



Full wwPDB NMR Structure Validation Report ⓘ

Dec 25, 2024 – 08:31 PM EST

PDB ID : 8X3A
BMRB ID : 12024
Title : Solution NMR structure of cellulosomal double-dockerin module of Clo1313_0689 from Clostridium thermocellum
Authors : Chen, C.; Feng, Y.
Deposited on : 2023-11-12

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.40

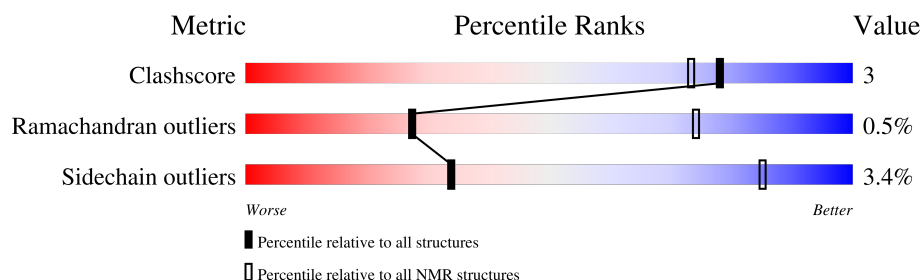
1 Overall quality at a glance

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	210492	14027
Ramachandran outliers	207382	12486
Sidechain outliers	206894	12463

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	152	

2 Ensemble composition and analysis

This entry contains 20 models. Model 17 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:2-A:141 (140)	0.68	17

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 6 clusters and 3 single-model clusters were found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2292 atoms, of which 1129 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Serine protease.

Mol	Chain	Residues	Atoms						Trace
1	A	151	Total	C	H	N	O	S	0
			2288	720	1129	203	233	3	

There are 10 discrepancies between the modelled and reference sequences:

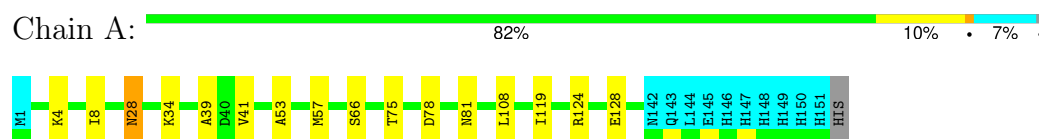
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q2HPT9
A	144	LEU	-	expression tag	UNP Q2HPT9
A	145	GLU	-	expression tag	UNP Q2HPT9
A	146	HIS	-	expression tag	UNP Q2HPT9
A	147	HIS	-	expression tag	UNP Q2HPT9
A	148	HIS	-	expression tag	UNP Q2HPT9
A	149	HIS	-	expression tag	UNP Q2HPT9
A	150	HIS	-	expression tag	UNP Q2HPT9
A	151	HIS	-	expression tag	UNP Q2HPT9
A	152	HIS	-	expression tag	UNP Q2HPT9

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	
2	A	4	Total	Ca
			4	4

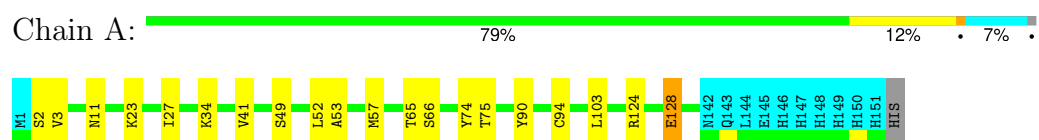
4.2.3 Score per residue for model 3

- Molecule 1: Serine protease



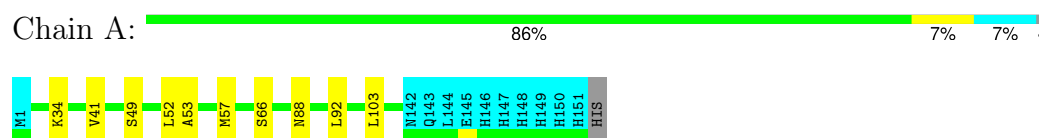
4.2.4 Score per residue for model 4

- Molecule 1: Serine protease



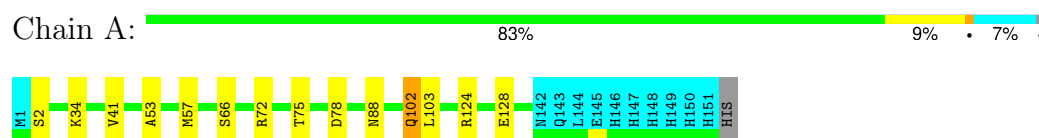
4.2.5 Score per residue for model 5

- Molecule 1: Serine protease



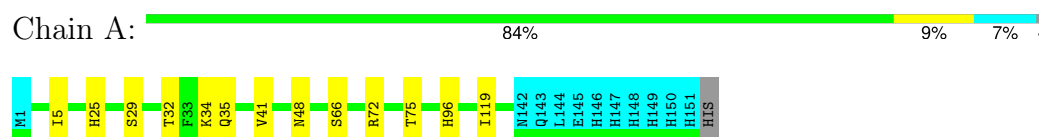
4.2.6 Score per residue for model 6

- Molecule 1: Serine protease



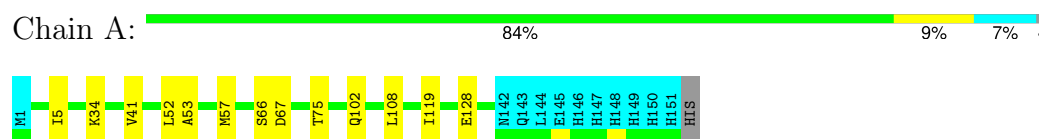
4.2.7 Score per residue for model 7

- Molecule 1: Serine protease



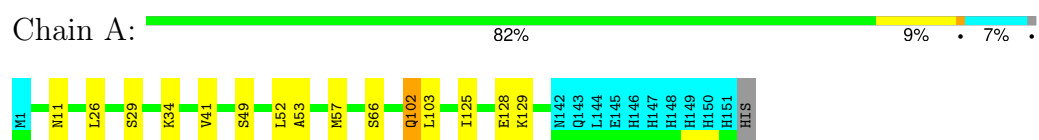
4.2.8 Score per residue for model 8

- Molecule 1: Serine protease



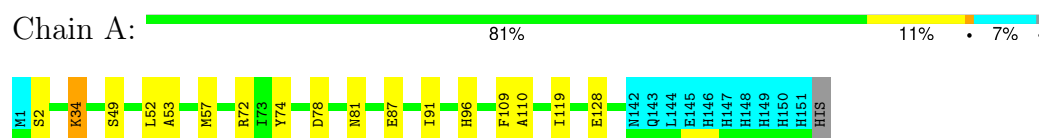
4.2.9 Score per residue for model 9

- Molecule 1: Serine protease



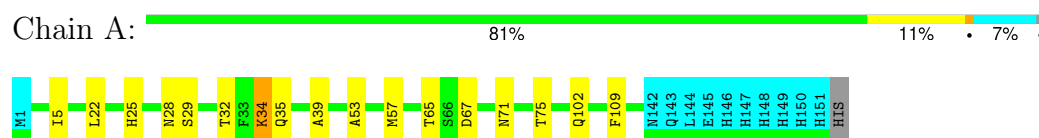
4.2.10 Score per residue for model 10

- Molecule 1: Serine protease



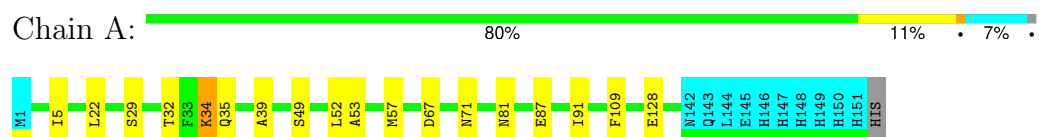
4.2.11 Score per residue for model 11

- Molecule 1: Serine protease



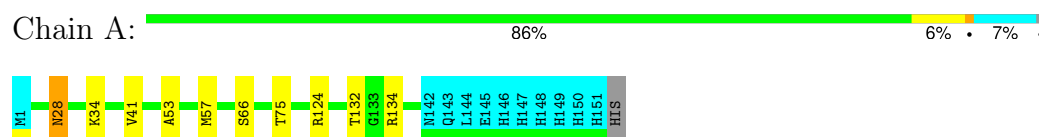
4.2.12 Score per residue for model 12

- Molecule 1: Serine protease



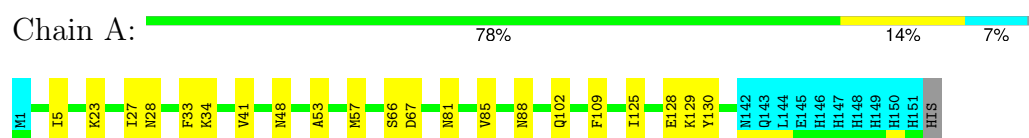
4.2.13 Score per residue for model 13

- Molecule 1: Serine protease



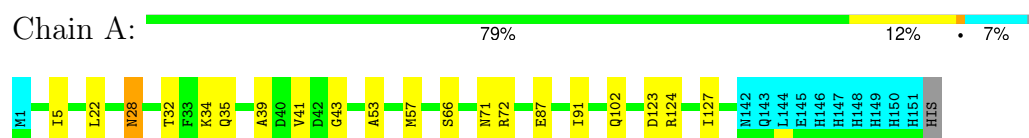
4.2.14 Score per residue for model 14

- Molecule 1: Serine protease



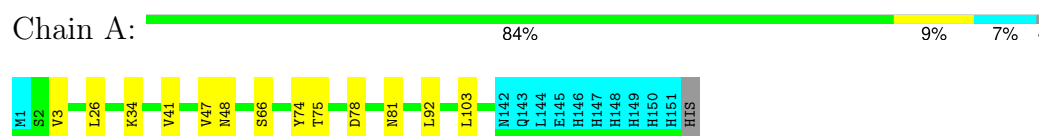
4.2.15 Score per residue for model 15

- Molecule 1: Serine protease



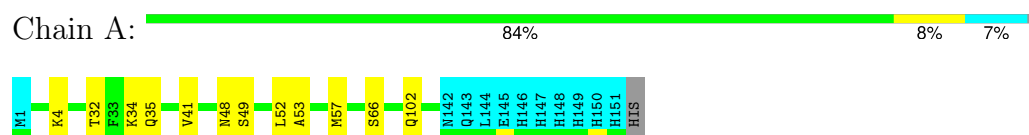
4.2.16 Score per residue for model 16

- Molecule 1: Serine protease



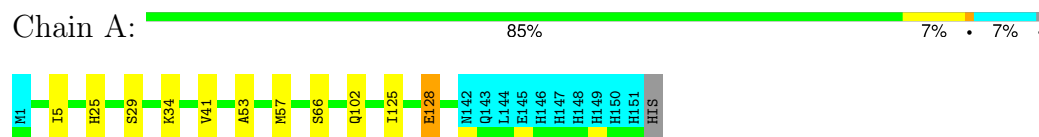
4.2.17 Score per residue for model 17 (medoid)

- Molecule 1: Serine protease



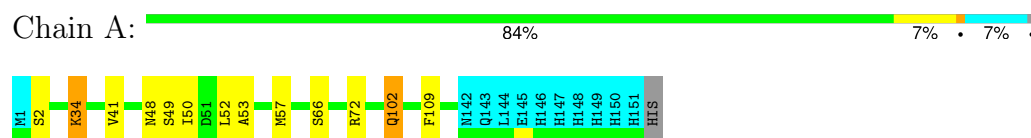
4.2.18 Score per residue for model 18

- Molecule 1: Serine protease



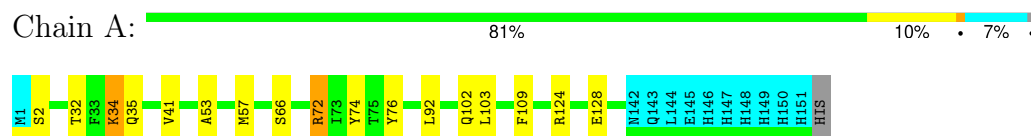
4.2.19 Score per residue for model 19

- Molecule 1: Serine protease



4.2.20 Score per residue for model 20

- Molecule 1: Serine protease



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CYANA	structure calculation	
CNS	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1786
Number of shifts mapped to atoms	1786
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 [i](#)

6.1 Standard geometry [i](#)

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

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1057	1039	1036	6±1
All	All	21220	20780	20712	114

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:25:HIS:HA	1:A:29:SER:O	0.54	2.02	11	4
1:A:94:CYS:SG	1:A:124:ARG:HD2	0.52	2.45	4	1
1:A:22:LEU:HD13	1:A:39:ALA:HB1	0.52	1.82	11	3
1:A:85:VAL:HB	1:A:130:TYR:CE1	0.52	2.39	14	1
1:A:32:THR:OG1	1:A:35:GLN:HG2	0.50	2.07	12	7
1:A:5:ILE:HB	1:A:67:ASP:O	0.49	2.08	14	6
1:A:26:LEU:HD21	1:A:47:VAL:HG12	0.49	1.85	16	1
1:A:53:ALA:O	1:A:57:MET:HG2	0.48	2.08	15	18
1:A:34:LYS:HG2	1:A:109:PHE:CZ	0.48	2.44	20	5
1:A:41:VAL:O	1:A:66:SER:HB3	0.48	2.08	16	14
1:A:96:HIS:CD2	1:A:119:ILE:HB	0.47	2.45	7	2
1:A:49:SER:O	1:A:52:LEU:HG	0.46	2.11	19	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:2:SER:HA	1:A:72:ARG:O	0.46	2.10	19	1
1:A:78:ASP:OD2	1:A:81:ASN:HA	0.46	2.11	3	2
1:A:8:ILE:CD1	1:A:39:ALA:HA	0.45	2.42	3	1
1:A:72:ARG:CZ	1:A:74:TYR:HB3	0.45	2.42	20	1
1:A:5:ILE:CG2	1:A:41:VAL:HA	0.45	2.41	15	3
1:A:102:GLN:N	1:A:102:GLN:HE21	0.44	2.10	19	2
1:A:26:LEU:HD12	1:A:52:LEU:HD23	0.44	1.89	9	1
1:A:75:THR:HB	1:A:78:ASP:HB3	0.44	1.88	1	3
1:A:23:LYS:O	1:A:27:ILE:HG13	0.44	2.12	14	4
1:A:90:TYR:CE1	1:A:128:GLU:HB3	0.44	2.48	4	1
1:A:43:GLY:HA2	1:A:72:ARG:NH2	0.44	2.28	15	1
1:A:87:GLU:O	1:A:91:ILE:HG13	0.43	2.12	15	3
1:A:41:VAL:O	1:A:66:SER:HB2	0.43	2.13	5	2
1:A:92:LEU:O	1:A:103:LEU:HD11	0.43	2.13	5	3
1:A:108:LEU:O	1:A:119:ILE:HD11	0.43	2.13	3	3
1:A:125:ILE:O	1:A:129:LYS:HG3	0.42	2.14	14	2
1:A:33:PHE:O	1:A:109:PHE:HB2	0.42	2.14	14	1
1:A:5:ILE:HD11	1:A:72:ARG:HG2	0.42	1.92	7	1
1:A:132:THR:OG1	1:A:134:ARG:HG2	0.42	2.14	13	1
1:A:48:ASN:ND2	1:A:50:ILE:HB	0.42	2.29	19	1
1:A:3:VAL:HG23	1:A:74:TYR:CE2	0.41	2.50	4	2
1:A:123:ASP:O	1:A:127:ILE:HG12	0.41	2.15	15	1
1:A:125:ILE:HA	1:A:128:GLU:HG3	0.40	1.91	9	1
1:A:102:GLN:HE21	1:A:102:GLN:N	0.40	2.14	6	1
1:A:74:TYR:CE2	1:A:110:ALA:HA	0.40	2.51	10	1
1:A:125:ILE:O	1:A:128:GLU:HG3	0.40	2.17	18	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	140/152 (92%)	132±2 (95±1%)	7±2 (5±1%)	1±1 (1±0%)	27	74
All	All	2800/3040 (92%)	2650 (95%)	135 (5%)	15 (1%)	27	74

All 5 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	28	ASN	6
1	A	2	SER	4
1	A	65	THR	2
1	A	29	SER	2
1	A	63	GLY	1

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	115/127 (91%)	111±1 (97±1%)	4±1 (3±1%)	34 85
All	All	2300/2540 (91%)	2222 (97%)	78 (3%)	34 85

All 15 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	34	LYS	20
1	A	102	GLN	10
1	A	128	GLU	9
1	A	75	THR	5
1	A	124	ARG	5
1	A	81	ASN	4
1	A	48	ASN	4
1	A	11	ASN	3
1	A	28	ASN	3
1	A	103	LEU	3
1	A	88	ASN	3
1	A	72	ARG	3
1	A	71	ASN	3
1	A	4	LYS	2
1	A	52	LEU	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 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 93% for the well-defined parts and 90% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	1786
Number of shifts mapped to atoms	1786
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	148	-0.35 ± 0.10	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	132	0.26 ± 0.09	None needed (< 0.5 ppm)
$^{13}\text{C}'$	143	-0.23 ± 0.10	None needed (< 0.5 ppm)
^{15}N	142	0.06 ± 0.43	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 93%, i.e. 1687 atoms were assigned a chemical shift out of a possible 1821. 0 out of 19 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	692/714 (97%)	286/295 (97%)	274/280 (98%)	132/139 (95%)
Sidechain	923/1000 (92%)	631/652 (97%)	273/316 (86%)	19/32 (59%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	72/107 (67%)	36/50 (72%)	36/51 (71%)	0/6 (0%)
Overall	1687/1821 (93%)	953/997 (96%)	583/647 (90%)	151/177 (85%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 90%, i.e. 1786 atoms were assigned a chemical shift out of a possible 1989. 0 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	739/769 (96%)	306/317 (97%)	291/302 (96%)	142/150 (95%)
Sidechain	975/1065 (92%)	666/694 (96%)	288/337 (85%)	21/34 (62%)
Aromatic	72/155 (46%)	36/74 (49%)	36/63 (57%)	0/18 (0%)
Overall	1786/1989 (90%)	1008/1085 (93%)	615/702 (88%)	163/202 (81%)

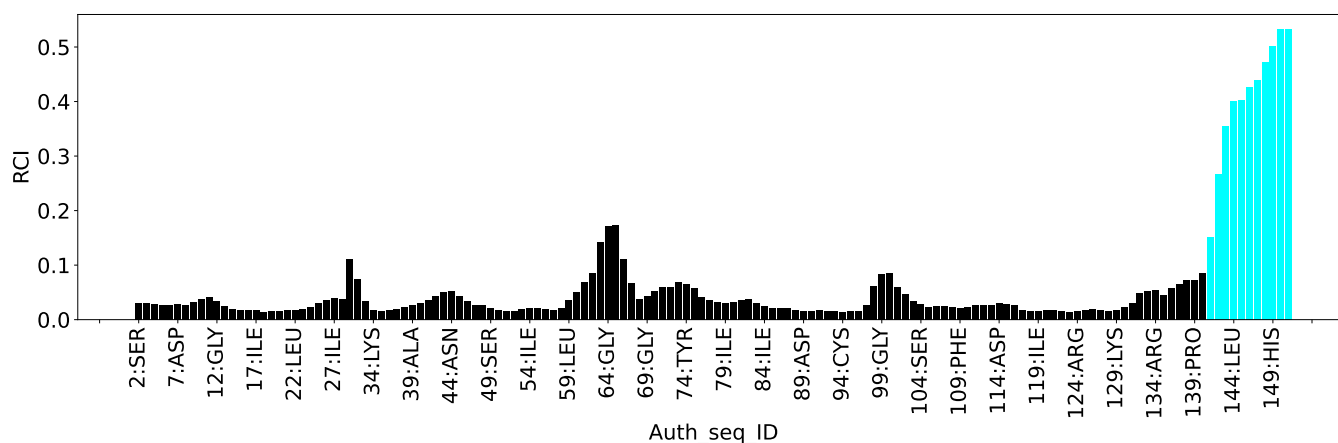
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	4119
Intra-residue ($ i-j =0$)	1456
Sequential ($ i-j =1$)	890
Medium range ($ i-j >1$ and $ i-j <5$)	587
Long range ($ i-j \geq 5$)	1098
Inter-chain	0
Hydrogen bond restraints	88
Disulfide bond restraints	0
Total dihedral-angle restraints	323
Number of unmapped restraints	0
Number of restraints per residue	28.7
Number of long range restraints per residue ¹	7.1

¹Long range hydrogen bonds and disulfide bonds are counted as long range restraints while calculating the number of long range restraints per residue

8.2 Residual restraint violations

This section provides the overview of the restraint violations analysis. The violations are binned as small, medium and large violations based on its absolute value. Average number of violations per model is calculated by dividing the total number of violations in each bin by the size of the ensemble.

8.2.1 Average number of distance violations per model

Distance violations less than 0.1 Å are not included in the calculation.

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	54.4	0.2
0.2-0.5 (Medium)	69.8	0.5
>0.5 (Large)	65.5	19.52

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)	10.7	4.41
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

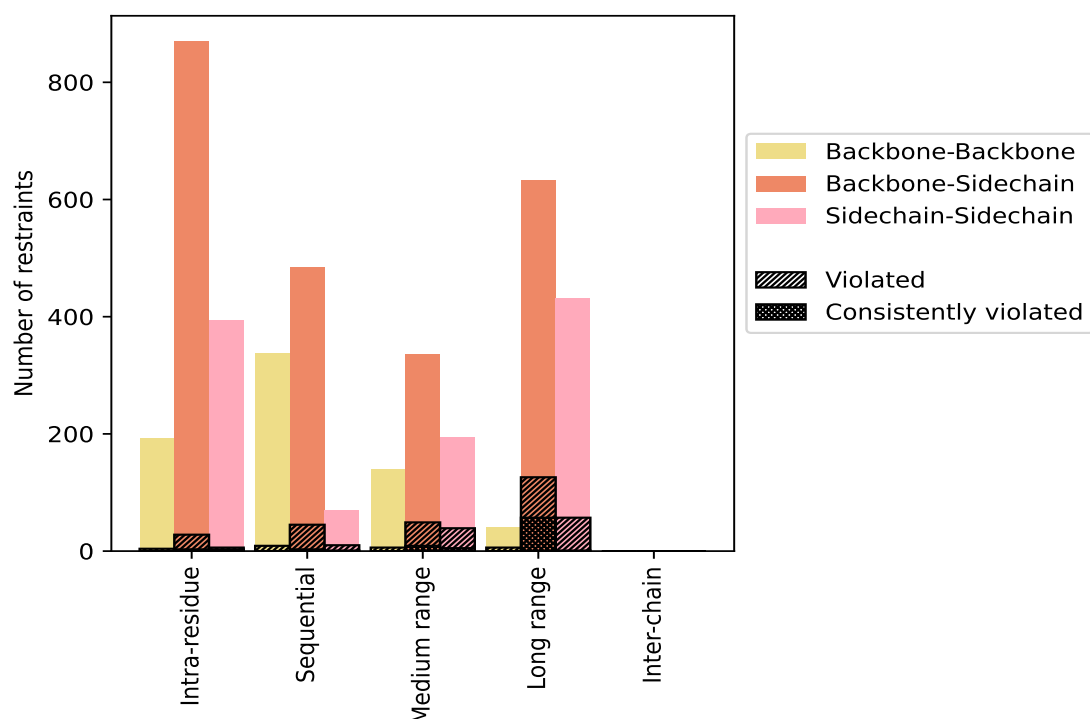
9.1 Summary of distance violations ⓘ

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)	1456	35.3	38	2.6	0.9	6	0.4	0.1
Backbone-Backbone	193	4.7	4	2.1	0.1	0	0.0	0.0
Backbone-Sidechain	870	21.1	28	3.2	0.7	3	0.3	0.1
Sidechain-Sidechain	393	9.5	6	1.5	0.1	3	0.8	0.1
Sequential (i-j =1)	890	21.6	64	7.2	1.6	4	0.4	0.1
Backbone-Backbone	337	8.2	9	2.7	0.2	0	0.0	0.0
Backbone-Sidechain	484	11.8	45	9.3	1.1	3	0.6	0.1
Sidechain-Sidechain	69	1.7	10	14.5	0.2	1	1.4	0.0
Medium range (i-j >1 & i-j <5)	587	14.3	93	15.8	2.3	14	2.4	0.3
Backbone-Backbone	139	3.4	6	4.3	0.1	0	0.0	0.0
Backbone-Sidechain	254	6.2	48	18.9	1.2	9	3.5	0.2
Sidechain-Sidechain	194	4.7	39	20.1	0.9	5	2.6	0.1
Long range (i-j ≥5)	1098	26.7	189	17.2	4.6	58	5.3	1.4
Backbone-Backbone	40	1.0	6	15.0	0.1	0	0.0	0.0
Backbone-Sidechain	627	15.2	126	20.1	3.1	57	9.1	1.4
Sidechain-Sidechain	431	10.5	57	13.2	1.4	1	0.2	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	88	2.1	1	1.1	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	4119	100.0	385	9.3	9.3	82	2.0	2.0
Backbone-Backbone	709	17.2	25	3.5	0.6	0	0.0	0.0
Backbone-Sidechain	2323	56.4	248	10.7	6.0	72	3.1	1.7
Sidechain-Sidechain	1087	26.4	112	10.3	2.7	10	0.9	0.2

¹ percentage calculated with respect to the total number of distance restraints, ² percentage calculated with respect to the number of restraints in a particular restraint category, ³ violated in at least one model, ⁴ violated in all the models

9.1.1 Bar chart : Distribution of distance restraints and violations [i](#)



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfied bonds are counted in their appropriate category on the x-axis

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

The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	26	24	28	107	0	185	4.08	18.26	6.44	0.36
2	23	36	34	100	0	193	4.11	19.24	6.68	0.33
3	17	33	44	105	0	199	3.89	18.49	6.46	0.3
4	21	24	39	106	0	190	4.02	19.02	6.49	0.31
5	22	27	35	105	0	189	4.09	18.45	6.59	0.31
6	21	27	41	97	0	186	4.15	18.16	6.59	0.33
7	18	28	42	107	0	195	3.95	18.82	6.46	0.33
8	21	40	38	105	0	204	3.88	19.2	6.53	0.31
9	18	33	40	103	0	194	4.04	18.38	6.57	0.32
10	18	31	35	105	0	189	3.86	18.3	6.22	0.33

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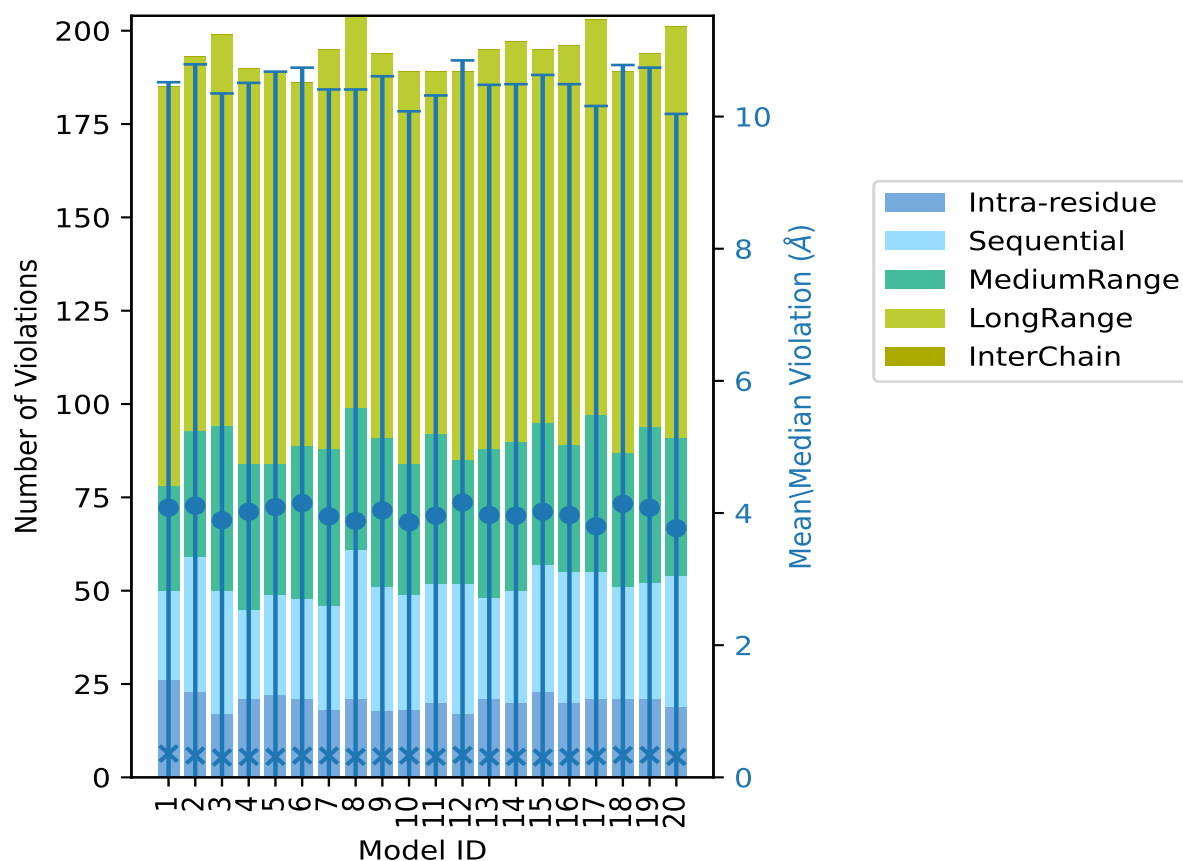
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	20	32	40	97	0	189	3.96	18.42	6.36	0.31
12	17	35	33	104	0	189	4.16	19.06	6.69	0.34
13	21	27	40	107	0	195	3.97	18.38	6.51	0.31
14	20	30	40	107	0	197	3.96	18.72	6.53	0.31
15	23	34	38	100	0	195	4.02	18.87	6.61	0.3
16	20	35	34	107	0	196	3.97	18.94	6.52	0.31
17	21	34	42	106	0	203	3.8	18.65	6.36	0.32
18	21	30	36	102	0	189	4.14	19.52	6.64	0.34
19	21	31	42	100	0	194	4.08	18.96	6.66	0.34
20	19	35	37	110	0	201	3.77	18.12	6.27	0.31

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

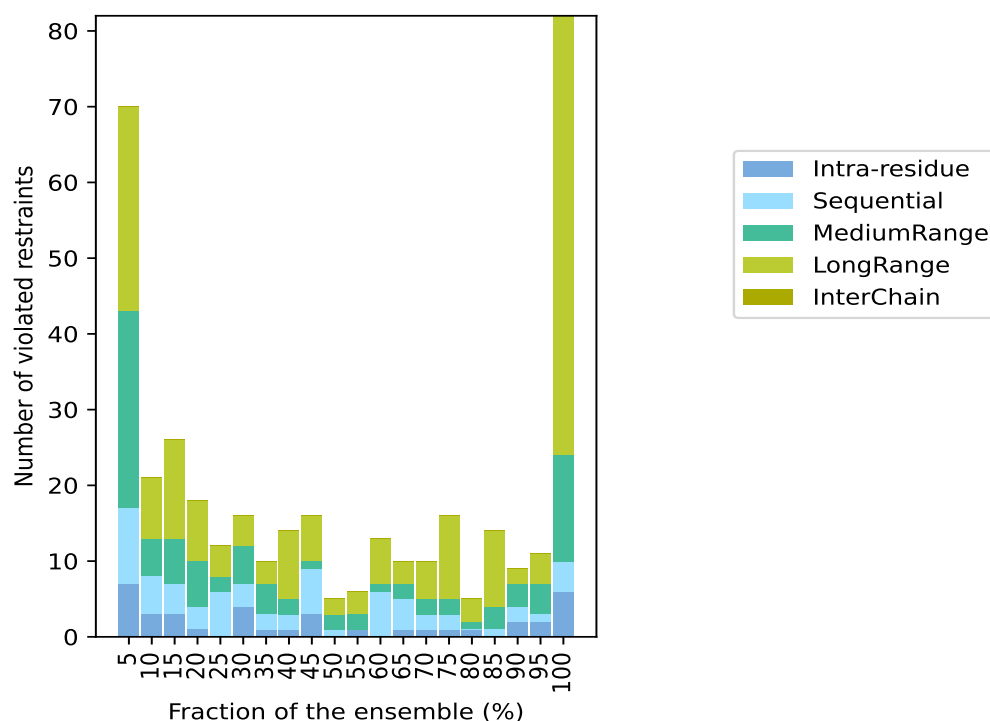
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 3647(IR:1418, SQ:826, MR:494, LR:909, IC:0) restraints are 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	%
7	10	26	27	0	70	1	5.0
3	5	5	8	0	21	2	10.0
3	4	6	13	0	26	3	15.0
1	3	6	8	0	18	4	20.0
0	6	2	4	0	12	5	25.0
4	3	5	4	0	16	6	30.0
1	2	4	3	0	10	7	35.0
1	2	2	9	0	14	8	40.0
3	6	1	6	0	16	9	45.0
0	1	2	2	0	5	10	50.0
1	0	2	3	0	6	11	55.0
0	6	1	6	0	13	12	60.0
1	4	2	3	0	10	13	65.0
1	2	2	5	0	10	14	70.0
1	2	2	11	0	16	15	75.0
1	0	1	3	0	5	16	80.0
0	1	3	10	0	14	17	85.0
2	2	3	2	0	9	18	90.0
2	1	4	4	0	11	19	95.0
6	4	14	58	0	82	20	100.0

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

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

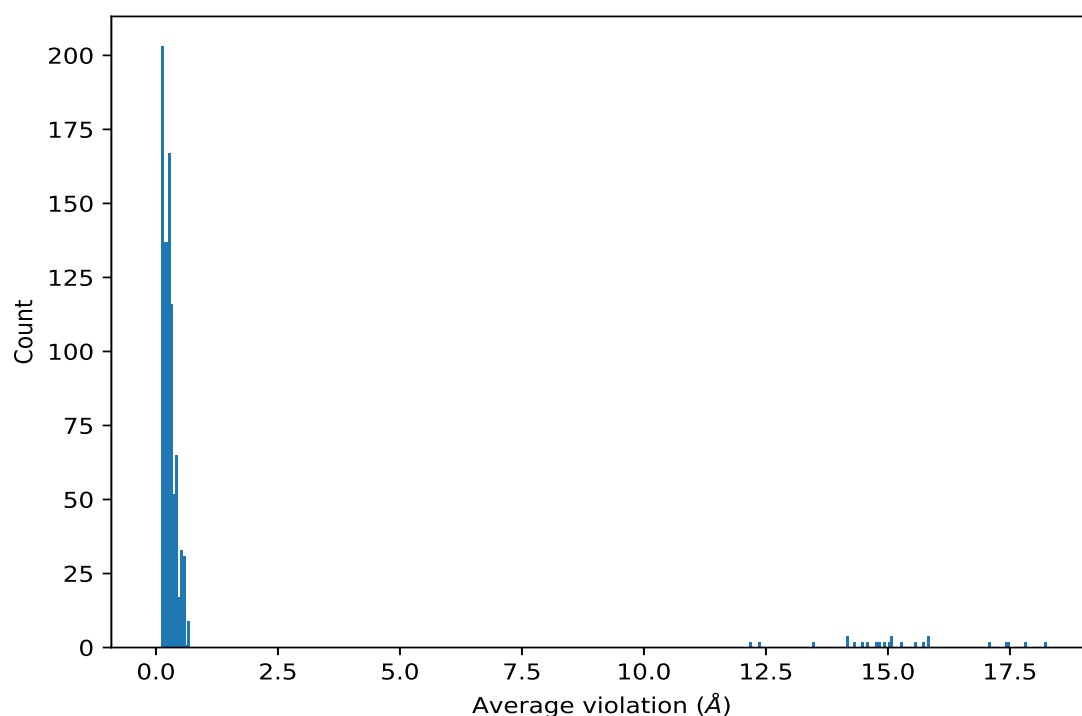
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,4006)	1:123:A:ASP:OD1	1:4:A:LYS:CA	20	18.21	0.67	18.34
(2,23)	1:123:A:ASP:OD1	1:4:A:LYS:CA	20	18.21	0.67	18.34
(1,4007)	1:123:A:ASP:OD2	1:4:A:LYS:CA	20	17.83	0.69	17.64
(2,24)	1:123:A:ASP:OD2	1:4:A:LYS:CA	20	17.83	0.69	17.64
(1,4003)	1:114:A:ASP:OD1	1:4:A:LYS:CA	20	17.49	0.82	17.21
(2,20)	1:114:A:ASP:OD1	1:4:A:LYS:CA	20	17.49	0.82	17.21
(1,4005)	1:118:A:VAL:O	1:4:A:LYS:CA	20	17.43	0.3	17.42
(2,22)	1:118:A:VAL:O	1:4:A:LYS:CA	20	17.43	0.3	17.42
(1,4004)	1:116:A:ASN:OD1	1:4:A:LYS:CA	20	17.06	0.33	17.1
(2,21)	1:116:A:ASN:OD1	1:4:A:LYS:CA	20	17.06	0.33	17.1
(1,3997)	1:80:A:ASP:OD1	1:3:A:VAL:CA	20	15.82	0.68	15.85
(2,14)	1:80:A:ASP:OD1	1:3:A:VAL:CA	20	15.82	0.68	15.85
(1,3998)	1:82:A:ASN:OD1	1:3:A:VAL:CA	20	15.82	0.6	15.78
(2,15)	1:82:A:ASN:OD1	1:3:A:VAL:CA	20	15.82	0.6	15.78
(1,4000)	1:89:A:ASP:OD1	1:3:A:VAL:CA	20	15.74	0.55	15.69
(2,17)	1:89:A:ASP:OD1	1:3:A:VAL:CA	20	15.74	0.55	15.69

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3999)	1:84:A:ILE:O	1:3:A:VAL:CA	20	15.56	0.53	15.46
(2,16)	1:84:A:ILE:O	1:3:A:VAL:CA	20	15.56	0.53	15.46
(1,4002)	1:112:A:ASP:OD1	1:4:A:LYS:CA	20	15.26	0.34	15.14
(2,19)	1:112:A:ASP:OD1	1:4:A:LYS:CA	20	15.26	0.34	15.14
(1,3988)	1:18:A:ASP:OD1	1:1:A:MET:CA	20	15.09	0.92	14.96
(2,5)	1:18:A:ASP:OD1	1:1:A:MET:CA	20	15.09	0.92	14.96
(1,3989)	1:18:A:ASP:OD2	1:1:A:MET:CA	20	15.06	1.07	15.16
(2,6)	1:18:A:ASP:OD2	1:1:A:MET:CA	20	15.06	1.07	15.16
(1,3985)	1:9:A:ASP:OD1	1:1:A:MET:CA	20	15.02	1.37	14.8
(2,2)	1:9:A:ASP:OD1	1:1:A:MET:CA	20	15.02	1.37	14.8
(1,4001)	1:89:A:ASP:OD2	1:3:A:VAL:CA	20	14.94	0.82	14.77
(2,18)	1:89:A:ASP:OD2	1:3:A:VAL:CA	20	14.94	0.82	14.77
(1,3992)	1:44:A:ASN:OD1	1:2:A:SER:CA	20	14.83	0.31	14.79
(2,9)	1:44:A:ASN:OD1	1:2:A:SER:CA	20	14.83	0.31	14.79
(1,3993)	1:46:A:TYR:O	1:2:A:SER:CA	20	14.75	0.44	14.78
(2,10)	1:46:A:TYR:O	1:2:A:SER:CA	20	14.75	0.44	14.78
(1,3995)	1:51:A:ASP:OD2	1:2:A:SER:CA	20	14.56	0.73	14.9
(2,12)	1:51:A:ASP:OD2	1:2:A:SER:CA	20	14.56	0.73	14.9
(1,3986)	1:11:A:ASN:OD1	1:1:A:MET:CA	20	14.48	1.07	14.67
(2,3)	1:11:A:ASN:OD1	1:1:A:MET:CA	20	14.48	1.07	14.67
(1,3987)	1:13:A:GLU:O	1:1:A:MET:CA	20	14.31	0.92	14.46
(2,4)	1:13:A:GLU:O	1:1:A:MET:CA	20	14.31	0.92	14.46
(1,3994)	1:51:A:ASP:OD1	1:2:A:SER:CA	20	14.17	0.78	13.68
(2,11)	1:51:A:ASP:OD1	1:2:A:SER:CA	20	14.17	0.78	13.68
(1,3991)	1:42:A:ASP:OD1	1:2:A:SER:CA	20	14.15	0.61	13.93
(2,8)	1:42:A:ASP:OD1	1:2:A:SER:CA	20	14.15	0.61	13.93
(1,3996)	1:78:A:ASP:OD1	1:3:A:VAL:CA	20	13.48	0.55	13.39
(2,13)	1:78:A:ASP:OD1	1:3:A:VAL:CA	20	13.48	0.55	13.39
(1,3984)	1:7:A:ASP:OD1	1:1:A:MET:CA	20	12.38	0.89	12.58
(2,1)	1:7:A:ASP:OD1	1:1:A:MET:CA	20	12.38	0.89	12.58
(1,3990)	1:40:A:ASP:OD1	1:2:A:SER:CA	20	12.19	0.24	12.24
(2,7)	1:40:A:ASP:OD1	1:2:A:SER:CA	20	12.19	0.24	12.24
(1,1032)	1:93:A:ILE:HD11	1:112:A:ASP:H	20	0.66	0.07	0.66
(1,1032)	1:93:A:ILE:HD12	1:112:A:ASP:H	20	0.66	0.07	0.66
(1,1032)	1:93:A:ILE:HD13	1:112:A:ASP:H	20	0.66	0.07	0.66
(1,1032)	1:79:A:ILE:HD11	1:112:A:ASP:H	20	0.66	0.07	0.66
(1,1032)	1:79:A:ILE:HD12	1:112:A:ASP:H	20	0.66	0.07	0.66
(1,1032)	1:79:A:ILE:HD13	1:112:A:ASP:H	20	0.66	0.07	0.66
(1,883)	1:59:A:LEU:HB3	1:61:A:GLY:H	20	0.64	0.08	0.64
(1,2522)	1:23:A:LYS:HA	1:22:A:LEU:HD21	20	0.6	0.07	0.6
(1,2522)	1:23:A:LYS:HA	1:22:A:LEU:HD22	20	0.6	0.07	0.6
(1,2522)	1:23:A:LYS:HA	1:22:A:LEU:HD23	20	0.6	0.07	0.6

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2522)	1:139:A:PRO:HD2	1:135:A:ILE:HG13	20	0.6	0.07	0.6
(1,2522)	1:139:A:PRO:HD3	1:135:A:ILE:HG13	20	0.6	0.07	0.6
(1,3386)	1:32:A:THR:HA	1:31:A:LEU:HD11	20	0.58	0.06	0.58
(1,3386)	1:32:A:THR:HA	1:31:A:LEU:HD12	20	0.58	0.06	0.58
(1,3386)	1:32:A:THR:HA	1:31:A:LEU:HD13	20	0.58	0.06	0.58
(1,3386)	1:18:A:ASP:HA	1:31:A:LEU:HD11	20	0.58	0.06	0.58
(1,3386)	1:18:A:ASP:HA	1:31:A:LEU:HD12	20	0.58	0.06	0.58
(1,3386)	1:18:A:ASP:HA	1:31:A:LEU:HD13	20	0.58	0.06	0.58
(1,3596)	1:15:A:SER:HB3	1:14:A:ILE:HD11	20	0.58	0.07	0.57
(1,3596)	1:15:A:SER:HB3	1:14:A:ILE:HD12	20	0.58	0.07	0.57
(1,3596)	1:15:A:SER:HB3	1:14:A:ILE:HD13	20	0.58	0.07	0.57
(1,3596)	1:38:A:ALA:HA	1:14:A:ILE:HD11	20	0.58	0.07	0.57
(1,3596)	1:38:A:ALA:HA	1:14:A:ILE:HD12	20	0.58	0.07	0.57
(1,3596)	1:38:A:ALA:HA	1:14:A:ILE:HD13	20	0.58	0.07	0.57
(1,2995)	1:70:A:LYS:HB3	1:5:A:ILE:HG21	20	0.54	0.18	0.56
(1,2995)	1:70:A:LYS:HB3	1:5:A:ILE:HG22	20	0.54	0.18	0.56
(1,2995)	1:70:A:LYS:HB3	1:5:A:ILE:HG23	20	0.54	0.18	0.56
(1,1353)	1:66:A:SER:H	1:68:A:ILE:HD11	20	0.54	0.11	0.57
(1,1353)	1:66:A:SER:H	1:68:A:ILE:HD12	20	0.54	0.11	0.57
(1,1353)	1:66:A:SER:H	1:68:A:ILE:HD13	20	0.54	0.11	0.57
(1,1353)	1:55:A:LEU:H	1:68:A:ILE:HD11	20	0.54	0.11	0.57
(1,1353)	1:55:A:LEU:H	1:68:A:ILE:HD12	20	0.54	0.11	0.57
(1,1353)	1:55:A:LEU:H	1:68:A:ILE:HD13	20	0.54	0.11	0.57
(1,2523)	1:8:A:ILE:HA	1:22:A:LEU:HD21	20	0.52	0.12	0.51
(1,2523)	1:8:A:ILE:HA	1:22:A:LEU:HD22	20	0.52	0.12	0.51
(1,2523)	1:8:A:ILE:HA	1:22:A:LEU:HD23	20	0.52	0.12	0.51
(1,2523)	1:137:A:HIS:HB3	1:135:A:ILE:HG13	20	0.52	0.12	0.51
(1,2306)	1:73:A:ILE:H	1:5:A:ILE:HG13	20	0.51	0.22	0.48
(1,2306)	1:71:A:ASN:H	1:5:A:ILE:HG13	20	0.51	0.22	0.48
(1,929)	1:3:A:VAL:HG21	1:34:A:LYS:H	20	0.48	0.15	0.48
(1,929)	1:3:A:VAL:HG22	1:34:A:LYS:H	20	0.48	0.15	0.48
(1,929)	1:3:A:VAL:HG23	1:34:A:LYS:H	20	0.48	0.15	0.48
(1,929)	1:3:A:VAL:HG11	1:34:A:LYS:H	20	0.48	0.15	0.48
(1,929)	1:3:A:VAL:HG12	1:34:A:LYS:H	20	0.48	0.15	0.48
(1,929)	1:3:A:VAL:HG13	1:34:A:LYS:H	20	0.48	0.15	0.48
(1,1505)	1:2:A:SER:HA	1:73:A:ILE:HD11	20	0.44	0.14	0.42
(1,1505)	1:2:A:SER:HA	1:73:A:ILE:HD12	20	0.44	0.14	0.42
(1,1505)	1:2:A:SER:HA	1:73:A:ILE:HD13	20	0.44	0.14	0.42
(1,1505)	1:72:A:ARG:HA	1:73:A:ILE:HD11	20	0.44	0.14	0.42
(1,1505)	1:72:A:ARG:HA	1:73:A:ILE:HD12	20	0.44	0.14	0.42
(1,1505)	1:72:A:ARG:HA	1:73:A:ILE:HD13	20	0.44	0.14	0.42
(1,1238)	1:59:A:LEU:HD21	1:20:A:ALA:H	20	0.42	0.17	0.48

