:LEU:HD11	4	1.2
(1,2963)	1:109:A:TYR:HD1	1:128:A:LEU:HD12	4	1.2
(1,2963)	1:109:A:TYR:HD1	1:128:A:LEU:HD13	4	1.2
(1,2963)	1:109:A:TYR:HD2	1:128:A:LEU:HD11	4	1.2
(1,2963)	1:109:A:TYR:HD2	1:128:A:LEU:HD12	4	1.2
(1,2963)	1:109:A:TYR:HD2	1:128:A:LEU:HD13	4	1.2
(1,2961)	1:83:A:VAL:HG11	1:109:A:TYR:HD1	6	1.2
(1,2961)	1:83:A:VAL:HG11	1:109:A:TYR:HD2	6	1.2
(1,2961)	1:83:A:VAL:HG12	1:109:A:TYR:HD1	6	1.2
(1,2961)	1:83:A:VAL:HG12	1:109:A:TYR:HD2	6	1.2
(1,2961)	1:83:A:VAL:HG13	1:109:A:TYR:HD1	6	1.2
(1,2961)	1:83:A:VAL:HG13	1:109:A:TYR:HD2	6	1.2
(1,1303)	1:56:A:ALA:H	1:55:A:LYS:HD2	6	1.2
(1,1015)	1:99:A:LEU:HD21	1:101:A:PRO:HD2	1	1.2
(1,1015)	1:99:A:LEU:HD22	1:101:A:PRO:HD2	1	1.2
(1,1015)	1:99:A:LEU:HD23	1:101:A:PRO:HD2	1	1.2
(1,643)	1:76:A:LYS:HD2	1:66:A:GLY:HA3	1	1.2
(1,643)	1:76:A:LYS:HD3	1:66:A:GLY:HA3	1	1.2
(1,551)	1:83:A:VAL:HG11	1:54:A:ALA:HA	6	1.2
(1,551)	1:83:A:VAL:HG12	1:54:A:ALA:HA	6	1.2
(1,551)	1:83:A:VAL:HG13	1:54:A:ALA:HA	6	1.2
(1,55)	1:17:A:GLN:HG3	1:12:A:SER:HB3	2	1.2
(1,3232)	1:112:A:ALA:H	1:126:A:VAL:HG13	6	1.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1079)	1:125:A:LYS:HE2	1:108:A:ASP:HA	4	1.19
(1,1079)	1:125:A:LYS:HE3	1:108:A:ASP:HA	4	1.19
(1,3252)	1:18:A:PHE:HD1	1:10:A:VAL:HG11	10	1.18
(1,3232)	1:53:A:ILE:HG21	1:112:A:ALA:H	7	1.18
(1,3108)	1:128:A:LEU:HB3	1:105:A:ALA:HA	6	1.18
(1,2413)	1:86:A:THR:H	1:52:A:VAL:HG21	2	1.18
(1,2413)	1:86:A:THR:H	1:52:A:VAL:HG22	2	1.18
(1,2413)	1:86:A:THR:H	1:52:A:VAL:HG23	2	1.18
(1,1702)	1:83:A:VAL:HG21	1:99:A:LEU:HD11	2	1.18
(1,1702)	1:83:A:VAL:HG21	1:99:A:LEU:HD12	2	1.18
(1,1702)	1:83:A:VAL:HG21	1:99:A:LEU:HD13	2	1.18
(1,1702)	1:83:A:VAL:HG22	1:99:A:LEU:HD11	2	1.18
(1,1702)	1:83:A:VAL:HG22	1:99:A:LEU:HD12	2	1.18
(1,1702)	1:83:A:VAL:HG22	1:99:A:LEU:HD13	2	1.18
(1,1702)	1:83:A:VAL:HG23	1:99:A:LEU:HD11	2	1.18
(1,1702)	1:83:A:VAL:HG23	1:99:A:LEU:HD12	2	1.18
(1,1702)	1:83:A:VAL:HG23	1:99:A:LEU:HD13	2	1.18
(1,33)	1:10:A:VAL:HB	1:36:A:LEU:HD21	1	1.18
(1,33)	1:10:A:VAL:HB	1:36:A:LEU:HD22	1	1.18
(1,33)	1:10:A:VAL:HB	1:36:A:LEU:HD23	1	1.18
(1,2961)	1:83:A:VAL:HG11	1:109:A:TYR:HD1	7	1.17
(1,2961)	1:83:A:VAL:HG11	1:109:A:TYR:HD2	7	1.17
(1,2961)	1:83:A:VAL:HG12	1:109:A:TYR:HD1	7	1.17
(1,2961)	1:83:A:VAL:HG12	1:109:A:TYR:HD2	7	1.17
(1,2961)	1:83:A:VAL:HG13	1:109:A:TYR:HD1	7	1.17
(1,2961)	1:83:A:VAL:HG13	1:109:A:TYR:HD2	7	1.17
(1,2303)	1:67:A:VAL:HG11	1:66:A:GLY:H	2	1.17
(1,2303)	1:67:A:VAL:HG12	1:66:A:GLY:H	2	1.17
(1,2303)	1:67:A:VAL:HG13	1:66:A:GLY:H	2	1.17
(1,1797)	1:15:A:ASN:HB3	1:13:A:ASN:HD21	6	1.17
(1,1715)	1:59:A:MET:HE1	1:114:A:THR:HG1	9	1.17
(1,1715)	1:59:A:MET:HE2	1:114:A:THR:HG1	9	1.17
(1,1715)	1:59:A:MET:HE3	1:114:A:THR:HG1	9	1.17
(1,1178)	1:115:A:PHE:HB3	1:88:A:LEU:HD21	7	1.17
(1,1178)	1:115:A:PHE:HB3	1:88:A:LEU:HD22	7	1.17
(1,1178)	1:115:A:PHE:HB3	1:88:A:LEU:HD23	7	1.17
(1,1039)	1:99:A:LEU:HD21	1:101:A:PRO:HG3	6	1.17
(1,1039)	1:99:A:LEU:HD22	1:101:A:PRO:HG3	6	1.17
(1,1039)	1:99:A:LEU:HD23	1:101:A:PRO:HG3	6	1.17
(1,766)	1:69:A:ALA:HA	1:77:A:PRO:HD2	10	1.17
(1,58)	1:17:A:GLN:HG3	1:12:A:SER:HB2	2	1.17
(1,2961)	1:83:A:VAL:HG11	1:109:A:TYR:HD1	4	1.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2961)	1:83:A:VAL:HG11	1:109:A:TYR:HD2	4	1.16
(1,2961)	1:83:A:VAL:HG12	1:109:A:TYR:HD1	4	1.16
(1,2961)	1:83:A:VAL:HG12	1:109:A:TYR:HD2	4	1.16
(1,2961)	1:83:A:VAL:HG13	1:109:A:TYR:HD1	4	1.16
(1,2961)	1:83:A:VAL:HG13	1:109:A:TYR:HD2	4	1.16
(1,2595)	1:74:A:TYR:HB3	1:50:A:ASN:HD21	10	1.16
(1,2303)	1:67:A:VAL:HG11	1:66:A:GLY:H	3	1.16
(1,2303)	1:67:A:VAL:HG12	1:66:A:GLY:H	3	1.16
(1,2303)	1:67:A:VAL:HG13	1:66:A:GLY:H	3	1.16
(1,1619)	1:109:A:TYR:HE1	1:104:A:LEU:HD21	5	1.16
(1,1619)	1:109:A:TYR:HE1	1:104:A:LEU:HD22	5	1.16
(1,1619)	1:109:A:TYR:HE1	1:104:A:LEU:HD23	5	1.16
(1,1619)	1:109:A:TYR:HE2	1:104:A:LEU:HD21	5	1.16
(1,1619)	1:109:A:TYR:HE2	1:104:A:LEU:HD22	5	1.16
(1,1619)	1:109:A:TYR:HE2	1:104:A:LEU:HD23	5	1.16
(1,1303)	1:56:A:ALA:H	1:55:A:LYS:HD2	10	1.16
(1,1014)	1:101:A:PRO:HD2	1:25:A:VAL:HG21	9	1.16
(1,1014)	1:101:A:PRO:HD2	1:25:A:VAL:HG22	9	1.16
(1,1014)	1:101:A:PRO:HD2	1:25:A:VAL:HG23	9	1.16
(1,3232)	1:53:A:ILE:HG23	1:112:A:ALA:H	8	1.15
(1,2303)	1:67:A:VAL:HG11	1:66:A:GLY:H	9	1.15
(1,2303)	1:67:A:VAL:HG12	1:66:A:GLY:H	9	1.15
(1,2303)	1:67:A:VAL:HG13	1:66:A:GLY:H	9	1.15
(1,2068)	1:91:A:GLY:HA3	1:40:A:GLY:H	7	1.15
(1,1552)	1:109:A:TYR:HE1	1:83:A:VAL:HG11	2	1.15
(1,1552)	1:109:A:TYR:HE1	1:83:A:VAL:HG12	2	1.15
(1,1552)	1:109:A:TYR:HE1	1:83:A:VAL:HG13	2	1.15
(1,1552)	1:109:A:TYR:HE2	1:83:A:VAL:HG11	2	1.15
(1,1552)	1:109:A:TYR:HE2	1:83:A:VAL:HG12	2	1.15
(1,1552)	1:109:A:TYR:HE2	1:83:A:VAL:HG13	2	1.15
(1,551)	1:83:A:VAL:HG11	1:54:A:ALA:HA	4	1.15
(1,551)	1:83:A:VAL:HG12	1:54:A:ALA:HA	4	1.15
(1,551)	1:83:A:VAL:HG13	1:54:A:ALA:HA	4	1.15
(1,3168)	1:24:A:GLN:H	1:34:A:ILE:HG12	9	1.14
(1,2880)	1:67:A:VAL:HG21	1:74:A:TYR:HD1	6	1.14
(1,2880)	1:67:A:VAL:HG21	1:74:A:TYR:HD2	6	1.14
(1,2880)	1:67:A:VAL:HG22	1:74:A:TYR:HD1	6	1.14
(1,2880)	1:67:A:VAL:HG22	1:74:A:TYR:HD2	6	1.14
(1,2880)	1:67:A:VAL:HG23	1:74:A:TYR:HD1	6	1.14
(1,2880)	1:67:A:VAL:HG23	1:74:A:TYR:HD2	6	1.14
(1,1680)	1:27:A:LYS:HG2	1:128:A:LEU:HD21	8	1.14
(1,1680)	1:27:A:LYS:HG2	1:128:A:LEU:HD22	8	1.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1680)	1:27:A:LYS:HG2	1:128:A:LEU:HD23	8	1.14
(1,1680)	1:27:A:LYS:HG3	1:128:A:LEU:HD21	8	1.14
(1,1680)	1:27:A:LYS:HG3	1:128:A:LEU:HD22	8	1.14
(1,1680)	1:27:A:LYS:HG3	1:128:A:LEU:HD23	8	1.14
(1,1436)	1:47:A:MET:HE1	1:118:A:HIS:HB2	3	1.14
(1,1436)	1:47:A:MET:HE2	1:118:A:HIS:HB2	3	1.14
(1,1436)	1:47:A:MET:HE3	1:118:A:HIS:HB2	3	1.14
(1,1413)	1:10:A:VAL:HG21	1:34:A:ILE:HG21	10	1.14
(1,1413)	1:10:A:VAL:HG21	1:34:A:ILE:HG22	10	1.14
(1,1413)	1:10:A:VAL:HG21	1:34:A:ILE:HG23	10	1.14
(1,1413)	1:10:A:VAL:HG22	1:34:A:ILE:HG21	10	1.14
(1,1413)	1:10:A:VAL:HG22	1:34:A:ILE:HG22	10	1.14
(1,1413)	1:10:A:VAL:HG22	1:34:A:ILE:HG23	10	1.14
(1,1413)	1:10:A:VAL:HG23	1:34:A:ILE:HG21	10	1.14
(1,1413)	1:10:A:VAL:HG23	1:34:A:ILE:HG22	10	1.14
(1,1413)	1:10:A:VAL:HG23	1:34:A:ILE:HG23	10	1.14
(1,3261)	1:104:A:LEU:HB2	1:109:A:TYR:HE1	10	1.13
(1,3132)	1:104:A:LEU:HD11	1:25:A:VAL:HG13	7	1.13
(1,2413)	1:86:A:THR:H	1:52:A:VAL:HG21	7	1.13
(1,2413)	1:86:A:THR:H	1:52:A:VAL:HG22	7	1.13
(1,2413)	1:86:A:THR:H	1:52:A:VAL:HG23	7	1.13
(1,753)	1:76:A:LYS:HD2	1:77:A:PRO:HD3	9	1.13
(1,753)	1:76:A:LYS:HD3	1:77:A:PRO:HD3	9	1.13
(1,2987)	1:126:A:VAL:HG11	1:111:A:PHE:HD1	4	1.12
(1,2987)	1:126:A:VAL:HG11	1:111:A:PHE:HD2	4	1.12
(1,2987)	1:126:A:VAL:HG12	1:111:A:PHE:HD1	4	1.12
(1,2987)	1:126:A:VAL:HG12	1:111:A:PHE:HD2	4	1.12
(1,2987)	1:126:A:VAL:HG13	1:111:A:PHE:HD1	4	1.12
(1,2987)	1:126:A:VAL:HG13	1:111:A:PHE:HD2	4	1.12
(1,2987)	1:126:A:VAL:HG11	1:111:A:PHE:HD1	8	1.12
(1,2987)	1:126:A:VAL:HG11	1:111:A:PHE:HD2	8	1.12
(1,2987)	1:126:A:VAL:HG12	1:111:A:PHE:HD1	8	1.12
(1,2987)	1:126:A:VAL:HG12	1:111:A:PHE:HD2	8	1.12
(1,2987)	1:126:A:VAL:HG13	1:111:A:PHE:HD1	8	1.12
(1,2987)	1:126:A:VAL:HG13	1:111:A:PHE:HD2	8	1.12
(1,2627)	1:111:A:PHE:H	1:126:A:VAL:HG11	2	1.12
(1,2627)	1:111:A:PHE:H	1:126:A:VAL:HG12	2	1.12
(1,2627)	1:111:A:PHE:H	1:126:A:VAL:HG13	2	1.12
(1,2627)	1:111:A:PHE:H	1:126:A:VAL:HG11	8	1.12
(1,2627)	1:111:A:PHE:H	1:126:A:VAL:HG12	8	1.12
(1,2627)	1:111:A:PHE:H	1:126:A:VAL:HG13	8	1.12
(1,2214)	1:83:A:VAL:HG11	1:55:A:LYS:H	6	1.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2214)	1:83:A:VAL:HG12	1:55:A:LYS:H	6	1.12
(1,2214)	1:83:A:VAL:HG13	1:55:A:LYS:H	6	1.12
(1,1705)	1:99:A:LEU:HD11	1:31:A:GLU:HB2	9	1.12
(1,1705)	1:99:A:LEU:HD12	1:31:A:GLU:HB2	9	1.12
(1,1705)	1:99:A:LEU:HD13	1:31:A:GLU:HB2	9	1.12
(1,823)	1:82:A:VAL:HG21	1:85:A:HIS:HB2	9	1.12
(1,823)	1:82:A:VAL:HG22	1:85:A:HIS:HB2	9	1.12
(1,823)	1:82:A:VAL:HG23	1:85:A:HIS:HB2	9	1.12
(1,473)	1:49:A:HIS:HA	1:88:A:LEU:HD21	7	1.12
(1,473)	1:49:A:HIS:HA	1:88:A:LEU:HD22	7	1.12
(1,473)	1:49:A:HIS:HA	1:88:A:LEU:HD23	7	1.12
(1,44)	1:39:A:THR:HG21	1:11:A:GLU:HG3	4	1.12
(1,44)	1:39:A:THR:HG22	1:11:A:GLU:HG3	4	1.12
(1,44)	1:39:A:THR:HG23	1:11:A:GLU:HG3	4	1.12
(1,3168)	1:24:A:GLN:H	1:34:A:ILE:HG12	7	1.11
(1,2959)	1:104:A:LEU:HB2	1:109:A:TYR:HD1	9	1.11
(1,2959)	1:104:A:LEU:HB2	1:109:A:TYR:HD2	9	1.11
(1,2919)	1:16:A:MET:HG2	1:49:A:HIS:HE1	1	1.11
(1,2884)	1:115:A:PHE:HB3	1:74:A:TYR:HD1	7	1.11
(1,2884)	1:115:A:PHE:HB3	1:74:A:TYR:HD2	7	1.11
(1,2880)	1:67:A:VAL:HG21	1:74:A:TYR:HD1	3	1.11
(1,2880)	1:67:A:VAL:HG21	1:74:A:TYR:HD2	3	1.11
(1,2880)	1:67:A:VAL:HG22	1:74:A:TYR:HD1	3	1.11
(1,2880)	1:67:A:VAL:HG22	1:74:A:TYR:HD2	3	1.11
(1,2880)	1:67:A:VAL:HG23	1:74:A:TYR:HD1	3	1.11
(1,2880)	1:67:A:VAL:HG23	1:74:A:TYR:HD2	3	1.11
(1,2413)	1:86:A:THR:H	1:52:A:VAL:HG21	8	1.11
(1,2413)	1:86:A:THR:H	1:52:A:VAL:HG22	8	1.11
(1,2413)	1:86:A:THR:H	1:52:A:VAL:HG23	8	1.11
(1,1778)	1:12:A:SER:H	1:10:A:VAL:HB	10	1.11
(1,1436)	1:47:A:MET:HE1	1:118:A:HIS:HB2	10	1.11
(1,1436)	1:47:A:MET:HE2	1:118:A:HIS:HB2	10	1.11
(1,1436)	1:47:A:MET:HE3	1:118:A:HIS:HB2	10	1.11
(1,1303)	1:56:A:ALA:H	1:55:A:LYS:HD2	9	1.11
(1,1015)	1:99:A:LEU:HD21	1:101:A:PRO:HD2	7	1.11
(1,1015)	1:99:A:LEU:HD22	1:101:A:PRO:HD2	7	1.11
(1,1015)	1:99:A:LEU:HD23	1:101:A:PRO:HD2	7	1.11
(1,1014)	1:101:A:PRO:HD2	1:25:A:VAL:HG21	5	1.11
(1,1014)	1:101:A:PRO:HD2	1:25:A:VAL:HG22	5	1.11
(1,1014)	1:101:A:PRO:HD2	1:25:A:VAL:HG23	5	1.11
(1,551)	1:83:A:VAL:HG11	1:54:A:ALA:HA	10	1.11
(1,551)	1:83:A:VAL:HG12	1:54:A:ALA:HA	10	1.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,551)	1:83:A:VAL:HG13	1:54:A:ALA:HA	10	1.11
(1,3232)	1:112:A:ALA:H	1:126:A:VAL:HG13	1	1.1
(1,2966)	1:109:A:TYR:HE1	1:128:A:LEU:HD11	7	1.1
(1,2966)	1:109:A:TYR:HE1	1:128:A:LEU:HD12	7	1.1
(1,2966)	1:109:A:TYR:HE1	1:128:A:LEU:HD13	7	1.1
(1,2966)	1:109:A:TYR:HE2	1:128:A:LEU:HD11	7	1.1
(1,2966)	1:109:A:TYR:HE2	1:128:A:LEU:HD12	7	1.1
(1,2966)	1:109:A:TYR:HE2	1:128:A:LEU:HD13	7	1.1
(1,2963)	1:109:A:TYR:HD1	1:128:A:LEU:HD11	5	1.1
(1,2963)	1:109:A:TYR:HD1	1:128:A:LEU:HD12	5	1.1
(1,2963)	1:109:A:TYR:HD1	1:128:A:LEU:HD13	5	1.1
(1,2963)	1:109:A:TYR:HD2	1:128:A:LEU:HD11	5	1.1
(1,2963)	1:109:A:TYR:HD2	1:128:A:LEU:HD12	5	1.1
(1,2963)	1:109:A:TYR:HD2	1:128:A:LEU:HD13	5	1.1
(1,2959)	1:104:A:LEU:HB2	1:109:A:TYR:HD1	6	1.1
(1,2959)	1:104:A:LEU:HB2	1:109:A:TYR:HD2	6	1.1
(1,2413)	1:86:A:THR:H	1:52:A:VAL:HG21	6	1.1
(1,2413)	1:86:A:THR:H	1:52:A:VAL:HG22	6	1.1
(1,2413)	1:86:A:THR:H	1:52:A:VAL:HG23	6	1.1
(1,2303)	1:67:A:VAL:HG11	1:66:A:GLY:H	7	1.1
(1,2303)	1:67:A:VAL:HG12	1:66:A:GLY:H	7	1.1
(1,2303)	1:67:A:VAL:HG13	1:66:A:GLY:H	7	1.1
(1,1436)	1:47:A:MET:HE1	1:118:A:HIS:HB2	8	1.1
(1,1436)	1:47:A:MET:HE2	1:118:A:HIS:HB2	8	1.1
(1,1436)	1:47:A:MET:HE3	1:118:A:HIS:HB2	8	1.1
(1,1389)	1:27:A:LYS:HA	1:25:A:VAL:HG21	1	1.1
(1,1389)	1:27:A:LYS:HA	1:25:A:VAL:HG22	1	1.1
(1,1389)	1:27:A:LYS:HA	1:25:A:VAL:HG23	1	1.1
(1,1061)	1:105:A:ALA:HA	1:128:A:LEU:HD11	7	1.1
(1,1061)	1:105:A:ALA:HA	1:128:A:LEU:HD12	7	1.1
(1,1061)	1:105:A:ALA:HA	1:128:A:LEU:HD13	7	1.1
(2,1)	1:6:A:CYS:SG	1:29:A:CYS:SG	3	1.09
(1,2274)	1:81:A:ARG:HB3	1:62:A:VAL:H	4	1.09
(1,1980)	1:99:A:LEU:HB3	1:32:A:PHE:H	4	1.09
(1,1705)	1:99:A:LEU:HD11	1:31:A:GLU:HB2	7	1.09
(1,1705)	1:99:A:LEU:HD12	1:31:A:GLU:HB2	7	1.09
(1,1705)	1:99:A:LEU:HD13	1:31:A:GLU:HB2	7	1.09
(1,1552)	1:109:A:TYR:HE1	1:83:A:VAL:HG11	6	1.09
(1,1552)	1:109:A:TYR:HE1	1:83:A:VAL:HG12	6	1.09
(1,1552)	1:109:A:TYR:HE1	1:83:A:VAL:HG13	6	1.09
(1,1552)	1:109:A:TYR:HE2	1:83:A:VAL:HG11	6	1.09
(1,1552)	1:109:A:TYR:HE2	1:83:A:VAL:HG12	6	1.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1552)	1:109:A:TYR:HE2	1:83:A:VAL:HG13	6	1.09
(1,1015)	1:99:A:LEU:HD21	1:101:A:PRO:HD2	5	1.09
(1,1015)	1:99:A:LEU:HD22	1:101:A:PRO:HD2	5	1.09
(1,1015)	1:99:A:LEU:HD23	1:101:A:PRO:HD2	5	1.09
(1,463)	1:88:A:LEU:HG	1:48:A:GLY:HA2	5	1.09
(1,2963)	1:109:A:TYR:HD1	1:128:A:LEU:HD11	2	1.08
(1,2963)	1:109:A:TYR:HD1	1:128:A:LEU:HD12	2	1.08
(1,2963)	1:109:A:TYR:HD1	1:128:A:LEU:HD13	2	1.08
(1,2963)	1:109:A:TYR:HD2	1:128:A:LEU:HD11	2	1.08
(1,2963)	1:109:A:TYR:HD2	1:128:A:LEU:HD12	2	1.08
(1,2963)	1:109:A:TYR:HD2	1:128:A:LEU:HD13	2	1.08
(1,2959)	1:104:A:LEU:HB2	1:109:A:TYR:HD1	5	1.08
(1,2959)	1:104:A:LEU:HB2	1:109:A:TYR:HD2	5	1.08
(1,2884)	1:115:A:PHE:HB3	1:74:A:TYR:HD1	6	1.08
(1,2884)	1:115:A:PHE:HB3	1:74:A:TYR:HD2	6	1.08
(1,2591)	1:106:A:ASP:H	1:128:A:LEU:HD11	1	1.08
(1,2591)	1:106:A:ASP:H	1:128:A:LEU:HD12	1	1.08
(1,2591)	1:106:A:ASP:H	1:128:A:LEU:HD13	1	1.08
(1,1870)	1:19:A:ASN:HD22	1:10:A:VAL:HA	4	1.08
(1,1436)	1:47:A:MET:HE1	1:118:A:HIS:HB2	6	1.08
(1,1436)	1:47:A:MET:HE2	1:118:A:HIS:HB2	6	1.08
(1,1436)	1:47:A:MET:HE3	1:118:A:HIS:HB2	6	1.08
(1,3208)	1:79:A:ASP:H	1:75:A:VAL:HB	5	1.07
(1,3208)	1:79:A:ASP:H	1:75:A:VAL:HB	8	1.07
(1,3132)	1:104:A:LEU:HD12	1:25:A:VAL:HG12	8	1.07
(1,2987)	1:126:A:VAL:HG11	1:111:A:PHE:HD1	2	1.07
(1,2987)	1:126:A:VAL:HG11	1:111:A:PHE:HD2	2	1.07
(1,2987)	1:126:A:VAL:HG12	1:111:A:PHE:HD1	2	1.07
(1,2987)	1:126:A:VAL:HG12	1:111:A:PHE:HD2	2	1.07
(1,2987)	1:126:A:VAL:HG13	1:111:A:PHE:HD1	2	1.07
(1,2987)	1:126:A:VAL:HG13	1:111:A:PHE:HD2	2	1.07
(1,2676)	1:75:A:VAL:HG21	1:114:A:THR:H	7	1.07
(1,2676)	1:75:A:VAL:HG22	1:114:A:THR:H	7	1.07
(1,2676)	1:75:A:VAL:HG23	1:114:A:THR:H	7	1.07
(1,2569)	1:104:A:LEU:HG	1:104:A:LEU:H	9	1.07
(1,2125)	1:47:A:MET:H	1:43:A:PRO:HD3	3	1.07
(1,2125)	1:47:A:MET:H	1:43:A:PRO:HD3	9	1.07
(1,1552)	1:109:A:TYR:HE1	1:83:A:VAL:HG11	8	1.07
(1,1552)	1:109:A:TYR:HE1	1:83:A:VAL:HG12	8	1.07
(1,1552)	1:109:A:TYR:HE1	1:83:A:VAL:HG13	8	1.07
(1,1552)	1:109:A:TYR:HE2	1:83:A:VAL:HG11	8	1.07
(1,1552)	1:109:A:TYR:HE2	1:83:A:VAL:HG12	8	1.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1552)	1:109:A:TYR:HE2	1:83:A:VAL:HG13	8	1.07
(1,551)	1:83:A:VAL:HG11	1:54:A:ALA:HA	8	1.07
(1,551)	1:83:A:VAL:HG12	1:54:A:ALA:HA	8	1.07
(1,551)	1:83:A:VAL:HG13	1:54:A:ALA:HA	8	1.07
(1,3232)	1:53:A:ILE:HG21	1:112:A:ALA:H	5	1.06
(1,3208)	1:79:A:ASP:H	1:75:A:VAL:HB	3	1.06
(1,2880)	1:67:A:VAL:HG21	1:74:A:TYR:HD1	2	1.06
(1,2880)	1:67:A:VAL:HG21	1:74:A:TYR:HD2	2	1.06
(1,2880)	1:67:A:VAL:HG22	1:74:A:TYR:HD1	2	1.06
(1,2880)	1:67:A:VAL:HG22	1:74:A:TYR:HD2	2	1.06
(1,2880)	1:67:A:VAL:HG23	1:74:A:TYR:HD1	2	1.06
(1,2880)	1:67:A:VAL:HG23	1:74:A:TYR:HD2	2	1.06
(1,2413)	1:86:A:THR:H	1:52:A:VAL:HG21	4	1.06
(1,2413)	1:86:A:THR:H	1:52:A:VAL:HG22	4	1.06
(1,2413)	1:86:A:THR:H	1:52:A:VAL:HG23	4	1.06
(1,2405)	1:85:A:HIS:HD2	1:84:A:ALA:H	5	1.06
(1,2214)	1:83:A:VAL:HG11	1:55:A:LYS:H	4	1.06
(1,2214)	1:83:A:VAL:HG12	1:55:A:LYS:H	4	1.06
(1,2214)	1:83:A:VAL:HG13	1:55:A:LYS:H	4	1.06
(1,1682)	1:104:A:LEU:HG	1:128:A:LEU:HD21	9	1.06
(1,1682)	1:104:A:LEU:HG	1:128:A:LEU:HD22	9	1.06
(1,1682)	1:104:A:LEU:HG	1:128:A:LEU:HD23	9	1.06
(1,1436)	1:47:A:MET:HE1	1:118:A:HIS:HB2	9	1.06
(1,1436)	1:47:A:MET:HE2	1:118:A:HIS:HB2	9	1.06
(1,1436)	1:47:A:MET:HE3	1:118:A:HIS:HB2	9	1.06
(1,1389)	1:27:A:LYS:HA	1:25:A:VAL:HG21	2	1.06
(1,1389)	1:27:A:LYS:HA	1:25:A:VAL:HG22	2	1.06
(1,1389)	1:27:A:LYS:HA	1:25:A:VAL:HG23	2	1.06
(1,1181)	1:116:A:PRO:HB2	1:67:A:VAL:HG11	5	1.06
(1,1181)	1:116:A:PRO:HB2	1:67:A:VAL:HG12	5	1.06
(1,1181)	1:116:A:PRO:HB2	1:67:A:VAL:HG13	5	1.06
(1,1061)	1:105:A:ALA:HA	1:128:A:LEU:HD11	5	1.06
(1,1061)	1:105:A:ALA:HA	1:128:A:LEU:HD12	5	1.06
(1,1061)	1:105:A:ALA:HA	1:128:A:LEU:HD13	5	1.06
(1,3232)	1:53:A:ILE:HG22	1:112:A:ALA:H	2	1.05
(1,3125)	1:20:A:THR:HG23	1:10:A:VAL:HG13	10	1.05
(1,2966)	1:109:A:TYR:HE1	1:128:A:LEU:HD11	1	1.05
(1,2966)	1:109:A:TYR:HE1	1:128:A:LEU:HD12	1	1.05
(1,2966)	1:109:A:TYR:HE1	1:128:A:LEU:HD13	1	1.05
(1,2966)	1:109:A:TYR:HE2	1:128:A:LEU:HD11	1	1.05
(1,2966)	1:109:A:TYR:HE2	1:128:A:LEU:HD12	1	1.05
(1,2966)	1:109:A:TYR:HE2	1:128:A:LEU:HD13	1	1.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2556)	1:104:A:LEU:HG	1:103:A:LYS:H	9	1.05
(1,2061)	1:38:A:HIS:HA	1:40:A:GLY:H	8	1.05
(1,2060)	1:93:A:GLU:H	1:40:A:GLY:H	7	1.05
(1,2060)	1:93:A:GLU:H	1:40:A:GLY:H	9	1.05
(1,1978)	1:31:A:GLU:H	1:30:A:LYS:HD3	9	1.05
(1,1671)	1:25:A:VAL:HB	1:126:A:VAL:HG11	5	1.05
(1,1671)	1:25:A:VAL:HB	1:126:A:VAL:HG12	5	1.05
(1,1671)	1:25:A:VAL:HB	1:126:A:VAL:HG13	5	1.05
(1,1619)	1:109:A:TYR:HE1	1:104:A:LEU:HD21	6	1.05
(1,1619)	1:109:A:TYR:HE1	1:104:A:LEU:HD22	6	1.05
(1,1619)	1:109:A:TYR:HE1	1:104:A:LEU:HD23	6	1.05
(1,1619)	1:109:A:TYR:HE2	1:104:A:LEU:HD21	6	1.05
(1,1619)	1:109:A:TYR:HE2	1:104:A:LEU:HD22	6	1.05
(1,1619)	1:109:A:TYR:HE2	1:104:A:LEU:HD23	6	1.05
(1,1389)	1:27:A:LYS:HA	1:25:A:VAL:HG21	9	1.05
(1,1389)	1:27:A:LYS:HA	1:25:A:VAL:HG22	9	1.05
(1,1389)	1:27:A:LYS:HA	1:25:A:VAL:HG23	9	1.05
(1,1132)	1:111:A:PHE:HB2	1:126:A:VAL:HG11	8	1.05
(1,1132)	1:111:A:PHE:HB2	1:126:A:VAL:HG12	8	1.05
(1,1132)	1:111:A:PHE:HB2	1:126:A:VAL:HG13	8	1.05
(1,1095)	1:110:A:LYS:HD3	1:109:A:TYR:HA	10	1.05
(1,1059)	1:104:A:LEU:HG	1:101:A:PRO:HA	8	1.05
(1,643)	1:76:A:LYS:HD2	1:66:A:GLY:HA3	6	1.05
(1,643)	1:76:A:LYS:HD3	1:66:A:GLY:HA3	6	1.05
(1,58)	1:17:A:GLN:HG3	1:12:A:SER:HB2	1	1.05
(1,3108)	1:128:A:LEU:HB3	1:105:A:ALA:HA	1	1.04
(1,2595)	1:74:A:TYR:HB3	1:50:A:ASN:HD21	2	1.04
(1,1978)	1:31:A:GLU:H	1:30:A:LYS:HD3	3	1.04
(1,2959)	1:104:A:LEU:HB2	1:109:A:TYR:HD1	8	1.03
(1,2959)	1:104:A:LEU:HB2	1:109:A:TYR:HD2	8	1.03
(1,2880)	1:67:A:VAL:HG21	1:74:A:TYR:HD1	5	1.03
(1,2880)	1:67:A:VAL:HG21	1:74:A:TYR:HD2	5	1.03
(1,2880)	1:67:A:VAL:HG22	1:74:A:TYR:HD1	5	1.03
(1,2880)	1:67:A:VAL:HG22	1:74:A:TYR:HD2	5	1.03
(1,2880)	1:67:A:VAL:HG23	1:74:A:TYR:HD1	5	1.03
(1,2880)	1:67:A:VAL:HG23	1:74:A:TYR:HD2	5	1.03
(1,2556)	1:104:A:LEU:HG	1:103:A:LYS:H	8	1.03
(1,2060)	1:93:A:GLU:H	1:40:A:GLY:H	1	1.03
(1,1836)	1:17:A:GLN:HE22	1:15:A:ASN:HB3	3	1.03
(1,1680)	1:27:A:LYS:HG2	1:128:A:LEU:HD21	1	1.03
(1,1680)	1:27:A:LYS:HG2	1:128:A:LEU:HD22	1	1.03
(1,1680)	1:27:A:LYS:HG2	1:128:A:LEU:HD23	1	1.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1680)	1:27:A:LYS:HG3	1:128:A:LEU:HD21	1	1.03
(1,1680)	1:27:A:LYS:HG3	1:128:A:LEU:HD22	1	1.03
(1,1680)	1:27:A:LYS:HG3	1:128:A:LEU:HD23	1	1.03
(1,1627)	1:83:A:VAL:HG21	1:104:A:LEU:HD11	2	1.03
(1,1627)	1:83:A:VAL:HG21	1:104:A:LEU:HD12	2	1.03
(1,1627)	1:83:A:VAL:HG21	1:104:A:LEU:HD13	2	1.03
(1,1627)	1:83:A:VAL:HG22	1:104:A:LEU:HD11	2	1.03
(1,1627)	1:83:A:VAL:HG22	1:104:A:LEU:HD12	2	1.03
(1,1627)	1:83:A:VAL:HG22	1:104:A:LEU:HD13	2	1.03
(1,1627)	1:83:A:VAL:HG23	1:104:A:LEU:HD11	2	1.03
(1,1627)	1:83:A:VAL:HG23	1:104:A:LEU:HD12	2	1.03
(1,1627)	1:83:A:VAL:HG23	1:104:A:LEU:HD13	2	1.03
(1,1389)	1:27:A:LYS:HA	1:25:A:VAL:HG21	4	1.03
(1,1389)	1:27:A:LYS:HA	1:25:A:VAL:HG22	4	1.03
(1,1389)	1:27:A:LYS:HA	1:25:A:VAL:HG23	4	1.03
(1,1061)	1:105:A:ALA:HA	1:128:A:LEU:HD11	10	1.03
(1,1061)	1:105:A:ALA:HA	1:128:A:LEU:HD12	10	1.03
(1,1061)	1:105:A:ALA:HA	1:128:A:LEU:HD13	10	1.03
(1,766)	1:69:A:ALA:HA	1:77:A:PRO:HD2	1	1.03
(1,3262)	1:109:A:TYR:HE2	1:55:A:LYS:HD2	3	1.02
(1,3139)	1:51:A:LEU:HB2	1:86:A:THR:HG23	5	1.02
(1,2961)	1:83:A:VAL:HG11	1:109:A:TYR:HD1	10	1.02
(1,2961)	1:83:A:VAL:HG11	1:109:A:TYR:HD2	10	1.02
(1,2961)	1:83:A:VAL:HG12	1:109:A:TYR:HD1	10	1.02
(1,2961)	1:83:A:VAL:HG12	1:109:A:TYR:HD2	10	1.02
(1,2961)	1:83:A:VAL:HG13	1:109:A:TYR:HD1	10	1.02
(1,2961)	1:83:A:VAL:HG13	1:109:A:TYR:HD2	10	1.02
(1,2627)	1:111:A:PHE:H	1:126:A:VAL:HG11	4	1.02
(1,2627)	1:111:A:PHE:H	1:126:A:VAL:HG12	4	1.02
(1,2627)	1:111:A:PHE:H	1:126:A:VAL:HG13	4	1.02
(1,2556)	1:104:A:LEU:HG	1:103:A:LYS:H	5	1.02
(1,2469)	1:92:A:GLY:H	1:38:A:HIS:HB2	5	1.02
(1,2061)	1:38:A:HIS:HA	1:40:A:GLY:H	3	1.02
(1,2061)	1:38:A:HIS:HA	1:40:A:GLY:H	4	1.02
(1,1980)	1:99:A:LEU:HB3	1:32:A:PHE:H	9	1.02
(2,1)	1:6:A:CYS:SG	1:29:A:CYS:SG	1	1.01
(1,3160)	1:10:A:VAL:H	1:9:A:THR:HG22	2	1.01
(1,2362)	1:79:A:ASP:H	1:76:A:LYS:HB2	2	1.01
(1,2209)	1:54:A:ALA:H	1:126:A:VAL:HG21	5	1.01
(1,2209)	1:54:A:ALA:H	1:126:A:VAL:HG22	5	1.01
(1,2209)	1:54:A:ALA:H	1:126:A:VAL:HG23	5	1.01
(1,1753)	1:36:A:LEU:HD21	1:10:A:VAL:H	6	1.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1753)	1:36:A:LEU:HD22	1:10:A:VAL:H	6	1.01
(1,1753)	1:36:A:LEU:HD23	1:10:A:VAL:H	6	1.01
(1,1682)	1:104:A:LEU:HG	1:128:A:LEU:HD21	6	1.01
(1,1682)	1:104:A:LEU:HG	1:128:A:LEU:HD22	6	1.01
(1,1682)	1:104:A:LEU:HG	1:128:A:LEU:HD23	6	1.01
(1,1667)	1:53:A:ILE:HB	1:126:A:VAL:HG21	6	1.01
(1,1667)	1:53:A:ILE:HB	1:126:A:VAL:HG22	6	1.01
(1,1667)	1:53:A:ILE:HB	1:126:A:VAL:HG23	6	1.01
(1,1555)	1:98:A:THR:H	1:84:A:ALA:HB1	10	1.01
(1,1555)	1:98:A:THR:H	1:84:A:ALA:HB2	10	1.01
(1,1555)	1:98:A:THR:H	1:84:A:ALA:HB3	10	1.01
(1,1231)	1:122:A:MET:HA	1:121:A:LEU:HD11	7	1.01
(1,1231)	1:122:A:MET:HA	1:121:A:LEU:HD12	7	1.01
(1,1231)	1:122:A:MET:HA	1:121:A:LEU:HD13	7	1.01
(1,994)	1:83:A:VAL:HG21	1:99:A:LEU:HB3	10	1.01
(1,994)	1:83:A:VAL:HG22	1:99:A:LEU:HB3	10	1.01
(1,994)	1:83:A:VAL:HG23	1:99:A:LEU:HB3	10	1.01
(1,211)	1:26:A:SER:HB3	1:25:A:VAL:HG21	6	1.01
(1,211)	1:26:A:SER:HB3	1:25:A:VAL:HG22	6	1.01
(1,211)	1:26:A:SER:HB3	1:25:A:VAL:HG23	6	1.01
(1,44)	1:39:A:THR:HG21	1:11:A:GLU:HG3	3	1.01
(1,44)	1:39:A:THR:HG22	1:11:A:GLU:HG3	3	1.01
(1,44)	1:39:A:THR:HG23	1:11:A:GLU:HG3	3	1.01
(1,3132)	1:104:A:LEU:HD13	1:25:A:VAL:HG12	6	1.0
(1,2274)	1:81:A:ARG:HB3	1:62:A:VAL:H	7	1.0
(1,1428)	1:18:A:PHE:HD1	1:36:A:LEU:HD21	4	1.0
(1,1428)	1:18:A:PHE:HD1	1:36:A:LEU:HD22	4	1.0
(1,1428)	1:18:A:PHE:HD1	1:36:A:LEU:HD23	4	1.0
(1,1428)	1:18:A:PHE:HD2	1:36:A:LEU:HD21	4	1.0
(1,1428)	1:18:A:PHE:HD2	1:36:A:LEU:HD22	4	1.0
(1,1428)	1:18:A:PHE:HD2	1:36:A:LEU:HD23	4	1.0
(1,1389)	1:27:A:LYS:HA	1:25:A:VAL:HG21	5	1.0
(1,1389)	1:27:A:LYS:HA	1:25:A:VAL:HG22	5	1.0
(1,1389)	1:27:A:LYS:HA	1:25:A:VAL:HG23	5	1.0
(1,1014)	1:101:A:PRO:HD2	1:25:A:VAL:HG21	8	1.0
(1,1014)	1:101:A:PRO:HD2	1:25:A:VAL:HG22	8	1.0
(1,1014)	1:101:A:PRO:HD2	1:25:A:VAL:HG23	8	1.0
(1,643)	1:76:A:LYS:HD2	1:66:A:GLY:HA3	10	1.0
(1,643)	1:76:A:LYS:HD3	1:66:A:GLY:HA3	10	1.0
(1,211)	1:26:A:SER:HB3	1:25:A:VAL:HG21	10	1.0
(1,211)	1:26:A:SER:HB3	1:25:A:VAL:HG22	10	1.0
(1,211)	1:26:A:SER:HB3	1:25:A:VAL:HG23	10	1.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,119)	1:20:A:THR:HB	1:10:A:VAL:HG11	10	1.0
(1,119)	1:20:A:THR:HB	1:10:A:VAL:HG12	10	1.0
(1,119)	1:20:A:THR:HB	1:10:A:VAL:HG13	10	1.0
(1,3166)	1:126:A:VAL:HG12	1:23:A:ILE:H	3	0.99
(1,2674)	1:52:A:VAL:HG21	1:114:A:THR:H	5	0.99
(1,2674)	1:52:A:VAL:HG22	1:114:A:THR:H	5	0.99
(1,2674)	1:52:A:VAL:HG23	1:114:A:THR:H	5	0.99
(1,2114)	1:46:A:SER:H	1:43:A:PRO:HD3	9	0.99
(1,2081)	1:91:A:GLY:HA2	1:42:A:GLN:H	8	0.99
(1,1014)	1:101:A:PRO:HD2	1:25:A:VAL:HG21	1	0.99
(1,1014)	1:101:A:PRO:HD2	1:25:A:VAL:HG22	1	0.99
(1,1014)	1:101:A:PRO:HD2	1:25:A:VAL:HG23	1	0.99
(1,822)	1:85:A:HIS:HB3	1:52:A:VAL:HG21	4	0.99
(1,822)	1:85:A:HIS:HB3	1:52:A:VAL:HG22	4	0.99
(1,822)	1:85:A:HIS:HB3	1:52:A:VAL:HG23	4	0.99
(1,253)	1:98:A:THR:HB	1:31:A:GLU:HG2	8	0.99
(1,253)	1:98:A:THR:HB	1:31:A:GLU:HG3	8	0.99
(1,211)	1:26:A:SER:HB3	1:25:A:VAL:HG21	8	0.99
(1,211)	1:26:A:SER:HB3	1:25:A:VAL:HG22	8	0.99
(1,211)	1:26:A:SER:HB3	1:25:A:VAL:HG23	8	0.99
(1,3198)	1:64:A:LYS:HD3	1:61:A:GLY:H	10	0.98
(1,3165)	1:24:A:GLN:HB3	1:23:A:ILE:H	3	0.98
(1,2959)	1:104:A:LEU:HB2	1:109:A:TYR:HD1	10	0.98
(1,2959)	1:104:A:LEU:HB2	1:109:A:TYR:HD2	10	0.98
(1,2647)	1:112:A:ALA:H	1:126:A:VAL:HG21	3	0.98
(1,2647)	1:112:A:ALA:H	1:126:A:VAL:HG22	3	0.98
(1,2647)	1:112:A:ALA:H	1:126:A:VAL:HG23	3	0.98
(1,2469)	1:92:A:GLY:H	1:38:A:HIS:HB2	10	0.98
(1,2363)	1:79:A:ASP:H	1:76:A:LYS:HB3	9	0.98
(1,1870)	1:19:A:ASN:HD22	1:10:A:VAL:HA	2	0.98
(1,1753)	1:36:A:LEU:HD21	1:10:A:VAL:H	4	0.98
(1,1753)	1:36:A:LEU:HD22	1:10:A:VAL:H	4	0.98
(1,1753)	1:36:A:LEU:HD23	1:10:A:VAL:H	4	0.98
(1,1753)	1:36:A:LEU:HD21	1:10:A:VAL:H	7	0.98
(1,1753)	1:36:A:LEU:HD22	1:10:A:VAL:H	7	0.98
(1,1753)	1:36:A:LEU:HD23	1:10:A:VAL:H	7	0.98
(1,1525)	1:114:A:THR:HG21	1:75:A:VAL:HG21	1	0.98
(1,1525)	1:114:A:THR:HG21	1:75:A:VAL:HG22	1	0.98
(1,1525)	1:114:A:THR:HG21	1:75:A:VAL:HG23	1	0.98
(1,1525)	1:114:A:THR:HG22	1:75:A:VAL:HG21	1	0.98
(1,1525)	1:114:A:THR:HG22	1:75:A:VAL:HG22	1	0.98
(1,1525)	1:114:A:THR:HG22	1:75:A:VAL:HG23	1	0.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1525)	1:114:A:THR:HG23	1:75:A:VAL:HG21	1	0.98
(1,1525)	1:114:A:THR:HG23	1:75:A:VAL:HG22	1	0.98
(1,1525)	1:114:A:THR:HG23	1:75:A:VAL:HG23	1	0.98
(1,1389)	1:27:A:LYS:HA	1:25:A:VAL:HG21	7	0.98
(1,1389)	1:27:A:LYS:HA	1:25:A:VAL:HG22	7	0.98
(1,1389)	1:27:A:LYS:HA	1:25:A:VAL:HG23	7	0.98
(1,1064)	1:107:A:GLY:HA2	1:55:A:LYS:HD3	10	0.98
(1,463)	1:88:A:LEU:HG	1:48:A:GLY:HA2	8	0.98
(1,253)	1:98:A:THR:HB	1:31:A:GLU:HG2	7	0.98
(1,253)	1:98:A:THR:HB	1:31:A:GLU:HG3	7	0.98
(1,3232)	1:53:A:ILE:HG22	1:112:A:ALA:H	4	0.97
(1,3232)	1:112:A:ALA:H	1:126:A:VAL:HG11	10	0.97
(1,3132)	1:104:A:LEU:HD11	1:25:A:VAL:HG12	5	0.97
(1,3108)	1:128:A:LEU:HB3	1:105:A:ALA:HA	7	0.97
(1,2516)	1:97:A:LEU:H	1:36:A:LEU:HD11	6	0.97
(1,2516)	1:97:A:LEU:H	1:36:A:LEU:HD12	6	0.97
(1,2516)	1:97:A:LEU:H	1:36:A:LEU:HD13	6	0.97
(1,2125)	1:47:A:MET:H	1:43:A:PRO:HD3	7	0.97
(1,2062)	1:40:A:GLY:H	1:13:A:ASN:HA	8	0.97
(1,1797)	1:15:A:ASN:HB3	1:13:A:ASN:HD21	4	0.97
(1,1619)	1:109:A:TYR:HE1	1:104:A:LEU:HD21	8	0.97
(1,1619)	1:109:A:TYR:HE1	1:104:A:LEU:HD22	8	0.97
(1,1619)	1:109:A:TYR:HE1	1:104:A:LEU:HD23	8	0.97
(1,1619)	1:109:A:TYR:HE2	1:104:A:LEU:HD21	8	0.97
(1,1619)	1:109:A:TYR:HE2	1:104:A:LEU:HD22	8	0.97
(1,1619)	1:109:A:TYR:HE2	1:104:A:LEU:HD23	8	0.97
(1,1552)	1:109:A:TYR:HE1	1:83:A:VAL:HG11	10	0.97
(1,1552)	1:109:A:TYR:HE1	1:83:A:VAL:HG12	10	0.97
(1,1552)	1:109:A:TYR:HE1	1:83:A:VAL:HG13	10	0.97
(1,1552)	1:109:A:TYR:HE2	1:83:A:VAL:HG11	10	0.97
(1,1552)	1:109:A:TYR:HE2	1:83:A:VAL:HG12	10	0.97
(1,1552)	1:109:A:TYR:HE2	1:83:A:VAL:HG13	10	0.97
(1,1461)	1:126:A:VAL:HG11	1:51:A:LEU:HD21	3	0.97
(1,1461)	1:126:A:VAL:HG11	1:51:A:LEU:HD22	3	0.97
(1,1461)	1:126:A:VAL:HG11	1:51:A:LEU:HD23	3	0.97
(1,1461)	1:126:A:VAL:HG12	1:51:A:LEU:HD21	3	0.97
(1,1461)	1:126:A:VAL:HG12	1:51:A:LEU:HD22	3	0.97
(1,1461)	1:126:A:VAL:HG12	1:51:A:LEU:HD23	3	0.97
(1,1461)	1:126:A:VAL:HG13	1:51:A:LEU:HD21	3	0.97
(1,1461)	1:126:A:VAL:HG13	1:51:A:LEU:HD22	3	0.97
(1,1461)	1:126:A:VAL:HG13	1:51:A:LEU:HD23	3	0.97
(1,1348)	1:19:A:ASN:H	1:10:A:VAL:HG11	10	0.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1348)	1:19:A:ASN:H	1:10:A:VAL:HG12	10	0.97
(1,1348)	1:19:A:ASN:H	1:10:A:VAL:HG13	10	0.97
(1,766)	1:69:A:ALA:HA	1:77:A:PRO:HD2	7	0.97
(1,3132)	1:104:A:LEU:HD11	1:25:A:VAL:HG12	9	0.96
(1,2961)	1:83:A:VAL:HG11	1:109:A:TYR:HD1	8	0.96
(1,2961)	1:83:A:VAL:HG11	1:109:A:TYR:HD2	8	0.96
(1,2961)	1:83:A:VAL:HG12	1:109:A:TYR:HD1	8	0.96
(1,2961)	1:83:A:VAL:HG12	1:109:A:TYR:HD2	8	0.96
(1,2961)	1:83:A:VAL:HG13	1:109:A:TYR:HD1	8	0.96
(1,2961)	1:83:A:VAL:HG13	1:109:A:TYR:HD2	8	0.96
(1,2959)	1:104:A:LEU:HB2	1:109:A:TYR:HD1	1	0.96
(1,2959)	1:104:A:LEU:HB2	1:109:A:TYR:HD2	1	0.96
(1,2529)	1:99:A:LEU:H	1:31:A:GLU:HB2	10	0.96
(1,2125)	1:47:A:MET:H	1:43:A:PRO:HD3	10	0.96
(1,1753)	1:36:A:LEU:HD21	1:10:A:VAL:H	10	0.96
(1,1753)	1:36:A:LEU:HD22	1:10:A:VAL:H	10	0.96
(1,1753)	1:36:A:LEU:HD23	1:10:A:VAL:H	10	0.96
(1,1683)	1:104:A:LEU:HD11	1:128:A:LEU:HD21	6	0.96
(1,1683)	1:104:A:LEU:HD11	1:128:A:LEU:HD22	6	0.96
(1,1683)	1:104:A:LEU:HD11	1:128:A:LEU:HD23	6	0.96
(1,1683)	1:104:A:LEU:HD12	1:128:A:LEU:HD21	6	0.96
(1,1683)	1:104:A:LEU:HD12	1:128:A:LEU:HD22	6	0.96
(1,1683)	1:104:A:LEU:HD12	1:128:A:LEU:HD23	6	0.96
(1,1683)	1:104:A:LEU:HD13	1:128:A:LEU:HD21	6	0.96
(1,1683)	1:104:A:LEU:HD13	1:128:A:LEU:HD22	6	0.96
(1,1683)	1:104:A:LEU:HD13	1:128:A:LEU:HD23	6	0.96
(1,1667)	1:53:A:ILE:HB	1:126:A:VAL:HG21	9	0.96
(1,1667)	1:53:A:ILE:HB	1:126:A:VAL:HG22	9	0.96
(1,1667)	1:53:A:ILE:HB	1:126:A:VAL:HG23	9	0.96
(1,1549)	1:83:A:VAL:HG21	1:104:A:LEU:HD21	6	0.96
(1,1549)	1:83:A:VAL:HG21	1:104:A:LEU:HD22	6	0.96
(1,1549)	1:83:A:VAL:HG21	1:104:A:LEU:HD23	6	0.96
(1,1549)	1:83:A:VAL:HG22	1:104:A:LEU:HD21	6	0.96
(1,1549)	1:83:A:VAL:HG22	1:104:A:LEU:HD22	6	0.96
(1,1549)	1:83:A:VAL:HG22	1:104:A:LEU:HD23	6	0.96
(1,1549)	1:83:A:VAL:HG23	1:104:A:LEU:HD21	6	0.96
(1,1549)	1:83:A:VAL:HG23	1:104:A:LEU:HD22	6	0.96
(1,1549)	1:83:A:VAL:HG23	1:104:A:LEU:HD23	6	0.96
(1,1549)	1:83:A:VAL:HG21	1:104:A:LEU:HD21	7	0.96
(1,1549)	1:83:A:VAL:HG21	1:104:A:LEU:HD22	7	0.96
(1,1549)	1:83:A:VAL:HG21	1:104:A:LEU:HD23	7	0.96
(1,1549)	1:83:A:VAL:HG22	1:104:A:LEU:HD21	7	0.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1549)	1:83:A:VAL:HG22	1:104:A:LEU:HD22	7	0.96
(1,1549)	1:83:A:VAL:HG22	1:104:A:LEU:HD23	7	0.96
(1,1549)	1:83:A:VAL:HG23	1:104:A:LEU:HD21	7	0.96
(1,1549)	1:83:A:VAL:HG23	1:104:A:LEU:HD22	7	0.96
(1,1549)	1:83:A:VAL:HG23	1:104:A:LEU:HD23	7	0.96
(1,1132)	1:111:A:PHE:HB2	1:126:A:VAL:HG11	2	0.96
(1,1132)	1:111:A:PHE:HB2	1:126:A:VAL:HG12	2	0.96
(1,1132)	1:111:A:PHE:HB2	1:126:A:VAL:HG13	2	0.96
(1,1132)	1:111:A:PHE:HB2	1:126:A:VAL:HG11	4	0.96
(1,1132)	1:111:A:PHE:HB2	1:126:A:VAL:HG12	4	0.96
(1,1132)	1:111:A:PHE:HB2	1:126:A:VAL:HG13	4	0.96
(1,3165)	1:24:A:GLN:HB3	1:23:A:ILE:H	4	0.95
(1,2781)	1:110:A:LYS:HG2	1:126:A:VAL:H	6	0.95
(1,2360)	1:76:A:LYS:HE2	1:79:A:ASP:H	10	0.95
(1,2360)	1:76:A:LYS:HE3	1:79:A:ASP:H	10	0.95
(1,1682)	1:104:A:LEU:HG	1:128:A:LEU:HD21	7	0.95
(1,1682)	1:104:A:LEU:HG	1:128:A:LEU:HD22	7	0.95
(1,1682)	1:104:A:LEU:HG	1:128:A:LEU:HD23	7	0.95
(1,1680)	1:27:A:LYS:HG2	1:128:A:LEU:HD21	5	0.95
(1,1680)	1:27:A:LYS:HG2	1:128:A:LEU:HD22	5	0.95
(1,1680)	1:27:A:LYS:HG2	1:128:A:LEU:HD23	5	0.95
(1,1680)	1:27:A:LYS:HG3	1:128:A:LEU:HD21	5	0.95
(1,1680)	1:27:A:LYS:HG3	1:128:A:LEU:HD22	5	0.95
(1,1680)	1:27:A:LYS:HG3	1:128:A:LEU:HD23	5	0.95
(1,1619)	1:109:A:TYR:HE1	1:104:A:LEU:HD21	9	0.95
(1,1619)	1:109:A:TYR:HE1	1:104:A:LEU:HD22	9	0.95
(1,1619)	1:109:A:TYR:HE1	1:104:A:LEU:HD23	9	0.95
(1,1619)	1:109:A:TYR:HE2	1:104:A:LEU:HD21	9	0.95
(1,1619)	1:109:A:TYR:HE2	1:104:A:LEU:HD22	9	0.95
(1,1619)	1:109:A:TYR:HE2	1:104:A:LEU:HD23	9	0.95
(1,1039)	1:99:A:LEU:HD21	1:101:A:PRO:HG3	2	0.95
(1,1039)	1:99:A:LEU:HD22	1:101:A:PRO:HG3	2	0.95
(1,1039)	1:99:A:LEU:HD23	1:101:A:PRO:HG3	2	0.95
(1,753)	1:76:A:LYS:HD2	1:77:A:PRO:HD3	5	0.95
(1,753)	1:76:A:LYS:HD3	1:77:A:PRO:HD3	5	0.95
(1,3208)	1:76:A:LYS:HD3	1:79:A:ASP:H	7	0.94
(1,2959)	1:104:A:LEU:HB2	1:109:A:TYR:HD1	4	0.94
(1,2959)	1:104:A:LEU:HB2	1:109:A:TYR:HD2	4	0.94
(1,2679)	1:115:A:PHE:H	1:88:A:LEU:HD21	7	0.94
(1,2679)	1:115:A:PHE:H	1:88:A:LEU:HD22	7	0.94
(1,2679)	1:115:A:PHE:H	1:88:A:LEU:HD23	7	0.94
(1,2241)	1:57:A:GLU:HG3	1:58:A:ASP:H	5	0.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2211)	1:55:A:LYS:H	1:83:A:VAL:HB	1	0.94
(1,2158)	1:50:A:ASN:HD21	1:88:A:LEU:HD21	7	0.94
(1,2158)	1:50:A:ASN:HD21	1:88:A:LEU:HD22	7	0.94
(1,2158)	1:50:A:ASN:HD21	1:88:A:LEU:HD23	7	0.94
(1,1753)	1:36:A:LEU:HD21	1:10:A:VAL:H	8	0.94
(1,1753)	1:36:A:LEU:HD22	1:10:A:VAL:H	8	0.94
(1,1753)	1:36:A:LEU:HD23	1:10:A:VAL:H	8	0.94
(1,1669)	1:25:A:VAL:HG11	1:126:A:VAL:HG21	9	0.94
(1,1669)	1:25:A:VAL:HG11	1:126:A:VAL:HG22	9	0.94
(1,1669)	1:25:A:VAL:HG11	1:126:A:VAL:HG23	9	0.94
(1,1669)	1:25:A:VAL:HG12	1:126:A:VAL:HG21	9	0.94
(1,1669)	1:25:A:VAL:HG12	1:126:A:VAL:HG22	9	0.94
(1,1669)	1:25:A:VAL:HG12	1:126:A:VAL:HG23	9	0.94
(1,1669)	1:25:A:VAL:HG13	1:126:A:VAL:HG21	9	0.94
(1,1669)	1:25:A:VAL:HG13	1:126:A:VAL:HG22	9	0.94
(1,1669)	1:25:A:VAL:HG13	1:126:A:VAL:HG23	9	0.94
(1,1436)	1:47:A:MET:HE1	1:118:A:HIS:HB2	1	0.94
(1,1436)	1:47:A:MET:HE2	1:118:A:HIS:HB2	1	0.94
(1,1436)	1:47:A:MET:HE3	1:118:A:HIS:HB2	1	0.94
(1,1039)	1:99:A:LEU:HD21	1:101:A:PRO:HG3	9	0.94
(1,1039)	1:99:A:LEU:HD22	1:101:A:PRO:HG3	9	0.94
(1,1039)	1:99:A:LEU:HD23	1:101:A:PRO:HG3	9	0.94
(1,1035)	1:101:A:PRO:HG3	1:25:A:VAL:HG21	3	0.94
(1,1035)	1:101:A:PRO:HG3	1:25:A:VAL:HG22	3	0.94
(1,1035)	1:101:A:PRO:HG3	1:25:A:VAL:HG23	3	0.94
(1,1016)	1:99:A:LEU:HD21	1:101:A:PRO:HD3	6	0.94
(1,1016)	1:99:A:LEU:HD22	1:101:A:PRO:HD3	6	0.94
(1,1016)	1:99:A:LEU:HD23	1:101:A:PRO:HD3	6	0.94
(1,795)	1:82:A:VAL:HB	1:75:A:VAL:HG11	6	0.94
(1,795)	1:82:A:VAL:HB	1:75:A:VAL:HG12	6	0.94
(1,795)	1:82:A:VAL:HB	1:75:A:VAL:HG13	6	0.94
(1,2961)	1:83:A:VAL:HG11	1:109:A:TYR:HD1	1	0.93
(1,2961)	1:83:A:VAL:HG11	1:109:A:TYR:HD2	1	0.93
(1,2961)	1:83:A:VAL:HG12	1:109:A:TYR:HD1	1	0.93
(1,2961)	1:83:A:VAL:HG12	1:109:A:TYR:HD2	1	0.93
(1,2961)	1:83:A:VAL:HG13	1:109:A:TYR:HD1	1	0.93
(1,2961)	1:83:A:VAL:HG13	1:109:A:TYR:HD2	1	0.93
(1,2960)	1:109:A:TYR:HD1	1:127:A:THR:HG21	2	0.93
(1,2960)	1:109:A:TYR:HD1	1:127:A:THR:HG22	2	0.93
(1,2960)	1:109:A:TYR:HD1	1:127:A:THR:HG23	2	0.93
(1,2960)	1:109:A:TYR:HD2	1:127:A:THR:HG21	2	0.93
(1,2960)	1:109:A:TYR:HD2	1:127:A:THR:HG22	2	0.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2960)	1:109:A:TYR:HD2	1:127:A:THR:HG23	2	0.93
(1,2884)	1:115:A:PHE:HB3	1:74:A:TYR:HD1	3	0.93
(1,2884)	1:115:A:PHE:HB3	1:74:A:TYR:HD2	3	0.93
(1,2362)	1:79:A:ASP:H	1:76:A:LYS:HB2	3	0.93
(1,2214)	1:83:A:VAL:HG11	1:55:A:LYS:H	2	0.93
(1,2214)	1:83:A:VAL:HG12	1:55:A:LYS:H	2	0.93
(1,2214)	1:83:A:VAL:HG13	1:55:A:LYS:H	2	0.93
(1,2209)	1:54:A:ALA:H	1:126:A:VAL:HG21	6	0.93
(1,2209)	1:54:A:ALA:H	1:126:A:VAL:HG22	6	0.93
(1,2209)	1:54:A:ALA:H	1:126:A:VAL:HG23	6	0.93
(1,1568)	1:88:A:LEU:HD11	1:44:A:LYS:HE2	7	0.93
(1,1568)	1:88:A:LEU:HD11	1:44:A:LYS:HE3	7	0.93
(1,1568)	1:88:A:LEU:HD12	1:44:A:LYS:HE2	7	0.93
(1,1568)	1:88:A:LEU:HD12	1:44:A:LYS:HE3	7	0.93
(1,1568)	1:88:A:LEU:HD13	1:44:A:LYS:HE2	7	0.93
(1,1568)	1:88:A:LEU:HD13	1:44:A:LYS:HE3	7	0.93
(1,1498)	1:62:A:VAL:HG11	1:54:A:ALA:H	9	0.93
(1,1498)	1:62:A:VAL:HG12	1:54:A:ALA:H	9	0.93
(1,1498)	1:62:A:VAL:HG13	1:54:A:ALA:H	9	0.93
(1,852)	1:88:A:LEU:HB3	1:73:A:ASP:H	1	0.93
(1,639)	1:67:A:VAL:HG11	1:64:A:LYS:HA	4	0.93
(1,639)	1:67:A:VAL:HG12	1:64:A:LYS:HA	4	0.93
(1,639)	1:67:A:VAL:HG13	1:64:A:LYS:HA	4	0.93
(1,3168)	1:24:A:GLN:H	1:34:A:ILE:HG12	6	0.92
(1,3139)	1:51:A:LEU:HB2	1:86:A:THR:HG21	7	0.92
(1,2966)	1:109:A:TYR:HE1	1:128:A:LEU:HD11	5	0.92
(1,2966)	1:109:A:TYR:HE1	1:128:A:LEU:HD12	5	0.92
(1,2966)	1:109:A:TYR:HE1	1:128:A:LEU:HD13	5	0.92
(1,2966)	1:109:A:TYR:HE2	1:128:A:LEU:HD11	5	0.92
(1,2966)	1:109:A:TYR:HE2	1:128:A:LEU:HD12	5	0.92
(1,2966)	1:109:A:TYR:HE2	1:128:A:LEU:HD13	5	0.92
(1,2959)	1:104:A:LEU:HB2	1:109:A:TYR:HD1	7	0.92
(1,2959)	1:104:A:LEU:HB2	1:109:A:TYR:HD2	7	0.92
(1,2944)	1:107:A:GLY:HA3	1:109:A:TYR:HD1	4	0.92
(1,2944)	1:107:A:GLY:HA3	1:109:A:TYR:HD2	4	0.92
(1,2241)	1:57:A:GLU:HG3	1:58:A:ASP:H	4	0.92
(1,1543)	1:85:A:HIS:HD2	1:82:A:VAL:HG21	6	0.92
(1,1543)	1:85:A:HIS:HD2	1:82:A:VAL:HG22	6	0.92
(1,1543)	1:85:A:HIS:HD2	1:82:A:VAL:HG23	6	0.92
(1,1035)	1:101:A:PRO:HG3	1:25:A:VAL:HG21	2	0.92
(1,1035)	1:101:A:PRO:HG3	1:25:A:VAL:HG22	2	0.92
(1,1035)	1:101:A:PRO:HG3	1:25:A:VAL:HG23	2	0.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,816)	1:85:A:HIS:HB3	1:53:A:ILE:H	5	0.92
(1,3165)	1:24:A:GLN:HB3	1:23:A:ILE:H	2	0.91
(1,3037)	1:16:A:MET:HE1	1:118:A:HIS:HD2	1	0.91
(1,3037)	1:16:A:MET:HE2	1:118:A:HIS:HD2	1	0.91
(1,3037)	1:16:A:MET:HE3	1:118:A:HIS:HD2	1	0.91
(1,2652)	1:113:A:CYS:H	1:111:A:PHE:HB3	3	0.91
(1,2647)	1:112:A:ALA:H	1:126:A:VAL:HG21	7	0.91
(1,2647)	1:112:A:ALA:H	1:126:A:VAL:HG22	7	0.91
(1,2647)	1:112:A:ALA:H	1:126:A:VAL:HG23	7	0.91
(1,2516)	1:97:A:LEU:H	1:36:A:LEU:HD11	1	0.91
(1,2516)	1:97:A:LEU:H	1:36:A:LEU:HD12	1	0.91
(1,2516)	1:97:A:LEU:H	1:36:A:LEU:HD13	1	0.91
(1,2264)	1:61:A:GLY:H	1:59:A:MET:HG2	7	0.91
(1,2264)	1:61:A:GLY:H	1:59:A:MET:HG3	7	0.91
(1,1870)	1:19:A:ASN:HD22	1:10:A:VAL:HA	10	0.91
(1,1753)	1:36:A:LEU:HD21	1:10:A:VAL:H	2	0.91
(1,1753)	1:36:A:LEU:HD22	1:10:A:VAL:H	2	0.91
(1,1753)	1:36:A:LEU:HD23	1:10:A:VAL:H	2	0.91
(1,1428)	1:18:A:PHE:HD1	1:36:A:LEU:HD21	3	0.91
(1,1428)	1:18:A:PHE:HD1	1:36:A:LEU:HD22	3	0.91
(1,1428)	1:18:A:PHE:HD1	1:36:A:LEU:HD23	3	0.91
(1,1428)	1:18:A:PHE:HD2	1:36:A:LEU:HD21	3	0.91
(1,1428)	1:18:A:PHE:HD2	1:36:A:LEU:HD22	3	0.91
(1,1428)	1:18:A:PHE:HD2	1:36:A:LEU:HD23	3	0.91
(1,1001)	1:100:A:ASP:HA	1:31:A:GLU:HB2	9	0.91
(1,822)	1:85:A:HIS:HB3	1:52:A:VAL:HG21	6	0.91
(1,822)	1:85:A:HIS:HB3	1:52:A:VAL:HG22	6	0.91
(1,822)	1:85:A:HIS:HB3	1:52:A:VAL:HG23	6	0.91
(1,448)	1:43:A:PRO:HG3	1:46:A:SER:HB2	9	0.91
(1,448)	1:43:A:PRO:HG3	1:46:A:SER:HB3	9	0.91
(1,3232)	1:112:A:ALA:H	1:126:A:VAL:HG13	9	0.9
(1,3143)	1:103:A:LYS:HB3	1:99:A:LEU:HD22	1	0.9
(1,2591)	1:106:A:ASP:H	1:128:A:LEU:HD11	9	0.9
(1,2591)	1:106:A:ASP:H	1:128:A:LEU:HD12	9	0.9
(1,2591)	1:106:A:ASP:H	1:128:A:LEU:HD13	9	0.9
(1,2542)	1:100:A:ASP:H	1:83:A:VAL:HA	9	0.9
(1,2209)	1:54:A:ALA:H	1:126:A:VAL:HG21	1	0.9
(1,2209)	1:54:A:ALA:H	1:126:A:VAL:HG22	1	0.9
(1,2209)	1:54:A:ALA:H	1:126:A:VAL:HG23	1	0.9
(1,2125)	1:47:A:MET:H	1:43:A:PRO:HD3	4	0.9
(1,1753)	1:36:A:LEU:HD21	1:10:A:VAL:H	9	0.9
(1,1753)	1:36:A:LEU:HD22	1:10:A:VAL:H	9	0.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1753)	1:36:A:LEU:HD23	1:10:A:VAL:H	9	0.9
(1,1669)	1:25:A:VAL:HG11	1:126:A:VAL:HG21	1	0.9
(1,1669)	1:25:A:VAL:HG11	1:126:A:VAL:HG22	1	0.9