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1238)	1:59:A:LEU:HD22	1:20:A:ALA:H	20	0.42	0.17	0.48
(1,1238)	1:59:A:LEU:HD23	1:20:A:ALA:H	20	0.42	0.17	0.48
(1,1238)	1:17:A:ILE:HD11	1:20:A:ALA:H	20	0.42	0.17	0.48
(1,1238)	1:17:A:ILE:HD12	1:20:A:ALA:H	20	0.42	0.17	0.48
(1,1238)	1:17:A:ILE:HD13	1:20:A:ALA:H	20	0.42	0.17	0.48
(1,1238)	1:21:A:ILE:HD11	1:20:A:ALA:H	20	0.42	0.17	0.48
(1,1238)	1:21:A:ILE:HD12	1:20:A:ALA:H	20	0.42	0.17	0.48
(1,1238)	1:21:A:ILE:HD13	1:20:A:ALA:H	20	0.42	0.17	0.48
(1,605)	1:90:A:TYR:HB2	1:93:A:ILE:H	20	0.41	0.07	0.41
(1,3568)	1:86:A:ASP:HB2	1:88:A:ASN:HB2	20	0.41	0.06	0.41
(1,3568)	1:89:A:ASP:HB2	1:88:A:ASN:HB2	20	0.41	0.06	0.41
(1,3568)	1:89:A:ASP:HB3	1:88:A:ASN:HB2	20	0.41	0.06	0.41
(1,2247)	1:70:A:LYS:HA	1:70:A:LYS:HD2	20	0.39	0.04	0.39
(1,228)	1:19:A:TYR:HD1	1:57:A:MET:H	20	0.39	0.09	0.38
(1,228)	1:19:A:TYR:HD2	1:57:A:MET:H	20	0.39	0.09	0.38
(1,971)	1:60:A:LEU:HD21	1:62:A:LYS:H	20	0.38	0.08	0.4
(1,971)	1:60:A:LEU:HD22	1:62:A:LYS:H	20	0.38	0.08	0.4
(1,971)	1:60:A:LEU:HD23	1:62:A:LYS:H	20	0.38	0.08	0.4
(1,587)	1:7:A:ASP:HB3	1:11:A:ASN:H	20	0.36	0.09	0.36
(1,587)	1:9:A:ASP:HB3	1:11:A:ASN:H	20	0.36	0.09	0.36
(1,2484)	1:56:A:GLN:HE22	1:60:A:LEU:HD21	20	0.35	0.12	0.38
(1,2484)	1:56:A:GLN:HE22	1:60:A:LEU:HD22	20	0.35	0.12	0.38
(1,2484)	1:56:A:GLN:HE22	1:60:A:LEU:HD23	20	0.35	0.12	0.38
(1,2484)	1:56:A:GLN:HE22	1:52:A:LEU:HD21	20	0.35	0.12	0.38
(1,2484)	1:56:A:GLN:HE22	1:52:A:LEU:HD22	20	0.35	0.12	0.38
(1,2484)	1:56:A:GLN:HE22	1:52:A:LEU:HD23	20	0.35	0.12	0.38
(1,3171)	1:53:A:ALA:HB1	1:54:A:ILE:HA	20	0.35	0.03	0.36
(1,3171)	1:53:A:ALA:HB2	1:54:A:ILE:HA	20	0.35	0.03	0.36
(1,3171)	1:53:A:ALA:HB3	1:54:A:ILE:HA	20	0.35	0.03	0.36
(1,3171)	1:20:A:ALA:HB1	1:21:A:ILE:HA	20	0.35	0.03	0.36
(1,3171)	1:20:A:ALA:HB2	1:21:A:ILE:HA	20	0.35	0.03	0.36
(1,3171)	1:20:A:ALA:HB3	1:21:A:ILE:HA	20	0.35	0.03	0.36
(1,3171)	1:103:A:LEU:HG	1:107:A:SER:HB3	20	0.35	0.03	0.36
(1,1357)	1:123:A:ASP:H	1:93:A:ILE:HD11	20	0.34	0.1	0.34
(1,1357)	1:123:A:ASP:H	1:93:A:ILE:HD12	20	0.34	0.1	0.34
(1,1357)	1:123:A:ASP:H	1:93:A:ILE:HD13	20	0.34	0.1	0.34
(1,1357)	1:90:A:TYR:H	1:93:A:ILE:HD11	20	0.34	0.1	0.34
(1,1357)	1:90:A:TYR:H	1:93:A:ILE:HD12	20	0.34	0.1	0.34
(1,1357)	1:90:A:TYR:H	1:93:A:ILE:HD13	20	0.34	0.1	0.34
(1,743)	1:34:A:LYS:HD2	1:34:A:LYS:H	20	0.33	0.05	0.34
(1,2844)	1:58:A:TYR:H	1:68:A:ILE:HG21	20	0.32	0.08	0.32
(1,2844)	1:58:A:TYR:H	1:68:A:ILE:HG22	20	0.32	0.08	0.32

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2844)	1:58:A:TYR:H	1:68:A:ILE:HG23	20	0.32	0.08	0.32
(1,2844)	1:59:A:LEU:H	1:68:A:ILE:HG21	20	0.32	0.08	0.32
(1,2844)	1:59:A:LEU:H	1:68:A:ILE:HG22	20	0.32	0.08	0.32
(1,2844)	1:59:A:LEU:H	1:68:A:ILE:HG23	20	0.32	0.08	0.32
(1,909)	1:73:A:ILE:HD11	1:73:A:ILE:H	20	0.3	0.07	0.32
(1,909)	1:73:A:ILE:HD12	1:73:A:ILE:H	20	0.3	0.07	0.32
(1,909)	1:73:A:ILE:HD13	1:73:A:ILE:H	20	0.3	0.07	0.32
(1,909)	1:73:A:ILE:HG21	1:73:A:ILE:H	20	0.3	0.07	0.32
(1,909)	1:73:A:ILE:HG22	1:73:A:ILE:H	20	0.3	0.07	0.32
(1,909)	1:73:A:ILE:HG23	1:73:A:ILE:H	20	0.3	0.07	0.32
(1,1019)	1:22:A:LEU:HD21	1:52:A:LEU:H	20	0.29	0.05	0.3
(1,1019)	1:22:A:LEU:HD22	1:52:A:LEU:H	20	0.29	0.05	0.3
(1,1019)	1:22:A:LEU:HD23	1:52:A:LEU:H	20	0.29	0.05	0.3
(1,3871)	1:79:A:ILE:H	1:80:A:ASP:HB3	20	0.28	0.07	0.28
(1,3871)	1:11:A:ASN:H	1:9:A:ASP:HB3	20	0.28	0.07	0.28
(1,3871)	1:11:A:ASN:H	1:7:A:ASP:HB3	20	0.28	0.07	0.28
(1,3871)	1:21:A:ILE:H	1:9:A:ASP:HB3	20	0.28	0.07	0.28
(1,2001)	1:82:A:ASN:HD22	1:82:A:ASN:HB3	20	0.27	0.02	0.28
(1,2001)	1:11:A:ASN:HD22	1:11:A:ASN:HB3	20	0.27	0.02	0.28
(1,2379)	1:107:A:SER:HA	1:108:A:LEU:HG	20	0.26	0.05	0.26
(1,2379)	1:102:A:GLN:HA	1:108:A:LEU:HG	20	0.26	0.05	0.26
(1,1022)	1:79:A:ILE:HG21	1:81:A:ASN:H	20	0.25	0.07	0.24
(1,1022)	1:79:A:ILE:HG22	1:81:A:ASN:H	20	0.25	0.07	0.24
(1,1022)	1:79:A:ILE:HG23	1:81:A:ASN:H	20	0.25	0.07	0.24
(1,1220)	1:131:A:ILE:HG21	1:133:A:GLY:H	20	0.25	0.1	0.22
(1,1220)	1:131:A:ILE:HG22	1:133:A:GLY:H	20	0.25	0.1	0.22
(1,1220)	1:131:A:ILE:HG23	1:133:A:GLY:H	20	0.25	0.1	0.22
(1,3581)	1:56:A:GLN:H	1:68:A:ILE:HD11	20	0.25	0.08	0.26
(1,3581)	1:56:A:GLN:H	1:68:A:ILE:HD12	20	0.25	0.08	0.26
(1,3581)	1:56:A:GLN:H	1:68:A:ILE:HD13	20	0.25	0.08	0.26
(1,3581)	1:67:A:ASP:H	1:68:A:ILE:HD11	20	0.25	0.08	0.26
(1,3581)	1:67:A:ASP:H	1:68:A:ILE:HD12	20	0.25	0.08	0.26
(1,3581)	1:67:A:ASP:H	1:68:A:ILE:HD13	20	0.25	0.08	0.26
(1,981)	1:84:A:ILE:HD11	1:82:A:ASN:H	20	0.2	0.04	0.21
(1,981)	1:84:A:ILE:HD12	1:82:A:ASN:H	20	0.2	0.04	0.21
(1,981)	1:84:A:ILE:HD13	1:82:A:ASN:H	20	0.2	0.04	0.21
(1,2180)	1:23:A:LYS:HD2	1:23:A:LYS:HB2	20	0.2	0.05	0.2
(1,2180)	1:20:A:ALA:HB1	1:23:A:LYS:HB2	20	0.2	0.05	0.2
(1,2180)	1:20:A:ALA:HB2	1:23:A:LYS:HB2	20	0.2	0.05	0.2
(1,2180)	1:20:A:ALA:HB3	1:23:A:LYS:HB2	20	0.2	0.05	0.2
(1,2273)	1:70:A:LYS:HB2	1:70:A:LYS:HD2	20	0.14	0.02	0.14
(1,2410)	1:102:A:GLN:HG3	1:108:A:LEU:HG	19	0.58	0.16	0.47

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1784)	1:130:A:TYR:H	1:129:A:LYS:HE2	19	0.56	0.1	0.58
(1,1784)	1:130:A:TYR:H	1:129:A:LYS:HE3	19	0.56	0.1	0.58
(1,1784)	1:125:A:ILE:H	1:129:A:LYS:HE2	19	0.56	0.1	0.58
(1,1784)	1:125:A:ILE:H	1:129:A:LYS:HE3	19	0.56	0.1	0.58
(1,3695)	1:108:A:LEU:HD21	1:102:A:GLN:HG2	19	0.54	0.1	0.56
(1,3695)	1:108:A:LEU:HD22	1:102:A:GLN:HG2	19	0.54	0.1	0.56
(1,3695)	1:108:A:LEU:HD23	1:102:A:GLN:HG2	19	0.54	0.1	0.56
(1,2586)	1:39:A:ALA:HB1	1:36:A:LEU:HD11	19	0.4	0.1	0.38
(1,2586)	1:39:A:ALA:HB1	1:36:A:LEU:HD12	19	0.4	0.1	0.38
(1,2586)	1:39:A:ALA:HB1	1:36:A:LEU:HD13	19	0.4	0.1	0.38
(1,2586)	1:39:A:ALA:HB2	1:36:A:LEU:HD11	19	0.4	0.1	0.38
(1,2586)	1:39:A:ALA:HB2	1:36:A:LEU:HD12	19	0.4	0.1	0.38
(1,2586)	1:39:A:ALA:HB2	1:36:A:LEU:HD13	19	0.4	0.1	0.38
(1,2586)	1:39:A:ALA:HB3	1:36:A:LEU:HD11	19	0.4	0.1	0.38
(1,2586)	1:39:A:ALA:HB3	1:36:A:LEU:HD12	19	0.4	0.1	0.38
(1,2586)	1:39:A:ALA:HB3	1:36:A:LEU:HD13	19	0.4	0.1	0.38
(1,2586)	1:106:A:ALA:HB1	1:36:A:LEU:HD11	19	0.4	0.1	0.38
(1,2586)	1:106:A:ALA:HB1	1:36:A:LEU:HD12	19	0.4	0.1	0.38
(1,2586)	1:106:A:ALA:HB1	1:36:A:LEU:HD13	19	0.4	0.1	0.38
(1,2586)	1:106:A:ALA:HB2	1:36:A:LEU:HD11	19	0.4	0.1	0.38
(1,2586)	1:106:A:ALA:HB2	1:36:A:LEU:HD12	19	0.4	0.1	0.38
(1,2586)	1:106:A:ALA:HB2	1:36:A:LEU:HD13	19	0.4	0.1	0.38
(1,2586)	1:106:A:ALA:HB3	1:36:A:LEU:HD11	19	0.4	0.1	0.38
(1,2586)	1:106:A:ALA:HB3	1:36:A:LEU:HD12	19	0.4	0.1	0.38
(1,2586)	1:106:A:ALA:HB3	1:36:A:LEU:HD13	19	0.4	0.1	0.38
(1,3238)	1:74:A:TYR:HB3	1:2:A:SER:HA	19	0.34	0.07	0.34
(1,2344)	1:19:A:TYR:H	1:59:A:LEU:HD21	19	0.31	0.12	0.32
(1,2344)	1:19:A:TYR:H	1:59:A:LEU:HD22	19	0.31	0.12	0.32
(1,2344)	1:19:A:TYR:H	1:59:A:LEU:HD23	19	0.31	0.12	0.32
(1,2344)	1:58:A:TYR:HD1	1:59:A:LEU:HD21	19	0.31	0.12	0.32
(1,2344)	1:58:A:TYR:HD1	1:59:A:LEU:HD22	19	0.31	0.12	0.32
(1,2344)	1:58:A:TYR:HD1	1:59:A:LEU:HD23	19	0.31	0.12	0.32
(1,2344)	1:58:A:TYR:HD2	1:59:A:LEU:HD21	19	0.31	0.12	0.32
(1,2344)	1:58:A:TYR:HD2	1:59:A:LEU:HD22	19	0.31	0.12	0.32
(1,2344)	1:58:A:TYR:HD2	1:59:A:LEU:HD23	19	0.31	0.12	0.32
(1,2344)	1:19:A:TYR:HD1	1:59:A:LEU:HD21	19	0.31	0.12	0.32
(1,2344)	1:19:A:TYR:HD1	1:59:A:LEU:HD22	19	0.31	0.12	0.32
(1,2344)	1:19:A:TYR:HD1	1:59:A:LEU:HD23	19	0.31	0.12	0.32
(1,2344)	1:19:A:TYR:HD2	1:59:A:LEU:HD21	19	0.31	0.12	0.32
(1,2344)	1:19:A:TYR:HD2	1:59:A:LEU:HD22	19	0.31	0.12	0.32
(1,2344)	1:19:A:TYR:HD2	1:59:A:LEU:HD23	19	0.31	0.12	0.32
(1,3371)	1:36:A:LEU:HA	1:36:A:LEU:HD11	19	0.26	0.03	0.27

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3371)	1:36:A:LEU:HA	1:36:A:LEU:HD12	19	0.26	0.03	0.27
(1,3371)	1:36:A:LEU:HA	1:36:A:LEU:HD13	19	0.26	0.03	0.27
(1,1163)	1:27:A:ILE:HD11	1:27:A:ILE:H	19	0.25	0.04	0.24
(1,1163)	1:27:A:ILE:HD12	1:27:A:ILE:H	19	0.25	0.04	0.24
(1,1163)	1:27:A:ILE:HD13	1:27:A:ILE:H	19	0.25	0.04	0.24
(1,3095)	1:57:A:MET:HE1	1:53:A:ALA:HA	19	0.2	0.05	0.21
(1,3095)	1:57:A:MET:HE2	1:53:A:ALA:HA	19	0.2	0.05	0.21
(1,3095)	1:57:A:MET:HE3	1:53:A:ALA:HA	19	0.2	0.05	0.21
(1,81)	1:58:A:TYR:H	1:61:A:GLY:H	19	0.2	0.08	0.18
(1,3834)	1:74:A:TYR:H	1:3:A:VAL:HG11	19	0.14	0.02	0.14
(1,3834)	1:74:A:TYR:H	1:3:A:VAL:HG12	19	0.14	0.02	0.14
(1,3834)	1:74:A:TYR:H	1:3:A:VAL:HG13	19	0.14	0.02	0.14
(1,1162)	1:79:A:ILE:HG21	1:111:A:ALA:H	18	0.52	0.16	0.5
(1,1162)	1:79:A:ILE:HG22	1:111:A:ALA:H	18	0.52	0.16	0.5
(1,1162)	1:79:A:ILE:HG23	1:111:A:ALA:H	18	0.52	0.16	0.5
(1,2483)	1:56:A:GLN:HE21	1:52:A:LEU:HD21	18	0.39	0.08	0.4
(1,2483)	1:56:A:GLN:HE21	1:52:A:LEU:HD22	18	0.39	0.08	0.4
(1,2483)	1:56:A:GLN:HE21	1:52:A:LEU:HD23	18	0.39	0.08	0.4
(1,2483)	1:56:A:GLN:HE21	1:60:A:LEU:HD21	18	0.39	0.08	0.4
(1,2483)	1:56:A:GLN:HE21	1:60:A:LEU:HD22	18	0.39	0.08	0.4
(1,2483)	1:56:A:GLN:HE21	1:60:A:LEU:HD23	18	0.39	0.08	0.4
(1,2546)	1:56:A:GLN:HB2	1:60:A:LEU:HD21	18	0.35	0.05	0.35
(1,2546)	1:56:A:GLN:HB2	1:60:A:LEU:HD22	18	0.35	0.05	0.35
(1,2546)	1:56:A:GLN:HB2	1:60:A:LEU:HD23	18	0.35	0.05	0.35
(1,2546)	1:56:A:GLN:HB3	1:60:A:LEU:HD21	18	0.35	0.05	0.35
(1,2546)	1:56:A:GLN:HB3	1:60:A:LEU:HD22	18	0.35	0.05	0.35
(1,2546)	1:56:A:GLN:HB3	1:60:A:LEU:HD23	18	0.35	0.05	0.35
(1,2546)	1:35:A:GLN:HB2	1:31:A:LEU:HD21	18	0.35	0.05	0.35
(1,2546)	1:35:A:GLN:HB2	1:31:A:LEU:HD22	18	0.35	0.05	0.35
(1,2546)	1:35:A:GLN:HB2	1:31:A:LEU:HD23	18	0.35	0.05	0.35
(1,2966)	1:94:A:CYS:HB3	1:97:A:ILE:HG21	18	0.34	0.13	0.32
(1,2966)	1:94:A:CYS:HB3	1:97:A:ILE:HG22	18	0.34	0.13	0.32
(1,2966)	1:94:A:CYS:HB3	1:97:A:ILE:HG23	18	0.34	0.13	0.32
(1,2966)	1:94:A:CYS:HB3	1:91:A:ILE:HG21	18	0.34	0.13	0.32
(1,2966)	1:94:A:CYS:HB3	1:91:A:ILE:HG22	18	0.34	0.13	0.32
(1,2966)	1:94:A:CYS:HB3	1:91:A:ILE:HG23	18	0.34	0.13	0.32
(1,2966)	1:95:A:ASN:HB3	1:91:A:ILE:HG21	18	0.34	0.13	0.32
(1,2966)	1:95:A:ASN:HB3	1:91:A:ILE:HG22	18	0.34	0.13	0.32
(1,2966)	1:95:A:ASN:HB3	1:91:A:ILE:HG23	18	0.34	0.13	0.32
(1,2966)	1:88:A:ASN:HB3	1:91:A:ILE:HG21	18	0.34	0.13	0.32
(1,2966)	1:88:A:ASN:HB3	1:91:A:ILE:HG22	18	0.34	0.13	0.32
(1,2966)	1:88:A:ASN:HB3	1:91:A:ILE:HG23	18	0.34	0.13	0.32

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2499)	1:135:A:ILE:HA	1:135:A:ILE:HG12	18	0.29	0.01	0.29
(1,2499)	1:62:A:LYS:HA	1:62:A:LYS:HG3	18	0.29	0.01	0.29
(1,1137)	1:97:A:ILE:HG21	1:96:A:HIS:H	18	0.25	0.07	0.24
(1,1137)	1:97:A:ILE:HG22	1:96:A:HIS:H	18	0.25	0.07	0.24
(1,1137)	1:97:A:ILE:HG23	1:96:A:HIS:H	18	0.25	0.07	0.24
(1,1137)	1:79:A:ILE:HD11	1:96:A:HIS:H	18	0.25	0.07	0.24
(1,1137)	1:79:A:ILE:HD12	1:96:A:HIS:H	18	0.25	0.07	0.24
(1,1137)	1:79:A:ILE:HD13	1:96:A:HIS:H	18	0.25	0.07	0.24
(1,582)	1:57:A:MET:HB3	1:58:A:TYR:H	18	0.15	0.03	0.14
(1,2352)	1:85:A:VAL:HA	1:84:A:ILE:HG13	18	0.15	0.02	0.15
(1,779)	1:62:A:LYS:HB3	1:62:A:LYS:H	18	0.13	0.02	0.13
(1,1067)	1:68:A:ILE:HD11	1:63:A:GLY:H	17	0.58	0.12	0.61
(1,1067)	1:68:A:ILE:HD12	1:63:A:GLY:H	17	0.58	0.12	0.61
(1,1067)	1:68:A:ILE:HD13	1:63:A:GLY:H	17	0.58	0.12	0.61
(1,1067)	1:60:A:LEU:HD21	1:63:A:GLY:H	17	0.58	0.12	0.61
(1,1067)	1:60:A:LEU:HD22	1:63:A:GLY:H	17	0.58	0.12	0.61
(1,1067)	1:60:A:LEU:HD23	1:63:A:GLY:H	17	0.58	0.12	0.61
(1,3180)	1:127:A:ILE:HB	1:79:A:ILE:HD11	17	0.37	0.11	0.38
(1,3180)	1:127:A:ILE:HB	1:79:A:ILE:HD12	17	0.37	0.11	0.38
(1,3180)	1:127:A:ILE:HB	1:79:A:ILE:HD13	17	0.37	0.11	0.38
(1,3040)	1:6:A:GLY:HA2	1:14:A:ILE:HG21	17	0.32	0.11	0.35
(1,3040)	1:6:A:GLY:HA2	1:14:A:ILE:HG22	17	0.32	0.11	0.35
(1,3040)	1:6:A:GLY:HA2	1:14:A:ILE:HG23	17	0.32	0.11	0.35
(1,3040)	1:18:A:ASP:HB2	1:14:A:ILE:HG21	17	0.32	0.11	0.35
(1,3040)	1:18:A:ASP:HB2	1:14:A:ILE:HG22	17	0.32	0.11	0.35
(1,3040)	1:18:A:ASP:HB2	1:14:A:ILE:HG23	17	0.32	0.11	0.35
(1,2537)	1:52:A:LEU:HA	1:55:A:LEU:HD11	17	0.31	0.12	0.33
(1,2537)	1:52:A:LEU:HA	1:55:A:LEU:HD12	17	0.31	0.12	0.33
(1,2537)	1:52:A:LEU:HA	1:55:A:LEU:HD13	17	0.31	0.12	0.33
(1,3724)	1:71:A:ASN:HB3	1:5:A:ILE:HG13	17	0.3	0.14	0.23
(1,1221)	1:62:A:LYS:HB3	1:63:A:GLY:H	17	0.28	0.07	0.28
(1,1221)	1:57:A:MET:HB2	1:63:A:GLY:H	17	0.28	0.07	0.28
(1,3840)	1:123:A:ASP:HB2	1:111:A:ALA:HB1	17	0.28	0.14	0.25
(1,3840)	1:123:A:ASP:HB2	1:111:A:ALA:HB2	17	0.28	0.14	0.25
(1,3840)	1:123:A:ASP:HB2	1:111:A:ALA:HB3	17	0.28	0.14	0.25
(1,3840)	1:112:A:ASP:HB3	1:111:A:ALA:HB1	17	0.28	0.14	0.25
(1,3840)	1:112:A:ASP:HB3	1:111:A:ALA:HB2	17	0.28	0.14	0.25
(1,3840)	1:112:A:ASP:HB3	1:111:A:ALA:HB3	17	0.28	0.14	0.25
(1,2832)	1:91:A:ILE:H	1:91:A:ILE:HG21	17	0.27	0.04	0.29
(1,2832)	1:91:A:ILE:H	1:91:A:ILE:HG22	17	0.27	0.04	0.29
(1,2832)	1:91:A:ILE:H	1:91:A:ILE:HG23	17	0.27	0.04	0.29
(1,2832)	1:131:A:ILE:H	1:131:A:ILE:HG21	17	0.27	0.04	0.29

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2832)	1:131:A:ILE:H	1:131:A:ILE:HG22	17	0.27	0.04	0.29
(1,2832)	1:131:A:ILE:H	1:131:A:ILE:HG23	17	0.27	0.04	0.29
(1,2832)	1:136:A:THR:H	1:135:A:ILE:HG21	17	0.27	0.04	0.29
(1,2832)	1:136:A:THR:H	1:135:A:ILE:HG22	17	0.27	0.04	0.29
(1,2832)	1:136:A:THR:H	1:135:A:ILE:HG23	17	0.27	0.04	0.29
(1,2832)	1:87:A:GLU:H	1:131:A:ILE:HG21	17	0.27	0.04	0.29
(1,2832)	1:87:A:GLU:H	1:131:A:ILE:HG22	17	0.27	0.04	0.29
(1,2832)	1:87:A:GLU:H	1:131:A:ILE:HG23	17	0.27	0.04	0.29
(1,980)	1:54:A:ILE:HD11	1:42:A:ASP:H	17	0.24	0.09	0.21
(1,980)	1:54:A:ILE:HD12	1:42:A:ASP:H	17	0.24	0.09	0.21
(1,980)	1:54:A:ILE:HD13	1:42:A:ASP:H	17	0.24	0.09	0.21
(1,2515)	1:92:A:LEU:HA	1:103:A:LEU:HD11	17	0.23	0.07	0.21
(1,2515)	1:92:A:LEU:HA	1:103:A:LEU:HD12	17	0.23	0.07	0.21
(1,2515)	1:92:A:LEU:HA	1:103:A:LEU:HD13	17	0.23	0.07	0.21
(1,2515)	1:93:A:ILE:HA	1:103:A:LEU:HD11	17	0.23	0.07	0.21
(1,2515)	1:93:A:ILE:HA	1:103:A:LEU:HD12	17	0.23	0.07	0.21
(1,2515)	1:93:A:ILE:HA	1:103:A:LEU:HD13	17	0.23	0.07	0.21
(1,3219)	1:93:A:ILE:HD11	1:119:A:ILE:HD11	17	0.23	0.04	0.24
(1,3219)	1:93:A:ILE:HD11	1:119:A:ILE:HD12	17	0.23	0.04	0.24
(1,3219)	1:93:A:ILE:HD11	1:119:A:ILE:HD13	17	0.23	0.04	0.24
(1,3219)	1:93:A:ILE:HD12	1:119:A:ILE:HD11	17	0.23	0.04	0.24
(1,3219)	1:93:A:ILE:HD12	1:119:A:ILE:HD12	17	0.23	0.04	0.24
(1,3219)	1:93:A:ILE:HD12	1:119:A:ILE:HD13	17	0.23	0.04	0.24
(1,3219)	1:93:A:ILE:HD13	1:119:A:ILE:HD11	17	0.23	0.04	0.24
(1,3219)	1:93:A:ILE:HD13	1:119:A:ILE:HD12	17	0.23	0.04	0.24
(1,3219)	1:93:A:ILE:HD13	1:119:A:ILE:HD13	17	0.23	0.04	0.24
(1,1042)	1:50:A:ILE:HD11	1:49:A:SER:H	17	0.22	0.07	0.21
(1,1042)	1:50:A:ILE:HD12	1:49:A:SER:H	17	0.22	0.07	0.21
(1,1042)	1:50:A:ILE:HD13	1:49:A:SER:H	17	0.22	0.07	0.21
(1,1042)	1:52:A:LEU:HD21	1:49:A:SER:H	17	0.22	0.07	0.21
(1,1042)	1:52:A:LEU:HD22	1:49:A:SER:H	17	0.22	0.07	0.21
(1,1042)	1:52:A:LEU:HD23	1:49:A:SER:H	17	0.22	0.07	0.21
(1,3543)	1:17:A:ILE:HA	1:21:A:ILE:HD11	17	0.19	0.04	0.18
(1,3543)	1:17:A:ILE:HA	1:21:A:ILE:HD12	17	0.19	0.04	0.18
(1,3543)	1:17:A:ILE:HA	1:21:A:ILE:HD13	17	0.19	0.04	0.18
(1,1195)	1:60:A:LEU:HD21	1:57:A:MET:H	17	0.18	0.04	0.17
(1,1195)	1:60:A:LEU:HD22	1:57:A:MET:H	17	0.18	0.04	0.17
(1,1195)	1:60:A:LEU:HD23	1:57:A:MET:H	17	0.18	0.04	0.17
(3,61)	1:109:A:PHE:H	1:105:A:ASP:O	17	0.13	0.02	0.13
(1,1150)	1:134:A:ARG:HG2	1:129:A:LYS:H	16	0.51	0.21	0.44
(1,1150)	1:134:A:ARG:HG3	1:129:A:LYS:H	16	0.51	0.21	0.44
(1,1150)	1:134:A:ARG:HB3	1:129:A:LYS:H	16	0.51	0.21	0.44

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3890)	1:73:A:ILE:H	1:2:A:SER:HB2	16	0.48	0.17	0.46
(1,3890)	1:4:A:LYS:H	1:2:A:SER:HB2	16	0.48	0.17	0.46
(1,3890)	1:71:A:ASN:H	1:2:A:SER:HB2	16	0.48	0.17	0.46
(1,386)	1:117:A:ASN:HA	1:119:A:ILE:H	16	0.28	0.09	0.29
(1,386)	1:96:A:HIS:HB3	1:119:A:ILE:H	16	0.28	0.09	0.29
(1,2350)	1:52:A:LEU:H	1:52:A:LEU:HD21	16	0.24	0.09	0.22
(1,2350)	1:52:A:LEU:H	1:52:A:LEU:HD22	16	0.24	0.09	0.22
(1,2350)	1:52:A:LEU:H	1:52:A:LEU:HD23	16	0.24	0.09	0.22
(1,2904)	1:3:A:VAL:HA	1:38:A:ALA:HB1	16	0.23	0.05	0.22
(1,2904)	1:3:A:VAL:HA	1:38:A:ALA:HB2	16	0.23	0.05	0.22
(1,2904)	1:3:A:VAL:HA	1:38:A:ALA:HB3	16	0.23	0.05	0.22
(1,2904)	1:6:A:GLY:HA3	1:38:A:ALA:HB1	16	0.23	0.05	0.22
(1,2904)	1:6:A:GLY:HA3	1:38:A:ALA:HB2	16	0.23	0.05	0.22
(1,2904)	1:6:A:GLY:HA3	1:38:A:ALA:HB3	16	0.23	0.05	0.22
(1,2697)	1:135:A:ILE:HB	1:136:A:THR:HG21	15	0.44	0.2	0.45
(1,2697)	1:135:A:ILE:HB	1:136:A:THR:HG22	15	0.44	0.2	0.45
(1,2697)	1:135:A:ILE:HB	1:136:A:THR:HG23	15	0.44	0.2	0.45
(1,2697)	1:128:A:GLU:HG2	1:132:A:THR:HG21	15	0.44	0.2	0.45
(1,2697)	1:128:A:GLU:HG2	1:132:A:THR:HG22	15	0.44	0.2	0.45
(1,2697)	1:128:A:GLU:HG2	1:132:A:THR:HG23	15	0.44	0.2	0.45
(1,2697)	1:128:A:GLU:HG3	1:132:A:THR:HG21	15	0.44	0.2	0.45
(1,2697)	1:128:A:GLU:HG3	1:132:A:THR:HG22	15	0.44	0.2	0.45
(1,2697)	1:128:A:GLU:HG3	1:132:A:THR:HG23	15	0.44	0.2	0.45
(1,2697)	1:57:A:MET:HB2	1:65:A:THR:HG21	15	0.44	0.2	0.45
(1,2697)	1:57:A:MET:HB2	1:65:A:THR:HG22	15	0.44	0.2	0.45
(1,2697)	1:57:A:MET:HB2	1:65:A:THR:HG23	15	0.44	0.2	0.45
(1,2697)	1:134:A:ARG:HB2	1:132:A:THR:HG21	15	0.44	0.2	0.45
(1,2697)	1:134:A:ARG:HB2	1:132:A:THR:HG22	15	0.44	0.2	0.45
(1,2697)	1:134:A:ARG:HB2	1:132:A:THR:HG23	15	0.44	0.2	0.45
(1,554)	1:4:A:LYS:HE2	1:4:A:LYS:H	15	0.42	0.13	0.48
(1,554)	1:4:A:LYS:HE3	1:4:A:LYS:H	15	0.42	0.13	0.48
(1,554)	1:34:A:LYS:HE2	1:4:A:LYS:H	15	0.42	0.13	0.48
(1,2962)	1:42:A:ASP:HB3	1:50:A:ILE:HG21	15	0.4	0.1	0.4
(1,2962)	1:42:A:ASP:HB3	1:50:A:ILE:HG22	15	0.4	0.1	0.4
(1,2962)	1:42:A:ASP:HB3	1:50:A:ILE:HG23	15	0.4	0.1	0.4
(1,2962)	1:42:A:ASP:HB3	1:54:A:ILE:HG21	15	0.4	0.1	0.4
(1,2962)	1:42:A:ASP:HB3	1:54:A:ILE:HG22	15	0.4	0.1	0.4
(1,2962)	1:42:A:ASP:HB3	1:54:A:ILE:HG23	15	0.4	0.1	0.4
(1,2970)	1:87:A:GLU:HG2	1:127:A:ILE:HG21	15	0.39	0.18	0.38
(1,2970)	1:87:A:GLU:HG2	1:127:A:ILE:HG22	15	0.39	0.18	0.38
(1,2970)	1:87:A:GLU:HG2	1:127:A:ILE:HG23	15	0.39	0.18	0.38
(1,1043)	1:21:A:ILE:HG21	1:32:A:THR:H	15	0.38	0.17	0.35

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1043)	1:21:A:ILE:HG22	1:32:A:THR:H	15	0.38	0.17	0.35
(1,1043)	1:21:A:ILE:HG23	1:32:A:THR:H	15	0.38	0.17	0.35
(1,1043)	1:8:A:ILE:HG21	1:32:A:THR:H	15	0.38	0.17	0.35
(1,1043)	1:8:A:ILE:HG22	1:32:A:THR:H	15	0.38	0.17	0.35
(1,1043)	1:8:A:ILE:HG23	1:32:A:THR:H	15	0.38	0.17	0.35
(1,1813)	1:35:A:GLN:HE21	1:34:A:LYS:HE2	15	0.37	0.13	0.36
(1,1813)	1:19:A:TYR:HD1	1:23:A:LYS:HE2	15	0.37	0.13	0.36
(1,1813)	1:19:A:TYR:HD2	1:23:A:LYS:HE2	15	0.37	0.13	0.36
(1,1806)	1:81:A:ASN:HD22	1:72:A:ARG:HD3	15	0.34	0.11	0.3
(1,1806)	1:74:A:TYR:HE2	1:72:A:ARG:HD3	15	0.34	0.11	0.3
(1,1806)	1:74:A:TYR:HE1	1:72:A:ARG:HD3	15	0.34	0.11	0.3
(1,3183)	1:90:A:TYR:HB2	1:79:A:ILE:HD11	15	0.29	0.1	0.31
(1,3183)	1:90:A:TYR:HB2	1:79:A:ILE:HD12	15	0.29	0.1	0.31
(1,3183)	1:90:A:TYR:HB2	1:79:A:ILE:HD13	15	0.29	0.1	0.31
(1,3183)	1:35:A:GLN:HG2	1:8:A:ILE:HD11	15	0.29	0.1	0.31
(1,3183)	1:35:A:GLN:HG2	1:8:A:ILE:HD12	15	0.29	0.1	0.31
(1,3183)	1:35:A:GLN:HG2	1:8:A:ILE:HD13	15	0.29	0.1	0.31
(1,3183)	1:88:A:ASN:HB3	1:79:A:ILE:HD11	15	0.29	0.1	0.31
(1,3183)	1:88:A:ASN:HB3	1:79:A:ILE:HD12	15	0.29	0.1	0.31
(1,3183)	1:88:A:ASN:HB3	1:79:A:ILE:HD13	15	0.29	0.1	0.31
(1,1132)	1:131:A:ILE:HG12	1:130:A:TYR:H	15	0.29	0.11	0.27
(1,1132)	1:134:A:ARG:HG2	1:130:A:TYR:H	15	0.29	0.11	0.27
(1,1132)	1:134:A:ARG:HG3	1:130:A:TYR:H	15	0.29	0.11	0.27
(1,3797)	1:93:A:ILE:H	1:79:A:ILE:HB	15	0.24	0.07	0.28
(1,3459)	1:74:A:TYR:HB3	1:73:A:ILE:HA	15	0.19	0.05	0.22
(1,2583)	1:126:A:LEU:HB2	1:138:A:LEU:HD21	15	0.19	0.06	0.18
(1,2583)	1:126:A:LEU:HB2	1:138:A:LEU:HD22	15	0.19	0.06	0.18
(1,2583)	1:126:A:LEU:HB2	1:138:A:LEU:HD23	15	0.19	0.06	0.18
(1,2583)	1:92:A:LEU:HG	1:103:A:LEU:HD11	15	0.19	0.06	0.18
(1,2583)	1:92:A:LEU:HG	1:103:A:LEU:HD12	15	0.19	0.06	0.18
(1,2583)	1:92:A:LEU:HG	1:103:A:LEU:HD13	15	0.19	0.06	0.18
(1,1197)	1:126:A:LEU:HD11	1:122:A:THR:H	15	0.18	0.04	0.18
(1,1197)	1:126:A:LEU:HD12	1:122:A:THR:H	15	0.18	0.04	0.18
(1,1197)	1:126:A:LEU:HD13	1:122:A:THR:H	15	0.18	0.04	0.18
(1,3843)	1:126:A:LEU:HA	1:113:A:ALA:HB1	15	0.18	0.03	0.17
(1,3843)	1:126:A:LEU:HA	1:113:A:ALA:HB2	15	0.18	0.03	0.17
(1,3843)	1:126:A:LEU:HA	1:113:A:ALA:HB3	15	0.18	0.03	0.17
(1,874)	1:139:A:PRO:HG2	1:115:A:GLY:H	15	0.14	0.02	0.14
(1,874)	1:139:A:PRO:HG3	1:115:A:GLY:H	15	0.14	0.02	0.14
(1,359)	1:45:A:GLY:HA3	1:45:A:GLY:H	15	0.11	0.01	0.11
(1,359)	1:83:A:GLY:HA3	1:83:A:GLY:H	15	0.11	0.01	0.11
(1,2942)	1:90:A:TYR:HB3	1:131:A:ILE:HG21	14	0.46	0.22	0.43

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2942)	1:90:A:TYR:HB3	1:131:A:ILE:HG22	14	0.46	0.22	0.43
(1,2942)	1:90:A:TYR:HB3	1:131:A:ILE:HG23	14	0.46	0.22	0.43
(1,2942)	1:86:A:ASP:HB2	1:131:A:ILE:HG21	14	0.46	0.22	0.43
(1,2942)	1:86:A:ASP:HB2	1:131:A:ILE:HG22	14	0.46	0.22	0.43
(1,2942)	1:86:A:ASP:HB2	1:131:A:ILE:HG23	14	0.46	0.22	0.43
(1,3457)	1:74:A:TYR:HB3	1:75:A:THR:HA	14	0.4	0.08	0.42
(1,1328)	1:97:A:ILE:HG21	1:121:A:GLN:H	14	0.29	0.08	0.29
(1,1328)	1:97:A:ILE:HG22	1:121:A:GLN:H	14	0.29	0.08	0.29
(1,1328)	1:97:A:ILE:HG23	1:121:A:GLN:H	14	0.29	0.08	0.29
(1,1511)	1:3:A:VAL:HA	1:5:A:ILE:HD11	14	0.26	0.05	0.25
(1,1511)	1:3:A:VAL:HA	1:5:A:ILE:HD12	14	0.26	0.05	0.25
(1,1511)	1:3:A:VAL:HA	1:5:A:ILE:HD13	14	0.26	0.05	0.25
(1,1326)	1:5:A:ILE:HD11	1:39:A:ALA:H	14	0.23	0.07	0.24
(1,1326)	1:5:A:ILE:HD12	1:39:A:ALA:H	14	0.23	0.07	0.24
(1,1326)	1:5:A:ILE:HD13	1:39:A:ALA:H	14	0.23	0.07	0.24
(1,1489)	1:70:A:LYS:H	1:5:A:ILE:HD11	14	0.21	0.08	0.18
(1,1489)	1:70:A:LYS:H	1:5:A:ILE:HD12	14	0.21	0.08	0.18
(1,1489)	1:70:A:LYS:H	1:5:A:ILE:HD13	14	0.21	0.08	0.18
(1,1091)	1:103:A:LEU:HD21	1:104:A:SER:H	14	0.21	0.09	0.18
(1,1091)	1:103:A:LEU:HD22	1:104:A:SER:H	14	0.21	0.09	0.18
(1,1091)	1:103:A:LEU:HD23	1:104:A:SER:H	14	0.21	0.09	0.18
(1,1091)	1:108:A:LEU:HD21	1:104:A:SER:H	14	0.21	0.09	0.18
(1,1091)	1:108:A:LEU:HD22	1:104:A:SER:H	14	0.21	0.09	0.18
(1,1091)	1:108:A:LEU:HD23	1:104:A:SER:H	14	0.21	0.09	0.18
(1,3049)	1:12:A:GLY:HA2	1:13:A:GLU:HG2	14	0.2	0.07	0.2
(1,3049)	1:12:A:GLY:HA2	1:13:A:GLU:HG3	14	0.2	0.07	0.2
(1,2248)	1:70:A:LYS:HA	1:70:A:LYS:HD3	14	0.18	0.03	0.18
(1,2630)	1:75:A:THR:H	1:75:A:THR:HG21	14	0.13	0.02	0.13
(1,2630)	1:75:A:THR:H	1:75:A:THR:HG22	14	0.13	0.02	0.13
(1,2630)	1:75:A:THR:H	1:75:A:THR:HG23	14	0.13	0.02	0.13
(1,962)	1:73:A:ILE:HD11	1:71:A:ASN:H	13	0.37	0.12	0.35
(1,962)	1:73:A:ILE:HD12	1:71:A:ASN:H	13	0.37	0.12	0.35
(1,962)	1:73:A:ILE:HD13	1:71:A:ASN:H	13	0.37	0.12	0.35
(1,962)	1:5:A:ILE:HD11	1:71:A:ASN:H	13	0.37	0.12	0.35
(1,962)	1:5:A:ILE:HD12	1:71:A:ASN:H	13	0.37	0.12	0.35
(1,962)	1:5:A:ILE:HD13	1:71:A:ASN:H	13	0.37	0.12	0.35
(1,2466)	1:24:A:SER:H	1:23:A:LYS:HG2	13	0.36	0.12	0.4
(1,3938)	1:14:A:ILE:HB	1:58:A:TYR:HD1	13	0.31	0.11	0.36
(1,3938)	1:14:A:ILE:HB	1:58:A:TYR:HD2	13	0.31	0.11	0.36
(1,1949)	1:136:A:THR:HG21	1:135:A:ILE:HB	13	0.3	0.08	0.27
(1,1949)	1:136:A:THR:HG22	1:135:A:ILE:HB	13	0.3	0.08	0.27
(1,1949)	1:136:A:THR:HG23	1:135:A:ILE:HB	13	0.3	0.08	0.27

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1949)	1:138:A:LEU:HG	1:135:A:ILE:HB	13	0.3	0.08	0.27
(1,870)	1:52:A:LEU:HG	1:56:A:GLN:HE21	13	0.29	0.11	0.27
(1,903)	1:41:A:VAL:HG21	1:48:A:ASN:H	13	0.24	0.09	0.21
(1,903)	1:41:A:VAL:HG22	1:48:A:ASN:H	13	0.24	0.09	0.21
(1,903)	1:41:A:VAL:HG23	1:48:A:ASN:H	13	0.24	0.09	0.21
(1,2761)	1:74:A:TYR:HB2	1:75:A:THR:HG21	13	0.21	0.06	0.21
(1,2761)	1:74:A:TYR:HB2	1:75:A:THR:HG22	13	0.21	0.06	0.21
(1,2761)	1:74:A:TYR:HB2	1:75:A:THR:HG23	13	0.21	0.06	0.21
(1,2980)	1:21:A:ILE:HB	1:20:A:ALA:HB1	13	0.15	0.03	0.16
(1,2980)	1:21:A:ILE:HB	1:20:A:ALA:HB2	13	0.15	0.03	0.16
(1,2980)	1:21:A:ILE:HB	1:20:A:ALA:HB3	13	0.15	0.03	0.16
(1,2980)	1:54:A:ILE:HB	1:53:A:ALA:HB1	13	0.15	0.03	0.16
(1,2980)	1:54:A:ILE:HB	1:53:A:ALA:HB2	13	0.15	0.03	0.16
(1,2980)	1:54:A:ILE:HB	1:53:A:ALA:HB3	13	0.15	0.03	0.16
(1,1939)	1:92:A:LEU:HD21	1:80:A:ASP:HB3	13	0.14	0.03	0.14
(1,1939)	1:92:A:LEU:HD22	1:80:A:ASP:HB3	13	0.14	0.03	0.14
(1,1939)	1:92:A:LEU:HD23	1:80:A:ASP:HB3	13	0.14	0.03	0.14
(1,2316)	1:121:A:GLN:H	1:121:A:GLN:HB3	13	0.14	0.02	0.14
(1,3408)	1:59:A:LEU:HD11	1:15:A:SER:HB3	12	0.7	0.16	0.75
(1,3408)	1:59:A:LEU:HD12	1:15:A:SER:HB3	12	0.7	0.16	0.75
(1,3408)	1:59:A:LEU:HD13	1:15:A:SER:HB3	12	0.7	0.16	0.75
(1,3635)	1:112:A:ASP:HB2	1:113:A:ALA:HA	12	0.47	0.09	0.5
(1,3635)	1:76:A:TYR:HB2	1:113:A:ALA:HA	12	0.47	0.09	0.5
(1,2765)	1:40:A:ASP:HB3	1:3:A:VAL:HG11	12	0.33	0.15	0.35
(1,2765)	1:40:A:ASP:HB3	1:3:A:VAL:HG12	12	0.33	0.15	0.35
(1,2765)	1:40:A:ASP:HB3	1:3:A:VAL:HG13	12	0.33	0.15	0.35
(1,2765)	1:74:A:TYR:HB2	1:3:A:VAL:HG21	12	0.33	0.15	0.35
(1,2765)	1:74:A:TYR:HB2	1:3:A:VAL:HG22	12	0.33	0.15	0.35
(1,2765)	1:74:A:TYR:HB2	1:3:A:VAL:HG23	12	0.33	0.15	0.35
(1,866)	1:27:A:ILE:HG13	1:24:A:SER:H	12	0.28	0.07	0.29
(1,866)	1:20:A:ALA:HB1	1:24:A:SER:H	12	0.28	0.07	0.29
(1,866)	1:20:A:ALA:HB2	1:24:A:SER:H	12	0.28	0.07	0.29
(1,866)	1:20:A:ALA:HB3	1:24:A:SER:H	12	0.28	0.07	0.29
(1,1117)	1:96:A:HIS:HA	1:102:A:GLN:H	12	0.26	0.11	0.24
(1,806)	1:53:A:ALA:HB1	1:57:A:MET:H	12	0.17	0.04	0.16
(1,806)	1:53:A:ALA:HB2	1:57:A:MET:H	12	0.17	0.04	0.16
(1,806)	1:53:A:ALA:HB3	1:57:A:MET:H	12	0.17	0.04	0.16
(1,2300)	1:49:A:SER:H	1:50:A:ILE:HG13	12	0.17	0.06	0.16
(1,931)	1:8:A:ILE:HG21	1:22:A:LEU:H	12	0.16	0.03	0.16
(1,931)	1:8:A:ILE:HG22	1:22:A:LEU:H	12	0.16	0.03	0.16
(1,931)	1:8:A:ILE:HG23	1:22:A:LEU:H	12	0.16	0.03	0.16
(1,1122)	1:93:A:ILE:HD11	1:94:A:CYS:H	12	0.15	0.03	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1122)	1:93:A:ILE:HD12	1:94:A:CYS:H	12	0.15	0.03	0.16
(1,1122)	1:93:A:ILE:HD13	1:94:A:CYS:H	12	0.15	0.03	0.16
(1,1122)	1:91:A:ILE:HG21	1:94:A:CYS:H	12	0.15	0.03	0.16
(1,1122)	1:91:A:ILE:HG22	1:94:A:CYS:H	12	0.15	0.03	0.16
(1,1122)	1:91:A:ILE:HG23	1:94:A:CYS:H	12	0.15	0.03	0.16
(1,3697)	1:101:A:GLY:HA2	1:102:A:GLN:HG3	12	0.15	0.03	0.14
(1,596)	1:95:A:ASN:HB3	1:95:A:ASN:H	12	0.14	0.02	0.15
(1,1182)	1:126:A:LEU:HD11	1:127:A:ILE:H	12	0.13	0.02	0.12
(1,1182)	1:126:A:LEU:HD12	1:127:A:ILE:H	12	0.13	0.02	0.12
(1,1182)	1:126:A:LEU:HD13	1:127:A:ILE:H	12	0.13	0.02	0.12
(1,1182)	1:126:A:LEU:HD21	1:127:A:ILE:H	12	0.13	0.02	0.12
(1,1182)	1:126:A:LEU:HD22	1:127:A:ILE:H	12	0.13	0.02	0.12
(1,1182)	1:126:A:LEU:HD23	1:127:A:ILE:H	12	0.13	0.02	0.12
(1,1482)	1:28:A:ASN:H	1:27:A:ILE:HA	12	0.11	0.01	0.11
(1,396)	1:39:A:ALA:HA	1:8:A:ILE:H	11	0.55	0.13	0.56
(1,2954)	1:9:A:ASP:HB3	1:20:A:ALA:HB1	11	0.34	0.13	0.36
(1,2954)	1:9:A:ASP:HB3	1:20:A:ALA:HB2	11	0.34	0.13	0.36
(1,2954)	1:9:A:ASP:HB3	1:20:A:ALA:HB3	11	0.34	0.13	0.36
(1,2954)	1:23:A:LYS:HE2	1:20:A:ALA:HB1	11	0.34	0.13	0.36
(1,2954)	1:23:A:LYS:HE2	1:20:A:ALA:HB2	11	0.34	0.13	0.36
(1,2954)	1:23:A:LYS:HE2	1:20:A:ALA:HB3	11	0.34	0.13	0.36
(1,3875)	1:55:A:LEU:HB3	1:8:A:ILE:HG12	11	0.33	0.22	0.21
(1,3875)	1:55:A:LEU:HB3	1:8:A:ILE:HG13	11	0.33	0.22	0.21
(1,3875)	1:35:A:GLN:HB2	1:8:A:ILE:HG12	11	0.33	0.22	0.21
(1,3875)	1:35:A:GLN:HB2	1:8:A:ILE:HG13	11	0.33	0.22	0.21
(1,2145)	1:2:A:SER:HB2	1:3:A:VAL:HB	11	0.29	0.13	0.25
(1,2145)	1:37:A:ALA:HA	1:3:A:VAL:HB	11	0.29	0.13	0.25
(1,1388)	1:103:A:LEU:HA	1:107:A:SER:HB3	11	0.25	0.06	0.25
(1,1222)	1:63:A:GLY:HA3	1:63:A:GLY:H	11	0.13	0.01	0.13
(1,2373)	1:55:A:LEU:HA	1:59:A:LEU:HD21	10	0.21	0.09	0.18
(1,2373)	1:55:A:LEU:HA	1:59:A:LEU:HD22	10	0.21	0.09	0.18
(1,2373)	1:55:A:LEU:HA	1:59:A:LEU:HD23	10	0.21	0.09	0.18
(1,823)	1:70:A:LYS:HG2	1:69:A:GLY:H	10	0.19	0.04	0.2
(1,823)	1:70:A:LYS:HG3	1:69:A:GLY:H	10	0.19	0.04	0.2
(1,2641)	1:123:A:ASP:H	1:113:A:ALA:HB1	10	0.17	0.03	0.18
(1,2641)	1:123:A:ASP:H	1:113:A:ALA:HB2	10	0.17	0.03	0.18
(1,2641)	1:123:A:ASP:H	1:113:A:ALA:HB3	10	0.17	0.03	0.18
(1,2641)	1:115:A:GLY:H	1:113:A:ALA:HB1	10	0.17	0.03	0.18
(1,2641)	1:115:A:GLY:H	1:113:A:ALA:HB2	10	0.17	0.03	0.18
(1,2641)	1:115:A:GLY:H	1:113:A:ALA:HB3	10	0.17	0.03	0.18
(1,1004)	1:59:A:LEU:HD21	1:16:A:SER:H	10	0.16	0.05	0.15
(1,1004)	1:59:A:LEU:HD22	1:16:A:SER:H	10	0.16	0.05	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1004)	1:59:A:LEU:HD23	1:16:A:SER:H	10	0.16	0.05	0.15
(1,1004)	1:59:A:LEU:HD11	1:16:A:SER:H	10	0.16	0.05	0.15
(1,1004)	1:59:A:LEU:HD12	1:16:A:SER:H	10	0.16	0.05	0.15
(1,1004)	1:59:A:LEU:HD13	1:16:A:SER:H	10	0.16	0.05	0.15
(1,2979)	1:57:A:MET:HE1	1:53:A:ALA:HB1	10	0.12	0.01	0.11
(1,2979)	1:57:A:MET:HE1	1:53:A:ALA:HB2	10	0.12	0.01	0.11
(1,2979)	1:57:A:MET:HE1	1:53:A:ALA:HB3	10	0.12	0.01	0.11
(1,2979)	1:57:A:MET:HE2	1:53:A:ALA:HB1	10	0.12	0.01	0.11
(1,2979)	1:57:A:MET:HE2	1:53:A:ALA:HB2	10	0.12	0.01	0.11
(1,2979)	1:57:A:MET:HE2	1:53:A:ALA:HB3	10	0.12	0.01	0.11
(1,2979)	1:57:A:MET:HE3	1:53:A:ALA:HB1	10	0.12	0.01	0.11
(1,2979)	1:57:A:MET:HE3	1:53:A:ALA:HB2	10	0.12	0.01	0.11
(1,2979)	1:57:A:MET:HE3	1:53:A:ALA:HB3	10	0.12	0.01	0.11
(1,2239)	1:104:A:SER:HA	1:102:A:GLN:HB2	9	0.55	0.06	0.56
(1,2239)	1:104:A:SER:HA	1:102:A:GLN:HB3	9	0.55	0.06	0.56
(1,572)	1:9:A:ASP:HB3	1:20:A:ALA:H	9	0.36	0.2	0.3
(1,2874)	1:19:A:TYR:HD1	1:20:A:ALA:HB1	9	0.34	0.1	0.31
(1,2874)	1:19:A:TYR:HD1	1:20:A:ALA:HB2	9	0.34	0.1	0.31
(1,2874)	1:19:A:TYR:HD1	1:20:A:ALA:HB3	9	0.34	0.1	0.31
(1,2874)	1:19:A:TYR:HD2	1:20:A:ALA:HB1	9	0.34	0.1	0.31
(1,2874)	1:19:A:TYR:HD2	1:20:A:ALA:HB2	9	0.34	0.1	0.31
(1,2874)	1:19:A:TYR:HD2	1:20:A:ALA:HB3	9	0.34	0.1	0.31
(1,925)	1:59:A:LEU:HD11	1:59:A:LEU:H	9	0.31	0.07	0.32
(1,925)	1:59:A:LEU:HD12	1:59:A:LEU:H	9	0.31	0.07	0.32
(1,925)	1:59:A:LEU:HD13	1:59:A:LEU:H	9	0.31	0.07	0.32
(1,3274)	1:73:A:ILE:HA	1:72:A:ARG:HD2	9	0.28	0.16	0.19
(1,3274)	1:106:A:ALA:HA	1:72:A:ARG:HD2	9	0.28	0.16	0.19
(1,3274)	1:43:A:GLY:HA2	1:72:A:ARG:HD2	9	0.28	0.16	0.19
(1,760)	1:97:A:ILE:HB	1:96:A:HIS:H	9	0.2	0.1	0.17
(1,2456)	1:23:A:LYS:H	1:52:A:LEU:HD11	9	0.2	0.09	0.16
(1,2456)	1:23:A:LYS:H	1:52:A:LEU:HD12	9	0.2	0.09	0.16
(1,2456)	1:23:A:LYS:H	1:52:A:LEU:HD13	9	0.2	0.09	0.16
(1,3164)	1:123:A:ASP:HB2	1:93:A:ILE:HD11	9	0.18	0.07	0.15
(1,3164)	1:123:A:ASP:HB2	1:93:A:ILE:HD12	9	0.18	0.07	0.15
(1,3164)	1:123:A:ASP:HB2	1:93:A:ILE:HD13	9	0.18	0.07	0.15
(1,3623)	1:135:A:ILE:HG12	1:134:A:ARG:HA	9	0.18	0.05	0.17
(1,2713)	1:80:A:ASP:HA	1:79:A:ILE:HG21	9	0.17	0.04	0.16
(1,2713)	1:80:A:ASP:HA	1:79:A:ILE:HG22	9	0.17	0.04	0.16
(1,2713)	1:80:A:ASP:HA	1:79:A:ILE:HG23	9	0.17	0.04	0.16
(1,741)	1:59:A:LEU:HB3	1:59:A:LEU:H	9	0.15	0.01	0.15
(1,1451)	1:119:A:ILE:HG21	1:93:A:ILE:HD11	9	0.14	0.03	0.13
(1,1451)	1:119:A:ILE:HG21	1:93:A:ILE:HD12	9	0.14	0.03	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1451)	1:119:A:ILE:HG21	1:93:A:ILE:HD13	9	0.14	0.03	0.13
(1,1451)	1:119:A:ILE:HG22	1:93:A:ILE:HD11	9	0.14	0.03	0.13
(1,1451)	1:119:A:ILE:HG22	1:93:A:ILE:HD12	9	0.14	0.03	0.13
(1,1451)	1:119:A:ILE:HG22	1:93:A:ILE:HD13	9	0.14	0.03	0.13
(1,1451)	1:119:A:ILE:HG23	1:93:A:ILE:HD11	9	0.14	0.03	0.13
(1,1451)	1:119:A:ILE:HG23	1:93:A:ILE:HD12	9	0.14	0.03	0.13
(1,1451)	1:119:A:ILE:HG23	1:93:A:ILE:HD13	9	0.14	0.03	0.13
(1,2652)	1:80:A:ASP:H	1:79:A:ILE:HG21	9	0.14	0.04	0.13
(1,2652)	1:80:A:ASP:H	1:79:A:ILE:HG22	9	0.14	0.04	0.13
(1,2652)	1:80:A:ASP:H	1:79:A:ILE:HG23	9	0.14	0.04	0.13
(1,2682)	1:38:A:ALA:H	1:3:A:VAL:HG11	9	0.13	0.02	0.13
(1,2682)	1:38:A:ALA:H	1:3:A:VAL:HG12	9	0.13	0.02	0.13
(1,2682)	1:38:A:ALA:H	1:3:A:VAL:HG13	9	0.13	0.02	0.13
(1,250)	1:102:A:GLN:HE22	1:101:A:GLY:H	9	0.12	0.01	0.12
(1,380)	1:61:A:GLY:HA3	1:61:A:GLY:H	9	0.11	0.01	0.11
(1,3696)	1:108:A:LEU:HD21	1:102:A:GLN:HG3	8	0.3	0.09	0.29
(1,3696)	1:108:A:LEU:HD22	1:102:A:GLN:HG3	8	0.3	0.09	0.29
(1,3696)	1:108:A:LEU:HD23	1:102:A:GLN:HG3	8	0.3	0.09	0.29
(1,3696)	1:108:A:LEU:HD11	1:102:A:GLN:HG3	8	0.3	0.09	0.29
(1,3696)	1:108:A:LEU:HD12	1:102:A:GLN:HG3	8	0.3	0.09	0.29
(1,3696)	1:108:A:LEU:HD13	1:102:A:GLN:HG3	8	0.3	0.09	0.29
(1,3758)	1:102:A:GLN:HG3	1:108:A:LEU:HD21	8	0.3	0.09	0.29
(1,3758)	1:102:A:GLN:HG3	1:108:A:LEU:HD22	8	0.3	0.09	0.29
(1,3758)	1:102:A:GLN:HG3	1:108:A:LEU:HD23	8	0.3	0.09	0.29
(1,3758)	1:102:A:GLN:HG3	1:108:A:LEU:HD11	8	0.3	0.09	0.29
(1,3758)	1:102:A:GLN:HG3	1:108:A:LEU:HD12	8	0.3	0.09	0.29
(1,3758)	1:102:A:GLN:HG3	1:108:A:LEU:HD13	8	0.3	0.09	0.29
(1,97)	1:144:A:LEU:H	1:143:A:GLN:H	8	0.29	0.08	0.29
(1,3074)	1:4:A:LYS:HB2	1:71:A:ASN:HA	8	0.25	0.06	0.26
(1,3074)	1:72:A:ARG:HB2	1:71:A:ASN:HA	8	0.25	0.06	0.26
(1,2830)	1:65:A:THR:H	1:54:A:ILE:HG21	8	0.24	0.09	0.24
(1,2830)	1:65:A:THR:H	1:54:A:ILE:HG22	8	0.24	0.09	0.24
(1,2830)	1:65:A:THR:H	1:54:A:ILE:HG23	8	0.24	0.09	0.24
(1,2830)	1:66:A:SER:H	1:54:A:ILE:HG21	8	0.24	0.09	0.24
(1,2830)	1:66:A:SER:H	1:54:A:ILE:HG22	8	0.24	0.09	0.24
(1,2830)	1:66:A:SER:H	1:54:A:ILE:HG23	8	0.24	0.09	0.24
(1,3712)	1:130:A:TYR:HE1	1:137:A:HIS:HB3	8	0.23	0.06	0.23
(1,3712)	1:130:A:TYR:HE2	1:137:A:HIS:HB3	8	0.23	0.06	0.23
(1,933)	1:52:A:LEU:HD21	1:26:A:LEU:H	8	0.2	0.05	0.2
(1,933)	1:52:A:LEU:HD22	1:26:A:LEU:H	8	0.2	0.05	0.2
(1,933)	1:52:A:LEU:HD23	1:26:A:LEU:H	8	0.2	0.05	0.2
(1,933)	1:47:A:VAL:HG11	1:26:A:LEU:H	8	0.2	0.05	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,933)	1:47:A:VAL:HG12	1:26:A:LEU:H	8	0.2	0.05	0.2
(1,933)	1:47:A:VAL:HG13	1:26:A:LEU:H	8	0.2	0.05	0.2
(1,1149)	1:135:A:ILE:HG12	1:129:A:LYS:H	8	0.19	0.05	0.2
(1,2752)	1:35:A:GLN:HB2	1:32:A:THR:HG21	8	0.19	0.07	0.17
(1,2752)	1:35:A:GLN:HB2	1:32:A:THR:HG22	8	0.19	0.07	0.17
(1,2752)	1:35:A:GLN:HB2	1:32:A:THR:HG23	8	0.19	0.07	0.17
(1,2752)	1:57:A:MET:HB3	1:65:A:THR:HG21	8	0.19	0.07	0.17
(1,2752)	1:57:A:MET:HB3	1:65:A:THR:HG22	8	0.19	0.07	0.17
(1,2752)	1:57:A:MET:HB3	1:65:A:THR:HG23	8	0.19	0.07	0.17
(1,772)	1:20:A:ALA:HB1	1:23:A:LYS:H	8	0.17	0.04	0.18
(1,772)	1:20:A:ALA:HB2	1:23:A:LYS:H	8	0.17	0.04	0.18
(1,772)	1:20:A:ALA:HB3	1:23:A:LYS:H	8	0.17	0.04	0.18
(1,772)	1:23:A:LYS:HD2	1:23:A:LYS:H	8	0.17	0.04	0.18
(1,1534)	1:20:A:ALA:HB1	1:17:A:ILE:HA	8	0.17	0.05	0.18
(1,1534)	1:20:A:ALA:HB2	1:17:A:ILE:HA	8	0.17	0.05	0.18
(1,1534)	1:20:A:ALA:HB3	1:17:A:ILE:HA	8	0.17	0.05	0.18
(1,1534)	1:17:A:ILE:HB	1:17:A:ILE:HA	8	0.17	0.05	0.18
(1,1177)	1:92:A:LEU:HD21	1:89:A:ASP:H	8	0.15	0.03	0.15
(1,1177)	1:92:A:LEU:HD22	1:89:A:ASP:H	8	0.15	0.03	0.15
(1,1177)	1:92:A:LEU:HD23	1:89:A:ASP:H	8	0.15	0.03	0.15
(1,1177)	1:92:A:LEU:HD11	1:89:A:ASP:H	8	0.15	0.03	0.15
(1,1177)	1:92:A:LEU:HD12	1:89:A:ASP:H	8	0.15	0.03	0.15
(1,1177)	1:92:A:LEU:HD13	1:89:A:ASP:H	8	0.15	0.03	0.15
(1,1177)	1:79:A:ILE:HD11	1:89:A:ASP:H	8	0.15	0.03	0.15
(1,1177)	1:79:A:ILE:HD12	1:89:A:ASP:H	8	0.15	0.03	0.15
(1,1177)	1:79:A:ILE:HD13	1:89:A:ASP:H	8	0.15	0.03	0.15
(1,1260)	1:51:A:ASP:H	1:41:A:VAL:H	8	0.13	0.02	0.12
(1,3520)	1:127:A:ILE:HD11	1:126:A:LEU:HB2	8	0.12	0.01	0.11
(1,3520)	1:127:A:ILE:HD12	1:126:A:LEU:HB2	8	0.12	0.01	0.11
(1,3520)	1:127:A:ILE:HD13	1:126:A:LEU:HB2	8	0.12	0.01	0.11
(1,3019)	1:54:A:ILE:HA	1:65:A:THR:HB	7	0.33	0.15	0.29
(1,3019)	1:63:A:GLY:HA2	1:65:A:THR:HB	7	0.33	0.15	0.29
(1,579)	1:142:A:ASN:HB3	1:143:A:GLN:H	7	0.28	0.1	0.32
(1,3943)	1:22:A:LEU:HD21	1:19:A:TYR:HD1	7	0.28	0.12	0.31
(1,3943)	1:22:A:LEU:HD21	1:19:A:TYR:HD2	7	0.28	0.12	0.31
(1,3943)	1:22:A:LEU:HD22	1:19:A:TYR:HD1	7	0.28	0.12	0.31
(1,3943)	1:22:A:LEU:HD22	1:19:A:TYR:HD2	7	0.28	0.12	0.31
(1,3943)	1:22:A:LEU:HD23	1:19:A:TYR:HD1	7	0.28	0.12	0.31
(1,3943)	1:22:A:LEU:HD23	1:19:A:TYR:HD2	7	0.28	0.12	0.31
(1,3943)	1:59:A:LEU:HD21	1:19:A:TYR:HD1	7	0.28	0.12	0.31
(1,3943)	1:59:A:LEU:HD21	1:19:A:TYR:HD2	7	0.28	0.12	0.31
(1,3943)	1:59:A:LEU:HD22	1:19:A:TYR:HD1	7	0.28	0.12	0.31

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3943)	1:59:A:LEU:HD22	1:19:A:TYR:HD2	7	0.28	0.12	0.31
(1,3943)	1:59:A:LEU:HD23	1:19:A:TYR:HD1	7	0.28	0.12	0.31
(1,3943)	1:59:A:LEU:HD23	1:19:A:TYR:HD2	7	0.28	0.12	0.31
(1,3937)	1:20:A:ALA:HB1	1:19:A:TYR:HD1	7	0.25	0.05	0.26
(1,3937)	1:20:A:ALA:HB1	1:19:A:TYR:HD2	7	0.25	0.05	0.26
(1,3937)	1:20:A:ALA:HB2	1:19:A:TYR:HD1	7	0.25	0.05	0.26
(1,3937)	1:20:A:ALA:HB2	1:19:A:TYR:HD2	7	0.25	0.05	0.26
(1,3937)	1:20:A:ALA:HB3	1:19:A:TYR:HD1	7	0.25	0.05	0.26
(1,3937)	1:20:A:ALA:HB3	1:19:A:TYR:HD2	7	0.25	0.05	0.26
(1,3937)	1:23:A:LYS:HD2	1:19:A:TYR:HD1	7	0.25	0.05	0.26
(1,3937)	1:23:A:LYS:HD2	1:19:A:TYR:HD2	7	0.25	0.05	0.26
(1,1859)	1:27:A:ILE:HD11	1:23:A:LYS:HE2	7	0.2	0.06	0.21
(1,1859)	1:27:A:ILE:HD12	1:23:A:LYS:HE2	7	0.2	0.06	0.21
(1,1859)	1:27:A:ILE:HD13	1:23:A:LYS:HE2	7	0.2	0.06	0.21
(1,1859)	1:60:A:LEU:HD21	1:62:A:LYS:HE2	7	0.2	0.06	0.21
(1,1859)	1:60:A:LEU:HD22	1:62:A:LYS:HE2	7	0.2	0.06	0.21
(1,1859)	1:60:A:LEU:HD23	1:62:A:LYS:HE2	7	0.2	0.06	0.21
(1,3177)	1:129:A:LYS:HE2	1:135:A:ILE:HD11	7	0.19	0.06	0.17
(1,3177)	1:129:A:LYS:HE2	1:135:A:ILE:HD12	7	0.19	0.06	0.17
(1,3177)	1:129:A:LYS:HE2	1:135:A:ILE:HD13	7	0.19	0.06	0.17
(1,3177)	1:129:A:LYS:HE3	1:135:A:ILE:HD11	7	0.19	0.06	0.17
(1,3177)	1:129:A:LYS:HE3	1:135:A:ILE:HD12	7	0.19	0.06	0.17
(1,3177)	1:129:A:LYS:HE3	1:135:A:ILE:HD13	7	0.19	0.06	0.17
(1,2829)	1:59:A:LEU:H	1:14:A:ILE:HG21	7	0.17	0.03	0.19
(1,2829)	1:59:A:LEU:H	1:14:A:ILE:HG22	7	0.17	0.03	0.19
(1,2829)	1:59:A:LEU:H	1:14:A:ILE:HG23	7	0.17	0.03	0.19
(1,2664)	1:52:A:LEU:H	1:41:A:VAL:HG21	7	0.13	0.03	0.12
(1,2664)	1:52:A:LEU:H	1:41:A:VAL:HG22	7	0.13	0.03	0.12
(1,2664)	1:52:A:LEU:H	1:41:A:VAL:HG23	7	0.13	0.03	0.12
(1,939)	1:91:A:ILE:HD11	1:91:A:ILE:H	7	0.12	0.02	0.12
(1,939)	1:91:A:ILE:HD12	1:91:A:ILE:H	7	0.12	0.02	0.12
(1,939)	1:91:A:ILE:HD13	1:91:A:ILE:H	7	0.12	0.02	0.12
(1,3707)	1:71:A:ASN:HA	1:72:A:ARG:HB2	7	0.11	0.01	0.11
(1,1056)	1:122:A:THR:HG21	1:114:A:ASP:H	6	0.35	0.14	0.4
(1,1056)	1:122:A:THR:HG22	1:114:A:ASP:H	6	0.35	0.14	0.4
(1,1056)	1:122:A:THR:HG23	1:114:A:ASP:H	6	0.35	0.14	0.4
(1,1792)	1:132:A:THR:H	1:134:A:ARG:HD2	6	0.27	0.09	0.28
(1,1792)	1:132:A:THR:H	1:134:A:ARG:HD3	6	0.27	0.09	0.28
(1,1792)	1:133:A:GLY:H	1:134:A:ARG:HD2	6	0.27	0.09	0.28
(1,1792)	1:133:A:GLY:H	1:134:A:ARG:HD3	6	0.27	0.09	0.28
(1,3791)	1:132:A:THR:H	1:134:A:ARG:HD2	6	0.27	0.09	0.28
(1,3791)	1:132:A:THR:H	1:134:A:ARG:HD3	6	0.27	0.09	0.28

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3791)	1:133:A:GLY:H	1:134:A:ARG:HD2	6	0.27	0.09	0.28
(1,3791)	1:133:A:GLY:H	1:134:A:ARG:HD3	6	0.27	0.09	0.28
(1,3805)	1:125:A:ILE:HG12	1:128:A:GLU:HG2	6	0.27	0.09	0.28
(1,3805)	1:125:A:ILE:HG12	1:128:A:GLU:HG3	6	0.27	0.09	0.28
(1,1024)	1:118:A:VAL:HG21	1:116:A:ASN:HD21	6	0.23	0.05	0.25
(1,1024)	1:118:A:VAL:HG22	1:116:A:ASN:HD21	6	0.23	0.05	0.25
(1,1024)	1:118:A:VAL:HG23	1:116:A:ASN:HD21	6	0.23	0.05	0.25
(1,3336)	1:126:A:LEU:HD11	1:139:A:PRO:HB3	6	0.23	0.06	0.24
(1,3336)	1:126:A:LEU:HD12	1:139:A:PRO:HB3	6	0.23	0.06	0.24
(1,3336)	1:126:A:LEU:HD13	1:139:A:PRO:HB3	6	0.23	0.06	0.24
(1,1549)	1:70:A:LYS:HB2	1:5:A:ILE:HD11	6	0.22	0.1	0.18
(1,1549)	1:70:A:LYS:HB2	1:5:A:ILE:HD12	6	0.22	0.1	0.18
(1,1549)	1:70:A:LYS:HB2	1:5:A:ILE:HD13	6	0.22	0.1	0.18
(1,1841)	1:62:A:LYS:HB3	1:62:A:LYS:HE3	6	0.19	0.04	0.2
(1,2550)	1:40:A:ASP:HB3	1:47:A:VAL:HG11	6	0.19	0.05	0.18
(1,2550)	1:40:A:ASP:HB3	1:47:A:VAL:HG12	6	0.19	0.05	0.18
(1,2550)	1:40:A:ASP:HB3	1:47:A:VAL:HG13	6	0.19	0.05	0.18
(1,2603)	1:26:A:LEU:HD11	1:22:A:LEU:HD21	6	0.19	0.05	0.19
(1,2603)	1:26:A:LEU:HD11	1:22:A:LEU:HD22	6	0.19	0.05	0.19
(1,2603)	1:26:A:LEU:HD11	1:22:A:LEU:HD23	6	0.19	0.05	0.19
(1,2603)	1:26:A:LEU:HD12	1:22:A:LEU:HD21	6	0.19	0.05	0.19
(1,2603)	1:26:A:LEU:HD12	1:22:A:LEU:HD22	6	0.19	0.05	0.19
(1,2603)	1:26:A:LEU:HD12	1:22:A:LEU:HD23	6	0.19	0.05	0.19
(1,2603)	1:26:A:LEU:HD13	1:22:A:LEU:HD21	6	0.19	0.05	0.19
(1,2603)	1:26:A:LEU:HD13	1:22:A:LEU:HD22	6	0.19	0.05	0.19
(1,2603)	1:26:A:LEU:HD13	1:22:A:LEU:HD23	6	0.19	0.05	0.19
(1,2449)	1:130:A:TYR:H	1:126:A:LEU:HD21	6	0.18	0.05	0.16
(1,2449)	1:130:A:TYR:H	1:126:A:LEU:HD22	6	0.18	0.05	0.16
(1,2449)	1:130:A:TYR:H	1:126:A:LEU:HD23	6	0.18	0.05	0.16
(1,2449)	1:59:A:LEU:H	1:60:A:LEU:HD21	6	0.18	0.05	0.16
(1,2449)	1:59:A:LEU:H	1:60:A:LEU:HD22	6	0.18	0.05	0.16
(1,2449)	1:59:A:LEU:H	1:60:A:LEU:HD23	6	0.18	0.05	0.16
(1,2215)	1:9:A:ASP:H	1:8:A:ILE:HG12	6	0.17	0.04	0.17
(1,2215)	1:9:A:ASP:H	1:8:A:ILE:HG13	6	0.17	0.04	0.17
(1,978)	1:131:A:ILE:HD11	1:131:A:ILE:H	6	0.16	0.03	0.16
(1,978)	1:131:A:ILE:HD12	1:131:A:ILE:H	6	0.16	0.03	0.16
(1,978)	1:131:A:ILE:HD13	1:131:A:ILE:H	6	0.16	0.03	0.16
(1,3263)	1:5:A:ILE:HG21	1:6:A:GLY:HA2	6	0.12	0.02	0.12
(1,3263)	1:5:A:ILE:HG22	1:6:A:GLY:HA2	6	0.12	0.02	0.12
(1,3263)	1:5:A:ILE:HG23	1:6:A:GLY:HA2	6	0.12	0.02	0.12
(1,1321)	1:23:A:LYS:HB3	1:23:A:LYS:H	6	0.12	0.01	0.12
(1,1639)	1:23:A:LYS:HD2	1:23:A:LYS:HA	6	0.12	0.01	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1225)	1:110:A:ALA:HA	1:76:A:TYR:H	5	0.37	0.1	0.38
(1,694)	1:9:A:ASP:HB3	1:35:A:GLN:HE22	5	0.31	0.07	0.35
(1,2277)	1:93:A:ILE:HB	1:127:A:ILE:HG12	5	0.21	0.1	0.21
(1,2277)	1:93:A:ILE:HB	1:127:A:ILE:HG13	5	0.21	0.1	0.21
(1,1141)	1:144:A:LEU:HG	1:143:A:GLN:H	5	0.18	0.03	0.18
(1,3212)	1:53:A:ALA:HB1	1:49:A:SER:HB2	5	0.18	0.06	0.16
(1,3212)	1:53:A:ALA:HB1	1:49:A:SER:HB3	5	0.18	0.06	0.16
(1,3212)	1:53:A:ALA:HB2	1:49:A:SER:HB2	5	0.18	0.06	0.16
(1,3212)	1:53:A:ALA:HB2	1:49:A:SER:HB3	5	0.18	0.06	0.16
(1,3212)	1:53:A:ALA:HB3	1:49:A:SER:HB2	5	0.18	0.06	0.16
(1,3212)	1:53:A:ALA:HB3	1:49:A:SER:HB3	5	0.18	0.06	0.16
(1,2509)	1:49:A:SER:HB2	1:52:A:LEU:HD11	5	0.15	0.02	0.16
(1,2509)	1:49:A:SER:HB2	1:52:A:LEU:HD12	5	0.15	0.02	0.16
(1,2509)	1:49:A:SER:HB2	1:52:A:LEU:HD13	5	0.15	0.02	0.16
(1,2509)	1:49:A:SER:HB3	1:52:A:LEU:HD11	5	0.15	0.02	0.16
(1,2509)	1:49:A:SER:HB3	1:52:A:LEU:HD12	5	0.15	0.02	0.16
(1,2509)	1:49:A:SER:HB3	1:52:A:LEU:HD13	5	0.15	0.02	0.16
(1,2509)	1:52:A:LEU:HA	1:52:A:LEU:HD11	5	0.15	0.02	0.16
(1,2509)	1:52:A:LEU:HA	1:52:A:LEU:HD12	5	0.15	0.02	0.16
(1,2509)	1:52:A:LEU:HA	1:52:A:LEU:HD13	5	0.15	0.02	0.16
(1,1840)	1:62:A:LYS:HB3	1:62:A:LYS:HE2	5	0.14	0.02	0.13
(1,1840)	1:57:A:MET:HE1	1:62:A:LYS:HE2	5	0.14	0.02	0.13
(1,1840)	1:57:A:MET:HE2	1:62:A:LYS:HE2	5	0.14	0.02	0.13
(1,1840)	1:57:A:MET:HE3	1:62:A:LYS:HE2	5	0.14	0.02	0.13
(1,3096)	1:79:A:ILE:HG21	1:80:A:ASP:HA	5	0.13	0.02	0.14
(1,3096)	1:79:A:ILE:HG22	1:80:A:ASP:HA	5	0.13	0.02	0.14
(1,3096)	1:79:A:ILE:HG23	1:80:A:ASP:HA	5	0.13	0.02	0.14
(1,3096)	1:92:A:LEU:HD21	1:80:A:ASP:HA	5	0.13	0.02	0.14
(1,3096)	1:92:A:LEU:HD22	1:80:A:ASP:HA	5	0.13	0.02	0.14
(1,3096)	1:92:A:LEU:HD23	1:80:A:ASP:HA	5	0.13	0.02	0.14
(1,1502)	1:26:A:LEU:HA	1:27:A:ILE:HA	5	0.13	0.03	0.11
(1,2763)	1:34:A:LYS:HE3	1:3:A:VAL:HG11	5	0.13	0.01	0.13
(1,2763)	1:34:A:LYS:HE3	1:3:A:VAL:HG12	5	0.13	0.01	0.13
(1,2763)	1:34:A:LYS:HE3	1:3:A:VAL:HG13	5	0.13	0.01	0.13
(1,3030)	1:58:A:TYR:H	1:57:A:MET:HE1	5	0.13	0.02	0.12
(1,3030)	1:58:A:TYR:H	1:57:A:MET:HE2	5	0.13	0.02	0.12
(1,3030)	1:58:A:TYR:H	1:57:A:MET:HE3	5	0.13	0.02	0.12
(1,391)	1:72:A:ARG:HD2	1:73:A:ILE:H	5	0.12	0.02	0.11
(1,2747)	1:72:A:ARG:HD2	1:3:A:VAL:HG11	4	0.43	0.16	0.42
(1,2747)	1:72:A:ARG:HD2	1:3:A:VAL:HG12	4	0.43	0.16	0.42
(1,2747)	1:72:A:ARG:HD2	1:3:A:VAL:HG13	4	0.43	0.16	0.42
(1,3812)	1:70:A:LYS:HA	1:4:A:LYS:HD2	4	0.39	0.14	0.44