(1,1669)	1:25:A:VAL:HG11	1:126:A:VAL:HG23	1	0.9
(1,1669)	1:25:A:VAL:HG12	1:126:A:VAL:HG21	1	0.9
(1,1669)	1:25:A:VAL:HG12	1:126:A:VAL:HG22	1	0.9
(1,1669)	1:25:A:VAL:HG12	1:126:A:VAL:HG23	1	0.9
(1,1669)	1:25:A:VAL:HG13	1:126:A:VAL:HG21	1	0.9
(1,1669)	1:25:A:VAL:HG13	1:126:A:VAL:HG22	1	0.9
(1,1669)	1:25:A:VAL:HG13	1:126:A:VAL:HG23	1	0.9
(1,1669)	1:25:A:VAL:HG11	1:126:A:VAL:HG21	7	0.9
(1,1669)	1:25:A:VAL:HG11	1:126:A:VAL:HG22	7	0.9
(1,1669)	1:25:A:VAL:HG11	1:126:A:VAL:HG23	7	0.9
(1,1669)	1:25:A:VAL:HG12	1:126:A:VAL:HG21	7	0.9
(1,1669)	1:25:A:VAL:HG12	1:126:A:VAL:HG22	7	0.9
(1,1669)	1:25:A:VAL:HG12	1:126:A:VAL:HG23	7	0.9
(1,1669)	1:25:A:VAL:HG13	1:126:A:VAL:HG21	7	0.9
(1,1669)	1:25:A:VAL:HG13	1:126:A:VAL:HG22	7	0.9
(1,1669)	1:25:A:VAL:HG13	1:126:A:VAL:HG23	7	0.9
(1,1428)	1:18:A:PHE:HD1	1:36:A:LEU:HD21	1	0.9
(1,1428)	1:18:A:PHE:HD1	1:36:A:LEU:HD22	1	0.9
(1,1428)	1:18:A:PHE:HD1	1:36:A:LEU:HD23	1	0.9
(1,1428)	1:18:A:PHE:HD2	1:36:A:LEU:HD21	1	0.9
(1,1428)	1:18:A:PHE:HD2	1:36:A:LEU:HD22	1	0.9
(1,1428)	1:18:A:PHE:HD2	1:36:A:LEU:HD23	1	0.9
(1,1389)	1:27:A:LYS:HA	1:25:A:VAL:HG21	10	0.9
(1,1389)	1:27:A:LYS:HA	1:25:A:VAL:HG22	10	0.9
(1,1389)	1:27:A:LYS:HA	1:25:A:VAL:HG23	10	0.9
(1,766)	1:69:A:ALA:HA	1:77:A:PRO:HD2	8	0.9
(1,580)	1:130:A:ASP:HA	1:128:A:LEU:HD21	5	0.9
(1,580)	1:130:A:ASP:HA	1:128:A:LEU:HD22	5	0.9
(1,580)	1:130:A:ASP:HA	1:128:A:LEU:HD23	5	0.9
(1,580)	1:130:A:ASP:HA	1:128:A:LEU:HD21	9	0.9
(1,580)	1:130:A:ASP:HA	1:128:A:LEU:HD22	9	0.9
(1,580)	1:130:A:ASP:HA	1:128:A:LEU:HD23	9	0.9
(1,3168)	1:24:A:GLN:H	1:34:A:ILE:HG12	10	0.89
(1,2966)	1:109:A:TYR:HE1	1:128:A:LEU:HD11	9	0.89
(1,2966)	1:109:A:TYR:HE1	1:128:A:LEU:HD12	9	0.89
(1,2966)	1:109:A:TYR:HE1	1:128:A:LEU:HD13	9	0.89
(1,2966)	1:109:A:TYR:HE2	1:128:A:LEU:HD11	9	0.89
(1,2966)	1:109:A:TYR:HE2	1:128:A:LEU:HD12	9	0.89
(1,2966)	1:109:A:TYR:HE2	1:128:A:LEU:HD13	9	0.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2884)	1:115:A:PHE:HB3	1:74:A:TYR:HD1	2	0.89
(1,2884)	1:115:A:PHE:HB3	1:74:A:TYR:HD2	2	0.89
(1,2626)	1:53:A:ILE:HG12	1:111:A:PHE:H	9	0.89
(1,2356)	1:78:A:ASP:H	1:76:A:LYS:HD2	7	0.89
(1,2356)	1:78:A:ASP:H	1:76:A:LYS:HD3	7	0.89
(1,2326)	1:88:A:LEU:HD11	1:73:A:ASP:H	7	0.89
(1,2326)	1:88:A:LEU:HD12	1:73:A:ASP:H	7	0.89
(1,2326)	1:88:A:LEU:HD13	1:73:A:ASP:H	7	0.89
(1,1779)	1:39:A:THR:HG21	1:12:A:SER:H	6	0.89
(1,1779)	1:39:A:THR:HG22	1:12:A:SER:H	6	0.89
(1,1779)	1:39:A:THR:HG23	1:12:A:SER:H	6	0.89
(1,1715)	1:59:A:MET:HE1	1:114:A:THR:HG1	2	0.89
(1,1715)	1:59:A:MET:HE2	1:114:A:THR:HG1	2	0.89
(1,1715)	1:59:A:MET:HE3	1:114:A:THR:HG1	2	0.89
(1,1506)	1:81:A:ARG:HB2	1:62:A:VAL:HG11	7	0.89
(1,1506)	1:81:A:ARG:HB2	1:62:A:VAL:HG12	7	0.89
(1,1506)	1:81:A:ARG:HB2	1:62:A:VAL:HG13	7	0.89
(1,1389)	1:27:A:LYS:HA	1:25:A:VAL:HG21	8	0.89
(1,1389)	1:27:A:LYS:HA	1:25:A:VAL:HG22	8	0.89
(1,1389)	1:27:A:LYS:HA	1:25:A:VAL:HG23	8	0.89
(1,580)	1:130:A:ASP:HA	1:128:A:LEU:HD21	2	0.89
(1,580)	1:130:A:ASP:HA	1:128:A:LEU:HD22	2	0.89
(1,580)	1:130:A:ASP:HA	1:128:A:LEU:HD23	2	0.89
(1,3156)	1:59:A:MET:HE3	1:110:A:LYS:HB2	6	0.88
(1,2960)	1:109:A:TYR:HD1	1:127:A:THR:HG21	3	0.88
(1,2960)	1:109:A:TYR:HD1	1:127:A:THR:HG22	3	0.88
(1,2960)	1:109:A:TYR:HD1	1:127:A:THR:HG23	3	0.88
(1,2960)	1:109:A:TYR:HD2	1:127:A:THR:HG21	3	0.88
(1,2960)	1:109:A:TYR:HD2	1:127:A:THR:HG22	3	0.88
(1,2960)	1:109:A:TYR:HD2	1:127:A:THR:HG23	3	0.88
(1,2647)	1:112:A:ALA:H	1:126:A:VAL:HG21	10	0.88
(1,2647)	1:112:A:ALA:H	1:126:A:VAL:HG22	10	0.88
(1,2647)	1:112:A:ALA:H	1:126:A:VAL:HG23	10	0.88
(1,2397)	1:83:A:VAL:HB	1:84:A:ALA:H	9	0.88
(1,2264)	1:61:A:GLY:H	1:59:A:MET:HG2	9	0.88
(1,2264)	1:61:A:GLY:H	1:59:A:MET:HG3	9	0.88
(1,1980)	1:99:A:LEU:HB3	1:32:A:PHE:H	10	0.88
(1,1526)	1:52:A:VAL:HG21	1:75:A:VAL:HG21	1	0.88
(1,1526)	1:52:A:VAL:HG21	1:75:A:VAL:HG22	1	0.88
(1,1526)	1:52:A:VAL:HG21	1:75:A:VAL:HG23	1	0.88
(1,1526)	1:52:A:VAL:HG22	1:75:A:VAL:HG21	1	0.88
(1,1526)	1:52:A:VAL:HG22	1:75:A:VAL:HG22	1	0.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1526)	1:52:A:VAL:HG22	1:75:A:VAL:HG23	1	0.88
(1,1526)	1:52:A:VAL:HG23	1:75:A:VAL:HG21	1	0.88
(1,1526)	1:52:A:VAL:HG23	1:75:A:VAL:HG22	1	0.88
(1,1526)	1:52:A:VAL:HG23	1:75:A:VAL:HG23	1	0.88
(1,1498)	1:62:A:VAL:HG11	1:54:A:ALA:H	6	0.88
(1,1498)	1:62:A:VAL:HG12	1:54:A:ALA:H	6	0.88
(1,1498)	1:62:A:VAL:HG13	1:54:A:ALA:H	6	0.88
(1,1039)	1:99:A:LEU:HD21	1:101:A:PRO:HG3	3	0.88
(1,1039)	1:99:A:LEU:HD22	1:101:A:PRO:HG3	3	0.88
(1,1039)	1:99:A:LEU:HD23	1:101:A:PRO:HG3	3	0.88
(1,2959)	1:104:A:LEU:HB2	1:109:A:TYR:HD1	2	0.87
(1,2959)	1:104:A:LEU:HB2	1:109:A:TYR:HD2	2	0.87
(1,2944)	1:107:A:GLY:HA3	1:109:A:TYR:HD1	10	0.87
(1,2944)	1:107:A:GLY:HA3	1:109:A:TYR:HD2	10	0.87
(1,2652)	1:113:A:CYS:H	1:111:A:PHE:HB3	2	0.87
(1,2595)	1:74:A:TYR:HB3	1:50:A:ASN:HD21	6	0.87
(1,1753)	1:36:A:LEU:HD21	1:10:A:VAL:H	3	0.87
(1,1753)	1:36:A:LEU:HD22	1:10:A:VAL:H	3	0.87
(1,1753)	1:36:A:LEU:HD23	1:10:A:VAL:H	3	0.87
(1,1753)	1:36:A:LEU:HD21	1:10:A:VAL:H	5	0.87
(1,1753)	1:36:A:LEU:HD22	1:10:A:VAL:H	5	0.87
(1,1753)	1:36:A:LEU:HD23	1:10:A:VAL:H	5	0.87
(1,1686)	1:128:A:LEU:HD11	1:127:A:THR:HG21	2	0.87
(1,1686)	1:128:A:LEU:HD11	1:127:A:THR:HG22	2	0.87
(1,1686)	1:128:A:LEU:HD11	1:127:A:THR:HG23	2	0.87
(1,1686)	1:128:A:LEU:HD12	1:127:A:THR:HG21	2	0.87
(1,1686)	1:128:A:LEU:HD12	1:127:A:THR:HG22	2	0.87
(1,1686)	1:128:A:LEU:HD12	1:127:A:THR:HG23	2	0.87
(1,1686)	1:128:A:LEU:HD13	1:127:A:THR:HG21	2	0.87
(1,1686)	1:128:A:LEU:HD13	1:127:A:THR:HG22	2	0.87
(1,1686)	1:128:A:LEU:HD13	1:127:A:THR:HG23	2	0.87
(1,1527)	1:82:A:VAL:HG11	1:75:A:VAL:HG21	1	0.87
(1,1527)	1:82:A:VAL:HG11	1:75:A:VAL:HG22	1	0.87
(1,1527)	1:82:A:VAL:HG11	1:75:A:VAL:HG23	1	0.87
(1,1527)	1:82:A:VAL:HG12	1:75:A:VAL:HG21	1	0.87
(1,1527)	1:82:A:VAL:HG12	1:75:A:VAL:HG22	1	0.87
(1,1527)	1:82:A:VAL:HG12	1:75:A:VAL:HG23	1	0.87
(1,1527)	1:82:A:VAL:HG13	1:75:A:VAL:HG21	1	0.87
(1,1527)	1:82:A:VAL:HG13	1:75:A:VAL:HG22	1	0.87
(1,1527)	1:82:A:VAL:HG13	1:75:A:VAL:HG23	1	0.87
(1,1389)	1:27:A:LYS:HA	1:25:A:VAL:HG21	3	0.87
(1,1389)	1:27:A:LYS:HA	1:25:A:VAL:HG22	3	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1389)	1:27:A:LYS:HA	1:25:A:VAL:HG23	3	0.87
(1,1074)	1:107:A:GLY:HA2	1:109:A:TYR:HE1	10	0.87
(1,1074)	1:107:A:GLY:HA2	1:109:A:TYR:HE2	10	0.87
(1,1035)	1:101:A:PRO:HG3	1:25:A:VAL:HG21	6	0.87
(1,1035)	1:101:A:PRO:HG3	1:25:A:VAL:HG22	6	0.87
(1,1035)	1:101:A:PRO:HG3	1:25:A:VAL:HG23	6	0.87
(1,551)	1:83:A:VAL:HG11	1:54:A:ALA:HA	1	0.87
(1,551)	1:83:A:VAL:HG12	1:54:A:ALA:HA	1	0.87
(1,551)	1:83:A:VAL:HG13	1:54:A:ALA:HA	1	0.87
(1,448)	1:43:A:PRO:HG3	1:46:A:SER:HB2	4	0.87
(1,448)	1:43:A:PRO:HG3	1:46:A:SER:HB3	4	0.87
(1,3165)	1:24:A:GLN:HB3	1:23:A:ILE:H	5	0.86
(1,2652)	1:113:A:CYS:H	1:111:A:PHE:HB3	10	0.86
(1,2170)	1:88:A:LEU:HB3	1:50:A:ASN:HD22	9	0.86
(1,2062)	1:40:A:GLY:H	1:13:A:ASN:HA	3	0.86
(1,1801)	1:13:A:ASN:HD22	1:17:A:GLN:HB3	7	0.86
(1,1680)	1:27:A:LYS:HG2	1:128:A:LEU:HD21	2	0.86
(1,1680)	1:27:A:LYS:HG2	1:128:A:LEU:HD22	2	0.86
(1,1680)	1:27:A:LYS:HG2	1:128:A:LEU:HD23	2	0.86
(1,1680)	1:27:A:LYS:HG3	1:128:A:LEU:HD21	2	0.86
(1,1680)	1:27:A:LYS:HG3	1:128:A:LEU:HD22	2	0.86
(1,1680)	1:27:A:LYS:HG3	1:128:A:LEU:HD23	2	0.86
(1,1680)	1:27:A:LYS:HG2	1:128:A:LEU:HD21	9	0.86
(1,1680)	1:27:A:LYS:HG2	1:128:A:LEU:HD22	9	0.86
(1,1680)	1:27:A:LYS:HG2	1:128:A:LEU:HD23	9	0.86
(1,1680)	1:27:A:LYS:HG3	1:128:A:LEU:HD21	9	0.86
(1,1680)	1:27:A:LYS:HG3	1:128:A:LEU:HD22	9	0.86
(1,1680)	1:27:A:LYS:HG3	1:128:A:LEU:HD23	9	0.86
(1,1547)	1:83:A:VAL:HG21	1:84:A:ALA:HB1	5	0.86
(1,1547)	1:83:A:VAL:HG21	1:84:A:ALA:HB2	5	0.86
(1,1547)	1:83:A:VAL:HG21	1:84:A:ALA:HB3	5	0.86
(1,1547)	1:83:A:VAL:HG22	1:84:A:ALA:HB1	5	0.86
(1,1547)	1:83:A:VAL:HG22	1:84:A:ALA:HB2	5	0.86
(1,1547)	1:83:A:VAL:HG22	1:84:A:ALA:HB3	5	0.86
(1,1547)	1:83:A:VAL:HG23	1:84:A:ALA:HB1	5	0.86
(1,1547)	1:83:A:VAL:HG23	1:84:A:ALA:HB2	5	0.86
(1,1547)	1:83:A:VAL:HG23	1:84:A:ALA:HB3	5	0.86
(1,1381)	1:104:A:LEU:HD11	1:25:A:VAL:HG21	8	0.86
(1,1381)	1:104:A:LEU:HD11	1:25:A:VAL:HG22	8	0.86
(1,1381)	1:104:A:LEU:HD11	1:25:A:VAL:HG23	8	0.86
(1,1381)	1:104:A:LEU:HD12	1:25:A:VAL:HG21	8	0.86
(1,1381)	1:104:A:LEU:HD12	1:25:A:VAL:HG22	8	0.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1381)	1:104:A:LEU:HD12	1:25:A:VAL:HG23	8	0.86
(1,1381)	1:104:A:LEU:HD13	1:25:A:VAL:HG21	8	0.86
(1,1381)	1:104:A:LEU:HD13	1:25:A:VAL:HG22	8	0.86
(1,1381)	1:104:A:LEU:HD13	1:25:A:VAL:HG23	8	0.86
(1,1074)	1:107:A:GLY:HA2	1:109:A:TYR:HE1	4	0.86
(1,1074)	1:107:A:GLY:HA2	1:109:A:TYR:HE2	4	0.86
(1,1059)	1:104:A:LEU:HG	1:101:A:PRO:HA	5	0.86
(1,639)	1:67:A:VAL:HG11	1:64:A:LYS:HA	2	0.86
(1,639)	1:67:A:VAL:HG12	1:64:A:LYS:HA	2	0.86
(1,639)	1:67:A:VAL:HG13	1:64:A:LYS:HA	2	0.86
(1,3220)	1:94:A:GLU:H	1:93:A:GLU:HB2	6	0.85
(1,3165)	1:24:A:GLN:HB3	1:23:A:ILE:H	6	0.85
(1,2944)	1:107:A:GLY:HA3	1:109:A:TYR:HD1	1	0.85
(1,2944)	1:107:A:GLY:HA3	1:109:A:TYR:HD2	1	0.85
(1,2623)	1:125:A:LYS:HD2	1:110:A:LYS:H	5	0.85
(1,2623)	1:125:A:LYS:HD3	1:110:A:LYS:H	5	0.85
(1,2516)	1:97:A:LEU:H	1:36:A:LEU:HD11	10	0.85
(1,2516)	1:97:A:LEU:H	1:36:A:LEU:HD12	10	0.85
(1,2516)	1:97:A:LEU:H	1:36:A:LEU:HD13	10	0.85
(1,2125)	1:47:A:MET:H	1:43:A:PRO:HD3	2	0.85
(1,2125)	1:47:A:MET:H	1:43:A:PRO:HD3	8	0.85
(1,1669)	1:25:A:VAL:HG11	1:126:A:VAL:HG21	10	0.85
(1,1669)	1:25:A:VAL:HG11	1:126:A:VAL:HG22	10	0.85
(1,1669)	1:25:A:VAL:HG11	1:126:A:VAL:HG23	10	0.85
(1,1669)	1:25:A:VAL:HG12	1:126:A:VAL:HG21	10	0.85
(1,1669)	1:25:A:VAL:HG12	1:126:A:VAL:HG22	10	0.85
(1,1669)	1:25:A:VAL:HG12	1:126:A:VAL:HG23	10	0.85
(1,1669)	1:25:A:VAL:HG13	1:126:A:VAL:HG21	10	0.85
(1,1669)	1:25:A:VAL:HG13	1:126:A:VAL:HG22	10	0.85
(1,1669)	1:25:A:VAL:HG13	1:126:A:VAL:HG23	10	0.85
(1,1436)	1:47:A:MET:HE1	1:118:A:HIS:HB2	5	0.85
(1,1436)	1:47:A:MET:HE2	1:118:A:HIS:HB2	5	0.85
(1,1436)	1:47:A:MET:HE3	1:118:A:HIS:HB2	5	0.85
(1,1035)	1:101:A:PRO:HG3	1:25:A:VAL:HG21	4	0.85
(1,1035)	1:101:A:PRO:HG3	1:25:A:VAL:HG22	4	0.85
(1,1035)	1:101:A:PRO:HG3	1:25:A:VAL:HG23	4	0.85
(1,851)	1:88:A:LEU:HB2	1:73:A:ASP:H	10	0.85
(1,493)	1:50:A:ASN:HA	1:36:A:LEU:HD11	1	0.85
(1,493)	1:50:A:ASN:HA	1:36:A:LEU:HD12	1	0.85
(1,493)	1:50:A:ASN:HA	1:36:A:LEU:HD13	1	0.85
(2,1)	1:6:A:CYS:SG	1:29:A:CYS:SG	4	0.84
(1,3139)	1:51:A:LEU:HB2	1:86:A:THR:HG22	8	0.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2529)	1:99:A:LEU:H	1:31:A:GLU:HB2	7	0.84
(1,2168)	1:74:A:TYR:HB3	1:50:A:ASN:HD22	7	0.84
(1,2125)	1:47:A:MET:H	1:43:A:PRO:HD3	1	0.84
(1,1702)	1:83:A:VAL:HG21	1:99:A:LEU:HD11	4	0.84
(1,1702)	1:83:A:VAL:HG21	1:99:A:LEU:HD12	4	0.84
(1,1702)	1:83:A:VAL:HG21	1:99:A:LEU:HD13	4	0.84
(1,1702)	1:83:A:VAL:HG22	1:99:A:LEU:HD11	4	0.84
(1,1702)	1:83:A:VAL:HG22	1:99:A:LEU:HD12	4	0.84
(1,1702)	1:83:A:VAL:HG22	1:99:A:LEU:HD13	4	0.84
(1,1702)	1:83:A:VAL:HG23	1:99:A:LEU:HD11	4	0.84
(1,1702)	1:83:A:VAL:HG23	1:99:A:LEU:HD12	4	0.84
(1,1702)	1:83:A:VAL:HG23	1:99:A:LEU:HD13	4	0.84
(1,1552)	1:109:A:TYR:HE1	1:83:A:VAL:HG11	5	0.84
(1,1552)	1:109:A:TYR:HE1	1:83:A:VAL:HG12	5	0.84
(1,1552)	1:109:A:TYR:HE1	1:83:A:VAL:HG13	5	0.84
(1,1552)	1:109:A:TYR:HE2	1:83:A:VAL:HG11	5	0.84
(1,1552)	1:109:A:TYR:HE2	1:83:A:VAL:HG12	5	0.84
(1,1552)	1:109:A:TYR:HE2	1:83:A:VAL:HG13	5	0.84
(1,1526)	1:52:A:VAL:HG21	1:75:A:VAL:HG21	5	0.84
(1,1526)	1:52:A:VAL:HG21	1:75:A:VAL:HG22	5	0.84
(1,1526)	1:52:A:VAL:HG21	1:75:A:VAL:HG23	5	0.84
(1,1526)	1:52:A:VAL:HG22	1:75:A:VAL:HG21	5	0.84
(1,1526)	1:52:A:VAL:HG22	1:75:A:VAL:HG22	5	0.84
(1,1526)	1:52:A:VAL:HG22	1:75:A:VAL:HG23	5	0.84
(1,1526)	1:52:A:VAL:HG23	1:75:A:VAL:HG21	5	0.84
(1,1526)	1:52:A:VAL:HG23	1:75:A:VAL:HG22	5	0.84
(1,1526)	1:52:A:VAL:HG23	1:75:A:VAL:HG23	5	0.84
(1,1498)	1:62:A:VAL:HG11	1:54:A:ALA:H	8	0.84
(1,1498)	1:62:A:VAL:HG12	1:54:A:ALA:H	8	0.84
(1,1498)	1:62:A:VAL:HG13	1:54:A:ALA:H	8	0.84
(1,1355)	1:18:A:PHE:HB2	1:10:A:VAL:HG11	10	0.84
(1,1355)	1:18:A:PHE:HB2	1:10:A:VAL:HG12	10	0.84
(1,1355)	1:18:A:PHE:HB2	1:10:A:VAL:HG13	10	0.84
(1,1035)	1:101:A:PRO:HG3	1:25:A:VAL:HG21	10	0.84
(1,1035)	1:101:A:PRO:HG3	1:25:A:VAL:HG22	10	0.84
(1,1035)	1:101:A:PRO:HG3	1:25:A:VAL:HG23	10	0.84
(1,639)	1:67:A:VAL:HG11	1:64:A:LYS:HA	10	0.84
(1,639)	1:67:A:VAL:HG12	1:64:A:LYS:HA	10	0.84
(1,639)	1:67:A:VAL:HG13	1:64:A:LYS:HA	10	0.84
(1,580)	1:130:A:ASP:HA	1:128:A:LEU:HD21	1	0.84
(1,580)	1:130:A:ASP:HA	1:128:A:LEU:HD22	1	0.84
(1,580)	1:130:A:ASP:HA	1:128:A:LEU:HD23	1	0.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,126)	1:21:A:LYS:HE2	1:21:A:LYS:HB2	2	0.84
(1,126)	1:21:A:LYS:HE3	1:21:A:LYS:HB2	2	0.84
(1,3165)	1:24:A:GLN:HB3	1:23:A:ILE:H	8	0.83
(1,3139)	1:51:A:LEU:HB2	1:86:A:THR:HG21	9	0.83
(1,3043)	1:19:A:ASN:HB3	1:11:A:GLU:HB3	7	0.83
(1,2961)	1:83:A:VAL:HG11	1:109:A:TYR:HD1	5	0.83
(1,2961)	1:83:A:VAL:HG11	1:109:A:TYR:HD2	5	0.83
(1,2961)	1:83:A:VAL:HG12	1:109:A:TYR:HD1	5	0.83
(1,2961)	1:83:A:VAL:HG12	1:109:A:TYR:HD2	5	0.83
(1,2961)	1:83:A:VAL:HG13	1:109:A:TYR:HD1	5	0.83
(1,2961)	1:83:A:VAL:HG13	1:109:A:TYR:HD2	5	0.83
(1,2696)	1:117:A:GLY:H	1:67:A:VAL:HG11	5	0.83
(1,2696)	1:117:A:GLY:H	1:67:A:VAL:HG12	5	0.83
(1,2696)	1:117:A:GLY:H	1:67:A:VAL:HG13	5	0.83
(1,2062)	1:40:A:GLY:H	1:13:A:ASN:HA	4	0.83
(1,2060)	1:93:A:GLU:H	1:40:A:GLY:H	6	0.83
(1,1497)	1:54:A:ALA:HB1	1:52:A:VAL:HG11	8	0.83
(1,1497)	1:54:A:ALA:HB1	1:52:A:VAL:HG12	8	0.83
(1,1497)	1:54:A:ALA:HB1	1:52:A:VAL:HG13	8	0.83
(1,1497)	1:54:A:ALA:HB2	1:52:A:VAL:HG11	8	0.83
(1,1497)	1:54:A:ALA:HB2	1:52:A:VAL:HG12	8	0.83
(1,1497)	1:54:A:ALA:HB2	1:52:A:VAL:HG13	8	0.83
(1,1497)	1:54:A:ALA:HB3	1:52:A:VAL:HG11	8	0.83
(1,1497)	1:54:A:ALA:HB3	1:52:A:VAL:HG12	8	0.83
(1,1497)	1:54:A:ALA:HB3	1:52:A:VAL:HG13	8	0.83
(1,795)	1:82:A:VAL:HB	1:75:A:VAL:HG11	3	0.83
(1,795)	1:82:A:VAL:HB	1:75:A:VAL:HG12	3	0.83
(1,795)	1:82:A:VAL:HB	1:75:A:VAL:HG13	3	0.83
(1,551)	1:83:A:VAL:HG11	1:54:A:ALA:HA	5	0.83
(1,551)	1:83:A:VAL:HG12	1:54:A:ALA:HA	5	0.83
(1,551)	1:83:A:VAL:HG13	1:54:A:ALA:HA	5	0.83
(1,126)	1:21:A:LYS:HE2	1:21:A:LYS:HB2	7	0.83
(1,126)	1:21:A:LYS:HE3	1:21:A:LYS:HB2	7	0.83
(1,3166)	1:126:A:VAL:HG12	1:23:A:ILE:H	5	0.82
(1,2652)	1:113:A:CYS:H	1:111:A:PHE:HB3	8	0.82
(1,2626)	1:53:A:ILE:HG12	1:111:A:PHE:H	6	0.82
(1,2569)	1:104:A:LEU:HG	1:104:A:LEU:H	7	0.82
(1,2326)	1:88:A:LEU:HD11	1:73:A:ASP:H	6	0.82
(1,2326)	1:88:A:LEU:HD12	1:73:A:ASP:H	6	0.82
(1,2326)	1:88:A:LEU:HD13	1:73:A:ASP:H	6	0.82
(1,2125)	1:47:A:MET:H	1:43:A:PRO:HD3	5	0.82
(1,1669)	1:25:A:VAL:HG11	1:126:A:VAL:HG21	6	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1669)	1:25:A:VAL:HG11	1:126:A:VAL:HG22	6	0.82
(1,1669)	1:25:A:VAL:HG11	1:126:A:VAL:HG23	6	0.82
(1,1669)	1:25:A:VAL:HG12	1:126:A:VAL:HG21	6	0.82
(1,1669)	1:25:A:VAL:HG12	1:126:A:VAL:HG22	6	0.82
(1,1669)	1:25:A:VAL:HG12	1:126:A:VAL:HG23	6	0.82
(1,1669)	1:25:A:VAL:HG13	1:126:A:VAL:HG21	6	0.82
(1,1669)	1:25:A:VAL:HG13	1:126:A:VAL:HG22	6	0.82
(1,1669)	1:25:A:VAL:HG13	1:126:A:VAL:HG23	6	0.82
(1,1660)	1:25:A:VAL:H	1:126:A:VAL:HG21	4	0.82
(1,1660)	1:25:A:VAL:H	1:126:A:VAL:HG22	4	0.82
(1,1660)	1:25:A:VAL:H	1:126:A:VAL:HG23	4	0.82
(1,1506)	1:81:A:ARG:HB2	1:62:A:VAL:HG11	10	0.82
(1,1506)	1:81:A:ARG:HB2	1:62:A:VAL:HG12	10	0.82
(1,1506)	1:81:A:ARG:HB2	1:62:A:VAL:HG13	10	0.82
(1,1503)	1:81:A:ARG:HD2	1:62:A:VAL:HG11	10	0.82
(1,1503)	1:81:A:ARG:HD2	1:62:A:VAL:HG12	10	0.82
(1,1503)	1:81:A:ARG:HD2	1:62:A:VAL:HG13	10	0.82
(1,984)	1:98:A:THR:HB	1:31:A:GLU:HB2	7	0.82
(1,741)	1:77:A:PRO:HA	1:75:A:VAL:HG11	1	0.82
(1,741)	1:77:A:PRO:HA	1:75:A:VAL:HG12	1	0.82
(1,741)	1:77:A:PRO:HA	1:75:A:VAL:HG13	1	0.82
(1,578)	1:56:A:ALA:HA	1:110:A:LYS:HD2	7	0.82
(1,493)	1:50:A:ASN:HA	1:36:A:LEU:HD11	5	0.82
(1,493)	1:50:A:ASN:HA	1:36:A:LEU:HD12	5	0.82
(1,493)	1:50:A:ASN:HA	1:36:A:LEU:HD13	5	0.82
(1,3139)	1:51:A:LEU:HB2	1:86:A:THR:HG22	2	0.81
(1,2959)	1:104:A:LEU:HB2	1:109:A:TYR:HD1	3	0.81
(1,2959)	1:104:A:LEU:HB2	1:109:A:TYR:HD2	3	0.81
(1,2880)	1:67:A:VAL:HG21	1:74:A:TYR:HD1	4	0.81
(1,2880)	1:67:A:VAL:HG21	1:74:A:TYR:HD2	4	0.81
(1,2880)	1:67:A:VAL:HG22	1:74:A:TYR:HD1	4	0.81
(1,2880)	1:67:A:VAL:HG22	1:74:A:TYR:HD2	4	0.81
(1,2880)	1:67:A:VAL:HG23	1:74:A:TYR:HD1	4	0.81
(1,2880)	1:67:A:VAL:HG23	1:74:A:TYR:HD2	4	0.81
(1,2880)	1:67:A:VAL:HG21	1:74:A:TYR:HD1	9	0.81
(1,2880)	1:67:A:VAL:HG21	1:74:A:TYR:HD2	9	0.81
(1,2880)	1:67:A:VAL:HG22	1:74:A:TYR:HD1	9	0.81
(1,2880)	1:67:A:VAL:HG22	1:74:A:TYR:HD2	9	0.81
(1,2880)	1:67:A:VAL:HG23	1:74:A:TYR:HD1	9	0.81
(1,2880)	1:67:A:VAL:HG23	1:74:A:TYR:HD2	9	0.81
(1,2569)	1:104:A:LEU:HG	1:104:A:LEU:H	6	0.81
(1,2214)	1:83:A:VAL:HG11	1:55:A:LYS:H	3	0.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2214)	1:83:A:VAL:HG12	1:55:A:LYS:H	3	0.81
(1,2214)	1:83:A:VAL:HG13	1:55:A:LYS:H	3	0.81
(1,2117)	1:46:A:SER:H	1:43:A:PRO:HB3	9	0.81
(1,2114)	1:46:A:SER:H	1:43:A:PRO:HD3	5	0.81
(1,1705)	1:99:A:LEU:HD11	1:31:A:GLU:HB2	2	0.81
(1,1705)	1:99:A:LEU:HD12	1:31:A:GLU:HB2	2	0.81
(1,1705)	1:99:A:LEU:HD13	1:31:A:GLU:HB2	2	0.81
(1,1547)	1:83:A:VAL:HG21	1:84:A:ALA:HB1	3	0.81
(1,1547)	1:83:A:VAL:HG21	1:84:A:ALA:HB2	3	0.81
(1,1547)	1:83:A:VAL:HG21	1:84:A:ALA:HB3	3	0.81
(1,1547)	1:83:A:VAL:HG22	1:84:A:ALA:HB1	3	0.81
(1,1547)	1:83:A:VAL:HG22	1:84:A:ALA:HB2	3	0.81
(1,1547)	1:83:A:VAL:HG22	1:84:A:ALA:HB3	3	0.81
(1,1547)	1:83:A:VAL:HG23	1:84:A:ALA:HB1	3	0.81
(1,1547)	1:83:A:VAL:HG23	1:84:A:ALA:HB2	3	0.81
(1,1547)	1:83:A:VAL:HG23	1:84:A:ALA:HB3	3	0.81
(1,1509)	1:62:A:VAL:HG21	1:114:A:THR:HG21	8	0.81
(1,1509)	1:62:A:VAL:HG21	1:114:A:THR:HG22	8	0.81
(1,1509)	1:62:A:VAL:HG21	1:114:A:THR:HG23	8	0.81
(1,1509)	1:62:A:VAL:HG22	1:114:A:THR:HG21	8	0.81
(1,1509)	1:62:A:VAL:HG22	1:114:A:THR:HG22	8	0.81
(1,1509)	1:62:A:VAL:HG22	1:114:A:THR:HG23	8	0.81
(1,1509)	1:62:A:VAL:HG23	1:114:A:THR:HG21	8	0.81
(1,1509)	1:62:A:VAL:HG23	1:114:A:THR:HG22	8	0.81
(1,1509)	1:62:A:VAL:HG23	1:114:A:THR:HG23	8	0.81
(1,1039)	1:99:A:LEU:HD21	1:101:A:PRO:HG3	10	0.81
(1,1039)	1:99:A:LEU:HD22	1:101:A:PRO:HG3	10	0.81
(1,1039)	1:99:A:LEU:HD23	1:101:A:PRO:HG3	10	0.81
(1,882)	1:91:A:GLY:HA3	1:38:A:HIS:HB2	2	0.81
(1,564)	1:55:A:LYS:HB2	1:58:A:ASP:H	5	0.81
(1,126)	1:21:A:LYS:HE2	1:21:A:LYS:HB2	9	0.81
(1,126)	1:21:A:LYS:HE3	1:21:A:LYS:HB2	9	0.81
(1,126)	1:21:A:LYS:HE2	1:21:A:LYS:HB2	10	0.81
(1,126)	1:21:A:LYS:HE3	1:21:A:LYS:HB2	10	0.81
(1,3165)	1:24:A:GLN:HB3	1:23:A:ILE:H	7	0.8
(1,2591)	1:106:A:ASP:H	1:128:A:LEU:HD11	4	0.8
(1,2591)	1:106:A:ASP:H	1:128:A:LEU:HD12	4	0.8
(1,2591)	1:106:A:ASP:H	1:128:A:LEU:HD13	4	0.8
(1,2105)	1:43:A:PRO:HB3	1:45:A:ALA:H	3	0.8
(1,1671)	1:25:A:VAL:HB	1:126:A:VAL:HG11	3	0.8
(1,1671)	1:25:A:VAL:HB	1:126:A:VAL:HG12	3	0.8
(1,1671)	1:25:A:VAL:HB	1:126:A:VAL:HG13	3	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1547)	1:83:A:VAL:HG21	1:84:A:ALA:HB1	2	0.8
(1,1547)	1:83:A:VAL:HG21	1:84:A:ALA:HB2	2	0.8
(1,1547)	1:83:A:VAL:HG21	1:84:A:ALA:HB3	2	0.8
(1,1547)	1:83:A:VAL:HG22	1:84:A:ALA:HB1	2	0.8
(1,1547)	1:83:A:VAL:HG22	1:84:A:ALA:HB2	2	0.8
(1,1547)	1:83:A:VAL:HG22	1:84:A:ALA:HB3	2	0.8
(1,1547)	1:83:A:VAL:HG23	1:84:A:ALA:HB1	2	0.8
(1,1547)	1:83:A:VAL:HG23	1:84:A:ALA:HB2	2	0.8
(1,1547)	1:83:A:VAL:HG23	1:84:A:ALA:HB3	2	0.8
(1,1547)	1:83:A:VAL:HG21	1:84:A:ALA:HB1	10	0.8
(1,1547)	1:83:A:VAL:HG21	1:84:A:ALA:HB2	10	0.8
(1,1547)	1:83:A:VAL:HG21	1:84:A:ALA:HB3	10	0.8
(1,1547)	1:83:A:VAL:HG22	1:84:A:ALA:HB1	10	0.8
(1,1547)	1:83:A:VAL:HG22	1:84:A:ALA:HB2	10	0.8
(1,1547)	1:83:A:VAL:HG22	1:84:A:ALA:HB3	10	0.8
(1,1547)	1:83:A:VAL:HG23	1:84:A:ALA:HB1	10	0.8
(1,1547)	1:83:A:VAL:HG23	1:84:A:ALA:HB2	10	0.8
(1,1547)	1:83:A:VAL:HG23	1:84:A:ALA:HB3	10	0.8
(1,1509)	1:62:A:VAL:HG21	1:114:A:THR:HG21	1	0.8
(1,1509)	1:62:A:VAL:HG21	1:114:A:THR:HG22	1	0.8
(1,1509)	1:62:A:VAL:HG21	1:114:A:THR:HG23	1	0.8
(1,1509)	1:62:A:VAL:HG22	1:114:A:THR:HG21	1	0.8
(1,1509)	1:62:A:VAL:HG22	1:114:A:THR:HG22	1	0.8
(1,1509)	1:62:A:VAL:HG22	1:114:A:THR:HG23	1	0.8
(1,1509)	1:62:A:VAL:HG23	1:114:A:THR:HG21	1	0.8
(1,1509)	1:62:A:VAL:HG23	1:114:A:THR:HG22	1	0.8
(1,1509)	1:62:A:VAL:HG23	1:114:A:THR:HG23	1	0.8
(1,1389)	1:27:A:LYS:HA	1:25:A:VAL:HG21	6	0.8
(1,1389)	1:27:A:LYS:HA	1:25:A:VAL:HG22	6	0.8
(1,1389)	1:27:A:LYS:HA	1:25:A:VAL:HG23	6	0.8
(1,493)	1:50:A:ASN:HA	1:36:A:LEU:HD11	10	0.8
(1,493)	1:50:A:ASN:HA	1:36:A:LEU:HD12	10	0.8
(1,493)	1:50:A:ASN:HA	1:36:A:LEU:HD13	10	0.8
(2,1)	1:6:A:CYS:SG	1:29:A:CYS:SG	10	0.79
(1,2840)	1:53:A:ILE:HD11	1:32:A:PHE:HD1	6	0.79
(1,2840)	1:53:A:ILE:HD11	1:32:A:PHE:HD2	6	0.79
(1,2840)	1:53:A:ILE:HD12	1:32:A:PHE:HD1	6	0.79
(1,2840)	1:53:A:ILE:HD12	1:32:A:PHE:HD2	6	0.79
(1,2840)	1:53:A:ILE:HD13	1:32:A:PHE:HD1	6	0.79
(1,2840)	1:53:A:ILE:HD13	1:32:A:PHE:HD2	6	0.79
(1,2674)	1:52:A:VAL:HG21	1:114:A:THR:H	9	0.79
(1,2674)	1:52:A:VAL:HG22	1:114:A:THR:H	9	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2674)	1:52:A:VAL:HG23	1:114:A:THR:H	9	0.79
(1,1547)	1:83:A:VAL:HG21	1:84:A:ALA:HB1	7	0.79
(1,1547)	1:83:A:VAL:HG21	1:84:A:ALA:HB2	7	0.79
(1,1547)	1:83:A:VAL:HG21	1:84:A:ALA:HB3	7	0.79
(1,1547)	1:83:A:VAL:HG22	1:84:A:ALA:HB1	7	0.79
(1,1547)	1:83:A:VAL:HG22	1:84:A:ALA:HB2	7	0.79
(1,1547)	1:83:A:VAL:HG22	1:84:A:ALA:HB3	7	0.79
(1,1547)	1:83:A:VAL:HG23	1:84:A:ALA:HB1	7	0.79
(1,1547)	1:83:A:VAL:HG23	1:84:A:ALA:HB2	7	0.79
(1,1547)	1:83:A:VAL:HG23	1:84:A:ALA:HB3	7	0.79
(1,1506)	1:81:A:ARG:HB2	1:62:A:VAL:HG11	1	0.79
(1,1506)	1:81:A:ARG:HB2	1:62:A:VAL:HG12	1	0.79
(1,1506)	1:81:A:ARG:HB2	1:62:A:VAL:HG13	1	0.79
(1,1506)	1:81:A:ARG:HB2	1:62:A:VAL:HG11	6	0.79
(1,1506)	1:81:A:ARG:HB2	1:62:A:VAL:HG12	6	0.79
(1,1506)	1:81:A:ARG:HB2	1:62:A:VAL:HG13	6	0.79
(1,1001)	1:100:A:ASP:HA	1:31:A:GLU:HB2	7	0.79
(1,3220)	1:94:A:GLU:H	1:93:A:GLU:HB2	10	0.78
(1,2966)	1:109:A:TYR:HE1	1:128:A:LEU:HD11	8	0.78
(1,2966)	1:109:A:TYR:HE1	1:128:A:LEU:HD12	8	0.78
(1,2966)	1:109:A:TYR:HE1	1:128:A:LEU:HD13	8	0.78
(1,2966)	1:109:A:TYR:HE2	1:128:A:LEU:HD11	8	0.78
(1,2966)	1:109:A:TYR:HE2	1:128:A:LEU:HD12	8	0.78
(1,2966)	1:109:A:TYR:HE2	1:128:A:LEU:HD13	8	0.78
(1,2880)	1:67:A:VAL:HG21	1:74:A:TYR:HD1	1	0.78
(1,2880)	1:67:A:VAL:HG21	1:74:A:TYR:HD2	1	0.78
(1,2880)	1:67:A:VAL:HG22	1:74:A:TYR:HD1	1	0.78
(1,2880)	1:67:A:VAL:HG22	1:74:A:TYR:HD2	1	0.78
(1,2880)	1:67:A:VAL:HG23	1:74:A:TYR:HD1	1	0.78
(1,2880)	1:67:A:VAL:HG23	1:74:A:TYR:HD2	1	0.78
(1,2808)	1:27:A:LYS:HE2	1:129:A:VAL:H	8	0.78
(1,2808)	1:27:A:LYS:HE3	1:129:A:VAL:H	8	0.78
(1,2569)	1:104:A:LEU:HG	1:104:A:LEU:H	5	0.78
(1,2569)	1:104:A:LEU:HG	1:104:A:LEU:H	8	0.78
(1,2214)	1:83:A:VAL:HG11	1:55:A:LYS:H	5	0.78
(1,2214)	1:83:A:VAL:HG12	1:55:A:LYS:H	5	0.78
(1,2214)	1:83:A:VAL:HG13	1:55:A:LYS:H	5	0.78
(1,2114)	1:46:A:SER:H	1:43:A:PRO:HD3	2	0.78
(1,1680)	1:27:A:LYS:HG2	1:128:A:LEU:HD21	10	0.78
(1,1680)	1:27:A:LYS:HG2	1:128:A:LEU:HD22	10	0.78
(1,1680)	1:27:A:LYS:HG2	1:128:A:LEU:HD23	10	0.78
(1,1680)	1:27:A:LYS:HG3	1:128:A:LEU:HD21	10	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1680)	1:27:A:LYS:HG3	1:128:A:LEU:HD22	10	0.78
(1,1680)	1:27:A:LYS:HG3	1:128:A:LEU:HD23	10	0.78
(1,1654)	1:122:A:MET:HG2	1:121:A:LEU:HD11	9	0.78
(1,1654)	1:122:A:MET:HG2	1:121:A:LEU:HD12	9	0.78
(1,1654)	1:122:A:MET:HG2	1:121:A:LEU:HD13	9	0.78
(1,1654)	1:122:A:MET:HG3	1:121:A:LEU:HD11	9	0.78
(1,1654)	1:122:A:MET:HG3	1:121:A:LEU:HD12	9	0.78
(1,1654)	1:122:A:MET:HG3	1:121:A:LEU:HD13	9	0.78
(1,1547)	1:83:A:VAL:HG21	1:84:A:ALA:HB1	1	0.78
(1,1547)	1:83:A:VAL:HG21	1:84:A:ALA:HB2	1	0.78
(1,1547)	1:83:A:VAL:HG21	1:84:A:ALA:HB3	1	0.78
(1,1547)	1:83:A:VAL:HG22	1:84:A:ALA:HB1	1	0.78
(1,1547)	1:83:A:VAL:HG22	1:84:A:ALA:HB2	1	0.78
(1,1547)	1:83:A:VAL:HG22	1:84:A:ALA:HB3	1	0.78
(1,1547)	1:83:A:VAL:HG23	1:84:A:ALA:HB1	1	0.78
(1,1547)	1:83:A:VAL:HG23	1:84:A:ALA:HB2	1	0.78
(1,1547)	1:83:A:VAL:HG23	1:84:A:ALA:HB3	1	0.78
(1,1547)	1:83:A:VAL:HG21	1:84:A:ALA:HB1	4	0.78
(1,1547)	1:83:A:VAL:HG21	1:84:A:ALA:HB2	4	0.78
(1,1547)	1:83:A:VAL:HG21	1:84:A:ALA:HB3	4	0.78
(1,1547)	1:83:A:VAL:HG22	1:84:A:ALA:HB1	4	0.78
(1,1547)	1:83:A:VAL:HG22	1:84:A:ALA:HB2	4	0.78
(1,1547)	1:83:A:VAL:HG22	1:84:A:ALA:HB3	4	0.78
(1,1547)	1:83:A:VAL:HG23	1:84:A:ALA:HB1	4	0.78
(1,1547)	1:83:A:VAL:HG23	1:84:A:ALA:HB2	4	0.78
(1,1547)	1:83:A:VAL:HG23	1:84:A:ALA:HB3	4	0.78
(1,1514)	1:75:A:VAL:HB	1:69:A:ALA:HB1	4	0.78
(1,1514)	1:75:A:VAL:HB	1:69:A:ALA:HB2	4	0.78
(1,1514)	1:75:A:VAL:HB	1:69:A:ALA:HB3	4	0.78
(1,1064)	1:107:A:GLY:HA2	1:55:A:LYS:HD3	8	0.78
(1,1017)	1:101:A:PRO:HD3	1:25:A:VAL:HG21	2	0.78
(1,1017)	1:101:A:PRO:HD3	1:25:A:VAL:HG22	2	0.78
(1,1017)	1:101:A:PRO:HD3	1:25:A:VAL:HG23	2	0.78
(1,1009)	1:101:A:PRO:HA	1:27:A:LYS:HA	5	0.78
(1,1009)	1:101:A:PRO:HA	1:27:A:LYS:HA	7	0.78
(1,882)	1:91:A:GLY:HA3	1:38:A:HIS:HB2	8	0.78
(1,643)	1:76:A:LYS:HD2	1:66:A:GLY:HA3	5	0.78
(1,643)	1:76:A:LYS:HD3	1:66:A:GLY:HA3	5	0.78
(1,2516)	1:97:A:LEU:H	1:36:A:LEU:HD11	9	0.77
(1,2516)	1:97:A:LEU:H	1:36:A:LEU:HD12	9	0.77
(1,2516)	1:97:A:LEU:H	1:36:A:LEU:HD13	9	0.77
(1,2209)	1:54:A:ALA:H	1:126:A:VAL:HG21	9	0.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2209)	1:54:A:ALA:H	1:126:A:VAL:HG22	9	0.77
(1,2209)	1:54:A:ALA:H	1:126:A:VAL:HG23	9	0.77
(1,1679)	1:27:A:LYS:HB2	1:128:A:LEU:HD21	3	0.77
(1,1679)	1:27:A:LYS:HB2	1:128:A:LEU:HD22	3	0.77
(1,1679)	1:27:A:LYS:HB2	1:128:A:LEU:HD23	3	0.77
(1,1679)	1:27:A:LYS:HB3	1:128:A:LEU:HD21	3	0.77
(1,1679)	1:27:A:LYS:HB3	1:128:A:LEU:HD22	3	0.77
(1,1679)	1:27:A:LYS:HB3	1:128:A:LEU:HD23	3	0.77
(1,1525)	1:114:A:THR:HG21	1:75:A:VAL:HG21	7	0.77
(1,1525)	1:114:A:THR:HG21	1:75:A:VAL:HG22	7	0.77
(1,1525)	1:114:A:THR:HG21	1:75:A:VAL:HG23	7	0.77
(1,1525)	1:114:A:THR:HG22	1:75:A:VAL:HG21	7	0.77
(1,1525)	1:114:A:THR:HG22	1:75:A:VAL:HG22	7	0.77
(1,1525)	1:114:A:THR:HG22	1:75:A:VAL:HG23	7	0.77
(1,1525)	1:114:A:THR:HG23	1:75:A:VAL:HG21	7	0.77
(1,1525)	1:114:A:THR:HG23	1:75:A:VAL:HG22	7	0.77
(1,1525)	1:114:A:THR:HG23	1:75:A:VAL:HG23	7	0.77
(1,1514)	1:75:A:VAL:HB	1:69:A:ALA:HB1	9	0.77
(1,1514)	1:75:A:VAL:HB	1:69:A:ALA:HB2	9	0.77
(1,1514)	1:75:A:VAL:HB	1:69:A:ALA:HB3	9	0.77
(1,1497)	1:54:A:ALA:HB1	1:52:A:VAL:HG11	6	0.77
(1,1497)	1:54:A:ALA:HB1	1:52:A:VAL:HG12	6	0.77
(1,1497)	1:54:A:ALA:HB1	1:52:A:VAL:HG13	6	0.77
(1,1497)	1:54:A:ALA:HB2	1:52:A:VAL:HG11	6	0.77
(1,1497)	1:54:A:ALA:HB2	1:52:A:VAL:HG12	6	0.77
(1,1497)	1:54:A:ALA:HB2	1:52:A:VAL:HG13	6	0.77
(1,1497)	1:54:A:ALA:HB3	1:52:A:VAL:HG11	6	0.77
(1,1497)	1:54:A:ALA:HB3	1:52:A:VAL:HG12	6	0.77
(1,1497)	1:54:A:ALA:HB3	1:52:A:VAL:HG13	6	0.77
(1,1428)	1:18:A:PHE:HD1	1:36:A:LEU:HD21	5	0.77
(1,1428)	1:18:A:PHE:HD1	1:36:A:LEU:HD22	5	0.77
(1,1428)	1:18:A:PHE:HD1	1:36:A:LEU:HD23	5	0.77
(1,1428)	1:18:A:PHE:HD2	1:36:A:LEU:HD21	5	0.77
(1,1428)	1:18:A:PHE:HD2	1:36:A:LEU:HD22	5	0.77
(1,1428)	1:18:A:PHE:HD2	1:36:A:LEU:HD23	5	0.77
(1,1064)	1:107:A:GLY:HA2	1:55:A:LYS:HD3	1	0.77
(1,1039)	1:99:A:LEU:HD21	1:101:A:PRO:HG3	4	0.77
(1,1039)	1:99:A:LEU:HD22	1:101:A:PRO:HG3	4	0.77
(1,1039)	1:99:A:LEU:HD23	1:101:A:PRO:HG3	4	0.77
(1,1035)	1:101:A:PRO:HG3	1:25:A:VAL:HG21	9	0.77
(1,1035)	1:101:A:PRO:HG3	1:25:A:VAL:HG22	9	0.77
(1,1035)	1:101:A:PRO:HG3	1:25:A:VAL:HG23	9	0.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,258)	1:6:A:CYS:HB2	1:32:A:PHE:HA	7	0.77
(1,3244)	1:123:A:ASN:HD21	1:122:A:MET:HB3	5	0.76
(1,3232)	1:53:A:ILE:HG22	1:112:A:ALA:H	3	0.76
(1,3166)	1:126:A:VAL:HG11	1:23:A:ILE:H	10	0.76
(1,2884)	1:115:A:PHE:HB3	1:74:A:TYR:HD1	4	0.76
(1,2884)	1:115:A:PHE:HB3	1:74:A:TYR:HD2	4	0.76
(1,2652)	1:113:A:CYS:H	1:111:A:PHE:HB3	1	0.76
(1,2652)	1:113:A:CYS:H	1:111:A:PHE:HB3	4	0.76
(1,2652)	1:113:A:CYS:H	1:111:A:PHE:HB3	7	0.76
(1,2652)	1:113:A:CYS:H	1:111:A:PHE:HB3	9	0.76
(1,2647)	1:112:A:ALA:H	1:126:A:VAL:HG21	6	0.76
(1,2647)	1:112:A:ALA:H	1:126:A:VAL:HG22	6	0.76
(1,2647)	1:112:A:ALA:H	1:126:A:VAL:HG23	6	0.76
(1,2179)	1:51:A:LEU:H	1:95:A:SER:HB2	3	0.76
(1,1715)	1:59:A:MET:HE1	1:114:A:THR:HG1	4	0.76
(1,1715)	1:59:A:MET:HE2	1:114:A:THR:HG1	4	0.76
(1,1715)	1:59:A:MET:HE3	1:114:A:THR:HG1	4	0.76
(1,1613)	1:101:A:PRO:HA	1:99:A:LEU:HD21	6	0.76
(1,1613)	1:101:A:PRO:HA	1:99:A:LEU:HD22	6	0.76
(1,1613)	1:101:A:PRO:HA	1:99:A:LEU:HD23	6	0.76
(1,1547)	1:83:A:VAL:HG21	1:84:A:ALA:HB1	8	0.76
(1,1547)	1:83:A:VAL:HG21	1:84:A:ALA:HB2	8	0.76
(1,1547)	1:83:A:VAL:HG21	1:84:A:ALA:HB3	8	0.76
(1,1547)	1:83:A:VAL:HG22	1:84:A:ALA:HB1	8	0.76
(1,1547)	1:83:A:VAL:HG22	1:84:A:ALA:HB2	8	0.76
(1,1547)	1:83:A:VAL:HG22	1:84:A:ALA:HB3	8	0.76
(1,1547)	1:83:A:VAL:HG23	1:84:A:ALA:HB1	8	0.76
(1,1547)	1:83:A:VAL:HG23	1:84:A:ALA:HB2	8	0.76
(1,1547)	1:83:A:VAL:HG23	1:84:A:ALA:HB3	8	0.76
(1,1513)	1:76:A:LYS:HB3	1:69:A:ALA:HB1	9	0.76
(1,1513)	1:76:A:LYS:HB3	1:69:A:ALA:HB2	9	0.76
(1,1513)	1:76:A:LYS:HB3	1:69:A:ALA:HB3	9	0.76
(1,1509)	1:62:A:VAL:HG21	1:114:A:THR:HG21	10	0.76
(1,1509)	1:62:A:VAL:HG21	1:114:A:THR:HG22	10	0.76
(1,1509)	1:62:A:VAL:HG21	1:114:A:THR:HG23	10	0.76
(1,1509)	1:62:A:VAL:HG22	1:114:A:THR:HG21	10	0.76
(1,1509)	1:62:A:VAL:HG22	1:114:A:THR:HG22	10	0.76
(1,1509)	1:62:A:VAL:HG22	1:114:A:THR:HG23	10	0.76
(1,1509)	1:62:A:VAL:HG23	1:114:A:THR:HG21	10	0.76
(1,1509)	1:62:A:VAL:HG23	1:114:A:THR:HG22	10	0.76
(1,1509)	1:62:A:VAL:HG23	1:114:A:THR:HG23	10	0.76
(1,760)	1:76:A:LYS:HD2	1:77:A:PRO:HD2	6	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,760)	1:76:A:LYS:HD3	1:77:A:PRO:HD2	6	0.76
(1,493)	1:50:A:ASN:HA	1:36:A:LEU:HD11	3	0.76
(1,493)	1:50:A:ASN:HA	1:36:A:LEU:HD12	3	0.76
(1,493)	1:50:A:ASN:HA	1:36:A:LEU:HD13	3	0.76
(1,493)	1:50:A:ASN:HA	1:36:A:LEU:HD11	8	0.76
(1,493)	1:50:A:ASN:HA	1:36:A:LEU:HD12	8	0.76
(1,493)	1:50:A:ASN:HA	1:36:A:LEU:HD13	8	0.76
(1,3208)	1:79:A:ASP:H	1:75:A:VAL:HB	10	0.75
(1,2966)	1:109:A:TYR:HE1	1:128:A:LEU:HD11	6	0.75
(1,2966)	1:109:A:TYR:HE1	1:128:A:LEU:HD12	6	0.75
(1,2966)	1:109:A:TYR:HE1	1:128:A:LEU:HD13	6	0.75
(1,2966)	1:109:A:TYR:HE2	1:128:A:LEU:HD11	6	0.75
(1,2966)	1:109:A:TYR:HE2	1:128:A:LEU:HD12	6	0.75
(1,2966)	1:109:A:TYR:HE2	1:128:A:LEU:HD13	6	0.75
(1,2963)	1:109:A:TYR:HD1	1:128:A:LEU:HD11	10	0.75
(1,2963)	1:109:A:TYR:HD1	1:128:A:LEU:HD12	10	0.75
(1,2963)	1:109:A:TYR:HD1	1:128:A:LEU:HD13	10	0.75
(1,2963)	1:109:A:TYR:HD2	1:128:A:LEU:HD11	10	0.75
(1,2963)	1:109:A:TYR:HD2	1:128:A:LEU:HD12	10	0.75
(1,2963)	1:109:A:TYR:HD2	1:128:A:LEU:HD13	10	0.75
(1,2884)	1:115:A:PHE:HB3	1:74:A:TYR:HD1	5	0.75
(1,2884)	1:115:A:PHE:HB3	1:74:A:TYR:HD2	5	0.75
(1,2696)	1:117:A:GLY:H	1:67:A:VAL:HG11	1	0.75
(1,2696)	1:117:A:GLY:H	1:67:A:VAL:HG12	1	0.75
(1,2696)	1:117:A:GLY:H	1:67:A:VAL:HG13	1	0.75
(1,2516)	1:97:A:LEU:H	1:36:A:LEU:HD11	2	0.75
(1,2516)	1:97:A:LEU:H	1:36:A:LEU:HD12	2	0.75
(1,2516)	1:97:A:LEU:H	1:36:A:LEU:HD13	2	0.75
(1,2359)	1:78:A:ASP:H	1:79:A:ASP:H	9	0.75
(1,2125)	1:47:A:MET:H	1:43:A:PRO:HD3	6	0.75
(1,2045)	1:94:A:GLU:HB2	1:38:A:HIS:H	7	0.75
(1,1753)	1:36:A:LEU:HD21	1:10:A:VAL:H	1	0.75
(1,1753)	1:36:A:LEU:HD22	1:10:A:VAL:H	1	0.75
(1,1753)	1:36:A:LEU:HD23	1:10:A:VAL:H	1	0.75
(1,1715)	1:59:A:MET:HE1	1:114:A:THR:HG1	1	0.75
(1,1715)	1:59:A:MET:HE2	1:114:A:THR:HG1	1	0.75
(1,1715)	1:59:A:MET:HE3	1:114:A:THR:HG1	1	0.75
(1,1660)	1:25:A:VAL:H	1:126:A:VAL:HG21	2	0.75
(1,1660)	1:25:A:VAL:H	1:126:A:VAL:HG22	2	0.75
(1,1660)	1:25:A:VAL:H	1:126:A:VAL:HG23	2	0.75
(1,1547)	1:83:A:VAL:HG21	1:84:A:ALA:HB1	6	0.75
(1,1547)	1:83:A:VAL:HG21	1:84:A:ALA:HB2	6	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1547)	1:83:A:VAL:HG21	1:84:A:ALA:HB3	6	0.75
(1,1547)	1:83:A:VAL:HG22	1:84:A:ALA:HB1	6	0.75
(1,1547)	1:83:A:VAL:HG22	1:84:A:ALA:HB2	6	0.75
(1,1547)	1:83:A:VAL:HG22	1:84:A:ALA:HB3	6	0.75
(1,1547)	1:83:A:VAL:HG23	1:84:A:ALA:HB1	6	0.75
(1,1547)	1:83:A:VAL:HG23	1:84:A:ALA:HB2	6	0.75
(1,1547)	1:83:A:VAL:HG23	1:84:A:ALA:HB3	6	0.75
(1,1526)	1:52:A:VAL:HG21	1:75:A:VAL:HG21	3	0.75
(1,1526)	1:52:A:VAL:HG21	1:75:A:VAL:HG22	3	0.75
(1,1526)	1:52:A:VAL:HG21	1:75:A:VAL:HG23	3	0.75
(1,1526)	1:52:A:VAL:HG22	1:75:A:VAL:HG21	3	0.75
(1,1526)	1:52:A:VAL:HG22	1:75:A:VAL:HG22	3	0.75
(1,1526)	1:52:A:VAL:HG22	1:75:A:VAL:HG23	3	0.75
(1,1526)	1:52:A:VAL:HG23	1:75:A:VAL:HG21	3	0.75
(1,1526)	1:52:A:VAL:HG23	1:75:A:VAL:HG22	3	0.75
(1,1526)	1:52:A:VAL:HG23	1:75:A:VAL:HG23	3	0.75
(1,1074)	1:107:A:GLY:HA2	1:109:A:TYR:HE1	5	0.75
(1,1074)	1:107:A:GLY:HA2	1:109:A:TYR:HE2	5	0.75
(1,117)	1:19:A:ASN:HB3	1:11:A:GLU:HB2	10	0.75
(1,3108)	1:128:A:LEU:HB3	1:105:A:ALA:HA	9	0.74
(1,2966)	1:109:A:TYR:HE1	1:128:A:LEU:HD11	4	0.74
(1,2966)	1:109:A:TYR:HE1	1:128:A:LEU:HD12	4	0.74
(1,2966)	1:109:A:TYR:HE1	1:128:A:LEU:HD13	4	0.74
(1,2966)	1:109:A:TYR:HE2	1:128:A:LEU:HD11	4	0.74
(1,2966)	1:109:A:TYR:HE2	1:128:A:LEU:HD12	4	0.74
(1,2966)	1:109:A:TYR:HE2	1:128:A:LEU:HD13	4	0.74
(1,2516)	1:97:A:LEU:H	1:36:A:LEU:HD11	7	0.74
(1,2516)	1:97:A:LEU:H	1:36:A:LEU:HD12	7	0.74
(1,2516)	1:97:A:LEU:H	1:36:A:LEU:HD13	7	0.74
(1,2179)	1:51:A:LEU:H	1:95:A:SER:HB2	2	0.74
(1,2114)	1:46:A:SER:H	1:43:A:PRO:HD3	10	0.74
(1,2058)	1:40:A:GLY:H	1:39:A:THR:H	3	0.74
(1,2058)	1:40:A:GLY:H	1:39:A:THR:H	8	0.74
(1,1870)	1:19:A:ASN:HD22	1:10:A:VAL:HA	8	0.74
(1,1609)	1:99:A:LEU:HD21	1:32:A:PHE:H	9	0.74
(1,1609)	1:99:A:LEU:HD22	1:32:A:PHE:H	9	0.74
(1,1609)	1:99:A:LEU:HD23	1:32:A:PHE:H	9	0.74
(1,1461)	1:126:A:VAL:HG11	1:51:A:LEU:HD21	2	0.74
(1,1461)	1:126:A:VAL:HG11	1:51:A:LEU:HD22	2	0.74
(1,1461)	1:126:A:VAL:HG11	1:51:A:LEU:HD23	2	0.74
(1,1461)	1:126:A:VAL:HG12	1:51:A:LEU:HD21	2	0.74
(1,1461)	1:126:A:VAL:HG12	1:51:A:LEU:HD22	2	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1461)	1:126:A:VAL:HG12	1:51:A:LEU:HD23	2	0.74
(1,1461)	1:126:A:VAL:HG13	1:51:A:LEU:HD21	2	0.74
(1,1461)	1:126:A:VAL:HG13	1:51:A:LEU:HD22	2	0.74
(1,1461)	1:126:A:VAL:HG13	1:51:A:LEU:HD23	2	0.74
(1,1428)	1:18:A:PHE:HD1	1:36:A:LEU:HD21	8	0.74
(1,1428)	1:18:A:PHE:HD1	1:36:A:LEU:HD22	8	0.74
(1,1428)	1:18:A:PHE:HD1	1:36:A:LEU:HD23	8	0.74
(1,1428)	1:18:A:PHE:HD2	1:36:A:LEU:HD21	8	0.74
(1,1428)	1:18:A:PHE:HD2	1:36:A:LEU:HD22	8	0.74
(1,1428)	1:18:A:PHE:HD2	1:36:A:LEU:HD23	8	0.74
(1,882)	1:91:A:GLY:HA3	1:38:A:HIS:HB2	4	0.74
(1,646)	1:76:A:LYS:HB3	1:66:A:GLY:HA3	6	0.74
(1,36)	1:38:A:HIS:HA	1:39:A:THR:HG21	6	0.74
(1,36)	1:38:A:HIS:HA	1:39:A:THR:HG22	6	0.74
(1,36)	1:38:A:HIS:HA	1:39:A:THR:HG23	6	0.74
(1,3220)	1:94:A:GLU:H	1:93:A:GLU:HG2	3	0.73
(1,3220)	1:94:A:GLU:H	1:93:A:GLU:HB2	4	0.73
(1,2884)	1:115:A:PHE:HB3	1:74:A:TYR:HD1	8	0.73
(1,2884)	1:115:A:PHE:HB3	1:74:A:TYR:HD2	8	0.73
(1,2747)	1:123:A:ASN:H	1:121:A:LEU:HD11	7	0.73
(1,2747)	1:123:A:ASN:H	1:121:A:LEU:HD12	7	0.73
(1,2747)	1:123:A:ASN:H	1:121:A:LEU:HD13	7	0.73
(1,2652)	1:113:A:CYS:H	1:111:A:PHE:HB3	5	0.73
(1,2542)	1:100:A:ASP:H	1:83:A:VAL:HA	10	0.73
(1,2516)	1:97:A:LEU:H	1:36:A:LEU:HD11	5	0.73
(1,2516)	1:97:A:LEU:H	1:36:A:LEU:HD12	5	0.73
(1,2516)	1:97:A:LEU:H	1:36:A:LEU:HD13	5	0.73
(1,2215)	1:83:A:VAL:HG21	1:55:A:LYS:H	9	0.73
(1,2215)	1:83:A:VAL:HG22	1:55:A:LYS:H	9	0.73
(1,2215)	1:83:A:VAL:HG23	1:55:A:LYS:H	9	0.73
(1,1683)	1:104:A:LEU:HD11	1:128:A:LEU:HD21	7	0.73
(1,1683)	1:104:A:LEU:HD11	1:128:A:LEU:HD22	7	0.73
(1,1683)	1:104:A:LEU:HD11	1:128:A:LEU:HD23	7	0.73
(1,1683)	1:104:A:LEU:HD12	1:128:A:LEU:HD21	7	0.73
(1,1683)	1:104:A:LEU:HD12	1:128:A:LEU:HD22	7	0.73
(1,1683)	1:104:A:LEU:HD12	1:128:A:LEU:HD23	7	0.73
(1,1683)	1:104:A:LEU:HD13	1:128:A:LEU:HD21	7	0.73
(1,1683)	1:104:A:LEU:HD13	1:128:A:LEU:HD22	7	0.73
(1,1683)	1:104:A:LEU:HD13	1:128:A:LEU:HD23	7	0.73
(1,1461)	1:126:A:VAL:HG11	1:51:A:LEU:HD21	8	0.73
(1,1461)	1:126:A:VAL:HG11	1:51:A:LEU:HD22	8	0.73
(1,1461)	1:126:A:VAL:HG11	1:51:A:LEU:HD23	8	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1461)	1:126:A:VAL:HG12	1:51:A:LEU:HD21	8	0.73
(1,1461)	1:126:A:VAL:HG12	1:51:A:LEU:HD22	8	0.73
(1,1461)	1:126:A:VAL:HG12	1:51:A:LEU:HD23	8	0.73
(1,1461)	1:126:A:VAL:HG13	1:51:A:LEU:HD21	8	0.73
(1,1461)	1:126:A:VAL:HG13	1:51:A:LEU:HD22	8	0.73
(1,1461)	1:126:A:VAL:HG13	1:51:A:LEU:HD23	8	0.73
(1,639)	1:67:A:VAL:HG11	1:64:A:LYS:HA	9	0.73
(1,639)	1:67:A:VAL:HG12	1:64:A:LYS:HA	9	0.73
(1,639)	1:67:A:VAL:HG13	1:64:A:LYS:HA	9	0.73
(1,3220)	1:94:A:GLU:H	1:93:A:GLU:HB2	9	0.72
(1,3167)	1:129:A:VAL:HG22	1:24:A:GLN:H	4	0.72
(1,3166)	1:126:A:VAL:HG13	1:23:A:ILE:H	9	0.72
(1,3165)	1:24:A:GLN:HB3	1:23:A:ILE:H	9	0.72
(1,2832)	1:18:A:PHE:HE1	1:12:A:SER:HB2	2	0.72
(1,2832)	1:18:A:PHE:HE2	1:12:A:SER:HB2	2	0.72
(1,2652)	1:113:A:CYS:H	1:111:A:PHE:HB3	6	0.72
(1,2623)	1:125:A:LYS:HD2	1:110:A:LYS:H	6	0.72
(1,2623)	1:125:A:LYS:HD3	1:110:A:LYS:H	6	0.72
(1,2591)	1:106:A:ASP:H	1:128:A:LEU:HD11	2	0.72
(1,2591)	1:106:A:ASP:H	1:128:A:LEU:HD12	2	0.72
(1,2591)	1:106:A:ASP:H	1:128:A:LEU:HD13	2	0.72
(1,2058)	1:40:A:GLY:H	1:39:A:THR:H	4	0.72
(1,1978)	1:31:A:GLU:H	1:30:A:LYS:HD3	10	0.72
(1,1680)	1:27:A:LYS:HG2	1:128:A:LEU:HD21	6	0.72
(1,1680)	1:27:A:LYS:HG2	1:128:A:LEU:HD22	6	0.72
(1,1680)	1:27:A:LYS:HG2	1:128:A:LEU:HD23	6	0.72
(1,1680)	1:27:A:LYS:HG3	1:128:A:LEU:HD21	6	0.72
(1,1680)	1:27:A:LYS:HG3	1:128:A:LEU:HD22	6	0.72
(1,1680)	1:27:A:LYS:HG3	1:128:A:LEU:HD23	6	0.72
(1,1609)	1:99:A:LEU:HD21	1:32:A:PHE:H	4	0.72
(1,1609)	1:99:A:LEU:HD22	1:32:A:PHE:H	4	0.72
(1,1609)	1:99:A:LEU:HD23	1:32:A:PHE:H	4	0.72
(1,1388)	1:101:A:PRO:HA	1:25:A:VAL:HG21	2	0.72
(1,1388)	1:101:A:PRO:HA	1:25:A:VAL:HG22	2	0.72
(1,1388)	1:101:A:PRO:HA	1:25:A:VAL:HG23	2	0.72
(1,1064)	1:107:A:GLY:HA2	1:55:A:LYS:HD3	3	0.72
(1,1061)	1:105:A:ALA:HA	1:128:A:LEU:HD11	6	0.72
(1,1061)	1:105:A:ALA:HA	1:128:A:LEU:HD12	6	0.72
(1,1061)	1:105:A:ALA:HA	1:128:A:LEU:HD13	6	0.72
(1,769)	1:77:A:PRO:HG2	1:72:A:THR:HG21	3	0.72
(1,769)	1:77:A:PRO:HG2	1:72:A:THR:HG22	3	0.72
(1,769)	1:77:A:PRO:HG2	1:72:A:THR:HG23	3	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,463)	1:88:A:LEU:HG	1:48:A:GLY:HA2	1	0.72
(2,1)	1:6:A:CYS:SG	1:29:A:CYS:SG	2	0.71
(1,3143)	1:103:A:LYS:HB2	1:99:A:LEU:HD23	3	0.71
(1,2955)	1:55:A:LYS:HB3	1:109:A:TYR:HE1	4	0.71
(1,2955)	1:55:A:LYS:HB3	1:109:A:TYR:HE2	4	0.71
(1,2880)	1:67:A:VAL:HG21	1:74:A:TYR:HD1	8	0.71
(1,2880)	1:67:A:VAL:HG21	1:74:A:TYR:HD2	8	0.71
(1,2880)	1:67:A:VAL:HG22	1:74:A:TYR:HD1	8	0.71
(1,2880)	1:67:A:VAL:HG22	1:74:A:TYR:HD2	8	0.71
(1,2880)	1:67:A:VAL:HG23	1:74:A:TYR:HD1	8	0.71
(1,2880)	1:67:A:VAL:HG23	1:74:A:TYR:HD2	8	0.71
(1,2876)	1:38:A:HIS:HE1	1:13:A:ASN:HB2	3	0.71
(1,2360)	1:76:A:LYS:HE2	1:79:A:ASP:H	6	0.71
(1,2360)	1:76:A:LYS:HE3	1:79:A:ASP:H	6	0.71
(1,1798)	1:15:A:ASN:HB2	1:13:A:ASN:HD21	4	0.71
(1,1686)	1:128:A:LEU:HD11	1:127:A:THR:HG21	7	0.71
(1,1686)	1:128:A:LEU:HD11	1:127:A:THR:HG22	7	0.71
(1,1686)	1:128:A:LEU:HD11	1:127:A:THR:HG23	7	0.71
(1,1686)	1:128:A:LEU:HD12	1:127:A:THR:HG21	7	0.71
(1,1686)	1:128:A:LEU:HD12	1:127:A:THR:HG22	7	0.71
(1,1686)	1:128:A:LEU:HD12	1:127:A:THR:HG23	7	0.71
(1,1686)	1:128:A:LEU:HD13	1:127:A:THR:HG21	7	0.71
(1,1686)	1:128:A:LEU:HD13	1:127:A:THR:HG22	7	0.71
(1,1686)	1:128:A:LEU:HD13	1:127:A:THR:HG23	7	0.71
(1,1686)	1:128:A:LEU:HD11	1:127:A:THR:HG21	10	0.71
(1,1686)	1:128:A:LEU:HD11	1:127:A:THR:HG22	10	0.71
(1,1686)	1:128:A:LEU:HD11	1:127:A:THR:HG23	10	0.71
(1,1686)	1:128:A:LEU:HD12	1:127:A:THR:HG21	10	0.71
(1,1686)	1:128:A:LEU:HD12	1:127:A:THR:HG22	10	0.71
(1,1686)	1:128:A:LEU:HD12	1:127:A:THR:HG23	10	0.71
(1,1686)	1:128:A:LEU:HD13	1:127:A:THR:HG21	10	0.71
(1,1686)	1:128:A:LEU:HD13	1:127:A:THR:HG22	10	0.71
(1,1686)	1:128:A:LEU:HD13	1:127:A:THR:HG23	10	0.71
(1,1498)	1:62:A:VAL:HG11	1:54:A:ALA:H	2	0.71
(1,1498)	1:62:A:VAL:HG12	1:54:A:ALA:H	2	0.71
(1,1498)	1:62:A:VAL:HG13	1:54:A:ALA:H	2	0.71
(1,1428)	1:18:A:PHE:HD1	1:36:A:LEU:HD21	2	0.71
(1,1428)	1:18:A:PHE:HD1	1:36:A:LEU:HD22	2	0.71
(1,1428)	1:18:A:PHE:HD1	1:36:A:LEU:HD23	2	0.71
(1,1428)	1:18:A:PHE:HD2	1:36:A:LEU:HD21	2	0.71
(1,1428)	1:18:A:PHE:HD2	1:36:A:LEU:HD22	2	0.71
(1,1428)	1:18:A:PHE:HD2	1:36:A:LEU:HD23	2	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1199)	1:116:A:PRO:HD2	1:67:A:VAL:HG11	5	0.71
(1,1199)	1:116:A:PRO:HD2	1:67:A:VAL:HG12	5	0.71
(1,1199)	1:116:A:PRO:HD2	1:67:A:VAL:HG13	5	0.71
(1,1064)	1:107:A:GLY:HA2	1:55:A:LYS:HD3	9	0.71
(1,984)	1:98:A:THR:HB	1:31:A:GLU:HB2	5	0.71
(1,889)	1:92:A:GLY:HA2	1:93:A:GLU:HG3	6	0.71
(1,802)	1:83:A:VAL:HB	1:104:A:LEU:HD21	9	0.71
(1,802)	1:83:A:VAL:HB	1:104:A:LEU:HD22	9	0.71
(1,802)	1:83:A:VAL:HB	1:104:A:LEU:HD23	9	0.71
(1,3165)	1:24:A:GLN:HB3	1:23:A:ILE:H	10	0.7
(1,3143)	1:103:A:LYS:HB2	1:99:A:LEU:HD21	7	0.7
(1,3139)	1:51:A:LEU:HB2	1:86:A:THR:HG23	6	0.7
(1,2032)	1:36:A:LEU:HD21	1:37:A:LYS:H	9	0.7
(1,2032)	1:36:A:LEU:HD22	1:37:A:LYS:H	9	0.7
(1,2032)	1:36:A:LEU:HD23	1:37:A:LYS:H	9	0.7
(1,1715)	1:59:A:MET:HE1	1:114:A:THR:HG1	5	0.7
(1,1715)	1:59:A:MET:HE2	1:114:A:THR:HG1	5	0.7
(1,1715)	1:59:A:MET:HE3	1:114:A:THR:HG1	5	0.7
(1,1686)	1:128:A:LEU:HD11	1:127:A:THR:HG21	5	0.7
(1,1686)	1:128:A:LEU:HD11	1:127:A:THR:HG22	5	0.7
(1,1686)	1:128:A:LEU:HD11	1:127:A:THR:HG23	5	0.7
(1,1686)	1:128:A:LEU:HD12	1:127:A:THR:HG21	5	0.7
(1,1686)	1:128:A:LEU:HD12	1:127:A:THR:HG22	5	0.7
(1,1686)	1:128:A:LEU:HD12	1:127:A:THR:HG23	5	0.7
(1,1686)	1:128:A:LEU:HD13	1:127:A:THR:HG21	5	0.7
(1,1686)	1:128:A:LEU:HD13	1:127:A:THR:HG22	5	0.7
(1,1686)	1:128:A:LEU:HD13	1:127:A:THR:HG23	5	0.7
(1,1506)	1:81:A:ARG:HB2	1:62:A:VAL:HG11	3	0.7
(1,1506)	1:81:A:ARG:HB2	1:62:A:VAL:HG12	3	0.7
(1,1506)	1:81:A:ARG:HB2	1:62:A:VAL:HG13	3	0.7
(1,1498)	1:62:A:VAL:HG11	1:54:A:ALA:H	3	0.7
(1,1498)	1:62:A:VAL:HG12	1:54:A:ALA:H	3	0.7
(1,1498)	1:62:A:VAL:HG13	1:54:A:ALA:H	3	0.7
(1,493)	1:50:A:ASN:HA	1:36:A:LEU:HD11	4	0.7
(1,493)	1:50:A:ASN:HA	1:36:A:LEU:HD12	4	0.7
(1,493)	1:50:A:ASN:HA	1:36:A:LEU:HD13	4	0.7
(1,45)	1:11:A:GLU:HG3	1:9:A:THR:HG21	8	0.7
(1,45)	1:11:A:GLU:HG3	1:9:A:THR:HG22	8	0.7
(1,45)	1:11:A:GLU:HG3	1:9:A:THR:HG23	8	0.7
(1,3165)	1:24:A:GLN:HB3	1:23:A:ILE:H	1	0.69
(1,3139)	1:51:A:LEU:HB2	1:86:A:THR:HG22	1	0.69
(1,3139)	1:51:A:LEU:HB2	1:86:A:THR:HG22	3	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2966)	1:109:A:TYR:HE1	1:128:A:LEU:HD11	2	0.69
(1,2966)	1:109:A:TYR:HE1	1:128:A:LEU:HD12	2	0.69
(1,2966)	1:109:A:TYR:HE1	1:128:A:LEU:HD13	2	0.69
(1,2966)	1:109:A:TYR:HE2	1:128:A:LEU:HD11	2	0.69
(1,2966)	1:109:A:TYR:HE2	1:128:A:LEU:HD12	2	0.69
(1,2966)	1:109:A:TYR:HE2	1:128:A:LEU:HD13	2	0.69
(1,2884)	1:115:A:PHE:HB3	1:74:A:TYR:HD1	9	0.69
(1,2884)	1:115:A:PHE:HB3	1:74:A:TYR:HD2	9	0.69
(1,2832)	1:18:A:PHE:HE1	1:12:A:SER:HB2	8	0.69
(1,2832)	1:18:A:PHE:HE2	1:12:A:SER:HB2	8	0.69
(1,2631)	1:110:A:LYS:HE2	1:111:A:PHE:H	10	0.69
(1,2631)	1:110:A:LYS:HE3	1:111:A:PHE:H	10	0.69
(1,2595)	1:74:A:TYR:HB3	1:50:A:ASN:HD21	9	0.69
(1,2363)	1:79:A:ASP:H	1:76:A:LYS:HB3	10	0.69
(1,2214)	1:83:A:VAL:HG11	1:55:A:LYS:H	10	0.69
(1,2214)	1:83:A:VAL:HG12	1:55:A:LYS:H	10	0.69
(1,2214)	1:83:A:VAL:HG13	1:55:A:LYS:H	10	0.69
(1,2062)	1:40:A:GLY:H	1:13:A:ASN:HA	9	0.69
(1,1879)	1:20:A:THR:H	1:19:A:ASN:HB3	10	0.69
(1,1715)	1:59:A:MET:HE1	1:114:A:THR:HG1	6	0.69
(1,1715)	1:59:A:MET:HE2	1:114:A:THR:HG1	6	0.69
(1,1715)	1:59:A:MET:HE3	1:114:A:THR:HG1	6	0.69
(1,1680)	1:27:A:LYS:HG2	1:128:A:LEU:HD21	7	0.69
(1,1680)	1:27:A:LYS:HG2	1:128:A:LEU:HD22	7	0.69
(1,1680)	1:27:A:LYS:HG2	1:128:A:LEU:HD23	7	0.69
(1,1680)	1:27:A:LYS:HG3	1:128:A:LEU:HD21	7	0.69
(1,1680)	1:27:A:LYS:HG3	1:128:A:LEU:HD22	7	0.69
(1,1680)	1:27:A:LYS:HG3	1:128:A:LEU:HD23	7	0.69
(1,1667)	1:53:A:ILE:HB	1:126:A:VAL:HG21	7	0.69
(1,1667)	1:53:A:ILE:HB	1:126:A:VAL:HG22	7	0.69
(1,1667)	1:53:A:ILE:HB	1:126:A:VAL:HG23	7	0.69
(1,1543)	1:85:A:HIS:HD2	1:82:A:VAL:HG21	4	0.69
(1,1543)	1:85:A:HIS:HD2	1:82:A:VAL:HG22	4	0.69
(1,1543)	1:85:A:HIS:HD2	1:82:A:VAL:HG23	4	0.69
(1,1514)	1:75:A:VAL:HB	1:69:A:ALA:HB1	1	0.69
(1,1514)	1:75:A:VAL:HB	1:69:A:ALA:HB2	1	0.69
(1,1514)	1:75:A:VAL:HB	1:69:A:ALA:HB3	1	0.69
(1,3264)	1:111:A:PHE:HD2	1:20:A:THR:HG21	5	0.68
(1,3167)	1:129:A:VAL:HG23	1:24:A:GLN:H	8	0.68
(1,3134)	1:23:A:ILE:HG12	1:34:A:ILE:HG22	4	0.68
(1,3043)	1:19:A:ASN:HB3	1:11:A:GLU:HB3	3	0.68
(1,2985)	1:53:A:ILE:HG13	1:111:A:PHE:HD1	9	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2985)	1:53:A:ILE:HG13	1:111:A:PHE:HD2	9	0.68
(1,2884)	1:115:A:PHE:HB3	1:74:A:TYR:HD1	10	0.68
(1,2884)	1:115:A:PHE:HB3	1:74:A:TYR:HD2	10	0.68
(1,2647)	1:112:A:ALA:H	1:126:A:VAL:HG21	1	0.68
(1,2647)	1:112:A:ALA:H	1:126:A:VAL:HG22	1	0.68
(1,2647)	1:112:A:ALA:H	1:126:A:VAL:HG23	1	0.68
(1,2647)	1:112:A:ALA:H	1:126:A:VAL:HG21	5	0.68
(1,2647)	1:112:A:ALA:H	1:126:A:VAL:HG22	5	0.68
(1,2647)	1:112:A:ALA:H	1:126:A:VAL:HG23	5	0.68
(1,2179)	1:51:A:LEU:H	1:95:A:SER:HB2	7	0.68
(1,2114)	1:46:A:SER:H	1:43:A:PRO:HD3	4	0.68
(1,2032)	1:36:A:LEU:HD21	1:37:A:LYS:H	10	0.68
(1,2032)	1:36:A:LEU:HD22	1:37:A:LYS:H	10	0.68
(1,2032)	1:36:A:LEU:HD23	1:37:A:LYS:H	10	0.68
(1,1879)	1:20:A:THR:H	1:19:A:ASN:HB3	1	0.68
(1,1686)	1:128:A:LEU:HD11	1:127:A:THR:HG21	4	0.68
(1,1686)	1:128:A:LEU:HD11	1:127:A:THR:HG22	4	0.68
(1,1686)	1:128:A:LEU:HD11	1:127:A:THR:HG23	4	0.68
(1,1686)	1:128:A:LEU:HD12	1:127:A:THR:HG21	4	0.68
(1,1686)	1:128:A:LEU:HD12	1:127:A:THR:HG22	4	0.68
(1,1686)	1:128:A:LEU:HD12	1:127:A:THR:HG23	4	0.68
(1,1686)	1:128:A:LEU:HD13	1:127:A:THR:HG21	4	0.68
(1,1686)	1:128:A:LEU:HD13	1:127:A:THR:HG22	4	0.68
(1,1686)	1:128:A:LEU:HD13	1:127:A:THR:HG23	4	0.68
(1,1686)	1:128:A:LEU:HD11	1:127:A:THR:HG21	6	0.68
(1,1686)	1:128:A:LEU:HD11	1:127:A:THR:HG22	6	0.68
(1,1686)	1:128:A:LEU:HD11	1:127:A:THR:HG23	6	0.68
(1,1686)	1:128:A:LEU:HD12	1:127:A:THR:HG21	6	0.68
(1,1686)	1:128:A:LEU:HD12	1:127:A:THR:HG22	6	0.68
(1,1686)	1:128:A:LEU:HD12	1:127:A:THR:HG23	6	0.68
(1,1686)	1:128:A:LEU:HD13	1:127:A:THR:HG21	6	0.68
(1,1686)	1:128:A:LEU:HD13	1:127:A:THR:HG22	6	0.68
(1,1686)	1:128:A:LEU:HD13	1:127:A:THR:HG23	6	0.68
(1,1669)	1:25:A:VAL:HG11	1:126:A:VAL:HG21	5	0.68
(1,1669)	1:25:A:VAL:HG11	1:126:A:VAL:HG22	5	0.68
(1,1669)	1:25:A:VAL:HG11	1:126:A:VAL:HG23	5	0.68
(1,1669)	1:25:A:VAL:HG12	1:126:A:VAL:HG21	5	0.68
(1,1669)	1:25:A:VAL:HG12	1:126:A:VAL:HG22	5	0.68
(1,1669)	1:25:A:VAL:HG12	1:126:A:VAL:HG23	5	0.68
(1,1669)	1:25:A:VAL:HG13	1:126:A:VAL:HG21	5	0.68
(1,1669)	1:25:A:VAL:HG13	1:126:A:VAL:HG22	5	0.68
(1,1669)	1:25:A:VAL:HG13	1:126:A:VAL:HG23	5	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1526)	1:52:A:VAL:HG21	1:75:A:VAL:HG21	9	0.68
(1,1526)	1:52:A:VAL:HG21	1:75:A:VAL:HG22	9	0.68
(1,1526)	1:52:A:VAL:HG21	1:75:A:VAL:HG23	9	0.68
(1,1526)	1:52:A:VAL:HG22	1:75:A:VAL:HG21	9	0.68
(1,1526)	1:52:A:VAL:HG22	1:75:A:VAL:HG22	9	0.68
(1,1526)	1:52:A:VAL:HG22	1:75:A:VAL:HG23	9	0.68
(1,1526)	1:52:A:VAL:HG23	1:75:A:VAL:HG21	9	0.68
(1,1526)	1:52:A:VAL:HG23	1:75:A:VAL:HG22	9	0.68
(1,1526)	1:52:A:VAL:HG23	1:75:A:VAL:HG23	9	0.68
(1,1064)	1:107:A:GLY:HA2	1:55:A:LYS:HD3	5	0.68
(1,1039)	1:99:A:LEU:HD21	1:101:A:PRO:HG3	8	0.68
(1,1039)	1:99:A:LEU:HD22	1:101:A:PRO:HG3	8	0.68
(1,1039)	1:99:A:LEU:HD23	1:101:A:PRO:HG3	8	0.68
(1,852)	1:88:A:LEU:HB3	1:73:A:ASP:H	4	0.68
(1,579)	1:56:A:ALA:HA	1:110:A:LYS:HD3	3	0.68
(1,493)	1:50:A:ASN:HA	1:36:A:LEU:HD11	6	0.68
(1,493)	1:50:A:ASN:HA	1:36:A:LEU:HD12	6	0.68
(1,493)	1:50:A:ASN:HA	1:36:A:LEU:HD13	6	0.68
(1,255)	1:98:A:THR:HG21	1:31:A:GLU:HG2	2	0.68
(1,255)	1:98:A:THR:HG21	1:31:A:GLU:HG3	2	0.68
(1,255)	1:98:A:THR:HG22	1:31:A:GLU:HG2	2	0.68
(1,255)	1:98:A:THR:HG22	1:31:A:GLU:HG3	2	0.68
(1,255)	1:98:A:THR:HG23	1:31:A:GLU:HG2	2	0.68
(1,255)	1:98:A:THR:HG23	1:31:A:GLU:HG3	2	0.68
(2,1)	1:6:A:CYS:SG	1:29:A:CYS:SG	7	0.67
(1,3148)	1:104:A:LEU:HD22	1:126:A:VAL:HG22	1	0.67
(1,2712)	1:121:A:LEU:HB3	1:120:A:ALA:H	7	0.67
(1,2478)	1:93:A:GLU:H	1:38:A:HIS:HB2	1	0.67
(1,2469)	1:92:A:GLY:H	1:38:A:HIS:HB2	4	0.67
(1,2170)	1:88:A:LEU:HB3	1:50:A:ASN:HD22	10	0.67
(1,1879)	1:20:A:THR:H	1:19:A:ASN:HB3	5	0.67
(1,1686)	1:128:A:LEU:HD11	1:127:A:THR:HG21	3	0.67
(1,1686)	1:128:A:LEU:HD11	1:127:A:THR:HG22	3	0.67
(1,1686)	1:128:A:LEU:HD11	1:127:A:THR:HG23	3	0.67
(1,1686)	1:128:A:LEU:HD12	1:127:A:THR:HG21	3	0.67
(1,1686)	1:128:A:LEU:HD12	1:127:A:THR:HG22	3	0.67
(1,1686)	1:128:A:LEU:HD12	1:127:A:THR:HG23	3	0.67
(1,1686)	1:128:A:LEU:HD13	1:127:A:THR:HG21	3	0.67
(1,1686)	1:128:A:LEU:HD13	1:127:A:THR:HG22	3	0.67
(1,1686)	1:128:A:LEU:HD13	1:127:A:THR:HG23	3	0.67
(1,1668)	1:23:A:ILE:HG21	1:126:A:VAL:HG21	2	0.67
(1,1668)	1:23:A:ILE:HG21	1:126:A:VAL:HG22	2	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1668)	1:23:A:ILE:HG21	1:126:A:VAL:HG23	2	0.67
(1,1668)	1:23:A:ILE:HG22	1:126:A:VAL:HG21	2	0.67
(1,1668)	1:23:A:ILE:HG22	1:126:A:VAL:HG22	2	0.67
(1,1668)	1:23:A:ILE:HG22	1:126:A:VAL:HG23	2	0.67
(1,1668)	1:23:A:ILE:HG23	1:126:A:VAL:HG21	2	0.67
(1,1668)	1:23:A:ILE:HG23	1:126:A:VAL:HG22	2	0.67
(1,1668)	1:23:A:ILE:HG23	1:126:A:VAL:HG23	2	0.67
(1,1525)	1:114:A:THR:HG21	1:75:A:VAL:HG21	3	0.67
(1,1525)	1:114:A:THR:HG21	1:75:A:VAL:HG22	3	0.67
(1,1525)	1:114:A:THR:HG21	1:75:A:VAL:HG23	3	0.67
(1,1525)	1:114:A:THR:HG22	1:75:A:VAL:HG21	3	0.67
(1,1525)	1:114:A:THR:HG22	1:75:A:VAL:HG22	3	0.67
(1,1525)	1:114:A:THR:HG22	1:75:A:VAL:HG23	3	0.67
(1,1525)	1:114:A:THR:HG23	1:75:A:VAL:HG21	3	0.67
(1,1525)	1:114:A:THR:HG23	1:75:A:VAL:HG22	3	0.67
(1,1525)	1:114:A:THR:HG23	1:75:A:VAL:HG23	3	0.67
(1,1497)	1:54:A:ALA:HB1	1:52:A:VAL:HG11	4	0.67
(1,1497)	1:54:A:ALA:HB1	1:52:A:VAL:HG12	4	0.67
(1,1497)	1:54:A:ALA:HB1	1:52:A:VAL:HG13	4	0.67
(1,1497)	1:54:A:ALA:HB2	1:52:A:VAL:HG11	4	0.67
(1,1497)	1:54:A:ALA:HB2	1:52:A:VAL:HG12	4	0.67
(1,1497)	1:54:A:ALA:HB2	1:52:A:VAL:HG13	4	0.67
(1,1497)	1:54:A:ALA:HB3	1:52:A:VAL:HG11	4	0.67
(1,1497)	1:54:A:ALA:HB3	1:52:A:VAL:HG12	4	0.67
(1,1497)	1:54:A:ALA:HB3	1:52:A:VAL:HG13	4	0.67
(1,1016)	1:99:A:LEU:HD21	1:101:A:PRO:HD3	9	0.67
(1,1016)	1:99:A:LEU:HD22	1:101:A:PRO:HD3	9	0.67
(1,1016)	1:99:A:LEU:HD23	1:101:A:PRO:HD3	9	0.67
(1,889)	1:92:A:GLY:HA2	1:93:A:GLU:HG3	9	0.67
(1,822)	1:85:A:HIS:HB3	1:52:A:VAL:HG21	7	0.67
(1,822)	1:85:A:HIS:HB3	1:52:A:VAL:HG22	7	0.67
(1,822)	1:85:A:HIS:HB3	1:52:A:VAL:HG23	7	0.67
(1,564)	1:55:A:LYS:HB2	1:58:A:ASP:H	8	0.67
(1,46)	1:12:A:SER:HA	1:36:A:LEU:HD21	4	0.67
(1,46)	1:12:A:SER:HA	1:36:A:LEU:HD22	4	0.67
(1,46)	1:12:A:SER:HA	1:36:A:LEU:HD23	4	0.67
(1,3177)	1:35:A:THR:HG23	1:35:A:THR:H	1	0.66
(1,2491)	1:37:A:LYS:HD2	1:95:A:SER:H	4	0.66
(1,2491)	1:37:A:LYS:HD3	1:95:A:SER:H	4	0.66
(1,2478)	1:93:A:GLU:H	1:38:A:HIS:HB2	8	0.66
(1,1797)	1:15:A:ASN:HB3	1:13:A:ASN:HD21	3	0.66
(1,1705)	1:99:A:LEU:HD11	1:31:A:GLU:HB2	6	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1705)	1:99:A:LEU:HD12	1:31:A:GLU:HB2	6	0.66
(1,1705)	1:99:A:LEU:HD13	1:31:A:GLU:HB2	6	0.66
(1,1514)	1:75:A:VAL:HB	1:69:A:ALA:HB1	7	0.66
(1,1514)	1:75:A:VAL:HB	1:69:A:ALA:HB2	7	0.66
(1,1514)	1:75:A:VAL:HB	1:69:A:ALA:HB3	7	0.66
(1,1428)	1:18:A:PHE:HD1	1:36:A:LEU:HD21	6	0.66
(1,1428)	1:18:A:PHE:HD1	1:36:A:LEU:HD22	6	0.66
(1,1428)	1:18:A:PHE:HD1	1:36:A:LEU:HD23	6	0.66
(1,1428)	1:18:A:PHE:HD2	1:36:A:LEU:HD21	6	0.66
(1,1428)	1:18:A:PHE:HD2	1:36:A:LEU:HD22	6	0.66
(1,1428)	1:18:A:PHE:HD2	1:36:A:LEU:HD23	6	0.66
(1,1388)	1:101:A:PRO:HA	1:25:A:VAL:HG21	3	0.66
(1,1388)	1:101:A:PRO:HA	1:25:A:VAL:HG22	3	0.66
(1,1388)	1:101:A:PRO:HA	1:25:A:VAL:HG23	3	0.66
(1,1381)	1:104:A:LEU:HD11	1:25:A:VAL:HG21	5	0.66
(1,1381)	1:104:A:LEU:HD11	1:25:A:VAL:HG22	5	0.66
(1,1381)	1:104:A:LEU:HD11	1:25:A:VAL:HG23	5	0.66
(1,1381)	1:104:A:LEU:HD12	1:25:A:VAL:HG21	5	0.66
(1,1381)	1:104:A:LEU:HD12	1:25:A:VAL:HG22	5	0.66
(1,1381)	1:104:A:LEU:HD12	1:25:A:VAL:HG23	5	0.66
(1,1381)	1:104:A:LEU:HD13	1:25:A:VAL:HG21	5	0.66
(1,1381)	1:104:A:LEU:HD13	1:25:A:VAL:HG22	5	0.66
(1,1381)	1:104:A:LEU:HD13	1:25:A:VAL:HG23	5	0.66
(1,1074)	1:107:A:GLY:HA2	1:109:A:TYR:HE1	1	0.66
(1,1074)	1:107:A:GLY:HA2	1:109:A:TYR:HE2	1	0.66
(1,1016)	1:99:A:LEU:HD21	1:101:A:PRO:HD3	2	0.66
(1,1016)	1:99:A:LEU:HD22	1:101:A:PRO:HD3	2	0.66
(1,1016)	1:99:A:LEU:HD23	1:101:A:PRO:HD3	2	0.66
(1,984)	1:98:A:THR:HB	1:31:A:GLU:HB2	10	0.66
(1,882)	1:91:A:GLY:HA3	1:38:A:HIS:HB2	3	0.66
(1,766)	1:69:A:ALA:HA	1:77:A:PRO:HD2	3	0.66
(1,639)	1:67:A:VAL:HG11	1:64:A:LYS:HA	3	0.66
(1,639)	1:67:A:VAL:HG12	1:64:A:LYS:HA	3	0.66
(1,639)	1:67:A:VAL:HG13	1:64:A:LYS:HA	3	0.66
(1,426)	1:43:A:PRO:HG3	1:46:A:SER:H	9	0.66
(1,3148)	1:53:A:ILE:HD13	1:104:A:LEU:HD22	4	0.65
(1,3134)	1:23:A:ILE:HG12	1:34:A:ILE:HG23	1	0.65
(1,3014)	1:115:A:PHE:HE1	1:48:A:GLY:HA2	6	0.65
(1,3014)	1:115:A:PHE:HE2	1:48:A:GLY:HA2	6	0.65
(1,2629)	1:125:A:LYS:HD2	1:111:A:PHE:H	1	0.65
(1,2629)	1:125:A:LYS:HD3	1:111:A:PHE:H	1	0.65
(1,2611)	1:110:A:LYS:HG2	1:109:A:TYR:H	10	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2538)	1:100:A:ASP:H	1:83:A:VAL:HB	9	0.65
(1,2516)	1:97:A:LEU:H	1:36:A:LEU:HD11	3	0.65
(1,2516)	1:97:A:LEU:H	1:36:A:LEU:HD12	3	0.65
(1,2516)	1:97:A:LEU:H	1:36:A:LEU:HD13	3	0.65
(1,2326)	1:88:A:LEU:HD11	1:73:A:ASP:H	3	0.65
(1,2326)	1:88:A:LEU:HD12	1:73:A:ASP:H	3	0.65
(1,2326)	1:88:A:LEU:HD13	1:73:A:ASP:H	3	0.65
(1,2179)	1:51:A:LEU:H	1:95:A:SER:HB2	6	0.65
(1,2142)	1:88:A:LEU:HD21	1:49:A:HIS:H	7	0.65
(1,2142)	1:88:A:LEU:HD22	1:49:A:HIS:H	7	0.65
(1,2142)	1:88:A:LEU:HD23	1:49:A:HIS:H	7	0.65
(1,2032)	1:36:A:LEU:HD21	1:37:A:LYS:H	5	0.65
(1,2032)	1:36:A:LEU:HD22	1:37:A:LYS:H	5	0.65
(1,2032)	1:36:A:LEU:HD23	1:37:A:LYS:H	5	0.65
(1,2032)	1:36:A:LEU:HD21	1:37:A:LYS:H	8	0.65
(1,2032)	1:36:A:LEU:HD22	1:37:A:LYS:H	8	0.65
(1,2032)	1:36:A:LEU:HD23	1:37:A:LYS:H	8	0.65
(1,1539)	1:82:A:VAL:H	1:82:A:VAL:HG11	5	0.65
(1,1539)	1:82:A:VAL:H	1:82:A:VAL:HG12	5	0.65
(1,1539)	1:82:A:VAL:H	1:82:A:VAL:HG13	5	0.65
(1,1428)	1:18:A:PHE:HD1	1:36:A:LEU:HD21	10	0.65
(1,1428)	1:18:A:PHE:HD1	1:36:A:LEU:HD22	10	0.65
(1,1428)	1:18:A:PHE:HD1	1:36:A:LEU:HD23	10	0.65
(1,1428)	1:18:A:PHE:HD2	1:36:A:LEU:HD21	10	0.65
(1,1428)	1:18:A:PHE:HD2	1:36:A:LEU:HD22	10	0.65
(1,1428)	1:18:A:PHE:HD2	1:36:A:LEU:HD23	10	0.65
(1,1079)	1:125:A:LYS:HE2	1:108:A:ASP:HA	3	0.65
(1,1079)	1:125:A:LYS:HE3	1:108:A:ASP:HA	3	0.65
(1,1017)	1:101:A:PRO:HD3	1:25:A:VAL:HG21	3	0.65
(1,1017)	1:101:A:PRO:HD3	1:25:A:VAL:HG22	3	0.65
(1,1017)	1:101:A:PRO:HD3	1:25:A:VAL:HG23	3	0.65
(1,1017)	1:101:A:PRO:HD3	1:25:A:VAL:HG21	6	0.65
(1,1017)	1:101:A:PRO:HD3	1:25:A:VAL:HG22	6	0.65
(1,1017)	1:101:A:PRO:HD3	1:25:A:VAL:HG23	6	0.65
(1,739)	1:77:A:PRO:HA	1:75:A:VAL:HB	6	0.65
(1,493)	1:50:A:ASN:HA	1:36:A:LEU:HD11	2	0.65
(1,493)	1:50:A:ASN:HA	1:36:A:LEU:HD12	2	0.65
(1,493)	1:50:A:ASN:HA	1:36:A:LEU:HD13	2	0.65
(1,464)	1:88:A:LEU:HD11	1:48:A:GLY:HA2	9	0.65
(1,464)	1:88:A:LEU:HD12	1:48:A:GLY:HA2	9	0.65
(1,464)	1:88:A:LEU:HD13	1:48:A:GLY:HA2	9	0.65
(1,3168)	1:24:A:GLN:H	1:34:A:ILE:HG12	5	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2876)	1:38:A:HIS:HE1	1:13:A:ASN:HB2	2	0.64
(1,2659)	1:124:A:GLY:H	1:113:A:CYS:H	1	0.64
(1,2647)	1:112:A:ALA:H	1:126:A:VAL:HG21	9	0.64
(1,2647)	1:112:A:ALA:H	1:126:A:VAL:HG22	9	0.64
(1,2647)	1:112:A:ALA:H	1:126:A:VAL:HG23	9	0.64
(1,2611)	1:110:A:LYS:HG2	1:109:A:TYR:H	3	0.64
(1,2591)	1:106:A:ASP:H	1:128:A:LEU:HD11	7	0.64
(1,2591)	1:106:A:ASP:H	1:128:A:LEU:HD12	7	0.64
(1,2591)	1:106:A:ASP:H	1:128:A:LEU:HD13	7	0.64
(1,2491)	1:37:A:LYS:HD2	1:95:A:SER:H	6	0.64
(1,2491)	1:37:A:LYS:HD3	1:95:A:SER:H	6	0.64
(1,2360)	1:76:A:LYS:HE2	1:79:A:ASP:H	8	0.64
(1,2360)	1:76:A:LYS:HE3	1:79:A:ASP:H	8	0.64
(1,2190)	1:85:A:HIS:HB3	1:52:A:VAL:H	5	0.64
(1,1980)	1:99:A:LEU:HB3	1:32:A:PHE:H	2	0.64
(1,1702)	1:83:A:VAL:HG21	1:99:A:LEU:HD11	5	0.64
(1,1702)	1:83:A:VAL:HG21	1:99:A:LEU:HD12	5	0.64
(1,1702)	1:83:A:VAL:HG21	1:99:A:LEU:HD13	5	0.64
(1,1702)	1:83:A:VAL:HG22	1:99:A:LEU:HD11	5	0.64
(1,1702)	1:83:A:VAL:HG22	1:99:A:LEU:HD12	5	0.64
(1,1702)	1:83:A:VAL:HG22	1:99:A:LEU:HD13	5	0.64
(1,1702)	1:83:A:VAL:HG23	1:99:A:LEU:HD11	5	0.64
(1,1702)	1:83:A:VAL:HG23	1:99:A:LEU:HD12	5	0.64
(1,1702)	1:83:A:VAL:HG23	1:99:A:LEU:HD13	5	0.64
(1,1613)	1:101:A:PRO:HA	1:99:A:LEU:HD21	3	0.64
(1,1613)	1:101:A:PRO:HA	1:99:A:LEU:HD22	3	0.64
(1,1613)	1:101:A:PRO:HA	1:99:A:LEU:HD23	3	0.64
(1,1543)	1:85:A:HIS:HD2	1:82:A:VAL:HG21	2	0.64
(1,1543)	1:85:A:HIS:HD2	1:82:A:VAL:HG22	2	0.64
(1,1543)	1:85:A:HIS:HD2	1:82:A:VAL:HG23	2	0.64
(1,1539)	1:82:A:VAL:H	1:82:A:VAL:HG11	7	0.64
(1,1539)	1:82:A:VAL:H	1:82:A:VAL:HG12	7	0.64
(1,1539)	1:82:A:VAL:H	1:82:A:VAL:HG13	7	0.64
(1,1093)	1:56:A:ALA:HB1	1:108:A:ASP:HB2	3	0.64
(1,1093)	1:56:A:ALA:HB2	1:108:A:ASP:HB2	3	0.64
(1,1093)	1:56:A:ALA:HB3	1:108:A:ASP:HB2	3	0.64
(1,795)	1:82:A:VAL:HB	1:75:A:VAL:HG11	7	0.64
(1,795)	1:82:A:VAL:HB	1:75:A:VAL:HG12	7	0.64
(1,795)	1:82:A:VAL:HB	1:75:A:VAL:HG13	7	0.64
(1,580)	1:130:A:ASP:HA	1:128:A:LEU:HD21	4	0.64
(1,580)	1:130:A:ASP:HA	1:128:A:LEU:HD22	4	0.64
(1,580)	1:130:A:ASP:HA	1:128:A:LEU:HD23	4	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,494)	1:50:A:ASN:HB3	1:88:A:LEU:HD21	7	0.64
(1,494)	1:50:A:ASN:HB3	1:88:A:LEU:HD22	7	0.64
(1,494)	1:50:A:ASN:HB3	1:88:A:LEU:HD23	7	0.64
(1,3178)	1:37:A:LYS:HG2	1:36:A:LEU:H	8	0.63
(1,3178)	1:37:A:LYS:HG3	1:36:A:LEU:H	8	0.63
(1,2623)	1:125:A:LYS:HD2	1:110:A:LYS:H	9	0.63
(1,2623)	1:125:A:LYS:HD3	1:110:A:LYS:H	9	0.63
(1,2304)	1:67:A:VAL:HG11	1:67:A:VAL:H	1	0.63
(1,2304)	1:67:A:VAL:HG12	1:67:A:VAL:H	1	0.63
(1,2304)	1:67:A:VAL:HG13	1:67:A:VAL:H	1	0.63
(1,2304)	1:67:A:VAL:HG11	1:67:A:VAL:H	4	0.63
(1,2304)	1:67:A:VAL:HG12	1:67:A:VAL:H	4	0.63
(1,2304)	1:67:A:VAL:HG13	1:67:A:VAL:H	4	0.63
(1,2304)	1:67:A:VAL:HG11	1:67:A:VAL:H	8	0.63
(1,2304)	1:67:A:VAL:HG12	1:67:A:VAL:H	8	0.63
(1,2304)	1:67:A:VAL:HG13	1:67:A:VAL:H	8	0.63
(1,2173)	1:51:A:LEU:H	1:36:A:LEU:HD11	5	0.63
(1,2173)	1:51:A:LEU:H	1:36:A:LEU:HD12	5	0.63
(1,2173)	1:51:A:LEU:H	1:36:A:LEU:HD13	5	0.63
(1,1801)	1:13:A:ASN:HD22	1:17:A:GLN:HB3	4	0.63
(1,1715)	1:59:A:MET:HE1	1:114:A:THR:HG1	8	0.63
(1,1715)	1:59:A:MET:HE2	1:114:A:THR:HG1	8	0.63
(1,1715)	1:59:A:MET:HE3	1:114:A:THR:HG1	8	0.63
(1,1702)	1:83:A:VAL:HG21	1:99:A:LEU:HD11	8	0.63
(1,1702)	1:83:A:VAL:HG21	1:99:A:LEU:HD12	8	0.63
(1,1702)	1:83:A:VAL:HG21	1:99:A:LEU:HD13	8	0.63
(1,1702)	1:83:A:VAL:HG22	1:99:A:LEU:HD11	8	0.63
(1,1702)	1:83:A:VAL:HG22	1:99:A:LEU:HD12	8	0.63
(1,1702)	1:83:A:VAL:HG22	1:99:A:LEU:HD13	8	0.63
(1,1702)	1:83:A:VAL:HG23	1:99:A:LEU:HD11	8	0.63
(1,1702)	1:83:A:VAL:HG23	1:99:A:LEU:HD12	8	0.63
(1,1702)	1:83:A:VAL:HG23	1:99:A:LEU:HD13	8	0.63
(1,1686)	1:128:A:LEU:HD11	1:127:A:THR:HG21	9	0.63
(1,1686)	1:128:A:LEU:HD11	1:127:A:THR:HG22	9	0.63
(1,1686)	1:128:A:LEU:HD11	1:127:A:THR:HG23	9	0.63
(1,1686)	1:128:A:LEU:HD12	1:127:A:THR:HG21	9	0.63
(1,1686)	1:128:A:LEU:HD12	1:127:A:THR:HG22	9	0.63
(1,1686)	1:128:A:LEU:HD12	1:127:A:THR:HG23	9	0.63
(1,1686)	1:128:A:LEU:HD13	1:127:A:THR:HG21	9	0.63
(1,1686)	1:128:A:LEU:HD13	1:127:A:THR:HG22	9	0.63
(1,1686)	1:128:A:LEU:HD13	1:127:A:THR:HG23	9	0.63
(1,1609)	1:99:A:LEU:HD21	1:32:A:PHE:H	10	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1609)	1:99:A:LEU:HD22	1:32:A:PHE:H	10	0.63
(1,1609)	1:99:A:LEU:HD23	1:32:A:PHE:H	10	0.63
(1,1509)	1:62:A:VAL:HG21	1:114:A:THR:HG21	7	0.63
(1,1509)	1:62:A:VAL:HG21	1:114:A:THR:HG22	7	0.63
(1,1509)	1:62:A:VAL:HG21	1:114:A:THR:HG23	7	0.63
(1,1509)	1:62:A:VAL:HG22	1:114:A:THR:HG21	7	0.63
(1,1509)	1:62:A:VAL:HG22	1:114:A:THR:HG22	7	0.63
(1,1509)	1:62:A:VAL:HG22	1:114:A:THR:HG23	7	0.63
(1,1509)	1:62:A:VAL:HG23	1:114:A:THR:HG21	7	0.63
(1,1509)	1:62:A:VAL:HG23	1:114:A:THR:HG22	7	0.63
(1,1509)	1:62:A:VAL:HG23	1:114:A:THR:HG23	7	0.63
(1,1253)	1:124:A:GLY:HA2	1:111:A:PHE:HZ	3	0.63
(1,1063)	1:107:A:GLY:HA2	1:55:A:LYS:HD2	10	0.63
(1,852)	1:88:A:LEU:HB3	1:73:A:ASP:H	5	0.63
(1,741)	1:77:A:PRO:HA	1:75:A:VAL:HG11	8	0.63
(1,741)	1:77:A:PRO:HA	1:75:A:VAL:HG12	8	0.63
(1,741)	1:77:A:PRO:HA	1:75:A:VAL:HG13	8	0.63
(1,646)	1:76:A:LYS:HB3	1:66:A:GLY:HA3	2	0.63
(1,564)	1:55:A:LYS:HB2	1:58:A:ASP:H	1	0.63
(1,3198)	1:64:A:LYS:HD3	1:61:A:GLY:H	7	0.62
(1,3166)	1:126:A:VAL:HG13	1:23:A:ILE:H	1	0.62
(1,2745)	1:123:A:ASN:H	1:21:A:LYS:HG2	2	0.62
(1,2745)	1:123:A:ASN:H	1:21:A:LYS:HG3	2	0.62
(1,2676)	1:75:A:VAL:HG21	1:114:A:THR:H	3	0.62
(1,2676)	1:75:A:VAL:HG22	1:114:A:THR:H	3	0.62
(1,2676)	1:75:A:VAL:HG23	1:114:A:THR:H	3	0.62
(1,2676)	1:75:A:VAL:HG21	1:114:A:THR:H	9	0.62
(1,2676)	1:75:A:VAL:HG22	1:114:A:THR:H	9	0.62
(1,2676)	1:75:A:VAL:HG23	1:114:A:THR:H	9	0.62
(1,2659)	1:124:A:GLY:H	1:113:A:CYS:H	2	0.62
(1,2659)	1:124:A:GLY:H	1:113:A:CYS:H	4	0.62
(1,2623)	1:125:A:LYS:HD2	1:110:A:LYS:H	1	0.62
(1,2623)	1:125:A:LYS:HD3	1:110:A:LYS:H	1	0.62
(1,2304)	1:67:A:VAL:HG11	1:67:A:VAL:H	2	0.62
(1,2304)	1:67:A:VAL:HG12	1:67:A:VAL:H	2	0.62
(1,2304)	1:67:A:VAL:HG13	1:67:A:VAL:H	2	0.62
(1,2304)	1:67:A:VAL:HG11	1:67:A:VAL:H	3	0.62
(1,2304)	1:67:A:VAL:HG12	1:67:A:VAL:H	3	0.62
(1,2304)	1:67:A:VAL:HG13	1:67:A:VAL:H	3	0.62
(1,2304)	1:67:A:VAL:HG11	1:67:A:VAL:H	6	0.62
(1,2304)	1:67:A:VAL:HG12	1:67:A:VAL:H	6	0.62
(1,2304)	1:67:A:VAL:HG13	1:67:A:VAL:H	6	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2304)	1:67:A:VAL:HG11	1:67:A:VAL:H	7	0.62
(1,2304)	1:67:A:VAL:HG12	1:67:A:VAL:H	7	0.62
(1,2304)	1:67:A:VAL:HG13	1:67:A:VAL:H	7	0.62
(1,2304)	1:67:A:VAL:HG11	1:67:A:VAL:H	9	0.62
(1,2304)	1:67:A:VAL:HG12	1:67:A:VAL:H	9	0.62
(1,2304)	1:67:A:VAL:HG13	1:67:A:VAL:H	9	0.62
(1,2304)	1:67:A:VAL:HG11	1:67:A:VAL:H	10	0.62
(1,2304)	1:67:A:VAL:HG12	1:67:A:VAL:H	10	0.62
(1,2304)	1:67:A:VAL:HG13	1:67:A:VAL:H	10	0.62
(1,2200)	1:53:A:ILE:H	1:52:A:VAL:HG21	1	0.62
(1,2200)	1:53:A:ILE:H	1:52:A:VAL:HG22	1	0.62
(1,2200)	1:53:A:ILE:H	1:52:A:VAL:HG23	1	0.62
(1,2061)	1:38:A:HIS:HA	1:40:A:GLY:H	9	0.62
(1,1879)	1:20:A:THR:H	1:19:A:ASN:HB3	9	0.62
(1,1865)	1:19:A:ASN:HD22	1:10:A:VAL:HG11	10	0.62
(1,1865)	1:19:A:ASN:HD22	1:10:A:VAL:HG12	10	0.62
(1,1865)	1:19:A:ASN:HD22	1:10:A:VAL:HG13	10	0.62
(1,1715)	1:59:A:MET:HE1	1:114:A:THR:HG1	10	0.62
(1,1715)	1:59:A:MET:HE2	1:114:A:THR:HG1	10	0.62
(1,1715)	1:59:A:MET:HE3	1:114:A:THR:HG1	10	0.62
(1,1705)	1:99:A:LEU:HD11	1:31:A:GLU:HB2	5	0.62
(1,1705)	1:99:A:LEU:HD12	1:31:A:GLU:HB2	5	0.62
(1,1705)	1:99:A:LEU:HD13	1:31:A:GLU:HB2	5	0.62
(1,1686)	1:128:A:LEU:HD11	1:127:A:THR:HG21	1	0.62
(1,1686)	1:128:A:LEU:HD11	1:127:A:THR:HG22	1	0.62
(1,1686)	1:128:A:LEU:HD11	1:127:A:THR:HG23	1	0.62
(1,1686)	1:128:A:LEU:HD12	1:127:A:THR:HG21	1	0.62
(1,1686)	1:128:A:LEU:HD12	1:127:A:THR:HG22	1	0.62
(1,1686)	1:128:A:LEU:HD12	1:127:A:THR:HG23	1	0.62
(1,1686)	1:128:A:LEU:HD13	1:127:A:THR:HG21	1	0.62
(1,1686)	1:128:A:LEU:HD13	1:127:A:THR:HG22	1	0.62
(1,1686)	1:128:A:LEU:HD13	1:127:A:THR:HG23	1	0.62
(1,1653)	1:121:A:LEU:HA	1:121:A:LEU:HD21	5	0.62
(1,1653)	1:121:A:LEU:HA	1:121:A:LEU:HD22	5	0.62
(1,1653)	1:121:A:LEU:HA	1:121:A:LEU:HD23	5	0.62
(1,1627)	1:83:A:VAL:HG21	1:104:A:LEU:HD11	10	0.62
(1,1627)	1:83:A:VAL:HG21	1:104:A:LEU:HD12	10	0.62
(1,1627)	1:83:A:VAL:HG21	1:104:A:LEU:HD13	10	0.62
(1,1627)	1:83:A:VAL:HG22	1:104:A:LEU:HD11	10	0.62
(1,1627)	1:83:A:VAL:HG22	1:104:A:LEU:HD12	10	0.62
(1,1627)	1:83:A:VAL:HG22	1:104:A:LEU:HD13	10	0.62
(1,1627)	1:83:A:VAL:HG23	1:104:A:LEU:HD11	10	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1627)	1:83:A:VAL:HG23	1:104:A:LEU:HD12	10	0.62
(1,1627)	1:83:A:VAL:HG23	1:104:A:LEU:HD13	10	0.62
(1,1614)	1:32:A:PHE:HB2	1:99:A:LEU:HD21	9	0.62
(1,1614)	1:32:A:PHE:HB2	1:99:A:LEU:HD22	9	0.62
(1,1614)	1:32:A:PHE:HB2	1:99:A:LEU:HD23	9	0.62
(1,1497)	1:54:A:ALA:HB1	1:52:A:VAL:HG11	7	0.62
(1,1497)	1:54:A:ALA:HB1	1:52:A:VAL:HG12	7	0.62
(1,1497)	1:54:A:ALA:HB1	1:52:A:VAL:HG13	7	0.62
(1,1497)	1:54:A:ALA:HB2	1:52:A:VAL:HG11	7	0.62
(1,1497)	1:54:A:ALA:HB2	1:52:A:VAL:HG12	7	0.62
(1,1497)	1:54:A:ALA:HB2	1:52:A:VAL:HG13	7	0.62
(1,1497)	1:54:A:ALA:HB3	1:52:A:VAL:HG11	7	0.62
(1,1497)	1:54:A:ALA:HB3	1:52:A:VAL:HG12	7	0.62
(1,1497)	1:54:A:ALA:HB3	1:52:A:VAL:HG13	7	0.62
(1,1461)	1:126:A:VAL:HG11	1:51:A:LEU:HD21	5	0.62
(1,1461)	1:126:A:VAL:HG11	1:51:A:LEU:HD22	5	0.62
(1,1461)	1:126:A:VAL:HG11	1:51:A:LEU:HD23	5	0.62
(1,1461)	1:126:A:VAL:HG12	1:51:A:LEU:HD21	5	0.62
(1,1461)	1:126:A:VAL:HG12	1:51:A:LEU:HD22	5	0.62
(1,1461)	1:126:A:VAL:HG12	1:51:A:LEU:HD23	5	0.62
(1,1461)	1:126:A:VAL:HG13	1:51:A:LEU:HD21	5	0.62
(1,1461)	1:126:A:VAL:HG13	1:51:A:LEU:HD22	5	0.62
(1,1461)	1:126:A:VAL:HG13	1:51:A:LEU:HD23	5	0.62
(1,1392)	1:127:A:THR:H	1:25:A:VAL:HG11	10	0.62
(1,1392)	1:127:A:THR:H	1:25:A:VAL:HG12	10	0.62
(1,1392)	1:127:A:THR:H	1:25:A:VAL:HG13	10	0.62
(1,1031)	1:101:A:PRO:HG2	1:29:A:CYS:HB2	7	0.62
(1,1031)	1:101:A:PRO:HG2	1:29:A:CYS:HB3	7	0.62
(1,1017)	1:101:A:PRO:HD3	1:25:A:VAL:HG21	4	0.62
(1,1017)	1:101:A:PRO:HD3	1:25:A:VAL:HG22	4	0.62
(1,1017)	1:101:A:PRO:HD3	1:25:A:VAL:HG23	4	0.62
(1,1016)	1:99:A:LEU:HD21	1:101:A:PRO:HD3	3	0.62
(1,1016)	1:99:A:LEU:HD22	1:101:A:PRO:HD3	3	0.62
(1,1016)	1:99:A:LEU:HD23	1:101:A:PRO:HD3	3	0.62
(1,952)	1:96:A:SER:HA	1:36:A:LEU:HB3	2	0.62
(1,882)	1:91:A:GLY:HA3	1:38:A:HIS:HB2	1	0.62
(1,822)	1:85:A:HIS:HB3	1:52:A:VAL:HG21	8	0.62
(1,822)	1:85:A:HIS:HB3	1:52:A:VAL:HG22	8	0.62
(1,822)	1:85:A:HIS:HB3	1:52:A:VAL:HG23	8	0.62
(1,426)	1:43:A:PRO:HG3	1:46:A:SER:H	5	0.62
(2,1)	1:6:A:CYS:SG	1:29:A:CYS:SG	5	0.61
(1,3220)	1:94:A:GLU:H	1:93:A:GLU:HB2	5	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3134)	1:23:A:ILE:HG12	1:34:A:ILE:HG23	8	0.61
(1,2676)	1:75:A:VAL:HG21	1:114:A:THR:H	1	0.61
(1,2676)	1:75:A:VAL:HG22	1:114:A:THR:H	1	0.61
(1,2676)	1:75:A:VAL:HG23	1:114:A:THR:H	1	0.61
(1,2508)	1:85:A:HIS:H	1:97:A:LEU:H	3	0.61
(1,2200)	1:53:A:ILE:H	1:52:A:VAL:HG21	3	0.61
(1,2200)	1:53:A:ILE:H	1:52:A:VAL:HG22	3	0.61
(1,2200)	1:53:A:ILE:H	1:52:A:VAL:HG23	3	0.61
(1,2200)	1:53:A:ILE:H	1:52:A:VAL:HG21	10	0.61
(1,2200)	1:53:A:ILE:H	1:52:A:VAL:HG22	10	0.61
(1,2200)	1:53:A:ILE:H	1:52:A:VAL:HG23	10	0.61
(1,1712)	1:59:A:MET:HE1	1:123:A:ASN:HB2	10	0.61
(1,1712)	1:59:A:MET:HE2	1:123:A:ASN:HB2	10	0.61
(1,1712)	1:59:A:MET:HE3	1:123:A:ASN:HB2	10	0.61
(1,1667)	1:53:A:ILE:HB	1:126:A:VAL:HG21	3	0.61
(1,1667)	1:53:A:ILE:HB	1:126:A:VAL:HG22	3	0.61
(1,1667)	1:53:A:ILE:HB	1:126:A:VAL:HG23	3	0.61
(1,1659)	1:127:A:THR:H	1:126:A:VAL:HG21	4	0.61
(1,1659)	1:127:A:THR:H	1:126:A:VAL:HG22	4	0.61
(1,1659)	1:127:A:THR:H	1:126:A:VAL:HG23	4	0.61
(1,1525)	1:114:A:THR:HG21	1:75:A:VAL:HG21	8	0.61
(1,1525)	1:114:A:THR:HG21	1:75:A:VAL:HG22	8	0.61
(1,1525)	1:114:A:THR:HG21	1:75:A:VAL:HG23	8	0.61
(1,1525)	1:114:A:THR:HG22	1:75:A:VAL:HG21	8	0.61
(1,1525)	1:114:A:THR:HG22	1:75:A:VAL:HG22	8	0.61
(1,1525)	1:114:A:THR:HG22	1:75:A:VAL:HG23	8	0.61
(1,1525)	1:114:A:THR:HG23	1:75:A:VAL:HG21	8	0.61
(1,1525)	1:114:A:THR:HG23	1:75:A:VAL:HG22	8	0.61
(1,1525)	1:114:A:THR:HG23	1:75:A:VAL:HG23	8	0.61
(1,1467)	1:85:A:HIS:HB2	1:52:A:VAL:HG11	5	0.61
(1,1467)	1:85:A:HIS:HB2	1:52:A:VAL:HG12	5	0.61
(1,1467)	1:85:A:HIS:HB2	1:52:A:VAL:HG13	5	0.61
(1,1253)	1:124:A:GLY:HA2	1:111:A:PHE:HZ	2	0.61
(1,1156)	1:52:A:VAL:HG21	1:113:A:CYS:HA	5	0.61
(1,1156)	1:52:A:VAL:HG22	1:113:A:CYS:HA	5	0.61
(1,1156)	1:52:A:VAL:HG23	1:113:A:CYS:HA	5	0.61
(1,1017)	1:101:A:PRO:HD3	1:25:A:VAL:HG21	9	0.61
(1,1017)	1:101:A:PRO:HD3	1:25:A:VAL:HG22	9	0.61
(1,1017)	1:101:A:PRO:HD3	1:25:A:VAL:HG23	9	0.61
(1,994)	1:83:A:VAL:HG21	1:99:A:LEU:HB3	3	0.61
(1,994)	1:83:A:VAL:HG22	1:99:A:LEU:HB3	3	0.61
(1,994)	1:83:A:VAL:HG23	1:99:A:LEU:HB3	3	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,769)	1:77:A:PRO:HG2	1:72:A:THR:HG21	2	0.61
(1,769)	1:77:A:PRO:HG2	1:72:A:THR:HG22	2	0.61
(1,769)	1:77:A:PRO:HG2	1:72:A:THR:HG23	2	0.61
(1,578)	1:56:A:ALA:HA	1:110:A:LYS:HD2	1	0.61
(1,258)	1:6:A:CYS:HB2	1:32:A:PHE:HA	2	0.61
(1,192)	1:27:A:LYS:HG2	1:26:A:SER:HA	4	0.61
(1,192)	1:27:A:LYS:HG3	1:26:A:SER:HA	4	0.61
(1,156)	1:126:A:VAL:HG11	1:23:A:ILE:HB	3	0.61
(1,156)	1:126:A:VAL:HG12	1:23:A:ILE:HB	3	0.61
(1,156)	1:126:A:VAL:HG13	1:23:A:ILE:HB	3	0.61
(1,3264)	1:111:A:PHE:HD1	1:20:A:THR:HG23	3	0.6
(1,3177)	1:35:A:THR:HG21	1:35:A:THR:H	2	0.6
(1,2342)	1:75:A:VAL:HB	1:74:A:TYR:H	5	0.6
(1,2179)	1:51:A:LEU:H	1:95:A:SER:HB2	9	0.6
(1,2105)	1:43:A:PRO:HB3	1:45:A:ALA:H	8	0.6
(1,2058)	1:40:A:GLY:H	1:39:A:THR:H	9	0.6
(1,2032)	1:36:A:LEU:HD21	1:37:A:LYS:H	6	0.6
(1,2032)	1:36:A:LEU:HD22	1:37:A:LYS:H	6	0.6
(1,2032)	1:36:A:LEU:HD23	1:37:A:LYS:H	6	0.6
(1,1683)	1:104:A:LEU:HD11	1:128:A:LEU:HD21	9	0.6
(1,1683)	1:104:A:LEU:HD11	1:128:A:LEU:HD22	9	0.6
(1,1683)	1:104:A:LEU:HD11	1:128:A:LEU:HD23	9	0.6
(1,1683)	1:104:A:LEU:HD12	1:128:A:LEU:HD21	9	0.6
(1,1683)	1:104:A:LEU:HD12	1:128:A:LEU:HD22	9	0.6
(1,1683)	1:104:A:LEU:HD12	1:128:A:LEU:HD23	9	0.6
(1,1683)	1:104:A:LEU:HD13	1:128:A:LEU:HD21	9	0.6
(1,1683)	1:104:A:LEU:HD13	1:128:A:LEU:HD22	9	0.6
(1,1683)	1:104:A:LEU:HD13	1:128:A:LEU:HD23	9	0.6
(1,1667)	1:53:A:ILE:HB	1:126:A:VAL:HG21	10	0.6
(1,1667)	1:53:A:ILE:HB	1:126:A:VAL:HG22	10	0.6
(1,1667)	1:53:A:ILE:HB	1:126:A:VAL:HG23	10	0.6
(1,1461)	1:126:A:VAL:HG11	1:51:A:LEU:HD21	4	0.6
(1,1461)	1:126:A:VAL:HG11	1:51:A:LEU:HD22	4	0.6
(1,1461)	1:126:A:VAL:HG11	1:51:A:LEU:HD23	4	0.6
(1,1461)	1:126:A:VAL:HG12	1:51:A:LEU:HD21	4	0.6
(1,1461)	1:126:A:VAL:HG12	1:51:A:LEU:HD22	4	0.6
(1,1461)	1:126:A:VAL:HG12	1:51:A:LEU:HD23	4	0.6
(1,1461)	1:126:A:VAL:HG13	1:51:A:LEU:HD21	4	0.6
(1,1461)	1:126:A:VAL:HG13	1:51:A:LEU:HD22	4	0.6
(1,1461)	1:126:A:VAL:HG13	1:51:A:LEU:HD23	4	0.6
(1,1388)	1:101:A:PRO:HA	1:25:A:VAL:HG21	5	0.6
(1,1388)	1:101:A:PRO:HA	1:25:A:VAL:HG22	5	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1388)	1:101:A:PRO:HA	1:25:A:VAL:HG23	5	0.6
(1,1231)	1:122:A:MET:HA	1:121:A:LEU:HD11	10	0.6
(1,1231)	1:122:A:MET:HA	1:121:A:LEU:HD12	10	0.6
(1,1231)	1:122:A:MET:HA	1:121:A:LEU:HD13	10	0.6
(1,882)	1:91:A:GLY:HA3	1:38:A:HIS:HB2	9	0.6
(1,805)	1:85:A:HIS:HA	1:52:A:VAL:HG21	7	0.6
(1,805)	1:85:A:HIS:HA	1:52:A:VAL:HG22	7	0.6
(1,805)	1:85:A:HIS:HA	1:52:A:VAL:HG23	7	0.6
(1,3243)	1:123:A:ASN:HD21	1:120:A:ALA:HB2	5	0.59
(1,3139)	1:51:A:LEU:HB2	1:86:A:THR:HG23	4	0.59
(1,2878)	1:38:A:HIS:HE1	1:47:A:MET:HG3	3	0.59
(1,2595)	1:74:A:TYR:HB3	1:50:A:ASN:HD21	8	0.59
(1,2478)	1:93:A:GLU:H	1:38:A:HIS:HB2	2	0.59
(1,2368)	1:80:A:ALA:H	1:79:A:ASP:HA	5	0.59
(1,1986)	1:101:A:PRO:HD2	1:32:A:PHE:H	6	0.59
(1,1980)	1:99:A:LEU:HB3	1:32:A:PHE:H	3	0.59
(1,1980)	1:99:A:LEU:HB3	1:32:A:PHE:H	8	0.59
(1,1685)	1:104:A:LEU:HD11	1:128:A:LEU:HD11	8	0.59
(1,1685)	1:104:A:LEU:HD11	1:128:A:LEU:HD12	8	0.59
(1,1685)	1:104:A:LEU:HD11	1:128:A:LEU:HD13	8	0.59
(1,1685)	1:104:A:LEU:HD12	1:128:A:LEU:HD11	8	0.59
(1,1685)	1:104:A:LEU:HD12	1:128:A:LEU:HD12	8	0.59
(1,1685)	1:104:A:LEU:HD12	1:128:A:LEU:HD13	8	0.59
(1,1685)	1:104:A:LEU:HD13	1:128:A:LEU:HD11	8	0.59
(1,1685)	1:104:A:LEU:HD13	1:128:A:LEU:HD12	8	0.59
(1,1685)	1:104:A:LEU:HD13	1:128:A:LEU:HD13	8	0.59
(1,1514)	1:75:A:VAL:HB	1:69:A:ALA:HB1	8	0.59
(1,1514)	1:75:A:VAL:HB	1:69:A:ALA:HB2	8	0.59
(1,1514)	1:75:A:VAL:HB	1:69:A:ALA:HB3	8	0.59
(1,1509)	1:62:A:VAL:HG21	1:114:A:THR:HG21	5	0.59
(1,1509)	1:62:A:VAL:HG21	1:114:A:THR:HG22	5	0.59
(1,1509)	1:62:A:VAL:HG21	1:114:A:THR:HG23	5	0.59
(1,1509)	1:62:A:VAL:HG22	1:114:A:THR:HG21	5	0.59
(1,1509)	1:62:A:VAL:HG22	1:114:A:THR:HG22	5	0.59
(1,1509)	1:62:A:VAL:HG22	1:114:A:THR:HG23	5	0.59
(1,1509)	1:62:A:VAL:HG23	1:114:A:THR:HG21	5	0.59
(1,1509)	1:62:A:VAL:HG23	1:114:A:THR:HG22	5	0.59
(1,1509)	1:62:A:VAL:HG23	1:114:A:THR:HG23	5	0.59
(1,1497)	1:54:A:ALA:HB1	1:52:A:VAL:HG11	2	0.59
(1,1497)	1:54:A:ALA:HB1	1:52:A:VAL:HG12	2	0.59
(1,1497)	1:54:A:ALA:HB1	1:52:A:VAL:HG13	2	0.59
(1,1497)	1:54:A:ALA:HB2	1:52:A:VAL:HG11	2	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1497)	1:54:A:ALA:HB2	1:52:A:VAL:HG12	2	0.59
(1,1497)	1:54:A:ALA:HB2	1:52:A:VAL:HG13	2	0.59
(1,1497)	1:54:A:ALA:HB3	1:52:A:VAL:HG11	2	0.59
(1,1497)	1:54:A:ALA:HB3	1:52:A:VAL:HG12	2	0.59
(1,1497)	1:54:A:ALA:HB3	1:52:A:VAL:HG13	2	0.59
(1,1388)	1:101:A:PRO:HA	1:25:A:VAL:HG21	8	0.59
(1,1388)	1:101:A:PRO:HA	1:25:A:VAL:HG22	8	0.59
(1,1388)	1:101:A:PRO:HA	1:25:A:VAL:HG23	8	0.59
(1,1074)	1:107:A:GLY:HA2	1:109:A:TYR:HE1	7	0.59
(1,1074)	1:107:A:GLY:HA2	1:109:A:TYR:HE2	7	0.59
(1,1017)	1:101:A:PRO:HD3	1:25:A:VAL:HG21	10	0.59
(1,1017)	1:101:A:PRO:HD3	1:25:A:VAL:HG22	10	0.59
(1,1017)	1:101:A:PRO:HD3	1:25:A:VAL:HG23	10	0.59
(1,580)	1:130:A:ASP:HA	1:128:A:LEU:HD21	8	0.59
(1,580)	1:130:A:ASP:HA	1:128:A:LEU:HD22	8	0.59
(1,580)	1:130:A:ASP:HA	1:128:A:LEU:HD23	8	0.59
(1,3220)	1:94:A:GLU:H	1:93:A:GLU:HB2	7	0.58
(1,3177)	1:9:A:THR:HG23	1:35:A:THR:H	4	0.58
(1,3134)	1:23:A:ILE:HG12	1:34:A:ILE:HG23	3	0.58
(1,2902)	1:49:A:HIS:HD2	1:90:A:GLY:HA3	2	0.58
(1,2876)	1:38:A:HIS:HE1	1:13:A:ASN:HB2	4	0.58
(1,2573)	1:105:A:ALA:H	1:128:A:LEU:HD11	1	0.58
(1,2573)	1:105:A:ALA:H	1:128:A:LEU:HD12	1	0.58
(1,2573)	1:105:A:ALA:H	1:128:A:LEU:HD13	1	0.58
(1,2529)	1:99:A:LEU:H	1:31:A:GLU:HB2	5	0.58
(1,2516)	1:97:A:LEU:H	1:36:A:LEU:HD11	4	0.58
(1,2516)	1:97:A:LEU:H	1:36:A:LEU:HD12	4	0.58
(1,2516)	1:97:A:LEU:H	1:36:A:LEU:HD13	4	0.58
(1,2362)	1:79:A:ASP:H	1:76:A:LYS:HB2	10	0.58
(1,2114)	1:46:A:SER:H	1:43:A:PRO:HD3	6	0.58
(1,2046)	1:37:A:LYS:HD2	1:38:A:HIS:H	6	0.58
(1,2046)	1:37:A:LYS:HD3	1:38:A:HIS:H	6	0.58
(1,1978)	1:31:A:GLU:H	1:30:A:LYS:HD3	2	0.58
(1,1801)	1:13:A:ASN:HD22	1:17:A:GLN:HB3	5	0.58
(1,1660)	1:25:A:VAL:H	1:126:A:VAL:HG21	8	0.58
(1,1660)	1:25:A:VAL:H	1:126:A:VAL:HG22	8	0.58
(1,1660)	1:25:A:VAL:H	1:126:A:VAL:HG23	8	0.58
(1,1627)	1:83:A:VAL:HG21	1:104:A:LEU:HD11	4	0.58
(1,1627)	1:83:A:VAL:HG21	1:104:A:LEU:HD12	4	0.58
(1,1627)	1:83:A:VAL:HG21	1:104:A:LEU:HD13	4	0.58
(1,1627)	1:83:A:VAL:HG22	1:104:A:LEU:HD11	4	0.58
(1,1627)	1:83:A:VAL:HG22	1:104:A:LEU:HD12	4	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1627)	1:83:A:VAL:HG22	1:104:A:LEU:HD13	4	0.58
(1,1627)	1:83:A:VAL:HG23	1:104:A:LEU:HD11	4	0.58
(1,1627)	1:83:A:VAL:HG23	1:104:A:LEU:HD12	4	0.58
(1,1627)	1:83:A:VAL:HG23	1:104:A:LEU:HD13	4	0.58
(1,1533)	1:50:A:ASN:HD22	1:75:A:VAL:HG21	4	0.58
(1,1533)	1:50:A:ASN:HD22	1:75:A:VAL:HG22	4	0.58
(1,1533)	1:50:A:ASN:HD22	1:75:A:VAL:HG23	4	0.58
(1,1503)	1:81:A:ARG:HD2	1:62:A:VAL:HG11	6	0.58
(1,1503)	1:81:A:ARG:HD2	1:62:A:VAL:HG12	6	0.58
(1,1503)	1:81:A:ARG:HD2	1:62:A:VAL:HG13	6	0.58
(1,1498)	1:62:A:VAL:HG11	1:54:A:ALA:H	5	0.58
(1,1498)	1:62:A:VAL:HG12	1:54:A:ALA:H	5	0.58
(1,1498)	1:62:A:VAL:HG13	1:54:A:ALA:H	5	0.58