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3812)	1:12:A:GLY:HA3	1:4:A:LYS:HD2	4	0.39	0.14	0.44
(1,2120)	1:74:A:TYR:HE1	1:72:A:ARG:HB2	4	0.3	0.06	0.32
(1,2120)	1:74:A:TYR:HE2	1:72:A:ARG:HB2	4	0.3	0.06	0.32
(1,2120)	1:81:A:ASN:HD22	1:72:A:ARG:HB2	4	0.3	0.06	0.32
(1,2367)	1:72:A:ARG:HA	1:73:A:ILE:HG12	4	0.26	0.1	0.26
(1,2367)	1:2:A:SER:HA	1:73:A:ILE:HG12	4	0.26	0.1	0.26
(1,2287)	1:119:A:ILE:HG21	1:93:A:ILE:HG13	4	0.26	0.11	0.22
(1,2287)	1:119:A:ILE:HG22	1:93:A:ILE:HG13	4	0.26	0.11	0.22
(1,2287)	1:119:A:ILE:HG23	1:93:A:ILE:HG13	4	0.26	0.11	0.22
(1,1115)	1:55:A:LEU:HD21	1:8:A:ILE:H	4	0.24	0.11	0.24
(1,1115)	1:55:A:LEU:HD22	1:8:A:ILE:H	4	0.24	0.11	0.24
(1,1115)	1:55:A:LEU:HD23	1:8:A:ILE:H	4	0.24	0.11	0.24
(1,871)	1:52:A:LEU:HG	1:56:A:GLN:HE22	4	0.21	0.06	0.24
(1,1843)	1:24:A:SER:HB2	1:23:A:LYS:HE2	4	0.2	0.06	0.18
(1,1843)	1:24:A:SER:HB3	1:23:A:LYS:HE2	4	0.2	0.06	0.18
(1,1843)	1:57:A:MET:HA	1:62:A:LYS:HE2	4	0.2	0.06	0.18
(1,746)	1:144:A:LEU:HG	1:144:A:LEU:H	4	0.19	0.03	0.2
(1,2260)	1:124:A:ARG:HA	1:127:A:ILE:HG12	4	0.18	0.08	0.14
(1,2260)	1:124:A:ARG:HA	1:127:A:ILE:HG13	4	0.18	0.08	0.14
(1,2260)	1:111:A:ALA:HA	1:127:A:ILE:HG12	4	0.18	0.08	0.14
(1,2260)	1:111:A:ALA:HA	1:127:A:ILE:HG13	4	0.18	0.08	0.14
(1,1140)	1:144:A:LEU:HD21	1:143:A:GLN:H	4	0.17	0.03	0.16
(1,1140)	1:144:A:LEU:HD22	1:143:A:GLN:H	4	0.17	0.03	0.16
(1,1140)	1:144:A:LEU:HD23	1:143:A:GLN:H	4	0.17	0.03	0.16
(1,2455)	1:143:A:GLN:H	1:144:A:LEU:HD21	4	0.17	0.03	0.16
(1,2455)	1:143:A:GLN:H	1:144:A:LEU:HD22	4	0.17	0.03	0.16
(1,2455)	1:143:A:GLN:H	1:144:A:LEU:HD23	4	0.17	0.03	0.16
(1,948)	1:5:A:ILE:HG21	1:70:A:LYS:H	4	0.16	0.01	0.16
(1,948)	1:5:A:ILE:HG22	1:70:A:LYS:H	4	0.16	0.01	0.16
(1,948)	1:5:A:ILE:HG23	1:70:A:LYS:H	4	0.16	0.01	0.16
(1,1651)	1:59:A:LEU:HD21	1:56:A:GLN:HA	4	0.15	0.02	0.16
(1,1651)	1:59:A:LEU:HD22	1:56:A:GLN:HA	4	0.15	0.02	0.16
(1,1651)	1:59:A:LEU:HD23	1:56:A:GLN:HA	4	0.15	0.02	0.16
(1,1651)	1:60:A:LEU:HD11	1:56:A:GLN:HA	4	0.15	0.02	0.16
(1,1651)	1:60:A:LEU:HD12	1:56:A:GLN:HA	4	0.15	0.02	0.16
(1,1651)	1:60:A:LEU:HD13	1:56:A:GLN:HA	4	0.15	0.02	0.16
(1,1417)	1:94:A:CYS:HB3	1:91:A:ILE:HA	4	0.14	0.01	0.14
(1,753)	1:129:A:LYS:HD2	1:128:A:GLU:H	4	0.14	0.01	0.14
(1,753)	1:129:A:LYS:HD3	1:128:A:GLU:H	4	0.14	0.01	0.14
(1,753)	1:124:A:ARG:HB2	1:128:A:GLU:H	4	0.14	0.01	0.14
(1,753)	1:124:A:ARG:HB3	1:128:A:GLU:H	4	0.14	0.01	0.14
(1,1205)	1:97:A:ILE:HD11	1:98:A:ASN:H	4	0.13	0.02	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1205)	1:97:A:ILE:HD12	1:98:A:ASN:H	4	0.13	0.02	0.13
(1,1205)	1:97:A:ILE:HD13	1:98:A:ASN:H	4	0.13	0.02	0.13
(1,1226)	1:68:A:ILE:HD11	1:58:A:TYR:H	4	0.12	0.01	0.12
(1,1226)	1:68:A:ILE:HD12	1:58:A:TYR:H	4	0.12	0.01	0.12
(1,1226)	1:68:A:ILE:HD13	1:58:A:TYR:H	4	0.12	0.01	0.12
(1,1097)	1:108:A:LEU:HD21	1:112:A:ASP:H	3	0.36	0.17	0.37
(1,1097)	1:108:A:LEU:HD22	1:112:A:ASP:H	3	0.36	0.17	0.37
(1,1097)	1:108:A:LEU:HD23	1:112:A:ASP:H	3	0.36	0.17	0.37
(1,1097)	1:103:A:LEU:HD21	1:112:A:ASP:H	3	0.36	0.17	0.37
(1,1097)	1:103:A:LEU:HD22	1:112:A:ASP:H	3	0.36	0.17	0.37
(1,1097)	1:103:A:LEU:HD23	1:112:A:ASP:H	3	0.36	0.17	0.37
(1,1780)	1:129:A:LYS:H	1:134:A:ARG:HD2	3	0.35	0.12	0.37
(1,1780)	1:129:A:LYS:H	1:134:A:ARG:HD3	3	0.35	0.12	0.37
(1,3431)	1:4:A:LYS:HG3	1:71:A:ASN:HA	3	0.31	0.13	0.25
(1,2170)	1:124:A:ARG:HB2	1:128:A:GLU:HG2	3	0.27	0.09	0.26
(1,2170)	1:124:A:ARG:HB2	1:128:A:GLU:HG3	3	0.27	0.09	0.26
(1,2170)	1:124:A:ARG:HB3	1:128:A:GLU:HG2	3	0.27	0.09	0.26
(1,2170)	1:124:A:ARG:HB3	1:128:A:GLU:HG3	3	0.27	0.09	0.26
(1,2482)	1:96:A:HIS:H	1:103:A:LEU:HD11	3	0.27	0.05	0.28
(1,2482)	1:96:A:HIS:H	1:103:A:LEU:HD12	3	0.27	0.05	0.28
(1,2482)	1:96:A:HIS:H	1:103:A:LEU:HD13	3	0.27	0.05	0.28
(1,2999)	1:50:A:ILE:HG12	1:53:A:ALA:HB1	3	0.24	0.09	0.22
(1,2999)	1:50:A:ILE:HG12	1:53:A:ALA:HB2	3	0.24	0.09	0.22
(1,2999)	1:50:A:ILE:HG12	1:53:A:ALA:HB3	3	0.24	0.09	0.22
(1,1358)	1:96:A:HIS:H	1:97:A:ILE:HD11	3	0.23	0.1	0.17
(1,1358)	1:96:A:HIS:H	1:97:A:ILE:HD12	3	0.23	0.1	0.17
(1,1358)	1:96:A:HIS:H	1:97:A:ILE:HD13	3	0.23	0.1	0.17
(1,1444)	1:41:A:VAL:HB	1:68:A:ILE:HD11	3	0.23	0.03	0.24
(1,1444)	1:41:A:VAL:HB	1:68:A:ILE:HD12	3	0.23	0.03	0.24
(1,1444)	1:41:A:VAL:HB	1:68:A:ILE:HD13	3	0.23	0.03	0.24
(1,1092)	1:103:A:LEU:HD21	1:111:A:ALA:H	3	0.22	0.08	0.26
(1,1092)	1:103:A:LEU:HD22	1:111:A:ALA:H	3	0.22	0.08	0.26
(1,1092)	1:103:A:LEU:HD23	1:111:A:ALA:H	3	0.22	0.08	0.26
(1,1822)	1:70:A:LYS:HA	1:70:A:LYS:HE2	3	0.21	0.02	0.2
(1,1822)	1:70:A:LYS:HA	1:70:A:LYS:HE3	3	0.21	0.02	0.2
(1,2472)	1:145:A:GLU:H	1:144:A:LEU:HD21	3	0.2	0.02	0.21
(1,2472)	1:145:A:GLU:H	1:144:A:LEU:HD22	3	0.2	0.02	0.21
(1,2472)	1:145:A:GLU:H	1:144:A:LEU:HD23	3	0.2	0.02	0.21
(1,2472)	1:144:A:LEU:H	1:144:A:LEU:HD21	3	0.2	0.02	0.21
(1,2472)	1:144:A:LEU:H	1:144:A:LEU:HD22	3	0.2	0.02	0.21
(1,2472)	1:144:A:LEU:H	1:144:A:LEU:HD23	3	0.2	0.02	0.21
(1,3404)	1:97:A:ILE:HA	1:119:A:ILE:HG21	3	0.2	0.1	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3404)	1:97:A:ILE:HA	1:119:A:ILE:HG22	3	0.2	0.1	0.14
(1,3404)	1:97:A:ILE:HA	1:119:A:ILE:HG23	3	0.2	0.1	0.14
(1,3404)	1:2:A:SER:HB3	1:73:A:ILE:HG21	3	0.2	0.1	0.14
(1,3404)	1:2:A:SER:HB3	1:73:A:ILE:HG22	3	0.2	0.1	0.14
(1,3404)	1:2:A:SER:HB3	1:73:A:ILE:HG23	3	0.2	0.1	0.14
(1,2182)	1:131:A:ILE:HD11	1:87:A:GLU:HG3	3	0.19	0.05	0.16
(1,2182)	1:131:A:ILE:HD12	1:87:A:GLU:HG3	3	0.19	0.05	0.16
(1,2182)	1:131:A:ILE:HD13	1:87:A:GLU:HG3	3	0.19	0.05	0.16
(1,2182)	1:131:A:ILE:HG21	1:87:A:GLU:HG3	3	0.19	0.05	0.16
(1,2182)	1:131:A:ILE:HG22	1:87:A:GLU:HG3	3	0.19	0.05	0.16
(1,2182)	1:131:A:ILE:HG23	1:87:A:GLU:HG3	3	0.19	0.05	0.16
(1,988)	1:85:A:VAL:HG21	1:78:A:ASP:H	3	0.18	0.03	0.17
(1,988)	1:85:A:VAL:HG22	1:78:A:ASP:H	3	0.18	0.03	0.17
(1,988)	1:85:A:VAL:HG23	1:78:A:ASP:H	3	0.18	0.03	0.17
(1,1768)	1:57:A:MET:HB2	1:64:A:GLY:HA2	3	0.17	0.05	0.18
(1,1768)	1:57:A:MET:HB2	1:64:A:GLY:HA3	3	0.17	0.05	0.18
(1,2560)	1:62:A:LYS:HE3	1:62:A:LYS:HG2	3	0.17	0.04	0.14
(1,2560)	1:62:A:LYS:HE2	1:62:A:LYS:HG2	3	0.17	0.04	0.14
(1,1021)	1:92:A:LEU:HD11	1:88:A:ASN:HD22	3	0.15	0.03	0.17
(1,1021)	1:92:A:LEU:HD12	1:88:A:ASN:HD22	3	0.15	0.03	0.17
(1,1021)	1:92:A:LEU:HD13	1:88:A:ASN:HD22	3	0.15	0.03	0.17
(1,1288)	1:121:A:GLN:HG2	1:122:A:THR:H	3	0.14	0.01	0.13
(1,1288)	1:121:A:GLN:HG3	1:122:A:THR:H	3	0.14	0.01	0.13
(1,2278)	1:50:A:ILE:HB	1:54:A:ILE:HG12	3	0.14	0.02	0.14
(1,2278)	1:50:A:ILE:HB	1:54:A:ILE:HG13	3	0.14	0.02	0.14
(1,2278)	1:57:A:MET:HB2	1:54:A:ILE:HG12	3	0.14	0.02	0.14
(1,2278)	1:57:A:MET:HB2	1:54:A:ILE:HG13	3	0.14	0.02	0.14
(1,2878)	1:40:A:ASP:H	1:38:A:ALA:HB1	3	0.14	0.01	0.14
(1,2878)	1:40:A:ASP:H	1:38:A:ALA:HB2	3	0.14	0.01	0.14
(1,2878)	1:40:A:ASP:H	1:38:A:ALA:HB3	3	0.14	0.01	0.14
(1,2978)	1:53:A:ALA:HB1	1:57:A:MET:HE1	3	0.13	0.02	0.14
(1,2978)	1:53:A:ALA:HB1	1:57:A:MET:HE2	3	0.13	0.02	0.14
(1,2978)	1:53:A:ALA:HB1	1:57:A:MET:HE3	3	0.13	0.02	0.14
(1,2978)	1:53:A:ALA:HB2	1:57:A:MET:HE1	3	0.13	0.02	0.14
(1,2978)	1:53:A:ALA:HB2	1:57:A:MET:HE2	3	0.13	0.02	0.14
(1,2978)	1:53:A:ALA:HB2	1:57:A:MET:HE3	3	0.13	0.02	0.14
(1,2978)	1:53:A:ALA:HB3	1:57:A:MET:HE1	3	0.13	0.02	0.14
(1,2978)	1:53:A:ALA:HB3	1:57:A:MET:HE2	3	0.13	0.02	0.14
(1,2978)	1:53:A:ALA:HB3	1:57:A:MET:HE3	3	0.13	0.02	0.14
(1,2400)	1:94:A:CYS:HB3	1:124:A:ARG:HG2	3	0.12	0.01	0.13
(1,3242)	1:144:A:LEU:H	1:144:A:LEU:HA	3	0.12	0.02	0.12
(1,977)	1:132:A:THR:HG21	1:131:A:ILE:H	3	0.12	0.01	0.11

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,977)	1:132:A:THR:HG22	1:131:A:ILE:H	3	0.12	0.01	0.11
(1,977)	1:132:A:THR:HG23	1:131:A:ILE:H	3	0.12	0.01	0.11
(1,2618)	1:131:A:ILE:H	1:132:A:THR:HG21	3	0.12	0.01	0.11
(1,2618)	1:131:A:ILE:H	1:132:A:THR:HG22	3	0.12	0.01	0.11
(1,2618)	1:131:A:ILE:H	1:132:A:THR:HG23	3	0.12	0.01	0.11
(1,2891)	1:58:A:TYR:HD1	1:54:A:ILE:HG21	3	0.12	0.0	0.12
(1,2891)	1:58:A:TYR:HD1	1:54:A:ILE:HG22	3	0.12	0.0	0.12
(1,2891)	1:58:A:TYR:HD1	1:54:A:ILE:HG23	3	0.12	0.0	0.12
(1,2891)	1:58:A:TYR:HD2	1:54:A:ILE:HG21	3	0.12	0.0	0.12
(1,2891)	1:58:A:TYR:HD2	1:54:A:ILE:HG22	3	0.12	0.0	0.12
(1,2891)	1:58:A:TYR:HD2	1:54:A:ILE:HG23	3	0.12	0.0	0.12
(1,3045)	1:133:A:GLY:HA2	1:136:A:THR:HG21	2	0.54	0.03	0.54
(1,3045)	1:133:A:GLY:HA2	1:136:A:THR:HG22	2	0.54	0.03	0.54
(1,3045)	1:133:A:GLY:HA2	1:136:A:THR:HG23	2	0.54	0.03	0.54
(1,3045)	1:64:A:GLY:HA2	1:65:A:THR:HG21	2	0.54	0.03	0.54
(1,3045)	1:64:A:GLY:HA2	1:65:A:THR:HG22	2	0.54	0.03	0.54
(1,3045)	1:64:A:GLY:HA2	1:65:A:THR:HG23	2	0.54	0.03	0.54
(1,3045)	1:64:A:GLY:HA3	1:65:A:THR:HG21	2	0.54	0.03	0.54
(1,3045)	1:64:A:GLY:HA3	1:65:A:THR:HG22	2	0.54	0.03	0.54
(1,3045)	1:64:A:GLY:HA3	1:65:A:THR:HG23	2	0.54	0.03	0.54
(1,3663)	1:68:A:ILE:HG21	1:4:A:LYS:HE2	2	0.38	0.22	0.38
(1,3663)	1:68:A:ILE:HG21	1:4:A:LYS:HE3	2	0.38	0.22	0.38
(1,3663)	1:68:A:ILE:HG22	1:4:A:LYS:HE2	2	0.38	0.22	0.38
(1,3663)	1:68:A:ILE:HG22	1:4:A:LYS:HE3	2	0.38	0.22	0.38
(1,3663)	1:68:A:ILE:HG23	1:4:A:LYS:HE2	2	0.38	0.22	0.38
(1,3663)	1:68:A:ILE:HG23	1:4:A:LYS:HE3	2	0.38	0.22	0.38
(1,1817)	1:132:A:THR:HB	1:134:A:ARG:HD2	2	0.34	0.05	0.34
(1,1817)	1:132:A:THR:HB	1:134:A:ARG:HD3	2	0.34	0.05	0.34
(1,3832)	1:116:A:ASN:H	1:140:A:VAL:HG21	2	0.32	0.04	0.32
(1,3832)	1:116:A:ASN:H	1:140:A:VAL:HG22	2	0.32	0.04	0.32
(1,3832)	1:116:A:ASN:H	1:140:A:VAL:HG23	2	0.32	0.04	0.32
(1,2356)	1:62:A:LYS:HA	1:62:A:LYS:HD2	2	0.29	0.03	0.29
(1,2356)	1:62:A:LYS:HA	1:62:A:LYS:HD3	2	0.29	0.03	0.29
(1,500)	1:83:A:GLY:HA2	1:82:A:ASN:HD22	2	0.26	0.01	0.26
(1,500)	1:8:A:ILE:HA	1:35:A:GLN:H	2	0.26	0.01	0.26
(1,970)	1:4:A:LYS:HB2	1:71:A:ASN:H	2	0.26	0.12	0.26
(1,970)	1:70:A:LYS:HD3	1:71:A:ASN:H	2	0.26	0.12	0.26
(1,446)	1:43:A:GLY:HA2	1:44:A:ASN:H	2	0.24	0.08	0.24
(1,774)	1:72:A:ARG:HB2	1:3:A:VAL:H	2	0.18	0.02	0.18
(1,1379)	1:130:A:TYR:HD1	1:135:A:ILE:HD11	2	0.18	0.07	0.18
(1,1379)	1:130:A:TYR:HD1	1:135:A:ILE:HD12	2	0.18	0.07	0.18
(1,1379)	1:130:A:TYR:HD1	1:135:A:ILE:HD13	2	0.18	0.07	0.18

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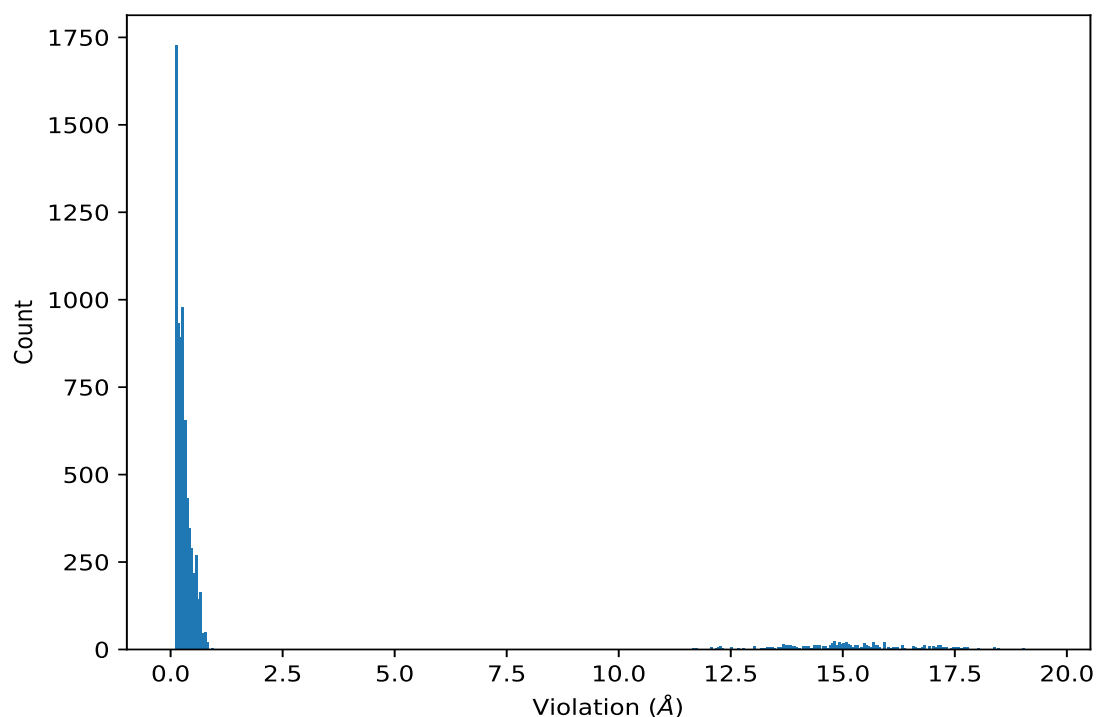
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1379)	1:130:A:TYR:HD2	1:135:A:ILE:HD11	2	0.18	0.07	0.18
(1,1379)	1:130:A:TYR:HD2	1:135:A:ILE:HD12	2	0.18	0.07	0.18
(1,1379)	1:130:A:TYR:HD2	1:135:A:ILE:HD13	2	0.18	0.07	0.18
(1,1510)	1:72:A:ARG:HA	1:5:A:ILE:HD11	2	0.15	0.0	0.15
(1,1510)	1:72:A:ARG:HA	1:5:A:ILE:HD12	2	0.15	0.0	0.15
(1,1510)	1:72:A:ARG:HA	1:5:A:ILE:HD13	2	0.15	0.0	0.15
(1,2743)	1:18:A:ASP:HB2	1:8:A:ILE:HG21	2	0.14	0.03	0.14
(1,2743)	1:18:A:ASP:HB2	1:8:A:ILE:HG22	2	0.14	0.03	0.14
(1,2743)	1:18:A:ASP:HB2	1:8:A:ILE:HG23	2	0.14	0.03	0.14
(1,1322)	1:117:A:ASN:HA	1:116:A:ASN:H	2	0.14	0.02	0.14
(1,1322)	1:112:A:ASP:HB3	1:116:A:ASN:H	2	0.14	0.02	0.14
(1,1853)	1:132:A:THR:HG21	1:134:A:ARG:HD2	2	0.14	0.03	0.14
(1,1853)	1:132:A:THR:HG21	1:134:A:ARG:HD3	2	0.14	0.03	0.14
(1,1853)	1:132:A:THR:HG22	1:134:A:ARG:HD2	2	0.14	0.03	0.14
(1,1853)	1:132:A:THR:HG22	1:134:A:ARG:HD3	2	0.14	0.03	0.14
(1,1853)	1:132:A:THR:HG23	1:134:A:ARG:HD2	2	0.14	0.03	0.14
(1,1853)	1:132:A:THR:HG23	1:134:A:ARG:HD3	2	0.14	0.03	0.14
(1,2721)	1:134:A:ARG:HD2	1:132:A:THR:HG21	2	0.14	0.03	0.14
(1,2721)	1:134:A:ARG:HD2	1:132:A:THR:HG22	2	0.14	0.03	0.14
(1,2721)	1:134:A:ARG:HD2	1:132:A:THR:HG23	2	0.14	0.03	0.14
(1,2721)	1:134:A:ARG:HD3	1:132:A:THR:HG21	2	0.14	0.03	0.14
(1,2721)	1:134:A:ARG:HD3	1:132:A:THR:HG22	2	0.14	0.03	0.14
(1,2721)	1:134:A:ARG:HD3	1:132:A:THR:HG23	2	0.14	0.03	0.14
(1,3337)	1:5:A:ILE:HG21	1:41:A:VAL:HB	2	0.14	0.01	0.14
(1,3337)	1:5:A:ILE:HG22	1:41:A:VAL:HB	2	0.14	0.01	0.14
(1,3337)	1:5:A:ILE:HG23	1:41:A:VAL:HB	2	0.14	0.01	0.14
(1,3205)	1:51:A:ASP:H	1:50:A:ILE:HD11	2	0.12	0.01	0.12
(1,3205)	1:51:A:ASP:H	1:50:A:ILE:HD12	2	0.12	0.01	0.12
(1,3205)	1:51:A:ASP:H	1:50:A:ILE:HD13	2	0.12	0.01	0.12
(1,798)	1:13:A:GLU:HG2	1:13:A:GLU:H	2	0.12	0.0	0.12
(1,798)	1:13:A:GLU:HG3	1:13:A:GLU:H	2	0.12	0.0	0.12
(1,3721)	1:7:A:ASP:H	1:4:A:LYS:HD2	2	0.12	0.0	0.12
(1,2337)	1:84:A:ILE:H	1:84:A:ILE:HG12	2	0.11	0.01	0.11
(1,1801)	1:144:A:LEU:H	1:144:A:LEU:HB2	2	0.11	0.0	0.11