(1,1303)	1:56:A:ALA:H	1:55:A:LYS:HD2	8	0.58
(1,1064)	1:107:A:GLY:HA2	1:55:A:LYS:HD3	2	0.58
(1,805)	1:85:A:HIS:HA	1:52:A:VAL:HG21	6	0.58
(1,805)	1:85:A:HIS:HA	1:52:A:VAL:HG22	6	0.58
(1,805)	1:85:A:HIS:HA	1:52:A:VAL:HG23	6	0.58
(1,315)	1:10:A:VAL:HB	1:36:A:LEU:HA	10	0.58
(1,258)	1:6:A:CYS:HB2	1:32:A:PHE:HA	5	0.58
(1,3177)	1:35:A:THR:HG21	1:35:A:THR:H	7	0.57
(1,2963)	1:109:A:TYR:HD1	1:128:A:LEU:HD11	3	0.57
(1,2963)	1:109:A:TYR:HD1	1:128:A:LEU:HD12	3	0.57
(1,2963)	1:109:A:TYR:HD1	1:128:A:LEU:HD13	3	0.57
(1,2963)	1:109:A:TYR:HD2	1:128:A:LEU:HD11	3	0.57
(1,2963)	1:109:A:TYR:HD2	1:128:A:LEU:HD12	3	0.57
(1,2963)	1:109:A:TYR:HD2	1:128:A:LEU:HD13	3	0.57
(1,2413)	1:86:A:THR:H	1:52:A:VAL:HG21	5	0.57
(1,2413)	1:86:A:THR:H	1:52:A:VAL:HG22	5	0.57
(1,2413)	1:86:A:THR:H	1:52:A:VAL:HG23	5	0.57
(1,1388)	1:101:A:PRO:HA	1:25:A:VAL:HG21	6	0.57
(1,1388)	1:101:A:PRO:HA	1:25:A:VAL:HG22	6	0.57
(1,1388)	1:101:A:PRO:HA	1:25:A:VAL:HG23	6	0.57
(1,1253)	1:124:A:GLY:HA2	1:111:A:PHE:HZ	6	0.57
(1,1070)	1:55:A:LYS:HE2	1:107:A:GLY:HA2	1	0.57
(1,1070)	1:55:A:LYS:HE3	1:107:A:GLY:HA2	1	0.57
(1,741)	1:77:A:PRO:HA	1:75:A:VAL:HG11	9	0.57
(1,741)	1:77:A:PRO:HA	1:75:A:VAL:HG12	9	0.57
(1,741)	1:77:A:PRO:HA	1:75:A:VAL:HG13	9	0.57
(1,564)	1:55:A:LYS:HB2	1:58:A:ASP:H	3	0.57
(1,258)	1:6:A:CYS:HB2	1:32:A:PHE:HA	10	0.57
(1,3166)	1:126:A:VAL:HG13	1:23:A:ILE:H	6	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3014)	1:115:A:PHE:HE1	1:48:A:GLY:HA2	8	0.56
(1,3014)	1:115:A:PHE:HE2	1:48:A:GLY:HA2	8	0.56
(1,2840)	1:53:A:ILE:HD11	1:32:A:PHE:HD1	3	0.56
(1,2840)	1:53:A:ILE:HD11	1:32:A:PHE:HD2	3	0.56
(1,2840)	1:53:A:ILE:HD12	1:32:A:PHE:HD1	3	0.56
(1,2840)	1:53:A:ILE:HD12	1:32:A:PHE:HD2	3	0.56
(1,2840)	1:53:A:ILE:HD13	1:32:A:PHE:HD1	3	0.56
(1,2840)	1:53:A:ILE:HD13	1:32:A:PHE:HD2	3	0.56
(1,2832)	1:18:A:PHE:HE1	1:12:A:SER:HB2	9	0.56
(1,2832)	1:18:A:PHE:HE2	1:12:A:SER:HB2	9	0.56
(1,2659)	1:124:A:GLY:H	1:113:A:CYS:H	3	0.56
(1,2659)	1:124:A:GLY:H	1:113:A:CYS:H	7	0.56
(1,2342)	1:75:A:VAL:HB	1:74:A:TYR:H	1	0.56
(1,2302)	1:76:A:LYS:HB3	1:66:A:GLY:H	8	0.56
(1,2173)	1:51:A:LEU:H	1:36:A:LEU:HD11	6	0.56
(1,2173)	1:51:A:LEU:H	1:36:A:LEU:HD12	6	0.56
(1,2173)	1:51:A:LEU:H	1:36:A:LEU:HD13	6	0.56
(1,2032)	1:36:A:LEU:HD21	1:37:A:LYS:H	3	0.56
(1,2032)	1:36:A:LEU:HD22	1:37:A:LYS:H	3	0.56
(1,2032)	1:36:A:LEU:HD23	1:37:A:LYS:H	3	0.56
(1,1797)	1:15:A:ASN:HB3	1:13:A:ASN:HD21	9	0.56
(1,1659)	1:127:A:THR:H	1:126:A:VAL:HG21	2	0.56
(1,1659)	1:127:A:THR:H	1:126:A:VAL:HG22	2	0.56
(1,1659)	1:127:A:THR:H	1:126:A:VAL:HG23	2	0.56
(1,1549)	1:83:A:VAL:HG21	1:104:A:LEU:HD21	8	0.56
(1,1549)	1:83:A:VAL:HG21	1:104:A:LEU:HD22	8	0.56
(1,1549)	1:83:A:VAL:HG21	1:104:A:LEU:HD23	8	0.56
(1,1549)	1:83:A:VAL:HG22	1:104:A:LEU:HD21	8	0.56
(1,1549)	1:83:A:VAL:HG22	1:104:A:LEU:HD22	8	0.56
(1,1549)	1:83:A:VAL:HG22	1:104:A:LEU:HD23	8	0.56
(1,1549)	1:83:A:VAL:HG23	1:104:A:LEU:HD21	8	0.56
(1,1549)	1:83:A:VAL:HG23	1:104:A:LEU:HD22	8	0.56
(1,1549)	1:83:A:VAL:HG23	1:104:A:LEU:HD23	8	0.56
(1,1514)	1:75:A:VAL:HB	1:69:A:ALA:HB1	6	0.56
(1,1514)	1:75:A:VAL:HB	1:69:A:ALA:HB2	6	0.56
(1,1514)	1:75:A:VAL:HB	1:69:A:ALA:HB3	6	0.56
(1,1428)	1:18:A:PHE:HD1	1:36:A:LEU:HD21	9	0.56
(1,1428)	1:18:A:PHE:HD1	1:36:A:LEU:HD22	9	0.56
(1,1428)	1:18:A:PHE:HD1	1:36:A:LEU:HD23	9	0.56
(1,1428)	1:18:A:PHE:HD2	1:36:A:LEU:HD21	9	0.56
(1,1428)	1:18:A:PHE:HD2	1:36:A:LEU:HD22	9	0.56
(1,1428)	1:18:A:PHE:HD2	1:36:A:LEU:HD23	9	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1303)	1:56:A:ALA:H	1:55:A:LYS:HD2	3	0.56
(1,1119)	1:125:A:LYS:HA	1:110:A:LYS:HG2	6	0.56
(1,1074)	1:107:A:GLY:HA2	1:109:A:TYR:HE1	8	0.56
(1,1074)	1:107:A:GLY:HA2	1:109:A:TYR:HE2	8	0.56
(1,1035)	1:101:A:PRO:HG3	1:25:A:VAL:HG21	1	0.56
(1,1035)	1:101:A:PRO:HG3	1:25:A:VAL:HG22	1	0.56
(1,1035)	1:101:A:PRO:HG3	1:25:A:VAL:HG23	1	0.56
(1,769)	1:77:A:PRO:HG2	1:72:A:THR:HG21	10	0.56
(1,769)	1:77:A:PRO:HG2	1:72:A:THR:HG22	10	0.56
(1,769)	1:77:A:PRO:HG2	1:72:A:THR:HG23	10	0.56
(1,126)	1:21:A:LYS:HE2	1:21:A:LYS:HB2	4	0.56
(1,126)	1:21:A:LYS:HE3	1:21:A:LYS:HB2	4	0.56
(1,95)	1:17:A:GLN:H	1:17:A:GLN:HG2	3	0.56
(1,3148)	1:53:A:ILE:HD11	1:104:A:LEU:HD21	3	0.55
(1,3139)	1:51:A:LEU:HB2	1:86:A:THR:HG23	10	0.55
(1,2985)	1:53:A:ILE:HG13	1:111:A:PHE:HD1	6	0.55
(1,2985)	1:53:A:ILE:HG13	1:111:A:PHE:HD2	6	0.55
(1,2884)	1:115:A:PHE:HB3	1:74:A:TYR:HD1	1	0.55
(1,2884)	1:115:A:PHE:HB3	1:74:A:TYR:HD2	1	0.55
(1,2880)	1:67:A:VAL:HG21	1:74:A:TYR:HD1	7	0.55
(1,2880)	1:67:A:VAL:HG21	1:74:A:TYR:HD2	7	0.55
(1,2880)	1:67:A:VAL:HG22	1:74:A:TYR:HD1	7	0.55
(1,2880)	1:67:A:VAL:HG22	1:74:A:TYR:HD2	7	0.55
(1,2880)	1:67:A:VAL:HG23	1:74:A:TYR:HD1	7	0.55
(1,2880)	1:67:A:VAL:HG23	1:74:A:TYR:HD2	7	0.55
(1,2573)	1:105:A:ALA:H	1:128:A:LEU:HD11	9	0.55
(1,2573)	1:105:A:ALA:H	1:128:A:LEU:HD12	9	0.55
(1,2573)	1:105:A:ALA:H	1:128:A:LEU:HD13	9	0.55
(1,2342)	1:75:A:VAL:HB	1:74:A:TYR:H	8	0.55
(1,2173)	1:51:A:LEU:H	1:36:A:LEU:HD11	1	0.55
(1,2173)	1:51:A:LEU:H	1:36:A:LEU:HD12	1	0.55
(1,2173)	1:51:A:LEU:H	1:36:A:LEU:HD13	1	0.55
(1,2117)	1:46:A:SER:H	1:43:A:PRO:HB3	5	0.55
(1,2105)	1:43:A:PRO:HB3	1:45:A:ALA:H	1	0.55
(1,1686)	1:128:A:LEU:HD11	1:127:A:THR:HG21	8	0.55
(1,1686)	1:128:A:LEU:HD11	1:127:A:THR:HG22	8	0.55
(1,1686)	1:128:A:LEU:HD11	1:127:A:THR:HG23	8	0.55
(1,1686)	1:128:A:LEU:HD12	1:127:A:THR:HG21	8	0.55
(1,1686)	1:128:A:LEU:HD12	1:127:A:THR:HG22	8	0.55
(1,1686)	1:128:A:LEU:HD12	1:127:A:THR:HG23	8	0.55
(1,1686)	1:128:A:LEU:HD13	1:127:A:THR:HG21	8	0.55
(1,1686)	1:128:A:LEU:HD13	1:127:A:THR:HG22	8	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1686)	1:128:A:LEU:HD13	1:127:A:THR:HG23	8	0.55
(1,1659)	1:127:A:THR:H	1:126:A:VAL:HG21	8	0.55
(1,1659)	1:127:A:THR:H	1:126:A:VAL:HG22	8	0.55
(1,1659)	1:127:A:THR:H	1:126:A:VAL:HG23	8	0.55
(1,1618)	1:109:A:TYR:HD1	1:104:A:LEU:HD21	7	0.55
(1,1618)	1:109:A:TYR:HD1	1:104:A:LEU:HD22	7	0.55
(1,1618)	1:109:A:TYR:HD1	1:104:A:LEU:HD23	7	0.55
(1,1618)	1:109:A:TYR:HD2	1:104:A:LEU:HD21	7	0.55
(1,1618)	1:109:A:TYR:HD2	1:104:A:LEU:HD22	7	0.55
(1,1618)	1:109:A:TYR:HD2	1:104:A:LEU:HD23	7	0.55
(1,1392)	1:127:A:THR:H	1:25:A:VAL:HG11	2	0.55
(1,1392)	1:127:A:THR:H	1:25:A:VAL:HG12	2	0.55
(1,1392)	1:127:A:THR:H	1:25:A:VAL:HG13	2	0.55
(1,1253)	1:124:A:GLY:HA2	1:111:A:PHE:HZ	8	0.55
(1,1156)	1:52:A:VAL:HG21	1:113:A:CYS:HA	9	0.55
(1,1156)	1:52:A:VAL:HG22	1:113:A:CYS:HA	9	0.55
(1,1156)	1:52:A:VAL:HG23	1:113:A:CYS:HA	9	0.55
(1,1009)	1:101:A:PRO:HA	1:27:A:LYS:HA	1	0.55
(1,830)	1:86:A:THR:HA	1:97:A:LEU:HB2	1	0.55
(1,805)	1:85:A:HIS:HA	1:52:A:VAL:HG21	4	0.55
(1,805)	1:85:A:HIS:HA	1:52:A:VAL:HG22	4	0.55
(1,805)	1:85:A:HIS:HA	1:52:A:VAL:HG23	4	0.55
(1,589)	1:57:A:GLU:HG3	1:57:A:GLU:H	6	0.55
(1,589)	1:57:A:GLU:HG3	1:57:A:GLU:H	8	0.55
(1,498)	1:50:A:ASN:HB2	1:51:A:LEU:H	7	0.55
(1,3177)	1:35:A:THR:HG23	1:35:A:THR:H	9	0.54
(1,3123)	1:23:A:ILE:HG12	1:10:A:VAL:HG21	10	0.54
(1,2902)	1:49:A:HIS:HD2	1:90:A:GLY:HA3	5	0.54
(1,2659)	1:124:A:GLY:H	1:113:A:CYS:H	5	0.54
(1,2611)	1:110:A:LYS:HG2	1:109:A:TYR:H	2	0.54
(1,2478)	1:93:A:GLU:H	1:38:A:HIS:HB2	6	0.54
(1,2362)	1:79:A:ASP:H	1:76:A:LYS:HB2	8	0.54
(1,2342)	1:75:A:VAL:HB	1:74:A:TYR:H	4	0.54
(1,2342)	1:75:A:VAL:HB	1:74:A:TYR:H	9	0.54
(1,2117)	1:46:A:SER:H	1:43:A:PRO:HB3	4	0.54
(1,2117)	1:46:A:SER:H	1:43:A:PRO:HB3	8	0.54
(1,2114)	1:46:A:SER:H	1:43:A:PRO:HD3	7	0.54
(1,2114)	1:46:A:SER:H	1:43:A:PRO:HD3	8	0.54
(1,2045)	1:94:A:GLU:HB2	1:38:A:HIS:H	1	0.54
(1,2032)	1:36:A:LEU:HD21	1:37:A:LYS:H	1	0.54
(1,2032)	1:36:A:LEU:HD22	1:37:A:LYS:H	1	0.54
(1,2032)	1:36:A:LEU:HD23	1:37:A:LYS:H	1	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2032)	1:36:A:LEU:HD21	1:37:A:LYS:H	7	0.54
(1,2032)	1:36:A:LEU:HD22	1:37:A:LYS:H	7	0.54
(1,2032)	1:36:A:LEU:HD23	1:37:A:LYS:H	7	0.54
(1,1678)	1:27:A:LYS:HA	1:128:A:LEU:HD21	3	0.54
(1,1678)	1:27:A:LYS:HA	1:128:A:LEU:HD22	3	0.54
(1,1678)	1:27:A:LYS:HA	1:128:A:LEU:HD23	3	0.54
(1,1539)	1:82:A:VAL:H	1:82:A:VAL:HG11	3	0.54
(1,1539)	1:82:A:VAL:H	1:82:A:VAL:HG12	3	0.54
(1,1539)	1:82:A:VAL:H	1:82:A:VAL:HG13	3	0.54
(1,1539)	1:82:A:VAL:H	1:82:A:VAL:HG11	4	0.54
(1,1539)	1:82:A:VAL:H	1:82:A:VAL:HG12	4	0.54
(1,1539)	1:82:A:VAL:H	1:82:A:VAL:HG13	4	0.54
(1,1539)	1:82:A:VAL:H	1:82:A:VAL:HG11	6	0.54
(1,1539)	1:82:A:VAL:H	1:82:A:VAL:HG12	6	0.54
(1,1539)	1:82:A:VAL:H	1:82:A:VAL:HG13	6	0.54
(1,1539)	1:82:A:VAL:H	1:82:A:VAL:HG11	9	0.54
(1,1539)	1:82:A:VAL:H	1:82:A:VAL:HG12	9	0.54
(1,1539)	1:82:A:VAL:H	1:82:A:VAL:HG13	9	0.54
(1,1467)	1:85:A:HIS:HB2	1:52:A:VAL:HG11	9	0.54
(1,1467)	1:85:A:HIS:HB2	1:52:A:VAL:HG12	9	0.54
(1,1467)	1:85:A:HIS:HB2	1:52:A:VAL:HG13	9	0.54
(1,1388)	1:101:A:PRO:HA	1:25:A:VAL:HG21	4	0.54
(1,1388)	1:101:A:PRO:HA	1:25:A:VAL:HG22	4	0.54
(1,1388)	1:101:A:PRO:HA	1:25:A:VAL:HG23	4	0.54
(1,1092)	1:56:A:ALA:HB1	1:108:A:ASP:HB3	8	0.54
(1,1092)	1:56:A:ALA:HB2	1:108:A:ASP:HB3	8	0.54
(1,1092)	1:56:A:ALA:HB3	1:108:A:ASP:HB3	8	0.54
(1,805)	1:85:A:HIS:HA	1:52:A:VAL:HG21	2	0.54
(1,805)	1:85:A:HIS:HA	1:52:A:VAL:HG22	2	0.54
(1,805)	1:85:A:HIS:HA	1:52:A:VAL:HG23	2	0.54
(1,805)	1:85:A:HIS:HA	1:52:A:VAL:HG21	8	0.54
(1,805)	1:85:A:HIS:HA	1:52:A:VAL:HG22	8	0.54
(1,805)	1:85:A:HIS:HA	1:52:A:VAL:HG23	8	0.54
(1,795)	1:82:A:VAL:HB	1:75:A:VAL:HG11	8	0.54
(1,795)	1:82:A:VAL:HB	1:75:A:VAL:HG12	8	0.54
(1,795)	1:82:A:VAL:HB	1:75:A:VAL:HG13	8	0.54
(1,741)	1:77:A:PRO:HA	1:75:A:VAL:HG11	3	0.54
(1,741)	1:77:A:PRO:HA	1:75:A:VAL:HG12	3	0.54
(1,741)	1:77:A:PRO:HA	1:75:A:VAL:HG13	3	0.54
(2,1)	1:6:A:CYS:SG	1:29:A:CYS:SG	6	0.53
(1,3220)	1:94:A:GLU:H	1:93:A:GLU:HB2	1	0.53
(1,3166)	1:126:A:VAL:HG12	1:23:A:ILE:H	7	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2214)	1:83:A:VAL:HG11	1:55:A:LYS:H	8	0.53
(1,2214)	1:83:A:VAL:HG12	1:55:A:LYS:H	8	0.53
(1,2214)	1:83:A:VAL:HG13	1:55:A:LYS:H	8	0.53
(1,1879)	1:20:A:THR:H	1:19:A:ASN:HB3	2	0.53
(1,1780)	1:12:A:SER:H	1:36:A:LEU:HD21	2	0.53
(1,1780)	1:12:A:SER:H	1:36:A:LEU:HD22	2	0.53
(1,1780)	1:12:A:SER:H	1:36:A:LEU:HD23	2	0.53
(1,1669)	1:25:A:VAL:HG11	1:126:A:VAL:HG21	3	0.53
(1,1669)	1:25:A:VAL:HG11	1:126:A:VAL:HG22	3	0.53
(1,1669)	1:25:A:VAL:HG11	1:126:A:VAL:HG23	3	0.53
(1,1669)	1:25:A:VAL:HG12	1:126:A:VAL:HG21	3	0.53
(1,1669)	1:25:A:VAL:HG12	1:126:A:VAL:HG22	3	0.53
(1,1669)	1:25:A:VAL:HG12	1:126:A:VAL:HG23	3	0.53
(1,1669)	1:25:A:VAL:HG13	1:126:A:VAL:HG21	3	0.53
(1,1669)	1:25:A:VAL:HG13	1:126:A:VAL:HG22	3	0.53
(1,1669)	1:25:A:VAL:HG13	1:126:A:VAL:HG23	3	0.53
(1,1539)	1:82:A:VAL:H	1:82:A:VAL:HG11	2	0.53
(1,1539)	1:82:A:VAL:H	1:82:A:VAL:HG12	2	0.53
(1,1539)	1:82:A:VAL:H	1:82:A:VAL:HG13	2	0.53
(1,1514)	1:75:A:VAL:HB	1:69:A:ALA:HB1	5	0.53
(1,1514)	1:75:A:VAL:HB	1:69:A:ALA:HB2	5	0.53
(1,1514)	1:75:A:VAL:HB	1:69:A:ALA:HB3	5	0.53
(1,1392)	1:127:A:THR:H	1:25:A:VAL:HG11	8	0.53
(1,1392)	1:127:A:THR:H	1:25:A:VAL:HG12	8	0.53
(1,1392)	1:127:A:THR:H	1:25:A:VAL:HG13	8	0.53
(1,1388)	1:101:A:PRO:HA	1:25:A:VAL:HG21	10	0.53
(1,1388)	1:101:A:PRO:HA	1:25:A:VAL:HG22	10	0.53
(1,1388)	1:101:A:PRO:HA	1:25:A:VAL:HG23	10	0.53
(1,1093)	1:56:A:ALA:HB1	1:108:A:ASP:HB2	2	0.53
(1,1093)	1:56:A:ALA:HB2	1:108:A:ASP:HB2	2	0.53
(1,1093)	1:56:A:ALA:HB3	1:108:A:ASP:HB2	2	0.53
(1,741)	1:77:A:PRO:HA	1:75:A:VAL:HG11	7	0.53
(1,741)	1:77:A:PRO:HA	1:75:A:VAL:HG12	7	0.53
(1,741)	1:77:A:PRO:HA	1:75:A:VAL:HG13	7	0.53
(1,646)	1:76:A:LYS:HB3	1:66:A:GLY:HA3	9	0.53
(1,643)	1:76:A:LYS:HD2	1:66:A:GLY:HA3	2	0.53
(1,643)	1:76:A:LYS:HD3	1:66:A:GLY:HA3	2	0.53
(1,580)	1:130:A:ASP:HA	1:128:A:LEU:HD21	10	0.53
(1,580)	1:130:A:ASP:HA	1:128:A:LEU:HD22	10	0.53
(1,580)	1:130:A:ASP:HA	1:128:A:LEU:HD23	10	0.53
(1,387)	1:41:A:THR:HA	1:91:A:GLY:HA2	4	0.53
(1,233)	1:30:A:LYS:HA	1:30:A:LYS:HD3	9	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,178)	1:25:A:VAL:H	1:24:A:GLN:HG3	10	0.53
(1,3143)	1:103:A:LYS:HB2	1:99:A:LEU:HD22	5	0.52
(1,3124)	1:18:A:PHE:HD1	1:10:A:VAL:HG11	10	0.52
(1,2676)	1:75:A:VAL:HG21	1:114:A:THR:H	8	0.52
(1,2676)	1:75:A:VAL:HG22	1:114:A:THR:H	8	0.52
(1,2676)	1:75:A:VAL:HG23	1:114:A:THR:H	8	0.52
(1,2516)	1:97:A:LEU:H	1:36:A:LEU:HD11	8	0.52
(1,2516)	1:97:A:LEU:H	1:36:A:LEU:HD12	8	0.52
(1,2516)	1:97:A:LEU:H	1:36:A:LEU:HD13	8	0.52
(1,2478)	1:93:A:GLU:H	1:38:A:HIS:HB2	4	0.52
(1,2407)	1:85:A:HIS:H	1:85:A:HIS:HD2	5	0.52
(1,2364)	1:82:A:VAL:HG11	1:79:A:ASP:H	2	0.52
(1,2364)	1:82:A:VAL:HG12	1:79:A:ASP:H	2	0.52
(1,2364)	1:82:A:VAL:HG13	1:79:A:ASP:H	2	0.52
(1,2342)	1:75:A:VAL:HB	1:74:A:TYR:H	7	0.52
(1,2264)	1:61:A:GLY:H	1:59:A:MET:HG2	1	0.52
(1,2264)	1:61:A:GLY:H	1:59:A:MET:HG3	1	0.52
(1,2032)	1:36:A:LEU:HD21	1:37:A:LYS:H	2	0.52
(1,2032)	1:36:A:LEU:HD22	1:37:A:LYS:H	2	0.52
(1,2032)	1:36:A:LEU:HD23	1:37:A:LYS:H	2	0.52
(1,1897)	1:25:A:VAL:HG11	1:24:A:GLN:H	3	0.52
(1,1897)	1:25:A:VAL:HG12	1:24:A:GLN:H	3	0.52
(1,1897)	1:25:A:VAL:HG13	1:24:A:GLN:H	3	0.52
(1,1682)	1:104:A:LEU:HG	1:128:A:LEU:HD21	5	0.52
(1,1682)	1:104:A:LEU:HG	1:128:A:LEU:HD22	5	0.52
(1,1682)	1:104:A:LEU:HG	1:128:A:LEU:HD23	5	0.52
(1,1654)	1:122:A:MET:HG2	1:121:A:LEU:HD11	8	0.52
(1,1654)	1:122:A:MET:HG2	1:121:A:LEU:HD12	8	0.52
(1,1654)	1:122:A:MET:HG2	1:121:A:LEU:HD13	8	0.52
(1,1654)	1:122:A:MET:HG3	1:121:A:LEU:HD11	8	0.52
(1,1654)	1:122:A:MET:HG3	1:121:A:LEU:HD12	8	0.52
(1,1654)	1:122:A:MET:HG3	1:121:A:LEU:HD13	8	0.52
(1,1653)	1:121:A:LEU:HA	1:121:A:LEU:HD21	6	0.52
(1,1653)	1:121:A:LEU:HA	1:121:A:LEU:HD22	6	0.52
(1,1653)	1:121:A:LEU:HA	1:121:A:LEU:HD23	6	0.52
(1,1539)	1:82:A:VAL:H	1:82:A:VAL:HG11	1	0.52
(1,1539)	1:82:A:VAL:H	1:82:A:VAL:HG12	1	0.52
(1,1539)	1:82:A:VAL:H	1:82:A:VAL:HG13	1	0.52
(1,1539)	1:82:A:VAL:H	1:82:A:VAL:HG11	8	0.52
(1,1539)	1:82:A:VAL:H	1:82:A:VAL:HG12	8	0.52
(1,1539)	1:82:A:VAL:H	1:82:A:VAL:HG13	8	0.52
(1,1539)	1:82:A:VAL:H	1:82:A:VAL:HG11	10	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1539)	1:82:A:VAL:H	1:82:A:VAL:HG12	10	0.52
(1,1539)	1:82:A:VAL:H	1:82:A:VAL:HG13	10	0.52
(1,1525)	1:114:A:THR:HG21	1:75:A:VAL:HG21	4	0.52
(1,1525)	1:114:A:THR:HG21	1:75:A:VAL:HG22	4	0.52
(1,1525)	1:114:A:THR:HG21	1:75:A:VAL:HG23	4	0.52
(1,1525)	1:114:A:THR:HG22	1:75:A:VAL:HG21	4	0.52
(1,1525)	1:114:A:THR:HG22	1:75:A:VAL:HG22	4	0.52
(1,1525)	1:114:A:THR:HG22	1:75:A:VAL:HG23	4	0.52
(1,1525)	1:114:A:THR:HG23	1:75:A:VAL:HG21	4	0.52
(1,1525)	1:114:A:THR:HG23	1:75:A:VAL:HG22	4	0.52
(1,1525)	1:114:A:THR:HG23	1:75:A:VAL:HG23	4	0.52
(1,1514)	1:75:A:VAL:HB	1:69:A:ALA:HB1	3	0.52
(1,1514)	1:75:A:VAL:HB	1:69:A:ALA:HB2	3	0.52
(1,1514)	1:75:A:VAL:HB	1:69:A:ALA:HB3	3	0.52
(1,1428)	1:18:A:PHE:HD1	1:36:A:LEU:HD21	7	0.52
(1,1428)	1:18:A:PHE:HD1	1:36:A:LEU:HD22	7	0.52
(1,1428)	1:18:A:PHE:HD1	1:36:A:LEU:HD23	7	0.52
(1,1428)	1:18:A:PHE:HD2	1:36:A:LEU:HD21	7	0.52
(1,1428)	1:18:A:PHE:HD2	1:36:A:LEU:HD22	7	0.52
(1,1428)	1:18:A:PHE:HD2	1:36:A:LEU:HD23	7	0.52
(1,1379)	1:53:A:ILE:HD11	1:23:A:ILE:HG21	3	0.52
(1,1379)	1:53:A:ILE:HD11	1:23:A:ILE:HG22	3	0.52
(1,1379)	1:53:A:ILE:HD11	1:23:A:ILE:HG23	3	0.52
(1,1379)	1:53:A:ILE:HD12	1:23:A:ILE:HG21	3	0.52
(1,1379)	1:53:A:ILE:HD12	1:23:A:ILE:HG22	3	0.52
(1,1379)	1:53:A:ILE:HD12	1:23:A:ILE:HG23	3	0.52
(1,1379)	1:53:A:ILE:HD13	1:23:A:ILE:HG21	3	0.52
(1,1379)	1:53:A:ILE:HD13	1:23:A:ILE:HG22	3	0.52
(1,1379)	1:53:A:ILE:HD13	1:23:A:ILE:HG23	3	0.52
(1,1095)	1:110:A:LYS:HD3	1:109:A:TYR:HA	4	0.52
(1,578)	1:56:A:ALA:HA	1:110:A:LYS:HD2	5	0.52
(1,3220)	1:94:A:GLU:H	1:93:A:GLU:HB2	8	0.51
(1,3178)	1:37:A:LYS:HG2	1:36:A:LEU:H	1	0.51
(1,3178)	1:37:A:LYS:HG3	1:36:A:LEU:H	1	0.51
(1,2817)	1:130:A:ASP:H	1:3:A:ALA:HB1	3	0.51
(1,2817)	1:130:A:ASP:H	1:3:A:ALA:HB2	3	0.51
(1,2817)	1:130:A:ASP:H	1:3:A:ALA:HB3	3	0.51
(1,2749)	1:123:A:ASN:HD21	1:119:A:GLY:HA2	5	0.51
(1,2696)	1:117:A:GLY:H	1:67:A:VAL:HG11	2	0.51
(1,2696)	1:117:A:GLY:H	1:67:A:VAL:HG12	2	0.51
(1,2696)	1:117:A:GLY:H	1:67:A:VAL:HG13	2	0.51
(1,2676)	1:75:A:VAL:HG21	1:114:A:THR:H	4	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2676)	1:75:A:VAL:HG22	1:114:A:THR:H	4	0.51
(1,2676)	1:75:A:VAL:HG23	1:114:A:THR:H	4	0.51
(1,2659)	1:124:A:GLY:H	1:113:A:CYS:H	6	0.51
(1,2508)	1:85:A:HIS:H	1:97:A:LEU:H	6	0.51
(1,2508)	1:85:A:HIS:H	1:97:A:LEU:H	10	0.51
(1,2342)	1:75:A:VAL:HB	1:74:A:TYR:H	3	0.51
(1,2117)	1:46:A:SER:H	1:43:A:PRO:HB3	6	0.51
(1,1715)	1:59:A:MET:HE1	1:114:A:THR:HG1	3	0.51
(1,1715)	1:59:A:MET:HE2	1:114:A:THR:HG1	3	0.51
(1,1715)	1:59:A:MET:HE3	1:114:A:THR:HG1	3	0.51
(1,1653)	1:121:A:LEU:HA	1:121:A:LEU:HD21	4	0.51
(1,1653)	1:121:A:LEU:HA	1:121:A:LEU:HD22	4	0.51
(1,1653)	1:121:A:LEU:HA	1:121:A:LEU:HD23	4	0.51
(1,1628)	1:101:A:PRO:HB2	1:104:A:LEU:HD11	6	0.51
(1,1628)	1:101:A:PRO:HB2	1:104:A:LEU:HD12	6	0.51
(1,1628)	1:101:A:PRO:HB2	1:104:A:LEU:HD13	6	0.51
(1,1543)	1:85:A:HIS:HD2	1:82:A:VAL:HG21	10	0.51
(1,1543)	1:85:A:HIS:HD2	1:82:A:VAL:HG22	10	0.51
(1,1543)	1:85:A:HIS:HD2	1:82:A:VAL:HG23	10	0.51
(1,1388)	1:101:A:PRO:HA	1:25:A:VAL:HG21	7	0.51
(1,1388)	1:101:A:PRO:HA	1:25:A:VAL:HG22	7	0.51
(1,1388)	1:101:A:PRO:HA	1:25:A:VAL:HG23	7	0.51
(1,1100)	1:110:A:LYS:HA	1:126:A:VAL:HG11	2	0.51
(1,1100)	1:110:A:LYS:HA	1:126:A:VAL:HG12	2	0.51
(1,1100)	1:110:A:LYS:HA	1:126:A:VAL:HG13	2	0.51
(1,889)	1:92:A:GLY:HA2	1:93:A:GLU:HG3	2	0.51
(1,579)	1:56:A:ALA:HA	1:110:A:LYS:HD3	2	0.51
(1,464)	1:88:A:LEU:HD11	1:48:A:GLY:HA2	4	0.51
(1,464)	1:88:A:LEU:HD12	1:48:A:GLY:HA2	4	0.51
(1,464)	1:88:A:LEU:HD13	1:48:A:GLY:HA2	4	0.51
(1,426)	1:43:A:PRO:HG3	1:46:A:SER:H	2	0.51
(1,426)	1:43:A:PRO:HG3	1:46:A:SER:H	10	0.51
(1,387)	1:41:A:THR:HA	1:91:A:GLY:HA2	3	0.51
(1,258)	1:6:A:CYS:HB2	1:32:A:PHE:HA	6	0.51
(1,126)	1:21:A:LYS:HE2	1:21:A:LYS:HB2	1	0.51
(1,126)	1:21:A:LYS:HE3	1:21:A:LYS:HB2	1	0.51
(2,1)	1:6:A:CYS:SG	1:29:A:CYS:SG	8	0.5
(1,3264)	1:111:A:PHE:HD1	1:20:A:THR:HG22	10	0.5
(1,3177)	1:35:A:THR:HG22	1:35:A:THR:H	6	0.5
(1,2659)	1:124:A:GLY:H	1:113:A:CYS:H	8	0.5
(1,2595)	1:74:A:TYR:HB3	1:50:A:ASN:HD21	3	0.5
(1,2173)	1:51:A:LEU:H	1:36:A:LEU:HD11	10	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2173)	1:51:A:LEU:H	1:36:A:LEU:HD12	10	0.5
(1,2173)	1:51:A:LEU:H	1:36:A:LEU:HD13	10	0.5
(1,1978)	1:31:A:GLU:H	1:30:A:LYS:HD3	4	0.5
(1,1653)	1:121:A:LEU:HA	1:121:A:LEU:HD21	2	0.5
(1,1653)	1:121:A:LEU:HA	1:121:A:LEU:HD22	2	0.5
(1,1653)	1:121:A:LEU:HA	1:121:A:LEU:HD23	2	0.5
(1,1613)	1:101:A:PRO:HA	1:99:A:LEU:HD21	2	0.5
(1,1613)	1:101:A:PRO:HA	1:99:A:LEU:HD22	2	0.5
(1,1613)	1:101:A:PRO:HA	1:99:A:LEU:HD23	2	0.5
(1,1379)	1:53:A:ILE:HD11	1:23:A:ILE:HG21	9	0.5
(1,1379)	1:53:A:ILE:HD11	1:23:A:ILE:HG22	9	0.5
(1,1379)	1:53:A:ILE:HD11	1:23:A:ILE:HG23	9	0.5
(1,1379)	1:53:A:ILE:HD12	1:23:A:ILE:HG21	9	0.5
(1,1379)	1:53:A:ILE:HD12	1:23:A:ILE:HG22	9	0.5
(1,1379)	1:53:A:ILE:HD12	1:23:A:ILE:HG23	9	0.5
(1,1379)	1:53:A:ILE:HD13	1:23:A:ILE:HG21	9	0.5
(1,1379)	1:53:A:ILE:HD13	1:23:A:ILE:HG22	9	0.5
(1,1379)	1:53:A:ILE:HD13	1:23:A:ILE:HG23	9	0.5
(1,1320)	1:47:A:MET:HE1	1:118:A:HIS:HE1	4	0.5
(1,1320)	1:47:A:MET:HE2	1:118:A:HIS:HE1	4	0.5
(1,1320)	1:47:A:MET:HE3	1:118:A:HIS:HE1	4	0.5
(1,1253)	1:124:A:GLY:HA2	1:111:A:PHE:HZ	1	0.5
(1,1253)	1:124:A:GLY:HA2	1:111:A:PHE:HZ	4	0.5
(1,1035)	1:101:A:PRO:HG3	1:25:A:VAL:HG21	8	0.5
(1,1035)	1:101:A:PRO:HG3	1:25:A:VAL:HG22	8	0.5
(1,1035)	1:101:A:PRO:HG3	1:25:A:VAL:HG23	8	0.5
(1,1001)	1:100:A:ASP:HA	1:31:A:GLU:HB2	2	0.5
(1,994)	1:83:A:VAL:HG21	1:99:A:LEU:HB3	2	0.5
(1,994)	1:83:A:VAL:HG22	1:99:A:LEU:HB3	2	0.5
(1,994)	1:83:A:VAL:HG23	1:99:A:LEU:HB3	2	0.5
(1,639)	1:67:A:VAL:HG11	1:64:A:LYS:HA	7	0.5
(1,639)	1:67:A:VAL:HG12	1:64:A:LYS:HA	7	0.5
(1,639)	1:67:A:VAL:HG13	1:64:A:LYS:HA	7	0.5
(1,589)	1:57:A:GLU:HG3	1:57:A:GLU:H	1	0.5
(1,3220)	1:94:A:GLU:H	1:93:A:GLU:HB2	2	0.49
(1,3075)	1:55:A:LYS:HB2	1:54:A:ALA:HB3	8	0.49
(1,3014)	1:115:A:PHE:HE1	1:48:A:GLY:HA2	7	0.49
(1,3014)	1:115:A:PHE:HE2	1:48:A:GLY:HA2	7	0.49
(1,2955)	1:55:A:LYS:HB3	1:109:A:TYR:HE1	6	0.49
(1,2955)	1:55:A:LYS:HB3	1:109:A:TYR:HE2	6	0.49
(1,2759)	1:123:A:ASN:HD22	1:21:A:LYS:HG2	2	0.49
(1,2759)	1:123:A:ASN:HD22	1:21:A:LYS:HG3	2	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2534)	1:100:A:ASP:H	1:83:A:VAL:HG21	10	0.49
(1,2534)	1:100:A:ASP:H	1:83:A:VAL:HG22	10	0.49
(1,2534)	1:100:A:ASP:H	1:83:A:VAL:HG23	10	0.49
(1,2469)	1:92:A:GLY:H	1:38:A:HIS:HB2	2	0.49
(1,2394)	1:84:A:ALA:H	1:104:A:LEU:HD21	6	0.49
(1,2394)	1:84:A:ALA:H	1:104:A:LEU:HD22	6	0.49
(1,2394)	1:84:A:ALA:H	1:104:A:LEU:HD23	6	0.49
(1,2032)	1:36:A:LEU:HD21	1:37:A:LYS:H	4	0.49
(1,2032)	1:36:A:LEU:HD22	1:37:A:LYS:H	4	0.49
(1,2032)	1:36:A:LEU:HD23	1:37:A:LYS:H	4	0.49
(1,1950)	1:27:A:LYS:HD2	1:28:A:ALA:H	2	0.49
(1,1950)	1:27:A:LYS:HD3	1:28:A:ALA:H	2	0.49
(1,1653)	1:121:A:LEU:HA	1:121:A:LEU:HD21	9	0.49
(1,1653)	1:121:A:LEU:HA	1:121:A:LEU:HD22	9	0.49
(1,1653)	1:121:A:LEU:HA	1:121:A:LEU:HD23	9	0.49
(1,830)	1:86:A:THR:HA	1:97:A:LEU:HB2	5	0.49
(1,586)	1:27:A:LYS:HE2	1:130:A:ASP:HA	3	0.49
(1,586)	1:27:A:LYS:HE3	1:130:A:ASP:HA	3	0.49
(1,498)	1:50:A:ASN:HB2	1:51:A:LEU:H	9	0.49
(1,426)	1:43:A:PRO:HG3	1:46:A:SER:H	6	0.49
(1,258)	1:6:A:CYS:HB2	1:32:A:PHE:HA	1	0.49
(1,258)	1:6:A:CYS:HB2	1:32:A:PHE:HA	8	0.49
(1,178)	1:25:A:VAL:H	1:24:A:GLN:HG3	5	0.49
(1,3190)	1:51:A:LEU:H	1:36:A:LEU:HB3	5	0.48
(1,2960)	1:109:A:TYR:HD1	1:127:A:THR:HG21	5	0.48
(1,2960)	1:109:A:TYR:HD1	1:127:A:THR:HG22	5	0.48
(1,2960)	1:109:A:TYR:HD1	1:127:A:THR:HG23	5	0.48
(1,2960)	1:109:A:TYR:HD2	1:127:A:THR:HG21	5	0.48
(1,2960)	1:109:A:TYR:HD2	1:127:A:THR:HG22	5	0.48
(1,2960)	1:109:A:TYR:HD2	1:127:A:THR:HG23	5	0.48
(1,2925)	1:63:A:PHE:HD1	1:112:A:ALA:HB1	9	0.48
(1,2925)	1:63:A:PHE:HD1	1:112:A:ALA:HB2	9	0.48
(1,2925)	1:63:A:PHE:HD1	1:112:A:ALA:HB3	9	0.48
(1,2925)	1:63:A:PHE:HD2	1:112:A:ALA:HB1	9	0.48
(1,2925)	1:63:A:PHE:HD2	1:112:A:ALA:HB2	9	0.48
(1,2925)	1:63:A:PHE:HD2	1:112:A:ALA:HB3	9	0.48
(1,2591)	1:106:A:ASP:H	1:128:A:LEU:HD11	5	0.48
(1,2591)	1:106:A:ASP:H	1:128:A:LEU:HD12	5	0.48
(1,2591)	1:106:A:ASP:H	1:128:A:LEU:HD13	5	0.48
(1,2538)	1:100:A:ASP:H	1:83:A:VAL:HB	10	0.48
(1,2529)	1:99:A:LEU:H	1:31:A:GLU:HB2	2	0.48
(1,2117)	1:46:A:SER:H	1:43:A:PRO:HB3	1	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2117)	1:46:A:SER:H	1:43:A:PRO:HB3	3	0.48
(1,1961)	1:101:A:PRO:HB2	1:29:A:CYS:H	5	0.48
(1,1653)	1:121:A:LEU:HA	1:121:A:LEU:HD21	3	0.48
(1,1653)	1:121:A:LEU:HA	1:121:A:LEU:HD22	3	0.48
(1,1653)	1:121:A:LEU:HA	1:121:A:LEU:HD23	3	0.48
(1,1613)	1:101:A:PRO:HA	1:99:A:LEU:HD21	8	0.48
(1,1613)	1:101:A:PRO:HA	1:99:A:LEU:HD22	8	0.48
(1,1613)	1:101:A:PRO:HA	1:99:A:LEU:HD23	8	0.48
(1,1533)	1:50:A:ASN:HD22	1:75:A:VAL:HG21	1	0.48
(1,1533)	1:50:A:ASN:HD22	1:75:A:VAL:HG22	1	0.48
(1,1533)	1:50:A:ASN:HD22	1:75:A:VAL:HG23	1	0.48
(1,1392)	1:127:A:THR:H	1:25:A:VAL:HG11	4	0.48
(1,1392)	1:127:A:THR:H	1:25:A:VAL:HG12	4	0.48
(1,1392)	1:127:A:THR:H	1:25:A:VAL:HG13	4	0.48
(1,1253)	1:124:A:GLY:HA2	1:111:A:PHE:HZ	9	0.48
(1,1095)	1:110:A:LYS:HD3	1:109:A:TYR:HA	9	0.48
(1,1074)	1:107:A:GLY:HA2	1:109:A:TYR:HE1	6	0.48
(1,1074)	1:107:A:GLY:HA2	1:109:A:TYR:HE2	6	0.48
(1,1067)	1:107:A:GLY:HA2	1:55:A:LYS:HG2	10	0.48
(1,1067)	1:107:A:GLY:HA2	1:55:A:LYS:HG3	10	0.48
(1,737)	1:76:A:LYS:HD2	1:65:A:ASP:HB2	1	0.48
(1,737)	1:76:A:LYS:HD3	1:65:A:ASP:HB2	1	0.48
(1,730)	1:75:A:VAL:HB	1:75:A:VAL:H	4	0.48
(1,643)	1:76:A:LYS:HD2	1:66:A:GLY:HA3	8	0.48
(1,643)	1:76:A:LYS:HD3	1:66:A:GLY:HA3	8	0.48
(1,639)	1:67:A:VAL:HG11	1:64:A:LYS:HA	6	0.48
(1,639)	1:67:A:VAL:HG12	1:64:A:LYS:HA	6	0.48
(1,639)	1:67:A:VAL:HG13	1:64:A:LYS:HA	6	0.48
(1,233)	1:30:A:LYS:HA	1:30:A:LYS:HD3	10	0.48
(1,82)	1:15:A:ASN:HB2	1:17:A:GLN:HB2	8	0.48
(1,2944)	1:107:A:GLY:HA3	1:109:A:TYR:HD1	9	0.47
(1,2944)	1:107:A:GLY:HA3	1:109:A:TYR:HD2	9	0.47
(1,2542)	1:100:A:ASP:H	1:83:A:VAL:HA	4	0.47
(1,2356)	1:78:A:ASP:H	1:76:A:LYS:HD2	8	0.47
(1,2356)	1:78:A:ASP:H	1:76:A:LYS:HD3	8	0.47
(1,2045)	1:94:A:GLU:HB2	1:38:A:HIS:H	8	0.47
(1,1698)	1:24:A:GLN:HG3	1:129:A:VAL:HG21	8	0.47
(1,1698)	1:24:A:GLN:HG3	1:129:A:VAL:HG22	8	0.47
(1,1698)	1:24:A:GLN:HG3	1:129:A:VAL:HG23	8	0.47
(1,1653)	1:121:A:LEU:HA	1:121:A:LEU:HD21	8	0.47
(1,1653)	1:121:A:LEU:HA	1:121:A:LEU:HD22	8	0.47
(1,1653)	1:121:A:LEU:HA	1:121:A:LEU:HD23	8	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1498)	1:62:A:VAL:HG11	1:54:A:ALA:H	4	0.47
(1,1498)	1:62:A:VAL:HG12	1:54:A:ALA:H	4	0.47
(1,1498)	1:62:A:VAL:HG13	1:54:A:ALA:H	4	0.47
(1,1392)	1:127:A:THR:H	1:25:A:VAL:HG11	6	0.47
(1,1392)	1:127:A:THR:H	1:25:A:VAL:HG12	6	0.47
(1,1392)	1:127:A:THR:H	1:25:A:VAL:HG13	6	0.47
(1,1392)	1:127:A:THR:H	1:25:A:VAL:HG11	7	0.47
(1,1392)	1:127:A:THR:H	1:25:A:VAL:HG12	7	0.47
(1,1392)	1:127:A:THR:H	1:25:A:VAL:HG13	7	0.47
(1,1381)	1:104:A:LEU:HD11	1:25:A:VAL:HG21	6	0.47
(1,1381)	1:104:A:LEU:HD11	1:25:A:VAL:HG22	6	0.47
(1,1381)	1:104:A:LEU:HD11	1:25:A:VAL:HG23	6	0.47
(1,1381)	1:104:A:LEU:HD12	1:25:A:VAL:HG21	6	0.47
(1,1381)	1:104:A:LEU:HD12	1:25:A:VAL:HG22	6	0.47
(1,1381)	1:104:A:LEU:HD12	1:25:A:VAL:HG23	6	0.47
(1,1381)	1:104:A:LEU:HD13	1:25:A:VAL:HG21	6	0.47
(1,1381)	1:104:A:LEU:HD13	1:25:A:VAL:HG22	6	0.47
(1,1381)	1:104:A:LEU:HD13	1:25:A:VAL:HG23	6	0.47
(1,1016)	1:99:A:LEU:HD21	1:101:A:PRO:HD3	4	0.47
(1,1016)	1:99:A:LEU:HD22	1:101:A:PRO:HD3	4	0.47
(1,1016)	1:99:A:LEU:HD23	1:101:A:PRO:HD3	4	0.47
(1,1016)	1:99:A:LEU:HD21	1:101:A:PRO:HD3	10	0.47
(1,1016)	1:99:A:LEU:HD22	1:101:A:PRO:HD3	10	0.47
(1,1016)	1:99:A:LEU:HD23	1:101:A:PRO:HD3	10	0.47
(1,1003)	1:100:A:ASP:HA	1:99:A:LEU:HD21	9	0.47
(1,1003)	1:100:A:ASP:HA	1:99:A:LEU:HD22	9	0.47
(1,1003)	1:100:A:ASP:HA	1:99:A:LEU:HD23	9	0.47
(1,952)	1:96:A:SER:HA	1:36:A:LEU:HB3	5	0.47
(1,822)	1:85:A:HIS:HB3	1:52:A:VAL:HG21	2	0.47
(1,822)	1:85:A:HIS:HB3	1:52:A:VAL:HG22	2	0.47
(1,822)	1:85:A:HIS:HB3	1:52:A:VAL:HG23	2	0.47
(1,730)	1:75:A:VAL:HB	1:75:A:VAL:H	5	0.47
(1,646)	1:76:A:LYS:HB3	1:66:A:GLY:HA3	10	0.47
(1,45)	1:11:A:GLU:HG3	1:9:A:THR:HG21	10	0.47
(1,45)	1:11:A:GLU:HG3	1:9:A:THR:HG22	10	0.47
(1,45)	1:11:A:GLU:HG3	1:9:A:THR:HG23	10	0.47
(1,3148)	1:53:A:ILE:HD11	1:104:A:LEU:HD22	10	0.46
(1,3075)	1:55:A:LYS:HB2	1:54:A:ALA:HB3	1	0.46
(1,2964)	1:109:A:TYR:HD1	1:128:A:LEU:HD21	7	0.46
(1,2964)	1:109:A:TYR:HD1	1:128:A:LEU:HD22	7	0.46
(1,2964)	1:109:A:TYR:HD1	1:128:A:LEU:HD23	7	0.46
(1,2964)	1:109:A:TYR:HD2	1:128:A:LEU:HD21	7	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2964)	1:109:A:TYR:HD2	1:128:A:LEU:HD22	7	0.46
(1,2964)	1:109:A:TYR:HD2	1:128:A:LEU:HD23	7	0.46
(1,2876)	1:38:A:HIS:HE1	1:13:A:ASN:HB2	10	0.46
(1,2214)	1:83:A:VAL:HG11	1:55:A:LYS:H	1	0.46
(1,2214)	1:83:A:VAL:HG12	1:55:A:LYS:H	1	0.46
(1,2214)	1:83:A:VAL:HG13	1:55:A:LYS:H	1	0.46
(1,1702)	1:83:A:VAL:HG21	1:99:A:LEU:HD11	7	0.46
(1,1702)	1:83:A:VAL:HG21	1:99:A:LEU:HD12	7	0.46
(1,1702)	1:83:A:VAL:HG21	1:99:A:LEU:HD13	7	0.46
(1,1702)	1:83:A:VAL:HG22	1:99:A:LEU:HD11	7	0.46
(1,1702)	1:83:A:VAL:HG22	1:99:A:LEU:HD12	7	0.46
(1,1702)	1:83:A:VAL:HG22	1:99:A:LEU:HD13	7	0.46
(1,1702)	1:83:A:VAL:HG23	1:99:A:LEU:HD11	7	0.46
(1,1702)	1:83:A:VAL:HG23	1:99:A:LEU:HD12	7	0.46
(1,1702)	1:83:A:VAL:HG23	1:99:A:LEU:HD13	7	0.46
(1,1562)	1:89:A:ILE:H	1:88:A:LEU:HD21	7	0.46
(1,1562)	1:89:A:ILE:H	1:88:A:LEU:HD22	7	0.46
(1,1562)	1:89:A:ILE:H	1:88:A:LEU:HD23	7	0.46
(1,1533)	1:50:A:ASN:HD22	1:75:A:VAL:HG21	3	0.46
(1,1533)	1:50:A:ASN:HD22	1:75:A:VAL:HG22	3	0.46
(1,1533)	1:50:A:ASN:HD22	1:75:A:VAL:HG23	3	0.46
(1,1381)	1:104:A:LEU:HD11	1:25:A:VAL:HG21	9	0.46
(1,1381)	1:104:A:LEU:HD11	1:25:A:VAL:HG22	9	0.46
(1,1381)	1:104:A:LEU:HD11	1:25:A:VAL:HG23	9	0.46
(1,1381)	1:104:A:LEU:HD12	1:25:A:VAL:HG21	9	0.46
(1,1381)	1:104:A:LEU:HD12	1:25:A:VAL:HG22	9	0.46
(1,1381)	1:104:A:LEU:HD12	1:25:A:VAL:HG23	9	0.46
(1,1381)	1:104:A:LEU:HD13	1:25:A:VAL:HG21	9	0.46
(1,1381)	1:104:A:LEU:HD13	1:25:A:VAL:HG22	9	0.46
(1,1381)	1:104:A:LEU:HD13	1:25:A:VAL:HG23	9	0.46
(1,1095)	1:110:A:LYS:HD3	1:109:A:TYR:HA	6	0.46
(1,1063)	1:107:A:GLY:HA2	1:55:A:LYS:HD2	2	0.46
(1,994)	1:83:A:VAL:HG21	1:99:A:LEU:HB3	4	0.46
(1,994)	1:83:A:VAL:HG22	1:99:A:LEU:HB3	4	0.46
(1,994)	1:83:A:VAL:HG23	1:99:A:LEU:HB3	4	0.46
(1,730)	1:75:A:VAL:HB	1:75:A:VAL:H	8	0.46
(1,646)	1:76:A:LYS:HB3	1:66:A:GLY:HA3	5	0.46
(1,643)	1:76:A:LYS:HD2	1:66:A:GLY:HA3	9	0.46
(1,643)	1:76:A:LYS:HD3	1:66:A:GLY:HA3	9	0.46
(1,255)	1:98:A:THR:HG21	1:31:A:GLU:HG2	6	0.46
(1,255)	1:98:A:THR:HG21	1:31:A:GLU:HG3	6	0.46
(1,255)	1:98:A:THR:HG22	1:31:A:GLU:HG2	6	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,255)	1:98:A:THR:HG22	1:31:A:GLU:HG3	6	0.46
(1,255)	1:98:A:THR:HG23	1:31:A:GLU:HG2	6	0.46
(1,255)	1:98:A:THR:HG23	1:31:A:GLU:HG3	6	0.46
(1,178)	1:25:A:VAL:H	1:24:A:GLN:HG3	3	0.46
(1,52)	1:49:A:HIS:HD2	1:12:A:SER:HB3	1	0.46
(1,3014)	1:115:A:PHE:HE1	1:48:A:GLY:HA2	9	0.45
(1,3014)	1:115:A:PHE:HE2	1:48:A:GLY:HA2	9	0.45
(1,2883)	1:88:A:LEU:HG	1:74:A:TYR:HD1	7	0.45
(1,2883)	1:88:A:LEU:HG	1:74:A:TYR:HD2	7	0.45
(1,2876)	1:38:A:HIS:HE1	1:13:A:ASN:HB2	9	0.45
(1,2623)	1:125:A:LYS:HD2	1:110:A:LYS:H	3	0.45
(1,2623)	1:125:A:LYS:HD3	1:110:A:LYS:H	3	0.45
(1,2173)	1:51:A:LEU:H	1:36:A:LEU:HD11	7	0.45
(1,2173)	1:51:A:LEU:H	1:36:A:LEU:HD12	7	0.45
(1,2173)	1:51:A:LEU:H	1:36:A:LEU:HD13	7	0.45
(1,1801)	1:13:A:ASN:HD22	1:17:A:GLN:HB3	10	0.45
(1,1525)	1:114:A:THR:HG21	1:75:A:VAL:HG21	10	0.45
(1,1525)	1:114:A:THR:HG21	1:75:A:VAL:HG22	10	0.45
(1,1525)	1:114:A:THR:HG21	1:75:A:VAL:HG23	10	0.45
(1,1525)	1:114:A:THR:HG22	1:75:A:VAL:HG21	10	0.45
(1,1525)	1:114:A:THR:HG22	1:75:A:VAL:HG22	10	0.45
(1,1525)	1:114:A:THR:HG22	1:75:A:VAL:HG23	10	0.45
(1,1525)	1:114:A:THR:HG23	1:75:A:VAL:HG21	10	0.45
(1,1525)	1:114:A:THR:HG23	1:75:A:VAL:HG22	10	0.45
(1,1525)	1:114:A:THR:HG23	1:75:A:VAL:HG23	10	0.45
(1,1303)	1:56:A:ALA:H	1:55:A:LYS:HD2	5	0.45
(1,1303)	1:56:A:ALA:H	1:55:A:LYS:HD2	7	0.45
(1,1085)	1:108:A:ASP:HB3	1:56:A:ALA:H	8	0.45
(1,994)	1:83:A:VAL:HG21	1:99:A:LEU:HB3	7	0.45
(1,994)	1:83:A:VAL:HG22	1:99:A:LEU:HB3	7	0.45
(1,994)	1:83:A:VAL:HG23	1:99:A:LEU:HB3	7	0.45
(1,952)	1:96:A:SER:HA	1:36:A:LEU:HB3	1	0.45
(1,730)	1:75:A:VAL:HB	1:75:A:VAL:H	7	0.45
(1,730)	1:75:A:VAL:HB	1:75:A:VAL:H	10	0.45
(1,390)	1:41:A:THR:HB	1:91:A:GLY:HA2	3	0.45
(1,390)	1:41:A:THR:HB	1:91:A:GLY:HA2	4	0.45
(1,82)	1:15:A:ASN:HB2	1:17:A:GLN:HB2	9	0.45
(1,52)	1:49:A:HIS:HD2	1:12:A:SER:HB3	5	0.45
(1,3246)	1:123:A:ASN:HD22	1:120:A:ALA:HB2	5	0.44
(1,3134)	1:23:A:ILE:HG12	1:34:A:ILE:HG22	6	0.44
(1,3014)	1:115:A:PHE:HE1	1:48:A:GLY:HA2	2	0.44
(1,3014)	1:115:A:PHE:HE2	1:48:A:GLY:HA2	2	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3014)	1:115:A:PHE:HE1	1:48:A:GLY:HA2	5	0.44
(1,3014)	1:115:A:PHE:HE2	1:48:A:GLY:HA2	5	0.44
(1,3014)	1:115:A:PHE:HE1	1:48:A:GLY:HA2	10	0.44
(1,3014)	1:115:A:PHE:HE2	1:48:A:GLY:HA2	10	0.44
(1,2902)	1:49:A:HIS:HD2	1:90:A:GLY:HA3	8	0.44
(1,2534)	1:100:A:ASP:H	1:83:A:VAL:HG21	2	0.44
(1,2534)	1:100:A:ASP:H	1:83:A:VAL:HG22	2	0.44
(1,2534)	1:100:A:ASP:H	1:83:A:VAL:HG23	2	0.44
(1,2349)	1:79:A:ASP:H	1:76:A:LYS:H	9	0.44
(1,2241)	1:57:A:GLU:HG3	1:58:A:ASP:H	6	0.44
(1,1980)	1:99:A:LEU:HB3	1:32:A:PHE:H	1	0.44
(1,1801)	1:13:A:ASN:HD22	1:17:A:GLN:HB3	6	0.44
(1,1755)	1:86:A:THR:HG21	1:10:A:VAL:H	3	0.44
(1,1755)	1:86:A:THR:HG22	1:10:A:VAL:H	3	0.44
(1,1755)	1:86:A:THR:HG23	1:10:A:VAL:H	3	0.44
(1,1755)	1:86:A:THR:HG21	1:10:A:VAL:H	10	0.44
(1,1755)	1:86:A:THR:HG22	1:10:A:VAL:H	10	0.44
(1,1755)	1:86:A:THR:HG23	1:10:A:VAL:H	10	0.44
(1,1705)	1:99:A:LEU:HD11	1:31:A:GLU:HB2	10	0.44
(1,1705)	1:99:A:LEU:HD12	1:31:A:GLU:HB2	10	0.44
(1,1705)	1:99:A:LEU:HD13	1:31:A:GLU:HB2	10	0.44
(1,1133)	1:111:A:PHE:HB2	1:126:A:VAL:HG21	7	0.44
(1,1133)	1:111:A:PHE:HB2	1:126:A:VAL:HG22	7	0.44
(1,1133)	1:111:A:PHE:HB2	1:126:A:VAL:HG23	7	0.44
(1,952)	1:96:A:SER:HA	1:36:A:LEU:HB3	6	0.44
(1,830)	1:86:A:THR:HA	1:97:A:LEU:HB2	6	0.44
(1,830)	1:86:A:THR:HA	1:97:A:LEU:HB2	8	0.44
(1,730)	1:75:A:VAL:HB	1:75:A:VAL:H	1	0.44
(1,730)	1:75:A:VAL:HB	1:75:A:VAL:H	9	0.44
(1,3048)	1:25:A:VAL:HB	1:23:A:ILE:HG21	7	0.43
(1,3014)	1:115:A:PHE:HE1	1:48:A:GLY:HA2	3	0.43
(1,3014)	1:115:A:PHE:HE2	1:48:A:GLY:HA2	3	0.43
(1,2955)	1:55:A:LYS:HB3	1:109:A:TYR:HE1	9	0.43
(1,2955)	1:55:A:LYS:HB3	1:109:A:TYR:HE2	9	0.43
(1,2944)	1:107:A:GLY:HA3	1:109:A:TYR:HD1	7	0.43
(1,2944)	1:107:A:GLY:HA3	1:109:A:TYR:HD2	7	0.43
(1,2764)	1:124:A:GLY:H	1:110:A:LYS:HE2	2	0.43
(1,2764)	1:124:A:GLY:H	1:110:A:LYS:HE3	2	0.43
(1,2745)	1:123:A:ASN:H	1:21:A:LYS:HG2	8	0.43
(1,2745)	1:123:A:ASN:H	1:21:A:LYS:HG3	8	0.43
(1,2696)	1:117:A:GLY:H	1:67:A:VAL:HG11	8	0.43
(1,2696)	1:117:A:GLY:H	1:67:A:VAL:HG12	8	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2696)	1:117:A:GLY:H	1:67:A:VAL:HG13	8	0.43
(1,2659)	1:124:A:GLY:H	1:113:A:CYS:H	10	0.43
(1,2528)	1:99:A:LEU:H	1:31:A:GLU:HG2	10	0.43
(1,2528)	1:99:A:LEU:H	1:31:A:GLU:HG3	10	0.43
(1,2508)	1:85:A:HIS:H	1:97:A:LEU:H	2	0.43
(1,2478)	1:93:A:GLU:H	1:38:A:HIS:HB2	10	0.43
(1,2362)	1:79:A:ASP:H	1:76:A:LYS:HB2	6	0.43
(1,2361)	1:82:A:VAL:HB	1:79:A:ASP:H	9	0.43
(1,2264)	1:61:A:GLY:H	1:59:A:MET:HG2	6	0.43
(1,2264)	1:61:A:GLY:H	1:59:A:MET:HG3	6	0.43
(1,2173)	1:51:A:LEU:H	1:36:A:LEU:HD11	8	0.43
(1,2173)	1:51:A:LEU:H	1:36:A:LEU:HD12	8	0.43
(1,2173)	1:51:A:LEU:H	1:36:A:LEU:HD13	8	0.43
(1,2173)	1:51:A:LEU:H	1:36:A:LEU:HD11	9	0.43
(1,2173)	1:51:A:LEU:H	1:36:A:LEU:HD12	9	0.43
(1,2173)	1:51:A:LEU:H	1:36:A:LEU:HD13	9	0.43
(1,2114)	1:46:A:SER:H	1:43:A:PRO:HD3	1	0.43
(1,2074)	1:91:A:GLY:HA2	1:41:A:THR:H	4	0.43
(1,1980)	1:99:A:LEU:HB3	1:32:A:PHE:H	7	0.43
(1,1897)	1:25:A:VAL:HG11	1:24:A:GLN:H	10	0.43
(1,1897)	1:25:A:VAL:HG12	1:24:A:GLN:H	10	0.43
(1,1897)	1:25:A:VAL:HG13	1:24:A:GLN:H	10	0.43
(1,1799)	1:13:A:ASN:HD21	1:17:A:GLN:HB3	9	0.43
(1,1654)	1:122:A:MET:HG2	1:121:A:LEU:HD11	7	0.43
(1,1654)	1:122:A:MET:HG2	1:121:A:LEU:HD12	7	0.43
(1,1654)	1:122:A:MET:HG2	1:121:A:LEU:HD13	7	0.43
(1,1654)	1:122:A:MET:HG3	1:121:A:LEU:HD11	7	0.43
(1,1654)	1:122:A:MET:HG3	1:121:A:LEU:HD12	7	0.43
(1,1654)	1:122:A:MET:HG3	1:121:A:LEU:HD13	7	0.43
(1,1535)	1:75:A:VAL:HG21	1:50:A:ASN:HD21	7	0.43
(1,1535)	1:75:A:VAL:HG22	1:50:A:ASN:HD21	7	0.43
(1,1535)	1:75:A:VAL:HG23	1:50:A:ASN:HD21	7	0.43
(1,1393)	1:25:A:VAL:H	1:25:A:VAL:HG11	4	0.43
(1,1393)	1:25:A:VAL:H	1:25:A:VAL:HG12	4	0.43
(1,1393)	1:25:A:VAL:H	1:25:A:VAL:HG13	4	0.43
(1,1393)	1:25:A:VAL:H	1:25:A:VAL:HG11	5	0.43
(1,1393)	1:25:A:VAL:H	1:25:A:VAL:HG12	5	0.43
(1,1393)	1:25:A:VAL:H	1:25:A:VAL:HG13	5	0.43
(1,1392)	1:127:A:THR:H	1:25:A:VAL:HG11	9	0.43
(1,1392)	1:127:A:THR:H	1:25:A:VAL:HG12	9	0.43
(1,1392)	1:127:A:THR:H	1:25:A:VAL:HG13	9	0.43
(1,1381)	1:104:A:LEU:HD11	1:25:A:VAL:HG21	7	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1381)	1:104:A:LEU:HD11	1:25:A:VAL:HG22	7	0.43
(1,1381)	1:104:A:LEU:HD11	1:25:A:VAL:HG23	7	0.43
(1,1381)	1:104:A:LEU:HD12	1:25:A:VAL:HG21	7	0.43
(1,1381)	1:104:A:LEU:HD12	1:25:A:VAL:HG22	7	0.43
(1,1381)	1:104:A:LEU:HD12	1:25:A:VAL:HG23	7	0.43
(1,1381)	1:104:A:LEU:HD13	1:25:A:VAL:HG21	7	0.43
(1,1381)	1:104:A:LEU:HD13	1:25:A:VAL:HG22	7	0.43
(1,1381)	1:104:A:LEU:HD13	1:25:A:VAL:HG23	7	0.43
(1,1003)	1:100:A:ASP:HA	1:99:A:LEU:HD21	4	0.43
(1,1003)	1:100:A:ASP:HA	1:99:A:LEU:HD22	4	0.43
(1,1003)	1:100:A:ASP:HA	1:99:A:LEU:HD23	4	0.43
(1,952)	1:96:A:SER:HA	1:36:A:LEU:HB3	10	0.43
(1,464)	1:88:A:LEU:HD11	1:48:A:GLY:HA2	10	0.43
(1,464)	1:88:A:LEU:HD12	1:48:A:GLY:HA2	10	0.43
(1,464)	1:88:A:LEU:HD13	1:48:A:GLY:HA2	10	0.43
(1,204)	1:26:A:SER:HB3	1:25:A:VAL:HA	8	0.43
(1,52)	1:49:A:HIS:HD2	1:12:A:SER:HB3	7	0.43
(1,35)	1:11:A:GLU:HA	1:36:A:LEU:HD21	2	0.43
(1,35)	1:11:A:GLU:HA	1:36:A:LEU:HD22	2	0.43
(1,35)	1:11:A:GLU:HA	1:36:A:LEU:HD23	2	0.43
(1,3264)	1:111:A:PHE:HD1	1:20:A:THR:HG21	6	0.42
(1,2944)	1:107:A:GLY:HA3	1:109:A:TYR:HD1	3	0.42
(1,2944)	1:107:A:GLY:HA3	1:109:A:TYR:HD2	3	0.42
(1,2876)	1:38:A:HIS:HE1	1:13:A:ASN:HB2	7	0.42
(1,2538)	1:100:A:ASP:H	1:83:A:VAL:HB	2	0.42
(1,2478)	1:93:A:GLU:H	1:38:A:HIS:HB2	7	0.42
(1,1960)	1:101:A:PRO:HG2	1:29:A:CYS:H	5	0.42
(1,1950)	1:27:A:LYS:HD2	1:28:A:ALA:H	4	0.42
(1,1950)	1:27:A:LYS:HD3	1:28:A:ALA:H	4	0.42
(1,1897)	1:25:A:VAL:HG11	1:24:A:GLN:H	2	0.42
(1,1897)	1:25:A:VAL:HG12	1:24:A:GLN:H	2	0.42
(1,1897)	1:25:A:VAL:HG13	1:24:A:GLN:H	2	0.42
(1,1897)	1:25:A:VAL:HG11	1:24:A:GLN:H	7	0.42
(1,1897)	1:25:A:VAL:HG12	1:24:A:GLN:H	7	0.42
(1,1897)	1:25:A:VAL:HG13	1:24:A:GLN:H	7	0.42
(1,1897)	1:25:A:VAL:HG11	1:24:A:GLN:H	9	0.42
(1,1897)	1:25:A:VAL:HG12	1:24:A:GLN:H	9	0.42
(1,1897)	1:25:A:VAL:HG13	1:24:A:GLN:H	9	0.42
(1,1797)	1:15:A:ASN:HB3	1:13:A:ASN:HD21	8	0.42
(1,1702)	1:83:A:VAL:HG21	1:99:A:LEU:HD11	6	0.42
(1,1702)	1:83:A:VAL:HG21	1:99:A:LEU:HD12	6	0.42
(1,1702)	1:83:A:VAL:HG21	1:99:A:LEU:HD13	6	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1702)	1:83:A:VAL:HG22	1:99:A:LEU:HD11	6	0.42
(1,1702)	1:83:A:VAL:HG22	1:99:A:LEU:HD12	6	0.42
(1,1702)	1:83:A:VAL:HG22	1:99:A:LEU:HD13	6	0.42
(1,1702)	1:83:A:VAL:HG23	1:99:A:LEU:HD11	6	0.42
(1,1702)	1:83:A:VAL:HG23	1:99:A:LEU:HD12	6	0.42
(1,1702)	1:83:A:VAL:HG23	1:99:A:LEU:HD13	6	0.42
(1,1628)	1:101:A:PRO:HB2	1:104:A:LEU:HD11	9	0.42
(1,1628)	1:101:A:PRO:HB2	1:104:A:LEU:HD12	9	0.42