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,20)	1:114:A:ASP:OD1	1:4:A:LYS:CA	18	19.52
(1,4003)	1:114:A:ASP:OD1	1:4:A:LYS:CA	18	19.52
(2,20)	1:114:A:ASP:OD1	1:4:A:LYS:CA	2	19.24
(1,4003)	1:114:A:ASP:OD1	1:4:A:LYS:CA	2	19.24
(2,23)	1:123:A:ASP:OD1	1:4:A:LYS:CA	8	19.2
(1,4006)	1:123:A:ASP:OD1	1:4:A:LYS:CA	8	19.2
(2,24)	1:123:A:ASP:OD2	1:4:A:LYS:CA	12	19.06
(1,4007)	1:123:A:ASP:OD2	1:4:A:LYS:CA	12	19.06
(2,23)	1:123:A:ASP:OD1	1:4:A:LYS:CA	18	19.03
(1,4006)	1:123:A:ASP:OD1	1:4:A:LYS:CA	18	19.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,23)	1:123:A:ASP:OD1	1:4:A:LYS:CA	4	19.02
(1,4006)	1:123:A:ASP:OD1	1:4:A:LYS:CA	4	19.02
(2,24)	1:123:A:ASP:OD2	1:4:A:LYS:CA	19	18.96
(1,4007)	1:123:A:ASP:OD2	1:4:A:LYS:CA	19	18.96
(2,23)	1:123:A:ASP:OD1	1:4:A:LYS:CA	16	18.94
(1,4006)	1:123:A:ASP:OD1	1:4:A:LYS:CA	16	18.94
(2,23)	1:123:A:ASP:OD1	1:4:A:LYS:CA	15	18.87
(1,4006)	1:123:A:ASP:OD1	1:4:A:LYS:CA	15	18.87
(2,23)	1:123:A:ASP:OD1	1:4:A:LYS:CA	7	18.82
(1,4006)	1:123:A:ASP:OD1	1:4:A:LYS:CA	7	18.82
(2,24)	1:123:A:ASP:OD2	1:4:A:LYS:CA	2	18.75
(1,4007)	1:123:A:ASP:OD2	1:4:A:LYS:CA	2	18.75
(2,24)	1:123:A:ASP:OD2	1:4:A:LYS:CA	14	18.72
(1,4007)	1:123:A:ASP:OD2	1:4:A:LYS:CA	14	18.72
(2,24)	1:123:A:ASP:OD2	1:4:A:LYS:CA	17	18.65
(1,4007)	1:123:A:ASP:OD2	1:4:A:LYS:CA	17	18.65
(2,23)	1:123:A:ASP:OD1	1:4:A:LYS:CA	3	18.49
(1,4006)	1:123:A:ASP:OD1	1:4:A:LYS:CA	3	18.49
(2,23)	1:123:A:ASP:OD1	1:4:A:LYS:CA	5	18.45
(1,4006)	1:123:A:ASP:OD1	1:4:A:LYS:CA	5	18.45
(2,23)	1:123:A:ASP:OD1	1:4:A:LYS:CA	11	18.42
(1,4006)	1:123:A:ASP:OD1	1:4:A:LYS:CA	11	18.42
(2,24)	1:123:A:ASP:OD2	1:4:A:LYS:CA	9	18.38
(2,20)	1:114:A:ASP:OD1	1:4:A:LYS:CA	13	18.38
(1,4007)	1:123:A:ASP:OD2	1:4:A:LYS:CA	9	18.38
(1,4003)	1:114:A:ASP:OD1	1:4:A:LYS:CA	13	18.38
(2,23)	1:123:A:ASP:OD1	1:4:A:LYS:CA	13	18.37
(1,4006)	1:123:A:ASP:OD1	1:4:A:LYS:CA	13	18.37
(2,23)	1:123:A:ASP:OD1	1:4:A:LYS:CA	10	18.3
(1,4006)	1:123:A:ASP:OD1	1:4:A:LYS:CA	10	18.3
(2,23)	1:123:A:ASP:OD1	1:4:A:LYS:CA	1	18.26
(1,4006)	1:123:A:ASP:OD1	1:4:A:LYS:CA	1	18.26
(2,20)	1:114:A:ASP:OD1	1:4:A:LYS:CA	14	18.2
(1,4003)	1:114:A:ASP:OD1	1:4:A:LYS:CA	14	18.2
(2,24)	1:123:A:ASP:OD2	1:4:A:LYS:CA	6	18.16
(1,4007)	1:123:A:ASP:OD2	1:4:A:LYS:CA	6	18.16
(2,23)	1:123:A:ASP:OD1	1:4:A:LYS:CA	20	18.12
(1,4006)	1:123:A:ASP:OD1	1:4:A:LYS:CA	20	18.12
(2,20)	1:114:A:ASP:OD1	1:4:A:LYS:CA	15	18.08
(1,4003)	1:114:A:ASP:OD1	1:4:A:LYS:CA	15	18.08
(2,24)	1:123:A:ASP:OD2	1:4:A:LYS:CA	8	18.04
(1,4007)	1:123:A:ASP:OD2	1:4:A:LYS:CA	8	18.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,23)	1:123:A:ASP:OD1	1:4:A:LYS:CA	14	18.03
(1,4006)	1:123:A:ASP:OD1	1:4:A:LYS:CA	14	18.03
(2,22)	1:118:A:VAL:O	1:4:A:LYS:CA	8	17.97
(1,4005)	1:118:A:VAL:O	1:4:A:LYS:CA	8	17.97
(2,22)	1:118:A:VAL:O	1:4:A:LYS:CA	12	17.81
(1,4005)	1:118:A:VAL:O	1:4:A:LYS:CA	12	17.81
(2,24)	1:123:A:ASP:OD2	1:4:A:LYS:CA	18	17.79
(1,4007)	1:123:A:ASP:OD2	1:4:A:LYS:CA	18	17.79
(2,22)	1:118:A:VAL:O	1:4:A:LYS:CA	7	17.78
(1,4005)	1:118:A:VAL:O	1:4:A:LYS:CA	7	17.78
(2,22)	1:118:A:VAL:O	1:4:A:LYS:CA	4	17.76
(2,20)	1:114:A:ASP:OD1	1:4:A:LYS:CA	16	17.76
(1,4005)	1:118:A:VAL:O	1:4:A:LYS:CA	4	17.76
(1,4003)	1:114:A:ASP:OD1	1:4:A:LYS:CA	16	17.76
(2,24)	1:123:A:ASP:OD2	1:4:A:LYS:CA	16	17.74
(1,4007)	1:123:A:ASP:OD2	1:4:A:LYS:CA	16	17.74
(2,23)	1:123:A:ASP:OD1	1:4:A:LYS:CA	12	17.71
(1,4006)	1:123:A:ASP:OD1	1:4:A:LYS:CA	12	17.71
(2,22)	1:118:A:VAL:O	1:4:A:LYS:CA	16	17.7
(1,4005)	1:118:A:VAL:O	1:4:A:LYS:CA	16	17.7
(2,20)	1:114:A:ASP:OD1	1:4:A:LYS:CA	8	17.68
(1,4003)	1:114:A:ASP:OD1	1:4:A:LYS:CA	8	17.68
(2,22)	1:118:A:VAL:O	1:4:A:LYS:CA	2	17.66
(1,4005)	1:118:A:VAL:O	1:4:A:LYS:CA	2	17.66
(2,20)	1:114:A:ASP:OD1	1:4:A:LYS:CA	20	17.65
(1,4003)	1:114:A:ASP:OD1	1:4:A:LYS:CA	20	17.65
(2,22)	1:118:A:VAL:O	1:4:A:LYS:CA	18	17.64
(1,4005)	1:118:A:VAL:O	1:4:A:LYS:CA	18	17.64
(2,22)	1:118:A:VAL:O	1:4:A:LYS:CA	14	17.57
(2,21)	1:116:A:ASN:OD1	1:4:A:LYS:CA	8	17.57
(1,4005)	1:118:A:VAL:O	1:4:A:LYS:CA	14	17.57
(1,4004)	1:116:A:ASN:OD1	1:4:A:LYS:CA	8	17.57
(2,20)	1:114:A:ASP:OD1	1:4:A:LYS:CA	5	17.56
(1,4003)	1:114:A:ASP:OD1	1:4:A:LYS:CA	5	17.56
(2,24)	1:123:A:ASP:OD2	1:4:A:LYS:CA	7	17.55
(1,4007)	1:123:A:ASP:OD2	1:4:A:LYS:CA	7	17.55
(2,24)	1:123:A:ASP:OD2	1:4:A:LYS:CA	15	17.52
(1,4007)	1:123:A:ASP:OD2	1:4:A:LYS:CA	15	17.52
(2,21)	1:116:A:ASN:OD1	1:4:A:LYS:CA	2	17.51
(2,21)	1:116:A:ASN:OD1	1:4:A:LYS:CA	16	17.51
(1,4004)	1:116:A:ASN:OD1	1:4:A:LYS:CA	2	17.51
(1,4004)	1:116:A:ASN:OD1	1:4:A:LYS:CA	16	17.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,24)	1:123:A:ASP:OD2	1:4:A:LYS:CA	4	17.5
(1,4007)	1:123:A:ASP:OD2	1:4:A:LYS:CA	4	17.5
(2,23)	1:123:A:ASP:OD1	1:4:A:LYS:CA	19	17.48
(2,22)	1:118:A:VAL:O	1:4:A:LYS:CA	3	17.48
(2,22)	1:118:A:VAL:O	1:4:A:LYS:CA	17	17.48
(1,4006)	1:123:A:ASP:OD1	1:4:A:LYS:CA	19	17.48
(1,4005)	1:118:A:VAL:O	1:4:A:LYS:CA	3	17.48
(1,4005)	1:118:A:VAL:O	1:4:A:LYS:CA	17	17.48
(2,23)	1:123:A:ASP:OD1	1:4:A:LYS:CA	2	17.46
(1,4006)	1:123:A:ASP:OD1	1:4:A:LYS:CA	2	17.46
(2,21)	1:116:A:ASN:OD1	1:4:A:LYS:CA	18	17.44
(1,4004)	1:116:A:ASN:OD1	1:4:A:LYS:CA	18	17.44
(2,21)	1:116:A:ASN:OD1	1:4:A:LYS:CA	12	17.43
(1,4004)	1:116:A:ASN:OD1	1:4:A:LYS:CA	12	17.43
(2,22)	1:118:A:VAL:O	1:4:A:LYS:CA	11	17.36
(1,4005)	1:118:A:VAL:O	1:4:A:LYS:CA	11	17.36
(2,22)	1:118:A:VAL:O	1:4:A:LYS:CA	15	17.33
(1,4005)	1:118:A:VAL:O	1:4:A:LYS:CA	15	17.33
(2,22)	1:118:A:VAL:O	1:4:A:LYS:CA	9	17.32
(1,4005)	1:118:A:VAL:O	1:4:A:LYS:CA	9	17.32
(2,2)	1:9:A:ASP:OD1	1:1:A:MET:CA	19	17.31
(1,3985)	1:9:A:ASP:OD1	1:1:A:MET:CA	19	17.31
(2,21)	1:116:A:ASN:OD1	1:4:A:LYS:CA	7	17.29
(1,4004)	1:116:A:ASN:OD1	1:4:A:LYS:CA	7	17.29
(2,20)	1:114:A:ASP:OD1	1:4:A:LYS:CA	4	17.26
(1,4003)	1:114:A:ASP:OD1	1:4:A:LYS:CA	4	17.26
(2,22)	1:118:A:VAL:O	1:4:A:LYS:CA	13	17.25
(2,22)	1:118:A:VAL:O	1:4:A:LYS:CA	19	17.25
(1,4005)	1:118:A:VAL:O	1:4:A:LYS:CA	13	17.25
(1,4005)	1:118:A:VAL:O	1:4:A:LYS:CA	19	17.25
(2,23)	1:123:A:ASP:OD1	1:4:A:LYS:CA	17	17.24
(1,4006)	1:123:A:ASP:OD1	1:4:A:LYS:CA	17	17.24
(2,21)	1:116:A:ASN:OD1	1:4:A:LYS:CA	4	17.22
(1,4004)	1:116:A:ASN:OD1	1:4:A:LYS:CA	4	17.22
(2,22)	1:118:A:VAL:O	1:4:A:LYS:CA	6	17.2
(1,4005)	1:118:A:VAL:O	1:4:A:LYS:CA	6	17.2
(2,24)	1:123:A:ASP:OD2	1:4:A:LYS:CA	20	17.19
(2,23)	1:123:A:ASP:OD1	1:4:A:LYS:CA	9	17.19
(2,14)	1:80:A:ASP:OD1	1:3:A:VAL:CA	12	17.19
(1,4007)	1:123:A:ASP:OD2	1:4:A:LYS:CA	20	17.19
(1,4006)	1:123:A:ASP:OD1	1:4:A:LYS:CA	9	17.19
(1,3997)	1:80:A:ASP:OD1	1:3:A:VAL:CA	12	17.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,24)	1:123:A:ASP:OD2	1:4:A:LYS:CA	13	17.17
(2,21)	1:116:A:ASN:OD1	1:4:A:LYS:CA	17	17.17
(1,4007)	1:123:A:ASP:OD2	1:4:A:LYS:CA	13	17.17
(1,4004)	1:116:A:ASN:OD1	1:4:A:LYS:CA	17	17.17
(2,20)	1:114:A:ASP:OD1	1:4:A:LYS:CA	12	17.16
(1,4003)	1:114:A:ASP:OD1	1:4:A:LYS:CA	12	17.16
(2,15)	1:82:A:ASN:OD1	1:3:A:VAL:CA	12	17.15
(1,3998)	1:82:A:ASN:OD1	1:3:A:VAL:CA	12	17.15
(2,24)	1:123:A:ASP:OD2	1:4:A:LYS:CA	3	17.14
(2,24)	1:123:A:ASP:OD2	1:4:A:LYS:CA	5	17.14
(2,21)	1:116:A:ASN:OD1	1:4:A:LYS:CA	3	17.14
(1,4007)	1:123:A:ASP:OD2	1:4:A:LYS:CA	3	17.14
(1,4007)	1:123:A:ASP:OD2	1:4:A:LYS:CA	5	17.14
(1,4004)	1:116:A:ASN:OD1	1:4:A:LYS:CA	3	17.14
(2,21)	1:116:A:ASN:OD1	1:4:A:LYS:CA	15	17.13
(1,4004)	1:116:A:ASN:OD1	1:4:A:LYS:CA	15	17.13
(2,22)	1:118:A:VAL:O	1:4:A:LYS:CA	5	17.1
(1,4005)	1:118:A:VAL:O	1:4:A:LYS:CA	5	17.1
(2,21)	1:116:A:ASN:OD1	1:4:A:LYS:CA	14	17.08
(1,4004)	1:116:A:ASN:OD1	1:4:A:LYS:CA	14	17.08
(2,24)	1:123:A:ASP:OD2	1:4:A:LYS:CA	11	17.07
(1,4007)	1:123:A:ASP:OD2	1:4:A:LYS:CA	11	17.07
(2,22)	1:118:A:VAL:O	1:4:A:LYS:CA	1	17.05
(1,4005)	1:118:A:VAL:O	1:4:A:LYS:CA	1	17.05
(2,24)	1:123:A:ASP:OD2	1:4:A:LYS:CA	10	17.04
(1,4007)	1:123:A:ASP:OD2	1:4:A:LYS:CA	10	17.04
(2,20)	1:114:A:ASP:OD1	1:4:A:LYS:CA	19	17.03
(2,18)	1:89:A:ASP:OD2	1:3:A:VAL:CA	12	17.03
(1,4003)	1:114:A:ASP:OD1	1:4:A:LYS:CA	19	17.03
(1,4001)	1:89:A:ASP:OD2	1:3:A:VAL:CA	12	17.03
(2,20)	1:114:A:ASP:OD1	1:4:A:LYS:CA	7	17.02
(1,4003)	1:114:A:ASP:OD1	1:4:A:LYS:CA	7	17.02
(2,22)	1:118:A:VAL:O	1:4:A:LYS:CA	10	17.0
(1,4005)	1:118:A:VAL:O	1:4:A:LYS:CA	10	17.0
(2,5)	1:18:A:ASP:OD1	1:1:A:MET:CA	2	16.99
(1,3988)	1:18:A:ASP:OD1	1:1:A:MET:CA	2	16.99
(2,24)	1:123:A:ASP:OD2	1:4:A:LYS:CA	1	16.94
(2,2)	1:9:A:ASP:OD1	1:1:A:MET:CA	3	16.94
(1,4007)	1:123:A:ASP:OD2	1:4:A:LYS:CA	1	16.94
(1,3985)	1:9:A:ASP:OD1	1:1:A:MET:CA	3	16.94
(2,20)	1:114:A:ASP:OD1	1:4:A:LYS:CA	6	16.93
(1,4003)	1:114:A:ASP:OD1	1:4:A:LYS:CA	6	16.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,21)	1:116:A:ASN:OD1	1:4:A:LYS:CA	9	16.92
(1,4004)	1:116:A:ASN:OD1	1:4:A:LYS:CA	9	16.92
(2,21)	1:116:A:ASN:OD1	1:4:A:LYS:CA	11	16.91
(1,4004)	1:116:A:ASN:OD1	1:4:A:LYS:CA	11	16.91
(2,15)	1:82:A:ASN:OD1	1:3:A:VAL:CA	19	16.85
(1,3998)	1:82:A:ASN:OD1	1:3:A:VAL:CA	19	16.85
(2,23)	1:123:A:ASP:OD1	1:4:A:LYS:CA	6	16.84
(2,22)	1:118:A:VAL:O	1:4:A:LYS:CA	20	16.84
(2,14)	1:80:A:ASP:OD1	1:3:A:VAL:CA	15	16.84
(1,4006)	1:123:A:ASP:OD1	1:4:A:LYS:CA	6	16.84
(1,4005)	1:118:A:VAL:O	1:4:A:LYS:CA	20	16.84
(1,3997)	1:80:A:ASP:OD1	1:3:A:VAL:CA	15	16.84
(2,21)	1:116:A:ASN:OD1	1:4:A:LYS:CA	10	16.83
(2,20)	1:114:A:ASP:OD1	1:4:A:LYS:CA	10	16.83
(2,20)	1:114:A:ASP:OD1	1:4:A:LYS:CA	17	16.83
(1,4004)	1:116:A:ASN:OD1	1:4:A:LYS:CA	10	16.83
(1,4003)	1:114:A:ASP:OD1	1:4:A:LYS:CA	10	16.83
(1,4003)	1:114:A:ASP:OD1	1:4:A:LYS:CA	17	16.83
(2,21)	1:116:A:ASN:OD1	1:4:A:LYS:CA	5	16.82
(1,4004)	1:116:A:ASN:OD1	1:4:A:LYS:CA	5	16.82
(2,20)	1:114:A:ASP:OD1	1:4:A:LYS:CA	9	16.78
(2,2)	1:9:A:ASP:OD1	1:1:A:MET:CA	6	16.78
(1,4003)	1:114:A:ASP:OD1	1:4:A:LYS:CA	9	16.78
(1,3985)	1:9:A:ASP:OD1	1:1:A:MET:CA	6	16.78
(2,14)	1:80:A:ASP:OD1	1:3:A:VAL:CA	19	16.76
(1,3997)	1:80:A:ASP:OD1	1:3:A:VAL:CA	19	16.76
(2,21)	1:116:A:ASN:OD1	1:4:A:LYS:CA	19	16.75
(1,4004)	1:116:A:ASN:OD1	1:4:A:LYS:CA	19	16.75
(2,17)	1:89:A:ASP:OD1	1:3:A:VAL:CA	19	16.74
(1,4000)	1:89:A:ASP:OD1	1:3:A:VAL:CA	19	16.74
(2,2)	1:9:A:ASP:OD1	1:1:A:MET:CA	16	16.73
(1,3985)	1:9:A:ASP:OD1	1:1:A:MET:CA	16	16.73
(2,20)	1:114:A:ASP:OD1	1:4:A:LYS:CA	3	16.69
(1,4003)	1:114:A:ASP:OD1	1:4:A:LYS:CA	3	16.69
(2,21)	1:116:A:ASN:OD1	1:4:A:LYS:CA	1	16.67
(1,4004)	1:116:A:ASN:OD1	1:4:A:LYS:CA	1	16.67
(2,21)	1:116:A:ASN:OD1	1:4:A:LYS:CA	13	16.65
(1,4004)	1:116:A:ASN:OD1	1:4:A:LYS:CA	13	16.65
(2,6)	1:18:A:ASP:OD2	1:1:A:MET:CA	9	16.63
(1,3989)	1:18:A:ASP:OD2	1:1:A:MET:CA	9	16.63
(2,20)	1:114:A:ASP:OD1	1:4:A:LYS:CA	1	16.6
(1,4003)	1:114:A:ASP:OD1	1:4:A:LYS:CA	1	16.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,16)	1:84:A:ILE:O	1:3:A:VAL:CA	12	16.59
(1,3999)	1:84:A:ILE:O	1:3:A:VAL:CA	12	16.59
(2,21)	1:116:A:ASN:OD1	1:4:A:LYS:CA	20	16.58
(2,20)	1:114:A:ASP:OD1	1:4:A:LYS:CA	11	16.58
(2,15)	1:82:A:ASN:OD1	1:3:A:VAL:CA	7	16.58
(1,4004)	1:116:A:ASN:OD1	1:4:A:LYS:CA	20	16.58
(1,4003)	1:114:A:ASP:OD1	1:4:A:LYS:CA	11	16.58
(1,3998)	1:82:A:ASN:OD1	1:3:A:VAL:CA	7	16.58
(2,18)	1:89:A:ASP:OD2	1:3:A:VAL:CA	15	16.56
(1,4001)	1:89:A:ASP:OD2	1:3:A:VAL:CA	15	16.56
(2,21)	1:116:A:ASN:OD1	1:4:A:LYS:CA	6	16.51
(1,4004)	1:116:A:ASN:OD1	1:4:A:LYS:CA	6	16.51
(2,16)	1:84:A:ILE:O	1:3:A:VAL:CA	19	16.48
(1,3999)	1:84:A:ILE:O	1:3:A:VAL:CA	19	16.48
(2,6)	1:18:A:ASP:OD2	1:1:A:MET:CA	8	16.44
(1,3989)	1:18:A:ASP:OD2	1:1:A:MET:CA	8	16.44
(2,17)	1:89:A:ASP:OD1	1:3:A:VAL:CA	14	16.38
(1,4000)	1:89:A:ASP:OD1	1:3:A:VAL:CA	14	16.38
(2,17)	1:89:A:ASP:OD1	1:3:A:VAL:CA	18	16.36
(1,4000)	1:89:A:ASP:OD1	1:3:A:VAL:CA	18	16.36
(2,17)	1:89:A:ASP:OD1	1:3:A:VAL:CA	7	16.34
(2,15)	1:82:A:ASN:OD1	1:3:A:VAL:CA	15	16.34
(1,4000)	1:89:A:ASP:OD1	1:3:A:VAL:CA	7	16.34
(1,3998)	1:82:A:ASN:OD1	1:3:A:VAL:CA	15	16.34
(2,3)	1:11:A:ASN:OD1	1:1:A:MET:CA	9	16.33
(1,3986)	1:11:A:ASN:OD1	1:1:A:MET:CA	9	16.33
(2,17)	1:89:A:ASP:OD1	1:3:A:VAL:CA	8	16.32
(2,2)	1:9:A:ASP:OD1	1:1:A:MET:CA	8	16.32
(1,4000)	1:89:A:ASP:OD1	1:3:A:VAL:CA	8	16.32
(1,3985)	1:9:A:ASP:OD1	1:1:A:MET:CA	8	16.32
(2,14)	1:80:A:ASP:OD1	1:3:A:VAL:CA	6	16.31
(2,5)	1:18:A:ASP:OD1	1:1:A:MET:CA	19	16.31
(1,3997)	1:80:A:ASP:OD1	1:3:A:VAL:CA	6	16.31
(1,3988)	1:18:A:ASP:OD1	1:1:A:MET:CA	19	16.31
(2,14)	1:80:A:ASP:OD1	1:3:A:VAL:CA	18	16.28
(1,3997)	1:80:A:ASP:OD1	1:3:A:VAL:CA	18	16.28
(2,14)	1:80:A:ASP:OD1	1:3:A:VAL:CA	9	16.24
(2,5)	1:18:A:ASP:OD1	1:1:A:MET:CA	16	16.24
(1,3997)	1:80:A:ASP:OD1	1:3:A:VAL:CA	9	16.24
(1,3988)	1:18:A:ASP:OD1	1:1:A:MET:CA	16	16.24
(2,15)	1:82:A:ASN:OD1	1:3:A:VAL:CA	13	16.21
(1,3998)	1:82:A:ASN:OD1	1:3:A:VAL:CA	13	16.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,18)	1:89:A:ASP:OD2	1:3:A:VAL:CA	13	16.19
(2,16)	1:84:A:ILE:O	1:3:A:VAL:CA	15	16.19
(2,15)	1:82:A:ASN:OD1	1:3:A:VAL:CA	5	16.19
(1,4001)	1:89:A:ASP:OD2	1:3:A:VAL:CA	13	16.19
(1,3999)	1:84:A:ILE:O	1:3:A:VAL:CA	15	16.19
(1,3998)	1:82:A:ASN:OD1	1:3:A:VAL:CA	5	16.19
(2,6)	1:18:A:ASP:OD2	1:1:A:MET:CA	5	16.17
(1,3989)	1:18:A:ASP:OD2	1:1:A:MET:CA	5	16.17
(2,14)	1:80:A:ASP:OD1	1:3:A:VAL:CA	14	16.13
(1,3997)	1:80:A:ASP:OD1	1:3:A:VAL:CA	14	16.13
(2,14)	1:80:A:ASP:OD1	1:3:A:VAL:CA	7	16.12
(1,3997)	1:80:A:ASP:OD1	1:3:A:VAL:CA	7	16.12
(2,17)	1:89:A:ASP:OD1	1:3:A:VAL:CA	5	16.11
(1,4000)	1:89:A:ASP:OD1	1:3:A:VAL:CA	5	16.11
(2,14)	1:80:A:ASP:OD1	1:3:A:VAL:CA	17	16.08
(1,3997)	1:80:A:ASP:OD1	1:3:A:VAL:CA	17	16.08
(2,16)	1:84:A:ILE:O	1:3:A:VAL:CA	7	16.05
(1,3999)	1:84:A:ILE:O	1:3:A:VAL:CA	7	16.05
(2,15)	1:82:A:ASN:OD1	1:3:A:VAL:CA	8	16.02
(1,3998)	1:82:A:ASN:OD1	1:3:A:VAL:CA	8	16.02
(2,16)	1:84:A:ILE:O	1:3:A:VAL:CA	8	16.01
(1,3999)	1:84:A:ILE:O	1:3:A:VAL:CA	8	16.01
(2,19)	1:112:A:ASP:OD1	1:4:A:LYS:CA	8	16.0
(1,4002)	1:112:A:ASP:OD1	1:4:A:LYS:CA	8	16.0
(2,5)	1:18:A:ASP:OD1	1:1:A:MET:CA	6	15.95
(1,3988)	1:18:A:ASP:OD1	1:1:A:MET:CA	6	15.95
(2,16)	1:84:A:ILE:O	1:3:A:VAL:CA	5	15.94
(2,15)	1:82:A:ASN:OD1	1:3:A:VAL:CA	14	15.94
(1,3999)	1:84:A:ILE:O	1:3:A:VAL:CA	5	15.94
(1,3998)	1:82:A:ASN:OD1	1:3:A:VAL:CA	14	15.94
(2,17)	1:89:A:ASP:OD1	1:3:A:VAL:CA	17	15.93
(2,15)	1:82:A:ASN:OD1	1:3:A:VAL:CA	17	15.93
(2,14)	1:80:A:ASP:OD1	1:3:A:VAL:CA	13	15.93
(1,4000)	1:89:A:ASP:OD1	1:3:A:VAL:CA	17	15.93
(1,3998)	1:82:A:ASN:OD1	1:3:A:VAL:CA	17	15.93
(1,3997)	1:80:A:ASP:OD1	1:3:A:VAL:CA	13	15.93
(2,6)	1:18:A:ASP:OD2	1:1:A:MET:CA	3	15.92
(2,6)	1:18:A:ASP:OD2	1:1:A:MET:CA	15	15.92
(1,3989)	1:18:A:ASP:OD2	1:1:A:MET:CA	3	15.92
(1,3989)	1:18:A:ASP:OD2	1:1:A:MET:CA	15	15.92
(2,15)	1:82:A:ASN:OD1	1:3:A:VAL:CA	18	15.9
(2,4)	1:13:A:GLU:O	1:1:A:MET:CA	2	15.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3998)	1:82:A:ASN:OD1	1:3:A:VAL:CA	18	15.9
(1,3987)	1:13:A:GLU:O	1:1:A:MET:CA	2	15.9
(2,17)	1:89:A:ASP:OD1	1:3:A:VAL:CA	4	15.87
(1,4000)	1:89:A:ASP:OD1	1:3:A:VAL:CA	4	15.87
(2,5)	1:18:A:ASP:OD1	1:1:A:MET:CA	12	15.84
(1,3988)	1:18:A:ASP:OD1	1:1:A:MET:CA	12	15.84
(2,5)	1:18:A:ASP:OD1	1:1:A:MET:CA	14	15.83
(1,3988)	1:18:A:ASP:OD1	1:1:A:MET:CA	14	15.83
(2,5)	1:18:A:ASP:OD1	1:1:A:MET:CA	9	15.8
(1,3988)	1:18:A:ASP:OD1	1:1:A:MET:CA	9	15.8
(2,16)	1:84:A:ILE:O	1:3:A:VAL:CA	14	15.79
(1,3999)	1:84:A:ILE:O	1:3:A:VAL:CA	14	15.79
(2,17)	1:89:A:ASP:OD1	1:3:A:VAL:CA	2	15.78
(1,4000)	1:89:A:ASP:OD1	1:3:A:VAL:CA	2	15.78
(2,14)	1:80:A:ASP:OD1	1:3:A:VAL:CA	5	15.77
(2,3)	1:11:A:ASN:OD1	1:1:A:MET:CA	2	15.77
(1,3997)	1:80:A:ASP:OD1	1:3:A:VAL:CA	5	15.77
(1,3986)	1:11:A:ASN:OD1	1:1:A:MET:CA	2	15.77
(2,5)	1:18:A:ASP:OD1	1:1:A:MET:CA	18	15.76
(2,2)	1:9:A:ASP:OD1	1:1:A:MET:CA	9	15.76
(1,3988)	1:18:A:ASP:OD1	1:1:A:MET:CA	18	15.76
(1,3985)	1:9:A:ASP:OD1	1:1:A:MET:CA	9	15.76
(2,6)	1:18:A:ASP:OD2	1:1:A:MET:CA	13	15.74
(2,2)	1:9:A:ASP:OD1	1:1:A:MET:CA	13	15.74
(1,3989)	1:18:A:ASP:OD2	1:1:A:MET:CA	13	15.74
(1,3985)	1:9:A:ASP:OD1	1:1:A:MET:CA	13	15.74
(2,19)	1:112:A:ASP:OD1	1:4:A:LYS:CA	16	15.73
(2,19)	1:112:A:ASP:OD1	1:4:A:LYS:CA	18	15.73
(2,3)	1:11:A:ASN:OD1	1:1:A:MET:CA	19	15.73
(1,4002)	1:112:A:ASP:OD1	1:4:A:LYS:CA	16	15.73
(1,4002)	1:112:A:ASP:OD1	1:4:A:LYS:CA	18	15.73
(1,3986)	1:11:A:ASN:OD1	1:1:A:MET:CA	19	15.73
(2,17)	1:89:A:ASP:OD1	1:3:A:VAL:CA	6	15.72
(1,4000)	1:89:A:ASP:OD1	1:3:A:VAL:CA	6	15.72
(2,16)	1:84:A:ILE:O	1:3:A:VAL:CA	13	15.7
(2,6)	1:18:A:ASP:OD2	1:1:A:MET:CA	2	15.7
(1,3999)	1:84:A:ILE:O	1:3:A:VAL:CA	13	15.7
(1,3989)	1:18:A:ASP:OD2	1:1:A:MET:CA	2	15.7
(2,11)	1:51:A:ASP:OD1	1:2:A:SER:CA	2	15.68
(1,3994)	1:51:A:ASP:OD1	1:2:A:SER:CA	2	15.68
(2,18)	1:89:A:ASP:OD2	1:3:A:VAL:CA	11	15.66
(2,17)	1:89:A:ASP:OD1	1:3:A:VAL:CA	3	15.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,17)	1:89:A:ASP:OD1	1:3:A:VAL:CA	12	15.66
(2,16)	1:84:A:ILE:O	1:3:A:VAL:CA	18	15.66
(2,15)	1:82:A:ASN:OD1	1:3:A:VAL:CA	6	15.66
(2,14)	1:80:A:ASP:OD1	1:3:A:VAL:CA	3	15.66
(1,4001)	1:89:A:ASP:OD2	1:3:A:VAL:CA	11	15.66
(1,4000)	1:89:A:ASP:OD1	1:3:A:VAL:CA	3	15.66
(1,4000)	1:89:A:ASP:OD1	1:3:A:VAL:CA	12	15.66
(1,3999)	1:84:A:ILE:O	1:3:A:VAL:CA	18	15.66
(1,3998)	1:82:A:ASN:OD1	1:3:A:VAL:CA	6	15.66
(1,3997)	1:80:A:ASP:OD1	1:3:A:VAL:CA	3	15.66
(2,8)	1:42:A:ASP:OD1	1:2:A:SER:CA	20	15.65
(1,3991)	1:42:A:ASP:OD1	1:2:A:SER:CA	20	15.65
(2,19)	1:112:A:ASP:OD1	1:4:A:LYS:CA	12	15.63
(2,10)	1:46:A:TYR:O	1:2:A:SER:CA	17	15.63
(1,4002)	1:112:A:ASP:OD1	1:4:A:LYS:CA	12	15.63
(1,3993)	1:46:A:TYR:O	1:2:A:SER:CA	17	15.63
(2,4)	1:13:A:GLU:O	1:1:A:MET:CA	9	15.62
(1,3987)	1:13:A:GLU:O	1:1:A:MET:CA	9	15.62
(2,17)	1:89:A:ASP:OD1	1:3:A:VAL:CA	1	15.61
(1,4000)	1:89:A:ASP:OD1	1:3:A:VAL:CA	1	15.61
(2,2)	1:9:A:ASP:OD1	1:1:A:MET:CA	2	15.6
(1,3985)	1:9:A:ASP:OD1	1:1:A:MET:CA	2	15.6
(2,19)	1:112:A:ASP:OD1	1:4:A:LYS:CA	2	15.59
(2,6)	1:18:A:ASP:OD2	1:1:A:MET:CA	1	15.59
(1,4002)	1:112:A:ASP:OD1	1:4:A:LYS:CA	2	15.59
(1,3989)	1:18:A:ASP:OD2	1:1:A:MET:CA	1	15.59
(2,19)	1:112:A:ASP:OD1	1:4:A:LYS:CA	7	15.58
(1,4002)	1:112:A:ASP:OD1	1:4:A:LYS:CA	7	15.58
(2,15)	1:82:A:ASN:OD1	1:3:A:VAL:CA	10	15.57
(1,3998)	1:82:A:ASN:OD1	1:3:A:VAL:CA	10	15.57
(2,17)	1:89:A:ASP:OD1	1:3:A:VAL:CA	16	15.54
(1,4000)	1:89:A:ASP:OD1	1:3:A:VAL:CA	16	15.54
(2,17)	1:89:A:ASP:OD1	1:3:A:VAL:CA	9	15.53
(2,15)	1:82:A:ASN:OD1	1:3:A:VAL:CA	9	15.53
(1,4000)	1:89:A:ASP:OD1	1:3:A:VAL:CA	9	15.53
(1,3998)	1:82:A:ASN:OD1	1:3:A:VAL:CA	9	15.53
(2,17)	1:89:A:ASP:OD1	1:3:A:VAL:CA	15	15.51
(2,14)	1:80:A:ASP:OD1	1:3:A:VAL:CA	4	15.51
(2,14)	1:80:A:ASP:OD1	1:3:A:VAL:CA	11	15.51
(1,4000)	1:89:A:ASP:OD1	1:3:A:VAL:CA	15	15.51
(1,3997)	1:80:A:ASP:OD1	1:3:A:VAL:CA	4	15.51
(1,3997)	1:80:A:ASP:OD1	1:3:A:VAL:CA	11	15.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,15)	1:82:A:ASN:OD1	1:3:A:VAL:CA	11	15.49
(2,9)	1:44:A:ASN:OD1	1:2:A:SER:CA	14	15.49
(1,3998)	1:82:A:ASN:OD1	1:3:A:VAL:CA	11	15.49
(1,3992)	1:44:A:ASN:OD1	1:2:A:SER:CA	14	15.49
(2,19)	1:112:A:ASP:OD1	1:4:A:LYS:CA	15	15.48
(2,12)	1:51:A:ASP:OD2	1:2:A:SER:CA	9	15.48
(1,4002)	1:112:A:ASP:OD1	1:4:A:LYS:CA	15	15.48
(1,3995)	1:51:A:ASP:OD2	1:2:A:SER:CA	9	15.48
(2,8)	1:42:A:ASP:OD1	1:2:A:SER:CA	5	15.47
(1,3991)	1:42:A:ASP:OD1	1:2:A:SER:CA	5	15.47
(2,16)	1:84:A:ILE:O	1:3:A:VAL:CA	2	15.46
(2,16)	1:84:A:ILE:O	1:3:A:VAL:CA	17	15.46
(2,6)	1:18:A:ASP:OD2	1:1:A:MET:CA	17	15.46
(2,3)	1:11:A:ASN:OD1	1:1:A:MET:CA	16	15.46
(1,3999)	1:84:A:ILE:O	1:3:A:VAL:CA	2	15.46
(1,3999)	1:84:A:ILE:O	1:3:A:VAL:CA	17	15.46
(1,3989)	1:18:A:ASP:OD2	1:1:A:MET:CA	17	15.46
(1,3986)	1:11:A:ASN:OD1	1:1:A:MET:CA	16	15.46
(2,12)	1:51:A:ASP:OD2	1:2:A:SER:CA	18	15.44
(1,3995)	1:51:A:ASP:OD2	1:2:A:SER:CA	18	15.44
(2,16)	1:84:A:ILE:O	1:3:A:VAL:CA	4	15.42
(1,3999)	1:84:A:ILE:O	1:3:A:VAL:CA	4	15.42
(2,16)	1:84:A:ILE:O	1:3:A:VAL:CA	6	15.4
(2,15)	1:82:A:ASN:OD1	1:3:A:VAL:CA	4	15.4
(1,3999)	1:84:A:ILE:O	1:3:A:VAL:CA	6	15.4
(1,3998)	1:82:A:ASN:OD1	1:3:A:VAL:CA	4	15.4
(2,17)	1:89:A:ASP:OD1	1:3:A:VAL:CA	10	15.39
(1,4000)	1:89:A:ASP:OD1	1:3:A:VAL:CA	10	15.39
(2,10)	1:46:A:TYR:O	1:2:A:SER:CA	2	15.37
(1,3993)	1:46:A:TYR:O	1:2:A:SER:CA	2	15.37
(2,14)	1:80:A:ASP:OD1	1:3:A:VAL:CA	8	15.35
(2,12)	1:51:A:ASP:OD2	1:2:A:SER:CA	13	15.35
(1,3997)	1:80:A:ASP:OD1	1:3:A:VAL:CA	8	15.35
(1,3995)	1:51:A:ASP:OD2	1:2:A:SER:CA	13	15.35
(2,2)	1:9:A:ASP:OD1	1:1:A:MET:CA	20	15.34
(1,3985)	1:9:A:ASP:OD1	1:1:A:MET:CA	20	15.34
(2,15)	1:82:A:ASN:OD1	1:3:A:VAL:CA	1	15.33
(2,15)	1:82:A:ASN:OD1	1:3:A:VAL:CA	3	15.33
(1,3998)	1:82:A:ASN:OD1	1:3:A:VAL:CA	1	15.33
(1,3998)	1:82:A:ASN:OD1	1:3:A:VAL:CA	3	15.33
(2,9)	1:44:A:ASN:OD1	1:2:A:SER:CA	17	15.31
(1,3992)	1:44:A:ASN:OD1	1:2:A:SER:CA	17	15.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,12)	1:51:A:ASP:OD2	1:2:A:SER:CA	14	15.3
(1,3995)	1:51:A:ASP:OD2	1:2:A:SER:CA	14	15.3
(2,18)	1:89:A:ASP:OD2	1:3:A:VAL:CA	19	15.29
(2,10)	1:46:A:TYR:O	1:2:A:SER:CA	3	15.29
(1,4001)	1:89:A:ASP:OD2	1:3:A:VAL:CA	19	15.29
(1,3993)	1:46:A:TYR:O	1:2:A:SER:CA	3	15.29
(2,19)	1:112:A:ASP:OD1	1:4:A:LYS:CA	17	15.28
(1,4002)	1:112:A:ASP:OD1	1:4:A:LYS:CA	17	15.28
(2,12)	1:51:A:ASP:OD2	1:2:A:SER:CA	15	15.27
(1,3995)	1:51:A:ASP:OD2	1:2:A:SER:CA	15	15.27
(2,16)	1:84:A:ILE:O	1:3:A:VAL:CA	11	15.26
(2,11)	1:51:A:ASP:OD1	1:2:A:SER:CA	17	15.26
(1,3999)	1:84:A:ILE:O	1:3:A:VAL:CA	11	15.26
(1,3994)	1:51:A:ASP:OD1	1:2:A:SER:CA	17	15.26
(2,12)	1:51:A:ASP:OD2	1:2:A:SER:CA	6	15.23
(2,3)	1:11:A:ASN:OD1	1:1:A:MET:CA	6	15.23
(1,3995)	1:51:A:ASP:OD2	1:2:A:SER:CA	6	15.23
(1,3986)	1:11:A:ASN:OD1	1:1:A:MET:CA	6	15.23
(2,15)	1:82:A:ASN:OD1	1:3:A:VAL:CA	2	15.22
(2,8)	1:42:A:ASP:OD1	1:2:A:SER:CA	19	15.22
(1,3998)	1:82:A:ASN:OD1	1:3:A:VAL:CA	2	15.22
(1,3991)	1:42:A:ASP:OD1	1:2:A:SER:CA	19	15.22
(2,16)	1:84:A:ILE:O	1:3:A:VAL:CA	10	15.2
(1,3999)	1:84:A:ILE:O	1:3:A:VAL:CA	10	15.2
(2,16)	1:84:A:ILE:O	1:3:A:VAL:CA	1	15.19
(1,3999)	1:84:A:ILE:O	1:3:A:VAL:CA	1	15.19
(2,19)	1:112:A:ASP:OD1	1:4:A:LYS:CA	3	15.18
(2,6)	1:18:A:ASP:OD2	1:1:A:MET:CA	4	15.18
(1,4002)	1:112:A:ASP:OD1	1:4:A:LYS:CA	3	15.18
(1,3989)	1:18:A:ASP:OD2	1:1:A:MET:CA	4	15.18
(2,11)	1:51:A:ASP:OD1	1:2:A:SER:CA	3	15.17
(1,3994)	1:51:A:ASP:OD1	1:2:A:SER:CA	3	15.17
(2,14)	1:80:A:ASP:OD1	1:3:A:VAL:CA	20	15.15
(1,3997)	1:80:A:ASP:OD1	1:3:A:VAL:CA	20	15.15
(2,19)	1:112:A:ASP:OD1	1:4:A:LYS:CA	4	15.14
(2,19)	1:112:A:ASP:OD1	1:4:A:LYS:CA	9	15.14
(2,19)	1:112:A:ASP:OD1	1:4:A:LYS:CA	14	15.14
(2,6)	1:18:A:ASP:OD2	1:1:A:MET:CA	20	15.14
(1,4002)	1:112:A:ASP:OD1	1:4:A:LYS:CA	4	15.14
(1,4002)	1:112:A:ASP:OD1	1:4:A:LYS:CA	9	15.14
(1,4002)	1:112:A:ASP:OD1	1:4:A:LYS:CA	14	15.14
(1,3989)	1:18:A:ASP:OD2	1:1:A:MET:CA	20	15.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,9)	1:44:A:ASN:OD1	1:2:A:SER:CA	3	15.13
(1,3992)	1:44:A:ASN:OD1	1:2:A:SER:CA	3	15.13
(2,9)	1:44:A:ASN:OD1	1:2:A:SER:CA	7	15.12
(1,3992)	1:44:A:ASN:OD1	1:2:A:SER:CA	7	15.12
(2,19)	1:112:A:ASP:OD1	1:4:A:LYS:CA	11	15.11
(2,6)	1:18:A:ASP:OD2	1:1:A:MET:CA	19	15.11
(1,4002)	1:112:A:ASP:OD1	1:4:A:LYS:CA	11	15.11
(1,3989)	1:18:A:ASP:OD2	1:1:A:MET:CA	19	15.11
(2,19)	1:112:A:ASP:OD1	1:4:A:LYS:CA	5	15.1
(2,17)	1:89:A:ASP:OD1	1:3:A:VAL:CA	20	15.1
(2,9)	1:44:A:ASN:OD1	1:2:A:SER:CA	10	15.1
(2,4)	1:13:A:GLU:O	1:1:A:MET:CA	8	15.1
(1,4002)	1:112:A:ASP:OD1	1:4:A:LYS:CA	5	15.1
(1,4000)	1:89:A:ASP:OD1	1:3:A:VAL:CA	20	15.1
(1,3992)	1:44:A:ASN:OD1	1:2:A:SER:CA	10	15.1
(1,3987)	1:13:A:GLU:O	1:1:A:MET:CA	8	15.1
(2,19)	1:112:A:ASP:OD1	1:4:A:LYS:CA	13	15.08
(2,6)	1:18:A:ASP:OD2	1:1:A:MET:CA	16	15.08
(1,4002)	1:112:A:ASP:OD1	1:4:A:LYS:CA	13	15.08
(1,3989)	1:18:A:ASP:OD2	1:1:A:MET:CA	16	15.08
(2,16)	1:84:A:ILE:O	1:3:A:VAL:CA	3	15.07
(1,3999)	1:84:A:ILE:O	1:3:A:VAL:CA	3	15.07
(2,16)	1:84:A:ILE:O	1:3:A:VAL:CA	9	15.06
(2,14)	1:80:A:ASP:OD1	1:3:A:VAL:CA	10	15.06
(2,10)	1:46:A:TYR:O	1:2:A:SER:CA	11	15.06
(2,9)	1:44:A:ASN:OD1	1:2:A:SER:CA	20	15.06
(1,3999)	1:84:A:ILE:O	1:3:A:VAL:CA	9	15.06
(1,3997)	1:80:A:ASP:OD1	1:3:A:VAL:CA	10	15.06
(1,3993)	1:46:A:TYR:O	1:2:A:SER:CA	11	15.06
(1,3992)	1:44:A:ASN:OD1	1:2:A:SER:CA	20	15.06
(2,12)	1:51:A:ASP:OD2	1:2:A:SER:CA	5	15.03
(1,3995)	1:51:A:ASP:OD2	1:2:A:SER:CA	5	15.03
(2,10)	1:46:A:TYR:O	1:2:A:SER:CA	14	15.02
(2,3)	1:11:A:ASN:OD1	1:1:A:MET:CA	1	15.02
(1,3993)	1:46:A:TYR:O	1:2:A:SER:CA	14	15.02
(1,3986)	1:11:A:ASN:OD1	1:1:A:MET:CA	1	15.02
(2,11)	1:51:A:ASP:OD1	1:2:A:SER:CA	16	15.01
(2,9)	1:44:A:ASN:OD1	1:2:A:SER:CA	2	15.01
(1,3994)	1:51:A:ASP:OD1	1:2:A:SER:CA	16	15.01
(1,3992)	1:44:A:ASN:OD1	1:2:A:SER:CA	2	15.01
(2,18)	1:89:A:ASP:OD2	1:3:A:VAL:CA	14	15.0
(2,18)	1:89:A:ASP:OD2	1:3:A:VAL:CA	18	15.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,12)	1:51:A:ASP:OD2	1:2:A:SER:CA	7	15.0
(2,4)	1:13:A:GLU:O	1:1:A:MET:CA	19	15.0
(1,4001)	1:89:A:ASP:OD2	1:3:A:VAL:CA	14	15.0
(1,4001)	1:89:A:ASP:OD2	1:3:A:VAL:CA	18	15.0
(1,3995)	1:51:A:ASP:OD2	1:2:A:SER:CA	7	15.0
(1,3987)	1:13:A:GLU:O	1:1:A:MET:CA	19	15.0
(2,19)	1:112:A:ASP:OD1	1:4:A:LYS:CA	10	14.99
(2,5)	1:18:A:ASP:OD1	1:1:A:MET:CA	3	14.99
(2,4)	1:13:A:GLU:O	1:1:A:MET:CA	6	14.99
(1,4002)	1:112:A:ASP:OD1	1:4:A:LYS:CA	10	14.99
(1,3988)	1:18:A:ASP:OD1	1:1:A:MET:CA	3	14.99
(1,3987)	1:13:A:GLU:O	1:1:A:MET:CA	6	14.99
(2,10)	1:46:A:TYR:O	1:2:A:SER:CA	6	14.98
(2,5)	1:18:A:ASP:OD1	1:1:A:MET:CA	5	14.98
(2,2)	1:9:A:ASP:OD1	1:1:A:MET:CA	5	14.98
(1,3993)	1:46:A:TYR:O	1:2:A:SER:CA	6	14.98
(1,3988)	1:18:A:ASP:OD1	1:1:A:MET:CA	5	14.98
(1,3985)	1:9:A:ASP:OD1	1:1:A:MET:CA	5	14.98
(2,6)	1:18:A:ASP:OD2	1:1:A:MET:CA	6	14.97
(1,3989)	1:18:A:ASP:OD2	1:1:A:MET:CA	6	14.97
(2,11)	1:51:A:ASP:OD1	1:2:A:SER:CA	8	14.96
(1,3994)	1:51:A:ASP:OD1	1:2:A:SER:CA	8	14.96
(2,5)	1:18:A:ASP:OD1	1:1:A:MET:CA	8	14.95
(1,3988)	1:18:A:ASP:OD1	1:1:A:MET:CA	8	14.95
(2,12)	1:51:A:ASP:OD2	1:2:A:SER:CA	11	14.94
(1,3995)	1:51:A:ASP:OD2	1:2:A:SER:CA	11	14.94
(2,15)	1:82:A:ASN:OD1	1:3:A:VAL:CA	16	14.93
(2,11)	1:51:A:ASP:OD1	1:2:A:SER:CA	10	14.93
(2,10)	1:46:A:TYR:O	1:2:A:SER:CA	18	14.93
(1,3998)	1:82:A:ASN:OD1	1:3:A:VAL:CA	16	14.93
(1,3994)	1:51:A:ASP:OD1	1:2:A:SER:CA	10	14.93
(1,3993)	1:46:A:TYR:O	1:2:A:SER:CA	18	14.93
(2,18)	1:89:A:ASP:OD2	1:3:A:VAL:CA	7	14.92
(2,14)	1:80:A:ASP:OD1	1:3:A:VAL:CA	2	14.92
(2,12)	1:51:A:ASP:OD2	1:2:A:SER:CA	4	14.92
(1,4001)	1:89:A:ASP:OD2	1:3:A:VAL:CA	7	14.92
(1,3997)	1:80:A:ASP:OD1	1:3:A:VAL:CA	2	14.92
(1,3995)	1:51:A:ASP:OD2	1:2:A:SER:CA	4	14.92
(2,19)	1:112:A:ASP:OD1	1:4:A:LYS:CA	1	14.91
(2,14)	1:80:A:ASP:OD1	1:3:A:VAL:CA	1	14.91
(2,3)	1:11:A:ASN:OD1	1:1:A:MET:CA	3	14.91
(1,4002)	1:112:A:ASP:OD1	1:4:A:LYS:CA	1	14.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3997)	1:80:A:ASP:OD1	1:3:A:VAL:CA	1	14.91
(1,3986)	1:11:A:ASN:OD1	1:1:A:MET:CA	3	14.91
(2,10)	1:46:A:TYR:O	1:2:A:SER:CA	15	14.89
(2,3)	1:11:A:ASN:OD1	1:1:A:MET:CA	15	14.89
(1,3993)	1:46:A:TYR:O	1:2:A:SER:CA	15	14.89
(1,3986)	1:11:A:ASN:OD1	1:1:A:MET:CA	15	14.89
(2,12)	1:51:A:ASP:OD2	1:2:A:SER:CA	1	14.88
(1,3995)	1:51:A:ASP:OD2	1:2:A:SER:CA	1	14.88
(2,16)	1:84:A:ILE:O	1:3:A:VAL:CA	16	14.87