(1,1628)	1:101:A:PRO:HB2	1:104:A:LEU:HD13	9	0.42
(1,1595)	1:53:A:ILE:HG12	1:97:A:LEU:HD11	10	0.42
(1,1595)	1:53:A:ILE:HG12	1:97:A:LEU:HD12	10	0.42
(1,1595)	1:53:A:ILE:HG12	1:97:A:LEU:HD13	10	0.42
(1,1498)	1:62:A:VAL:HG11	1:54:A:ALA:H	7	0.42
(1,1498)	1:62:A:VAL:HG12	1:54:A:ALA:H	7	0.42
(1,1498)	1:62:A:VAL:HG13	1:54:A:ALA:H	7	0.42
(1,1461)	1:126:A:VAL:HG11	1:51:A:LEU:HD21	6	0.42
(1,1461)	1:126:A:VAL:HG11	1:51:A:LEU:HD22	6	0.42
(1,1461)	1:126:A:VAL:HG11	1:51:A:LEU:HD23	6	0.42
(1,1461)	1:126:A:VAL:HG12	1:51:A:LEU:HD21	6	0.42
(1,1461)	1:126:A:VAL:HG12	1:51:A:LEU:HD22	6	0.42
(1,1461)	1:126:A:VAL:HG12	1:51:A:LEU:HD23	6	0.42
(1,1461)	1:126:A:VAL:HG13	1:51:A:LEU:HD21	6	0.42
(1,1461)	1:126:A:VAL:HG13	1:51:A:LEU:HD22	6	0.42
(1,1461)	1:126:A:VAL:HG13	1:51:A:LEU:HD23	6	0.42
(1,1393)	1:25:A:VAL:H	1:25:A:VAL:HG11	6	0.42
(1,1393)	1:25:A:VAL:H	1:25:A:VAL:HG12	6	0.42
(1,1393)	1:25:A:VAL:H	1:25:A:VAL:HG13	6	0.42
(1,1393)	1:25:A:VAL:H	1:25:A:VAL:HG11	7	0.42
(1,1393)	1:25:A:VAL:H	1:25:A:VAL:HG12	7	0.42
(1,1393)	1:25:A:VAL:H	1:25:A:VAL:HG13	7	0.42
(1,1393)	1:25:A:VAL:H	1:25:A:VAL:HG11	9	0.42
(1,1393)	1:25:A:VAL:H	1:25:A:VAL:HG12	9	0.42
(1,1393)	1:25:A:VAL:H	1:25:A:VAL:HG13	9	0.42
(1,1392)	1:127:A:THR:H	1:25:A:VAL:HG11	5	0.42
(1,1392)	1:127:A:THR:H	1:25:A:VAL:HG12	5	0.42
(1,1392)	1:127:A:THR:H	1:25:A:VAL:HG13	5	0.42
(1,1093)	1:56:A:ALA:HB1	1:108:A:ASP:HB2	4	0.42
(1,1093)	1:56:A:ALA:HB2	1:108:A:ASP:HB2	4	0.42
(1,1093)	1:56:A:ALA:HB3	1:108:A:ASP:HB2	4	0.42
(1,1001)	1:100:A:ASP:HA	1:31:A:GLU:HB2	10	0.42
(1,830)	1:86:A:THR:HA	1:97:A:LEU:HB2	3	0.42
(1,741)	1:77:A:PRO:HA	1:75:A:VAL:HG11	5	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,741)	1:77:A:PRO:HA	1:75:A:VAL:HG12	5	0.42
(1,741)	1:77:A:PRO:HA	1:75:A:VAL:HG13	5	0.42
(1,678)	1:68:A:GLY:HA3	1:67:A:VAL:HG21	8	0.42
(1,678)	1:68:A:GLY:HA3	1:67:A:VAL:HG22	8	0.42
(1,678)	1:68:A:GLY:HA3	1:67:A:VAL:HG23	8	0.42
(1,426)	1:43:A:PRO:HG3	1:46:A:SER:H	4	0.42
(1,230)	1:29:A:CYS:HB2	1:25:A:VAL:HG21	2	0.42
(1,230)	1:29:A:CYS:HB2	1:25:A:VAL:HG22	2	0.42
(1,230)	1:29:A:CYS:HB2	1:25:A:VAL:HG23	2	0.42
(1,230)	1:29:A:CYS:HB3	1:25:A:VAL:HG21	2	0.42
(1,230)	1:29:A:CYS:HB3	1:25:A:VAL:HG22	2	0.42
(1,230)	1:29:A:CYS:HB3	1:25:A:VAL:HG23	2	0.42
(1,204)	1:26:A:SER:HB3	1:25:A:VAL:HA	6	0.42
(1,3249)	1:128:A:LEU:HB2	1:129:A:VAL:H	8	0.41
(1,3177)	1:9:A:THR:HG21	1:35:A:THR:H	3	0.41
(1,3167)	1:129:A:VAL:HG22	1:24:A:GLN:H	2	0.41
(1,2945)	1:105:A:ALA:HA	1:109:A:TYR:HE1	5	0.41
(1,2945)	1:105:A:ALA:HA	1:109:A:TYR:HE2	5	0.41
(1,2759)	1:123:A:ASN:HD22	1:21:A:LYS:HG2	10	0.41
(1,2759)	1:123:A:ASN:HD22	1:21:A:LYS:HG3	10	0.41
(1,2747)	1:123:A:ASN:H	1:121:A:LEU:HD11	10	0.41
(1,2747)	1:123:A:ASN:H	1:121:A:LEU:HD12	10	0.41
(1,2747)	1:123:A:ASN:H	1:121:A:LEU:HD13	10	0.41
(1,2659)	1:124:A:GLY:H	1:113:A:CYS:H	9	0.41
(1,2469)	1:92:A:GLY:H	1:38:A:HIS:HB2	3	0.41
(1,2350)	1:76:A:LYS:H	1:65:A:ASP:HB2	8	0.41
(1,2179)	1:51:A:LEU:H	1:95:A:SER:HB2	1	0.41
(1,2138)	1:88:A:LEU:HD11	1:48:A:GLY:H	9	0.41
(1,2138)	1:88:A:LEU:HD12	1:48:A:GLY:H	9	0.41
(1,2138)	1:88:A:LEU:HD13	1:48:A:GLY:H	9	0.41
(1,1950)	1:27:A:LYS:HD2	1:28:A:ALA:H	9	0.41
(1,1950)	1:27:A:LYS:HD3	1:28:A:ALA:H	9	0.41
(1,1867)	1:19:A:ASN:HD22	1:11:A:GLU:HG2	8	0.41
(1,1801)	1:13:A:ASN:HD22	1:17:A:GLN:HB3	1	0.41
(1,1755)	1:86:A:THR:HG21	1:10:A:VAL:H	7	0.41
(1,1755)	1:86:A:THR:HG22	1:10:A:VAL:H	7	0.41
(1,1755)	1:86:A:THR:HG23	1:10:A:VAL:H	7	0.41
(1,1667)	1:53:A:ILE:HB	1:126:A:VAL:HG21	5	0.41
(1,1667)	1:53:A:ILE:HB	1:126:A:VAL:HG22	5	0.41
(1,1667)	1:53:A:ILE:HB	1:126:A:VAL:HG23	5	0.41
(1,1533)	1:50:A:ASN:HD22	1:75:A:VAL:HG21	5	0.41
(1,1533)	1:50:A:ASN:HD22	1:75:A:VAL:HG22	5	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1533)	1:50:A:ASN:HD22	1:75:A:VAL:HG23	5	0.41
(1,1514)	1:75:A:VAL:HB	1:69:A:ALA:HB1	10	0.41
(1,1514)	1:75:A:VAL:HB	1:69:A:ALA:HB2	10	0.41
(1,1514)	1:75:A:VAL:HB	1:69:A:ALA:HB3	10	0.41
(1,1420)	1:51:A:LEU:H	1:34:A:ILE:HG21	4	0.41
(1,1420)	1:51:A:LEU:H	1:34:A:ILE:HG22	4	0.41
(1,1420)	1:51:A:LEU:H	1:34:A:ILE:HG23	4	0.41
(1,1393)	1:25:A:VAL:H	1:25:A:VAL:HG11	2	0.41
(1,1393)	1:25:A:VAL:H	1:25:A:VAL:HG12	2	0.41
(1,1393)	1:25:A:VAL:H	1:25:A:VAL:HG13	2	0.41
(1,1393)	1:25:A:VAL:H	1:25:A:VAL:HG11	8	0.41
(1,1393)	1:25:A:VAL:H	1:25:A:VAL:HG12	8	0.41
(1,1393)	1:25:A:VAL:H	1:25:A:VAL:HG13	8	0.41
(1,1393)	1:25:A:VAL:H	1:25:A:VAL:HG11	10	0.41
(1,1393)	1:25:A:VAL:H	1:25:A:VAL:HG12	10	0.41
(1,1393)	1:25:A:VAL:H	1:25:A:VAL:HG13	10	0.41
(1,1063)	1:107:A:GLY:HA2	1:55:A:LYS:HD2	7	0.41
(1,760)	1:76:A:LYS:HD2	1:77:A:PRO:HD2	7	0.41
(1,760)	1:76:A:LYS:HD3	1:77:A:PRO:HD2	7	0.41
(1,759)	1:77:A:PRO:HD2	1:69:A:ALA:HB1	4	0.41
(1,759)	1:77:A:PRO:HD2	1:69:A:ALA:HB2	4	0.41
(1,759)	1:77:A:PRO:HD2	1:69:A:ALA:HB3	4	0.41
(1,564)	1:55:A:LYS:HB2	1:58:A:ASP:H	7	0.41
(1,426)	1:43:A:PRO:HG3	1:46:A:SER:H	8	0.41
(1,2964)	1:109:A:TYR:HD1	1:128:A:LEU:HD21	6	0.4
(1,2964)	1:109:A:TYR:HD1	1:128:A:LEU:HD22	6	0.4
(1,2964)	1:109:A:TYR:HD1	1:128:A:LEU:HD23	6	0.4
(1,2964)	1:109:A:TYR:HD2	1:128:A:LEU:HD21	6	0.4
(1,2964)	1:109:A:TYR:HD2	1:128:A:LEU:HD22	6	0.4
(1,2964)	1:109:A:TYR:HD2	1:128:A:LEU:HD23	6	0.4
(1,2944)	1:107:A:GLY:HA3	1:109:A:TYR:HD1	8	0.4
(1,2944)	1:107:A:GLY:HA3	1:109:A:TYR:HD2	8	0.4
(1,2902)	1:49:A:HIS:HD2	1:90:A:GLY:HA3	1	0.4
(1,2836)	1:18:A:PHE:HE1	1:36:A:LEU:HD21	5	0.4
(1,2836)	1:18:A:PHE:HE1	1:36:A:LEU:HD22	5	0.4
(1,2836)	1:18:A:PHE:HE1	1:36:A:LEU:HD23	5	0.4
(1,2836)	1:18:A:PHE:HE2	1:36:A:LEU:HD21	5	0.4
(1,2836)	1:18:A:PHE:HE2	1:36:A:LEU:HD22	5	0.4
(1,2836)	1:18:A:PHE:HE2	1:36:A:LEU:HD23	5	0.4
(1,2623)	1:125:A:LYS:HD2	1:110:A:LYS:H	2	0.4
(1,2623)	1:125:A:LYS:HD3	1:110:A:LYS:H	2	0.4
(1,2478)	1:93:A:GLU:H	1:38:A:HIS:HB2	5	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2468)	1:92:A:GLY:H	1:39:A:THR:HA	7	0.4
(1,2173)	1:51:A:LEU:H	1:36:A:LEU:HD11	4	0.4
(1,2173)	1:51:A:LEU:H	1:36:A:LEU:HD12	4	0.4
(1,2173)	1:51:A:LEU:H	1:36:A:LEU:HD13	4	0.4
(1,1897)	1:25:A:VAL:HG11	1:24:A:GLN:H	4	0.4
(1,1897)	1:25:A:VAL:HG12	1:24:A:GLN:H	4	0.4
(1,1897)	1:25:A:VAL:HG13	1:24:A:GLN:H	4	0.4
(1,1897)	1:25:A:VAL:HG11	1:24:A:GLN:H	5	0.4
(1,1897)	1:25:A:VAL:HG12	1:24:A:GLN:H	5	0.4
(1,1897)	1:25:A:VAL:HG13	1:24:A:GLN:H	5	0.4
(1,1867)	1:19:A:ASN:HD22	1:11:A:GLU:HG2	6	0.4
(1,1755)	1:86:A:THR:HG21	1:10:A:VAL:H	1	0.4
(1,1755)	1:86:A:THR:HG22	1:10:A:VAL:H	1	0.4
(1,1755)	1:86:A:THR:HG23	1:10:A:VAL:H	1	0.4
(1,1667)	1:53:A:ILE:HB	1:126:A:VAL:HG21	1	0.4
(1,1667)	1:53:A:ILE:HB	1:126:A:VAL:HG22	1	0.4
(1,1667)	1:53:A:ILE:HB	1:126:A:VAL:HG23	1	0.4
(1,1613)	1:101:A:PRO:HA	1:99:A:LEU:HD21	10	0.4
(1,1613)	1:101:A:PRO:HA	1:99:A:LEU:HD22	10	0.4
(1,1613)	1:101:A:PRO:HA	1:99:A:LEU:HD23	10	0.4
(1,1609)	1:99:A:LEU:HD21	1:32:A:PHE:H	2	0.4
(1,1609)	1:99:A:LEU:HD22	1:32:A:PHE:H	2	0.4
(1,1609)	1:99:A:LEU:HD23	1:32:A:PHE:H	2	0.4
(1,1550)	1:83:A:VAL:HG11	1:104:A:LEU:HD21	6	0.4
(1,1550)	1:83:A:VAL:HG11	1:104:A:LEU:HD22	6	0.4
(1,1550)	1:83:A:VAL:HG11	1:104:A:LEU:HD23	6	0.4
(1,1550)	1:83:A:VAL:HG12	1:104:A:LEU:HD21	6	0.4
(1,1550)	1:83:A:VAL:HG12	1:104:A:LEU:HD22	6	0.4
(1,1550)	1:83:A:VAL:HG12	1:104:A:LEU:HD23	6	0.4
(1,1550)	1:83:A:VAL:HG13	1:104:A:LEU:HD21	6	0.4
(1,1550)	1:83:A:VAL:HG13	1:104:A:LEU:HD22	6	0.4
(1,1550)	1:83:A:VAL:HG13	1:104:A:LEU:HD23	6	0.4
(1,1535)	1:75:A:VAL:HG21	1:50:A:ASN:HD21	6	0.4
(1,1535)	1:75:A:VAL:HG22	1:50:A:ASN:HD21	6	0.4
(1,1535)	1:75:A:VAL:HG23	1:50:A:ASN:HD21	6	0.4
(1,1393)	1:25:A:VAL:H	1:25:A:VAL:HG11	1	0.4
(1,1393)	1:25:A:VAL:H	1:25:A:VAL:HG12	1	0.4
(1,1393)	1:25:A:VAL:H	1:25:A:VAL:HG13	1	0.4
(1,1350)	1:11:A:GLU:H	1:10:A:VAL:HG11	10	0.4
(1,1350)	1:11:A:GLU:H	1:10:A:VAL:HG12	10	0.4
(1,1350)	1:11:A:GLU:H	1:10:A:VAL:HG13	10	0.4
(1,1093)	1:56:A:ALA:HB1	1:108:A:ASP:HB2	6	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1093)	1:56:A:ALA:HB2	1:108:A:ASP:HB2	6	0.4
(1,1093)	1:56:A:ALA:HB3	1:108:A:ASP:HB2	6	0.4
(1,1074)	1:107:A:GLY:HA2	1:109:A:TYR:HE1	9	0.4
(1,1074)	1:107:A:GLY:HA2	1:109:A:TYR:HE2	9	0.4
(1,1067)	1:107:A:GLY:HA2	1:55:A:LYS:HG2	1	0.4
(1,1067)	1:107:A:GLY:HA2	1:55:A:LYS:HG3	1	0.4
(1,1003)	1:100:A:ASP:HA	1:99:A:LEU:HD21	10	0.4
(1,1003)	1:100:A:ASP:HA	1:99:A:LEU:HD22	10	0.4
(1,1003)	1:100:A:ASP:HA	1:99:A:LEU:HD23	10	0.4
(1,741)	1:77:A:PRO:HA	1:75:A:VAL:HG11	10	0.4
(1,741)	1:77:A:PRO:HA	1:75:A:VAL:HG12	10	0.4
(1,741)	1:77:A:PRO:HA	1:75:A:VAL:HG13	10	0.4
(1,740)	1:77:A:PRO:HA	1:72:A:THR:HG21	4	0.4
(1,740)	1:77:A:PRO:HA	1:72:A:THR:HG22	4	0.4
(1,740)	1:77:A:PRO:HA	1:72:A:THR:HG23	4	0.4
(1,241)	1:98:A:THR:HG21	1:31:A:GLU:HB3	1	0.4
(1,241)	1:98:A:THR:HG22	1:31:A:GLU:HB3	1	0.4
(1,241)	1:98:A:THR:HG23	1:31:A:GLU:HB3	1	0.4
(1,178)	1:25:A:VAL:H	1:24:A:GLN:HG3	7	0.4
(1,3014)	1:115:A:PHE:HE1	1:48:A:GLY:HA2	1	0.39
(1,3014)	1:115:A:PHE:HE2	1:48:A:GLY:HA2	1	0.39
(1,2955)	1:55:A:LYS:HB3	1:109:A:TYR:HE1	2	0.39
(1,2955)	1:55:A:LYS:HB3	1:109:A:TYR:HE2	2	0.39
(1,2646)	1:112:A:ALA:H	1:52:A:VAL:HG21	5	0.39
(1,2646)	1:112:A:ALA:H	1:52:A:VAL:HG22	5	0.39
(1,2646)	1:112:A:ALA:H	1:52:A:VAL:HG23	5	0.39
(1,2573)	1:105:A:ALA:H	1:128:A:LEU:HD11	4	0.39
(1,2573)	1:105:A:ALA:H	1:128:A:LEU:HD12	4	0.39
(1,2573)	1:105:A:ALA:H	1:128:A:LEU:HD13	4	0.39
(1,2542)	1:100:A:ASP:H	1:83:A:VAL:HA	6	0.39
(1,2117)	1:46:A:SER:H	1:43:A:PRO:HB3	10	0.39
(1,2105)	1:43:A:PRO:HB3	1:45:A:ALA:H	6	0.39
(1,2057)	1:93:A:GLU:H	1:39:A:THR:H	7	0.39
(1,1984)	1:100:A:ASP:HB2	1:32:A:PHE:H	4	0.39
(1,1980)	1:99:A:LEU:HB3	1:32:A:PHE:H	5	0.39
(1,1980)	1:99:A:LEU:HB3	1:32:A:PHE:H	6	0.39
(1,1950)	1:27:A:LYS:HD2	1:28:A:ALA:H	1	0.39
(1,1950)	1:27:A:LYS:HD3	1:28:A:ALA:H	1	0.39
(1,1801)	1:13:A:ASN:HD22	1:17:A:GLN:HB3	2	0.39
(1,1698)	1:24:A:GLN:HG3	1:129:A:VAL:HG21	6	0.39
(1,1698)	1:24:A:GLN:HG3	1:129:A:VAL:HG22	6	0.39
(1,1698)	1:24:A:GLN:HG3	1:129:A:VAL:HG23	6	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1618)	1:109:A:TYR:HD1	1:104:A:LEU:HD21	6	0.39
(1,1618)	1:109:A:TYR:HD1	1:104:A:LEU:HD22	6	0.39
(1,1618)	1:109:A:TYR:HD1	1:104:A:LEU:HD23	6	0.39
(1,1618)	1:109:A:TYR:HD2	1:104:A:LEU:HD21	6	0.39
(1,1618)	1:109:A:TYR:HD2	1:104:A:LEU:HD22	6	0.39
(1,1618)	1:109:A:TYR:HD2	1:104:A:LEU:HD23	6	0.39
(1,1533)	1:50:A:ASN:HD22	1:75:A:VAL:HG21	8	0.39
(1,1533)	1:50:A:ASN:HD22	1:75:A:VAL:HG22	8	0.39
(1,1533)	1:50:A:ASN:HD22	1:75:A:VAL:HG23	8	0.39
(1,1379)	1:53:A:ILE:HD11	1:23:A:ILE:HG21	6	0.39
(1,1379)	1:53:A:ILE:HD11	1:23:A:ILE:HG22	6	0.39
(1,1379)	1:53:A:ILE:HD11	1:23:A:ILE:HG23	6	0.39
(1,1379)	1:53:A:ILE:HD12	1:23:A:ILE:HG21	6	0.39
(1,1379)	1:53:A:ILE:HD12	1:23:A:ILE:HG22	6	0.39
(1,1379)	1:53:A:ILE:HD12	1:23:A:ILE:HG23	6	0.39
(1,1379)	1:53:A:ILE:HD13	1:23:A:ILE:HG21	6	0.39
(1,1379)	1:53:A:ILE:HD13	1:23:A:ILE:HG22	6	0.39
(1,1379)	1:53:A:ILE:HD13	1:23:A:ILE:HG23	6	0.39
(1,1361)	1:111:A:PHE:HZ	1:20:A:THR:HG21	2	0.39
(1,1361)	1:111:A:PHE:HZ	1:20:A:THR:HG22	2	0.39
(1,1361)	1:111:A:PHE:HZ	1:20:A:THR:HG23	2	0.39
(1,1357)	1:20:A:THR:HG21	1:10:A:VAL:HG11	10	0.39
(1,1357)	1:20:A:THR:HG21	1:10:A:VAL:HG12	10	0.39
(1,1357)	1:20:A:THR:HG21	1:10:A:VAL:HG13	10	0.39
(1,1357)	1:20:A:THR:HG22	1:10:A:VAL:HG11	10	0.39
(1,1357)	1:20:A:THR:HG22	1:10:A:VAL:HG12	10	0.39
(1,1357)	1:20:A:THR:HG22	1:10:A:VAL:HG13	10	0.39
(1,1357)	1:20:A:THR:HG23	1:10:A:VAL:HG11	10	0.39
(1,1357)	1:20:A:THR:HG23	1:10:A:VAL:HG12	10	0.39
(1,1357)	1:20:A:THR:HG23	1:10:A:VAL:HG13	10	0.39
(1,1187)	1:116:A:PRO:HD2	1:74:A:TYR:HD1	7	0.39
(1,1187)	1:116:A:PRO:HD2	1:74:A:TYR:HD2	7	0.39
(1,1003)	1:100:A:ASP:HA	1:99:A:LEU:HD21	2	0.39
(1,1003)	1:100:A:ASP:HA	1:99:A:LEU:HD22	2	0.39
(1,1003)	1:100:A:ASP:HA	1:99:A:LEU:HD23	2	0.39
(1,994)	1:83:A:VAL:HG21	1:99:A:LEU:HB3	5	0.39
(1,994)	1:83:A:VAL:HG22	1:99:A:LEU:HB3	5	0.39
(1,994)	1:83:A:VAL:HG23	1:99:A:LEU:HB3	5	0.39
(1,830)	1:86:A:THR:HA	1:97:A:LEU:HB2	2	0.39
(1,830)	1:86:A:THR:HA	1:97:A:LEU:HB2	9	0.39
(1,730)	1:75:A:VAL:HB	1:75:A:VAL:H	3	0.39
(1,646)	1:76:A:LYS:HB3	1:66:A:GLY:HA3	7	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,204)	1:26:A:SER:HB3	1:25:A:VAL:HA	10	0.39
(1,3148)	1:53:A:ILE:HD12	1:104:A:LEU:HD23	2	0.38
(1,3134)	1:23:A:ILE:HG12	1:34:A:ILE:HG23	2	0.38
(1,3048)	1:25:A:VAL:HB	1:23:A:ILE:HG23	9	0.38
(1,2955)	1:55:A:LYS:HB3	1:109:A:TYR:HE1	10	0.38
(1,2955)	1:55:A:LYS:HB3	1:109:A:TYR:HE2	10	0.38
(1,2945)	1:105:A:ALA:HA	1:109:A:TYR:HE1	6	0.38
(1,2945)	1:105:A:ALA:HA	1:109:A:TYR:HE2	6	0.38
(1,2728)	1:122:A:MET:H	1:118:A:HIS:HB2	7	0.38
(1,2611)	1:110:A:LYS:HG2	1:109:A:TYR:H	6	0.38
(1,2264)	1:61:A:GLY:H	1:59:A:MET:HG2	2	0.38
(1,2264)	1:61:A:GLY:H	1:59:A:MET:HG3	2	0.38
(1,2241)	1:57:A:GLU:HG3	1:58:A:ASP:H	1	0.38
(1,2216)	1:58:A:ASP:HB2	1:55:A:LYS:H	5	0.38
(1,2045)	1:94:A:GLU:HB2	1:38:A:HIS:H	9	0.38
(1,1960)	1:101:A:PRO:HG2	1:29:A:CYS:H	7	0.38
(1,1897)	1:25:A:VAL:HG11	1:24:A:GLN:H	8	0.38
(1,1897)	1:25:A:VAL:HG12	1:24:A:GLN:H	8	0.38
(1,1897)	1:25:A:VAL:HG13	1:24:A:GLN:H	8	0.38
(1,1706)	1:53:A:ILE:HB	1:99:A:LEU:HD11	10	0.38
(1,1706)	1:53:A:ILE:HB	1:99:A:LEU:HD12	10	0.38
(1,1706)	1:53:A:ILE:HB	1:99:A:LEU:HD13	10	0.38
(1,1614)	1:32:A:PHE:HB2	1:99:A:LEU:HD21	4	0.38
(1,1614)	1:32:A:PHE:HB2	1:99:A:LEU:HD22	4	0.38
(1,1614)	1:32:A:PHE:HB2	1:99:A:LEU:HD23	4	0.38
(1,1613)	1:101:A:PRO:HA	1:99:A:LEU:HD21	4	0.38
(1,1613)	1:101:A:PRO:HA	1:99:A:LEU:HD22	4	0.38
(1,1613)	1:101:A:PRO:HA	1:99:A:LEU:HD23	4	0.38
(1,1532)	1:114:A:THR:HG1	1:75:A:VAL:HG21	7	0.38
(1,1532)	1:114:A:THR:HG1	1:75:A:VAL:HG22	7	0.38
(1,1532)	1:114:A:THR:HG1	1:75:A:VAL:HG23	7	0.38
(1,1393)	1:25:A:VAL:H	1:25:A:VAL:HG11	3	0.38
(1,1393)	1:25:A:VAL:H	1:25:A:VAL:HG12	3	0.38
(1,1393)	1:25:A:VAL:H	1:25:A:VAL:HG13	3	0.38
(1,1333)	1:49:A:HIS:HE1	1:47:A:MET:HG2	9	0.38
(1,1304)	1:55:A:LYS:HD2	1:55:A:LYS:H	1	0.38
(1,1293)	1:130:A:ASP:HB3	1:130:A:ASP:H	5	0.38
(1,1253)	1:124:A:GLY:HA2	1:111:A:PHE:HZ	7	0.38
(1,1103)	1:110:A:LYS:HA	1:125:A:LYS:HD2	10	0.38
(1,1103)	1:110:A:LYS:HA	1:125:A:LYS:HD3	10	0.38
(1,1017)	1:101:A:PRO:HD3	1:25:A:VAL:HG21	1	0.38
(1,1017)	1:101:A:PRO:HD3	1:25:A:VAL:HG22	1	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1017)	1:101:A:PRO:HD3	1:25:A:VAL:HG23	1	0.38
(1,1003)	1:100:A:ASP:HA	1:99:A:LEU:HD21	1	0.38
(1,1003)	1:100:A:ASP:HA	1:99:A:LEU:HD22	1	0.38
(1,1003)	1:100:A:ASP:HA	1:99:A:LEU:HD23	1	0.38
(1,1003)	1:100:A:ASP:HA	1:99:A:LEU:HD21	3	0.38
(1,1003)	1:100:A:ASP:HA	1:99:A:LEU:HD22	3	0.38
(1,1003)	1:100:A:ASP:HA	1:99:A:LEU:HD23	3	0.38
(1,952)	1:96:A:SER:HA	1:36:A:LEU:HB3	8	0.38
(1,952)	1:96:A:SER:HA	1:36:A:LEU:HB3	9	0.38
(1,864)	1:44:A:LYS:HB2	1:90:A:GLY:HA2	7	0.38
(1,678)	1:68:A:GLY:HA3	1:67:A:VAL:HG21	7	0.38
(1,678)	1:68:A:GLY:HA3	1:67:A:VAL:HG22	7	0.38
(1,678)	1:68:A:GLY:HA3	1:67:A:VAL:HG23	7	0.38
(1,52)	1:49:A:HIS:HD2	1:12:A:SER:HB3	6	0.38
(1,3198)	1:64:A:LYS:HD2	1:61:A:GLY:H	2	0.37
(1,3030)	1:47:A:MET:HE1	1:118:A:HIS:HD2	4	0.37
(1,3030)	1:47:A:MET:HE2	1:118:A:HIS:HD2	4	0.37
(1,3030)	1:47:A:MET:HE3	1:118:A:HIS:HD2	4	0.37
(1,2945)	1:105:A:ALA:HA	1:109:A:TYR:HE1	7	0.37
(1,2945)	1:105:A:ALA:HA	1:109:A:TYR:HE2	7	0.37
(1,2836)	1:18:A:PHE:HE1	1:36:A:LEU:HD21	4	0.37
(1,2836)	1:18:A:PHE:HE1	1:36:A:LEU:HD22	4	0.37
(1,2836)	1:18:A:PHE:HE1	1:36:A:LEU:HD23	4	0.37
(1,2836)	1:18:A:PHE:HE2	1:36:A:LEU:HD21	4	0.37
(1,2836)	1:18:A:PHE:HE2	1:36:A:LEU:HD22	4	0.37
(1,2836)	1:18:A:PHE:HE2	1:36:A:LEU:HD23	4	0.37
(1,2595)	1:74:A:TYR:HB3	1:50:A:ASN:HD21	4	0.37
(1,2173)	1:51:A:LEU:H	1:36:A:LEU:HD11	3	0.37
(1,2173)	1:51:A:LEU:H	1:36:A:LEU:HD12	3	0.37
(1,2173)	1:51:A:LEU:H	1:36:A:LEU:HD13	3	0.37
(1,1897)	1:25:A:VAL:HG11	1:24:A:GLN:H	1	0.37
(1,1897)	1:25:A:VAL:HG12	1:24:A:GLN:H	1	0.37
(1,1897)	1:25:A:VAL:HG13	1:24:A:GLN:H	1	0.37
(1,1755)	1:86:A:THR:HG21	1:10:A:VAL:H	8	0.37
(1,1755)	1:86:A:THR:HG22	1:10:A:VAL:H	8	0.37
(1,1755)	1:86:A:THR:HG23	1:10:A:VAL:H	8	0.37
(1,1702)	1:83:A:VAL:HG21	1:99:A:LEU:HD11	1	0.37
(1,1702)	1:83:A:VAL:HG21	1:99:A:LEU:HD12	1	0.37
(1,1702)	1:83:A:VAL:HG21	1:99:A:LEU:HD13	1	0.37
(1,1702)	1:83:A:VAL:HG22	1:99:A:LEU:HD11	1	0.37
(1,1702)	1:83:A:VAL:HG22	1:99:A:LEU:HD12	1	0.37
(1,1702)	1:83:A:VAL:HG22	1:99:A:LEU:HD13	1	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1702)	1:83:A:VAL:HG23	1:99:A:LEU:HD11	1	0.37
(1,1702)	1:83:A:VAL:HG23	1:99:A:LEU:HD12	1	0.37
(1,1702)	1:83:A:VAL:HG23	1:99:A:LEU:HD13	1	0.37
(1,1526)	1:52:A:VAL:HG21	1:75:A:VAL:HG21	10	0.37
(1,1526)	1:52:A:VAL:HG21	1:75:A:VAL:HG22	10	0.37
(1,1526)	1:52:A:VAL:HG21	1:75:A:VAL:HG23	10	0.37
(1,1526)	1:52:A:VAL:HG22	1:75:A:VAL:HG21	10	0.37
(1,1526)	1:52:A:VAL:HG22	1:75:A:VAL:HG22	10	0.37
(1,1526)	1:52:A:VAL:HG22	1:75:A:VAL:HG23	10	0.37
(1,1526)	1:52:A:VAL:HG23	1:75:A:VAL:HG21	10	0.37
(1,1526)	1:52:A:VAL:HG23	1:75:A:VAL:HG22	10	0.37
(1,1526)	1:52:A:VAL:HG23	1:75:A:VAL:HG23	10	0.37
(1,1379)	1:53:A:ILE:HD11	1:23:A:ILE:HG21	7	0.37
(1,1379)	1:53:A:ILE:HD11	1:23:A:ILE:HG22	7	0.37
(1,1379)	1:53:A:ILE:HD11	1:23:A:ILE:HG23	7	0.37
(1,1379)	1:53:A:ILE:HD12	1:23:A:ILE:HG21	7	0.37
(1,1379)	1:53:A:ILE:HD12	1:23:A:ILE:HG22	7	0.37
(1,1379)	1:53:A:ILE:HD12	1:23:A:ILE:HG23	7	0.37
(1,1379)	1:53:A:ILE:HD13	1:23:A:ILE:HG21	7	0.37
(1,1379)	1:53:A:ILE:HD13	1:23:A:ILE:HG22	7	0.37
(1,1379)	1:53:A:ILE:HD13	1:23:A:ILE:HG23	7	0.37
(1,1309)	1:114:A:THR:HG1	1:50:A:ASN:HB2	3	0.37
(1,1301)	1:55:A:LYS:HA	1:55:A:LYS:HD2	2	0.37
(1,1293)	1:130:A:ASP:HB3	1:130:A:ASP:H	8	0.37
(1,1074)	1:107:A:GLY:HA2	1:109:A:TYR:HE1	3	0.37
(1,1074)	1:107:A:GLY:HA2	1:109:A:TYR:HE2	3	0.37
(1,1066)	1:107:A:GLY:HA3	1:55:A:LYS:HG2	4	0.37
(1,1066)	1:107:A:GLY:HA3	1:55:A:LYS:HG3	4	0.37
(1,1009)	1:101:A:PRO:HA	1:27:A:LYS:HA	9	0.37
(1,1003)	1:100:A:ASP:HA	1:99:A:LEU:HD21	8	0.37
(1,1003)	1:100:A:ASP:HA	1:99:A:LEU:HD22	8	0.37
(1,1003)	1:100:A:ASP:HA	1:99:A:LEU:HD23	8	0.37
(1,830)	1:86:A:THR:HA	1:97:A:LEU:HB2	10	0.37
(1,678)	1:68:A:GLY:HA3	1:67:A:VAL:HG21	4	0.37
(1,678)	1:68:A:GLY:HA3	1:67:A:VAL:HG22	4	0.37
(1,678)	1:68:A:GLY:HA3	1:67:A:VAL:HG23	4	0.37
(1,464)	1:88:A:LEU:HD11	1:48:A:GLY:HA2	5	0.37
(1,464)	1:88:A:LEU:HD12	1:48:A:GLY:HA2	5	0.37
(1,464)	1:88:A:LEU:HD13	1:48:A:GLY:HA2	5	0.37
(1,228)	1:6:A:CYS:HB2	1:29:A:CYS:HB2	5	0.37
(1,228)	1:6:A:CYS:HB2	1:29:A:CYS:HB3	5	0.37
(1,178)	1:25:A:VAL:H	1:24:A:GLN:HG3	1	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,178)	1:25:A:VAL:H	1:24:A:GLN:HG3	2	0.37
(1,178)	1:25:A:VAL:H	1:24:A:GLN:HG3	9	0.37
(1,3259)	1:16:A:MET:HB3	1:49:A:HIS:HE1	1	0.36
(1,3177)	1:9:A:THR:HG21	1:35:A:THR:H	5	0.36
(1,2876)	1:38:A:HIS:HE1	1:13:A:ASN:HB2	5	0.36
(1,2840)	1:53:A:ILE:HD11	1:32:A:PHE:HD1	10	0.36
(1,2840)	1:53:A:ILE:HD11	1:32:A:PHE:HD2	10	0.36
(1,2840)	1:53:A:ILE:HD12	1:32:A:PHE:HD1	10	0.36
(1,2840)	1:53:A:ILE:HD12	1:32:A:PHE:HD2	10	0.36
(1,2840)	1:53:A:ILE:HD13	1:32:A:PHE:HD1	10	0.36
(1,2840)	1:53:A:ILE:HD13	1:32:A:PHE:HD2	10	0.36
(1,2540)	1:100:A:ASP:H	1:100:A:ASP:HB3	4	0.36
(1,2380)	1:82:A:VAL:H	1:79:A:ASP:HB2	1	0.36
(1,2380)	1:82:A:VAL:H	1:79:A:ASP:HB3	1	0.36
(1,2264)	1:61:A:GLY:H	1:59:A:MET:HG2	4	0.36
(1,2264)	1:61:A:GLY:H	1:59:A:MET:HG3	4	0.36
(1,2117)	1:46:A:SER:H	1:43:A:PRO:HB3	2	0.36
(1,2105)	1:43:A:PRO:HB3	1:45:A:ALA:H	10	0.36
(1,2074)	1:91:A:GLY:HA2	1:41:A:THR:H	3	0.36
(1,1897)	1:25:A:VAL:HG11	1:24:A:GLN:H	6	0.36
(1,1897)	1:25:A:VAL:HG12	1:24:A:GLN:H	6	0.36
(1,1897)	1:25:A:VAL:HG13	1:24:A:GLN:H	6	0.36
(1,1698)	1:24:A:GLN:HG3	1:129:A:VAL:HG21	4	0.36
(1,1698)	1:24:A:GLN:HG3	1:129:A:VAL:HG22	4	0.36
(1,1698)	1:24:A:GLN:HG3	1:129:A:VAL:HG23	4	0.36
(1,1527)	1:82:A:VAL:HG11	1:75:A:VAL:HG21	7	0.36
(1,1527)	1:82:A:VAL:HG11	1:75:A:VAL:HG22	7	0.36
(1,1527)	1:82:A:VAL:HG11	1:75:A:VAL:HG23	7	0.36
(1,1527)	1:82:A:VAL:HG12	1:75:A:VAL:HG21	7	0.36
(1,1527)	1:82:A:VAL:HG12	1:75:A:VAL:HG22	7	0.36
(1,1527)	1:82:A:VAL:HG12	1:75:A:VAL:HG23	7	0.36
(1,1527)	1:82:A:VAL:HG13	1:75:A:VAL:HG21	7	0.36
(1,1527)	1:82:A:VAL:HG13	1:75:A:VAL:HG22	7	0.36
(1,1527)	1:82:A:VAL:HG13	1:75:A:VAL:HG23	7	0.36
(1,1426)	1:86:A:THR:HG21	1:36:A:LEU:HD11	1	0.36
(1,1426)	1:86:A:THR:HG21	1:36:A:LEU:HD12	1	0.36
(1,1426)	1:86:A:THR:HG21	1:36:A:LEU:HD13	1	0.36
(1,1426)	1:86:A:THR:HG22	1:36:A:LEU:HD11	1	0.36
(1,1426)	1:86:A:THR:HG22	1:36:A:LEU:HD12	1	0.36
(1,1426)	1:86:A:THR:HG22	1:36:A:LEU:HD13	1	0.36
(1,1426)	1:86:A:THR:HG23	1:36:A:LEU:HD11	1	0.36
(1,1426)	1:86:A:THR:HG23	1:36:A:LEU:HD12	1	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1426)	1:86:A:THR:HG23	1:36:A:LEU:HD13	1	0.36
(1,1249)	1:123:A:ASN:HB3	1:124:A:GLY:H	7	0.36
(1,973)	1:98:A:THR:H	1:97:A:LEU:HB3	10	0.36
(1,852)	1:88:A:LEU:HB3	1:73:A:ASP:H	8	0.36
(1,846)	1:73:A:ASP:HB2	1:88:A:LEU:HB3	9	0.36
(1,846)	1:73:A:ASP:HB3	1:88:A:LEU:HB3	9	0.36
(1,678)	1:68:A:GLY:HA3	1:67:A:VAL:HG21	1	0.36
(1,678)	1:68:A:GLY:HA3	1:67:A:VAL:HG22	1	0.36
(1,678)	1:68:A:GLY:HA3	1:67:A:VAL:HG23	1	0.36
(1,3196)	1:59:A:MET:HG3	1:59:A:MET:H	1	0.35
(1,3196)	1:59:A:MET:HG3	1:59:A:MET:H	2	0.35
(1,3177)	1:9:A:THR:HG23	1:35:A:THR:H	10	0.35
(1,3134)	1:23:A:ILE:HG12	1:34:A:ILE:HG23	10	0.35
(1,2955)	1:55:A:LYS:HB3	1:109:A:TYR:HE1	7	0.35
(1,2955)	1:55:A:LYS:HB3	1:109:A:TYR:HE2	7	0.35
(1,2749)	1:123:A:ASN:HD21	1:119:A:GLY:HA2	10	0.35
(1,2628)	1:110:A:LYS:HB3	1:111:A:PHE:H	6	0.35
(1,2572)	1:105:A:ALA:H	1:104:A:LEU:HD21	9	0.35
(1,2572)	1:105:A:ALA:H	1:104:A:LEU:HD22	9	0.35
(1,2572)	1:105:A:ALA:H	1:104:A:LEU:HD23	9	0.35
(1,2342)	1:75:A:VAL:HB	1:74:A:TYR:H	10	0.35
(1,2105)	1:43:A:PRO:HB3	1:45:A:ALA:H	2	0.35
(1,2078)	1:42:A:GLN:H	1:41:A:THR:H	10	0.35
(1,2074)	1:91:A:GLY:HA2	1:41:A:THR:H	2	0.35
(1,2045)	1:94:A:GLU:HB2	1:38:A:HIS:H	5	0.35
(1,1755)	1:86:A:THR:HG21	1:10:A:VAL:H	4	0.35
(1,1755)	1:86:A:THR:HG22	1:10:A:VAL:H	4	0.35
(1,1755)	1:86:A:THR:HG23	1:10:A:VAL:H	4	0.35
(1,1683)	1:104:A:LEU:HD11	1:128:A:LEU:HD21	5	0.35
(1,1683)	1:104:A:LEU:HD11	1:128:A:LEU:HD22	5	0.35
(1,1683)	1:104:A:LEU:HD11	1:128:A:LEU:HD23	5	0.35
(1,1683)	1:104:A:LEU:HD12	1:128:A:LEU:HD21	5	0.35
(1,1683)	1:104:A:LEU:HD12	1:128:A:LEU:HD22	5	0.35
(1,1683)	1:104:A:LEU:HD12	1:128:A:LEU:HD23	5	0.35
(1,1683)	1:104:A:LEU:HD13	1:128:A:LEU:HD21	5	0.35
(1,1683)	1:104:A:LEU:HD13	1:128:A:LEU:HD22	5	0.35
(1,1683)	1:104:A:LEU:HD13	1:128:A:LEU:HD23	5	0.35
(1,1498)	1:62:A:VAL:HG11	1:54:A:ALA:H	10	0.35
(1,1498)	1:62:A:VAL:HG12	1:54:A:ALA:H	10	0.35
(1,1498)	1:62:A:VAL:HG13	1:54:A:ALA:H	10	0.35
(1,1341)	1:51:A:LEU:HG	1:10:A:VAL:HG21	10	0.35
(1,1341)	1:51:A:LEU:HG	1:10:A:VAL:HG22	10	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1341)	1:51:A:LEU:HG	1:10:A:VAL:HG23	10	0.35
(1,1127)	1:111:A:PHE:HA	1:126:A:VAL:HG21	3	0.35
(1,1127)	1:111:A:PHE:HA	1:126:A:VAL:HG22	3	0.35
(1,1127)	1:111:A:PHE:HA	1:126:A:VAL:HG23	3	0.35
(1,1064)	1:107:A:GLY:HA2	1:55:A:LYS:HD3	6	0.35
(1,1032)	1:32:A:PHE:HB2	1:101:A:PRO:HG2	7	0.35
(1,973)	1:98:A:THR:H	1:97:A:LEU:HB3	9	0.35
(1,785)	1:81:A:ARG:HD2	1:62:A:VAL:HG21	1	0.35
(1,785)	1:81:A:ARG:HD2	1:62:A:VAL:HG22	1	0.35
(1,785)	1:81:A:ARG:HD2	1:62:A:VAL:HG23	1	0.35
(1,759)	1:77:A:PRO:HD2	1:69:A:ALA:HB1	6	0.35
(1,759)	1:77:A:PRO:HD2	1:69:A:ALA:HB2	6	0.35
(1,759)	1:77:A:PRO:HD2	1:69:A:ALA:HB3	6	0.35
(1,426)	1:43:A:PRO:HG3	1:46:A:SER:H	7	0.35
(1,233)	1:30:A:LYS:HA	1:30:A:LYS:HD3	8	0.35
(1,178)	1:25:A:VAL:H	1:24:A:GLN:HG3	4	0.35
(1,46)	1:12:A:SER:HA	1:36:A:LEU:HD21	10	0.35
(1,46)	1:12:A:SER:HA	1:36:A:LEU:HD22	10	0.35
(1,46)	1:12:A:SER:HA	1:36:A:LEU:HD23	10	0.35
(1,3243)	1:123:A:ASN:HD21	1:120:A:ALA:HB2	9	0.34
(1,3198)	1:81:A:ARG:HB3	1:61:A:GLY:H	6	0.34
(1,3196)	1:59:A:MET:HG3	1:59:A:MET:H	4	0.34
(1,3134)	1:23:A:ILE:HG12	1:34:A:ILE:HG23	9	0.34
(1,2965)	1:109:A:TYR:HE1	1:83:A:VAL:HG21	9	0.34
(1,2965)	1:109:A:TYR:HE1	1:83:A:VAL:HG22	9	0.34
(1,2965)	1:109:A:TYR:HE1	1:83:A:VAL:HG23	9	0.34
(1,2965)	1:109:A:TYR:HE2	1:83:A:VAL:HG21	9	0.34
(1,2965)	1:109:A:TYR:HE2	1:83:A:VAL:HG22	9	0.34
(1,2965)	1:109:A:TYR:HE2	1:83:A:VAL:HG23	9	0.34
(1,2944)	1:107:A:GLY:HA3	1:109:A:TYR:HD1	2	0.34
(1,2944)	1:107:A:GLY:HA3	1:109:A:TYR:HD2	2	0.34
(1,2878)	1:38:A:HIS:HE1	1:47:A:MET:HG3	7	0.34
(1,2832)	1:18:A:PHE:HE1	1:12:A:SER:HB2	3	0.34
(1,2832)	1:18:A:PHE:HE2	1:12:A:SER:HB2	3	0.34
(1,2629)	1:125:A:LYS:HD2	1:111:A:PHE:H	9	0.34
(1,2629)	1:125:A:LYS:HD3	1:111:A:PHE:H	9	0.34
(1,2595)	1:74:A:TYR:HB3	1:50:A:ASN:HD21	5	0.34
(1,2395)	1:83:A:VAL:HG21	1:84:A:ALA:H	9	0.34
(1,2395)	1:83:A:VAL:HG22	1:84:A:ALA:H	9	0.34
(1,2395)	1:83:A:VAL:HG23	1:84:A:ALA:H	9	0.34
(1,2394)	1:84:A:ALA:H	1:104:A:LEU:HD21	5	0.34
(1,2394)	1:84:A:ALA:H	1:104:A:LEU:HD22	5	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2394)	1:84:A:ALA:H	1:104:A:LEU:HD23	5	0.34
(1,2302)	1:76:A:LYS:HB3	1:66:A:GLY:H	2	0.34
(1,2264)	1:61:A:GLY:H	1:59:A:MET:HG2	10	0.34
(1,2264)	1:61:A:GLY:H	1:59:A:MET:HG3	10	0.34
(1,2081)	1:91:A:GLY:HA2	1:42:A:GLN:H	6	0.34
(1,1930)	1:26:A:SER:H	1:25:A:VAL:HG21	2	0.34
(1,1930)	1:26:A:SER:H	1:25:A:VAL:HG22	2	0.34
(1,1930)	1:26:A:SER:H	1:25:A:VAL:HG23	2	0.34
(1,1755)	1:86:A:THR:HG21	1:10:A:VAL:H	9	0.34
(1,1755)	1:86:A:THR:HG22	1:10:A:VAL:H	9	0.34
(1,1755)	1:86:A:THR:HG23	1:10:A:VAL:H	9	0.34
(1,1628)	1:101:A:PRO:HB2	1:104:A:LEU:HD11	3	0.34
(1,1628)	1:101:A:PRO:HB2	1:104:A:LEU:HD12	3	0.34
(1,1628)	1:101:A:PRO:HB2	1:104:A:LEU:HD13	3	0.34
(1,1614)	1:32:A:PHE:HB2	1:99:A:LEU:HD21	2	0.34
(1,1614)	1:32:A:PHE:HB2	1:99:A:LEU:HD22	2	0.34
(1,1614)	1:32:A:PHE:HB2	1:99:A:LEU:HD23	2	0.34
(1,1309)	1:114:A:THR:HG1	1:50:A:ASN:HB2	6	0.34
(1,1249)	1:123:A:ASN:HB3	1:124:A:GLY:H	8	0.34
(1,1182)	1:116:A:PRO:HB3	1:67:A:VAL:HG11	5	0.34
(1,1182)	1:116:A:PRO:HB3	1:67:A:VAL:HG12	5	0.34
(1,1182)	1:116:A:PRO:HB3	1:67:A:VAL:HG13	5	0.34
(1,1017)	1:101:A:PRO:HD3	1:25:A:VAL:HG21	7	0.34
(1,1017)	1:101:A:PRO:HD3	1:25:A:VAL:HG22	7	0.34
(1,1017)	1:101:A:PRO:HD3	1:25:A:VAL:HG23	7	0.34
(1,952)	1:96:A:SER:HA	1:36:A:LEU:HB3	3	0.34
(1,813)	1:85:A:HIS:HB3	1:86:A:THR:H	5	0.34
(1,426)	1:43:A:PRO:HG3	1:46:A:SER:H	1	0.34
(1,233)	1:30:A:LYS:HA	1:30:A:LYS:HD3	7	0.34
(1,3196)	1:59:A:MET:HG3	1:59:A:MET:H	3	0.33
(1,3196)	1:59:A:MET:HG3	1:59:A:MET:H	6	0.33
(1,3196)	1:59:A:MET:HG3	1:59:A:MET:H	10	0.33
(1,3177)	1:9:A:THR:HG21	1:35:A:THR:H	8	0.33
(1,2712)	1:121:A:LEU:HB3	1:120:A:ALA:H	10	0.33
(1,2540)	1:100:A:ASP:H	1:100:A:ASP:HB3	9	0.33
(1,2508)	1:85:A:HIS:H	1:97:A:LEU:H	9	0.33
(1,2350)	1:76:A:LYS:H	1:65:A:ASP:HB2	1	0.33
(1,1930)	1:26:A:SER:H	1:25:A:VAL:HG21	6	0.33
(1,1930)	1:26:A:SER:H	1:25:A:VAL:HG22	6	0.33
(1,1930)	1:26:A:SER:H	1:25:A:VAL:HG23	6	0.33
(1,1755)	1:86:A:THR:HG21	1:10:A:VAL:H	2	0.33
(1,1755)	1:86:A:THR:HG22	1:10:A:VAL:H	2	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1755)	1:86:A:THR:HG23	1:10:A:VAL:H	2	0.33
(1,1553)	1:83:A:VAL:HG11	1:83:A:VAL:H	3	0.33
(1,1553)	1:83:A:VAL:HG12	1:83:A:VAL:H	3	0.33
(1,1553)	1:83:A:VAL:HG13	1:83:A:VAL:H	3	0.33
(1,1553)	1:83:A:VAL:HG11	1:83:A:VAL:H	4	0.33
(1,1553)	1:83:A:VAL:HG12	1:83:A:VAL:H	4	0.33
(1,1553)	1:83:A:VAL:HG13	1:83:A:VAL:H	4	0.33
(1,1553)	1:83:A:VAL:HG11	1:83:A:VAL:H	8	0.33
(1,1553)	1:83:A:VAL:HG12	1:83:A:VAL:H	8	0.33
(1,1553)	1:83:A:VAL:HG13	1:83:A:VAL:H	8	0.33
(1,1388)	1:101:A:PRO:HA	1:25:A:VAL:HG21	1	0.33
(1,1388)	1:101:A:PRO:HA	1:25:A:VAL:HG22	1	0.33
(1,1388)	1:101:A:PRO:HA	1:25:A:VAL:HG23	1	0.33
(1,1133)	1:111:A:PHE:HB2	1:126:A:VAL:HG21	6	0.33
(1,1133)	1:111:A:PHE:HB2	1:126:A:VAL:HG22	6	0.33
(1,1133)	1:111:A:PHE:HB2	1:126:A:VAL:HG23	6	0.33
(1,1067)	1:107:A:GLY:HA2	1:55:A:LYS:HG2	9	0.33
(1,1067)	1:107:A:GLY:HA2	1:55:A:LYS:HG3	9	0.33
(1,889)	1:92:A:GLY:HA2	1:93:A:GLU:HG3	10	0.33
(1,678)	1:68:A:GLY:HA3	1:67:A:VAL:HG21	9	0.33
(1,678)	1:68:A:GLY:HA3	1:67:A:VAL:HG22	9	0.33
(1,678)	1:68:A:GLY:HA3	1:67:A:VAL:HG23	9	0.33
(1,426)	1:43:A:PRO:HG3	1:46:A:SER:H	3	0.33
(1,418)	1:43:A:PRO:HD3	1:42:A:GLN:HB2	2	0.33
(1,418)	1:43:A:PRO:HD3	1:42:A:GLN:HB3	2	0.33
(1,357)	1:37:A:LYS:HD2	1:35:A:THR:HG21	7	0.33
(1,357)	1:37:A:LYS:HD2	1:35:A:THR:HG22	7	0.33
(1,357)	1:37:A:LYS:HD2	1:35:A:THR:HG23	7	0.33
(1,357)	1:37:A:LYS:HD3	1:35:A:THR:HG21	7	0.33
(1,357)	1:37:A:LYS:HD3	1:35:A:THR:HG22	7	0.33
(1,357)	1:37:A:LYS:HD3	1:35:A:THR:HG23	7	0.33
(1,3196)	1:59:A:MET:HG3	1:59:A:MET:H	5	0.32
(1,3014)	1:115:A:PHE:HE1	1:48:A:GLY:HA2	4	0.32
(1,3014)	1:115:A:PHE:HE2	1:48:A:GLY:HA2	4	0.32
(1,2944)	1:107:A:GLY:HA3	1:109:A:TYR:HD1	5	0.32
(1,2944)	1:107:A:GLY:HA3	1:109:A:TYR:HD2	5	0.32
(1,2902)	1:49:A:HIS:HD2	1:90:A:GLY:HA3	10	0.32
(1,2836)	1:18:A:PHE:HE1	1:36:A:LEU:HD21	3	0.32
(1,2836)	1:18:A:PHE:HE1	1:36:A:LEU:HD22	3	0.32
(1,2836)	1:18:A:PHE:HE1	1:36:A:LEU:HD23	3	0.32
(1,2836)	1:18:A:PHE:HE2	1:36:A:LEU:HD21	3	0.32
(1,2836)	1:18:A:PHE:HE2	1:36:A:LEU:HD22	3	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2836)	1:18:A:PHE:HE2	1:36:A:LEU:HD23	3	0.32
(1,2823)	1:52:A:VAL:HG11	1:114:A:THR:H	10	0.32
(1,2823)	1:52:A:VAL:HG12	1:114:A:THR:H	10	0.32
(1,2823)	1:52:A:VAL:HG13	1:114:A:THR:H	10	0.32
(1,2808)	1:27:A:LYS:HE2	1:129:A:VAL:H	5	0.32
(1,2808)	1:27:A:LYS:HE3	1:129:A:VAL:H	5	0.32
(1,2542)	1:100:A:ASP:H	1:83:A:VAL:HA	3	0.32
(1,2170)	1:88:A:LEU:HB3	1:50:A:ASN:HD22	8	0.32
(1,2117)	1:46:A:SER:H	1:43:A:PRO:HB3	7	0.32
(1,2114)	1:46:A:SER:H	1:43:A:PRO:HD3	3	0.32
(1,2068)	1:91:A:GLY:HA3	1:40:A:GLY:H	10	0.32
(1,1930)	1:26:A:SER:H	1:25:A:VAL:HG21	9	0.32
(1,1930)	1:26:A:SER:H	1:25:A:VAL:HG22	9	0.32
(1,1930)	1:26:A:SER:H	1:25:A:VAL:HG23	9	0.32
(1,1618)	1:109:A:TYR:HD1	1:104:A:LEU:HD21	5	0.32
(1,1618)	1:109:A:TYR:HD1	1:104:A:LEU:HD22	5	0.32
(1,1618)	1:109:A:TYR:HD1	1:104:A:LEU:HD23	5	0.32
(1,1618)	1:109:A:TYR:HD2	1:104:A:LEU:HD21	5	0.32
(1,1618)	1:109:A:TYR:HD2	1:104:A:LEU:HD22	5	0.32
(1,1618)	1:109:A:TYR:HD2	1:104:A:LEU:HD23	5	0.32
(1,1609)	1:99:A:LEU:HD21	1:32:A:PHE:H	8	0.32
(1,1609)	1:99:A:LEU:HD22	1:32:A:PHE:H	8	0.32
(1,1609)	1:99:A:LEU:HD23	1:32:A:PHE:H	8	0.32
(1,1553)	1:83:A:VAL:HG11	1:83:A:VAL:H	2	0.32
(1,1553)	1:83:A:VAL:HG12	1:83:A:VAL:H	2	0.32
(1,1553)	1:83:A:VAL:HG13	1:83:A:VAL:H	2	0.32
(1,1388)	1:101:A:PRO:HA	1:25:A:VAL:HG21	9	0.32
(1,1388)	1:101:A:PRO:HA	1:25:A:VAL:HG22	9	0.32
(1,1388)	1:101:A:PRO:HA	1:25:A:VAL:HG23	9	0.32
(1,1379)	1:53:A:ILE:HD11	1:23:A:ILE:HG21	10	0.32
(1,1379)	1:53:A:ILE:HD11	1:23:A:ILE:HG22	10	0.32
(1,1379)	1:53:A:ILE:HD11	1:23:A:ILE:HG23	10	0.32
(1,1379)	1:53:A:ILE:HD12	1:23:A:ILE:HG21	10	0.32
(1,1379)	1:53:A:ILE:HD12	1:23:A:ILE:HG22	10	0.32
(1,1379)	1:53:A:ILE:HD12	1:23:A:ILE:HG23	10	0.32
(1,1379)	1:53:A:ILE:HD13	1:23:A:ILE:HG21	10	0.32
(1,1379)	1:53:A:ILE:HD13	1:23:A:ILE:HG22	10	0.32
(1,1379)	1:53:A:ILE:HD13	1:23:A:ILE:HG23	10	0.32
(1,1253)	1:124:A:GLY:HA2	1:111:A:PHE:HZ	5	0.32
(1,1253)	1:124:A:GLY:HA2	1:111:A:PHE:HZ	10	0.32
(1,496)	1:114:A:THR:HG1	1:50:A:ASN:HB3	10	0.32
(1,418)	1:43:A:PRO:HD3	1:42:A:GLN:HB2	3	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,418)	1:43:A:PRO:HD3	1:42:A:GLN:HB3	3	0.32
(1,250)	1:32:A:PHE:H	1:31:A:GLU:HG2	4	0.32
(1,250)	1:32:A:PHE:H	1:31:A:GLU:HG3	4	0.32
(1,46)	1:12:A:SER:HA	1:36:A:LEU:HD21	2	0.32
(1,46)	1:12:A:SER:HA	1:36:A:LEU:HD22	2	0.32
(1,46)	1:12:A:SER:HA	1:36:A:LEU:HD23	2	0.32
(1,3198)	1:64:A:LYS:HD3	1:61:A:GLY:H	1	0.31
(1,3134)	1:23:A:ILE:HG12	1:34:A:ILE:HG22	5	0.31
(1,2925)	1:63:A:PHE:HD1	1:112:A:ALA:HB1	7	0.31
(1,2925)	1:63:A:PHE:HD1	1:112:A:ALA:HB2	7	0.31
(1,2925)	1:63:A:PHE:HD1	1:112:A:ALA:HB3	7	0.31
(1,2925)	1:63:A:PHE:HD2	1:112:A:ALA:HB1	7	0.31
(1,2925)	1:63:A:PHE:HD2	1:112:A:ALA:HB2	7	0.31
(1,2925)	1:63:A:PHE:HD2	1:112:A:ALA:HB3	7	0.31
(1,2478)	1:93:A:GLU:H	1:38:A:HIS:HB2	3	0.31
(1,2302)	1:76:A:LYS:HB3	1:66:A:GLY:H	3	0.31
(1,2302)	1:76:A:LYS:HB3	1:66:A:GLY:H	6	0.31
(1,2302)	1:76:A:LYS:HB3	1:66:A:GLY:H	9	0.31
(1,2241)	1:57:A:GLU:HG3	1:58:A:ASP:H	8	0.31
(1,2227)	1:110:A:LYS:HD3	1:56:A:ALA:H	4	0.31
(1,2105)	1:43:A:PRO:HB3	1:45:A:ALA:H	7	0.31
(1,2078)	1:42:A:GLN:H	1:41:A:THR:H	2	0.31
(1,2077)	1:38:A:HIS:HE1	1:41:A:THR:H	2	0.31
(1,1930)	1:26:A:SER:H	1:25:A:VAL:HG21	5	0.31
(1,1930)	1:26:A:SER:H	1:25:A:VAL:HG22	5	0.31
(1,1930)	1:26:A:SER:H	1:25:A:VAL:HG23	5	0.31
(1,1930)	1:26:A:SER:H	1:25:A:VAL:HG21	7	0.31
(1,1930)	1:26:A:SER:H	1:25:A:VAL:HG22	7	0.31
(1,1930)	1:26:A:SER:H	1:25:A:VAL:HG23	7	0.31
(1,1930)	1:26:A:SER:H	1:25:A:VAL:HG21	10	0.31
(1,1930)	1:26:A:SER:H	1:25:A:VAL:HG22	10	0.31
(1,1930)	1:26:A:SER:H	1:25:A:VAL:HG23	10	0.31
(1,1786)	1:38:A:HIS:HB3	1:13:A:ASN:H	10	0.31
(1,1755)	1:86:A:THR:HG21	1:10:A:VAL:H	6	0.31
(1,1755)	1:86:A:THR:HG22	1:10:A:VAL:H	6	0.31
(1,1755)	1:86:A:THR:HG23	1:10:A:VAL:H	6	0.31
(1,1654)	1:122:A:MET:HG2	1:121:A:LEU:HD11	3	0.31
(1,1654)	1:122:A:MET:HG2	1:121:A:LEU:HD12	3	0.31
(1,1654)	1:122:A:MET:HG2	1:121:A:LEU:HD13	3	0.31
(1,1654)	1:122:A:MET:HG3	1:121:A:LEU:HD11	3	0.31
(1,1654)	1:122:A:MET:HG3	1:121:A:LEU:HD12	3	0.31
(1,1654)	1:122:A:MET:HG3	1:121:A:LEU:HD13	3	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1553)	1:83:A:VAL:HG11	1:83:A:VAL:H	1	0.31
(1,1553)	1:83:A:VAL:HG12	1:83:A:VAL:H	1	0.31
(1,1553)	1:83:A:VAL:HG13	1:83:A:VAL:H	1	0.31
(1,1553)	1:83:A:VAL:HG11	1:83:A:VAL:H	5	0.31
(1,1553)	1:83:A:VAL:HG12	1:83:A:VAL:H	5	0.31
(1,1553)	1:83:A:VAL:HG13	1:83:A:VAL:H	5	0.31
(1,1553)	1:83:A:VAL:HG11	1:83:A:VAL:H	6	0.31
(1,1553)	1:83:A:VAL:HG12	1:83:A:VAL:H	6	0.31
(1,1553)	1:83:A:VAL:HG13	1:83:A:VAL:H	6	0.31
(1,1553)	1:83:A:VAL:HG11	1:83:A:VAL:H	7	0.31
(1,1553)	1:83:A:VAL:HG12	1:83:A:VAL:H	7	0.31
(1,1553)	1:83:A:VAL:HG13	1:83:A:VAL:H	7	0.31
(1,1553)	1:83:A:VAL:HG11	1:83:A:VAL:H	10	0.31
(1,1553)	1:83:A:VAL:HG12	1:83:A:VAL:H	10	0.31
(1,1553)	1:83:A:VAL:HG13	1:83:A:VAL:H	10	0.31
(1,1532)	1:114:A:THR:HG1	1:75:A:VAL:HG21	1	0.31
(1,1532)	1:114:A:THR:HG1	1:75:A:VAL:HG22	1	0.31
(1,1532)	1:114:A:THR:HG1	1:75:A:VAL:HG23	1	0.31
(1,1379)	1:53:A:ILE:HD11	1:23:A:ILE:HG21	4	0.31
(1,1379)	1:53:A:ILE:HD11	1:23:A:ILE:HG22	4	0.31
(1,1379)	1:53:A:ILE:HD11	1:23:A:ILE:HG23	4	0.31
(1,1379)	1:53:A:ILE:HD12	1:23:A:ILE:HG21	4	0.31
(1,1379)	1:53:A:ILE:HD12	1:23:A:ILE:HG22	4	0.31
(1,1379)	1:53:A:ILE:HD12	1:23:A:ILE:HG23	4	0.31
(1,1379)	1:53:A:ILE:HD13	1:23:A:ILE:HG21	4	0.31
(1,1379)	1:53:A:ILE:HD13	1:23:A:ILE:HG22	4	0.31
(1,1379)	1:53:A:ILE:HD13	1:23:A:ILE:HG23	4	0.31
(1,1309)	1:114:A:THR:HG1	1:50:A:ASN:HB2	10	0.31
(1,1301)	1:55:A:LYS:HA	1:55:A:LYS:HD2	6	0.31
(1,1074)	1:107:A:GLY:HA2	1:109:A:TYR:HE1	2	0.31
(1,1074)	1:107:A:GLY:HA2	1:109:A:TYR:HE2	2	0.31
(1,1042)	1:104:A:LEU:HA	1:104:A:LEU:HD21	5	0.31
(1,1042)	1:104:A:LEU:HA	1:104:A:LEU:HD22	5	0.31
(1,1042)	1:104:A:LEU:HA	1:104:A:LEU:HD23	5	0.31
(1,1042)	1:104:A:LEU:HA	1:104:A:LEU:HD21	8	0.31
(1,1042)	1:104:A:LEU:HA	1:104:A:LEU:HD22	8	0.31
(1,1042)	1:104:A:LEU:HA	1:104:A:LEU:HD23	8	0.31
(1,1039)	1:99:A:LEU:HD21	1:101:A:PRO:HG3	1	0.31
(1,1039)	1:99:A:LEU:HD22	1:101:A:PRO:HG3	1	0.31
(1,1039)	1:99:A:LEU:HD23	1:101:A:PRO:HG3	1	0.31
(1,1017)	1:101:A:PRO:HD3	1:25:A:VAL:HG21	8	0.31
(1,1017)	1:101:A:PRO:HD3	1:25:A:VAL:HG22	8	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1017)	1:101:A:PRO:HD3	1:25:A:VAL:HG23	8	0.31
(1,678)	1:68:A:GLY:HA3	1:67:A:VAL:HG21	10	0.31
(1,678)	1:68:A:GLY:HA3	1:67:A:VAL:HG22	10	0.31
(1,678)	1:68:A:GLY:HA3	1:67:A:VAL:HG23	10	0.31
(1,646)	1:76:A:LYS:HB3	1:66:A:GLY:HA3	8	0.31
(1,448)	1:43:A:PRO:HG3	1:46:A:SER:HB2	3	0.31
(1,448)	1:43:A:PRO:HG3	1:46:A:SER:HB3	3	0.31
(1,387)	1:41:A:THR:HA	1:91:A:GLY:HA2	8	0.31
(1,357)	1:37:A:LYS:HD2	1:35:A:THR:HG21	4	0.31
(1,357)	1:37:A:LYS:HD2	1:35:A:THR:HG22	4	0.31
(1,357)	1:37:A:LYS:HD2	1:35:A:THR:HG23	4	0.31
(1,357)	1:37:A:LYS:HD3	1:35:A:THR:HG21	4	0.31
(1,357)	1:37:A:LYS:HD3	1:35:A:THR:HG22	4	0.31
(1,357)	1:37:A:LYS:HD3	1:35:A:THR:HG23	4	0.31
(1,228)	1:6:A:CYS:HB2	1:29:A:CYS:HB2	2	0.31
(1,228)	1:6:A:CYS:HB2	1:29:A:CYS:HB3	2	0.31
(1,178)	1:25:A:VAL:H	1:24:A:GLN:HG3	8	0.31
(1,2964)	1:109:A:TYR:HD1	1:128:A:LEU:HD21	9	0.3
(1,2964)	1:109:A:TYR:HD1	1:128:A:LEU:HD22	9	0.3
(1,2964)	1:109:A:TYR:HD1	1:128:A:LEU:HD23	9	0.3
(1,2964)	1:109:A:TYR:HD2	1:128:A:LEU:HD21	9	0.3
(1,2964)	1:109:A:TYR:HD2	1:128:A:LEU:HD22	9	0.3
(1,2964)	1:109:A:TYR:HD2	1:128:A:LEU:HD23	9	0.3
(1,2541)	1:100:A:ASP:H	1:100:A:ASP:HB2	6	0.3
(1,2469)	1:92:A:GLY:H	1:38:A:HIS:HB2	8	0.3
(1,2264)	1:61:A:GLY:H	1:59:A:MET:HG2	3	0.3
(1,2264)	1:61:A:GLY:H	1:59:A:MET:HG3	3	0.3
(1,2077)	1:38:A:HIS:HE1	1:41:A:THR:H	10	0.3
(1,1930)	1:26:A:SER:H	1:25:A:VAL:HG21	4	0.3
(1,1930)	1:26:A:SER:H	1:25:A:VAL:HG22	4	0.3
(1,1930)	1:26:A:SER:H	1:25:A:VAL:HG23	4	0.3
(1,1846)	1:18:A:PHE:H	1:122:A:MET:HG2	6	0.3
(1,1846)	1:18:A:PHE:H	1:122:A:MET:HG3	6	0.3
(1,1613)	1:101:A:PRO:HA	1:99:A:LEU:HD21	9	0.3
(1,1613)	1:101:A:PRO:HA	1:99:A:LEU:HD22	9	0.3
(1,1613)	1:101:A:PRO:HA	1:99:A:LEU:HD23	9	0.3
(1,1095)	1:110:A:LYS:HD3	1:109:A:TYR:HA	7	0.3
(1,1042)	1:104:A:LEU:HA	1:104:A:LEU:HD21	7	0.3
(1,1042)	1:104:A:LEU:HA	1:104:A:LEU:HD22	7	0.3
(1,1042)	1:104:A:LEU:HA	1:104:A:LEU:HD23	7	0.3
(1,1042)	1:104:A:LEU:HA	1:104:A:LEU:HD21	9	0.3
(1,1042)	1:104:A:LEU:HA	1:104:A:LEU:HD22	9	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1042)	1:104:A:LEU:HA	1:104:A:LEU:HD23	9	0.3
(1,1003)	1:100:A:ASP:HA	1:99:A:LEU:HD21	6	0.3
(1,1003)	1:100:A:ASP:HA	1:99:A:LEU:HD22	6	0.3
(1,1003)	1:100:A:ASP:HA	1:99:A:LEU:HD23	6	0.3
(1,973)	1:98:A:THR:H	1:97:A:LEU:HB3	4	0.3
(1,973)	1:98:A:THR:H	1:97:A:LEU:HB3	6	0.3
(1,248)	1:31:A:GLU:HB2	1:32:A:PHE:H	9	0.3
(1,228)	1:6:A:CYS:HB2	1:29:A:CYS:HB2	7	0.3
(1,228)	1:6:A:CYS:HB2	1:29:A:CYS:HB3	7	0.3
(1,52)	1:49:A:HIS:HD2	1:12:A:SER:HB3	10	0.3
(1,47)	1:17:A:GLN:HG3	1:12:A:SER:HA	3	0.3
(1,35)	1:11:A:GLU:HA	1:36:A:LEU:HD21	5	0.3
(1,35)	1:11:A:GLU:HA	1:36:A:LEU:HD22	5	0.3
(1,35)	1:11:A:GLU:HA	1:36:A:LEU:HD23	5	0.3
(1,2967)	1:109:A:TYR:HD1	1:126:A:VAL:HG21	7	0.29
(1,2967)	1:109:A:TYR:HD1	1:126:A:VAL:HG22	7	0.29
(1,2967)	1:109:A:TYR:HD1	1:126:A:VAL:HG23	7	0.29
(1,2967)	1:109:A:TYR:HD2	1:126:A:VAL:HG21	7	0.29
(1,2967)	1:109:A:TYR:HD2	1:126:A:VAL:HG22	7	0.29
(1,2967)	1:109:A:TYR:HD2	1:126:A:VAL:HG23	7	0.29
(1,2925)	1:63:A:PHE:HD1	1:112:A:ALA:HB1	2	0.29
(1,2925)	1:63:A:PHE:HD1	1:112:A:ALA:HB2	2	0.29
(1,2925)	1:63:A:PHE:HD1	1:112:A:ALA:HB3	2	0.29
(1,2925)	1:63:A:PHE:HD2	1:112:A:ALA:HB1	2	0.29
(1,2925)	1:63:A:PHE:HD2	1:112:A:ALA:HB2	2	0.29
(1,2925)	1:63:A:PHE:HD2	1:112:A:ALA:HB3	2	0.29
(1,2836)	1:18:A:PHE:HE1	1:36:A:LEU:HD21	6	0.29
(1,2836)	1:18:A:PHE:HE1	1:36:A:LEU:HD22	6	0.29
(1,2836)	1:18:A:PHE:HE1	1:36:A:LEU:HD23	6	0.29
(1,2836)	1:18:A:PHE:HE2	1:36:A:LEU:HD21	6	0.29
(1,2836)	1:18:A:PHE:HE2	1:36:A:LEU:HD22	6	0.29
(1,2836)	1:18:A:PHE:HE2	1:36:A:LEU:HD23	6	0.29
(1,2836)	1:18:A:PHE:HE1	1:36:A:LEU:HD21	8	0.29
(1,2836)	1:18:A:PHE:HE1	1:36:A:LEU:HD22	8	0.29
(1,2836)	1:18:A:PHE:HE1	1:36:A:LEU:HD23	8	0.29
(1,2836)	1:18:A:PHE:HE2	1:36:A:LEU:HD21	8	0.29
(1,2836)	1:18:A:PHE:HE2	1:36:A:LEU:HD22	8	0.29
(1,2836)	1:18:A:PHE:HE2	1:36:A:LEU:HD23	8	0.29
(1,2629)	1:125:A:LYS:HD2	1:111:A:PHE:H	6	0.29
(1,2629)	1:125:A:LYS:HD3	1:111:A:PHE:H	6	0.29
(1,2540)	1:100:A:ASP:H	1:100:A:ASP:HB3	5	0.29
(1,2528)	1:99:A:LEU:H	1:31:A:GLU:HG2	9	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2528)	1:99:A:LEU:H	1:31:A:GLU:HG3	9	0.29
(1,2496)	1:96:A:SER:H	1:36:A:LEU:HB3	8	0.29
(1,2395)	1:83:A:VAL:HG21	1:84:A:ALA:H	1	0.29
(1,2395)	1:83:A:VAL:HG22	1:84:A:ALA:H	1	0.29
(1,2395)	1:83:A:VAL:HG23	1:84:A:ALA:H	1	0.29
(1,2395)	1:83:A:VAL:HG21	1:84:A:ALA:H	10	0.29
(1,2395)	1:83:A:VAL:HG22	1:84:A:ALA:H	10	0.29
(1,2395)	1:83:A:VAL:HG23	1:84:A:ALA:H	10	0.29
(1,2380)	1:82:A:VAL:H	1:79:A:ASP:HB2	10	0.29
(1,2380)	1:82:A:VAL:H	1:79:A:ASP:HB3	10	0.29
(1,2179)	1:51:A:LEU:H	1:95:A:SER:HB2	5	0.29
(1,2077)	1:38:A:HIS:HE1	1:41:A:THR:H	4	0.29
(1,1930)	1:26:A:SER:H	1:25:A:VAL:HG21	8	0.29
(1,1930)	1:26:A:SER:H	1:25:A:VAL:HG22	8	0.29
(1,1930)	1:26:A:SER:H	1:25:A:VAL:HG23	8	0.29
(1,1903)	1:24:A:GLN:HG2	1:24:A:GLN:H	6	0.29
(1,1848)	1:18:A:PHE:H	1:10:A:VAL:HG11	10	0.29
(1,1848)	1:18:A:PHE:H	1:10:A:VAL:HG12	10	0.29
(1,1848)	1:18:A:PHE:H	1:10:A:VAL:HG13	10	0.29
(1,1392)	1:127:A:THR:H	1:25:A:VAL:HG11	1	0.29
(1,1392)	1:127:A:THR:H	1:25:A:VAL:HG12	1	0.29
(1,1392)	1:127:A:THR:H	1:25:A:VAL:HG13	1	0.29
(1,1309)	1:114:A:THR:HG1	1:50:A:ASN:HB2	2	0.29
(1,1309)	1:114:A:THR:HG1	1:50:A:ASN:HB2	4	0.29
(1,1309)	1:114:A:THR:HG1	1:50:A:ASN:HB2	8	0.29
(1,1268)	1:127:A:THR:HB	1:24:A:GLN:HG3	7	0.29
(1,1249)	1:123:A:ASN:HB3	1:124:A:GLY:H	1	0.29
(1,1133)	1:111:A:PHE:HB2	1:126:A:VAL:HG21	3	0.29
(1,1133)	1:111:A:PHE:HB2	1:126:A:VAL:HG22	3	0.29
(1,1133)	1:111:A:PHE:HB2	1:126:A:VAL:HG23	3	0.29
(1,1042)	1:104:A:LEU:HA	1:104:A:LEU:HD21	6	0.29
(1,1042)	1:104:A:LEU:HA	1:104:A:LEU:HD22	6	0.29
(1,1042)	1:104:A:LEU:HA	1:104:A:LEU:HD23	6	0.29
(1,1031)	1:101:A:PRO:HG2	1:29:A:CYS:HB2	5	0.29
(1,1031)	1:101:A:PRO:HG2	1:29:A:CYS:HB3	5	0.29
(1,1003)	1:100:A:ASP:HA	1:99:A:LEU:HD21	5	0.29
(1,1003)	1:100:A:ASP:HA	1:99:A:LEU:HD22	5	0.29
(1,1003)	1:100:A:ASP:HA	1:99:A:LEU:HD23	5	0.29
(1,882)	1:91:A:GLY:HA3	1:38:A:HIS:HB2	6	0.29
(1,178)	1:25:A:VAL:H	1:24:A:GLN:HG3	6	0.29
(1,3077)	1:59:A:MET:HG2	1:56:A:ALA:HA	8	0.28
(1,3075)	1:55:A:LYS:HB2	1:54:A:ALA:HB2	3	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2987)	1:126:A:VAL:HG11	1:111:A:PHE:HD1	3	0.28
(1,2987)	1:126:A:VAL:HG11	1:111:A:PHE:HD2	3	0.28
(1,2987)	1:126:A:VAL:HG12	1:111:A:PHE:HD1	3	0.28
(1,2987)	1:126:A:VAL:HG12	1:111:A:PHE:HD2	3	0.28
(1,2987)	1:126:A:VAL:HG13	1:111:A:PHE:HD1	3	0.28
(1,2987)	1:126:A:VAL:HG13	1:111:A:PHE:HD2	3	0.28
(1,2836)	1:18:A:PHE:HE1	1:36:A:LEU:HD21	1	0.28
(1,2836)	1:18:A:PHE:HE1	1:36:A:LEU:HD22	1	0.28
(1,2836)	1:18:A:PHE:HE1	1:36:A:LEU:HD23	1	0.28
(1,2836)	1:18:A:PHE:HE2	1:36:A:LEU:HD21	1	0.28
(1,2836)	1:18:A:PHE:HE2	1:36:A:LEU:HD22	1	0.28
(1,2836)	1:18:A:PHE:HE2	1:36:A:LEU:HD23	1	0.28
(1,2529)	1:99:A:LEU:H	1:31:A:GLU:HB2	6	0.28
(1,2413)	1:86:A:THR:H	1:52:A:VAL:HG21	9	0.28
(1,2413)	1:86:A:THR:H	1:52:A:VAL:HG22	9	0.28
(1,2413)	1:86:A:THR:H	1:52:A:VAL:HG23	9	0.28
(1,2165)	1:74:A:TYR:HD1	1:50:A:ASN:HD22	9	0.28
(1,2165)	1:74:A:TYR:HD2	1:50:A:ASN:HD22	9	0.28
(1,2105)	1:43:A:PRO:HB3	1:45:A:ALA:H	4	0.28
(1,2105)	1:43:A:PRO:HB3	1:45:A:ALA:H	5	0.28
(1,2068)	1:91:A:GLY:HA3	1:40:A:GLY:H	2	0.28
(1,1780)	1:12:A:SER:H	1:36:A:LEU:HD21	10	0.28
(1,1780)	1:12:A:SER:H	1:36:A:LEU:HD22	10	0.28
(1,1780)	1:12:A:SER:H	1:36:A:LEU:HD23	10	0.28
(1,1595)	1:53:A:ILE:HG12	1:97:A:LEU:HD11	5	0.28
(1,1595)	1:53:A:ILE:HG12	1:97:A:LEU:HD12	5	0.28
(1,1595)	1:53:A:ILE:HG12	1:97:A:LEU:HD13	5	0.28
(1,1249)	1:123:A:ASN:HB3	1:124:A:GLY:H	9	0.28
(1,1125)	1:53:A:ILE:HG13	1:111:A:PHE:HA	6	0.28
(1,1003)	1:100:A:ASP:HA	1:99:A:LEU:HD21	7	0.28
(1,1003)	1:100:A:ASP:HA	1:99:A:LEU:HD22	7	0.28
(1,1003)	1:100:A:ASP:HA	1:99:A:LEU:HD23	7	0.28
(1,830)	1:86:A:THR:HA	1:97:A:LEU:HB2	4	0.28
(1,795)	1:82:A:VAL:HB	1:75:A:VAL:HG11	5	0.28
(1,795)	1:82:A:VAL:HB	1:75:A:VAL:HG12	5	0.28
(1,795)	1:82:A:VAL:HB	1:75:A:VAL:HG13	5	0.28
(1,766)	1:69:A:ALA:HA	1:77:A:PRO:HD2	2	0.28
(1,678)	1:68:A:GLY:HA3	1:67:A:VAL:HG21	6	0.28
(1,678)	1:68:A:GLY:HA3	1:67:A:VAL:HG22	6	0.28
(1,678)	1:68:A:GLY:HA3	1:67:A:VAL:HG23	6	0.28
(1,233)	1:30:A:LYS:HA	1:30:A:LYS:HD3	6	0.28
(1,3249)	1:128:A:LEU:HB2	1:129:A:VAL:H	5	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3213)	1:89:A:ILE:H	1:49:A:HIS:HB3	9	0.27
(1,3134)	1:36:A:LEU:HB3	1:34:A:ILE:HG22	7	0.27
(1,2812)	1:129:A:VAL:H	1:104:A:LEU:HD11	3	0.27
(1,2812)	1:129:A:VAL:H	1:104:A:LEU:HD12	3	0.27
(1,2812)	1:129:A:VAL:H	1:104:A:LEU:HD13	3	0.27
(1,2676)	1:75:A:VAL:HG21	1:114:A:THR:H	10	0.27
(1,2676)	1:75:A:VAL:HG22	1:114:A:THR:H	10	0.27
(1,2676)	1:75:A:VAL:HG23	1:114:A:THR:H	10	0.27
(1,2591)	1:106:A:ASP:H	1:128:A:LEU:HD11	10	0.27
(1,2591)	1:106:A:ASP:H	1:128:A:LEU:HD12	10	0.27
(1,2591)	1:106:A:ASP:H	1:128:A:LEU:HD13	10	0.27
(1,2557)	1:103:A:LYS:H	1:83:A:VAL:HG21	2	0.27
(1,2557)	1:103:A:LYS:H	1:83:A:VAL:HG22	2	0.27
(1,2557)	1:103:A:LYS:H	1:83:A:VAL:HG23	2	0.27
(1,2395)	1:83:A:VAL:HG21	1:84:A:ALA:H	3	0.27
(1,2395)	1:83:A:VAL:HG22	1:84:A:ALA:H	3	0.27
(1,2395)	1:83:A:VAL:HG23	1:84:A:ALA:H	3	0.27
(1,1984)	1:100:A:ASP:HB2	1:32:A:PHE:H	9	0.27
(1,1879)	1:20:A:THR:H	1:19:A:ASN:HB3	4	0.27
(1,1764)	1:19:A:ASN:HB2	1:11:A:GLU:H	6	0.27
(1,1654)	1:122:A:MET:HG2	1:121:A:LEU:HD11	10	0.27
(1,1654)	1:122:A:MET:HG2	1:121:A:LEU:HD12	10	0.27
(1,1654)	1:122:A:MET:HG2	1:121:A:LEU:HD13	10	0.27
(1,1654)	1:122:A:MET:HG3	1:121:A:LEU:HD11	10	0.27
(1,1654)	1:122:A:MET:HG3	1:121:A:LEU:HD12	10	0.27
(1,1654)	1:122:A:MET:HG3	1:121:A:LEU:HD13	10	0.27
(1,1613)	1:101:A:PRO:HA	1:99:A:LEU:HD21	1	0.27
(1,1613)	1:101:A:PRO:HA	1:99:A:LEU:HD22	1	0.27
(1,1613)	1:101:A:PRO:HA	1:99:A:LEU:HD23	1	0.27
(1,1613)	1:101:A:PRO:HA	1:99:A:LEU:HD21	7	0.27
(1,1613)	1:101:A:PRO:HA	1:99:A:LEU:HD22	7	0.27
(1,1613)	1:101:A:PRO:HA	1:99:A:LEU:HD23	7	0.27
(1,1527)	1:82:A:VAL:HG11	1:75:A:VAL:HG21	3	0.27
(1,1527)	1:82:A:VAL:HG11	1:75:A:VAL:HG22	3	0.27
(1,1527)	1:82:A:VAL:HG11	1:75:A:VAL:HG23	3	0.27
(1,1527)	1:82:A:VAL:HG12	1:75:A:VAL:HG21	3	0.27
(1,1527)	1:82:A:VAL:HG12	1:75:A:VAL:HG22	3	0.27
(1,1527)	1:82:A:VAL:HG12	1:75:A:VAL:HG23	3	0.27
(1,1527)	1:82:A:VAL:HG13	1:75:A:VAL:HG21	3	0.27
(1,1527)	1:82:A:VAL:HG13	1:75:A:VAL:HG22	3	0.27
(1,1527)	1:82:A:VAL:HG13	1:75:A:VAL:HG23	3	0.27
(1,1509)	1:62:A:VAL:HG21	1:114:A:THR:HG21	4	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1509)	1:62:A:VAL:HG21	1:114:A:THR:HG22	4	0.27
(1,1509)	1:62:A:VAL:HG21	1:114:A:THR:HG23	4	0.27
(1,1509)	1:62:A:VAL:HG22	1:114:A:THR:HG21	4	0.27
(1,1509)	1:62:A:VAL:HG22	1:114:A:THR:HG22	4	0.27
(1,1509)	1:62:A:VAL:HG22	1:114:A:THR:HG23	4	0.27
(1,1509)	1:62:A:VAL:HG23	1:114:A:THR:HG21	4	0.27
(1,1509)	1:62:A:VAL:HG23	1:114:A:THR:HG22	4	0.27
(1,1509)	1:62:A:VAL:HG23	1:114:A:THR:HG23	4	0.27
(1,1426)	1:86:A:THR:HG21	1:36:A:LEU:HD11	7	0.27
(1,1426)	1:86:A:THR:HG21	1:36:A:LEU:HD12	7	0.27
(1,1426)	1:86:A:THR:HG21	1:36:A:LEU:HD13	7	0.27
(1,1426)	1:86:A:THR:HG22	1:36:A:LEU:HD11	7	0.27
(1,1426)	1:86:A:THR:HG22	1:36:A:LEU:HD12	7	0.27
(1,1426)	1:86:A:THR:HG22	1:36:A:LEU:HD13	7	0.27
(1,1426)	1:86:A:THR:HG23	1:36:A:LEU:HD11	7	0.27
(1,1426)	1:86:A:THR:HG23	1:36:A:LEU:HD12	7	0.27
(1,1426)	1:86:A:THR:HG23	1:36:A:LEU:HD13	7	0.27
(1,1192)	1:116:A:PRO:HD2	1:74:A:TYR:HA	7	0.27
(1,1132)	1:111:A:PHE:HB2	1:126:A:VAL:HG11	3	0.27
(1,1132)	1:111:A:PHE:HB2	1:126:A:VAL:HG12	3	0.27
(1,1132)	1:111:A:PHE:HB2	1:126:A:VAL:HG13	3	0.27
(1,1127)	1:111:A:PHE:HA	1:126:A:VAL:HG21	10	0.27
(1,1127)	1:111:A:PHE:HA	1:126:A:VAL:HG22	10	0.27
(1,1127)	1:111:A:PHE:HA	1:126:A:VAL:HG23	10	0.27
(1,1100)	1:110:A:LYS:HA	1:126:A:VAL:HG11	4	0.27
(1,1100)	1:110:A:LYS:HA	1:126:A:VAL:HG12	4	0.27
(1,1100)	1:110:A:LYS:HA	1:126:A:VAL:HG13	4	0.27
(1,1016)	1:99:A:LEU:HD21	1:101:A:PRO:HD3	8	0.27
(1,1016)	1:99:A:LEU:HD22	1:101:A:PRO:HD3	8	0.27
(1,1016)	1:99:A:LEU:HD23	1:101:A:PRO:HD3	8	0.27
(1,973)	1:98:A:THR:H	1:97:A:LEU:HB3	2	0.27
(1,973)	1:98:A:THR:H	1:97:A:LEU:HB3	3	0.27
(1,813)	1:85:A:HIS:HB3	1:86:A:THR:H	10	0.27
(1,748)	1:77:A:PRO:HA	1:78:A:ASP:H	6	0.27
(1,639)	1:67:A:VAL:HG11	1:64:A:LYS:HA	1	0.27
(1,639)	1:67:A:VAL:HG12	1:64:A:LYS:HA	1	0.27
(1,639)	1:67:A:VAL:HG13	1:64:A:LYS:HA	1	0.27
(1,468)	1:88:A:LEU:HG	1:48:A:GLY:HA3	4	0.27
(1,387)	1:41:A:THR:HA	1:91:A:GLY:HA2	6	0.27
(1,357)	1:37:A:LYS:HD2	1:35:A:THR:HG21	8	0.27
(1,357)	1:37:A:LYS:HD2	1:35:A:THR:HG22	8	0.27
(1,357)	1:37:A:LYS:HD2	1:35:A:THR:HG23	8	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,357)	1:37:A:LYS:HD3	1:35:A:THR:HG21	8	0.27
(1,357)	1:37:A:LYS:HD3	1:35:A:THR:HG22	8	0.27
(1,357)	1:37:A:LYS:HD3	1:35:A:THR:HG23	8	0.27
(1,344)	1:37:A:LYS:HB3	1:11:A:GLU:HG3	6	0.27
(1,230)	1:29:A:CYS:HB2	1:25:A:VAL:HG21	10	0.27
(1,230)	1:29:A:CYS:HB2	1:25:A:VAL:HG22	10	0.27
(1,230)	1:29:A:CYS:HB2	1:25:A:VAL:HG23	10	0.27
(1,230)	1:29:A:CYS:HB3	1:25:A:VAL:HG21	10	0.27
(1,230)	1:29:A:CYS:HB3	1:25:A:VAL:HG22	10	0.27
(1,230)	1:29:A:CYS:HB3	1:25:A:VAL:HG23	10	0.27
(1,3243)	1:123:A:ASN:HD21	1:120:A:ALA:HB1	1	0.26
(1,3190)	1:51:A:LEU:H	1:36:A:LEU:HB3	8	0.26
(1,2876)	1:38:A:HIS:HE1	1:13:A:ASN:HB2	8	0.26
(1,2840)	1:53:A:ILE:HD11	1:32:A:PHE:HD1	4	0.26
(1,2840)	1:53:A:ILE:HD11	1:32:A:PHE:HD2	4	0.26
(1,2840)	1:53:A:ILE:HD12	1:32:A:PHE:HD1	4	0.26
(1,2840)	1:53:A:ILE:HD12	1:32:A:PHE:HD2	4	0.26
(1,2840)	1:53:A:ILE:HD13	1:32:A:PHE:HD1	4	0.26
(1,2840)	1:53:A:ILE:HD13	1:32:A:PHE:HD2	4	0.26
(1,2568)	1:104:A:LEU:HB3	1:104:A:LEU:H	4	0.26
(1,2508)	1:85:A:HIS:H	1:97:A:LEU:H	1	0.26
(1,2508)	1:85:A:HIS:H	1:97:A:LEU:H	4	0.26
(1,2508)	1:85:A:HIS:H	1:97:A:LEU:H	7	0.26
(1,2394)	1:84:A:ALA:H	1:104:A:LEU:HD21	9	0.26
(1,2394)	1:84:A:ALA:H	1:104:A:LEU:HD22	9	0.26
(1,2394)	1:84:A:ALA:H	1:104:A:LEU:HD23	9	0.26
(1,2200)	1:53:A:ILE:H	1:52:A:VAL:HG21	8	0.26
(1,2200)	1:53:A:ILE:H	1:52:A:VAL:HG22	8	0.26
(1,2200)	1:53:A:ILE:H	1:52:A:VAL:HG23	8	0.26
(1,2081)	1:91:A:GLY:HA2	1:42:A:GLN:H	1	0.26
(1,2081)	1:91:A:GLY:HA2	1:42:A:GLN:H	3	0.26
(1,2060)	1:93:A:GLU:H	1:40:A:GLY:H	5	0.26
(1,1930)	1:26:A:SER:H	1:25:A:VAL:HG21	3	0.26
(1,1930)	1:26:A:SER:H	1:25:A:VAL:HG22	3	0.26
(1,1930)	1:26:A:SER:H	1:25:A:VAL:HG23	3	0.26
(1,1780)	1:12:A:SER:H	1:36:A:LEU:HD21	4	0.26
(1,1780)	1:12:A:SER:H	1:36:A:LEU:HD22	4	0.26
(1,1780)	1:12:A:SER:H	1:36:A:LEU:HD23	4	0.26
(1,1618)	1:109:A:TYR:HD1	1:104:A:LEU:HD21	8	0.26
(1,1618)	1:109:A:TYR:HD1	1:104:A:LEU:HD22	8	0.26
(1,1618)	1:109:A:TYR:HD1	1:104:A:LEU:HD23	8	0.26
(1,1618)	1:109:A:TYR:HD2	1:104:A:LEU:HD21	8	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1618)	1:109:A:TYR:HD2	1:104:A:LEU:HD22	8	0.26
(1,1618)	1:109:A:TYR:HD2	1:104:A:LEU:HD23	8	0.26
(1,1509)	1:62:A:VAL:HG21	1:114:A:THR:HG21	6	0.26
(1,1509)	1:62:A:VAL:HG21	1:114:A:THR:HG22	6	0.26
(1,1509)	1:62:A:VAL:HG21	1:114:A:THR:HG23	6	0.26
(1,1509)	1:62:A:VAL:HG22	1:114:A:THR:HG21	6	0.26
(1,1509)	1:62:A:VAL:HG22	1:114:A:THR:HG22	6	0.26
(1,1509)	1:62:A:VAL:HG22	1:114:A:THR:HG23	6	0.26
(1,1509)	1:62:A:VAL:HG23	1:114:A:THR:HG21	6	0.26
(1,1509)	1:62:A:VAL:HG23	1:114:A:THR:HG22	6	0.26
(1,1509)	1:62:A:VAL:HG23	1:114:A:THR:HG23	6	0.26
(1,711)	1:74:A:TYR:HB3	1:88:A:LEU:HD11	6	0.26
(1,711)	1:74:A:TYR:HB3	1:88:A:LEU:HD12	6	0.26
(1,711)	1:74:A:TYR:HB3	1:88:A:LEU:HD13	6	0.26
(1,678)	1:68:A:GLY:HA3	1:67:A:VAL:HG21	2	0.26
(1,678)	1:68:A:GLY:HA3	1:67:A:VAL:HG22	2	0.26
(1,678)	1:68:A:GLY:HA3	1:67:A:VAL:HG23	2	0.26
(1,643)	1:76:A:LYS:HD2	1:66:A:GLY:HA3	7	0.26
(1,643)	1:76:A:LYS:HD3	1:66:A:GLY:HA3	7	0.26
(1,405)	1:43:A:PRO:HD3	1:42:A:GLN:HG3	2	0.26
(1,228)	1:6:A:CYS:HB2	1:29:A:CYS:HB2	9	0.26
(1,228)	1:6:A:CYS:HB2	1:29:A:CYS:HB3	9	0.26
(1,46)	1:12:A:SER:HA	1:36:A:LEU:HD21	5	0.26
(1,46)	1:12:A:SER:HA	1:36:A:LEU:HD22	5	0.26
(1,46)	1:12:A:SER:HA	1:36:A:LEU:HD23	5	0.26
(1,3249)	1:27:A:LYS:HG2	1:129:A:VAL:H	3	0.25
(1,3206)	1:78:A:ASP:HA	1:78:A:ASP:H	6	0.25
(1,3196)	1:59:A:MET:HG3	1:59:A:MET:H	8	0.25
(1,2970)	1:109:A:TYR:HD1	1:53:A:ILE:HD11	7	0.25
(1,2970)	1:109:A:TYR:HD1	1:53:A:ILE:HD12	7	0.25
(1,2970)	1:109:A:TYR:HD1	1:53:A:ILE:HD13	7	0.25
(1,2970)	1:109:A:TYR:HD2	1:53:A:ILE:HD11	7	0.25
(1,2970)	1:109:A:TYR:HD2	1:53:A:ILE:HD12	7	0.25
(1,2970)	1:109:A:TYR:HD2	1:53:A:ILE:HD13	7	0.25
(1,2779)	1:126:A:VAL:HG11	1:126:A:VAL:H	4	0.25
(1,2779)	1:126:A:VAL:HG12	1:126:A:VAL:H	4	0.25
(1,2779)	1:126:A:VAL:HG13	1:126:A:VAL:H	4	0.25
(1,2728)	1:122:A:MET:H	1:118:A:HIS:HB2	5	0.25
(1,2710)	1:120:A:ALA:H	1:121:A:LEU:HD11	9	0.25
(1,2710)	1:120:A:ALA:H	1:121:A:LEU:HD12	9	0.25
(1,2710)	1:120:A:ALA:H	1:121:A:LEU:HD13	9	0.25
(1,2624)	1:110:A:LYS:HG2	1:110:A:LYS:H	5	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2611)	1:110:A:LYS:HG2	1:109:A:TYR:H	1	0.25
(1,2302)	1:76:A:LYS:HB3	1:66:A:GLY:H	7	0.25
(1,2216)	1:58:A:ASP:HB2	1:55:A:LYS:H	4	0.25
(1,2138)	1:88:A:LEU:HD11	1:48:A:GLY:H	4	0.25
(1,2138)	1:88:A:LEU:HD12	1:48:A:GLY:H	4	0.25
(1,2138)	1:88:A:LEU:HD13	1:48:A:GLY:H	4	0.25
(1,2065)	1:40:A:GLY:H	1:38:A:HIS:HB2	3	0.25
(1,2065)	1:40:A:GLY:H	1:38:A:HIS:HB2	8	0.25
(1,2046)	1:37:A:LYS:HD2	1:38:A:HIS:H	4	0.25
(1,2046)	1:37:A:LYS:HD3	1:38:A:HIS:H	4	0.25
(1,1930)	1:26:A:SER:H	1:25:A:VAL:HG21	1	0.25
(1,1930)	1:26:A:SER:H	1:25:A:VAL:HG22	1	0.25
(1,1930)	1:26:A:SER:H	1:25:A:VAL:HG23	1	0.25
(1,1706)	1:53:A:ILE:HB	1:99:A:LEU:HD11	3	0.25
(1,1706)	1:53:A:ILE:HB	1:99:A:LEU:HD12	3	0.25
(1,1706)	1:53:A:ILE:HB	1:99:A:LEU:HD13	3	0.25
(1,1654)	1:122:A:MET:HG2	1:121:A:LEU:HD11	6	0.25
(1,1654)	1:122:A:MET:HG2	1:121:A:LEU:HD12	6	0.25
(1,1654)	1:122:A:MET:HG2	1:121:A:LEU:HD13	6	0.25
(1,1654)	1:122:A:MET:HG3	1:121:A:LEU:HD11	6	0.25
(1,1654)	1:122:A:MET:HG3	1:121:A:LEU:HD12	6	0.25
(1,1654)	1:122:A:MET:HG3	1:121:A:LEU:HD13	6	0.25
(1,1526)	1:52:A:VAL:HG21	1:75:A:VAL:HG21	6	0.25
(1,1526)	1:52:A:VAL:HG21	1:75:A:VAL:HG22	6	0.25
(1,1526)	1:52:A:VAL:HG21	1:75:A:VAL:HG23	6	0.25
(1,1526)	1:52:A:VAL:HG22	1:75:A:VAL:HG21	6	0.25
(1,1526)	1:52:A:VAL:HG22	1:75:A:VAL:HG22	6	0.25
(1,1526)	1:52:A:VAL:HG22	1:75:A:VAL:HG23	6	0.25
(1,1526)	1:52:A:VAL:HG23	1:75:A:VAL:HG21	6	0.25
(1,1526)	1:52:A:VAL:HG23	1:75:A:VAL:HG22	6	0.25
(1,1526)	1:52:A:VAL:HG23	1:75:A:VAL:HG23	6	0.25
(1,1509)	1:62:A:VAL:HG21	1:114:A:THR:HG21	9	0.25
(1,1509)	1:62:A:VAL:HG21	1:114:A:THR:HG22	9	0.25
(1,1509)	1:62:A:VAL:HG21	1:114:A:THR:HG23	9	0.25
(1,1509)	1:62:A:VAL:HG22	1:114:A:THR:HG21	9	0.25
(1,1509)	1:62:A:VAL:HG22	1:114:A:THR:HG22	9	0.25
(1,1509)	1:62:A:VAL:HG22	1:114:A:THR:HG23	9	0.25
(1,1509)	1:62:A:VAL:HG23	1:114:A:THR:HG21	9	0.25
(1,1509)	1:62:A:VAL:HG23	1:114:A:THR:HG22	9	0.25
(1,1509)	1:62:A:VAL:HG23	1:114:A:THR:HG23	9	0.25
(1,1461)	1:126:A:VAL:HG11	1:51:A:LEU:HD21	7	0.25
(1,1461)	1:126:A:VAL:HG11	1:51:A:LEU:HD22	7	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1461)	1:126:A:VAL:HG11	1:51:A:LEU:HD23	7	0.25
(1,1461)	1:126:A:VAL:HG12	1:51:A:LEU:HD21	7	0.25
(1,1461)	1:126:A:VAL:HG12	1:51:A:LEU:HD22	7	0.25
(1,1461)	1:126:A:VAL:HG12	1:51:A:LEU:HD23	7	0.25
(1,1461)	1:126:A:VAL:HG13	1:51:A:LEU:HD21	7	0.25
(1,1461)	1:126:A:VAL:HG13	1:51:A:LEU:HD22	7	0.25
(1,1461)	1:126:A:VAL:HG13	1:51:A:LEU:HD23	7	0.25
(1,1426)	1:86:A:THR:HG21	1:36:A:LEU:HD11	5	0.25
(1,1426)	1:86:A:THR:HG21	1:36:A:LEU:HD12	5	0.25
(1,1426)	1:86:A:THR:HG21	1:36:A:LEU:HD13	5	0.25
(1,1426)	1:86:A:THR:HG22	1:36:A:LEU:HD11	5	0.25
(1,1426)	1:86:A:THR:HG22	1:36:A:LEU:HD12	5	0.25
(1,1426)	1:86:A:THR:HG22	1:36:A:LEU:HD13	5	0.25
(1,1426)	1:86:A:THR:HG23	1:36:A:LEU:HD11	5	0.25
(1,1426)	1:86:A:THR:HG23	1:36:A:LEU:HD12	5	0.25
(1,1426)	1:86:A:THR:HG23	1:36:A:LEU:HD13	5	0.25
(1,1426)	1:86:A:THR:HG21	1:36:A:LEU:HD11	9	0.25
(1,1426)	1:86:A:THR:HG21	1:36:A:LEU:HD12	9	0.25
(1,1426)	1:86:A:THR:HG21	1:36:A:LEU:HD13	9	0.25
(1,1426)	1:86:A:THR:HG22	1:36:A:LEU:HD11	9	0.25
(1,1426)	1:86:A:THR:HG22	1:36:A:LEU:HD12	9	0.25
(1,1426)	1:86:A:THR:HG22	1:36:A:LEU:HD13	9	0.25
(1,1426)	1:86:A:THR:HG23	1:36:A:LEU:HD11	9	0.25
(1,1426)	1:86:A:THR:HG23	1:36:A:LEU:HD12	9	0.25
(1,1426)	1:86:A:THR:HG23	1:36:A:LEU:HD13	9	0.25
(1,1379)	1:53:A:ILE:HD11	1:23:A:ILE:HG21	2	0.25
(1,1379)	1:53:A:ILE:HD11	1:23:A:ILE:HG22	2	0.25
(1,1379)	1:53:A:ILE:HD11	1:23:A:ILE:HG23	2	0.25
(1,1379)	1:53:A:ILE:HD12	1:23:A:ILE:HG21	2	0.25
(1,1379)	1:53:A:ILE:HD12	1:23:A:ILE:HG22	2	0.25
(1,1379)	1:53:A:ILE:HD12	1:23:A:ILE:HG23	2	0.25
(1,1379)	1:53:A:ILE:HD13	1:23:A:ILE:HG21	2	0.25
(1,1379)	1:53:A:ILE:HD13	1:23:A:ILE:HG22	2	0.25
(1,1379)	1:53:A:ILE:HD13	1:23:A:ILE:HG23	2	0.25
(1,1345)	1:10:A:VAL:HG21	1:9:A:THR:H	10	0.25
(1,1345)	1:10:A:VAL:HG22	1:9:A:THR:H	10	0.25
(1,1345)	1:10:A:VAL:HG23	1:9:A:THR:H	10	0.25
(1,1315)	1:49:A:HIS:HD2	1:12:A:SER:HB2	4	0.25
(1,1301)	1:55:A:LYS:HA	1:55:A:LYS:HD2	10	0.25
(1,1249)	1:123:A:ASN:HB3	1:124:A:GLY:H	6	0.25
(1,991)	1:83:A:VAL:HG21	1:99:A:LEU:HB2	10	0.25
(1,991)	1:83:A:VAL:HG22	1:99:A:LEU:HB2	10	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,991)	1:83:A:VAL:HG23	1:99:A:LEU:HB2	10	0.25
(1,973)	1:98:A:THR:H	1:97:A:LEU:HB3	5	0.25
(1,973)	1:98:A:THR:H	1:97:A:LEU:HB3	7	0.25
(1,813)	1:85:A:HIS:HB3	1:86:A:THR:H	4	0.25
(1,711)	1:74:A:TYR:HB3	1:88:A:LEU:HD11	2	0.25
(1,711)	1:74:A:TYR:HB3	1:88:A:LEU:HD12	2	0.25
(1,711)	1:74:A:TYR:HB3	1:88:A:LEU:HD13	2	0.25
(1,678)	1:68:A:GLY:HA3	1:67:A:VAL:HG21	3	0.25
(1,678)	1:68:A:GLY:HA3	1:67:A:VAL:HG22	3	0.25
(1,678)	1:68:A:GLY:HA3	1:67:A:VAL:HG23	3	0.25
(1,646)	1:76:A:LYS:HB3	1:66:A:GLY:HA3	3	0.25
(1,639)	1:67:A:VAL:HG11	1:64:A:LYS:HA	8	0.25
(1,639)	1:67:A:VAL:HG12	1:64:A:LYS:HA	8	0.25
(1,639)	1:67:A:VAL:HG13	1:64:A:LYS:HA	8	0.25
(1,418)	1:43:A:PRO:HD3	1:42:A:GLN:HB2	6	0.25
(1,418)	1:43:A:PRO:HD3	1:42:A:GLN:HB3	6	0.25
(1,248)	1:31:A:GLU:HB2	1:32:A:PHE:H	2	0.25
(1,230)	1:29:A:CYS:HB2	1:25:A:VAL:HG21	9	0.25
(1,230)	1:29:A:CYS:HB2	1:25:A:VAL:HG22	9	0.25
(1,230)	1:29:A:CYS:HB2	1:25:A:VAL:HG23	9	0.25
(1,230)	1:29:A:CYS:HB3	1:25:A:VAL:HG21	9	0.25
(1,230)	1:29:A:CYS:HB3	1:25:A:VAL:HG22	9	0.25
(1,230)	1:29:A:CYS:HB3	1:25:A:VAL:HG23	9	0.25
(1,156)	1:126:A:VAL:HG11	1:23:A:ILE:HB	5	0.25
(1,156)	1:126:A:VAL:HG12	1:23:A:ILE:HB	5	0.25
(1,156)	1:126:A:VAL:HG13	1:23:A:ILE:HB	5	0.25
(1,21)	1:10:A:VAL:HB	1:9:A:THR:HA	7	0.25
(1,3263)	1:23:A:ILE:HG12	1:111:A:PHE:HD1	9	0.24
(1,3226)	1:100:A:ASP:H	1:99:A:LEU:HB3	6	0.24
(1,3221)	1:94:A:GLU:HB3	1:95:A:SER:H	8	0.24
(1,3213)	1:89:A:ILE:H	1:49:A:HIS:HB3	7	0.24
(1,3206)	1:78:A:ASP:HA	1:78:A:ASP:H	4	0.24
(1,3190)	1:51:A:LEU:H	1:36:A:LEU:HB3	4	0.24
(1,3086)	1:75:A:VAL:HB	1:52:A:VAL:HG22	6	0.24
(1,2962)	1:53:A:ILE:HG12	1:109:A:TYR:HD1	9	0.24
(1,2962)	1:53:A:ILE:HG12	1:109:A:TYR:HD2	9	0.24
(1,2955)	1:55:A:LYS:HB3	1:109:A:TYR:HE1	5	0.24
(1,2955)	1:55:A:LYS:HB3	1:109:A:TYR:HE2	5	0.24
(1,2629)	1:125:A:LYS:HD2	1:111:A:PHE:H	5	0.24
(1,2629)	1:125:A:LYS:HD3	1:111:A:PHE:H	5	0.24
(1,2568)	1:104:A:LEU:HB3	1:104:A:LEU:H	1	0.24
(1,2568)	1:104:A:LEU:HB3	1:104:A:LEU:H	2	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2568)	1:104:A:LEU:HB3	1:104:A:LEU:H	10	0.24
(1,2496)	1:96:A:SER:H	1:36:A:LEU:HB3	2	0.24
(1,2364)	1:82:A:VAL:HG11	1:79:A:ASP:H	6	0.24
(1,2364)	1:82:A:VAL:HG12	1:79:A:ASP:H	6	0.24
(1,2364)	1:82:A:VAL:HG13	1:79:A:ASP:H	6	0.24
(1,2293)	1:65:A:ASP:HB3	1:65:A:ASP:H	10	0.24
(1,2200)	1:53:A:ILE:H	1:52:A:VAL:HG21	7	0.24
(1,2200)	1:53:A:ILE:H	1:52:A:VAL:HG22	7	0.24
(1,2200)	1:53:A:ILE:H	1:52:A:VAL:HG23	7	0.24
(1,1986)	1:101:A:PRO:HD2	1:32:A:PHE:H	3	0.24
(1,1786)	1:38:A:HIS:HB3	1:13:A:ASN:H	7	0.24
(1,1763)	1:11:A:GLU:HG3	1:11:A:GLU:H	8	0.24
(1,1698)	1:24:A:GLN:HG3	1:129:A:VAL:HG21	7	0.24
(1,1698)	1:24:A:GLN:HG3	1:129:A:VAL:HG22	7	0.24
(1,1698)	1:24:A:GLN:HG3	1:129:A:VAL:HG23	7	0.24
(1,1614)	1:32:A:PHE:HB2	1:99:A:LEU:HD21	10	0.24
(1,1614)	1:32:A:PHE:HB2	1:99:A:LEU:HD22	10	0.24
(1,1614)	1:32:A:PHE:HB2	1:99:A:LEU:HD23	10	0.24
(1,1609)	1:99:A:LEU:HD21	1:32:A:PHE:H	3	0.24
(1,1609)	1:99:A:LEU:HD22	1:32:A:PHE:H	3	0.24
(1,1609)	1:99:A:LEU:HD23	1:32:A:PHE:H	3	0.24
(1,1461)	1:126:A:VAL:HG11	1:51:A:LEU:HD21	1	0.24
(1,1461)	1:126:A:VAL:HG11	1:51:A:LEU:HD22	1	0.24
(1,1461)	1:126:A:VAL:HG11	1:51:A:LEU:HD23	1	0.24
(1,1461)	1:126:A:VAL:HG12	1:51:A:LEU:HD21	1	0.24
(1,1461)	1:126:A:VAL:HG12	1:51:A:LEU:HD22	1	0.24
(1,1461)	1:126:A:VAL:HG12	1:51:A:LEU:HD23	1	0.24
(1,1461)	1:126:A:VAL:HG13	1:51:A:LEU:HD21	1	0.24
(1,1461)	1:126:A:VAL:HG13	1:51:A:LEU:HD22	1	0.24
(1,1461)	1:126:A:VAL:HG13	1:51:A:LEU:HD23	1	0.24
(1,1426)	1:86:A:THR:HG21	1:36:A:LEU:HD11	2	0.24
(1,1426)	1:86:A:THR:HG21	1:36:A:LEU:HD12	2	0.24
(1,1426)	1:86:A:THR:HG21	1:36:A:LEU:HD13	2	0.24
(1,1426)	1:86:A:THR:HG22	1:36:A:LEU:HD11	2	0.24
(1,1426)	1:86:A:THR:HG22	1:36:A:LEU:HD12	2	0.24
(1,1426)	1:86:A:THR:HG22	1:36:A:LEU:HD13	2	0.24
(1,1426)	1:86:A:THR:HG23	1:36:A:LEU:HD11	2	0.24
(1,1426)	1:86:A:THR:HG23	1:36:A:LEU:HD12	2	0.24
(1,1426)	1:86:A:THR:HG23	1:36:A:LEU:HD13	2	0.24
(1,1087)	1:108:A:ASP:H	1:108:A:ASP:HB3	1	0.24
(1,835)	1:87:A:LYS:HD2	1:87:A:LYS:HA	6	0.24
(1,835)	1:87:A:LYS:HD3	1:87:A:LYS:HA	6	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,813)	1:85:A:HIS:HB3	1:86:A:THR:H	6	0.24
(1,748)	1:77:A:PRO:HA	1:78:A:ASP:H	4	0.24
(1,581)	1:27:A:LYS:HB2	1:130:A:ASP:HA	2	0.24
(1,581)	1:27:A:LYS:HB3	1:130:A:ASP:HA	2	0.24
(1,390)	1:41:A:THR:HB	1:91:A:GLY:HA2	6	0.24
(1,73)	1:14:A:ASP:HA	1:47:A:MET:HG3	3	0.24
(1,21)	1:10:A:VAL:HB	1:9:A:THR:HA	6	0.24
(1,21)	1:10:A:VAL:HB	1:9:A:THR:HA	10	0.24
(1,3108)	1:128:A:LEU:HB3	1:105:A:ALA:HA	8	0.23
(1,2944)	1:107:A:GLY:HA3	1:109:A:TYR:HD1	6	0.23
(1,2944)	1:107:A:GLY:HA3	1:109:A:TYR:HD2	6	0.23
(1,2779)	1:126:A:VAL:HG11	1:126:A:VAL:H	8	0.23
(1,2779)	1:126:A:VAL:HG12	1:126:A:VAL:H	8	0.23
(1,2779)	1:126:A:VAL:HG13	1:126:A:VAL:H	8	0.23
(1,2745)	1:123:A:ASN:H	1:21:A:LYS:HG2	7	0.23
(1,2745)	1:123:A:ASN:H	1:21:A:LYS:HG3	7	0.23
(1,2728)	1:122:A:MET:H	1:118:A:HIS:HB2	3	0.23
(1,2646)	1:112:A:ALA:H	1:52:A:VAL:HG21	9	0.23
(1,2646)	1:112:A:ALA:H	1:52:A:VAL:HG22	9	0.23
(1,2646)	1:112:A:ALA:H	1:52:A:VAL:HG23	9	0.23
(1,2568)	1:104:A:LEU:HB3	1:104:A:LEU:H	3	0.23
(1,2538)	1:100:A:ASP:H	1:83:A:VAL:HB	4	0.23
(1,2534)	1:100:A:ASP:H	1:83:A:VAL:HG21	4	0.23
(1,2534)	1:100:A:ASP:H	1:83:A:VAL:HG22	4	0.23
(1,2534)	1:100:A:ASP:H	1:83:A:VAL:HG23	4	0.23
(1,2508)	1:85:A:HIS:H	1:97:A:LEU:H	8	0.23
(1,2395)	1:83:A:VAL:HG21	1:84:A:ALA:H	5	0.23
(1,2395)	1:83:A:VAL:HG22	1:84:A:ALA:H	5	0.23
(1,2395)	1:83:A:VAL:HG23	1:84:A:ALA:H	5	0.23
(1,2395)	1:83:A:VAL:HG21	1:84:A:ALA:H	7	0.23
(1,2395)	1:83:A:VAL:HG22	1:84:A:ALA:H	7	0.23
(1,2395)	1:83:A:VAL:HG23	1:84:A:ALA:H	7	0.23
(1,2380)	1:82:A:VAL:H	1:79:A:ASP:HB2	3	0.23
(1,2380)	1:82:A:VAL:H	1:79:A:ASP:HB3	3	0.23
(1,2264)	1:61:A:GLY:H	1:59:A:MET:HG2	5	0.23
(1,2264)	1:61:A:GLY:H	1:59:A:MET:HG3	5	0.23
(1,2241)	1:57:A:GLU:HG3	1:58:A:ASP:H	7	0.23
(1,2172)	1:50:A:ASN:HD22	1:88:A:LEU:HD21	9	0.23
(1,2172)	1:50:A:ASN:HD22	1:88:A:LEU:HD22	9	0.23
(1,2172)	1:50:A:ASN:HD22	1:88:A:LEU:HD23	9	0.23
(1,2089)	1:42:A:GLN:HE21	1:42:A:GLN:HB2	4	0.23
(1,2089)	1:42:A:GLN:HE21	1:42:A:GLN:HB3	4	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2081)	1:91:A:GLY:HA2	1:42:A:GLN:H	4	0.23
(1,2045)	1:94:A:GLU:HB2	1:38:A:HIS:H	2	0.23
(1,1903)	1:24:A:GLN:HG2	1:24:A:GLN:H	8	0.23
(1,1901)	1:23:A:ILE:HG13	1:24:A:GLN:H	4	0.23
(1,1851)	1:19:A:ASN:H	1:11:A:GLU:HB2	8	0.23
(1,1780)	1:12:A:SER:H	1:36:A:LEU:HD21	6	0.23
(1,1780)	1:12:A:SER:H	1:36:A:LEU:HD22	6	0.23
(1,1780)	1:12:A:SER:H	1:36:A:LEU:HD23	6	0.23
(1,1763)	1:11:A:GLU:HG3	1:11:A:GLU:H	10	0.23
(1,1627)	1:83:A:VAL:HG21	1:104:A:LEU:HD11	1	0.23
(1,1627)	1:83:A:VAL:HG21	1:104:A:LEU:HD12	1	0.23
(1,1627)	1:83:A:VAL:HG21	1:104:A:LEU:HD13	1	0.23
(1,1627)	1:83:A:VAL:HG22	1:104:A:LEU:HD11	1	0.23
(1,1627)	1:83:A:VAL:HG22	1:104:A:LEU:HD12	1	0.23
(1,1627)	1:83:A:VAL:HG22	1:104:A:LEU:HD13	1	0.23
(1,1627)	1:83:A:VAL:HG23	1:104:A:LEU:HD11	1	0.23
(1,1627)	1:83:A:VAL:HG23	1:104:A:LEU:HD12	1	0.23
(1,1627)	1:83:A:VAL:HG23	1:104:A:LEU:HD13	1	0.23
(1,1506)	1:81:A:ARG:HB2	1:62:A:VAL:HG11	9	0.23
(1,1506)	1:81:A:ARG:HB2	1:62:A:VAL:HG12	9	0.23
(1,1506)	1:81:A:ARG:HB2	1:62:A:VAL:HG13	9	0.23
(1,1426)	1:86:A:THR:HG21	1:36:A:LEU:HD11	3	0.23
(1,1426)	1:86:A:THR:HG21	1:36:A:LEU:HD12	3	0.23
(1,1426)	1:86:A:THR:HG21	1:36:A:LEU:HD13	3	0.23
(1,1426)	1:86:A:THR:HG22	1:36:A:LEU:HD11	3	0.23
(1,1426)	1:86:A:THR:HG22	1:36:A:LEU:HD12	3	0.23
(1,1426)	1:86:A:THR:HG22	1:36:A:LEU:HD13	3	0.23
(1,1426)	1:86:A:THR:HG23	1:36:A:LEU:HD11	3	0.23
(1,1426)	1:86:A:THR:HG23	1:36:A:LEU:HD12	3	0.23
(1,1426)	1:86:A:THR:HG23	1:36:A:LEU:HD13	3	0.23
(1,1426)	1:86:A:THR:HG21	1:36:A:LEU:HD11	10	0.23
(1,1426)	1:86:A:THR:HG21	1:36:A:LEU:HD12	10	0.23
(1,1426)	1:86:A:THR:HG21	1:36:A:LEU:HD13	10	0.23
(1,1426)	1:86:A:THR:HG22	1:36:A:LEU:HD11	10	0.23
(1,1426)	1:86:A:THR:HG22	1:36:A:LEU:HD12	10	0.23
(1,1426)	1:86:A:THR:HG22	1:36:A:LEU:HD13	10	0.23
(1,1426)	1:86:A:THR:HG23	1:36:A:LEU:HD11	10	0.23
(1,1426)	1:86:A:THR:HG23	1:36:A:LEU:HD12	10	0.23
(1,1426)	1:86:A:THR:HG23	1:36:A:LEU:HD13	10	0.23
(1,1420)	1:51:A:LEU:H	1:34:A:ILE:HG21	5	0.23
(1,1420)	1:51:A:LEU:H	1:34:A:ILE:HG22	5	0.23
(1,1420)	1:51:A:LEU:H	1:34:A:ILE:HG23	5	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1301)	1:55:A:LYS:HA	1:55:A:LYS:HD2	9	0.23
(1,1133)	1:111:A:PHE:HB2	1:126:A:VAL:HG21	10	0.23
(1,1133)	1:111:A:PHE:HB2	1:126:A:VAL:HG22	10	0.23
(1,1133)	1:111:A:PHE:HB2	1:126:A:VAL:HG23	10	0.23
(1,1125)	1:53:A:ILE:HG13	1:111:A:PHE:HA	9	0.23
(1,1087)	1:108:A:ASP:H	1:108:A:ASP:HB3	10	0.23
(1,582)	1:27:A:LYS:HD2	1:130:A:ASP:HA	4	0.23
(1,582)	1:27:A:LYS:HD3	1:130:A:ASP:HA	4	0.23
(1,230)	1:29:A:CYS:HB2	1:25:A:VAL:HG21	5	0.23
(1,230)	1:29:A:CYS:HB2	1:25:A:VAL:HG22	5	0.23
(1,230)	1:29:A:CYS:HB2	1:25:A:VAL:HG23	5	0.23
(1,230)	1:29:A:CYS:HB3	1:25:A:VAL:HG21	5	0.23
(1,230)	1:29:A:CYS:HB3	1:25:A:VAL:HG22	5	0.23
(1,230)	1:29:A:CYS:HB3	1:25:A:VAL:HG23	5	0.23
(1,72)	1:14:A:ASP:HA	1:47:A:MET:HG2	4	0.23
(1,46)	1:12:A:SER:HA	1:36:A:LEU:HD21	1	0.23
(1,46)	1:12:A:SER:HA	1:36:A:LEU:HD22	1	0.23
(1,46)	1:12:A:SER:HA	1:36:A:LEU:HD23	1	0.23
(1,46)	1:12:A:SER:HA	1:36:A:LEU:HD21	7	0.23
(1,46)	1:12:A:SER:HA	1:36:A:LEU:HD22	7	0.23
(1,46)	1:12:A:SER:HA	1:36:A:LEU:HD23	7	0.23
(1,3264)	1:111:A:PHE:HD2	1:20:A:THR:HG22	9	0.22
(1,3249)	1:128:A:LEU:HB2	1:129:A:VAL:H	2	0.22
(1,3221)	1:94:A:GLU:HB3	1:95:A:SER:H	5	0.22
(1,3206)	1:78:A:ASP:HA	1:78:A:ASP:H	9	0.22
(1,3206)	1:78:A:ASP:HA	1:78:A:ASP:H	10	0.22
(1,3048)	1:25:A:VAL:HB	1:23:A:ILE:HG21	6	0.22
(1,2967)	1:109:A:TYR:HD1	1:126:A:VAL:HG21	3	0.22
(1,2967)	1:109:A:TYR:HD1	1:126:A:VAL:HG22	3	0.22
(1,2967)	1:109:A:TYR:HD1	1:126:A:VAL:HG23	3	0.22
(1,2967)	1:109:A:TYR:HD2	1:126:A:VAL:HG21	3	0.22
(1,2967)	1:109:A:TYR:HD2	1:126:A:VAL:HG22	3	0.22
(1,2967)	1:109:A:TYR:HD2	1:126:A:VAL:HG23	3	0.22
(1,2964)	1:109:A:TYR:HD1	1:128:A:LEU:HD21	1	0.22
(1,2964)	1:109:A:TYR:HD1	1:128:A:LEU:HD22	1	0.22
(1,2964)	1:109:A:TYR:HD1	1:128:A:LEU:HD23	1	0.22
(1,2964)	1:109:A:TYR:HD2	1:128:A:LEU:HD21	1	0.22
(1,2964)	1:109:A:TYR:HD2	1:128:A:LEU:HD22	1	0.22
(1,2964)	1:109:A:TYR:HD2	1:128:A:LEU:HD23	1	0.22
(1,2962)	1:53:A:ILE:HG12	1:109:A:TYR:HD1	6	0.22
(1,2962)	1:53:A:ILE:HG12	1:109:A:TYR:HD2	6	0.22
(1,2926)	1:63:A:PHE:HE1	1:59:A:MET:HB3	10	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2926)	1:63:A:PHE:HE2	1:59:A:MET:HB3	10	0.22
(1,2925)	1:63:A:PHE:HD1	1:112:A:ALA:HB1	5	0.22
(1,2925)	1:63:A:PHE:HD1	1:112:A:ALA:HB2	5	0.22
(1,2925)	1:63:A:PHE:HD1	1:112:A:ALA:HB3	5	0.22
(1,2925)	1:63:A:PHE:HD2	1:112:A:ALA:HB1	5	0.22
(1,2925)	1:63:A:PHE:HD2	1:112:A:ALA:HB2	5	0.22
(1,2925)	1:63:A:PHE:HD2	1:112:A:ALA:HB3	5	0.22
(1,2925)	1:63:A:PHE:HD1	1:112:A:ALA:HB1	6	0.22
(1,2925)	1:63:A:PHE:HD1	1:112:A:ALA:HB2	6	0.22
(1,2925)	1:63:A:PHE:HD1	1:112:A:ALA:HB3	6	0.22
(1,2925)	1:63:A:PHE:HD2	1:112:A:ALA:HB1	6	0.22
(1,2925)	1:63:A:PHE:HD2	1:112:A:ALA:HB2	6	0.22
(1,2925)	1:63:A:PHE:HD2	1:112:A:ALA:HB3	6	0.22
(1,2902)	1:49:A:HIS:HD2	1:90:A:GLY:HA3	9	0.22
(1,2794)	1:109:A:TYR:HB3	1:127:A:THR:H	3	0.22
(1,2779)	1:126:A:VAL:HG11	1:126:A:VAL:H	2	0.22
(1,2779)	1:126:A:VAL:HG12	1:126:A:VAL:H	2	0.22
(1,2779)	1:126:A:VAL:HG13	1:126:A:VAL:H	2	0.22
(1,2394)	1:84:A:ALA:H	1:104:A:LEU:HD21	7	0.22
(1,2394)	1:84:A:ALA:H	1:104:A:LEU:HD22	7	0.22
(1,2394)	1:84:A:ALA:H	1:104:A:LEU:HD23	7	0.22
(1,2293)	1:65:A:ASP:HB3	1:65:A:ASP:H	3	0.22
(1,2065)	1:40:A:GLY:H	1:38:A:HIS:HB2	4	0.22
(1,1824)	1:121:A:LEU:HD11	1:17:A:GLN:H	9	0.22
(1,1824)	1:121:A:LEU:HD12	1:17:A:GLN:H	9	0.22
(1,1824)	1:121:A:LEU:HD13	1:17:A:GLN:H	9	0.22
(1,1755)	1:86:A:THR:HG21	1:10:A:VAL:H	5	0.22
(1,1755)	1:86:A:THR:HG22	1:10:A:VAL:H	5	0.22
(1,1755)	1:86:A:THR:HG23	1:10:A:VAL:H	5	0.22
(1,1627)	1:83:A:VAL:HG21	1:104:A:LEU:HD11	3	0.22
(1,1627)	1:83:A:VAL:HG21	1:104:A:LEU:HD12	3	0.22
(1,1627)	1:83:A:VAL:HG21	1:104:A:LEU:HD13	3	0.22
(1,1627)	1:83:A:VAL:HG22	1:104:A:LEU:HD11	3	0.22
(1,1627)	1:83:A:VAL:HG22	1:104:A:LEU:HD12	3	0.22
(1,1627)	1:83:A:VAL:HG22	1:104:A:LEU:HD13	3	0.22
(1,1627)	1:83:A:VAL:HG23	1:104:A:LEU:HD11	3	0.22
(1,1627)	1:83:A:VAL:HG23	1:104:A:LEU:HD12	3	0.22
(1,1627)	1:83:A:VAL:HG23	1:104:A:LEU:HD13	3	0.22
(1,1618)	1:109:A:TYR:HD1	1:104:A:LEU:HD21	9	0.22
(1,1618)	1:109:A:TYR:HD1	1:104:A:LEU:HD22	9	0.22
(1,1618)	1:109:A:TYR:HD1	1:104:A:LEU:HD23	9	0.22
(1,1618)	1:109:A:TYR:HD2	1:104:A:LEU:HD21	9	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1618)	1:109:A:TYR:HD2	1:104:A:LEU:HD22	9	0.22
(1,1618)	1:109:A:TYR:HD2	1:104:A:LEU:HD23	9	0.22
(1,1543)	1:85:A:HIS:HD2	1:82:A:VAL:HG21	9	0.22
(1,1543)	1:85:A:HIS:HD2	1:82:A:VAL:HG22	9	0.22
(1,1543)	1:85:A:HIS:HD2	1:82:A:VAL:HG23	9	0.22
(1,1426)	1:86:A:THR:HG21	1:36:A:LEU:HD11	6	0.22
(1,1426)	1:86:A:THR:HG21	1:36:A:LEU:HD12	6	0.22
(1,1426)	1:86:A:THR:HG21	1:36:A:LEU:HD13	6	0.22
(1,1426)	1:86:A:THR:HG22	1:36:A:LEU:HD11	6	0.22
(1,1426)	1:86:A:THR:HG22	1:36:A:LEU:HD12	6	0.22
(1,1426)	1:86:A:THR:HG22	1:36:A:LEU:HD13	6	0.22
(1,1426)	1:86:A:THR:HG23	1:36:A:LEU:HD11	6	0.22
(1,1426)	1:86:A:THR:HG23	1:36:A:LEU:HD12	6	0.22
(1,1426)	1:86:A:THR:HG23	1:36:A:LEU:HD13	6	0.22
(1,1303)	1:56:A:ALA:H	1:55:A:LYS:HD2	1	0.22
(1,1268)	1:127:A:THR:HB	1:24:A:GLN:HG3	9	0.22
(1,1192)	1:116:A:PRO:HD2	1:74:A:TYR:HA	4	0.22
(1,1087)	1:108:A:ASP:H	1:108:A:ASP:HB3	7	0.22
(1,1086)	1:108:A:ASP:HB2	1:56:A:ALA:H	4	0.22
(1,973)	1:98:A:THR:H	1:97:A:LEU:HB3	8	0.22
(1,959)	1:96:A:SER:HB3	1:33:A:THR:HG21	10	0.22
(1,959)	1:96:A:SER:HB3	1:33:A:THR:HG22	10	0.22
(1,959)	1:96:A:SER:HB3	1:33:A:THR:HG23	10	0.22
(1,813)	1:85:A:HIS:HB3	1:86:A:THR:H	9	0.22
(1,747)	1:77:A:PRO:HA	1:79:A:ASP:H	9	0.22
(1,711)	1:74:A:TYR:HB3	1:88:A:LEU:HD11	3	0.22
(1,711)	1:74:A:TYR:HB3	1:88:A:LEU:HD12	3	0.22
(1,711)	1:74:A:TYR:HB3	1:88:A:LEU:HD13	3	0.22
(1,35)	1:11:A:GLU:HA	1:36:A:LEU:HD21	6	0.22
(1,35)	1:11:A:GLU:HA	1:36:A:LEU:HD22	6	0.22
(1,35)	1:11:A:GLU:HA	1:36:A:LEU:HD23	6	0.22
(1,35)	1:11:A:GLU:HA	1:36:A:LEU:HD21	8	0.22
(1,35)	1:11:A:GLU:HA	1:36:A:LEU:HD22	8	0.22
(1,35)	1:11:A:GLU:HA	1:36:A:LEU:HD23	8	0.22
(1,3264)	1:111:A:PHE:HD1	1:20:A:THR:HG23	4	0.21
(1,3246)	1:123:A:ASN:HD22	1:120:A:ALA:HB1	1	0.21
(1,3243)	1:123:A:ASN:HD21	1:120:A:ALA:HB2	10	0.21
(1,3226)	1:100:A:ASP:H	1:99:A:LEU:HB3	7	0.21
(1,2970)	1:109:A:TYR:HD1	1:53:A:ILE:HD11	3	0.21
(1,2970)	1:109:A:TYR:HD1	1:53:A:ILE:HD12	3	0.21
(1,2970)	1:109:A:TYR:HD1	1:53:A:ILE:HD13	3	0.21
(1,2970)	1:109:A:TYR:HD2	1:53:A:ILE:HD11	3	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2970)	1:109:A:TYR:HD2	1:53:A:ILE:HD12	3	0.21
(1,2970)	1:109:A:TYR:HD2	1:53:A:ILE:HD13	3	0.21
(1,2925)	1:63:A:PHE:HD1	1:112:A:ALA:HB1	1	0.21
(1,2925)	1:63:A:PHE:HD1	1:112:A:ALA:HB2	1	0.21
(1,2925)	1:63:A:PHE:HD1	1:112:A:ALA:HB3	1	0.21
(1,2925)	1:63:A:PHE:HD2	1:112:A:ALA:HB1	1	0.21
(1,2925)	1:63:A:PHE:HD2	1:112:A:ALA:HB2	1	0.21
(1,2925)	1:63:A:PHE:HD2	1:112:A:ALA:HB3	1	0.21
(1,2925)	1:63:A:PHE:HD1	1:112:A:ALA:HB1	10	0.21
(1,2925)	1:63:A:PHE:HD1	1:112:A:ALA:HB2	10	0.21
(1,2925)	1:63:A:PHE:HD1	1:112:A:ALA:HB3	10	0.21
(1,2925)	1:63:A:PHE:HD2	1:112:A:ALA:HB1	10	0.21
(1,2925)	1:63:A:PHE:HD2	1:112:A:ALA:HB2	10	0.21
(1,2925)	1:63:A:PHE:HD2	1:112:A:ALA:HB3	10	0.21
(1,2889)	1:66:A:GLY:HA3	1:74:A:TYR:HD1	3	0.21
(1,2889)	1:66:A:GLY:HA3	1:74:A:TYR:HD2	3	0.21
(1,2728)	1:122:A:MET:H	1:118:A:HIS:HB2	8	0.21
(1,2710)	1:120:A:ALA:H	1:121:A:LEU:HD11	6	0.21
(1,2710)	1:120:A:ALA:H	1:121:A:LEU:HD12	6	0.21
(1,2710)	1:120:A:ALA:H	1:121:A:LEU:HD13	6	0.21
(1,2676)	1:75:A:VAL:HG21	1:114:A:THR:H	5	0.21
(1,2676)	1:75:A:VAL:HG22	1:114:A:THR:H	5	0.21
(1,2676)	1:75:A:VAL:HG23	1:114:A:THR:H	5	0.21
(1,2528)	1:99:A:LEU:H	1:31:A:GLU:HG2	3	0.21
(1,2528)	1:99:A:LEU:H	1:31:A:GLU:HG3	3	0.21
(1,2469)	1:92:A:GLY:H	1:38:A:HIS:HB2	9	0.21
(1,2364)	1:82:A:VAL:HG11	1:79:A:ASP:H	8	0.21
(1,2364)	1:82:A:VAL:HG12	1:79:A:ASP:H	8	0.21
(1,2364)	1:82:A:VAL:HG13	1:79:A:ASP:H	8	0.21
(1,2293)	1:65:A:ASP:HB3	1:65:A:ASP:H	4	0.21
(1,2105)	1:43:A:PRO:HB3	1:45:A:ALA:H	9	0.21
(1,2048)	1:39:A:THR:HG21	1:39:A:THR:H	6	0.21
(1,2048)	1:39:A:THR:HG22	1:39:A:THR:H	6	0.21
(1,2048)	1:39:A:THR:HG23	1:39:A:THR:H	6	0.21
(1,2045)	1:94:A:GLU:HB2	1:38:A:HIS:H	3	0.21
(1,1834)	1:17:A:GLN:HE21	1:17:A:GLN:HB2	1	0.21
(1,1689)	1:128:A:LEU:H	1:128:A:LEU:HD11	8	0.21
(1,1689)	1:128:A:LEU:H	1:128:A:LEU:HD12	8	0.21
(1,1689)	1:128:A:LEU:H	1:128:A:LEU:HD13	8	0.21
(1,1555)	1:98:A:THR:H	1:84:A:ALA:HB1	3	0.21
(1,1555)	1:98:A:THR:H	1:84:A:ALA:HB2	3	0.21
(1,1555)	1:98:A:THR:H	1:84:A:ALA:HB3	3	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1461)	1:126:A:VAL:HG11	1:51:A:LEU:HD21	9	0.21
(1,1461)	1:126:A:VAL:HG11	1:51:A:LEU:HD22	9	0.21
(1,1461)	1:126:A:VAL:HG11	1:51:A:LEU:HD23	9	0.21
(1,1461)	1:126:A:VAL:HG12	1:51:A:LEU:HD21	9	0.21
(1,1461)	1:126:A:VAL:HG12	1:51:A:LEU:HD22	9	0.21
(1,1461)	1:126:A:VAL:HG12	1:51:A:LEU:HD23	9	0.21
(1,1461)	1:126:A:VAL:HG13	1:51:A:LEU:HD21	9	0.21
(1,1461)	1:126:A:VAL:HG13	1:51:A:LEU:HD22	9	0.21
(1,1461)	1:126:A:VAL:HG13	1:51:A:LEU:HD23	9	0.21
(1,1392)	1:127:A:THR:H	1:25:A:VAL:HG11	3	0.21
(1,1392)	1:127:A:THR:H	1:25:A:VAL:HG12	3	0.21
(1,1392)	1:127:A:THR:H	1:25:A:VAL:HG13	3	0.21
(1,973)	1:98:A:THR:H	1:97:A:LEU:HB3	1	0.21
(1,813)	1:85:A:HIS:HB3	1:86:A:THR:H	1	0.21
(1,468)	1:88:A:LEU:HG	1:48:A:GLY:HA3	9	0.21
(1,418)	1:43:A:PRO:HD3	1:42:A:GLN:HB2	7	0.21
(1,418)	1:43:A:PRO:HD3	1:42:A:GLN:HB3	7	0.21
(1,357)	1:37:A:LYS:HD2	1:35:A:THR:HG21	1	0.21
(1,357)	1:37:A:LYS:HD2	1:35:A:THR:HG22	1	0.21
(1,357)	1:37:A:LYS:HD2	1:35:A:THR:HG23	1	0.21
(1,357)	1:37:A:LYS:HD3	1:35:A:THR:HG21	1	0.21
(1,357)	1:37:A:LYS:HD3	1:35:A:THR:HG22	1	0.21
(1,357)	1:37:A:LYS:HD3	1:35:A:THR:HG23	1	0.21
(1,248)	1:31:A:GLU:HB2	1:32:A:PHE:H	4	0.21
(1,230)	1:29:A:CYS:HB2	1:25:A:VAL:HG21	4	0.21
(1,230)	1:29:A:CYS:HB2	1:25:A:VAL:HG22	4	0.21
(1,230)	1:29:A:CYS:HB2	1:25:A:VAL:HG23	4	0.21
(1,230)	1:29:A:CYS:HB3	1:25:A:VAL:HG21	4	0.21
(1,230)	1:29:A:CYS:HB3	1:25:A:VAL:HG22	4	0.21
(1,230)	1:29:A:CYS:HB3	1:25:A:VAL:HG23	4	0.21
(1,211)	1:26:A:SER:HB3	1:25:A:VAL:HG21	9	0.21
(1,211)	1:26:A:SER:HB3	1:25:A:VAL:HG22	9	0.21
(1,211)	1:26:A:SER:HB3	1:25:A:VAL:HG23	9	0.21
(1,61)	1:18:A:PHE:HD1	1:12:A:SER:HB2	8	0.21
(1,61)	1:18:A:PHE:HD2	1:12:A:SER:HB2	8	0.21