(2,5)	1:18:A:ASP:OD1	1:1:A:MET:CA	7	14.87
(1,3999)	1:84:A:ILE:O	1:3:A:VAL:CA	16	14.87
(1,3988)	1:18:A:ASP:OD1	1:1:A:MET:CA	7	14.87
(2,18)	1:89:A:ASP:OD2	1:3:A:VAL:CA	8	14.86
(1,4001)	1:89:A:ASP:OD2	1:3:A:VAL:CA	8	14.86
(2,17)	1:89:A:ASP:OD1	1:3:A:VAL:CA	13	14.85
(2,10)	1:46:A:TYR:O	1:2:A:SER:CA	10	14.85
(2,4)	1:13:A:GLU:O	1:1:A:MET:CA	12	14.85
(1,4000)	1:89:A:ASP:OD1	1:3:A:VAL:CA	13	14.85
(1,3993)	1:46:A:TYR:O	1:2:A:SER:CA	10	14.85
(1,3987)	1:13:A:GLU:O	1:1:A:MET:CA	12	14.85
(2,11)	1:51:A:ASP:OD1	1:2:A:SER:CA	20	14.83
(2,10)	1:46:A:TYR:O	1:2:A:SER:CA	4	14.83
(2,9)	1:44:A:ASN:OD1	1:2:A:SER:CA	9	14.83
(2,3)	1:11:A:ASN:OD1	1:1:A:MET:CA	12	14.83
(1,3994)	1:51:A:ASP:OD1	1:2:A:SER:CA	20	14.83
(1,3993)	1:46:A:TYR:O	1:2:A:SER:CA	4	14.83
(1,3992)	1:44:A:ASN:OD1	1:2:A:SER:CA	9	14.83
(1,3986)	1:11:A:ASN:OD1	1:1:A:MET:CA	12	14.83
(2,19)	1:112:A:ASP:OD1	1:4:A:LYS:CA	20	14.82
(2,9)	1:44:A:ASN:OD1	1:2:A:SER:CA	8	14.82
(1,4002)	1:112:A:ASP:OD1	1:4:A:LYS:CA	20	14.82
(1,3992)	1:44:A:ASN:OD1	1:2:A:SER:CA	8	14.82
(2,19)	1:112:A:ASP:OD1	1:4:A:LYS:CA	6	14.81
(2,9)	1:44:A:ASN:OD1	1:2:A:SER:CA	4	14.81
(1,4002)	1:112:A:ASP:OD1	1:4:A:LYS:CA	6	14.81
(1,3992)	1:44:A:ASN:OD1	1:2:A:SER:CA	4	14.81
(2,11)	1:51:A:ASP:OD1	1:2:A:SER:CA	19	14.8
(1,3994)	1:51:A:ASP:OD1	1:2:A:SER:CA	19	14.8
(2,18)	1:89:A:ASP:OD2	1:3:A:VAL:CA	17	14.79
(1,4001)	1:89:A:ASP:OD2	1:3:A:VAL:CA	17	14.79
(2,9)	1:44:A:ASN:OD1	1:2:A:SER:CA	11	14.77
(2,9)	1:44:A:ASN:OD1	1:2:A:SER:CA	18	14.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3)	1:11:A:ASN:OD1	1:1:A:MET:CA	8	14.77
(1,3992)	1:44:A:ASN:OD1	1:2:A:SER:CA	11	14.77
(1,3992)	1:44:A:ASN:OD1	1:2:A:SER:CA	18	14.77
(1,3986)	1:11:A:ASN:OD1	1:1:A:MET:CA	8	14.77
(2,9)	1:44:A:ASN:OD1	1:2:A:SER:CA	15	14.76
(2,4)	1:13:A:GLU:O	1:1:A:MET:CA	15	14.76
(1,3992)	1:44:A:ASN:OD1	1:2:A:SER:CA	15	14.76
(1,3987)	1:13:A:GLU:O	1:1:A:MET:CA	15	14.76
(2,19)	1:112:A:ASP:OD1	1:4:A:LYS:CA	19	14.75
(2,18)	1:89:A:ASP:OD2	1:3:A:VAL:CA	5	14.75
(2,15)	1:82:A:ASN:OD1	1:3:A:VAL:CA	20	14.75
(1,4002)	1:112:A:ASP:OD1	1:4:A:LYS:CA	19	14.75
(1,4001)	1:89:A:ASP:OD2	1:3:A:VAL:CA	5	14.75
(1,3998)	1:82:A:ASN:OD1	1:3:A:VAL:CA	20	14.75
(2,9)	1:44:A:ASN:OD1	1:2:A:SER:CA	16	14.74
(1,3992)	1:44:A:ASN:OD1	1:2:A:SER:CA	16	14.74
(2,18)	1:89:A:ASP:OD2	1:3:A:VAL:CA	4	14.73
(2,10)	1:46:A:TYR:O	1:2:A:SER:CA	13	14.73
(2,10)	1:46:A:TYR:O	1:2:A:SER:CA	20	14.73
(1,4001)	1:89:A:ASP:OD2	1:3:A:VAL:CA	4	14.73
(1,3993)	1:46:A:TYR:O	1:2:A:SER:CA	13	14.73
(1,3993)	1:46:A:TYR:O	1:2:A:SER:CA	20	14.73
(2,10)	1:46:A:TYR:O	1:2:A:SER:CA	16	14.72
(1,3993)	1:46:A:TYR:O	1:2:A:SER:CA	16	14.72
(2,13)	1:78:A:ASP:OD1	1:3:A:VAL:CA	12	14.71
(1,3996)	1:78:A:ASP:OD1	1:3:A:VAL:CA	12	14.71
(2,10)	1:46:A:TYR:O	1:2:A:SER:CA	7	14.68
(1,3993)	1:46:A:TYR:O	1:2:A:SER:CA	7	14.68
(2,14)	1:80:A:ASP:OD1	1:3:A:VAL:CA	16	14.66
(1,3997)	1:80:A:ASP:OD1	1:3:A:VAL:CA	16	14.66
(2,12)	1:51:A:ASP:OD2	1:2:A:SER:CA	12	14.64
(1,3995)	1:51:A:ASP:OD2	1:2:A:SER:CA	12	14.64
(2,2)	1:9:A:ASP:OD1	1:1:A:MET:CA	15	14.63
(1,3985)	1:9:A:ASP:OD1	1:1:A:MET:CA	15	14.63
(2,9)	1:44:A:ASN:OD1	1:2:A:SER:CA	13	14.62
(2,8)	1:42:A:ASP:OD1	1:2:A:SER:CA	14	14.62
(2,4)	1:13:A:GLU:O	1:1:A:MET:CA	1	14.62
(1,3992)	1:44:A:ASN:OD1	1:2:A:SER:CA	13	14.62
(1,3991)	1:42:A:ASP:OD1	1:2:A:SER:CA	14	14.62
(1,3987)	1:13:A:GLU:O	1:1:A:MET:CA	1	14.62
(2,9)	1:44:A:ASN:OD1	1:2:A:SER:CA	6	14.6
(2,4)	1:13:A:GLU:O	1:1:A:MET:CA	16	14.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3992)	1:44:A:ASN:OD1	1:2:A:SER:CA	6	14.6
(1,3987)	1:13:A:GLU:O	1:1:A:MET:CA	16	14.6
(2,9)	1:44:A:ASN:OD1	1:2:A:SER:CA	5	14.57
(2,3)	1:11:A:ASN:OD1	1:1:A:MET:CA	5	14.57
(1,3992)	1:44:A:ASN:OD1	1:2:A:SER:CA	5	14.57
(1,3986)	1:11:A:ASN:OD1	1:1:A:MET:CA	5	14.57
(2,10)	1:46:A:TYR:O	1:2:A:SER:CA	12	14.56
(1,3993)	1:46:A:TYR:O	1:2:A:SER:CA	12	14.56
(2,10)	1:46:A:TYR:O	1:2:A:SER:CA	9	14.53
(1,3993)	1:46:A:TYR:O	1:2:A:SER:CA	9	14.53
(2,5)	1:18:A:ASP:OD1	1:1:A:MET:CA	11	14.49
(1,3988)	1:18:A:ASP:OD1	1:1:A:MET:CA	11	14.49
(2,16)	1:84:A:ILE:O	1:3:A:VAL:CA	20	14.48
(2,5)	1:18:A:ASP:OD1	1:1:A:MET:CA	15	14.48
(2,2)	1:9:A:ASP:OD1	1:1:A:MET:CA	12	14.48
(1,3999)	1:84:A:ILE:O	1:3:A:VAL:CA	20	14.48
(1,3988)	1:18:A:ASP:OD1	1:1:A:MET:CA	15	14.48
(1,3985)	1:9:A:ASP:OD1	1:1:A:MET:CA	12	14.48
(2,4)	1:13:A:GLU:O	1:1:A:MET:CA	18	14.47
(1,3987)	1:13:A:GLU:O	1:1:A:MET:CA	18	14.47
(2,3)	1:11:A:ASN:OD1	1:1:A:MET:CA	4	14.46
(1,3986)	1:11:A:ASN:OD1	1:1:A:MET:CA	4	14.46
(2,13)	1:78:A:ASP:OD1	1:3:A:VAL:CA	19	14.45
(2,6)	1:18:A:ASP:OD2	1:1:A:MET:CA	14	14.45
(1,3996)	1:78:A:ASP:OD1	1:3:A:VAL:CA	19	14.45
(1,3989)	1:18:A:ASP:OD2	1:1:A:MET:CA	14	14.45
(2,18)	1:89:A:ASP:OD2	1:3:A:VAL:CA	3	14.44
(2,10)	1:46:A:TYR:O	1:2:A:SER:CA	8	14.44
(2,9)	1:44:A:ASN:OD1	1:2:A:SER:CA	12	14.44
(2,4)	1:13:A:GLU:O	1:1:A:MET:CA	13	14.44
(1,4001)	1:89:A:ASP:OD2	1:3:A:VAL:CA	3	14.44
(1,3993)	1:46:A:TYR:O	1:2:A:SER:CA	8	14.44
(1,3992)	1:44:A:ASN:OD1	1:2:A:SER:CA	12	14.44
(1,3987)	1:13:A:GLU:O	1:1:A:MET:CA	13	14.44
(2,4)	1:13:A:GLU:O	1:1:A:MET:CA	5	14.4
(1,3987)	1:13:A:GLU:O	1:1:A:MET:CA	5	14.4
(2,18)	1:89:A:ASP:OD2	1:3:A:VAL:CA	2	14.39
(1,4001)	1:89:A:ASP:OD2	1:3:A:VAL:CA	2	14.39
(2,18)	1:89:A:ASP:OD2	1:3:A:VAL:CA	6	14.38
(2,17)	1:89:A:ASP:OD1	1:3:A:VAL:CA	11	14.38
(1,4001)	1:89:A:ASP:OD2	1:3:A:VAL:CA	6	14.38
(1,4000)	1:89:A:ASP:OD1	1:3:A:VAL:CA	11	14.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2)	1:9:A:ASP:OD1	1:1:A:MET:CA	1	14.37
(2,2)	1:9:A:ASP:OD1	1:1:A:MET:CA	14	14.37
(1,3985)	1:9:A:ASP:OD1	1:1:A:MET:CA	1	14.37
(1,3985)	1:9:A:ASP:OD1	1:1:A:MET:CA	14	14.37
(2,9)	1:44:A:ASN:OD1	1:2:A:SER:CA	1	14.36
(1,3992)	1:44:A:ASN:OD1	1:2:A:SER:CA	1	14.36
(2,18)	1:89:A:ASP:OD2	1:3:A:VAL:CA	1	14.35
(1,4001)	1:89:A:ASP:OD2	1:3:A:VAL:CA	1	14.35
(2,5)	1:18:A:ASP:OD1	1:1:A:MET:CA	4	14.31
(1,3988)	1:18:A:ASP:OD1	1:1:A:MET:CA	4	14.31
(2,5)	1:18:A:ASP:OD1	1:1:A:MET:CA	13	14.28
(1,3988)	1:18:A:ASP:OD1	1:1:A:MET:CA	13	14.28
(2,8)	1:42:A:ASP:OD1	1:2:A:SER:CA	17	14.27
(1,3991)	1:42:A:ASP:OD1	1:2:A:SER:CA	17	14.27
(2,6)	1:18:A:ASP:OD2	1:1:A:MET:CA	12	14.24
(2,3)	1:11:A:ASN:OD1	1:1:A:MET:CA	13	14.24
(1,3989)	1:18:A:ASP:OD2	1:1:A:MET:CA	12	14.24
(1,3986)	1:11:A:ASN:OD1	1:1:A:MET:CA	13	14.24
(2,18)	1:89:A:ASP:OD2	1:3:A:VAL:CA	16	14.23
(1,4001)	1:89:A:ASP:OD2	1:3:A:VAL:CA	16	14.23
(2,9)	1:44:A:ASN:OD1	1:2:A:SER:CA	19	14.22
(2,3)	1:11:A:ASN:OD1	1:1:A:MET:CA	18	14.22
(1,3992)	1:44:A:ASN:OD1	1:2:A:SER:CA	19	14.22
(1,3986)	1:11:A:ASN:OD1	1:1:A:MET:CA	18	14.22
(2,2)	1:9:A:ASP:OD1	1:1:A:MET:CA	18	14.2
(1,3985)	1:9:A:ASP:OD1	1:1:A:MET:CA	18	14.2
(2,4)	1:13:A:GLU:O	1:1:A:MET:CA	3	14.19
(1,3987)	1:13:A:GLU:O	1:1:A:MET:CA	3	14.19
(2,18)	1:89:A:ASP:OD2	1:3:A:VAL:CA	9	14.18
(2,5)	1:18:A:ASP:OD1	1:1:A:MET:CA	1	14.18
(1,4001)	1:89:A:ASP:OD2	1:3:A:VAL:CA	9	14.18
(1,3988)	1:18:A:ASP:OD1	1:1:A:MET:CA	1	14.18
(2,13)	1:78:A:ASP:OD1	1:3:A:VAL:CA	15	14.15
(1,3996)	1:78:A:ASP:OD1	1:3:A:VAL:CA	15	14.15
(2,8)	1:42:A:ASP:OD1	1:2:A:SER:CA	9	14.14
(2,8)	1:42:A:ASP:OD1	1:2:A:SER:CA	10	14.14
(1,3991)	1:42:A:ASP:OD1	1:2:A:SER:CA	9	14.14
(1,3991)	1:42:A:ASP:OD1	1:2:A:SER:CA	10	14.14
(2,8)	1:42:A:ASP:OD1	1:2:A:SER:CA	8	14.13
(1,3991)	1:42:A:ASP:OD1	1:2:A:SER:CA	8	14.13
(2,2)	1:9:A:ASP:OD1	1:1:A:MET:CA	4	14.12
(1,3985)	1:9:A:ASP:OD1	1:1:A:MET:CA	4	14.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,18)	1:89:A:ASP:OD2	1:3:A:VAL:CA	10	14.11
(1,4001)	1:89:A:ASP:OD2	1:3:A:VAL:CA	10	14.11
(2,8)	1:42:A:ASP:OD1	1:2:A:SER:CA	7	14.09
(1,3991)	1:42:A:ASP:OD1	1:2:A:SER:CA	7	14.09
(2,6)	1:18:A:ASP:OD2	1:1:A:MET:CA	18	14.04
(1,3989)	1:18:A:ASP:OD2	1:1:A:MET:CA	18	14.04
(2,10)	1:46:A:TYR:O	1:2:A:SER:CA	5	14.02
(1,3993)	1:46:A:TYR:O	1:2:A:SER:CA	5	14.02
(2,13)	1:78:A:ASP:OD1	1:3:A:VAL:CA	7	13.99
(1,3996)	1:78:A:ASP:OD1	1:3:A:VAL:CA	7	13.99
(2,10)	1:46:A:TYR:O	1:2:A:SER:CA	1	13.97
(2,5)	1:18:A:ASP:OD1	1:1:A:MET:CA	17	13.97
(1,3993)	1:46:A:TYR:O	1:2:A:SER:CA	1	13.97
(1,3988)	1:18:A:ASP:OD1	1:1:A:MET:CA	17	13.97
(2,8)	1:42:A:ASP:OD1	1:2:A:SER:CA	2	13.95
(1,3991)	1:42:A:ASP:OD1	1:2:A:SER:CA	2	13.95
(2,11)	1:51:A:ASP:OD1	1:2:A:SER:CA	14	13.94
(1,3994)	1:51:A:ASP:OD1	1:2:A:SER:CA	14	13.94
(2,2)	1:9:A:ASP:OD1	1:1:A:MET:CA	17	13.93
(1,3985)	1:9:A:ASP:OD1	1:1:A:MET:CA	17	13.93
(2,8)	1:42:A:ASP:OD1	1:2:A:SER:CA	13	13.92
(1,3991)	1:42:A:ASP:OD1	1:2:A:SER:CA	13	13.92
(2,8)	1:42:A:ASP:OD1	1:2:A:SER:CA	16	13.91
(1,3991)	1:42:A:ASP:OD1	1:2:A:SER:CA	16	13.91
(2,8)	1:42:A:ASP:OD1	1:2:A:SER:CA	15	13.88
(2,8)	1:42:A:ASP:OD1	1:2:A:SER:CA	18	13.88
(1,3991)	1:42:A:ASP:OD1	1:2:A:SER:CA	15	13.88
(1,3991)	1:42:A:ASP:OD1	1:2:A:SER:CA	18	13.88
(2,5)	1:18:A:ASP:OD1	1:1:A:MET:CA	20	13.87
(1,3988)	1:18:A:ASP:OD1	1:1:A:MET:CA	20	13.87
(2,18)	1:89:A:ASP:OD2	1:3:A:VAL:CA	20	13.86
(2,12)	1:51:A:ASP:OD2	1:2:A:SER:CA	2	13.86
(1,4001)	1:89:A:ASP:OD2	1:3:A:VAL:CA	20	13.86
(1,3995)	1:51:A:ASP:OD2	1:2:A:SER:CA	2	13.86
(2,12)	1:51:A:ASP:OD2	1:2:A:SER:CA	17	13.85
(1,3995)	1:51:A:ASP:OD2	1:2:A:SER:CA	17	13.85
(2,10)	1:46:A:TYR:O	1:2:A:SER:CA	19	13.84
(2,4)	1:13:A:GLU:O	1:1:A:MET:CA	17	13.84
(2,3)	1:11:A:ASN:OD1	1:1:A:MET:CA	17	13.84
(1,3993)	1:46:A:TYR:O	1:2:A:SER:CA	19	13.84
(1,3987)	1:13:A:GLU:O	1:1:A:MET:CA	17	13.84
(1,3986)	1:11:A:ASN:OD1	1:1:A:MET:CA	17	13.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,13)	1:78:A:ASP:OD1	1:3:A:VAL:CA	5	13.82
(2,4)	1:13:A:GLU:O	1:1:A:MET:CA	20	13.82
(1,3996)	1:78:A:ASP:OD1	1:3:A:VAL:CA	5	13.82
(1,3987)	1:13:A:GLU:O	1:1:A:MET:CA	20	13.82
(2,4)	1:13:A:GLU:O	1:1:A:MET:CA	4	13.8
(1,3987)	1:13:A:GLU:O	1:1:A:MET:CA	4	13.8
(2,13)	1:78:A:ASP:OD1	1:3:A:VAL:CA	13	13.78
(1,3996)	1:78:A:ASP:OD1	1:3:A:VAL:CA	13	13.78
(2,13)	1:78:A:ASP:OD1	1:3:A:VAL:CA	14	13.76
(2,8)	1:42:A:ASP:OD1	1:2:A:SER:CA	1	13.76
(2,3)	1:11:A:ASN:OD1	1:1:A:MET:CA	14	13.76
(2,1)	1:7:A:ASP:OD1	1:1:A:MET:CA	9	13.76
(1,3996)	1:78:A:ASP:OD1	1:3:A:VAL:CA	14	13.76
(1,3991)	1:42:A:ASP:OD1	1:2:A:SER:CA	1	13.76
(1,3986)	1:11:A:ASN:OD1	1:1:A:MET:CA	14	13.76
(1,3984)	1:7:A:ASP:OD1	1:1:A:MET:CA	9	13.76
(2,12)	1:51:A:ASP:OD2	1:2:A:SER:CA	10	13.75
(1,3995)	1:51:A:ASP:OD2	1:2:A:SER:CA	10	13.75
(2,8)	1:42:A:ASP:OD1	1:2:A:SER:CA	3	13.73
(2,2)	1:9:A:ASP:OD1	1:1:A:MET:CA	7	13.73
(1,3991)	1:42:A:ASP:OD1	1:2:A:SER:CA	3	13.73
(1,3985)	1:9:A:ASP:OD1	1:1:A:MET:CA	7	13.73
(2,8)	1:42:A:ASP:OD1	1:2:A:SER:CA	4	13.72
(2,8)	1:42:A:ASP:OD1	1:2:A:SER:CA	11	13.72
(1,3991)	1:42:A:ASP:OD1	1:2:A:SER:CA	4	13.72
(1,3991)	1:42:A:ASP:OD1	1:2:A:SER:CA	11	13.72
(2,12)	1:51:A:ASP:OD2	1:2:A:SER:CA	20	13.71
(2,1)	1:7:A:ASP:OD1	1:1:A:MET:CA	2	13.71
(1,3995)	1:51:A:ASP:OD2	1:2:A:SER:CA	20	13.71
(1,3984)	1:7:A:ASP:OD1	1:1:A:MET:CA	2	13.71
(2,13)	1:78:A:ASP:OD1	1:3:A:VAL:CA	8	13.7
(2,12)	1:51:A:ASP:OD2	1:2:A:SER:CA	8	13.7
(2,12)	1:51:A:ASP:OD2	1:2:A:SER:CA	16	13.7
(1,3996)	1:78:A:ASP:OD1	1:3:A:VAL:CA	8	13.7
(1,3995)	1:51:A:ASP:OD2	1:2:A:SER:CA	8	13.7
(1,3995)	1:51:A:ASP:OD2	1:2:A:SER:CA	16	13.7
(2,6)	1:18:A:ASP:OD2	1:1:A:MET:CA	7	13.69
(1,3989)	1:18:A:ASP:OD2	1:1:A:MET:CA	7	13.69
(2,12)	1:51:A:ASP:OD2	1:2:A:SER:CA	3	13.68
(2,11)	1:51:A:ASP:OD1	1:2:A:SER:CA	9	13.68
(1,3995)	1:51:A:ASP:OD2	1:2:A:SER:CA	3	13.68
(1,3994)	1:51:A:ASP:OD1	1:2:A:SER:CA	9	13.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,11)	1:51:A:ASP:OD1	1:2:A:SER:CA	13	13.67
(1,3994)	1:51:A:ASP:OD1	1:2:A:SER:CA	13	13.67
(2,11)	1:51:A:ASP:OD1	1:2:A:SER:CA	11	13.66
(1,3994)	1:51:A:ASP:OD1	1:2:A:SER:CA	11	13.66
(2,5)	1:18:A:ASP:OD1	1:1:A:MET:CA	10	13.63
(1,3988)	1:18:A:ASP:OD1	1:1:A:MET:CA	10	13.63
(2,13)	1:78:A:ASP:OD1	1:3:A:VAL:CA	18	13.62
(1,3996)	1:78:A:ASP:OD1	1:3:A:VAL:CA	18	13.62
(2,4)	1:13:A:GLU:O	1:1:A:MET:CA	14	13.61
(1,3987)	1:13:A:GLU:O	1:1:A:MET:CA	14	13.61
(2,11)	1:51:A:ASP:OD1	1:2:A:SER:CA	18	13.6
(1,3994)	1:51:A:ASP:OD1	1:2:A:SER:CA	18	13.6
(2,11)	1:51:A:ASP:OD1	1:2:A:SER:CA	7	13.58
(1,3994)	1:51:A:ASP:OD1	1:2:A:SER:CA	7	13.58
(2,3)	1:11:A:ASN:OD1	1:1:A:MET:CA	20	13.56
(1,3986)	1:11:A:ASN:OD1	1:1:A:MET:CA	20	13.56
(2,11)	1:51:A:ASP:OD1	1:2:A:SER:CA	5	13.55
(1,3994)	1:51:A:ASP:OD1	1:2:A:SER:CA	5	13.55
(2,11)	1:51:A:ASP:OD1	1:2:A:SER:CA	6	13.51
(1,3994)	1:51:A:ASP:OD1	1:2:A:SER:CA	6	13.51
(2,11)	1:51:A:ASP:OD1	1:2:A:SER:CA	15	13.48
(1,3994)	1:51:A:ASP:OD1	1:2:A:SER:CA	15	13.48
(2,13)	1:78:A:ASP:OD1	1:3:A:VAL:CA	17	13.47
(1,3996)	1:78:A:ASP:OD1	1:3:A:VAL:CA	17	13.47
(2,11)	1:51:A:ASP:OD1	1:2:A:SER:CA	4	13.45
(1,3994)	1:51:A:ASP:OD1	1:2:A:SER:CA	4	13.45
(2,8)	1:42:A:ASP:OD1	1:2:A:SER:CA	12	13.44
(2,3)	1:11:A:ASN:OD1	1:1:A:MET:CA	7	13.44
(1,3991)	1:42:A:ASP:OD1	1:2:A:SER:CA	12	13.44
(1,3986)	1:11:A:ASN:OD1	1:1:A:MET:CA	7	13.44
(2,4)	1:13:A:GLU:O	1:1:A:MET:CA	7	13.41
(1,3987)	1:13:A:GLU:O	1:1:A:MET:CA	7	13.41
(2,12)	1:51:A:ASP:OD2	1:2:A:SER:CA	19	13.38
(1,3995)	1:51:A:ASP:OD2	1:2:A:SER:CA	19	13.38
(2,11)	1:51:A:ASP:OD1	1:2:A:SER:CA	12	13.36
(2,6)	1:18:A:ASP:OD2	1:1:A:MET:CA	11	13.36
(1,3994)	1:51:A:ASP:OD1	1:2:A:SER:CA	12	13.36
(1,3989)	1:18:A:ASP:OD2	1:1:A:MET:CA	11	13.36
(2,8)	1:42:A:ASP:OD1	1:2:A:SER:CA	6	13.35
(1,3991)	1:42:A:ASP:OD1	1:2:A:SER:CA	6	13.35
(2,13)	1:78:A:ASP:OD1	1:3:A:VAL:CA	6	13.3
(2,2)	1:9:A:ASP:OD1	1:1:A:MET:CA	11	13.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3996)	1:78:A:ASP:OD1	1:3:A:VAL:CA	6	13.3
(1,3985)	1:9:A:ASP:OD1	1:1:A:MET:CA	11	13.3
(2,1)	1:7:A:ASP:OD1	1:1:A:MET:CA	19	13.27
(1,3984)	1:7:A:ASP:OD1	1:1:A:MET:CA	19	13.27
(2,3)	1:11:A:ASN:OD1	1:1:A:MET:CA	11	13.26
(1,3986)	1:11:A:ASN:OD1	1:1:A:MET:CA	11	13.26
(2,11)	1:51:A:ASP:OD1	1:2:A:SER:CA	1	13.24
(1,3994)	1:51:A:ASP:OD1	1:2:A:SER:CA	1	13.24
(2,13)	1:78:A:ASP:OD1	1:3:A:VAL:CA	4	13.23
(1,3996)	1:78:A:ASP:OD1	1:3:A:VAL:CA	4	13.23
(2,13)	1:78:A:ASP:OD1	1:3:A:VAL:CA	2	13.19
(1,3996)	1:78:A:ASP:OD1	1:3:A:VAL:CA	2	13.19
(2,4)	1:13:A:GLU:O	1:1:A:MET:CA	11	13.17
(1,3987)	1:13:A:GLU:O	1:1:A:MET:CA	11	13.17
(2,13)	1:78:A:ASP:OD1	1:3:A:VAL:CA	11	13.11
(1,3996)	1:78:A:ASP:OD1	1:3:A:VAL:CA	11	13.11
(2,13)	1:78:A:ASP:OD1	1:3:A:VAL:CA	10	13.07
(1,3996)	1:78:A:ASP:OD1	1:3:A:VAL:CA	10	13.07
(2,13)	1:78:A:ASP:OD1	1:3:A:VAL:CA	1	13.04
(1,3996)	1:78:A:ASP:OD1	1:3:A:VAL:CA	1	13.04
(2,13)	1:78:A:ASP:OD1	1:3:A:VAL:CA	3	13.03
(1,3996)	1:78:A:ASP:OD1	1:3:A:VAL:CA	3	13.03
(2,13)	1:78:A:ASP:OD1	1:3:A:VAL:CA	9	13.02
(2,1)	1:7:A:ASP:OD1	1:1:A:MET:CA	6	13.02
(2,1)	1:7:A:ASP:OD1	1:1:A:MET:CA	16	13.02
(1,3996)	1:78:A:ASP:OD1	1:3:A:VAL:CA	9	13.02
(1,3984)	1:7:A:ASP:OD1	1:1:A:MET:CA	6	13.02
(1,3984)	1:7:A:ASP:OD1	1:1:A:MET:CA	16	13.02
(2,1)	1:7:A:ASP:OD1	1:1:A:MET:CA	3	12.82
(1,3984)	1:7:A:ASP:OD1	1:1:A:MET:CA	3	12.82
(2,13)	1:78:A:ASP:OD1	1:3:A:VAL:CA	16	12.78
(1,3996)	1:78:A:ASP:OD1	1:3:A:VAL:CA	16	12.78
(2,1)	1:7:A:ASP:OD1	1:1:A:MET:CA	5	12.75
(1,3984)	1:7:A:ASP:OD1	1:1:A:MET:CA	5	12.75
(2,1)	1:7:A:ASP:OD1	1:1:A:MET:CA	8	12.72
(1,3984)	1:7:A:ASP:OD1	1:1:A:MET:CA	8	12.72
(2,1)	1:7:A:ASP:OD1	1:1:A:MET:CA	12	12.66
(1,3984)	1:7:A:ASP:OD1	1:1:A:MET:CA	12	12.66
(2,1)	1:7:A:ASP:OD1	1:1:A:MET:CA	15	12.65
(1,3984)	1:7:A:ASP:OD1	1:1:A:MET:CA	15	12.65
(2,7)	1:40:A:ASP:OD1	1:2:A:SER:CA	2	12.63
(1,3990)	1:40:A:ASP:OD1	1:2:A:SER:CA	2	12.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,7)	1:40:A:ASP:OD1	1:2:A:SER:CA	3	12.53
(2,7)	1:40:A:ASP:OD1	1:2:A:SER:CA	14	12.53
(1,3990)	1:40:A:ASP:OD1	1:2:A:SER:CA	3	12.53
(1,3990)	1:40:A:ASP:OD1	1:2:A:SER:CA	14	12.53
(2,1)	1:7:A:ASP:OD1	1:1:A:MET:CA	1	12.52
(1,3984)	1:7:A:ASP:OD1	1:1:A:MET:CA	1	12.52
(2,13)	1:78:A:ASP:OD1	1:3:A:VAL:CA	20	12.46
(1,3996)	1:78:A:ASP:OD1	1:3:A:VAL:CA	20	12.46
(2,7)	1:40:A:ASP:OD1	1:2:A:SER:CA	20	12.4
(1,3990)	1:40:A:ASP:OD1	1:2:A:SER:CA	20	12.4
(2,7)	1:40:A:ASP:OD1	1:2:A:SER:CA	10	12.35
(1,3990)	1:40:A:ASP:OD1	1:2:A:SER:CA	10	12.35
(2,6)	1:18:A:ASP:OD2	1:1:A:MET:CA	10	12.32
(1,3989)	1:18:A:ASP:OD2	1:1:A:MET:CA	10	12.32
(2,7)	1:40:A:ASP:OD1	1:2:A:SER:CA	8	12.29
(2,7)	1:40:A:ASP:OD1	1:2:A:SER:CA	18	12.29
(1,3990)	1:40:A:ASP:OD1	1:2:A:SER:CA	8	12.29
(1,3990)	1:40:A:ASP:OD1	1:2:A:SER:CA	18	12.29
(2,7)	1:40:A:ASP:OD1	1:2:A:SER:CA	11	12.27
(1,3990)	1:40:A:ASP:OD1	1:2:A:SER:CA	11	12.27
(2,1)	1:7:A:ASP:OD1	1:1:A:MET:CA	18	12.26
(1,3984)	1:7:A:ASP:OD1	1:1:A:MET:CA	18	12.26
(2,7)	1:40:A:ASP:OD1	1:2:A:SER:CA	15	12.25
(1,3990)	1:40:A:ASP:OD1	1:2:A:SER:CA	15	12.25
(2,7)	1:40:A:ASP:OD1	1:2:A:SER:CA	9	12.24
(2,7)	1:40:A:ASP:OD1	1:2:A:SER:CA	13	12.24
(1,3990)	1:40:A:ASP:OD1	1:2:A:SER:CA	9	12.24
(1,3990)	1:40:A:ASP:OD1	1:2:A:SER:CA	13	12.24
(2,1)	1:7:A:ASP:OD1	1:1:A:MET:CA	13	12.22
(1,3984)	1:7:A:ASP:OD1	1:1:A:MET:CA	13	12.22
(2,7)	1:40:A:ASP:OD1	1:2:A:SER:CA	4	12.19
(1,3990)	1:40:A:ASP:OD1	1:2:A:SER:CA	4	12.19
(2,7)	1:40:A:ASP:OD1	1:2:A:SER:CA	16	12.17
(1,3990)	1:40:A:ASP:OD1	1:2:A:SER:CA	16	12.17
(2,7)	1:40:A:ASP:OD1	1:2:A:SER:CA	6	12.12
(1,3990)	1:40:A:ASP:OD1	1:2:A:SER:CA	6	12.12
(2,7)	1:40:A:ASP:OD1	1:2:A:SER:CA	7	12.1
(2,1)	1:7:A:ASP:OD1	1:1:A:MET:CA	4	12.1
(1,3990)	1:40:A:ASP:OD1	1:2:A:SER:CA	7	12.1
(1,3984)	1:7:A:ASP:OD1	1:1:A:MET:CA	4	12.1
(2,7)	1:40:A:ASP:OD1	1:2:A:SER:CA	5	12.07
(1,3990)	1:40:A:ASP:OD1	1:2:A:SER:CA	5	12.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1)	1:7:A:ASP:OD1	1:1:A:MET:CA	14	12.02
(1,3984)	1:7:A:ASP:OD1	1:1:A:MET:CA	14	12.02
(2,7)	1:40:A:ASP:OD1	1:2:A:SER:CA	12	11.92
(1,3990)	1:40:A:ASP:OD1	1:2:A:SER:CA	12	11.92
(2,1)	1:7:A:ASP:OD1	1:1:A:MET:CA	17	11.88
(1,3984)	1:7:A:ASP:OD1	1:1:A:MET:CA	17	11.88
(2,7)	1:40:A:ASP:OD1	1:2:A:SER:CA	17	11.8
(1,3990)	1:40:A:ASP:OD1	1:2:A:SER:CA	17	11.8
(2,7)	1:40:A:ASP:OD1	1:2:A:SER:CA	19	11.77
(1,3990)	1:40:A:ASP:OD1	1:2:A:SER:CA	19	11.77
(2,2)	1:9:A:ASP:OD1	1:1:A:MET:CA	10	11.73
(1,3985)	1:9:A:ASP:OD1	1:1:A:MET:CA	10	11.73
(2,1)	1:7:A:ASP:OD1	1:1:A:MET:CA	20	11.72
(1,3984)	1:7:A:ASP:OD1	1:1:A:MET:CA	20	11.72
(2,7)	1:40:A:ASP:OD1	1:2:A:SER:CA	1	11.7
(1,3990)	1:40:A:ASP:OD1	1:2:A:SER:CA	1	11.7
(2,4)	1:13:A:GLU:O	1:1:A:MET:CA	10	11.65
(1,3987)	1:13:A:GLU:O	1:1:A:MET:CA	10	11.65
(2,1)	1:7:A:ASP:OD1	1:1:A:MET:CA	7	11.52
(1,3984)	1:7:A:ASP:OD1	1:1:A:MET:CA	7	11.52
(2,3)	1:11:A:ASN:OD1	1:1:A:MET:CA	10	11.4
(1,3986)	1:11:A:ASN:OD1	1:1:A:MET:CA	10	11.4
(2,1)	1:7:A:ASP:OD1	1:1:A:MET:CA	11	11.24
(1,3984)	1:7:A:ASP:OD1	1:1:A:MET:CA	11	11.24
(2,1)	1:7:A:ASP:OD1	1:1:A:MET:CA	10	9.74
(1,3984)	1:7:A:ASP:OD1	1:1:A:MET:CA	10	9.74
(1,2306)	1:71:A:ASN:H	1:5:A:ILE:HG13	9	0.97
(1,2306)	1:71:A:ASN:H	1:5:A:ILE:HG13	7	0.92
(1,2995)	1:70:A:LYS:HB3	1:5:A:ILE:HG21	17	0.9
(1,2995)	1:70:A:LYS:HB3	1:5:A:ILE:HG22	17	0.9
(1,2995)	1:70:A:LYS:HB3	1:5:A:ILE:HG23	17	0.9
(1,3890)	1:73:A:ILE:H	1:2:A:SER:HB2	16	0.87
(1,1150)	1:134:A:ARG:HG2	1:129:A:LYS:H	6	0.85
(1,1150)	1:134:A:ARG:HG3	1:129:A:LYS:H	6	0.85
(1,3408)	1:59:A:LEU:HD11	1:15:A:SER:HB3	7	0.83
(1,3408)	1:59:A:LEU:HD12	1:15:A:SER:HB3	7	0.83
(1,3408)	1:59:A:LEU:HD13	1:15:A:SER:HB3	7	0.83
(1,2942)	1:90:A:TYR:HB3	1:131:A:ILE:HG21	1	0.83
(1,2942)	1:90:A:TYR:HB3	1:131:A:ILE:HG22	1	0.83
(1,2942)	1:90:A:TYR:HB3	1:131:A:ILE:HG23	1	0.83
(1,2410)	1:102:A:GLN:HG3	1:108:A:LEU:HG	18	0.83
(1,1150)	1:134:A:ARG:HB3	1:129:A:LYS:H	15	0.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,883)	1:59:A:LEU:HB3	1:61:A:GLY:H	4	0.83
(1,1505)	1:2:A:SER:HA	1:73:A:ILE:HD11	1	0.82
(1,1505)	1:2:A:SER:HA	1:73:A:ILE:HD12	1	0.82
(1,1505)	1:2:A:SER:HA	1:73:A:ILE:HD13	1	0.82
(1,3890)	1:71:A:ASN:H	1:2:A:SER:HB2	19	0.81
(1,2410)	1:102:A:GLN:HG3	1:108:A:LEU:HG	17	0.81
(1,2410)	1:102:A:GLN:HG3	1:108:A:LEU:HG	19	0.81
(1,2306)	1:71:A:ASN:H	1:5:A:ILE:HG13	3	0.81
(1,1162)	1:79:A:ILE:HG21	1:111:A:ALA:H	19	0.81
(1,1162)	1:79:A:ILE:HG22	1:111:A:ALA:H	19	0.81
(1,1162)	1:79:A:ILE:HG23	1:111:A:ALA:H	19	0.81
(1,3408)	1:59:A:LEU:HD11	1:15:A:SER:HB3	2	0.79
(1,3408)	1:59:A:LEU:HD12	1:15:A:SER:HB3	2	0.79
(1,3408)	1:59:A:LEU:HD13	1:15:A:SER:HB3	2	0.79
(1,572)	1:9:A:ASP:HB3	1:20:A:ALA:H	8	0.79
(1,3408)	1:59:A:LEU:HD11	1:15:A:SER:HB3	1	0.78
(1,3408)	1:59:A:LEU:HD12	1:15:A:SER:HB3	1	0.78
(1,3408)	1:59:A:LEU:HD13	1:15:A:SER:HB3	1	0.78
(1,2697)	1:128:A:GLU:HG2	1:132:A:THR:HG21	7	0.78
(1,2697)	1:128:A:GLU:HG2	1:132:A:THR:HG22	7	0.78
(1,2697)	1:128:A:GLU:HG2	1:132:A:THR:HG23	7	0.78
(1,2697)	1:128:A:GLU:HG3	1:132:A:THR:HG21	7	0.78
(1,2697)	1:128:A:GLU:HG3	1:132:A:THR:HG22	7	0.78
(1,2697)	1:128:A:GLU:HG3	1:132:A:THR:HG23	7	0.78
(1,3408)	1:59:A:LEU:HD11	1:15:A:SER:HB3	16	0.77
(1,3408)	1:59:A:LEU:HD12	1:15:A:SER:HB3	16	0.77
(1,3408)	1:59:A:LEU:HD13	1:15:A:SER:HB3	16	0.77
(1,1150)	1:134:A:ARG:HG2	1:129:A:LYS:H	8	0.77
(1,1150)	1:134:A:ARG:HG3	1:129:A:LYS:H	8	0.77
(1,883)	1:59:A:LEU:HB3	1:61:A:GLY:H	5	0.77
(1,3408)	1:59:A:LEU:HD11	1:15:A:SER:HB3	13	0.76
(1,3408)	1:59:A:LEU:HD12	1:15:A:SER:HB3	13	0.76
(1,3408)	1:59:A:LEU:HD13	1:15:A:SER:HB3	13	0.76
(1,2995)	1:70:A:LYS:HB3	1:5:A:ILE:HG21	2	0.76
(1,2995)	1:70:A:LYS:HB3	1:5:A:ILE:HG22	2	0.76
(1,2995)	1:70:A:LYS:HB3	1:5:A:ILE:HG23	2	0.76
(1,2410)	1:102:A:GLN:HG3	1:108:A:LEU:HG	11	0.76
(1,2410)	1:102:A:GLN:HG3	1:108:A:LEU:HG	14	0.76
(1,1032)	1:93:A:ILE:HD11	1:112:A:ASP:H	5	0.76
(1,1032)	1:93:A:ILE:HD12	1:112:A:ASP:H	5	0.76
(1,1032)	1:93:A:ILE:HD13	1:112:A:ASP:H	5	0.76
(1,1032)	1:79:A:ILE:HD11	1:112:A:ASP:H	7	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1032)	1:79:A:ILE:HD12	1:112:A:ASP:H	7	0.76
(1,1032)	1:79:A:ILE:HD13	1:112:A:ASP:H	7	0.76
(1,3408)	1:59:A:LEU:HD11	1:15:A:SER:HB3	14	0.75
(1,3408)	1:59:A:LEU:HD12	1:15:A:SER:HB3	14	0.75
(1,3408)	1:59:A:LEU:HD13	1:15:A:SER:HB3	14	0.75
(1,3408)	1:59:A:LEU:HD11	1:15:A:SER:HB3	20	0.75
(1,3408)	1:59:A:LEU:HD12	1:15:A:SER:HB3	20	0.75
(1,3408)	1:59:A:LEU:HD13	1:15:A:SER:HB3	20	0.75
(1,2306)	1:73:A:ILE:H	1:5:A:ILE:HG13	1	0.75
(1,1162)	1:79:A:ILE:HG21	1:111:A:ALA:H	12	0.75
(1,1162)	1:79:A:ILE:HG22	1:111:A:ALA:H	12	0.75
(1,1162)	1:79:A:ILE:HG23	1:111:A:ALA:H	12	0.75
(1,1162)	1:79:A:ILE:HG21	1:111:A:ALA:H	13	0.75
(1,1162)	1:79:A:ILE:HG22	1:111:A:ALA:H	13	0.75
(1,1162)	1:79:A:ILE:HG23	1:111:A:ALA:H	13	0.75
(1,1032)	1:93:A:ILE:HD11	1:112:A:ASP:H	1	0.75
(1,1032)	1:93:A:ILE:HD12	1:112:A:ASP:H	1	0.75
(1,1032)	1:93:A:ILE:HD13	1:112:A:ASP:H	1	0.75
(1,396)	1:39:A:ALA:HA	1:8:A:ILE:H	18	0.75
(1,2970)	1:87:A:GLU:HG2	1:127:A:ILE:HG21	12	0.74
(1,2970)	1:87:A:GLU:HG2	1:127:A:ILE:HG22	12	0.74
(1,2970)	1:87:A:GLU:HG2	1:127:A:ILE:HG23	12	0.74
(1,2410)	1:102:A:GLN:HG3	1:108:A:LEU:HG	8	0.74
(1,883)	1:59:A:LEU:HB3	1:61:A:GLY:H	15	0.74
(1,2942)	1:86:A:ASP:HB2	1:131:A:ILE:HG21	14	0.73
(1,2942)	1:86:A:ASP:HB2	1:131:A:ILE:HG22	14	0.73
(1,2942)	1:86:A:ASP:HB2	1:131:A:ILE:HG23	14	0.73
(1,1162)	1:79:A:ILE:HG21	1:111:A:ALA:H	15	0.73
(1,1162)	1:79:A:ILE:HG22	1:111:A:ALA:H	15	0.73
(1,1162)	1:79:A:ILE:HG23	1:111:A:ALA:H	15	0.73
(1,1150)	1:134:A:ARG:HG2	1:129:A:LYS:H	16	0.73
(1,1150)	1:134:A:ARG:HG3	1:129:A:LYS:H	16	0.73
(1,3875)	1:55:A:LEU:HB3	1:8:A:ILE:HG12	7	0.72
(1,3875)	1:55:A:LEU:HB3	1:8:A:ILE:HG13	7	0.72
(1,3596)	1:38:A:ALA:HA	1:14:A:ILE:HD11	10	0.72
(1,3596)	1:38:A:ALA:HA	1:14:A:ILE:HD12	10	0.72
(1,3596)	1:38:A:ALA:HA	1:14:A:ILE:HD13	10	0.72
(1,2942)	1:86:A:ASP:HB2	1:131:A:ILE:HG21	2	0.72
(1,2942)	1:86:A:ASP:HB2	1:131:A:ILE:HG22	2	0.72
(1,2942)	1:86:A:ASP:HB2	1:131:A:ILE:HG23	2	0.72
(1,2523)	1:137:A:HIS:HB3	1:135:A:ILE:HG13	16	0.72
(1,2522)	1:139:A:PRO:HD2	1:135:A:ILE:HG13	11	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2522)	1:139:A:PRO:HD3	1:135:A:ILE:HG13	11	0.72
(1,1353)	1:55:A:LEU:H	1:68:A:ILE:HD11	20	0.72
(1,1353)	1:55:A:LEU:H	1:68:A:ILE:HD12	20	0.72
(1,1353)	1:55:A:LEU:H	1:68:A:ILE:HD13	20	0.72
(1,1032)	1:93:A:ILE:HD11	1:112:A:ASP:H	3	0.72
(1,1032)	1:93:A:ILE:HD12	1:112:A:ASP:H	3	0.72
(1,1032)	1:93:A:ILE:HD13	1:112:A:ASP:H	3	0.72
(1,3408)	1:59:A:LEU:HD11	1:15:A:SER:HB3	12	0.71
(1,3408)	1:59:A:LEU:HD12	1:15:A:SER:HB3	12	0.71
(1,3408)	1:59:A:LEU:HD13	1:15:A:SER:HB3	12	0.71
(1,3408)	1:59:A:LEU:HD11	1:15:A:SER:HB3	17	0.71
(1,3408)	1:59:A:LEU:HD12	1:15:A:SER:HB3	17	0.71
(1,3408)	1:59:A:LEU:HD13	1:15:A:SER:HB3	17	0.71
(1,2522)	1:139:A:PRO:HD2	1:135:A:ILE:HG13	7	0.71
(1,2522)	1:139:A:PRO:HD3	1:135:A:ILE:HG13	7	0.71
(1,2410)	1:102:A:GLN:HG3	1:108:A:LEU:HG	15	0.71
(1,1067)	1:68:A:ILE:HD11	1:63:A:GLY:H	10	0.71
(1,1067)	1:68:A:ILE:HD12	1:63:A:GLY:H	10	0.71
(1,1067)	1:68:A:ILE:HD13	1:63:A:GLY:H	10	0.71
(1,929)	1:3:A:VAL:HG21	1:34:A:LYS:H	8	0.71
(1,929)	1:3:A:VAL:HG22	1:34:A:LYS:H	8	0.71
(1,929)	1:3:A:VAL:HG23	1:34:A:LYS:H	8	0.71
(1,929)	1:3:A:VAL:HG21	1:34:A:LYS:H	20	0.71
(1,929)	1:3:A:VAL:HG22	1:34:A:LYS:H	20	0.71
(1,929)	1:3:A:VAL:HG23	1:34:A:LYS:H	20	0.71
(1,3695)	1:108:A:LEU:HD21	1:102:A:GLN:HG2	19	0.7
(1,3695)	1:108:A:LEU:HD22	1:102:A:GLN:HG2	19	0.7
(1,3695)	1:108:A:LEU:HD23	1:102:A:GLN:HG2	19	0.7
(1,3408)	1:59:A:LEU:HD11	1:15:A:SER:HB3	10	0.7
(1,3408)	1:59:A:LEU:HD12	1:15:A:SER:HB3	10	0.7
(1,3408)	1:59:A:LEU:HD13	1:15:A:SER:HB3	10	0.7
(1,3386)	1:32:A:THR:HA	1:31:A:LEU:HD11	8	0.7
(1,3386)	1:32:A:THR:HA	1:31:A:LEU:HD12	8	0.7
(1,3386)	1:32:A:THR:HA	1:31:A:LEU:HD13	8	0.7
(1,2995)	1:70:A:LYS:HB3	1:5:A:ILE:HG21	9	0.7
(1,2995)	1:70:A:LYS:HB3	1:5:A:ILE:HG22	9	0.7
(1,2995)	1:70:A:LYS:HB3	1:5:A:ILE:HG23	9	0.7
(1,2697)	1:135:A:ILE:HB	1:136:A:THR:HG21	1	0.7
(1,2697)	1:135:A:ILE:HB	1:136:A:THR:HG22	1	0.7
(1,2697)	1:135:A:ILE:HB	1:136:A:THR:HG23	1	0.7
(1,2523)	1:137:A:HIS:HB3	1:135:A:ILE:HG13	18	0.7
(1,2306)	1:71:A:ASN:H	1:5:A:ILE:HG13	2	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1353)	1:66:A:SER:H	1:68:A:ILE:HD11	14	0.7
(1,1353)	1:66:A:SER:H	1:68:A:ILE:HD12	14	0.7
(1,1353)	1:66:A:SER:H	1:68:A:ILE:HD13	14	0.7
(1,1162)	1:79:A:ILE:HG21	1:111:A:ALA:H	18	0.7
(1,1162)	1:79:A:ILE:HG22	1:111:A:ALA:H	18	0.7
(1,1162)	1:79:A:ILE:HG23	1:111:A:ALA:H	18	0.7
(1,1067)	1:68:A:ILE:HD11	1:63:A:GLY:H	3	0.7
(1,1067)	1:68:A:ILE:HD12	1:63:A:GLY:H	3	0.7
(1,1067)	1:68:A:ILE:HD13	1:63:A:GLY:H	3	0.7
(1,1043)	1:8:A:ILE:HG21	1:32:A:THR:H	4	0.7
(1,1043)	1:8:A:ILE:HG22	1:32:A:THR:H	4	0.7
(1,1043)	1:8:A:ILE:HG23	1:32:A:THR:H	4	0.7
(1,1032)	1:79:A:ILE:HD11	1:112:A:ASP:H	2	0.7
(1,1032)	1:79:A:ILE:HD12	1:112:A:ASP:H	2	0.7
(1,1032)	1:79:A:ILE:HD13	1:112:A:ASP:H	2	0.7
(1,883)	1:59:A:LEU:HB3	1:61:A:GLY:H	17	0.7
(1,883)	1:59:A:LEU:HB3	1:61:A:GLY:H	19	0.7
(1,2995)	1:70:A:LYS:HB3	1:5:A:ILE:HG21	3	0.69
(1,2995)	1:70:A:LYS:HB3	1:5:A:ILE:HG22	3	0.69
(1,2995)	1:70:A:LYS:HB3	1:5:A:ILE:HG23	3	0.69
(1,2942)	1:86:A:ASP:HB2	1:131:A:ILE:HG21	20	0.69
(1,2942)	1:86:A:ASP:HB2	1:131:A:ILE:HG22	20	0.69
(1,2942)	1:86:A:ASP:HB2	1:131:A:ILE:HG23	20	0.69
(1,2522)	1:23:A:LYS:HA	1:22:A:LEU:HD21	9	0.69
(1,2522)	1:23:A:LYS:HA	1:22:A:LEU:HD22	9	0.69
(1,2522)	1:23:A:LYS:HA	1:22:A:LEU:HD23	9	0.69
(1,1784)	1:130:A:TYR:H	1:129:A:LYS:HE2	18	0.69
(1,1784)	1:130:A:TYR:H	1:129:A:LYS:HE3	18	0.69
(1,1032)	1:93:A:ILE:HD11	1:112:A:ASP:H	13	0.69
(1,1032)	1:93:A:ILE:HD12	1:112:A:ASP:H	13	0.69
(1,1032)	1:93:A:ILE:HD13	1:112:A:ASP:H	13	0.69
(1,883)	1:59:A:LEU:HB3	1:61:A:GLY:H	1	0.69
(1,3875)	1:55:A:LEU:HB3	1:8:A:ILE:HG12	18	0.68
(1,3875)	1:55:A:LEU:HB3	1:8:A:ILE:HG13	18	0.68
(1,3695)	1:108:A:LEU:HD21	1:102:A:GLN:HG2	1	0.68
(1,3695)	1:108:A:LEU:HD22	1:102:A:GLN:HG2	1	0.68
(1,3695)	1:108:A:LEU:HD23	1:102:A:GLN:HG2	1	0.68
(1,3596)	1:15:A:SER:HB3	1:14:A:ILE:HD11	8	0.68
(1,3596)	1:15:A:SER:HB3	1:14:A:ILE:HD12	8	0.68
(1,3596)	1:15:A:SER:HB3	1:14:A:ILE:HD13	8	0.68
(1,3596)	1:15:A:SER:HB3	1:14:A:ILE:HD11	14	0.68
(1,3596)	1:15:A:SER:HB3	1:14:A:ILE:HD12	14	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3596)	1:15:A:SER:HB3	1:14:A:ILE:HD13	14	0.68
(1,2966)	1:95:A:ASN:HB3	1:91:A:ILE:HG21	19	0.68
(1,2966)	1:95:A:ASN:HB3	1:91:A:ILE:HG22	19	0.68
(1,2966)	1:95:A:ASN:HB3	1:91:A:ILE:HG23	19	0.68
(1,2410)	1:102:A:GLN:HG3	1:108:A:LEU:HG	9	0.68
(1,1505)	1:72:A:ARG:HA	1:73:A:ILE:HD11	15	0.68
(1,1505)	1:72:A:ARG:HA	1:73:A:ILE:HD12	15	0.68
(1,1505)	1:72:A:ARG:HA	1:73:A:ILE:HD13	15	0.68
(1,1067)	1:60:A:LEU:HD21	1:63:A:GLY:H	7	0.68
(1,1067)	1:60:A:LEU:HD22	1:63:A:GLY:H	7	0.68
(1,1067)	1:60:A:LEU:HD23	1:63:A:GLY:H	7	0.68
(1,1032)	1:93:A:ILE:HD11	1:112:A:ASP:H	14	0.68
(1,1032)	1:93:A:ILE:HD12	1:112:A:ASP:H	14	0.68
(1,1032)	1:93:A:ILE:HD13	1:112:A:ASP:H	14	0.68
(1,1032)	1:93:A:ILE:HD11	1:112:A:ASP:H	16	0.68
(1,1032)	1:93:A:ILE:HD12	1:112:A:ASP:H	16	0.68
(1,1032)	1:93:A:ILE:HD13	1:112:A:ASP:H	16	0.68
(1,1032)	1:93:A:ILE:HD11	1:112:A:ASP:H	18	0.68
(1,1032)	1:93:A:ILE:HD12	1:112:A:ASP:H	18	0.68
(1,1032)	1:93:A:ILE:HD13	1:112:A:ASP:H	18	0.68
(1,929)	1:3:A:VAL:HG21	1:34:A:LYS:H	14	0.68
(1,929)	1:3:A:VAL:HG22	1:34:A:LYS:H	14	0.68
(1,929)	1:3:A:VAL:HG23	1:34:A:LYS:H	14	0.68
(1,929)	1:3:A:VAL:HG21	1:34:A:LYS:H	17	0.68
(1,929)	1:3:A:VAL:HG22	1:34:A:LYS:H	17	0.68
(1,929)	1:3:A:VAL:HG23	1:34:A:LYS:H	17	0.68
(1,396)	1:39:A:ALA:HA	1:8:A:ILE:H	1	0.68
(1,3386)	1:32:A:THR:HA	1:31:A:LEU:HD11	2	0.67
(1,3386)	1:32:A:THR:HA	1:31:A:LEU:HD12	2	0.67
(1,3386)	1:32:A:THR:HA	1:31:A:LEU:HD13	2	0.67
(1,2523)	1:8:A:ILE:HA	1:22:A:LEU:HD21	11	0.67
(1,2523)	1:8:A:ILE:HA	1:22:A:LEU:HD22	11	0.67
(1,2523)	1:8:A:ILE:HA	1:22:A:LEU:HD23	11	0.67
(1,2522)	1:23:A:LYS:HA	1:22:A:LEU:HD21	12	0.67
(1,2522)	1:23:A:LYS:HA	1:22:A:LEU:HD22	12	0.67
(1,2522)	1:23:A:LYS:HA	1:22:A:LEU:HD23	12	0.67
(1,1067)	1:68:A:ILE:HD11	1:63:A:GLY:H	9	0.67
(1,1067)	1:68:A:ILE:HD12	1:63:A:GLY:H	9	0.67
(1,1067)	1:68:A:ILE:HD13	1:63:A:GLY:H	9	0.67
(1,1032)	1:93:A:ILE:HD11	1:112:A:ASP:H	10	0.67
(1,1032)	1:93:A:ILE:HD12	1:112:A:ASP:H	10	0.67
(1,1032)	1:93:A:ILE:HD13	1:112:A:ASP:H	10	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,883)	1:59:A:LEU:HB3	1:61:A:GLY:H	9	0.67
(1,883)	1:59:A:LEU:HB3	1:61:A:GLY:H	11	0.67
(1,396)	1:39:A:ALA:HA	1:8:A:ILE:H	2	0.67
(1,3596)	1:15:A:SER:HB3	1:14:A:ILE:HD11	13	0.66
(1,3596)	1:15:A:SER:HB3	1:14:A:ILE:HD12	13	0.66
(1,3596)	1:15:A:SER:HB3	1:14:A:ILE:HD13	13	0.66
(1,3386)	1:32:A:THR:HA	1:31:A:LEU:HD11	4	0.66
(1,3386)	1:32:A:THR:HA	1:31:A:LEU:HD12	4	0.66
(1,3386)	1:32:A:THR:HA	1:31:A:LEU:HD13	4	0.66
(1,2523)	1:8:A:ILE:HA	1:22:A:LEU:HD21	6	0.66
(1,2523)	1:8:A:ILE:HA	1:22:A:LEU:HD22	6	0.66
(1,2523)	1:8:A:ILE:HA	1:22:A:LEU:HD23	6	0.66
(1,2522)	1:23:A:LYS:HA	1:22:A:LEU:HD21	6	0.66
(1,2522)	1:23:A:LYS:HA	1:22:A:LEU:HD22	6	0.66
(1,2522)	1:23:A:LYS:HA	1:22:A:LEU:HD23	6	0.66
(1,1784)	1:130:A:TYR:H	1:129:A:LYS:HE2	11	0.66
(1,1784)	1:130:A:TYR:H	1:129:A:LYS:HE3	11	0.66
(1,1784)	1:130:A:TYR:H	1:129:A:LYS:HE2	16	0.66
(1,1784)	1:130:A:TYR:H	1:129:A:LYS:HE3	16	0.66
(1,1238)	1:21:A:ILE:HD11	1:20:A:ALA:H	15	0.66
(1,1238)	1:21:A:ILE:HD12	1:20:A:ALA:H	15	0.66
(1,1238)	1:21:A:ILE:HD13	1:20:A:ALA:H	15	0.66
(1,1150)	1:134:A:ARG:HG2	1:129:A:LYS:H	3	0.66
(1,1150)	1:134:A:ARG:HG3	1:129:A:LYS:H	3	0.66
(1,1067)	1:68:A:ILE:HD11	1:63:A:GLY:H	1	0.66
(1,1067)	1:68:A:ILE:HD12	1:63:A:GLY:H	1	0.66
(1,1067)	1:68:A:ILE:HD13	1:63:A:GLY:H	1	0.66
(1,1043)	1:21:A:ILE:HG21	1:32:A:THR:H	2	0.66
(1,1043)	1:21:A:ILE:HG22	1:32:A:THR:H	2	0.66
(1,1043)	1:21:A:ILE:HG23	1:32:A:THR:H	2	0.66
(1,1032)	1:93:A:ILE:HD11	1:112:A:ASP:H	8	0.66
(1,1032)	1:93:A:ILE:HD12	1:112:A:ASP:H	8	0.66
(1,1032)	1:93:A:ILE:HD13	1:112:A:ASP:H	8	0.66
(1,1032)	1:93:A:ILE:HD11	1:112:A:ASP:H	11	0.66
(1,1032)	1:93:A:ILE:HD12	1:112:A:ASP:H	11	0.66
(1,1032)	1:93:A:ILE:HD13	1:112:A:ASP:H	11	0.66
(1,3386)	1:32:A:THR:HA	1:31:A:LEU:HD11	13	0.65
(1,3386)	1:32:A:THR:HA	1:31:A:LEU:HD12	13	0.65
(1,3386)	1:32:A:THR:HA	1:31:A:LEU:HD13	13	0.65
(1,3274)	1:73:A:ILE:HA	1:72:A:ARG:HD2	7	0.65
(1,2970)	1:87:A:GLU:HG2	1:127:A:ILE:HG21	17	0.65
(1,2970)	1:87:A:GLU:HG2	1:127:A:ILE:HG22	17	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2970)	1:87:A:GLU:HG2	1:127:A:ILE:HG23	17	0.65
(1,2522)	1:23:A:LYS:HA	1:22:A:LEU:HD21	20	0.65
(1,2522)	1:23:A:LYS:HA	1:22:A:LEU:HD22	20	0.65
(1,2522)	1:23:A:LYS:HA	1:22:A:LEU:HD23	20	0.65
(1,2239)	1:104:A:SER:HA	1:102:A:GLN:HB2	14	0.65
(1,2239)	1:104:A:SER:HA	1:102:A:GLN:HB3	14	0.65
(1,1784)	1:130:A:TYR:H	1:129:A:LYS:HE2	19	0.65
(1,1784)	1:130:A:TYR:H	1:129:A:LYS:HE3	19	0.65
(1,1032)	1:93:A:ILE:HD11	1:112:A:ASP:H	12	0.65
(1,1032)	1:93:A:ILE:HD12	1:112:A:ASP:H	12	0.65
(1,1032)	1:93:A:ILE:HD13	1:112:A:ASP:H	12	0.65
(1,1032)	1:93:A:ILE:HD11	1:112:A:ASP:H	20	0.65
(1,1032)	1:93:A:ILE:HD12	1:112:A:ASP:H	20	0.65
(1,1032)	1:93:A:ILE:HD13	1:112:A:ASP:H	20	0.65
(1,929)	1:3:A:VAL:HG21	1:34:A:LYS:H	3	0.65
(1,929)	1:3:A:VAL:HG22	1:34:A:LYS:H	3	0.65
(1,929)	1:3:A:VAL:HG23	1:34:A:LYS:H	3	0.65
(1,554)	1:4:A:LYS:HE2	1:4:A:LYS:H	15	0.65
(1,554)	1:4:A:LYS:HE3	1:4:A:LYS:H	15	0.65
(1,396)	1:39:A:ALA:HA	1:8:A:ILE:H	9	0.65
(1,3890)	1:71:A:ASN:H	1:2:A:SER:HB2	4	0.64
(1,3760)	1:35:A:GLN:H	1:31:A:LEU:HD11	8	0.64
(1,3760)	1:35:A:GLN:H	1:31:A:LEU:HD12	8	0.64
(1,3760)	1:35:A:GLN:H	1:31:A:LEU:HD13	8	0.64
(1,3386)	1:32:A:THR:HA	1:31:A:LEU:HD11	1	0.64
(1,3386)	1:32:A:THR:HA	1:31:A:LEU:HD12	1	0.64
(1,3386)	1:32:A:THR:HA	1:31:A:LEU:HD13	1	0.64
(1,3019)	1:54:A:ILE:HA	1:65:A:THR:HB	5	0.64
(1,2995)	1:70:A:LYS:HB3	1:5:A:ILE:HG21	7	0.64
(1,2995)	1:70:A:LYS:HB3	1:5:A:ILE:HG22	7	0.64
(1,2995)	1:70:A:LYS:HB3	1:5:A:ILE:HG23	7	0.64
(1,2995)	1:70:A:LYS:HB3	1:5:A:ILE:HG21	12	0.64
(1,2995)	1:70:A:LYS:HB3	1:5:A:ILE:HG22	12	0.64
(1,2995)	1:70:A:LYS:HB3	1:5:A:ILE:HG23	12	0.64
(1,2697)	1:135:A:ILE:HB	1:136:A:THR:HG21	13	0.64
(1,2697)	1:135:A:ILE:HB	1:136:A:THR:HG22	13	0.64
(1,2697)	1:135:A:ILE:HB	1:136:A:THR:HG23	13	0.64
(1,2522)	1:139:A:PRO:HD2	1:135:A:ILE:HG13	3	0.64
(1,2522)	1:139:A:PRO:HD3	1:135:A:ILE:HG13	3	0.64
(1,2522)	1:23:A:LYS:HA	1:22:A:LEU:HD21	8	0.64
(1,2522)	1:23:A:LYS:HA	1:22:A:LEU:HD22	8	0.64
(1,2522)	1:23:A:LYS:HA	1:22:A:LEU:HD23	8	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1784)	1:125:A:ILE:H	1:129:A:LYS:HE2	3	0.64
(1,1784)	1:125:A:ILE:H	1:129:A:LYS:HE3	3	0.64
(1,1150)	1:134:A:ARG:HG2	1:129:A:LYS:H	20	0.64
(1,1150)	1:134:A:ARG:HG3	1:129:A:LYS:H	20	0.64
(1,1067)	1:60:A:LEU:HD21	1:63:A:GLY:H	2	0.64
(1,1067)	1:60:A:LEU:HD22	1:63:A:GLY:H	2	0.64
(1,1067)	1:60:A:LEU:HD23	1:63:A:GLY:H	2	0.64
(1,1067)	1:68:A:ILE:HD11	1:63:A:GLY:H	17	0.64
(1,1067)	1:68:A:ILE:HD12	1:63:A:GLY:H	17	0.64
(1,1067)	1:68:A:ILE:HD13	1:63:A:GLY:H	17	0.64
(1,883)	1:59:A:LEU:HB3	1:61:A:GLY:H	8	0.64
(1,883)	1:59:A:LEU:HB3	1:61:A:GLY:H	14	0.64
(1,883)	1:59:A:LEU:HB3	1:61:A:GLY:H	16	0.64
(1,3840)	1:123:A:ASP:HB2	1:111:A:ALA:HB1	19	0.63
(1,3840)	1:123:A:ASP:HB2	1:111:A:ALA:HB2	19	0.63
(1,3840)	1:123:A:ASP:HB2	1:111:A:ALA:HB3	19	0.63
(1,3596)	1:15:A:SER:HB3	1:14:A:ILE:HD11	19	0.63
(1,3596)	1:15:A:SER:HB3	1:14:A:ILE:HD12	19	0.63
(1,3596)	1:15:A:SER:HB3	1:14:A:ILE:HD13	19	0.63
(1,3386)	1:32:A:THR:HA	1:31:A:LEU:HD11	11	0.63
(1,3386)	1:32:A:THR:HA	1:31:A:LEU:HD12	11	0.63
(1,3386)	1:32:A:THR:HA	1:31:A:LEU:HD13	11	0.63
(1,2522)	1:139:A:PRO:HD2	1:135:A:ILE:HG13	19	0.63
(1,2522)	1:139:A:PRO:HD3	1:135:A:ILE:HG13	19	0.63
(1,1784)	1:125:A:ILE:H	1:129:A:LYS:HE2	6	0.63
(1,1784)	1:125:A:ILE:H	1:129:A:LYS:HE3	6	0.63
(1,1353)	1:55:A:LEU:H	1:68:A:ILE:HD11	11	0.63
(1,1353)	1:55:A:LEU:H	1:68:A:ILE:HD12	11	0.63
(1,1353)	1:55:A:LEU:H	1:68:A:ILE:HD13	11	0.63
(1,1353)	1:66:A:SER:H	1:68:A:ILE:HD11	13	0.63
(1,1353)	1:66:A:SER:H	1:68:A:ILE:HD12	13	0.63
(1,1353)	1:66:A:SER:H	1:68:A:ILE:HD13	13	0.63
(1,1353)	1:55:A:LEU:H	1:68:A:ILE:HD11	16	0.63
(1,1353)	1:55:A:LEU:H	1:68:A:ILE:HD12	16	0.63
(1,1353)	1:55:A:LEU:H	1:68:A:ILE:HD13	16	0.63
(1,1238)	1:17:A:ILE:HD11	1:20:A:ALA:H	11	0.63
(1,1238)	1:17:A:ILE:HD12	1:20:A:ALA:H	11	0.63
(1,1238)	1:17:A:ILE:HD13	1:20:A:ALA:H	11	0.63
(1,1032)	1:93:A:ILE:HD11	1:112:A:ASP:H	15	0.63
(1,1032)	1:93:A:ILE:HD12	1:112:A:ASP:H	15	0.63
(1,1032)	1:93:A:ILE:HD13	1:112:A:ASP:H	15	0.63
(1,883)	1:59:A:LEU:HB3	1:61:A:GLY:H	18	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3695)	1:108:A:LEU:HD21	1:102:A:GLN:HG2	7	0.62
(1,3695)	1:108:A:LEU:HD22	1:102:A:GLN:HG2	7	0.62
(1,3695)	1:108:A:LEU:HD23	1:102:A:GLN:HG2	7	0.62
(1,3695)	1:108:A:LEU:HD21	1:102:A:GLN:HG2	10	0.62
(1,3695)	1:108:A:LEU:HD22	1:102:A:GLN:HG2	10	0.62
(1,3695)	1:108:A:LEU:HD23	1:102:A:GLN:HG2	10	0.62
(1,3408)	1:59:A:LEU:HD11	1:15:A:SER:HB3	18	0.62
(1,3408)	1:59:A:LEU:HD12	1:15:A:SER:HB3	18	0.62
(1,3408)	1:59:A:LEU:HD13	1:15:A:SER:HB3	18	0.62
(1,2995)	1:70:A:LYS:HB3	1:5:A:ILE:HG21	4	0.62
(1,2995)	1:70:A:LYS:HB3	1:5:A:ILE:HG22	4	0.62
(1,2995)	1:70:A:LYS:HB3	1:5:A:ILE:HG23	4	0.62
(1,2586)	1:39:A:ALA:HB1	1:36:A:LEU:HD11	10	0.62
(1,2586)	1:39:A:ALA:HB1	1:36:A:LEU:HD12	10	0.62
(1,2586)	1:39:A:ALA:HB1	1:36:A:LEU:HD13	10	0.62
(1,2586)	1:39:A:ALA:HB2	1:36:A:LEU:HD11	10	0.62
(1,2586)	1:39:A:ALA:HB2	1:36:A:LEU:HD12	10	0.62
(1,2586)	1:39:A:ALA:HB2	1:36:A:LEU:HD13	10	0.62
(1,2586)	1:39:A:ALA:HB3	1:36:A:LEU:HD11	10	0.62
(1,2586)	1:39:A:ALA:HB3	1:36:A:LEU:HD12	10	0.62
(1,2586)	1:39:A:ALA:HB3	1:36:A:LEU:HD13	10	0.62
(1,2523)	1:137:A:HIS:HB3	1:135:A:ILE:HG13	17	0.62
(1,1784)	1:130:A:TYR:H	1:129:A:LYS:HE2	2	0.62
(1,1784)	1:130:A:TYR:H	1:129:A:LYS:HE3	2	0.62
(1,1238)	1:17:A:ILE:HD11	1:20:A:ALA:H	3	0.62
(1,1238)	1:17:A:ILE:HD12	1:20:A:ALA:H	3	0.62
(1,1238)	1:17:A:ILE:HD13	1:20:A:ALA:H	3	0.62
(1,1067)	1:68:A:ILE:HD11	1:63:A:GLY:H	18	0.62
(1,1067)	1:68:A:ILE:HD12	1:63:A:GLY:H	18	0.62
(1,1067)	1:68:A:ILE:HD13	1:63:A:GLY:H	18	0.62
(1,1043)	1:21:A:ILE:HG21	1:32:A:THR:H	3	0.62
(1,1043)	1:21:A:ILE:HG22	1:32:A:THR:H	3	0.62
(1,1043)	1:21:A:ILE:HG23	1:32:A:THR:H	3	0.62
(1,1032)	1:93:A:ILE:HD11	1:112:A:ASP:H	17	0.62
(1,1032)	1:93:A:ILE:HD12	1:112:A:ASP:H	17	0.62
(1,1032)	1:93:A:ILE:HD13	1:112:A:ASP:H	17	0.62
(1,870)	1:52:A:LEU:HG	1:56:A:GLN:HE21	10	0.62
(1,3663)	1:68:A:ILE:HG21	1:4:A:LYS:HE2	10	0.61
(1,3663)	1:68:A:ILE:HG21	1:4:A:LYS:HE3	10	0.61
(1,3663)	1:68:A:ILE:HG22	1:4:A:LYS:HE2	10	0.61
(1,3663)	1:68:A:ILE:HG22	1:4:A:LYS:HE3	10	0.61
(1,3663)	1:68:A:ILE:HG23	1:4:A:LYS:HE2	10	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3663)	1:68:A:ILE:HG23	1:4:A:LYS:HE3	10	0.61
(1,3596)	1:15:A:SER:HB3	1:14:A:ILE:HD11	11	0.61
(1,3596)	1:15:A:SER:HB3	1:14:A:ILE:HD12	11	0.61
(1,3596)	1:15:A:SER:HB3	1:14:A:ILE:HD13	11	0.61
(1,3596)	1:15:A:SER:HB3	1:14:A:ILE:HD11	17	0.61
(1,3596)	1:15:A:SER:HB3	1:14:A:ILE:HD12	17	0.61
(1,3596)	1:15:A:SER:HB3	1:14:A:ILE:HD13	17	0.61
(1,3386)	1:32:A:THR:HA	1:31:A:LEU:HD11	7	0.61
(1,3386)	1:32:A:THR:HA	1:31:A:LEU:HD12	7	0.61
(1,3386)	1:32:A:THR:HA	1:31:A:LEU:HD13	7	0.61
(1,2942)	1:86:A:ASP:HB2	1:131:A:ILE:HG21	11	0.61
(1,2942)	1:86:A:ASP:HB2	1:131:A:ILE:HG22	11	0.61
(1,2942)	1:86:A:ASP:HB2	1:131:A:ILE:HG23	11	0.61
(1,2747)	1:72:A:ARG:HD2	1:3:A:VAL:HG11	3	0.61
(1,2747)	1:72:A:ARG:HD2	1:3:A:VAL:HG12	3	0.61
(1,2747)	1:72:A:ARG:HD2	1:3:A:VAL:HG13	3	0.61
(1,2523)	1:8:A:ILE:HA	1:22:A:LEU:HD21	8	0.61
(1,2523)	1:8:A:ILE:HA	1:22:A:LEU:HD22	8	0.61
(1,2523)	1:8:A:ILE:HA	1:22:A:LEU:HD23	8	0.61
(1,2306)	1:71:A:ASN:H	1:5:A:ILE:HG13	12	0.61
(1,2239)	1:104:A:SER:HA	1:102:A:GLN:HB2	18	0.61
(1,2239)	1:104:A:SER:HA	1:102:A:GLN:HB3	18	0.61
(1,1784)	1:125:A:ILE:H	1:129:A:LYS:HE2	4	0.61
(1,1784)	1:125:A:ILE:H	1:129:A:LYS:HE3	4	0.61
(1,1353)	1:55:A:LEU:H	1:68:A:ILE:HD11	2	0.61
(1,1353)	1:55:A:LEU:H	1:68:A:ILE:HD12	2	0.61
(1,1353)	1:55:A:LEU:H	1:68:A:ILE:HD13	2	0.61
(1,1353)	1:55:A:LEU:H	1:68:A:ILE:HD11	17	0.61
(1,1353)	1:55:A:LEU:H	1:68:A:ILE:HD12	17	0.61
(1,1353)	1:55:A:LEU:H	1:68:A:ILE:HD13	17	0.61
(1,1067)	1:68:A:ILE:HD11	1:63:A:GLY:H	11	0.61
(1,1067)	1:68:A:ILE:HD12	1:63:A:GLY:H	11	0.61
(1,1067)	1:68:A:ILE:HD13	1:63:A:GLY:H	11	0.61
(1,962)	1:73:A:ILE:HD11	1:71:A:ASN:H	12	0.61
(1,962)	1:73:A:ILE:HD12	1:71:A:ASN:H	12	0.61
(1,962)	1:73:A:ILE:HD13	1:71:A:ASN:H	12	0.61
(1,883)	1:59:A:LEU:HB3	1:61:A:GLY:H	7	0.61
(1,396)	1:39:A:ALA:HA	1:8:A:ILE:H	7	0.61
(1,3695)	1:108:A:LEU:HD21	1:102:A:GLN:HG2	2	0.6
(1,3695)	1:108:A:LEU:HD22	1:102:A:GLN:HG2	2	0.6
(1,3695)	1:108:A:LEU:HD23	1:102:A:GLN:HG2	2	0.6
(1,3386)	1:32:A:THR:HA	1:31:A:LEU:HD11	14	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3386)	1:32:A:THR:HA	1:31:A:LEU:HD12	14	0.6
(1,3386)	1:32:A:THR:HA	1:31:A:LEU:HD13	14	0.6
(1,3386)	1:32:A:THR:HA	1:31:A:LEU:HD11	17	0.6
(1,3386)	1:32:A:THR:HA	1:31:A:LEU:HD12	17	0.6
(1,3386)	1:32:A:THR:HA	1:31:A:LEU:HD13	17	0.6
(1,2995)	1:70:A:LYS:HB3	1:5:A:ILE:HG21	11	0.6
(1,2995)	1:70:A:LYS:HB3	1:5:A:ILE:HG22	11	0.6
(1,2995)	1:70:A:LYS:HB3	1:5:A:ILE:HG23	11	0.6
(1,2522)	1:23:A:LYS:HA	1:22:A:LEU:HD21	4	0.6
(1,2522)	1:23:A:LYS:HA	1:22:A:LEU:HD22	4	0.6
(1,2522)	1:23:A:LYS:HA	1:22:A:LEU:HD23	4	0.6
(1,2145)	1:2:A:SER:HB2	1:3:A:VAL:HB	2	0.6
(1,1784)	1:125:A:ILE:H	1:129:A:LYS:HE2	5	0.6
(1,1784)	1:125:A:ILE:H	1:129:A:LYS:HE3	5	0.6
(1,1505)	1:72:A:ARG:HA	1:73:A:ILE:HD11	3	0.6
(1,1505)	1:72:A:ARG:HA	1:73:A:ILE:HD12	3	0.6
(1,1505)	1:72:A:ARG:HA	1:73:A:ILE:HD13	3	0.6
(1,1238)	1:17:A:ILE:HD11	1:20:A:ALA:H	4	0.6
(1,1238)	1:17:A:ILE:HD12	1:20:A:ALA:H	4	0.6
(1,1238)	1:17:A:ILE:HD13	1:20:A:ALA:H	4	0.6
(1,1067)	1:68:A:ILE:HD11	1:63:A:GLY:H	6	0.6
(1,1067)	1:68:A:ILE:HD12	1:63:A:GLY:H	6	0.6
(1,1067)	1:68:A:ILE:HD13	1:63:A:GLY:H	6	0.6
(1,1032)	1:93:A:ILE:HD11	1:112:A:ASP:H	19	0.6
(1,1032)	1:93:A:ILE:HD12	1:112:A:ASP:H	19	0.6
(1,1032)	1:93:A:ILE:HD13	1:112:A:ASP:H	19	0.6
(1,883)	1:59:A:LEU:HB3	1:61:A:GLY:H	12	0.6
(1,883)	1:59:A:LEU:HB3	1:61:A:GLY:H	20	0.6
(1,605)	1:90:A:TYR:HB2	1:93:A:ILE:H	14	0.6
(1,3695)	1:108:A:LEU:HD21	1:102:A:GLN:HG2	20	0.59
(1,3695)	1:108:A:LEU:HD22	1:102:A:GLN:HG2	20	0.59
(1,3695)	1:108:A:LEU:HD23	1:102:A:GLN:HG2	20	0.59
(1,3596)	1:15:A:SER:HB3	1:14:A:ILE:HD11	4	0.59
(1,3596)	1:15:A:SER:HB3	1:14:A:ILE:HD12	4	0.59
(1,3596)	1:15:A:SER:HB3	1:14:A:ILE:HD13	4	0.59
(1,3596)	1:15:A:SER:HB3	1:14:A:ILE:HD11	5	0.59
(1,3596)	1:15:A:SER:HB3	1:14:A:ILE:HD12	5	0.59
(1,3596)	1:15:A:SER:HB3	1:14:A:ILE:HD13	5	0.59
(1,2962)	1:42:A:ASP:HB3	1:54:A:ILE:HG21	18	0.59
(1,2962)	1:42:A:ASP:HB3	1:54:A:ILE:HG22	18	0.59
(1,2962)	1:42:A:ASP:HB3	1:54:A:ILE:HG23	18	0.59
(1,2765)	1:74:A:TYR:HB2	1:3:A:VAL:HG21	2	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2765)	1:74:A:TYR:HB2	1:3:A:VAL:HG22	2	0.59
(1,2765)	1:74:A:TYR:HB2	1:3:A:VAL:HG23	2	0.59
(1,2523)	1:8:A:ILE:HA	1:22:A:LEU:HD21	2	0.59
(1,2523)	1:8:A:ILE:HA	1:22:A:LEU:HD22	2	0.59
(1,2523)	1:8:A:ILE:HA	1:22:A:LEU:HD23	2	0.59
(1,2522)	1:23:A:LYS:HA	1:22:A:LEU:HD21	14	0.59
(1,2522)	1:23:A:LYS:HA	1:22:A:LEU:HD22	14	0.59
(1,2522)	1:23:A:LYS:HA	1:22:A:LEU:HD23	14	0.59
(1,1357)	1:123:A:ASP:H	1:93:A:ILE:HD11	19	0.59
(1,1357)	1:123:A:ASP:H	1:93:A:ILE:HD12	19	0.59
(1,1357)	1:123:A:ASP:H	1:93:A:ILE:HD13	19	0.59
(1,1032)	1:93:A:ILE:HD11	1:112:A:ASP:H	4	0.59
(1,1032)	1:93:A:ILE:HD12	1:112:A:ASP:H	4	0.59
(1,1032)	1:93:A:ILE:HD13	1:112:A:ASP:H	4	0.59
(1,883)	1:59:A:LEU:HB3	1:61:A:GLY:H	3	0.59
(1,3695)	1:108:A:LEU:HD21	1:102:A:GLN:HG2	5	0.58
(1,3695)	1:108:A:LEU:HD22	1:102:A:GLN:HG2	5	0.58
(1,3695)	1:108:A:LEU:HD23	1:102:A:GLN:HG2	5	0.58
(1,3596)	1:15:A:SER:HB3	1:14:A:ILE:HD11	16	0.58
(1,3596)	1:15:A:SER:HB3	1:14:A:ILE:HD12	16	0.58
(1,3596)	1:15:A:SER:HB3	1:14:A:ILE:HD13	16	0.58
(1,3386)	1:32:A:THR:HA	1:31:A:LEU:HD11	3	0.58
(1,3386)	1:32:A:THR:HA	1:31:A:LEU:HD12	3	0.58
(1,3386)	1:32:A:THR:HA	1:31:A:LEU:HD13	3	0.58
(1,3386)	1:32:A:THR:HA	1:31:A:LEU:HD11	6	0.58
(1,3386)	1:32:A:THR:HA	1:31:A:LEU:HD12	6	0.58
(1,3386)	1:32:A:THR:HA	1:31:A:LEU:HD13	6	0.58
(1,2995)	1:70:A:LYS:HB3	1:5:A:ILE:HG21	20	0.58
(1,2995)	1:70:A:LYS:HB3	1:5:A:ILE:HG22	20	0.58
(1,2995)	1:70:A:LYS:HB3	1:5:A:ILE:HG23	20	0.58
(1,2970)	1:87:A:GLU:HG2	1:127:A:ILE:HG21	6	0.58
(1,2970)	1:87:A:GLU:HG2	1:127:A:ILE:HG22	6	0.58
(1,2970)	1:87:A:GLU:HG2	1:127:A:ILE:HG23	6	0.58
(1,2697)	1:128:A:GLU:HG2	1:132:A:THR:HG21	2	0.58
(1,2697)	1:128:A:GLU:HG2	1:132:A:THR:HG22	2	0.58
(1,2697)	1:128:A:GLU:HG2	1:132:A:THR:HG23	2	0.58
(1,2697)	1:128:A:GLU:HG3	1:132:A:THR:HG21	2	0.58
(1,2697)	1:128:A:GLU:HG3	1:132:A:THR:HG22	2	0.58
(1,2697)	1:128:A:GLU:HG3	1:132:A:THR:HG23	2	0.58
(1,2697)	1:57:A:MET:HB2	1:65:A:THR:HG21	9	0.58
(1,2697)	1:57:A:MET:HB2	1:65:A:THR:HG22	9	0.58
(1,2697)	1:57:A:MET:HB2	1:65:A:THR:HG23	9	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2697)	1:134:A:ARG:HB2	1:132:A:THR:HG21	15	0.58
(1,2697)	1:134:A:ARG:HB2	1:132:A:THR:HG22	15	0.58
(1,2697)	1:134:A:ARG:HB2	1:132:A:THR:HG23	15	0.58
(1,2586)	1:106:A:ALA:HB1	1:36:A:LEU:HD11	6	0.58
(1,2586)	1:106:A:ALA:HB1	1:36:A:LEU:HD12	6	0.58
(1,2586)	1:106:A:ALA:HB1	1:36:A:LEU:HD13	6	0.58
(1,2586)	1:106:A:ALA:HB2	1:36:A:LEU:HD11	6	0.58
(1,2586)	1:106:A:ALA:HB2	1:36:A:LEU:HD12	6	0.58
(1,2586)	1:106:A:ALA:HB2	1:36:A:LEU:HD13	6	0.58
(1,2586)	1:106:A:ALA:HB3	1:36:A:LEU:HD11	6	0.58
(1,2586)	1:106:A:ALA:HB3	1:36:A:LEU:HD12	6	0.58
(1,2586)	1:106:A:ALA:HB3	1:36:A:LEU:HD13	6	0.58
(1,2239)	1:104:A:SER:HA	1:102:A:GLN:HB2	6	0.58
(1,2239)	1:104:A:SER:HA	1:102:A:GLN:HB3	6	0.58
(1,1784)	1:130:A:TYR:H	1:129:A:LYS:HE2	1	0.58
(1,1784)	1:130:A:TYR:H	1:129:A:LYS:HE3	1	0.58
(1,1784)	1:125:A:ILE:H	1:129:A:LYS:HE2	17	0.58
(1,1784)	1:125:A:ILE:H	1:129:A:LYS:HE3	17	0.58
(1,1353)	1:66:A:SER:H	1:68:A:ILE:HD11	8	0.58
(1,1353)	1:66:A:SER:H	1:68:A:ILE:HD12	8	0.58
(1,1353)	1:66:A:SER:H	1:68:A:ILE:HD13	8	0.58
(1,1353)	1:55:A:LEU:H	1:68:A:ILE:HD11	18	0.58
(1,1353)	1:55:A:LEU:H	1:68:A:ILE:HD12	18	0.58
(1,1353)	1:55:A:LEU:H	1:68:A:ILE:HD13	18	0.58
(1,3875)	1:55:A:LEU:HB3	1:8:A:ILE:HG12	6	0.57
(1,3875)	1:55:A:LEU:HB3	1:8:A:ILE:HG13	6	0.57
(1,3840)	1:123:A:ASP:HB2	1:111:A:ALA:HB1	14	0.57
(1,3840)	1:123:A:ASP:HB2	1:111:A:ALA:HB2	14	0.57
(1,3840)	1:123:A:ASP:HB2	1:111:A:ALA:HB3	14	0.57
(1,3695)	1:108:A:LEU:HD21	1:102:A:GLN:HG2	14	0.57
(1,3695)	1:108:A:LEU:HD22	1:102:A:GLN:HG2	14	0.57
(1,3695)	1:108:A:LEU:HD23	1:102:A:GLN:HG2	14	0.57
(1,3596)	1:15:A:SER:HB3	1:14:A:ILE:HD11	6	0.57
(1,3596)	1:15:A:SER:HB3	1:14:A:ILE:HD12	6	0.57
(1,3596)	1:15:A:SER:HB3	1:14:A:ILE:HD13	6	0.57
(1,3596)	1:15:A:SER:HB3	1:14:A:ILE:HD11	7	0.57
(1,3596)	1:15:A:SER:HB3	1:14:A:ILE:HD12	7	0.57
(1,3596)	1:15:A:SER:HB3	1:14:A:ILE:HD13	7	0.57
(1,3596)	1:15:A:SER:HB3	1:14:A:ILE:HD11	9	0.57
(1,3596)	1:15:A:SER:HB3	1:14:A:ILE:HD12	9	0.57
(1,3596)	1:15:A:SER:HB3	1:14:A:ILE:HD13	9	0.57
(1,3386)	1:32:A:THR:HA	1:31:A:LEU:HD11	9	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3386)	1:32:A:THR:HA	1:31:A:LEU:HD12	9	0.57
(1,3386)	1:32:A:THR:HA	1:31:A:LEU:HD13	9	0.57
(1,3386)	1:32:A:THR:HA	1:31:A:LEU:HD11	20	0.57
(1,3386)	1:32:A:THR:HA	1:31:A:LEU:HD12	20	0.57
(1,3386)	1:32:A:THR:HA	1:31:A:LEU:HD13	20	0.57
(1,3045)	1:64:A:GLY:HA2	1:65:A:THR:HG21	10	0.57
(1,3045)	1:64:A:GLY:HA2	1:65:A:THR:HG22	10	0.57
(1,3045)	1:64:A:GLY:HA2	1:65:A:THR:HG23	10	0.57
(1,3045)	1:64:A:GLY:HA3	1:65:A:THR:HG21	10	0.57
(1,3045)	1:64:A:GLY:HA3	1:65:A:THR:HG22	10	0.57
(1,3045)	1:64:A:GLY:HA3	1:65:A:THR:HG23	10	0.57
(1,2966)	1:88:A:ASN:HB3	1:91:A:ILE:HG21	14	0.57
(1,2966)	1:88:A:ASN:HB3	1:91:A:ILE:HG22	14	0.57
(1,2966)	1:88:A:ASN:HB3	1:91:A:ILE:HG23	14	0.57
(1,2962)	1:42:A:ASP:HB3	1:50:A:ILE:HG21	19	0.57
(1,2962)	1:42:A:ASP:HB3	1:50:A:ILE:HG22	19	0.57
(1,2962)	1:42:A:ASP:HB3	1:50:A:ILE:HG23	19	0.57
(1,2522)	1:23:A:LYS:HA	1:22:A:LEU:HD21	13	0.57
(1,2522)	1:23:A:LYS:HA	1:22:A:LEU:HD22	13	0.57
(1,2522)	1:23:A:LYS:HA	1:22:A:LEU:HD23	13	0.57
(1,2484)	1:56:A:GLN:HE22	1:60:A:LEU:HD21	13	0.57
(1,2484)	1:56:A:GLN:HE22	1:60:A:LEU:HD22	13	0.57
(1,2484)	1:56:A:GLN:HE22	1:60:A:LEU:HD23	13	0.57
(1,1784)	1:125:A:ILE:H	1:129:A:LYS:HE2	10	0.57
(1,1784)	1:125:A:ILE:H	1:129:A:LYS:HE3	10	0.57
(1,1353)	1:55:A:LEU:H	1:68:A:ILE:HD11	7	0.57
(1,1353)	1:55:A:LEU:H	1:68:A:ILE:HD12	7	0.57
(1,1353)	1:55:A:LEU:H	1:68:A:ILE:HD13	7	0.57
(1,1353)	1:55:A:LEU:H	1:68:A:ILE:HD11	9	0.57
(1,1353)	1:55:A:LEU:H	1:68:A:ILE:HD12	9	0.57
(1,1353)	1:55:A:LEU:H	1:68:A:ILE:HD13	9	0.57
(1,1097)	1:103:A:LEU:HD21	1:112:A:ASP:H	4	0.57
(1,1097)	1:103:A:LEU:HD22	1:112:A:ASP:H	4	0.57
(1,1097)	1:103:A:LEU:HD23	1:112:A:ASP:H	4	0.57
(1,3890)	1:4:A:LYS:H	1:2:A:SER:HB2	8	0.56
(1,3890)	1:71:A:ASN:H	1:2:A:SER:HB2	18	0.56
(1,3695)	1:108:A:LEU:HD21	1:102:A:GLN:HG2	11	0.56
(1,3695)	1:108:A:LEU:HD22	1:102:A:GLN:HG2	11	0.56
(1,3695)	1:108:A:LEU:HD23	1:102:A:GLN:HG2	11	0.56
(1,3695)	1:108:A:LEU:HD21	1:102:A:GLN:HG2	16	0.56
(1,3695)	1:108:A:LEU:HD22	1:102:A:GLN:HG2	16	0.56
(1,3695)	1:108:A:LEU:HD23	1:102:A:GLN:HG2	16	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3635)	1:112:A:ASP:HB2	1:113:A:ALA:HA	1	0.56
(1,3596)	1:15:A:SER:HB3	1:14:A:ILE:HD11	3	0.56
(1,3596)	1:15:A:SER:HB3	1:14:A:ILE:HD12	3	0.56
(1,3596)	1:15:A:SER:HB3	1:14:A:ILE:HD13	3	0.56
(1,3386)	1:18:A:ASP:HA	1:31:A:LEU:HD11	5	0.56
(1,3386)	1:18:A:ASP:HA	1:31:A:LEU:HD12	5	0.56
(1,3386)	1:18:A:ASP:HA	1:31:A:LEU:HD13	5	0.56
(1,2995)	1:70:A:LYS:HB3	1:5:A:ILE:HG21	6	0.56
(1,2995)	1:70:A:LYS:HB3	1:5:A:ILE:HG22	6	0.56
(1,2995)	1:70:A:LYS:HB3	1:5:A:ILE:HG23	6	0.56
(1,2995)	1:70:A:LYS:HB3	1:5:A:ILE:HG21	19	0.56
(1,2995)	1:70:A:LYS:HB3	1:5:A:ILE:HG22	19	0.56
(1,2995)	1:70:A:LYS:HB3	1:5:A:ILE:HG23	19	0.56
(1,2954)	1:23:A:LYS:HE2	1:20:A:ALA:HB1	10	0.56
(1,2954)	1:23:A:LYS:HE2	1:20:A:ALA:HB2	10	0.56
(1,2954)	1:23:A:LYS:HE2	1:20:A:ALA:HB3	10	0.56
(1,2747)	1:72:A:ARG:HD2	1:3:A:VAL:HG11	1	0.56
(1,2747)	1:72:A:ARG:HD2	1:3:A:VAL:HG12	1	0.56
(1,2747)	1:72:A:ARG:HD2	1:3:A:VAL:HG13	1	0.56
(1,2697)	1:128:A:GLU:HG2	1:132:A:THR:HG21	12	0.56
(1,2697)	1:128:A:GLU:HG2	1:132:A:THR:HG22	12	0.56
(1,2697)	1:128:A:GLU:HG2	1:132:A:THR:HG23	12	0.56
(1,2697)	1:128:A:GLU:HG3	1:132:A:THR:HG21	12	0.56
(1,2697)	1:128:A:GLU:HG3	1:132:A:THR:HG22	12	0.56
(1,2697)	1:128:A:GLU:HG3	1:132:A:THR:HG23	12	0.56
(1,2344)	1:19:A:TYR:H	1:59:A:LEU:HD21	14	0.56
(1,2344)	1:19:A:TYR:H	1:59:A:LEU:HD22	14	0.56
(1,2344)	1:19:A:TYR:H	1:59:A:LEU:HD23	14	0.56
(1,2239)	1:104:A:SER:HA	1:102:A:GLN:HB2	9	0.56
(1,2239)	1:104:A:SER:HA	1:102:A:GLN:HB3	9	0.56
(1,2239)	1:104:A:SER:HA	1:102:A:GLN:HB2	17	0.56
(1,2239)	1:104:A:SER:HA	1:102:A:GLN:HB3	17	0.56
(1,1238)	1:21:A:ILE:HD11	1:20:A:ALA:H	5	0.56
(1,1238)	1:21:A:ILE:HD12	1:20:A:ALA:H	5	0.56
(1,1238)	1:21:A:ILE:HD13	1:20:A:ALA:H	5	0.56
(1,1238)	1:17:A:ILE:HD11	1:20:A:ALA:H	6	0.56
(1,1238)	1:17:A:ILE:HD12	1:20:A:ALA:H	6	0.56
(1,1238)	1:17:A:ILE:HD13	1:20:A:ALA:H	6	0.56
(1,1162)	1:79:A:ILE:HG21	1:111:A:ALA:H	17	0.56
(1,1162)	1:79:A:ILE:HG22	1:111:A:ALA:H	17	0.56
(1,1162)	1:79:A:ILE:HG23	1:111:A:ALA:H	17	0.56
(1,883)	1:59:A:LEU:HB3	1:61:A:GLY:H	6	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,396)	1:39:A:ALA:HA	1:8:A:ILE:H	6	0.56
(1,396)	1:39:A:ALA:HA	1:8:A:ILE:H	20	0.56
(1,3695)	1:108:A:LEU:HD21	1:102:A:GLN:HG2	12	0.55
(1,3695)	1:108:A:LEU:HD22	1:102:A:GLN:HG2	12	0.55
(1,3695)	1:108:A:LEU:HD23	1:102:A:GLN:HG2	12	0.55
(1,3695)	1:108:A:LEU:HD21	1:102:A:GLN:HG2	18	0.55
(1,3695)	1:108:A:LEU:HD22	1:102:A:GLN:HG2	18	0.55
(1,3695)	1:108:A:LEU:HD23	1:102:A:GLN:HG2	18	0.55
(1,3386)	1:32:A:THR:HA	1:31:A:LEU:HD11	10	0.55
(1,3386)	1:32:A:THR:HA	1:31:A:LEU:HD12	10	0.55
(1,3386)	1:32:A:THR:HA	1:31:A:LEU:HD13	10	0.55
(1,2995)	1:70:A:LYS:HB3	1:5:A:ILE:HG21	1	0.55
(1,2995)	1:70:A:LYS:HB3	1:5:A:ILE:HG22	1	0.55
(1,2995)	1:70:A:LYS:HB3	1:5:A:ILE:HG23	1	0.55
(1,2586)	1:39:A:ALA:HB1	1:36:A:LEU:HD11	11	0.55
(1,2586)	1:39:A:ALA:HB1	1:36:A:LEU:HD12	11	0.55
(1,2586)	1:39:A:ALA:HB1	1:36:A:LEU:HD13	11	0.55
(1,2586)	1:39:A:ALA:HB2	1:36:A:LEU:HD11	11	0.55
(1,2586)	1:39:A:ALA:HB2	1:36:A:LEU:HD12	11	0.55
(1,2586)	1:39:A:ALA:HB2	1:36:A:LEU:HD13	11	0.55
(1,2586)	1:39:A:ALA:HB3	1:36:A:LEU:HD11	11	0.55
(1,2586)	1:39:A:ALA:HB3	1:36:A:LEU:HD12	11	0.55
(1,2586)	1:39:A:ALA:HB3	1:36:A:LEU:HD13	11	0.55
(1,2523)	1:8:A:ILE:HA	1:22:A:LEU:HD21	1	0.55
(1,2523)	1:8:A:ILE:HA	1:22:A:LEU:HD22	1	0.55
(1,2523)	1:8:A:ILE:HA	1:22:A:LEU:HD23	1	0.55
(1,2522)	1:23:A:LYS:HA	1:22:A:LEU:HD21	2	0.55
(1,2522)	1:23:A:LYS:HA	1:22:A:LEU:HD22	2	0.55
(1,2522)	1:23:A:LYS:HA	1:22:A:LEU:HD23	2	0.55
(1,2484)	1:56:A:GLN:HE22	1:52:A:LEU:HD21	8	0.55
(1,2484)	1:56:A:GLN:HE22	1:52:A:LEU:HD22	8	0.55
(1,2484)	1:56:A:GLN:HE22	1:52:A:LEU:HD23	8	0.55
(1,2306)	1:71:A:ASN:H	1:5:A:ILE:HG13	10	0.55
(1,2306)	1:71:A:ASN:H	1:5:A:ILE:HG13	20	0.55
(1,2239)	1:104:A:SER:HA	1:102:A:GLN:HB2	19	0.55
(1,2239)	1:104:A:SER:HA	1:102:A:GLN:HB3	19	0.55
(1,1505)	1:72:A:ARG:HA	1:73:A:ILE:HD11	14	0.55
(1,1505)	1:72:A:ARG:HA	1:73:A:ILE:HD12	14	0.55
(1,1505)	1:72:A:ARG:HA	1:73:A:ILE:HD13	14	0.55
(1,1067)	1:68:A:ILE:HD11	1:63:A:GLY:H	4	0.55
(1,1067)	1:68:A:ILE:HD12	1:63:A:GLY:H	4	0.55
(1,1067)	1:68:A:ILE:HD13	1:63:A:GLY:H	4	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1067)	1:60:A:LEU:HD21	1:63:A:GLY:H	5	0.55
(1,1067)	1:60:A:LEU:HD22	1:63:A:GLY:H	5	0.55
(1,1067)	1:60:A:LEU:HD23	1:63:A:GLY:H	5	0.55
(1,1067)	1:68:A:ILE:HD11	1:63:A:GLY:H	12	0.55
(1,1067)	1:68:A:ILE:HD12	1:63:A:GLY:H	12	0.55
(1,1067)	1:68:A:ILE:HD13	1:63:A:GLY:H	12	0.55
(1,883)	1:59:A:LEU:HB3	1:61:A:GLY:H	2	0.55
(1,587)	1:9:A:ASP:HB3	1:11:A:ASN:H	16	0.55
(1,572)	1:9:A:ASP:HB3	1:20:A:ALA:H	13	0.55
(1,554)	1:4:A:LYS:HE2	1:4:A:LYS:H	17	0.55
(1,554)	1:4:A:LYS:HE3	1:4:A:LYS:H	17	0.55
(1,554)	1:4:A:LYS:HE2	1:4:A:LYS:H	18	0.55
(1,554)	1:4:A:LYS:HE3	1:4:A:LYS:H	18	0.55
(1,3890)	1:73:A:ILE:H	1:2:A:SER:HB2	1	0.54
(1,3386)	1:32:A:THR:HA	1:31:A:LEU:HD11	15	0.54
(1,3386)	1:32:A:THR:HA	1:31:A:LEU:HD12	15	0.54
(1,3386)	1:32:A:THR:HA	1:31:A:LEU:HD13	15	0.54
(1,2874)	1:19:A:TYR:HD1	1:20:A:ALA:HB1	20	0.54
(1,2874)	1:19:A:TYR:HD1	1:20:A:ALA:HB2	20	0.54
(1,2874)	1:19:A:TYR:HD1	1:20:A:ALA:HB3	20	0.54
(1,2874)	1:19:A:TYR:HD2	1:20:A:ALA:HB1	20	0.54
(1,2874)	1:19:A:TYR:HD2	1:20:A:ALA:HB2	20	0.54