(1,52)	1:49:A:HIS:HD2	1:12:A:SER:HB3	8	0.21
(1,21)	1:10:A:VAL:HB	1:9:A:THR:HA	3	0.21
(1,21)	1:10:A:VAL:HB	1:9:A:THR:HA	9	0.21
(1,3249)	1:128:A:LEU:HB2	1:129:A:VAL:H	9	0.2
(1,3206)	1:78:A:ASP:HA	1:78:A:ASP:H	2	0.2
(1,3143)	1:103:A:LYS:HB3	1:99:A:LEU:HD21	8	0.2
(1,3075)	1:55:A:LYS:HB2	1:54:A:ALA:HB3	5	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3058)	1:37:A:LYS:HB3	1:11:A:GLU:HG2	10	0.2
(1,2967)	1:109:A:TYR:HD1	1:126:A:VAL:HG21	4	0.2
(1,2967)	1:109:A:TYR:HD1	1:126:A:VAL:HG22	4	0.2
(1,2967)	1:109:A:TYR:HD1	1:126:A:VAL:HG23	4	0.2
(1,2967)	1:109:A:TYR:HD2	1:126:A:VAL:HG21	4	0.2
(1,2967)	1:109:A:TYR:HD2	1:126:A:VAL:HG22	4	0.2
(1,2967)	1:109:A:TYR:HD2	1:126:A:VAL:HG23	4	0.2
(1,2925)	1:63:A:PHE:HD1	1:112:A:ALA:HB1	3	0.2
(1,2925)	1:63:A:PHE:HD1	1:112:A:ALA:HB2	3	0.2
(1,2925)	1:63:A:PHE:HD1	1:112:A:ALA:HB3	3	0.2
(1,2925)	1:63:A:PHE:HD2	1:112:A:ALA:HB1	3	0.2
(1,2925)	1:63:A:PHE:HD2	1:112:A:ALA:HB2	3	0.2
(1,2925)	1:63:A:PHE:HD2	1:112:A:ALA:HB3	3	0.2
(1,2889)	1:66:A:GLY:HA3	1:74:A:TYR:HD1	8	0.2
(1,2889)	1:66:A:GLY:HA3	1:74:A:TYR:HD2	8	0.2
(1,2882)	1:74:A:TYR:HD1	1:88:A:LEU:HD11	6	0.2
(1,2882)	1:74:A:TYR:HD1	1:88:A:LEU:HD12	6	0.2
(1,2882)	1:74:A:TYR:HD1	1:88:A:LEU:HD13	6	0.2
(1,2882)	1:74:A:TYR:HD2	1:88:A:LEU:HD11	6	0.2
(1,2882)	1:74:A:TYR:HD2	1:88:A:LEU:HD12	6	0.2
(1,2882)	1:74:A:TYR:HD2	1:88:A:LEU:HD13	6	0.2
(1,2763)	1:123:A:ASN:HB2	1:124:A:GLY:H	10	0.2
(1,2595)	1:74:A:TYR:HB3	1:50:A:ASN:HD21	1	0.2
(1,2395)	1:83:A:VAL:HG21	1:84:A:ALA:H	2	0.2
(1,2395)	1:83:A:VAL:HG22	1:84:A:ALA:H	2	0.2
(1,2395)	1:83:A:VAL:HG23	1:84:A:ALA:H	2	0.2
(1,2395)	1:83:A:VAL:HG21	1:84:A:ALA:H	4	0.2
(1,2395)	1:83:A:VAL:HG22	1:84:A:ALA:H	4	0.2
(1,2395)	1:83:A:VAL:HG23	1:84:A:ALA:H	4	0.2
(1,2293)	1:65:A:ASP:HB3	1:65:A:ASP:H	5	0.2
(1,2170)	1:88:A:LEU:HB3	1:50:A:ASN:HD22	7	0.2
(1,1961)	1:101:A:PRO:HB2	1:29:A:CYS:H	7	0.2
(1,1950)	1:27:A:LYS:HD2	1:28:A:ALA:H	7	0.2
(1,1950)	1:27:A:LYS:HD3	1:28:A:ALA:H	7	0.2
(1,1767)	1:19:A:ASN:HD22	1:11:A:GLU:H	8	0.2
(1,1534)	1:75:A:VAL:H	1:75:A:VAL:HG21	6	0.2
(1,1534)	1:75:A:VAL:H	1:75:A:VAL:HG22	6	0.2
(1,1534)	1:75:A:VAL:H	1:75:A:VAL:HG23	6	0.2
(1,1304)	1:55:A:LYS:HD2	1:55:A:LYS:H	8	0.2
(1,1064)	1:107:A:GLY:HA2	1:55:A:LYS:HD3	7	0.2
(1,1056)	1:104:A:LEU:HB3	1:128:A:LEU:HD11	8	0.2
(1,1056)	1:104:A:LEU:HB3	1:128:A:LEU:HD12	8	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1056)	1:104:A:LEU:HB3	1:128:A:LEU:HD13	8	0.2
(1,994)	1:83:A:VAL:HG21	1:99:A:LEU:HB3	1	0.2
(1,994)	1:83:A:VAL:HG22	1:99:A:LEU:HB3	1	0.2
(1,994)	1:83:A:VAL:HG23	1:99:A:LEU:HB3	1	0.2
(1,813)	1:85:A:HIS:HB3	1:86:A:THR:H	2	0.2
(1,748)	1:77:A:PRO:HA	1:78:A:ASP:H	9	0.2
(1,572)	1:109:A:TYR:HE1	1:55:A:LYS:HD3	3	0.2
(1,572)	1:109:A:TYR:HE2	1:55:A:LYS:HD3	3	0.2
(1,496)	1:114:A:THR:HG1	1:50:A:ASN:HB3	2	0.2
(1,35)	1:11:A:GLU:HA	1:36:A:LEU:HD21	10	0.2
(1,35)	1:11:A:GLU:HA	1:36:A:LEU:HD22	10	0.2
(1,35)	1:11:A:GLU:HA	1:36:A:LEU:HD23	10	0.2
(1,21)	1:10:A:VAL:HB	1:9:A:THR:HA	8	0.2
(1,3264)	1:111:A:PHE:HD2	1:20:A:THR:HG21	1	0.19
(1,3262)	1:109:A:TYR:HE2	1:55:A:LYS:HD2	10	0.19
(1,3227)	1:103:A:LYS:HG2	1:102:A:ALA:H	7	0.19
(1,3221)	1:94:A:GLU:HB3	1:95:A:SER:H	9	0.19
(1,3164)	1:17:A:GLN:H	1:17:A:GLN:HB2	9	0.19
(1,2966)	1:109:A:TYR:HE1	1:128:A:LEU:HD11	3	0.19
(1,2966)	1:109:A:TYR:HE1	1:128:A:LEU:HD12	3	0.19
(1,2966)	1:109:A:TYR:HE1	1:128:A:LEU:HD13	3	0.19
(1,2966)	1:109:A:TYR:HE2	1:128:A:LEU:HD11	3	0.19
(1,2966)	1:109:A:TYR:HE2	1:128:A:LEU:HD12	3	0.19
(1,2966)	1:109:A:TYR:HE2	1:128:A:LEU:HD13	3	0.19
(1,2889)	1:66:A:GLY:HA3	1:74:A:TYR:HD1	7	0.19
(1,2889)	1:66:A:GLY:HA3	1:74:A:TYR:HD2	7	0.19
(1,2710)	1:120:A:ALA:H	1:121:A:LEU:HD11	8	0.19
(1,2710)	1:120:A:ALA:H	1:121:A:LEU:HD12	8	0.19
(1,2710)	1:120:A:ALA:H	1:121:A:LEU:HD13	8	0.19
(1,2629)	1:125:A:LYS:HD2	1:111:A:PHE:H	3	0.19
(1,2629)	1:125:A:LYS:HD3	1:111:A:PHE:H	3	0.19
(1,2624)	1:110:A:LYS:HG2	1:110:A:LYS:H	1	0.19
(1,2573)	1:105:A:ALA:H	1:128:A:LEU:HD11	2	0.19
(1,2573)	1:105:A:ALA:H	1:128:A:LEU:HD12	2	0.19
(1,2573)	1:105:A:ALA:H	1:128:A:LEU:HD13	2	0.19
(1,2469)	1:92:A:GLY:H	1:38:A:HIS:HB2	6	0.19
(1,2293)	1:65:A:ASP:HB3	1:65:A:ASP:H	2	0.19
(1,2293)	1:65:A:ASP:HB3	1:65:A:ASP:H	7	0.19
(1,1979)	1:32:A:PHE:H	1:25:A:VAL:HG21	4	0.19
(1,1979)	1:32:A:PHE:H	1:25:A:VAL:HG22	4	0.19
(1,1979)	1:32:A:PHE:H	1:25:A:VAL:HG23	4	0.19
(1,1903)	1:24:A:GLN:HG2	1:24:A:GLN:H	4	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1847)	1:18:A:PHE:H	1:20:A:THR:HG21	2	0.19
(1,1847)	1:18:A:PHE:H	1:20:A:THR:HG22	2	0.19
(1,1847)	1:18:A:PHE:H	1:20:A:THR:HG23	2	0.19
(1,1844)	1:18:A:PHE:H	1:17:A:GLN:HB2	3	0.19
(1,1786)	1:38:A:HIS:HB3	1:13:A:ASN:H	4	0.19
(1,1525)	1:114:A:THR:HG21	1:75:A:VAL:HG21	5	0.19
(1,1525)	1:114:A:THR:HG21	1:75:A:VAL:HG22	5	0.19
(1,1525)	1:114:A:THR:HG21	1:75:A:VAL:HG23	5	0.19
(1,1525)	1:114:A:THR:HG22	1:75:A:VAL:HG21	5	0.19
(1,1525)	1:114:A:THR:HG22	1:75:A:VAL:HG22	5	0.19
(1,1525)	1:114:A:THR:HG22	1:75:A:VAL:HG23	5	0.19
(1,1525)	1:114:A:THR:HG23	1:75:A:VAL:HG21	5	0.19
(1,1525)	1:114:A:THR:HG23	1:75:A:VAL:HG22	5	0.19
(1,1525)	1:114:A:THR:HG23	1:75:A:VAL:HG23	5	0.19
(1,1432)	1:47:A:MET:HE1	1:42:A:GLN:HE22	1	0.19
(1,1432)	1:47:A:MET:HE2	1:42:A:GLN:HE22	1	0.19
(1,1432)	1:47:A:MET:HE3	1:42:A:GLN:HE22	1	0.19
(1,1420)	1:51:A:LEU:H	1:34:A:ILE:HG21	7	0.19
(1,1420)	1:51:A:LEU:H	1:34:A:ILE:HG22	7	0.19
(1,1420)	1:51:A:LEU:H	1:34:A:ILE:HG23	7	0.19
(1,1385)	1:128:A:LEU:HB2	1:25:A:VAL:HG21	8	0.19
(1,1385)	1:128:A:LEU:HB2	1:25:A:VAL:HG22	8	0.19
(1,1385)	1:128:A:LEU:HB2	1:25:A:VAL:HG23	8	0.19
(1,1249)	1:123:A:ASN:HB3	1:124:A:GLY:H	4	0.19
(1,1063)	1:107:A:GLY:HA2	1:55:A:LYS:HD2	3	0.19
(1,1024)	1:31:A:GLU:HA	1:101:A:PRO:HG2	7	0.19
(1,830)	1:86:A:THR:HA	1:97:A:LEU:HB2	7	0.19
(1,754)	1:77:A:PRO:HD3	1:69:A:ALA:HB1	4	0.19
(1,754)	1:77:A:PRO:HD3	1:69:A:ALA:HB2	4	0.19
(1,754)	1:77:A:PRO:HD3	1:69:A:ALA:HB3	4	0.19
(1,586)	1:27:A:LYS:HE2	1:130:A:ASP:HA	8	0.19
(1,586)	1:27:A:LYS:HE3	1:130:A:ASP:HA	8	0.19
(1,468)	1:88:A:LEU:HG	1:48:A:GLY:HA3	10	0.19
(1,418)	1:43:A:PRO:HD3	1:42:A:GLN:HB2	4	0.19
(1,418)	1:43:A:PRO:HD3	1:42:A:GLN:HB3	4	0.19
(1,418)	1:43:A:PRO:HD3	1:42:A:GLN:HB2	5	0.19
(1,418)	1:43:A:PRO:HD3	1:42:A:GLN:HB3	5	0.19
(1,248)	1:31:A:GLU:HB2	1:32:A:PHE:H	7	0.19
(1,21)	1:10:A:VAL:HB	1:9:A:THR:HA	5	0.19
(1,3249)	1:128:A:LEU:HB2	1:129:A:VAL:H	6	0.18
(1,3226)	1:100:A:ASP:H	1:99:A:LEU:HB3	1	0.18
(1,3164)	1:17:A:GLN:H	1:17:A:GLN:HB2	8	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2983)	1:21:A:LYS:HG2	1:111:A:PHE:HZ	2	0.18
(1,2983)	1:21:A:LYS:HG3	1:111:A:PHE:HZ	2	0.18
(1,2902)	1:49:A:HIS:HD2	1:90:A:GLY:HA3	6	0.18
(1,2889)	1:66:A:GLY:HA3	1:74:A:TYR:HD1	10	0.18
(1,2889)	1:66:A:GLY:HA3	1:74:A:TYR:HD2	10	0.18
(1,2840)	1:53:A:ILE:HD11	1:32:A:PHE:HD1	2	0.18
(1,2840)	1:53:A:ILE:HD11	1:32:A:PHE:HD2	2	0.18
(1,2840)	1:53:A:ILE:HD12	1:32:A:PHE:HD1	2	0.18
(1,2840)	1:53:A:ILE:HD12	1:32:A:PHE:HD2	2	0.18
(1,2840)	1:53:A:ILE:HD13	1:32:A:PHE:HD1	2	0.18
(1,2840)	1:53:A:ILE:HD13	1:32:A:PHE:HD2	2	0.18
(1,2736)	1:123:A:ASN:H	1:18:A:PHE:HE1	2	0.18
(1,2736)	1:123:A:ASN:H	1:18:A:PHE:HE2	2	0.18
(1,2736)	1:123:A:ASN:H	1:18:A:PHE:HE1	10	0.18
(1,2736)	1:123:A:ASN:H	1:18:A:PHE:HE2	10	0.18
(1,2710)	1:120:A:ALA:H	1:121:A:LEU:HD11	1	0.18
(1,2710)	1:120:A:ALA:H	1:121:A:LEU:HD12	1	0.18
(1,2710)	1:120:A:ALA:H	1:121:A:LEU:HD13	1	0.18
(1,2710)	1:120:A:ALA:H	1:121:A:LEU:HD11	4	0.18
(1,2710)	1:120:A:ALA:H	1:121:A:LEU:HD12	4	0.18
(1,2710)	1:120:A:ALA:H	1:121:A:LEU:HD13	4	0.18
(1,2651)	1:113:A:CYS:H	1:52:A:VAL:HG11	1	0.18
(1,2651)	1:113:A:CYS:H	1:52:A:VAL:HG12	1	0.18
(1,2651)	1:113:A:CYS:H	1:52:A:VAL:HG13	1	0.18
(1,2651)	1:113:A:CYS:H	1:52:A:VAL:HG11	10	0.18
(1,2651)	1:113:A:CYS:H	1:52:A:VAL:HG12	10	0.18
(1,2651)	1:113:A:CYS:H	1:52:A:VAL:HG13	10	0.18
(1,2631)	1:110:A:LYS:HE2	1:111:A:PHE:H	2	0.18
(1,2631)	1:110:A:LYS:HE3	1:111:A:PHE:H	2	0.18
(1,2629)	1:125:A:LYS:HD2	1:111:A:PHE:H	7	0.18
(1,2629)	1:125:A:LYS:HD3	1:111:A:PHE:H	7	0.18
(1,2624)	1:110:A:LYS:HG2	1:110:A:LYS:H	3	0.18
(1,2497)	1:96:A:SER:H	1:36:A:LEU:HB2	7	0.18
(1,2293)	1:65:A:ASP:HB3	1:65:A:ASP:H	9	0.18
(1,2200)	1:53:A:ILE:H	1:52:A:VAL:HG21	6	0.18
(1,2200)	1:53:A:ILE:H	1:52:A:VAL:HG22	6	0.18
(1,2200)	1:53:A:ILE:H	1:52:A:VAL:HG23	6	0.18
(1,1944)	1:27:A:LYS:HG2	1:27:A:LYS:H	4	0.18
(1,1944)	1:27:A:LYS:HG3	1:27:A:LYS:H	4	0.18
(1,1879)	1:20:A:THR:H	1:19:A:ASN:HB3	7	0.18
(1,1628)	1:101:A:PRO:HB2	1:104:A:LEU:HD11	8	0.18
(1,1628)	1:101:A:PRO:HB2	1:104:A:LEU:HD12	8	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1628)	1:101:A:PRO:HB2	1:104:A:LEU:HD13	8	0.18
(1,1617)	1:104:A:LEU:H	1:104:A:LEU:HD21	9	0.18
(1,1617)	1:104:A:LEU:H	1:104:A:LEU:HD22	9	0.18
(1,1617)	1:104:A:LEU:H	1:104:A:LEU:HD23	9	0.18
(1,1552)	1:109:A:TYR:HE1	1:83:A:VAL:HG11	9	0.18
(1,1552)	1:109:A:TYR:HE1	1:83:A:VAL:HG12	9	0.18
(1,1552)	1:109:A:TYR:HE1	1:83:A:VAL:HG13	9	0.18
(1,1552)	1:109:A:TYR:HE2	1:83:A:VAL:HG11	9	0.18
(1,1552)	1:109:A:TYR:HE2	1:83:A:VAL:HG12	9	0.18
(1,1552)	1:109:A:TYR:HE2	1:83:A:VAL:HG13	9	0.18
(1,1383)	1:128:A:LEU:HD11	1:25:A:VAL:HG21	1	0.18
(1,1383)	1:128:A:LEU:HD11	1:25:A:VAL:HG22	1	0.18
(1,1383)	1:128:A:LEU:HD11	1:25:A:VAL:HG23	1	0.18
(1,1383)	1:128:A:LEU:HD12	1:25:A:VAL:HG21	1	0.18
(1,1383)	1:128:A:LEU:HD12	1:25:A:VAL:HG22	1	0.18
(1,1383)	1:128:A:LEU:HD12	1:25:A:VAL:HG23	1	0.18
(1,1383)	1:128:A:LEU:HD13	1:25:A:VAL:HG21	1	0.18
(1,1383)	1:128:A:LEU:HD13	1:25:A:VAL:HG22	1	0.18
(1,1383)	1:128:A:LEU:HD13	1:25:A:VAL:HG23	1	0.18
(1,1309)	1:114:A:THR:HG1	1:50:A:ASN:HB2	5	0.18
(1,1268)	1:127:A:THR:HB	1:24:A:GLN:HG3	5	0.18
(1,1127)	1:111:A:PHE:HA	1:126:A:VAL:HG21	7	0.18
(1,1127)	1:111:A:PHE:HA	1:126:A:VAL:HG22	7	0.18
(1,1127)	1:111:A:PHE:HA	1:126:A:VAL:HG23	7	0.18
(1,1069)	1:107:A:GLY:HA3	1:108:A:ASP:HB3	7	0.18
(1,935)	1:86:A:THR:HA	1:95:A:SER:HB2	8	0.18
(1,826)	1:85:A:HIS:HB3	1:114:A:THR:HG21	5	0.18
(1,826)	1:85:A:HIS:HB3	1:114:A:THR:HG22	5	0.18
(1,826)	1:85:A:HIS:HB3	1:114:A:THR:HG23	5	0.18
(1,813)	1:85:A:HIS:HB3	1:86:A:THR:H	7	0.18
(1,586)	1:27:A:LYS:HE2	1:130:A:ASP:HA	5	0.18
(1,586)	1:27:A:LYS:HE3	1:130:A:ASP:HA	5	0.18
(1,418)	1:43:A:PRO:HD3	1:42:A:GLN:HB2	1	0.18
(1,418)	1:43:A:PRO:HD3	1:42:A:GLN:HB3	1	0.18
(1,418)	1:43:A:PRO:HD3	1:42:A:GLN:HB2	8	0.18
(1,418)	1:43:A:PRO:HD3	1:42:A:GLN:HB3	8	0.18
(1,52)	1:49:A:HIS:HD2	1:12:A:SER:HB3	9	0.18
(1,3249)	1:128:A:LEU:HB2	1:129:A:VAL:H	4	0.17
(1,3048)	1:25:A:VAL:HB	1:23:A:ILE:HG21	5	0.17
(1,2925)	1:63:A:PHE:HD1	1:112:A:ALA:HB1	8	0.17
(1,2925)	1:63:A:PHE:HD1	1:112:A:ALA:HB2	8	0.17
(1,2925)	1:63:A:PHE:HD1	1:112:A:ALA:HB3	8	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2925)	1:63:A:PHE:HD2	1:112:A:ALA:HB1	8	0.17
(1,2925)	1:63:A:PHE:HD2	1:112:A:ALA:HB2	8	0.17
(1,2925)	1:63:A:PHE:HD2	1:112:A:ALA:HB3	8	0.17
(1,2889)	1:66:A:GLY:HA3	1:74:A:TYR:HD1	4	0.17
(1,2889)	1:66:A:GLY:HA3	1:74:A:TYR:HD2	4	0.17
(1,2836)	1:18:A:PHE:HE1	1:36:A:LEU:HD21	10	0.17
(1,2836)	1:18:A:PHE:HE1	1:36:A:LEU:HD22	10	0.17
(1,2836)	1:18:A:PHE:HE1	1:36:A:LEU:HD23	10	0.17
(1,2836)	1:18:A:PHE:HE2	1:36:A:LEU:HD21	10	0.17
(1,2836)	1:18:A:PHE:HE2	1:36:A:LEU:HD22	10	0.17
(1,2836)	1:18:A:PHE:HE2	1:36:A:LEU:HD23	10	0.17
(1,2709)	1:119:A:GLY:H	1:112:A:ALA:HB1	10	0.17
(1,2709)	1:119:A:GLY:H	1:112:A:ALA:HB2	10	0.17
(1,2709)	1:119:A:GLY:H	1:112:A:ALA:HB3	10	0.17
(1,2568)	1:104:A:LEU:HB3	1:104:A:LEU:H	9	0.17
(1,2400)	1:84:A:ALA:H	1:85:A:HIS:HB2	3	0.17
(1,2395)	1:83:A:VAL:HG21	1:84:A:ALA:H	8	0.17
(1,2395)	1:83:A:VAL:HG22	1:84:A:ALA:H	8	0.17
(1,2395)	1:83:A:VAL:HG23	1:84:A:ALA:H	8	0.17
(1,1978)	1:31:A:GLU:H	1:30:A:LYS:HD3	1	0.17
(1,1698)	1:24:A:GLN:HG3	1:129:A:VAL:HG21	2	0.17
(1,1698)	1:24:A:GLN:HG3	1:129:A:VAL:HG22	2	0.17
(1,1698)	1:24:A:GLN:HG3	1:129:A:VAL:HG23	2	0.17
(1,1525)	1:114:A:THR:HG21	1:75:A:VAL:HG21	9	0.17
(1,1525)	1:114:A:THR:HG21	1:75:A:VAL:HG22	9	0.17
(1,1525)	1:114:A:THR:HG21	1:75:A:VAL:HG23	9	0.17
(1,1525)	1:114:A:THR:HG22	1:75:A:VAL:HG21	9	0.17
(1,1525)	1:114:A:THR:HG22	1:75:A:VAL:HG22	9	0.17
(1,1525)	1:114:A:THR:HG22	1:75:A:VAL:HG23	9	0.17
(1,1525)	1:114:A:THR:HG23	1:75:A:VAL:HG21	9	0.17
(1,1525)	1:114:A:THR:HG23	1:75:A:VAL:HG22	9	0.17
(1,1525)	1:114:A:THR:HG23	1:75:A:VAL:HG23	9	0.17
(1,1523)	1:72:A:THR:HG21	1:72:A:THR:HA	3	0.17
(1,1523)	1:72:A:THR:HG22	1:72:A:THR:HA	3	0.17
(1,1523)	1:72:A:THR:HG23	1:72:A:THR:HA	3	0.17
(1,1506)	1:81:A:ARG:HB2	1:62:A:VAL:HG11	2	0.17
(1,1506)	1:81:A:ARG:HB2	1:62:A:VAL:HG12	2	0.17
(1,1506)	1:81:A:ARG:HB2	1:62:A:VAL:HG13	2	0.17
(1,1061)	1:105:A:ALA:HA	1:128:A:LEU:HD11	3	0.17
(1,1061)	1:105:A:ALA:HA	1:128:A:LEU:HD12	3	0.17
(1,1061)	1:105:A:ALA:HA	1:128:A:LEU:HD13	3	0.17
(1,1017)	1:101:A:PRO:HD3	1:25:A:VAL:HG21	5	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1017)	1:101:A:PRO:HD3	1:25:A:VAL:HG22	5	0.17
(1,1017)	1:101:A:PRO:HD3	1:25:A:VAL:HG23	5	0.17
(1,1001)	1:100:A:ASP:HA	1:31:A:GLU:HB2	6	0.17
(1,952)	1:96:A:SER:HA	1:36:A:LEU:HB3	4	0.17
(1,813)	1:85:A:HIS:HB3	1:86:A:THR:H	8	0.17
(1,581)	1:27:A:LYS:HB2	1:130:A:ASP:HA	3	0.17
(1,581)	1:27:A:LYS:HB3	1:130:A:ASP:HA	3	0.17
(1,487)	1:50:A:ASN:HD22	1:50:A:ASN:HA	3	0.17
(1,487)	1:50:A:ASN:HD22	1:50:A:ASN:HA	4	0.17
(1,487)	1:50:A:ASN:HD22	1:50:A:ASN:HA	6	0.17
(1,487)	1:50:A:ASN:HD22	1:50:A:ASN:HA	8	0.17
(1,382)	1:38:A:HIS:HE1	1:40:A:GLY:HA2	8	0.17
(1,21)	1:10:A:VAL:HB	1:9:A:THR:HA	1	0.17
(1,3249)	1:128:A:LEU:HB2	1:129:A:VAL:H	10	0.16
(1,3226)	1:100:A:ASP:H	1:99:A:LEU:HB3	5	0.16
(1,3221)	1:94:A:GLU:HG2	1:95:A:SER:H	10	0.16
(1,3048)	1:25:A:VAL:HB	1:23:A:ILE:HG22	8	0.16
(1,2916)	1:122:A:MET:HE1	1:49:A:HIS:HE1	1	0.16
(1,2916)	1:122:A:MET:HE2	1:49:A:HIS:HE1	1	0.16
(1,2916)	1:122:A:MET:HE3	1:49:A:HIS:HE1	1	0.16
(1,2840)	1:53:A:ILE:HD11	1:32:A:PHE:HD1	1	0.16
(1,2840)	1:53:A:ILE:HD11	1:32:A:PHE:HD2	1	0.16
(1,2840)	1:53:A:ILE:HD12	1:32:A:PHE:HD1	1	0.16
(1,2840)	1:53:A:ILE:HD12	1:32:A:PHE:HD2	1	0.16
(1,2840)	1:53:A:ILE:HD13	1:32:A:PHE:HD1	1	0.16
(1,2840)	1:53:A:ILE:HD13	1:32:A:PHE:HD2	1	0.16
(1,2823)	1:52:A:VAL:HG11	1:114:A:THR:H	1	0.16
(1,2823)	1:52:A:VAL:HG12	1:114:A:THR:H	1	0.16
(1,2823)	1:52:A:VAL:HG13	1:114:A:THR:H	1	0.16
(1,2611)	1:110:A:LYS:HG2	1:109:A:TYR:H	5	0.16
(1,2572)	1:105:A:ALA:H	1:104:A:LEU:HD21	7	0.16
(1,2572)	1:105:A:ALA:H	1:104:A:LEU:HD22	7	0.16
(1,2572)	1:105:A:ALA:H	1:104:A:LEU:HD23	7	0.16
(1,2508)	1:85:A:HIS:H	1:97:A:LEU:H	5	0.16
(1,2496)	1:96:A:SER:H	1:36:A:LEU:HB3	5	0.16
(1,2496)	1:96:A:SER:H	1:36:A:LEU:HB3	6	0.16
(1,2478)	1:93:A:GLU:H	1:38:A:HIS:HB2	9	0.16
(1,2200)	1:53:A:ILE:H	1:52:A:VAL:HG21	4	0.16
(1,2200)	1:53:A:ILE:H	1:52:A:VAL:HG22	4	0.16
(1,2200)	1:53:A:ILE:H	1:52:A:VAL:HG23	4	0.16
(1,2177)	1:50:A:ASN:HB3	1:51:A:LEU:H	9	0.16
(1,2138)	1:88:A:LEU:HD11	1:48:A:GLY:H	10	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2138)	1:88:A:LEU:HD12	1:48:A:GLY:H	10	0.16
(1,2138)	1:88:A:LEU:HD13	1:48:A:GLY:H	10	0.16
(1,1786)	1:38:A:HIS:HB3	1:13:A:ASN:H	5	0.16
(1,1614)	1:32:A:PHE:HB2	1:99:A:LEU:HD21	8	0.16
(1,1614)	1:32:A:PHE:HB2	1:99:A:LEU:HD22	8	0.16
(1,1614)	1:32:A:PHE:HB2	1:99:A:LEU:HD23	8	0.16
(1,1543)	1:85:A:HIS:HD2	1:82:A:VAL:HG21	8	0.16
(1,1543)	1:85:A:HIS:HD2	1:82:A:VAL:HG22	8	0.16
(1,1543)	1:85:A:HIS:HD2	1:82:A:VAL:HG23	8	0.16
(1,1523)	1:72:A:THR:HG21	1:72:A:THR:HA	6	0.16
(1,1523)	1:72:A:THR:HG22	1:72:A:THR:HA	6	0.16
(1,1523)	1:72:A:THR:HG23	1:72:A:THR:HA	6	0.16
(1,1513)	1:76:A:LYS:HB3	1:69:A:ALA:HB1	6	0.16
(1,1513)	1:76:A:LYS:HB3	1:69:A:ALA:HB2	6	0.16
(1,1513)	1:76:A:LYS:HB3	1:69:A:ALA:HB3	6	0.16
(1,1509)	1:62:A:VAL:HG21	1:114:A:THR:HG21	3	0.16
(1,1509)	1:62:A:VAL:HG21	1:114:A:THR:HG22	3	0.16
(1,1509)	1:62:A:VAL:HG21	1:114:A:THR:HG23	3	0.16
(1,1509)	1:62:A:VAL:HG22	1:114:A:THR:HG21	3	0.16
(1,1509)	1:62:A:VAL:HG22	1:114:A:THR:HG22	3	0.16
(1,1509)	1:62:A:VAL:HG22	1:114:A:THR:HG23	3	0.16
(1,1509)	1:62:A:VAL:HG23	1:114:A:THR:HG21	3	0.16
(1,1509)	1:62:A:VAL:HG23	1:114:A:THR:HG22	3	0.16
(1,1509)	1:62:A:VAL:HG23	1:114:A:THR:HG23	3	0.16
(1,1420)	1:51:A:LEU:H	1:34:A:ILE:HG21	8	0.16
(1,1420)	1:51:A:LEU:H	1:34:A:ILE:HG22	8	0.16
(1,1420)	1:51:A:LEU:H	1:34:A:ILE:HG23	8	0.16
(1,1341)	1:51:A:LEU:HG	1:10:A:VAL:HG21	7	0.16
(1,1341)	1:51:A:LEU:HG	1:10:A:VAL:HG22	7	0.16
(1,1341)	1:51:A:LEU:HG	1:10:A:VAL:HG23	7	0.16
(1,1268)	1:127:A:THR:HB	1:24:A:GLN:HG3	1	0.16
(1,1268)	1:127:A:THR:HB	1:24:A:GLN:HG3	10	0.16
(1,1133)	1:111:A:PHE:HB2	1:126:A:VAL:HG21	1	0.16
(1,1133)	1:111:A:PHE:HB2	1:126:A:VAL:HG22	1	0.16
(1,1133)	1:111:A:PHE:HB2	1:126:A:VAL:HG23	1	0.16
(1,1095)	1:110:A:LYS:HD3	1:109:A:TYR:HA	8	0.16
(1,876)	1:90:A:GLY:HA2	1:38:A:HIS:HD2	7	0.16
(1,769)	1:77:A:PRO:HG2	1:72:A:THR:HG21	9	0.16
(1,769)	1:77:A:PRO:HG2	1:72:A:THR:HG22	9	0.16
(1,769)	1:77:A:PRO:HG2	1:72:A:THR:HG23	9	0.16
(1,581)	1:27:A:LYS:HB2	1:130:A:ASP:HA	5	0.16
(1,581)	1:27:A:LYS:HB3	1:130:A:ASP:HA	5	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,496)	1:114:A:THR:HG1	1:50:A:ASN:HB3	3	0.16
(1,496)	1:114:A:THR:HG1	1:50:A:ASN:HB3	4	0.16
(1,496)	1:114:A:THR:HG1	1:50:A:ASN:HB3	8	0.16
(1,487)	1:50:A:ASN:HD22	1:50:A:ASN:HA	1	0.16
(1,487)	1:50:A:ASN:HD22	1:50:A:ASN:HA	5	0.16
(1,175)	1:24:A:GLN:HG3	1:129:A:VAL:HG11	5	0.16
(1,175)	1:24:A:GLN:HG3	1:129:A:VAL:HG12	5	0.16
(1,175)	1:24:A:GLN:HG3	1:129:A:VAL:HG13	5	0.16
(1,52)	1:49:A:HIS:HD2	1:12:A:SER:HB3	3	0.16
(1,44)	1:39:A:THR:HG21	1:11:A:GLU:HG3	9	0.16
(1,44)	1:39:A:THR:HG22	1:11:A:GLU:HG3	9	0.16
(1,44)	1:39:A:THR:HG23	1:11:A:GLU:HG3	9	0.16
(1,3262)	1:109:A:TYR:HE1	1:104:A:LEU:HD12	7	0.15
(1,3249)	1:128:A:LEU:HB2	1:129:A:VAL:H	1	0.15
(1,3221)	1:94:A:GLU:HB3	1:95:A:SER:H	1	0.15
(1,2952)	1:83:A:VAL:HB	1:109:A:TYR:HD1	9	0.15
(1,2952)	1:83:A:VAL:HB	1:109:A:TYR:HD2	9	0.15
(1,2902)	1:49:A:HIS:HD2	1:90:A:GLY:HA3	3	0.15
(1,2624)	1:110:A:LYS:HG2	1:110:A:LYS:H	10	0.15
(1,2568)	1:104:A:LEU:HB3	1:104:A:LEU:H	8	0.15
(1,2531)	1:99:A:LEU:H	1:98:A:THR:HG21	6	0.15
(1,2531)	1:99:A:LEU:H	1:98:A:THR:HG22	6	0.15
(1,2531)	1:99:A:LEU:H	1:98:A:THR:HG23	6	0.15
(1,2400)	1:84:A:ALA:H	1:85:A:HIS:HB2	1	0.15
(1,2400)	1:84:A:ALA:H	1:85:A:HIS:HB2	2	0.15
(1,2395)	1:83:A:VAL:HG21	1:84:A:ALA:H	6	0.15
(1,2395)	1:83:A:VAL:HG22	1:84:A:ALA:H	6	0.15
(1,2395)	1:83:A:VAL:HG23	1:84:A:ALA:H	6	0.15
(1,2368)	1:80:A:ALA:H	1:79:A:ASP:HA	7	0.15
(1,2227)	1:110:A:LYS:HD3	1:56:A:ALA:H	7	0.15
(1,2173)	1:51:A:LEU:H	1:36:A:LEU:HD11	2	0.15
(1,2173)	1:51:A:LEU:H	1:36:A:LEU:HD12	2	0.15
(1,2173)	1:51:A:LEU:H	1:36:A:LEU:HD13	2	0.15
(1,2066)	1:40:A:GLY:H	1:13:A:ASN:HB3	3	0.15
(1,1950)	1:27:A:LYS:HD2	1:28:A:ALA:H	3	0.15
(1,1950)	1:27:A:LYS:HD3	1:28:A:ALA:H	3	0.15
(1,1903)	1:24:A:GLN:HG2	1:24:A:GLN:H	9	0.15
(1,1810)	1:14:A:ASP:H	1:13:A:ASN:HB2	4	0.15
(1,1776)	1:12:A:SER:H	1:11:A:GLU:HB3	8	0.15
(1,1535)	1:75:A:VAL:HG21	1:50:A:ASN:HD21	4	0.15
(1,1535)	1:75:A:VAL:HG22	1:50:A:ASN:HD21	4	0.15
(1,1535)	1:75:A:VAL:HG23	1:50:A:ASN:HD21	4	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1523)	1:72:A:THR:HG21	1:72:A:THR:HA	5	0.15
(1,1523)	1:72:A:THR:HG22	1:72:A:THR:HA	5	0.15
(1,1523)	1:72:A:THR:HG23	1:72:A:THR:HA	5	0.15
(1,1523)	1:72:A:THR:HG21	1:72:A:THR:HA	7	0.15
(1,1523)	1:72:A:THR:HG22	1:72:A:THR:HA	7	0.15
(1,1523)	1:72:A:THR:HG23	1:72:A:THR:HA	7	0.15
(1,813)	1:85:A:HIS:HB3	1:86:A:THR:H	3	0.15
(1,619)	1:65:A:ASP:HB3	1:62:A:VAL:HA	9	0.15
(1,487)	1:50:A:ASN:HD22	1:50:A:ASN:HA	10	0.15
(1,258)	1:6:A:CYS:HB2	1:32:A:PHE:HA	4	0.15
(1,230)	1:29:A:CYS:HB2	1:25:A:VAL:HG21	7	0.15
(1,230)	1:29:A:CYS:HB2	1:25:A:VAL:HG22	7	0.15
(1,230)	1:29:A:CYS:HB2	1:25:A:VAL:HG23	7	0.15
(1,230)	1:29:A:CYS:HB3	1:25:A:VAL:HG21	7	0.15
(1,230)	1:29:A:CYS:HB3	1:25:A:VAL:HG22	7	0.15
(1,230)	1:29:A:CYS:HB3	1:25:A:VAL:HG23	7	0.15
(1,21)	1:10:A:VAL:HB	1:9:A:THR:HA	2	0.15
(1,21)	1:10:A:VAL:HB	1:9:A:THR:HA	4	0.15
(1,3263)	1:23:A:ILE:HG12	1:111:A:PHE:HD1	6	0.14
(1,3221)	1:94:A:GLU:HB3	1:95:A:SER:H	2	0.14
(1,3221)	1:94:A:GLU:HG2	1:95:A:SER:H	3	0.14
(1,3164)	1:17:A:GLN:H	1:17:A:GLN:HB2	6	0.14
(1,2916)	1:122:A:MET:HE1	1:49:A:HIS:HE1	6	0.14
(1,2916)	1:122:A:MET:HE2	1:49:A:HIS:HE1	6	0.14
(1,2916)	1:122:A:MET:HE3	1:49:A:HIS:HE1	6	0.14
(1,2591)	1:106:A:ASP:H	1:128:A:LEU:HD11	6	0.14
(1,2591)	1:106:A:ASP:H	1:128:A:LEU:HD12	6	0.14
(1,2591)	1:106:A:ASP:H	1:128:A:LEU:HD13	6	0.14
(1,2568)	1:104:A:LEU:HB3	1:104:A:LEU:H	5	0.14
(1,2568)	1:104:A:LEU:HB3	1:104:A:LEU:H	6	0.14
(1,2568)	1:104:A:LEU:HB3	1:104:A:LEU:H	7	0.14
(1,2380)	1:82:A:VAL:H	1:79:A:ASP:HB2	2	0.14
(1,2380)	1:82:A:VAL:H	1:79:A:ASP:HB3	2	0.14
(1,2291)	1:64:A:LYS:HG3	1:64:A:LYS:H	9	0.14
(1,2200)	1:53:A:ILE:H	1:52:A:VAL:HG21	2	0.14
(1,2200)	1:53:A:ILE:H	1:52:A:VAL:HG22	2	0.14
(1,2200)	1:53:A:ILE:H	1:52:A:VAL:HG23	2	0.14
(1,2177)	1:50:A:ASN:HB3	1:51:A:LEU:H	7	0.14
(1,1613)	1:101:A:PRO:HA	1:99:A:LEU:HD21	5	0.14
(1,1613)	1:101:A:PRO:HA	1:99:A:LEU:HD22	5	0.14
(1,1613)	1:101:A:PRO:HA	1:99:A:LEU:HD23	5	0.14
(1,1586)	1:87:A:LYS:HE2	1:89:A:ILE:HG21	10	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1586)	1:87:A:LYS:HE2	1:89:A:ILE:HG22	10	0.14
(1,1586)	1:87:A:LYS:HE2	1:89:A:ILE:HG23	10	0.14
(1,1586)	1:87:A:LYS:HE3	1:89:A:ILE:HG21	10	0.14
(1,1586)	1:87:A:LYS:HE3	1:89:A:ILE:HG22	10	0.14
(1,1586)	1:87:A:LYS:HE3	1:89:A:ILE:HG23	10	0.14
(1,1535)	1:75:A:VAL:HG21	1:50:A:ASN:HD21	5	0.14
(1,1535)	1:75:A:VAL:HG22	1:50:A:ASN:HD21	5	0.14
(1,1535)	1:75:A:VAL:HG23	1:50:A:ASN:HD21	5	0.14
(1,1526)	1:52:A:VAL:HG21	1:75:A:VAL:HG21	2	0.14
(1,1526)	1:52:A:VAL:HG21	1:75:A:VAL:HG22	2	0.14
(1,1526)	1:52:A:VAL:HG21	1:75:A:VAL:HG23	2	0.14
(1,1526)	1:52:A:VAL:HG22	1:75:A:VAL:HG21	2	0.14
(1,1526)	1:52:A:VAL:HG22	1:75:A:VAL:HG22	2	0.14
(1,1526)	1:52:A:VAL:HG22	1:75:A:VAL:HG23	2	0.14
(1,1526)	1:52:A:VAL:HG23	1:75:A:VAL:HG21	2	0.14
(1,1526)	1:52:A:VAL:HG23	1:75:A:VAL:HG22	2	0.14
(1,1526)	1:52:A:VAL:HG23	1:75:A:VAL:HG23	2	0.14
(1,1509)	1:62:A:VAL:HG21	1:114:A:THR:HG21	2	0.14
(1,1509)	1:62:A:VAL:HG21	1:114:A:THR:HG22	2	0.14
(1,1509)	1:62:A:VAL:HG21	1:114:A:THR:HG23	2	0.14
(1,1509)	1:62:A:VAL:HG22	1:114:A:THR:HG21	2	0.14
(1,1509)	1:62:A:VAL:HG22	1:114:A:THR:HG22	2	0.14
(1,1509)	1:62:A:VAL:HG22	1:114:A:THR:HG23	2	0.14
(1,1509)	1:62:A:VAL:HG23	1:114:A:THR:HG21	2	0.14
(1,1509)	1:62:A:VAL:HG23	1:114:A:THR:HG22	2	0.14
(1,1509)	1:62:A:VAL:HG23	1:114:A:THR:HG23	2	0.14
(1,1309)	1:114:A:THR:HG1	1:50:A:ASN:HB2	1	0.14
(1,1281)	1:128:A:LEU:HB3	1:129:A:VAL:H	9	0.14
(1,1268)	1:127:A:THR:HB	1:24:A:GLN:HG3	6	0.14
(1,1143)	1:111:A:PHE:HB3	1:112:A:ALA:H	2	0.14
(1,1143)	1:111:A:PHE:HB3	1:112:A:ALA:H	3	0.14
(1,1133)	1:111:A:PHE:HB2	1:126:A:VAL:HG21	5	0.14
(1,1133)	1:111:A:PHE:HB2	1:126:A:VAL:HG22	5	0.14
(1,1133)	1:111:A:PHE:HB2	1:126:A:VAL:HG23	5	0.14
(1,1133)	1:111:A:PHE:HB2	1:126:A:VAL:HG21	9	0.14
(1,1133)	1:111:A:PHE:HB2	1:126:A:VAL:HG22	9	0.14
(1,1133)	1:111:A:PHE:HB2	1:126:A:VAL:HG23	9	0.14
(1,1086)	1:108:A:ASP:HB2	1:56:A:ALA:H	3	0.14
(1,1052)	1:104:A:LEU:HB3	1:101:A:PRO:HA	4	0.14
(1,581)	1:27:A:LYS:HB2	1:130:A:ASP:HA	9	0.14
(1,581)	1:27:A:LYS:HB3	1:130:A:ASP:HA	9	0.14
(1,487)	1:50:A:ASN:HD22	1:50:A:ASN:HA	2	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,248)	1:31:A:GLU:HB2	1:32:A:PHE:H	5	0.14
(1,61)	1:18:A:PHE:HD1	1:12:A:SER:HB2	2	0.14
(1,61)	1:18:A:PHE:HD2	1:12:A:SER:HB2	2	0.14
(1,35)	1:11:A:GLU:HA	1:36:A:LEU:HD21	1	0.14
(1,35)	1:11:A:GLU:HA	1:36:A:LEU:HD22	1	0.14
(1,35)	1:11:A:GLU:HA	1:36:A:LEU:HD23	1	0.14
(1,3245)	1:123:A:ASN:HD22	1:120:A:ALA:HA	5	0.13
(1,3208)	1:76:A:LYS:HD3	1:79:A:ASP:H	1	0.13
(1,3192)	1:53:A:ILE:HD11	1:53:A:ILE:H	8	0.13
(1,3164)	1:17:A:GLN:H	1:17:A:GLN:HB2	1	0.13
(1,2966)	1:109:A:TYR:HE1	1:128:A:LEU:HD11	10	0.13
(1,2966)	1:109:A:TYR:HE1	1:128:A:LEU:HD12	10	0.13
(1,2966)	1:109:A:TYR:HE1	1:128:A:LEU:HD13	10	0.13
(1,2966)	1:109:A:TYR:HE2	1:128:A:LEU:HD11	10	0.13
(1,2966)	1:109:A:TYR:HE2	1:128:A:LEU:HD12	10	0.13
(1,2966)	1:109:A:TYR:HE2	1:128:A:LEU:HD13	10	0.13
(1,2950)	1:109:A:TYR:HE1	1:109:A:TYR:HB2	8	0.13
(1,2950)	1:109:A:TYR:HE2	1:109:A:TYR:HB2	8	0.13
(1,2950)	1:109:A:TYR:HE1	1:109:A:TYR:HB2	9	0.13
(1,2950)	1:109:A:TYR:HE2	1:109:A:TYR:HB2	9	0.13
(1,2926)	1:63:A:PHE:HE1	1:59:A:MET:HB3	5	0.13
(1,2926)	1:63:A:PHE:HE2	1:59:A:MET:HB3	5	0.13
(1,2916)	1:122:A:MET:HE1	1:49:A:HIS:HE1	2	0.13
(1,2916)	1:122:A:MET:HE2	1:49:A:HIS:HE1	2	0.13
(1,2916)	1:122:A:MET:HE3	1:49:A:HIS:HE1	2	0.13
(1,2916)	1:122:A:MET:HE1	1:49:A:HIS:HE1	4	0.13
(1,2916)	1:122:A:MET:HE2	1:49:A:HIS:HE1	4	0.13
(1,2916)	1:122:A:MET:HE3	1:49:A:HIS:HE1	4	0.13
(1,2889)	1:66:A:GLY:HA3	1:74:A:TYR:HD1	1	0.13
(1,2889)	1:66:A:GLY:HA3	1:74:A:TYR:HD2	1	0.13
(1,2882)	1:74:A:TYR:HD1	1:88:A:LEU:HD11	2	0.13
(1,2882)	1:74:A:TYR:HD1	1:88:A:LEU:HD12	2	0.13
(1,2882)	1:74:A:TYR:HD1	1:88:A:LEU:HD13	2	0.13
(1,2882)	1:74:A:TYR:HD2	1:88:A:LEU:HD11	2	0.13
(1,2882)	1:74:A:TYR:HD2	1:88:A:LEU:HD12	2	0.13
(1,2882)	1:74:A:TYR:HD2	1:88:A:LEU:HD13	2	0.13
(1,2836)	1:18:A:PHE:HE1	1:36:A:LEU:HD21	2	0.13
(1,2836)	1:18:A:PHE:HE1	1:36:A:LEU:HD22	2	0.13
(1,2836)	1:18:A:PHE:HE1	1:36:A:LEU:HD23	2	0.13
(1,2836)	1:18:A:PHE:HE2	1:36:A:LEU:HD21	2	0.13
(1,2836)	1:18:A:PHE:HE2	1:36:A:LEU:HD22	2	0.13
(1,2836)	1:18:A:PHE:HE2	1:36:A:LEU:HD23	2	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2575)	1:105:A:ALA:H	1:104:A:LEU:HB3	1	0.13
(1,1994)	1:6:A:CYS:HB2	1:33:A:THR:H	7	0.13
(1,1901)	1:23:A:ILE:HG13	1:24:A:GLN:H	3	0.13
(1,1668)	1:23:A:ILE:HG21	1:126:A:VAL:HG21	4	0.13
(1,1668)	1:23:A:ILE:HG21	1:126:A:VAL:HG22	4	0.13
(1,1668)	1:23:A:ILE:HG21	1:126:A:VAL:HG23	4	0.13
(1,1668)	1:23:A:ILE:HG22	1:126:A:VAL:HG21	4	0.13
(1,1668)	1:23:A:ILE:HG22	1:126:A:VAL:HG22	4	0.13
(1,1668)	1:23:A:ILE:HG22	1:126:A:VAL:HG23	4	0.13
(1,1668)	1:23:A:ILE:HG23	1:126:A:VAL:HG21	4	0.13
(1,1668)	1:23:A:ILE:HG23	1:126:A:VAL:HG22	4	0.13
(1,1668)	1:23:A:ILE:HG23	1:126:A:VAL:HG23	4	0.13
(1,1598)	1:53:A:ILE:HG12	1:97:A:LEU:HD21	10	0.13
(1,1598)	1:53:A:ILE:HG12	1:97:A:LEU:HD22	10	0.13
(1,1598)	1:53:A:ILE:HG12	1:97:A:LEU:HD23	10	0.13
(1,1595)	1:53:A:ILE:HG12	1:97:A:LEU:HD11	3	0.13
(1,1595)	1:53:A:ILE:HG12	1:97:A:LEU:HD12	3	0.13
(1,1595)	1:53:A:ILE:HG12	1:97:A:LEU:HD13	3	0.13
(1,1532)	1:114:A:THR:HG1	1:75:A:VAL:HG21	4	0.13
(1,1532)	1:114:A:THR:HG1	1:75:A:VAL:HG22	4	0.13
(1,1532)	1:114:A:THR:HG1	1:75:A:VAL:HG23	4	0.13
(1,1521)	1:72:A:THR:HG21	1:72:A:THR:H	9	0.13
(1,1521)	1:72:A:THR:HG22	1:72:A:THR:H	9	0.13
(1,1521)	1:72:A:THR:HG23	1:72:A:THR:H	9	0.13
(1,1506)	1:81:A:ARG:HB2	1:62:A:VAL:HG11	8	0.13
(1,1506)	1:81:A:ARG:HB2	1:62:A:VAL:HG12	8	0.13
(1,1506)	1:81:A:ARG:HB2	1:62:A:VAL:HG13	8	0.13
(1,1426)	1:86:A:THR:HG21	1:36:A:LEU:HD11	8	0.13
(1,1426)	1:86:A:THR:HG21	1:36:A:LEU:HD12	8	0.13
(1,1426)	1:86:A:THR:HG21	1:36:A:LEU:HD13	8	0.13
(1,1426)	1:86:A:THR:HG22	1:36:A:LEU:HD11	8	0.13
(1,1426)	1:86:A:THR:HG22	1:36:A:LEU:HD12	8	0.13
(1,1426)	1:86:A:THR:HG22	1:36:A:LEU:HD13	8	0.13
(1,1426)	1:86:A:THR:HG23	1:36:A:LEU:HD11	8	0.13
(1,1426)	1:86:A:THR:HG23	1:36:A:LEU:HD12	8	0.13
(1,1426)	1:86:A:THR:HG23	1:36:A:LEU:HD13	8	0.13
(1,1304)	1:55:A:LYS:HD2	1:55:A:LYS:H	5	0.13
(1,1143)	1:111:A:PHE:HB3	1:112:A:ALA:H	9	0.13
(1,768)	1:77:A:PRO:HG3	1:72:A:THR:HG21	4	0.13
(1,768)	1:77:A:PRO:HG3	1:72:A:THR:HG22	4	0.13
(1,768)	1:77:A:PRO:HG3	1:72:A:THR:HG23	4	0.13
(1,743)	1:77:A:PRO:HG3	1:77:A:PRO:HA	10	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,463)	1:88:A:LEU:HG	1:48:A:GLY:HA2	3	0.13
(1,418)	1:43:A:PRO:HD3	1:42:A:GLN:HB2	10	0.13
(1,418)	1:43:A:PRO:HD3	1:42:A:GLN:HB3	10	0.13
(1,230)	1:29:A:CYS:HB2	1:25:A:VAL:HG21	8	0.13
(1,230)	1:29:A:CYS:HB2	1:25:A:VAL:HG22	8	0.13
(1,230)	1:29:A:CYS:HB2	1:25:A:VAL:HG23	8	0.13
(1,230)	1:29:A:CYS:HB3	1:25:A:VAL:HG21	8	0.13
(1,230)	1:29:A:CYS:HB3	1:25:A:VAL:HG22	8	0.13
(1,230)	1:29:A:CYS:HB3	1:25:A:VAL:HG23	8	0.13
(1,211)	1:26:A:SER:HB3	1:25:A:VAL:HG21	2	0.13
(1,211)	1:26:A:SER:HB3	1:25:A:VAL:HG22	2	0.13
(1,211)	1:26:A:SER:HB3	1:25:A:VAL:HG23	2	0.13
(1,3226)	1:100:A:ASP:H	1:99:A:LEU:HB3	9	0.12
(1,3147)	1:128:A:LEU:H	1:104:A:LEU:HD22	2	0.12
(1,3122)	1:23:A:ILE:HG12	1:8:A:ALA:HB2	4	0.12
(1,3029)	1:118:A:HIS:HD2	1:47:A:MET:HG3	9	0.12
(1,2988)	1:53:A:ILE:HD11	1:111:A:PHE:HD1	7	0.12
(1,2988)	1:53:A:ILE:HD11	1:111:A:PHE:HD2	7	0.12
(1,2988)	1:53:A:ILE:HD12	1:111:A:PHE:HD1	7	0.12
(1,2988)	1:53:A:ILE:HD12	1:111:A:PHE:HD2	7	0.12
(1,2988)	1:53:A:ILE:HD13	1:111:A:PHE:HD1	7	0.12
(1,2988)	1:53:A:ILE:HD13	1:111:A:PHE:HD2	7	0.12
(1,2950)	1:109:A:TYR:HE1	1:109:A:TYR:HB2	1	0.12
(1,2950)	1:109:A:TYR:HE2	1:109:A:TYR:HB2	1	0.12
(1,2950)	1:109:A:TYR:HE1	1:109:A:TYR:HB2	5	0.12
(1,2950)	1:109:A:TYR:HE2	1:109:A:TYR:HB2	5	0.12
(1,2945)	1:105:A:ALA:HA	1:109:A:TYR:HE1	8	0.12
(1,2945)	1:105:A:ALA:HA	1:109:A:TYR:HE2	8	0.12
(1,2926)	1:63:A:PHE:HE1	1:59:A:MET:HB3	4	0.12
(1,2926)	1:63:A:PHE:HE2	1:59:A:MET:HB3	4	0.12
(1,2575)	1:105:A:ALA:H	1:104:A:LEU:HB3	4	0.12
(1,2573)	1:105:A:ALA:H	1:128:A:LEU:HD11	10	0.12
(1,2573)	1:105:A:ALA:H	1:128:A:LEU:HD12	10	0.12
(1,2573)	1:105:A:ALA:H	1:128:A:LEU:HD13	10	0.12
(1,2400)	1:84:A:ALA:H	1:85:A:HIS:HB2	8	0.12
(1,2374)	1:81:A:ARG:H	1:81:A:ARG:HB3	8	0.12
(1,2291)	1:64:A:LYS:HG3	1:64:A:LYS:H	4	0.12
(1,2068)	1:91:A:GLY:HA3	1:40:A:GLY:H	5	0.12
(1,2045)	1:94:A:GLU:HB2	1:38:A:HIS:H	10	0.12
(1,1994)	1:6:A:CYS:HB2	1:33:A:THR:H	8	0.12
(1,1994)	1:6:A:CYS:HB2	1:33:A:THR:H	10	0.12
(1,1986)	1:101:A:PRO:HD2	1:32:A:PHE:H	2	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1903)	1:24:A:GLN:HG2	1:24:A:GLN:H	7	0.12
(1,1901)	1:23:A:ILE:HG13	1:24:A:GLN:H	9	0.12
(1,1834)	1:17:A:GLN:HE21	1:17:A:GLN:HB2	3	0.12
(1,1786)	1:38:A:HIS:HB3	1:13:A:ASN:H	2	0.12
(1,1609)	1:99:A:LEU:HD21	1:32:A:PHE:H	6	0.12
(1,1609)	1:99:A:LEU:HD22	1:32:A:PHE:H	6	0.12
(1,1609)	1:99:A:LEU:HD23	1:32:A:PHE:H	6	0.12
(1,1598)	1:53:A:ILE:HG12	1:97:A:LEU:HD21	5	0.12
(1,1598)	1:53:A:ILE:HG12	1:97:A:LEU:HD22	5	0.12
(1,1598)	1:53:A:ILE:HG12	1:97:A:LEU:HD23	5	0.12
(1,1527)	1:82:A:VAL:HG11	1:75:A:VAL:HG21	8	0.12
(1,1527)	1:82:A:VAL:HG11	1:75:A:VAL:HG22	8	0.12
(1,1527)	1:82:A:VAL:HG11	1:75:A:VAL:HG23	8	0.12
(1,1527)	1:82:A:VAL:HG12	1:75:A:VAL:HG21	8	0.12
(1,1527)	1:82:A:VAL:HG12	1:75:A:VAL:HG22	8	0.12
(1,1527)	1:82:A:VAL:HG12	1:75:A:VAL:HG23	8	0.12
(1,1527)	1:82:A:VAL:HG13	1:75:A:VAL:HG21	8	0.12
(1,1527)	1:82:A:VAL:HG13	1:75:A:VAL:HG22	8	0.12
(1,1527)	1:82:A:VAL:HG13	1:75:A:VAL:HG23	8	0.12
(1,1281)	1:128:A:LEU:HB3	1:129:A:VAL:H	2	0.12
(1,1281)	1:128:A:LEU:HB3	1:129:A:VAL:H	5	0.12
(1,1249)	1:123:A:ASN:HB3	1:124:A:GLY:H	3	0.12
(1,1143)	1:111:A:PHE:HB3	1:112:A:ALA:H	8	0.12
(1,1087)	1:108:A:ASP:H	1:108:A:ASP:HB3	9	0.12
(1,1079)	1:125:A:LYS:HE2	1:108:A:ASP:HA	6	0.12
(1,1079)	1:125:A:LYS:HE3	1:108:A:ASP:HA	6	0.12
(1,1063)	1:107:A:GLY:HA2	1:55:A:LYS:HD2	5	0.12
(1,942)	1:87:A:LYS:HG2	1:95:A:SER:HB3	3	0.12
(1,942)	1:87:A:LYS:HG3	1:95:A:SER:HB3	3	0.12
(1,743)	1:77:A:PRO:HG3	1:77:A:PRO:HA	8	0.12
(1,496)	1:114:A:THR:HG1	1:50:A:ASN:HB3	5	0.12
(1,175)	1:24:A:GLN:HG3	1:129:A:VAL:HG11	1	0.12
(1,175)	1:24:A:GLN:HG3	1:129:A:VAL:HG12	1	0.12
(1,175)	1:24:A:GLN:HG3	1:129:A:VAL:HG13	1	0.12
(1,3249)	1:128:A:LEU:HB2	1:129:A:VAL:H	7	0.11
(1,3226)	1:100:A:ASP:H	1:99:A:LEU:HB3	4	0.11
(1,3192)	1:53:A:ILE:HD12	1:53:A:ILE:H	5	0.11
(1,3164)	1:17:A:GLN:H	1:17:A:GLN:HB2	10	0.11
(1,2970)	1:109:A:TYR:HD1	1:53:A:ILE:HD11	4	0.11
(1,2970)	1:109:A:TYR:HD1	1:53:A:ILE:HD12	4	0.11
(1,2970)	1:109:A:TYR:HD1	1:53:A:ILE:HD13	4	0.11
(1,2970)	1:109:A:TYR:HD2	1:53:A:ILE:HD11	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2970)	1:109:A:TYR:HD2	1:53:A:ILE:HD12	4	0.11
(1,2970)	1:109:A:TYR:HD2	1:53:A:ILE:HD13	4	0.11
(1,2951)	1:55:A:LYS:HB3	1:109:A:TYR:HD1	4	0.11
(1,2951)	1:55:A:LYS:HB3	1:109:A:TYR:HD2	4	0.11
(1,2950)	1:109:A:TYR:HE1	1:109:A:TYR:HB2	7	0.11
(1,2950)	1:109:A:TYR:HE2	1:109:A:TYR:HB2	7	0.11
(1,2946)	1:107:A:GLY:HA2	1:109:A:TYR:HD1	10	0.11
(1,2946)	1:107:A:GLY:HA2	1:109:A:TYR:HD2	10	0.11
(1,2882)	1:74:A:TYR:HD1	1:88:A:LEU:HD11	3	0.11
(1,2882)	1:74:A:TYR:HD1	1:88:A:LEU:HD12	3	0.11
(1,2882)	1:74:A:TYR:HD1	1:88:A:LEU:HD13	3	0.11
(1,2882)	1:74:A:TYR:HD2	1:88:A:LEU:HD11	3	0.11
(1,2882)	1:74:A:TYR:HD2	1:88:A:LEU:HD12	3	0.11
(1,2882)	1:74:A:TYR:HD2	1:88:A:LEU:HD13	3	0.11
(1,2573)	1:105:A:ALA:H	1:128:A:LEU:HD11	7	0.11
(1,2573)	1:105:A:ALA:H	1:128:A:LEU:HD12	7	0.11
(1,2573)	1:105:A:ALA:H	1:128:A:LEU:HD13	7	0.11
(1,2520)	1:98:A:THR:HB	1:98:A:THR:H	6	0.11
(1,2496)	1:96:A:SER:H	1:36:A:LEU:HB3	9	0.11
(1,2393)	1:83:A:VAL:H	1:104:A:LEU:HD21	5	0.11
(1,2393)	1:83:A:VAL:H	1:104:A:LEU:HD22	5	0.11
(1,2393)	1:83:A:VAL:H	1:104:A:LEU:HD23	5	0.11
(1,2364)	1:82:A:VAL:HG11	1:79:A:ASP:H	7	0.11
(1,2364)	1:82:A:VAL:HG12	1:79:A:ASP:H	7	0.11
(1,2364)	1:82:A:VAL:HG13	1:79:A:ASP:H	7	0.11
(1,2331)	1:72:A:THR:HA	1:73:A:ASP:H	2	0.11
(1,2264)	1:61:A:GLY:H	1:59:A:MET:HG2	8	0.11
(1,2264)	1:61:A:GLY:H	1:59:A:MET:HG3	8	0.11
(1,1986)	1:101:A:PRO:HD2	1:32:A:PHE:H	9	0.11
(1,1901)	1:23:A:ILE:HG13	1:24:A:GLN:H	1	0.11
(1,1803)	1:15:A:ASN:HB3	1:13:A:ASN:HD22	5	0.11
(1,1780)	1:12:A:SER:H	1:36:A:LEU:HD21	5	0.11
(1,1780)	1:12:A:SER:H	1:36:A:LEU:HD22	5	0.11
(1,1780)	1:12:A:SER:H	1:36:A:LEU:HD23	5	0.11
(1,1698)	1:24:A:GLN:HG3	1:129:A:VAL:HG21	10	0.11
(1,1698)	1:24:A:GLN:HG3	1:129:A:VAL:HG22	10	0.11
(1,1698)	1:24:A:GLN:HG3	1:129:A:VAL:HG23	10	0.11
(1,1420)	1:51:A:LEU:H	1:34:A:ILE:HG21	9	0.11
(1,1420)	1:51:A:LEU:H	1:34:A:ILE:HG22	9	0.11
(1,1420)	1:51:A:LEU:H	1:34:A:ILE:HG23	9	0.11
(1,1383)	1:128:A:LEU:HD11	1:25:A:VAL:HG21	9	0.11
(1,1383)	1:128:A:LEU:HD11	1:25:A:VAL:HG22	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1383)	1:128:A:LEU:HD11	1:25:A:VAL:HG23	9	0.11
(1,1383)	1:128:A:LEU:HD12	1:25:A:VAL:HG21	9	0.11
(1,1383)	1:128:A:LEU:HD12	1:25:A:VAL:HG22	9	0.11
(1,1383)	1:128:A:LEU:HD12	1:25:A:VAL:HG23	9	0.11
(1,1383)	1:128:A:LEU:HD13	1:25:A:VAL:HG21	9	0.11
(1,1383)	1:128:A:LEU:HD13	1:25:A:VAL:HG22	9	0.11
(1,1383)	1:128:A:LEU:HD13	1:25:A:VAL:HG23	9	0.11
(1,1320)	1:47:A:MET:HE1	1:118:A:HIS:HE1	7	0.11
(1,1320)	1:47:A:MET:HE2	1:118:A:HIS:HE1	7	0.11
(1,1320)	1:47:A:MET:HE3	1:118:A:HIS:HE1	7	0.11
(1,1304)	1:55:A:LYS:HD2	1:55:A:LYS:H	9	0.11
(1,1294)	1:130:A:ASP:HB2	1:130:A:ASP:H	9	0.11
(1,1281)	1:128:A:LEU:HB3	1:129:A:VAL:H	4	0.11
(1,1281)	1:128:A:LEU:HB3	1:129:A:VAL:H	8	0.11
(1,823)	1:82:A:VAL:HG21	1:85:A:HIS:HB2	5	0.11
(1,823)	1:82:A:VAL:HG22	1:85:A:HIS:HB2	5	0.11
(1,823)	1:82:A:VAL:HG23	1:85:A:HIS:HB2	5	0.11
(1,743)	1:77:A:PRO:HG3	1:77:A:PRO:HA	2	0.11
(1,670)	1:68:A:GLY:H	1:67:A:VAL:HB	5	0.11
(1,619)	1:65:A:ASP:HB3	1:62:A:VAL:HA	3	0.11
(1,580)	1:130:A:ASP:HA	1:128:A:LEU:HD21	7	0.11
(1,580)	1:130:A:ASP:HA	1:128:A:LEU:HD22	7	0.11
(1,580)	1:130:A:ASP:HA	1:128:A:LEU:HD23	7	0.11
(1,463)	1:88:A:LEU:HG	1:48:A:GLY:HA2	2	0.11
(1,228)	1:6:A:CYS:HB2	1:29:A:CYS:HB2	1	0.11
(1,228)	1:6:A:CYS:HB2	1:29:A:CYS:HB3	1	0.11
(1,228)	1:6:A:CYS:HB2	1:29:A:CYS:HB2	3	0.11
(1,228)	1:6:A:CYS:HB2	1:29:A:CYS:HB3	3	0.11
(1,175)	1:24:A:GLN:HG3	1:129:A:VAL:HG11	10	0.11
(1,175)	1:24:A:GLN:HG3	1:129:A:VAL:HG12	10	0.11
(1,175)	1:24:A:GLN:HG3	1:129:A:VAL:HG13	10	0.11
(1,156)	1:126:A:VAL:HG11	1:23:A:ILE:HB	10	0.11
(1,156)	1:126:A:VAL:HG12	1:23:A:ILE:HB	10	0.11
(1,156)	1:126:A:VAL:HG13	1:23:A:ILE:HB	10	0.11
(1,61)	1:18:A:PHE:HD1	1:12:A:SER:HB2	3	0.11
(1,61)	1:18:A:PHE:HD2	1:12:A:SER:HB2	3	0.11
(1,41)	1:10:A:VAL:HA	1:11:A:GLU:HG3	8	0.11
(1,3206)	1:78:A:ASP:HA	1:78:A:ASP:H	3	0.1
(1,3190)	1:51:A:LEU:H	1:36:A:LEU:HB3	6	0.1
(1,3164)	1:17:A:GLN:H	1:17:A:GLN:HB2	4	0.1
(1,2728)	1:122:A:MET:H	1:118:A:HIS:HB2	9	0.1
(1,2575)	1:105:A:ALA:H	1:104:A:LEU:HB3	10	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2542)	1:100:A:ASP:H	1:83:A:VAL:HA	8	0.1
(1,1689)	1:128:A:LEU:H	1:128:A:LEU:HD11	4	0.1
(1,1689)	1:128:A:LEU:H	1:128:A:LEU:HD12	4	0.1
(1,1689)	1:128:A:LEU:H	1:128:A:LEU:HD13	4	0.1
(1,1595)	1:53:A:ILE:HG12	1:97:A:LEU:HD11	1	0.1
(1,1595)	1:53:A:ILE:HG12	1:97:A:LEU:HD12	1	0.1
(1,1595)	1:53:A:ILE:HG12	1:97:A:LEU:HD13	1	0.1
(1,1550)	1:83:A:VAL:HG11	1:104:A:LEU:HD21	5	0.1
(1,1550)	1:83:A:VAL:HG11	1:104:A:LEU:HD22	5	0.1
(1,1550)	1:83:A:VAL:HG11	1:104:A:LEU:HD23	5	0.1
(1,1550)	1:83:A:VAL:HG12	1:104:A:LEU:HD21	5	0.1
(1,1550)	1:83:A:VAL:HG12	1:104:A:LEU:HD22	5	0.1
(1,1550)	1:83:A:VAL:HG12	1:104:A:LEU:HD23	5	0.1
(1,1550)	1:83:A:VAL:HG13	1:104:A:LEU:HD21	5	0.1
(1,1550)	1:83:A:VAL:HG13	1:104:A:LEU:HD22	5	0.1
(1,1550)	1:83:A:VAL:HG13	1:104:A:LEU:HD23	5	0.1
(1,1272)	1:104:A:LEU:HD11	1:128:A:LEU:HA	5	0.1
(1,1272)	1:104:A:LEU:HD12	1:128:A:LEU:HA	5	0.1
(1,1272)	1:104:A:LEU:HD13	1:128:A:LEU:HA	5	0.1
(1,1127)	1:111:A:PHE:HA	1:126:A:VAL:HG21	6	0.1
(1,1127)	1:111:A:PHE:HA	1:126:A:VAL:HG22	6	0.1
(1,1127)	1:111:A:PHE:HA	1:126:A:VAL:HG23	6	0.1
(1,1093)	1:56:A:ALA:HB1	1:108:A:ASP:HB2	5	0.1
(1,1093)	1:56:A:ALA:HB2	1:108:A:ASP:HB2	5	0.1
(1,1093)	1:56:A:ALA:HB3	1:108:A:ASP:HB2	5	0.1
(1,952)	1:96:A:SER:HA	1:36:A:LEU:HB3	7	0.1
(1,619)	1:65:A:ASP:HB3	1:62:A:VAL:HA	7	0.1
(1,608)	1:63:A:PHE:HB3	1:60:A:ASP:HA	8	0.1
(1,496)	1:114:A:THR:HG1	1:50:A:ASN:HB3	1	0.1

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

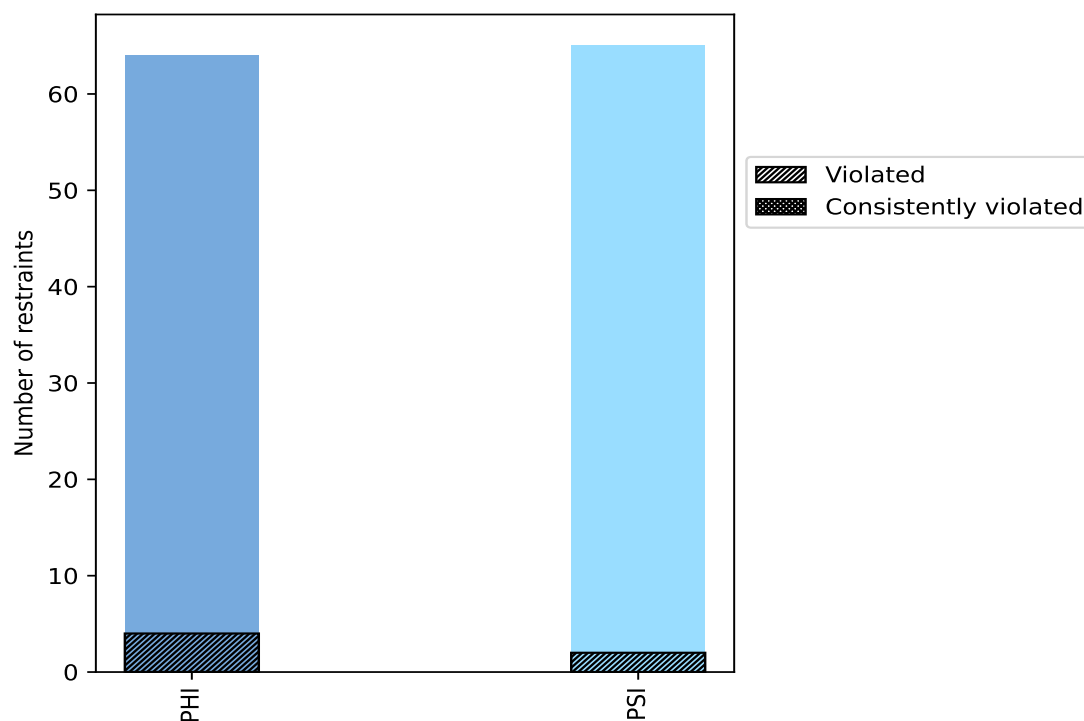
10.1 Summary of dihedral-angle violations [i](#)

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	64	49.6	4	6.2	3.1	0	0.0	0.0
PSI	65	50.4	2	3.1	1.6	0	0.0	0.0
Total	129	100.0	6	4.7	4.7	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](#)



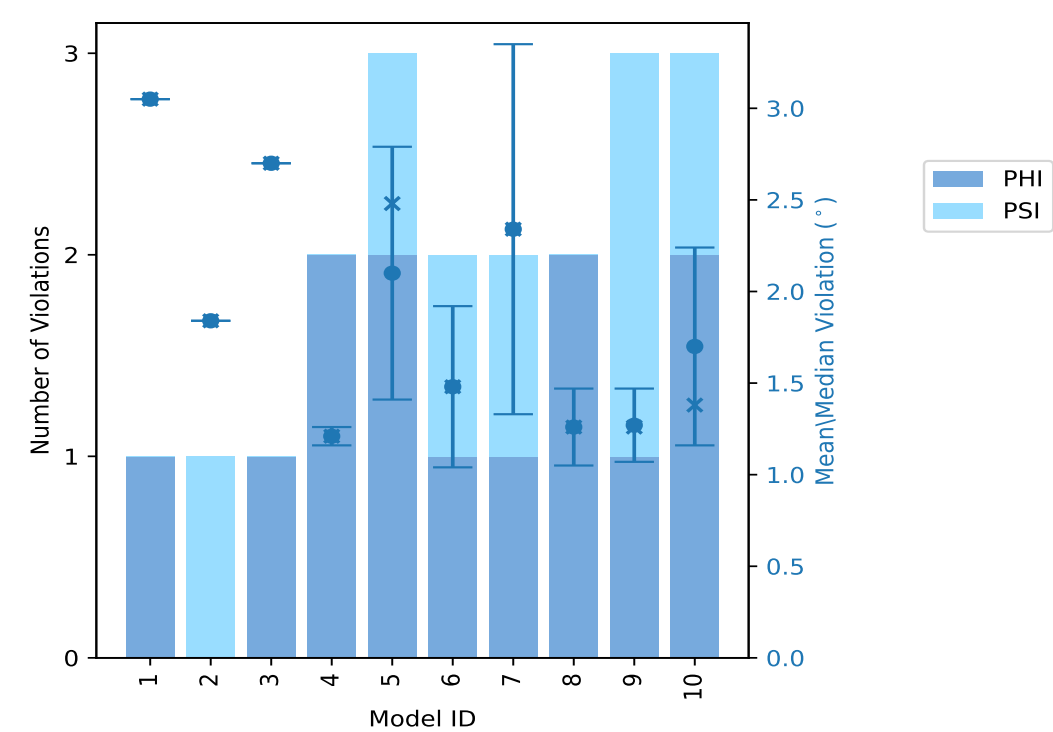
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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	1	0	1	3.05	3.05	0.0	3.05
2	0	1	1	1.84	1.84	0.0	1.84
3	1	0	1	2.7	2.7	0.0	2.7
4	2	0	2	1.21	1.26	0.05	1.21
5	2	1	3	2.1	2.7	0.69	2.48
6	1	1	2	1.48	1.92	0.44	1.48
7	1	1	2	2.34	3.35	1.01	2.34
8	2	0	2	1.26	1.47	0.21	1.26
9	1	2	3	1.27	1.52	0.2	1.26
10	2	1	3	1.7	2.47	0.54	1.38

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

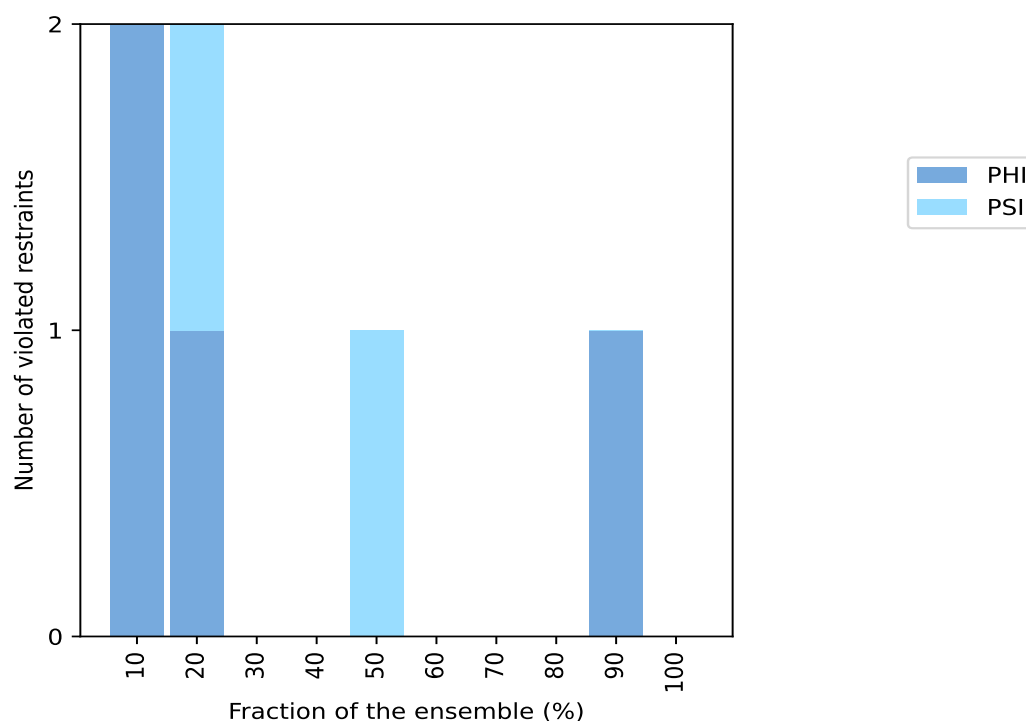
10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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

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

¹ Number of models with violations

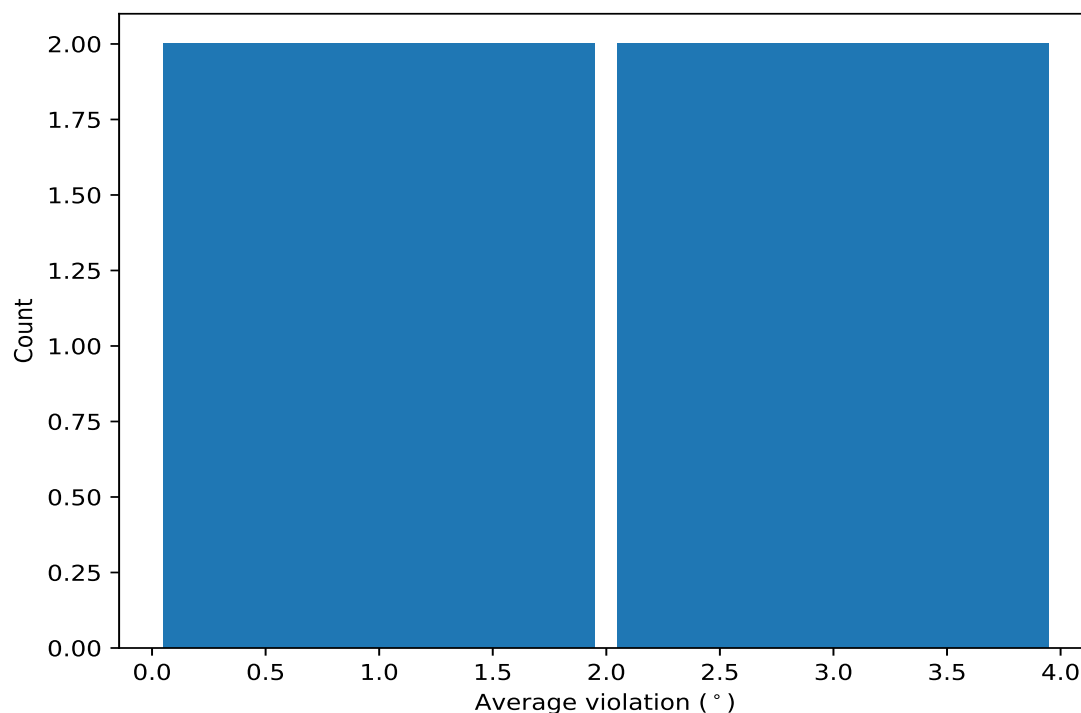
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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

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

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



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

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

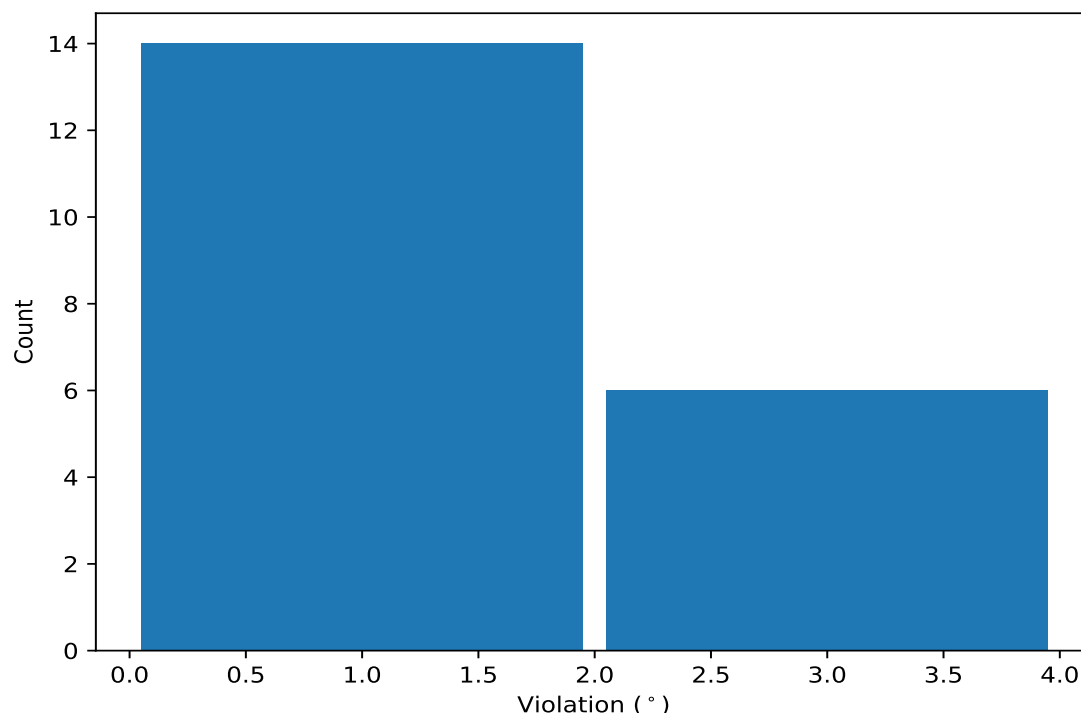
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,106)	1:108:A:ASP:C	1:109:A:TYR:N	1:109:A:TYR:CA	1:109:A:TYR:C	9	2.05	0.65	1.92
(1,12)	1:12:A:SER:N	1:12:A:SER:CA	1:12:A:SER:C	1:13:A:ASN:N	5	2.01	0.83	1.84
(1,53)	1:57:A:GLU:C	1:58:A:ASP:N	1:58:A:ASP:CA	1:58:A:ASP:C	2	1.19	0.07	1.19
(1,34)	1:38:A:HIS:N	1:38:A:HIS:CA	1:38:A:HIS:C	1:39:A:THR:N	2	1.15	0.11	1.15

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

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

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

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



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,12)	1:12:A:SER:N	1:12:A:SER:CA	1:12:A:SER:C	1:13:A:ASN:N	7	3.35
(1,106)	1:108:A:ASP:C	1:109:A:TYR:N	1:109:A:TYR:CA	1:109:A:TYR:C	1	3.05
(1,106)	1:108:A:ASP:C	1:109:A:TYR:N	1:109:A:TYR:CA	1:109:A:TYR:C	3	2.7
(1,106)	1:108:A:ASP:C	1:109:A:TYR:N	1:109:A:TYR:CA	1:109:A:TYR:C	5	2.7
(1,12)	1:12:A:SER:N	1:12:A:SER:CA	1:12:A:SER:C	1:13:A:ASN:N	5	2.48
(1,106)	1:108:A:ASP:C	1:109:A:TYR:N	1:109:A:TYR:CA	1:109:A:TYR:C	10	2.47
(1,106)	1:108:A:ASP:C	1:109:A:TYR:N	1:109:A:TYR:CA	1:109:A:TYR:C	6	1.92
(1,12)	1:12:A:SER:N	1:12:A:SER:CA	1:12:A:SER:C	1:13:A:ASN:N	2	1.84
(1,106)	1:108:A:ASP:C	1:109:A:TYR:N	1:109:A:TYR:CA	1:109:A:TYR:C	9	1.52
(1,106)	1:108:A:ASP:C	1:109:A:TYR:N	1:109:A:TYR:CA	1:109:A:TYR:C	8	1.47
(1,12)	1:12:A:SER:N	1:12:A:SER:CA	1:12:A:SER:C	1:13:A:ASN:N	10	1.38
(1,106)	1:108:A:ASP:C	1:109:A:TYR:N	1:109:A:TYR:CA	1:109:A:TYR:C	7	1.33
(1,106)	1:108:A:ASP:C	1:109:A:TYR:N	1:109:A:TYR:CA	1:109:A:TYR:C	4	1.26
(1,53)	1:57:A:GLU:C	1:58:A:ASP:N	1:58:A:ASP:CA	1:58:A:ASP:C	10	1.26

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,34)	1:38:A:HIS:N	1:38:A:HIS:CA	1:38:A:HIS:C	1:39:A:THR:N	9	1.26
(1,91)	1:95:A:SER:C	1:96:A:SER:N	1:96:A:SER:CA	1:96:A:SER:C	4	1.16
(1,53)	1:57:A:GLU:C	1:58:A:ASP:N	1:58:A:ASP:CA	1:58:A:ASP:C	5	1.13
(1,17)	1:23:A:ILE:C	1:24:A:GLN:N	1:24:A:GLN:CA	1:24:A:GLN:C	8	1.05
(1,34)	1:38:A:HIS:N	1:38:A:HIS:CA	1:38:A:HIS:C	1:39:A:THR:N	6	1.04
(1,12)	1:12:A:SER:N	1:12:A:SER:CA	1:12:A:SER:C	1:13:A:ASN:N	9	1.02