(1,2874)	1:19:A:TYR:HD2	1:20:A:ALA:HB3	20	0.54
(1,2522)	1:23:A:LYS:HA	1:22:A:LEU:HD21	1	0.54
(1,2522)	1:23:A:LYS:HA	1:22:A:LEU:HD22	1	0.54
(1,2522)	1:23:A:LYS:HA	1:22:A:LEU:HD23	1	0.54
(1,2344)	1:58:A:TYR:HD1	1:59:A:LEU:HD21	8	0.54
(1,2344)	1:58:A:TYR:HD1	1:59:A:LEU:HD22	8	0.54
(1,2344)	1:58:A:TYR:HD1	1:59:A:LEU:HD23	8	0.54
(1,2344)	1:58:A:TYR:HD2	1:59:A:LEU:HD21	8	0.54
(1,2344)	1:58:A:TYR:HD2	1:59:A:LEU:HD22	8	0.54
(1,2344)	1:58:A:TYR:HD2	1:59:A:LEU:HD23	8	0.54
(1,1813)	1:35:A:GLN:HE21	1:34:A:LYS:HE2	6	0.54
(1,1813)	1:19:A:TYR:HD1	1:23:A:LYS:HE2	20	0.54
(1,1813)	1:19:A:TYR:HD2	1:23:A:LYS:HE2	20	0.54
(1,1784)	1:125:A:ILE:H	1:129:A:LYS:HE2	20	0.54
(1,1784)	1:125:A:ILE:H	1:129:A:LYS:HE3	20	0.54
(1,1505)	1:72:A:ARG:HA	1:73:A:ILE:HD11	18	0.54
(1,1505)	1:72:A:ARG:HA	1:73:A:ILE:HD12	18	0.54
(1,1505)	1:72:A:ARG:HA	1:73:A:ILE:HD13	18	0.54
(1,1353)	1:55:A:LEU:H	1:68:A:ILE:HD11	5	0.54
(1,1353)	1:55:A:LEU:H	1:68:A:ILE:HD12	5	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1353)	1:55:A:LEU:H	1:68:A:ILE:HD13	5	0.54
(1,1353)	1:55:A:LEU:H	1:68:A:ILE:HD11	15	0.54
(1,1353)	1:55:A:LEU:H	1:68:A:ILE:HD12	15	0.54
(1,1353)	1:55:A:LEU:H	1:68:A:ILE:HD13	15	0.54
(1,1162)	1:79:A:ILE:HG21	1:111:A:ALA:H	7	0.54
(1,1162)	1:79:A:ILE:HG22	1:111:A:ALA:H	7	0.54
(1,1162)	1:79:A:ILE:HG23	1:111:A:ALA:H	7	0.54
(1,1162)	1:79:A:ILE:HG21	1:111:A:ALA:H	9	0.54
(1,1162)	1:79:A:ILE:HG22	1:111:A:ALA:H	9	0.54
(1,1162)	1:79:A:ILE:HG23	1:111:A:ALA:H	9	0.54
(1,1032)	1:93:A:ILE:HD11	1:112:A:ASP:H	6	0.54
(1,1032)	1:93:A:ILE:HD12	1:112:A:ASP:H	6	0.54
(1,1032)	1:93:A:ILE:HD13	1:112:A:ASP:H	6	0.54
(1,929)	1:3:A:VAL:HG11	1:34:A:LYS:H	10	0.54
(1,929)	1:3:A:VAL:HG12	1:34:A:LYS:H	10	0.54
(1,929)	1:3:A:VAL:HG13	1:34:A:LYS:H	10	0.54
(1,883)	1:59:A:LEU:HB3	1:61:A:GLY:H	13	0.54
(1,228)	1:19:A:TYR:HD1	1:57:A:MET:H	17	0.54
(1,228)	1:19:A:TYR:HD2	1:57:A:MET:H	17	0.54
(1,228)	1:19:A:TYR:HD1	1:57:A:MET:H	18	0.54
(1,228)	1:19:A:TYR:HD2	1:57:A:MET:H	18	0.54
(1,3890)	1:71:A:ASN:H	1:2:A:SER:HB2	5	0.53
(1,3812)	1:12:A:GLY:HA3	1:4:A:LYS:HD2	20	0.53
(1,3695)	1:108:A:LEU:HD21	1:102:A:GLN:HG2	13	0.53
(1,3695)	1:108:A:LEU:HD22	1:102:A:GLN:HG2	13	0.53
(1,3695)	1:108:A:LEU:HD23	1:102:A:GLN:HG2	13	0.53
(1,3635)	1:112:A:ASP:HB2	1:113:A:ALA:HA	10	0.53
(1,3635)	1:112:A:ASP:HB2	1:113:A:ALA:HA	17	0.53
(1,3386)	1:32:A:THR:HA	1:31:A:LEU:HD11	12	0.53
(1,3386)	1:32:A:THR:HA	1:31:A:LEU:HD12	12	0.53
(1,3386)	1:32:A:THR:HA	1:31:A:LEU:HD13	12	0.53
(1,3180)	1:127:A:ILE:HB	1:79:A:ILE:HD11	16	0.53
(1,3180)	1:127:A:ILE:HB	1:79:A:ILE:HD12	16	0.53
(1,3180)	1:127:A:ILE:HB	1:79:A:ILE:HD13	16	0.53
(1,2995)	1:70:A:LYS:HB3	1:5:A:ILE:HG21	14	0.53
(1,2995)	1:70:A:LYS:HB3	1:5:A:ILE:HG22	14	0.53
(1,2995)	1:70:A:LYS:HB3	1:5:A:ILE:HG23	14	0.53
(1,2942)	1:86:A:ASP:HB2	1:131:A:ILE:HG21	13	0.53
(1,2942)	1:86:A:ASP:HB2	1:131:A:ILE:HG22	13	0.53
(1,2942)	1:86:A:ASP:HB2	1:131:A:ILE:HG23	13	0.53
(1,2523)	1:8:A:ILE:HA	1:22:A:LEU:HD21	20	0.53
(1,2523)	1:8:A:ILE:HA	1:22:A:LEU:HD22	20	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2523)	1:8:A:ILE:HA	1:22:A:LEU:HD23	20	0.53
(1,2522)	1:139:A:PRO:HD2	1:135:A:ILE:HG13	15	0.53
(1,2522)	1:139:A:PRO:HD3	1:135:A:ILE:HG13	15	0.53
(1,1813)	1:35:A:GLN:HE21	1:34:A:LYS:HE2	12	0.53
(1,1784)	1:125:A:ILE:H	1:129:A:LYS:HE2	12	0.53
(1,1784)	1:125:A:ILE:H	1:129:A:LYS:HE3	12	0.53
(1,1357)	1:123:A:ASP:H	1:93:A:ILE:HD11	4	0.53
(1,1357)	1:123:A:ASP:H	1:93:A:ILE:HD12	4	0.53
(1,1357)	1:123:A:ASP:H	1:93:A:ILE:HD13	4	0.53
(1,1150)	1:134:A:ARG:HG2	1:129:A:LYS:H	12	0.53
(1,1150)	1:134:A:ARG:HG3	1:129:A:LYS:H	12	0.53
(1,1132)	1:131:A:ILE:HG12	1:130:A:TYR:H	1	0.53
(1,929)	1:3:A:VAL:HG21	1:34:A:LYS:H	19	0.53
(1,929)	1:3:A:VAL:HG22	1:34:A:LYS:H	19	0.53
(1,929)	1:3:A:VAL:HG23	1:34:A:LYS:H	19	0.53
(1,587)	1:7:A:ASP:HB3	1:11:A:ASN:H	18	0.53
(1,3724)	1:71:A:ASN:HB3	1:5:A:ILE:HG13	7	0.52
(1,3635)	1:112:A:ASP:HB2	1:113:A:ALA:HA	6	0.52
(1,3596)	1:15:A:SER:HB3	1:14:A:ILE:HD11	12	0.52
(1,3596)	1:15:A:SER:HB3	1:14:A:ILE:HD12	12	0.52
(1,3596)	1:15:A:SER:HB3	1:14:A:ILE:HD13	12	0.52
(1,3180)	1:127:A:ILE:HB	1:79:A:ILE:HD11	13	0.52
(1,3180)	1:127:A:ILE:HB	1:79:A:ILE:HD12	13	0.52
(1,3180)	1:127:A:ILE:HB	1:79:A:ILE:HD13	13	0.52
(1,2537)	1:52:A:LEU:HA	1:55:A:LEU:HD11	16	0.52
(1,2537)	1:52:A:LEU:HA	1:55:A:LEU:HD12	16	0.52
(1,2537)	1:52:A:LEU:HA	1:55:A:LEU:HD13	16	0.52
(1,2523)	1:8:A:ILE:HA	1:22:A:LEU:HD21	15	0.52
(1,2523)	1:8:A:ILE:HA	1:22:A:LEU:HD22	15	0.52
(1,2523)	1:8:A:ILE:HA	1:22:A:LEU:HD23	15	0.52
(1,2522)	1:23:A:LYS:HA	1:22:A:LEU:HD21	10	0.52
(1,2522)	1:23:A:LYS:HA	1:22:A:LEU:HD22	10	0.52
(1,2522)	1:23:A:LYS:HA	1:22:A:LEU:HD23	10	0.52
(1,2522)	1:23:A:LYS:HA	1:22:A:LEU:HD21	17	0.52
(1,2522)	1:23:A:LYS:HA	1:22:A:LEU:HD22	17	0.52
(1,2522)	1:23:A:LYS:HA	1:22:A:LEU:HD23	17	0.52
(1,2522)	1:23:A:LYS:HA	1:22:A:LEU:HD21	18	0.52
(1,2522)	1:23:A:LYS:HA	1:22:A:LEU:HD22	18	0.52
(1,2522)	1:23:A:LYS:HA	1:22:A:LEU:HD23	18	0.52
(1,2306)	1:71:A:ASN:H	1:5:A:ILE:HG13	14	0.52
(1,2306)	1:71:A:ASN:H	1:5:A:ILE:HG13	17	0.52
(1,1238)	1:21:A:ILE:HD11	1:20:A:ALA:H	8	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1238)	1:21:A:ILE:HD12	1:20:A:ALA:H	8	0.52
(1,1238)	1:21:A:ILE:HD13	1:20:A:ALA:H	8	0.52
(1,1238)	1:17:A:ILE:HD11	1:20:A:ALA:H	9	0.52
(1,1238)	1:17:A:ILE:HD12	1:20:A:ALA:H	9	0.52
(1,1238)	1:17:A:ILE:HD13	1:20:A:ALA:H	9	0.52
(1,1238)	1:59:A:LEU:HD21	1:20:A:ALA:H	18	0.52
(1,1238)	1:59:A:LEU:HD22	1:20:A:ALA:H	18	0.52
(1,1238)	1:59:A:LEU:HD23	1:20:A:ALA:H	18	0.52
(1,1162)	1:79:A:ILE:HG21	1:111:A:ALA:H	20	0.52
(1,1162)	1:79:A:ILE:HG22	1:111:A:ALA:H	20	0.52
(1,1162)	1:79:A:ILE:HG23	1:111:A:ALA:H	20	0.52
(1,1067)	1:68:A:ILE:HD11	1:63:A:GLY:H	19	0.52
(1,1067)	1:68:A:ILE:HD12	1:63:A:GLY:H	19	0.52
(1,1067)	1:68:A:ILE:HD13	1:63:A:GLY:H	19	0.52
(1,962)	1:73:A:ILE:HD11	1:71:A:ASN:H	2	0.52
(1,962)	1:73:A:ILE:HD12	1:71:A:ASN:H	2	0.52
(1,962)	1:73:A:ILE:HD13	1:71:A:ASN:H	2	0.52
(1,929)	1:3:A:VAL:HG21	1:34:A:LYS:H	7	0.52
(1,929)	1:3:A:VAL:HG22	1:34:A:LYS:H	7	0.52
(1,929)	1:3:A:VAL:HG23	1:34:A:LYS:H	7	0.52
(1,883)	1:59:A:LEU:HB3	1:61:A:GLY:H	10	0.52
(1,554)	1:34:A:LYS:HE2	1:4:A:LYS:H	4	0.52
(1,554)	1:4:A:LYS:HE2	1:4:A:LYS:H	12	0.52
(1,554)	1:4:A:LYS:HE3	1:4:A:LYS:H	12	0.52
(1,3695)	1:108:A:LEU:HD21	1:102:A:GLN:HG2	15	0.51
(1,3695)	1:108:A:LEU:HD22	1:102:A:GLN:HG2	15	0.51
(1,3695)	1:108:A:LEU:HD23	1:102:A:GLN:HG2	15	0.51
(1,3635)	1:112:A:ASP:HB2	1:113:A:ALA:HA	5	0.51
(1,3635)	1:112:A:ASP:HB2	1:113:A:ALA:HA	11	0.51
(1,3596)	1:15:A:SER:HB3	1:14:A:ILE:HD11	20	0.51
(1,3596)	1:15:A:SER:HB3	1:14:A:ILE:HD12	20	0.51
(1,3596)	1:15:A:SER:HB3	1:14:A:ILE:HD13	20	0.51
(1,3568)	1:86:A:ASP:HB2	1:88:A:ASN:HB2	8	0.51
(1,3386)	1:32:A:THR:HA	1:31:A:LEU:HD11	16	0.51
(1,3386)	1:32:A:THR:HA	1:31:A:LEU:HD12	16	0.51
(1,3386)	1:32:A:THR:HA	1:31:A:LEU:HD13	16	0.51
(1,3045)	1:133:A:GLY:HA2	1:136:A:THR:HG21	16	0.51
(1,3045)	1:133:A:GLY:HA2	1:136:A:THR:HG22	16	0.51
(1,3045)	1:133:A:GLY:HA2	1:136:A:THR:HG23	16	0.51
(1,3040)	1:18:A:ASP:HB2	1:14:A:ILE:HG21	19	0.51
(1,3040)	1:18:A:ASP:HB2	1:14:A:ILE:HG22	19	0.51
(1,3040)	1:18:A:ASP:HB2	1:14:A:ILE:HG23	19	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2970)	1:87:A:GLU:HG2	1:127:A:ILE:HG21	13	0.51
(1,2970)	1:87:A:GLU:HG2	1:127:A:ILE:HG22	13	0.51
(1,2970)	1:87:A:GLU:HG2	1:127:A:ILE:HG23	13	0.51
(1,2466)	1:24:A:SER:H	1:23:A:LYS:HG2	20	0.51
(1,2410)	1:102:A:GLN:HG3	1:108:A:LEU:HG	20	0.51
(1,2239)	1:104:A:SER:HA	1:102:A:GLN:HB2	15	0.51
(1,2239)	1:104:A:SER:HA	1:102:A:GLN:HB3	15	0.51
(1,1813)	1:19:A:TYR:HD1	1:23:A:LYS:HE2	16	0.51
(1,1813)	1:19:A:TYR:HD2	1:23:A:LYS:HE2	16	0.51
(1,1813)	1:35:A:GLN:HE21	1:34:A:LYS:HE2	18	0.51
(1,1067)	1:68:A:ILE:HD11	1:63:A:GLY:H	16	0.51
(1,1067)	1:68:A:ILE:HD12	1:63:A:GLY:H	16	0.51
(1,1067)	1:68:A:ILE:HD13	1:63:A:GLY:H	16	0.51
(1,929)	1:3:A:VAL:HG21	1:34:A:LYS:H	16	0.51
(1,929)	1:3:A:VAL:HG22	1:34:A:LYS:H	16	0.51
(1,929)	1:3:A:VAL:HG23	1:34:A:LYS:H	16	0.51
(1,605)	1:90:A:TYR:HB2	1:93:A:ILE:H	5	0.51
(1,554)	1:4:A:LYS:HE2	1:4:A:LYS:H	2	0.51
(1,554)	1:4:A:LYS:HE3	1:4:A:LYS:H	2	0.51
(1,228)	1:19:A:TYR:HD1	1:57:A:MET:H	20	0.51
(1,228)	1:19:A:TYR:HD2	1:57:A:MET:H	20	0.51
(1,3812)	1:12:A:GLY:HA3	1:4:A:LYS:HD2	4	0.5
(1,3695)	1:108:A:LEU:HD21	1:102:A:GLN:HG2	8	0.5
(1,3695)	1:108:A:LEU:HD22	1:102:A:GLN:HG2	8	0.5
(1,3695)	1:108:A:LEU:HD23	1:102:A:GLN:HG2	8	0.5
(1,3635)	1:112:A:ASP:HB2	1:113:A:ALA:HA	8	0.5
(1,3635)	1:112:A:ASP:HB2	1:113:A:ALA:HA	20	0.5
(1,3568)	1:89:A:ASP:HB2	1:88:A:ASN:HB2	7	0.5
(1,3568)	1:89:A:ASP:HB3	1:88:A:ASN:HB2	7	0.5
(1,3457)	1:74:A:TYR:HB3	1:75:A:THR:HA	9	0.5
(1,2995)	1:70:A:LYS:HB3	1:5:A:ILE:HG21	18	0.5
(1,2995)	1:70:A:LYS:HB3	1:5:A:ILE:HG22	18	0.5
(1,2995)	1:70:A:LYS:HB3	1:5:A:ILE:HG23	18	0.5
(1,2962)	1:42:A:ASP:HB3	1:54:A:ILE:HG21	9	0.5
(1,2962)	1:42:A:ASP:HB3	1:54:A:ILE:HG22	9	0.5
(1,2962)	1:42:A:ASP:HB3	1:54:A:ILE:HG23	9	0.5
(1,2962)	1:42:A:ASP:HB3	1:50:A:ILE:HG21	15	0.5
(1,2962)	1:42:A:ASP:HB3	1:50:A:ILE:HG22	15	0.5
(1,2962)	1:42:A:ASP:HB3	1:50:A:ILE:HG23	15	0.5
(1,2954)	1:9:A:ASP:HB3	1:20:A:ALA:HB1	5	0.5
(1,2954)	1:9:A:ASP:HB3	1:20:A:ALA:HB2	5	0.5
(1,2954)	1:9:A:ASP:HB3	1:20:A:ALA:HB3	5	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2844)	1:58:A:TYR:H	1:68:A:ILE:HG21	1	0.5
(1,2844)	1:58:A:TYR:H	1:68:A:ILE:HG22	1	0.5
(1,2844)	1:58:A:TYR:H	1:68:A:ILE:HG23	1	0.5
(1,2523)	1:8:A:ILE:HA	1:22:A:LEU:HD21	19	0.5
(1,2523)	1:8:A:ILE:HA	1:22:A:LEU:HD22	19	0.5
(1,2523)	1:8:A:ILE:HA	1:22:A:LEU:HD23	19	0.5
(1,1806)	1:81:A:ASN:HD22	1:72:A:ARG:HD3	4	0.5
(1,1784)	1:125:A:ILE:H	1:129:A:LYS:HE2	7	0.5
(1,1784)	1:125:A:ILE:H	1:129:A:LYS:HE3	7	0.5
(1,1505)	1:72:A:ARG:HA	1:73:A:ILE:HD11	4	0.5
(1,1505)	1:72:A:ARG:HA	1:73:A:ILE:HD12	4	0.5
(1,1505)	1:72:A:ARG:HA	1:73:A:ILE:HD13	4	0.5
(1,1505)	1:72:A:ARG:HA	1:73:A:ILE:HD11	17	0.5
(1,1505)	1:72:A:ARG:HA	1:73:A:ILE:HD12	17	0.5
(1,1505)	1:72:A:ARG:HA	1:73:A:ILE:HD13	17	0.5
(1,1225)	1:110:A:ALA:HA	1:76:A:TYR:H	10	0.5
(1,971)	1:60:A:LEU:HD21	1:62:A:LYS:H	12	0.5
(1,971)	1:60:A:LEU:HD22	1:62:A:LYS:H	12	0.5
(1,971)	1:60:A:LEU:HD23	1:62:A:LYS:H	12	0.5
(1,929)	1:3:A:VAL:HG21	1:34:A:LYS:H	15	0.5
(1,929)	1:3:A:VAL:HG22	1:34:A:LYS:H	15	0.5
(1,929)	1:3:A:VAL:HG23	1:34:A:LYS:H	15	0.5
(1,3890)	1:4:A:LYS:H	1:2:A:SER:HB2	12	0.49
(1,3724)	1:71:A:ASN:HB3	1:5:A:ILE:HG13	10	0.49
(1,3695)	1:108:A:LEU:HD21	1:102:A:GLN:HG2	3	0.49
(1,3695)	1:108:A:LEU:HD22	1:102:A:GLN:HG2	3	0.49
(1,3695)	1:108:A:LEU:HD23	1:102:A:GLN:HG2	3	0.49
(1,3431)	1:4:A:LYS:HG3	1:71:A:ASN:HA	5	0.49
(1,3386)	1:32:A:THR:HA	1:31:A:LEU:HD11	18	0.49
(1,3386)	1:32:A:THR:HA	1:31:A:LEU:HD12	18	0.49
(1,3386)	1:32:A:THR:HA	1:31:A:LEU:HD13	18	0.49
(1,3180)	1:127:A:ILE:HB	1:79:A:ILE:HD11	11	0.49
(1,3180)	1:127:A:ILE:HB	1:79:A:ILE:HD12	11	0.49
(1,3180)	1:127:A:ILE:HB	1:79:A:ILE:HD13	11	0.49
(1,2586)	1:106:A:ALA:HB1	1:36:A:LEU:HD11	12	0.49
(1,2586)	1:106:A:ALA:HB1	1:36:A:LEU:HD12	12	0.49
(1,2586)	1:106:A:ALA:HB1	1:36:A:LEU:HD13	12	0.49
(1,2586)	1:106:A:ALA:HB2	1:36:A:LEU:HD11	12	0.49
(1,2586)	1:106:A:ALA:HB2	1:36:A:LEU:HD12	12	0.49
(1,2586)	1:106:A:ALA:HB2	1:36:A:LEU:HD13	12	0.49
(1,2586)	1:106:A:ALA:HB3	1:36:A:LEU:HD11	12	0.49
(1,2586)	1:106:A:ALA:HB3	1:36:A:LEU:HD12	12	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2586)	1:106:A:ALA:HB3	1:36:A:LEU:HD13	12	0.49
(1,2523)	1:8:A:ILE:HA	1:22:A:LEU:HD21	12	0.49
(1,2523)	1:8:A:ILE:HA	1:22:A:LEU:HD22	12	0.49
(1,2523)	1:8:A:ILE:HA	1:22:A:LEU:HD23	12	0.49
(1,2483)	1:56:A:GLN:HE21	1:52:A:LEU:HD21	1	0.49
(1,2483)	1:56:A:GLN:HE21	1:52:A:LEU:HD22	1	0.49
(1,2483)	1:56:A:GLN:HE21	1:52:A:LEU:HD23	1	0.49
(1,2483)	1:56:A:GLN:HE21	1:60:A:LEU:HD21	14	0.49
(1,2483)	1:56:A:GLN:HE21	1:60:A:LEU:HD22	14	0.49
(1,2483)	1:56:A:GLN:HE21	1:60:A:LEU:HD23	14	0.49
(1,1784)	1:125:A:ILE:H	1:129:A:LYS:HE2	13	0.49
(1,1784)	1:125:A:ILE:H	1:129:A:LYS:HE3	13	0.49
(1,1780)	1:129:A:LYS:H	1:134:A:ARG:HD2	17	0.49
(1,1780)	1:129:A:LYS:H	1:134:A:ARG:HD3	17	0.49
(1,1238)	1:17:A:ILE:HD11	1:20:A:ALA:H	19	0.49
(1,1238)	1:17:A:ILE:HD12	1:20:A:ALA:H	19	0.49
(1,1238)	1:17:A:ILE:HD13	1:20:A:ALA:H	19	0.49
(1,1132)	1:131:A:ILE:HG12	1:130:A:TYR:H	2	0.49
(1,1056)	1:122:A:THR:HG21	1:114:A:ASP:H	14	0.49
(1,1056)	1:122:A:THR:HG22	1:114:A:ASP:H	14	0.49
(1,1056)	1:122:A:THR:HG23	1:114:A:ASP:H	14	0.49
(1,1043)	1:21:A:ILE:HG21	1:32:A:THR:H	18	0.49
(1,1043)	1:21:A:ILE:HG22	1:32:A:THR:H	18	0.49
(1,1043)	1:21:A:ILE:HG23	1:32:A:THR:H	18	0.49
(1,1032)	1:93:A:ILE:HD11	1:112:A:ASP:H	9	0.49
(1,1032)	1:93:A:ILE:HD12	1:112:A:ASP:H	9	0.49
(1,1032)	1:93:A:ILE:HD13	1:112:A:ASP:H	9	0.49
(1,3758)	1:102:A:GLN:HG3	1:108:A:LEU:HD21	18	0.48
(1,3758)	1:102:A:GLN:HG3	1:108:A:LEU:HD22	18	0.48
(1,3758)	1:102:A:GLN:HG3	1:108:A:LEU:HD23	18	0.48
(1,3696)	1:108:A:LEU:HD21	1:102:A:GLN:HG3	18	0.48
(1,3696)	1:108:A:LEU:HD22	1:102:A:GLN:HG3	18	0.48
(1,3696)	1:108:A:LEU:HD23	1:102:A:GLN:HG3	18	0.48
(1,3635)	1:112:A:ASP:HB2	1:113:A:ALA:HA	2	0.48
(1,3635)	1:112:A:ASP:HB2	1:113:A:ALA:HA	7	0.48
(1,3596)	1:15:A:SER:HB3	1:14:A:ILE:HD11	1	0.48
(1,3596)	1:15:A:SER:HB3	1:14:A:ILE:HD12	1	0.48
(1,3596)	1:15:A:SER:HB3	1:14:A:ILE:HD13	1	0.48
(1,3596)	1:15:A:SER:HB3	1:14:A:ILE:HD11	15	0.48
(1,3596)	1:15:A:SER:HB3	1:14:A:ILE:HD12	15	0.48
(1,3596)	1:15:A:SER:HB3	1:14:A:ILE:HD13	15	0.48
(1,2765)	1:74:A:TYR:HB2	1:3:A:VAL:HG21	18	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2765)	1:74:A:TYR:HB2	1:3:A:VAL:HG22	18	0.48
(1,2765)	1:74:A:TYR:HB2	1:3:A:VAL:HG23	18	0.48
(1,2522)	1:23:A:LYS:HA	1:22:A:LEU:HD21	5	0.48
(1,2522)	1:23:A:LYS:HA	1:22:A:LEU:HD22	5	0.48
(1,2522)	1:23:A:LYS:HA	1:22:A:LEU:HD23	5	0.48
(1,2522)	1:23:A:LYS:HA	1:22:A:LEU:HD21	16	0.48
(1,2522)	1:23:A:LYS:HA	1:22:A:LEU:HD22	16	0.48
(1,2522)	1:23:A:LYS:HA	1:22:A:LEU:HD23	16	0.48
(1,2484)	1:56:A:GLN:HE22	1:60:A:LEU:HD21	6	0.48
(1,2484)	1:56:A:GLN:HE22	1:60:A:LEU:HD22	6	0.48
(1,2484)	1:56:A:GLN:HE22	1:60:A:LEU:HD23	6	0.48
(1,2483)	1:56:A:GLN:HE21	1:52:A:LEU:HD21	2	0.48
(1,2483)	1:56:A:GLN:HE21	1:52:A:LEU:HD22	2	0.48
(1,2483)	1:56:A:GLN:HE21	1:52:A:LEU:HD23	2	0.48
(1,2466)	1:24:A:SER:H	1:23:A:LYS:HG2	16	0.48
(1,1813)	1:35:A:GLN:HE21	1:34:A:LYS:HE2	15	0.48
(1,1806)	1:81:A:ASN:HD22	1:72:A:ARG:HD3	3	0.48
(1,1806)	1:74:A:TYR:HE2	1:72:A:ARG:HD3	16	0.48
(1,1784)	1:125:A:ILE:H	1:129:A:LYS:HE2	8	0.48
(1,1784)	1:125:A:ILE:H	1:129:A:LYS:HE3	8	0.48
(1,1505)	1:72:A:ARG:HA	1:73:A:ILE:HD11	9	0.48
(1,1505)	1:72:A:ARG:HA	1:73:A:ILE:HD12	9	0.48
(1,1505)	1:72:A:ARG:HA	1:73:A:ILE:HD13	9	0.48
(1,1505)	1:72:A:ARG:HA	1:73:A:ILE:HD11	19	0.48
(1,1505)	1:72:A:ARG:HA	1:73:A:ILE:HD12	19	0.48
(1,1505)	1:72:A:ARG:HA	1:73:A:ILE:HD13	19	0.48
(1,1056)	1:122:A:THR:HG21	1:114:A:ASP:H	7	0.48
(1,1056)	1:122:A:THR:HG22	1:114:A:ASP:H	7	0.48
(1,1056)	1:122:A:THR:HG23	1:114:A:ASP:H	7	0.48
(1,587)	1:9:A:ASP:HB3	1:11:A:ASN:H	11	0.48
(1,554)	1:4:A:LYS:HE2	1:4:A:LYS:H	1	0.48
(1,554)	1:4:A:LYS:HE3	1:4:A:LYS:H	1	0.48
(1,554)	1:34:A:LYS:HE2	1:4:A:LYS:H	19	0.48
(1,3938)	1:14:A:ILE:HB	1:58:A:TYR:HD1	14	0.47
(1,3938)	1:14:A:ILE:HB	1:58:A:TYR:HD2	14	0.47
(1,3871)	1:79:A:ILE:H	1:80:A:ASP:HB3	18	0.47
(1,3724)	1:71:A:ASN:HB3	1:5:A:ILE:HG13	9	0.47
(1,3695)	1:108:A:LEU:HD21	1:102:A:GLN:HG2	4	0.47
(1,3695)	1:108:A:LEU:HD22	1:102:A:GLN:HG2	4	0.47
(1,3695)	1:108:A:LEU:HD23	1:102:A:GLN:HG2	4	0.47
(1,3596)	1:15:A:SER:HB3	1:14:A:ILE:HD11	18	0.47
(1,3596)	1:15:A:SER:HB3	1:14:A:ILE:HD12	18	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3596)	1:15:A:SER:HB3	1:14:A:ILE:HD13	18	0.47
(1,3568)	1:86:A:ASP:HB2	1:88:A:ASN:HB2	9	0.47
(1,3568)	1:86:A:ASP:HB2	1:88:A:ASN:HB2	11	0.47
(1,3568)	1:89:A:ASP:HB2	1:88:A:ASN:HB2	19	0.47
(1,3568)	1:89:A:ASP:HB3	1:88:A:ASN:HB2	19	0.47
(1,3180)	1:127:A:ILE:HB	1:79:A:ILE:HD11	6	0.47
(1,3180)	1:127:A:ILE:HB	1:79:A:ILE:HD12	6	0.47
(1,3180)	1:127:A:ILE:HB	1:79:A:ILE:HD13	6	0.47
(1,2995)	1:70:A:LYS:HB3	1:5:A:ILE:HG21	8	0.47
(1,2995)	1:70:A:LYS:HB3	1:5:A:ILE:HG22	8	0.47
(1,2995)	1:70:A:LYS:HB3	1:5:A:ILE:HG23	8	0.47
(1,2970)	1:87:A:GLU:HG2	1:127:A:ILE:HG21	11	0.47
(1,2970)	1:87:A:GLU:HG2	1:127:A:ILE:HG22	11	0.47
(1,2970)	1:87:A:GLU:HG2	1:127:A:ILE:HG23	11	0.47
(1,2523)	1:8:A:ILE:HA	1:22:A:LEU:HD21	4	0.47
(1,2523)	1:8:A:ILE:HA	1:22:A:LEU:HD22	4	0.47
(1,2523)	1:8:A:ILE:HA	1:22:A:LEU:HD23	4	0.47
(1,2523)	1:8:A:ILE:HA	1:22:A:LEU:HD21	5	0.47
(1,2523)	1:8:A:ILE:HA	1:22:A:LEU:HD22	5	0.47
(1,2523)	1:8:A:ILE:HA	1:22:A:LEU:HD23	5	0.47
(1,2523)	1:8:A:ILE:HA	1:22:A:LEU:HD21	14	0.47
(1,2523)	1:8:A:ILE:HA	1:22:A:LEU:HD22	14	0.47
(1,2523)	1:8:A:ILE:HA	1:22:A:LEU:HD23	14	0.47
(1,2484)	1:56:A:GLN:HE22	1:60:A:LEU:HD21	2	0.47
(1,2484)	1:56:A:GLN:HE22	1:60:A:LEU:HD22	2	0.47
(1,2484)	1:56:A:GLN:HE22	1:60:A:LEU:HD23	2	0.47
(1,2410)	1:102:A:GLN:HG3	1:108:A:LEU:HG	5	0.47
(1,2410)	1:102:A:GLN:HG3	1:108:A:LEU:HG	12	0.47
(1,2247)	1:70:A:LYS:HA	1:70:A:LYS:HD2	17	0.47
(1,2239)	1:104:A:SER:HA	1:102:A:GLN:HB2	11	0.47
(1,2239)	1:104:A:SER:HA	1:102:A:GLN:HB3	11	0.47
(1,1238)	1:59:A:LEU:HD21	1:20:A:ALA:H	14	0.47
(1,1238)	1:59:A:LEU:HD22	1:20:A:ALA:H	14	0.47
(1,1238)	1:59:A:LEU:HD23	1:20:A:ALA:H	14	0.47
(1,1162)	1:79:A:ILE:HG21	1:111:A:ALA:H	3	0.47
(1,1162)	1:79:A:ILE:HG22	1:111:A:ALA:H	3	0.47
(1,1162)	1:79:A:ILE:HG23	1:111:A:ALA:H	3	0.47
(1,971)	1:60:A:LEU:HD21	1:62:A:LYS:H	14	0.47
(1,971)	1:60:A:LEU:HD22	1:62:A:LYS:H	14	0.47
(1,971)	1:60:A:LEU:HD23	1:62:A:LYS:H	14	0.47
(1,971)	1:60:A:LEU:HD21	1:62:A:LYS:H	18	0.47
(1,971)	1:60:A:LEU:HD22	1:62:A:LYS:H	18	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,971)	1:60:A:LEU:HD23	1:62:A:LYS:H	18	0.47
(1,971)	1:60:A:LEU:HD21	1:62:A:LYS:H	19	0.47
(1,971)	1:60:A:LEU:HD22	1:62:A:LYS:H	19	0.47
(1,971)	1:60:A:LEU:HD23	1:62:A:LYS:H	19	0.47
(1,962)	1:73:A:ILE:HD11	1:71:A:ASN:H	7	0.47
(1,962)	1:73:A:ILE:HD12	1:71:A:ASN:H	7	0.47
(1,962)	1:73:A:ILE:HD13	1:71:A:ASN:H	7	0.47
(1,929)	1:3:A:VAL:HG21	1:34:A:LYS:H	2	0.47
(1,929)	1:3:A:VAL:HG22	1:34:A:LYS:H	2	0.47
(1,929)	1:3:A:VAL:HG23	1:34:A:LYS:H	2	0.47
(1,605)	1:90:A:TYR:HB2	1:93:A:ILE:H	2	0.47
(1,605)	1:90:A:TYR:HB2	1:93:A:ILE:H	12	0.47
(1,605)	1:90:A:TYR:HB2	1:93:A:ILE:H	17	0.47
(1,396)	1:39:A:ALA:HA	1:8:A:ILE:H	10	0.47
(1,3724)	1:71:A:ASN:HB3	1:5:A:ILE:HG13	3	0.46
(1,3596)	1:15:A:SER:HB3	1:14:A:ILE:HD11	2	0.46
(1,3596)	1:15:A:SER:HB3	1:14:A:ILE:HD12	2	0.46
(1,3596)	1:15:A:SER:HB3	1:14:A:ILE:HD13	2	0.46
(1,3568)	1:89:A:ASP:HB2	1:88:A:ASN:HB2	13	0.46
(1,3568)	1:89:A:ASP:HB3	1:88:A:ASN:HB2	13	0.46
(1,3238)	1:74:A:TYR:HB3	1:2:A:SER:HA	11	0.46
(1,3183)	1:90:A:TYR:HB2	1:79:A:ILE:HD11	4	0.46
(1,3183)	1:90:A:TYR:HB2	1:79:A:ILE:HD12	4	0.46
(1,3183)	1:90:A:TYR:HB2	1:79:A:ILE:HD13	4	0.46
(1,3180)	1:127:A:ILE:HB	1:79:A:ILE:HD11	19	0.46
(1,3180)	1:127:A:ILE:HB	1:79:A:ILE:HD12	19	0.46
(1,3180)	1:127:A:ILE:HB	1:79:A:ILE:HD13	19	0.46
(1,3040)	1:18:A:ASP:HB2	1:14:A:ILE:HG21	7	0.46
(1,3040)	1:18:A:ASP:HB2	1:14:A:ILE:HG22	7	0.46
(1,3040)	1:18:A:ASP:HB2	1:14:A:ILE:HG23	7	0.46
(1,2765)	1:40:A:ASP:HB3	1:3:A:VAL:HG11	19	0.46
(1,2765)	1:40:A:ASP:HB3	1:3:A:VAL:HG12	19	0.46
(1,2765)	1:40:A:ASP:HB3	1:3:A:VAL:HG13	19	0.46
(1,2586)	1:39:A:ALA:HB1	1:36:A:LEU:HD11	1	0.46
(1,2586)	1:39:A:ALA:HB1	1:36:A:LEU:HD12	1	0.46
(1,2586)	1:39:A:ALA:HB1	1:36:A:LEU:HD13	1	0.46
(1,2586)	1:39:A:ALA:HB2	1:36:A:LEU:HD11	1	0.46
(1,2586)	1:39:A:ALA:HB2	1:36:A:LEU:HD12	1	0.46
(1,2586)	1:39:A:ALA:HB2	1:36:A:LEU:HD13	1	0.46
(1,2586)	1:39:A:ALA:HB3	1:36:A:LEU:HD11	1	0.46
(1,2586)	1:39:A:ALA:HB3	1:36:A:LEU:HD12	1	0.46
(1,2586)	1:39:A:ALA:HB3	1:36:A:LEU:HD13	1	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2483)	1:56:A:GLN:HE21	1:52:A:LEU:HD21	13	0.46
(1,2483)	1:56:A:GLN:HE21	1:52:A:LEU:HD22	13	0.46
(1,2483)	1:56:A:GLN:HE21	1:52:A:LEU:HD23	13	0.46
(1,2483)	1:56:A:GLN:HE21	1:60:A:LEU:HD21	16	0.46
(1,2483)	1:56:A:GLN:HE21	1:60:A:LEU:HD22	16	0.46
(1,2483)	1:56:A:GLN:HE21	1:60:A:LEU:HD23	16	0.46
(1,2466)	1:24:A:SER:H	1:23:A:LYS:HG2	6	0.46
(1,2410)	1:102:A:GLN:HG3	1:108:A:LEU:HG	1	0.46
(1,2410)	1:102:A:GLN:HG3	1:108:A:LEU:HG	16	0.46
(1,1806)	1:81:A:ASN:HD22	1:72:A:ARG:HD3	10	0.46
(1,1353)	1:55:A:LEU:H	1:68:A:ILE:HD11	3	0.46
(1,1353)	1:55:A:LEU:H	1:68:A:ILE:HD12	3	0.46
(1,1353)	1:55:A:LEU:H	1:68:A:ILE:HD13	3	0.46
(1,1150)	1:134:A:ARG:HG2	1:129:A:LYS:H	2	0.46
(1,1150)	1:134:A:ARG:HG3	1:129:A:LYS:H	2	0.46
(1,1056)	1:122:A:THR:HG21	1:114:A:ASP:H	12	0.46
(1,1056)	1:122:A:THR:HG22	1:114:A:ASP:H	12	0.46
(1,1056)	1:122:A:THR:HG23	1:114:A:ASP:H	12	0.46
(1,971)	1:60:A:LEU:HD21	1:62:A:LYS:H	6	0.46
(1,971)	1:60:A:LEU:HD22	1:62:A:LYS:H	6	0.46
(1,971)	1:60:A:LEU:HD23	1:62:A:LYS:H	6	0.46
(1,962)	1:5:A:ILE:HD11	1:71:A:ASN:H	14	0.46
(1,962)	1:5:A:ILE:HD12	1:71:A:ASN:H	14	0.46
(1,962)	1:5:A:ILE:HD13	1:71:A:ASN:H	14	0.46
(1,587)	1:7:A:ASP:HB3	1:11:A:ASN:H	1	0.46
(1,386)	1:96:A:HIS:HB3	1:119:A:ILE:H	10	0.46
(1,228)	1:19:A:TYR:HD1	1:57:A:MET:H	16	0.46
(1,228)	1:19:A:TYR:HD2	1:57:A:MET:H	16	0.46
(1,3938)	1:14:A:ILE:HB	1:58:A:TYR:HD1	5	0.45
(1,3938)	1:14:A:ILE:HB	1:58:A:TYR:HD2	5	0.45
(1,3568)	1:89:A:ASP:HB2	1:88:A:ASN:HB2	17	0.45
(1,3568)	1:89:A:ASP:HB3	1:88:A:ASN:HB2	17	0.45
(1,3457)	1:74:A:TYR:HB3	1:75:A:THR:HA	13	0.45
(1,3457)	1:74:A:TYR:HB3	1:75:A:THR:HA	17	0.45
(1,3386)	1:32:A:THR:HA	1:31:A:LEU:HD11	19	0.45
(1,3386)	1:32:A:THR:HA	1:31:A:LEU:HD12	19	0.45
(1,3386)	1:32:A:THR:HA	1:31:A:LEU:HD13	19	0.45
(1,3183)	1:90:A:TYR:HB2	1:79:A:ILE:HD11	20	0.45
(1,3183)	1:90:A:TYR:HB2	1:79:A:ILE:HD12	20	0.45
(1,3183)	1:90:A:TYR:HB2	1:79:A:ILE:HD13	20	0.45
(1,3040)	1:18:A:ASP:HB2	1:14:A:ILE:HG21	14	0.45
(1,3040)	1:18:A:ASP:HB2	1:14:A:ILE:HG22	14	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3040)	1:18:A:ASP:HB2	1:14:A:ILE:HG23	14	0.45
(1,2954)	1:9:A:ASP:HB3	1:20:A:ALA:HB1	9	0.45
(1,2954)	1:9:A:ASP:HB3	1:20:A:ALA:HB2	9	0.45
(1,2954)	1:9:A:ASP:HB3	1:20:A:ALA:HB3	9	0.45
(1,2942)	1:86:A:ASP:HB2	1:131:A:ILE:HG21	4	0.45
(1,2942)	1:86:A:ASP:HB2	1:131:A:ILE:HG22	4	0.45
(1,2942)	1:86:A:ASP:HB2	1:131:A:ILE:HG23	4	0.45
(1,2697)	1:57:A:MET:HB2	1:65:A:THR:HG21	5	0.45
(1,2697)	1:57:A:MET:HB2	1:65:A:THR:HG22	5	0.45
(1,2697)	1:57:A:MET:HB2	1:65:A:THR:HG23	5	0.45
(1,2586)	1:39:A:ALA:HB1	1:36:A:LEU:HD11	5	0.45
(1,2586)	1:39:A:ALA:HB1	1:36:A:LEU:HD12	5	0.45
(1,2586)	1:39:A:ALA:HB1	1:36:A:LEU:HD13	5	0.45
(1,2586)	1:39:A:ALA:HB2	1:36:A:LEU:HD11	5	0.45
(1,2586)	1:39:A:ALA:HB2	1:36:A:LEU:HD12	5	0.45
(1,2586)	1:39:A:ALA:HB2	1:36:A:LEU:HD13	5	0.45
(1,2586)	1:39:A:ALA:HB3	1:36:A:LEU:HD11	5	0.45
(1,2586)	1:39:A:ALA:HB3	1:36:A:LEU:HD12	5	0.45
(1,2586)	1:39:A:ALA:HB3	1:36:A:LEU:HD13	5	0.45
(1,2537)	1:52:A:LEU:HA	1:55:A:LEU:HD11	2	0.45
(1,2537)	1:52:A:LEU:HA	1:55:A:LEU:HD12	2	0.45
(1,2537)	1:52:A:LEU:HA	1:55:A:LEU:HD13	2	0.45
(1,2523)	1:8:A:ILE:HA	1:22:A:LEU:HD21	7	0.45
(1,2523)	1:8:A:ILE:HA	1:22:A:LEU:HD22	7	0.45
(1,2523)	1:8:A:ILE:HA	1:22:A:LEU:HD23	7	0.45
(1,2410)	1:102:A:GLN:HG3	1:108:A:LEU:HG	10	0.45
(1,2350)	1:52:A:LEU:H	1:52:A:LEU:HD21	8	0.45
(1,2350)	1:52:A:LEU:H	1:52:A:LEU:HD22	8	0.45
(1,2350)	1:52:A:LEU:H	1:52:A:LEU:HD23	8	0.45
(1,2287)	1:119:A:ILE:HG21	1:93:A:ILE:HG13	9	0.45
(1,2287)	1:119:A:ILE:HG22	1:93:A:ILE:HG13	9	0.45
(1,2287)	1:119:A:ILE:HG23	1:93:A:ILE:HG13	9	0.45
(1,2247)	1:70:A:LYS:HA	1:70:A:LYS:HD2	19	0.45
(1,1949)	1:136:A:THR:HG21	1:135:A:ILE:HB	12	0.45
(1,1949)	1:136:A:THR:HG22	1:135:A:ILE:HB	12	0.45
(1,1949)	1:136:A:THR:HG23	1:135:A:ILE:HB	12	0.45
(1,1806)	1:81:A:ASN:HD22	1:72:A:ARG:HD3	6	0.45
(1,1353)	1:66:A:SER:H	1:68:A:ILE:HD11	19	0.45
(1,1353)	1:66:A:SER:H	1:68:A:ILE:HD12	19	0.45
(1,1353)	1:66:A:SER:H	1:68:A:ILE:HD13	19	0.45
(1,1220)	1:131:A:ILE:HG21	1:133:A:GLY:H	9	0.45
(1,1220)	1:131:A:ILE:HG22	1:133:A:GLY:H	9	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1220)	1:131:A:ILE:HG23	1:133:A:GLY:H	9	0.45
(1,1220)	1:131:A:ILE:HG21	1:133:A:GLY:H	10	0.45
(1,1220)	1:131:A:ILE:HG22	1:133:A:GLY:H	10	0.45
(1,1220)	1:131:A:ILE:HG23	1:133:A:GLY:H	10	0.45
(1,1117)	1:96:A:HIS:HA	1:102:A:GLN:H	1	0.45
(1,929)	1:3:A:VAL:HG21	1:34:A:LYS:H	6	0.45
(1,929)	1:3:A:VAL:HG22	1:34:A:LYS:H	6	0.45
(1,929)	1:3:A:VAL:HG23	1:34:A:LYS:H	6	0.45
(1,929)	1:3:A:VAL:HG21	1:34:A:LYS:H	12	0.45
(1,929)	1:3:A:VAL:HG22	1:34:A:LYS:H	12	0.45
(1,929)	1:3:A:VAL:HG23	1:34:A:LYS:H	12	0.45
(1,605)	1:90:A:TYR:HB2	1:93:A:ILE:H	8	0.45
(1,554)	1:4:A:LYS:HE2	1:4:A:LYS:H	7	0.45
(1,554)	1:4:A:LYS:HE3	1:4:A:LYS:H	7	0.45
(1,228)	1:19:A:TYR:HD1	1:57:A:MET:H	2	0.45
(1,228)	1:19:A:TYR:HD2	1:57:A:MET:H	2	0.45
(1,228)	1:19:A:TYR:HD1	1:57:A:MET:H	13	0.45
(1,228)	1:19:A:TYR:HD2	1:57:A:MET:H	13	0.45
(1,3890)	1:4:A:LYS:H	1:2:A:SER:HB2	2	0.44
(1,3724)	1:71:A:ASN:HB3	1:5:A:ILE:HG13	14	0.44
(1,3695)	1:108:A:LEU:HD21	1:102:A:GLN:HG2	17	0.44
(1,3695)	1:108:A:LEU:HD22	1:102:A:GLN:HG2	17	0.44
(1,3695)	1:108:A:LEU:HD23	1:102:A:GLN:HG2	17	0.44
(1,3457)	1:74:A:TYR:HB3	1:75:A:THR:HA	5	0.44
(1,3457)	1:74:A:TYR:HB3	1:75:A:THR:HA	15	0.44
(1,2995)	1:70:A:LYS:HB3	1:5:A:ILE:HG21	5	0.44
(1,2995)	1:70:A:LYS:HB3	1:5:A:ILE:HG22	5	0.44
(1,2995)	1:70:A:LYS:HB3	1:5:A:ILE:HG23	5	0.44
(1,2970)	1:87:A:GLU:HG2	1:127:A:ILE:HG21	9	0.44
(1,2970)	1:87:A:GLU:HG2	1:127:A:ILE:HG22	9	0.44
(1,2970)	1:87:A:GLU:HG2	1:127:A:ILE:HG23	9	0.44
(1,2962)	1:42:A:ASP:HB3	1:50:A:ILE:HG21	6	0.44
(1,2962)	1:42:A:ASP:HB3	1:50:A:ILE:HG22	6	0.44
(1,2962)	1:42:A:ASP:HB3	1:50:A:ILE:HG23	6	0.44
(1,2874)	1:19:A:TYR:HD1	1:20:A:ALA:HB1	16	0.44
(1,2874)	1:19:A:TYR:HD1	1:20:A:ALA:HB2	16	0.44
(1,2874)	1:19:A:TYR:HD1	1:20:A:ALA:HB3	16	0.44
(1,2874)	1:19:A:TYR:HD2	1:20:A:ALA:HB1	16	0.44
(1,2874)	1:19:A:TYR:HD2	1:20:A:ALA:HB2	16	0.44
(1,2874)	1:19:A:TYR:HD2	1:20:A:ALA:HB3	16	0.44
(1,2484)	1:56:A:GLN:HE22	1:60:A:LEU:HD21	1	0.44
(1,2484)	1:56:A:GLN:HE22	1:60:A:LEU:HD22	1	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2484)	1:56:A:GLN:HE22	1:60:A:LEU:HD23	1	0.44
(1,2483)	1:56:A:GLN:HE21	1:52:A:LEU:HD21	12	0.44
(1,2483)	1:56:A:GLN:HE21	1:52:A:LEU:HD22	12	0.44
(1,2483)	1:56:A:GLN:HE21	1:52:A:LEU:HD23	12	0.44
(1,2466)	1:24:A:SER:H	1:23:A:LYS:HG2	17	0.44
(1,2410)	1:102:A:GLN:HG3	1:108:A:LEU:HG	7	0.44
(1,2306)	1:71:A:ASN:H	1:5:A:ILE:HG13	11	0.44
(1,2239)	1:104:A:SER:HA	1:102:A:GLN:HB2	8	0.44
(1,2239)	1:104:A:SER:HA	1:102:A:GLN:HB3	8	0.44
(1,1949)	1:136:A:THR:HG21	1:135:A:ILE:HB	3	0.44
(1,1949)	1:136:A:THR:HG22	1:135:A:ILE:HB	3	0.44
(1,1949)	1:136:A:THR:HG23	1:135:A:ILE:HB	3	0.44
(1,1505)	1:72:A:ARG:HA	1:73:A:ILE:HD11	8	0.44
(1,1505)	1:72:A:ARG:HA	1:73:A:ILE:HD12	8	0.44
(1,1505)	1:72:A:ARG:HA	1:73:A:ILE:HD13	8	0.44
(1,1489)	1:70:A:LYS:H	1:5:A:ILE:HD11	2	0.44
(1,1489)	1:70:A:LYS:H	1:5:A:ILE:HD12	2	0.44
(1,1489)	1:70:A:LYS:H	1:5:A:ILE:HD13	2	0.44
(1,1353)	1:55:A:LEU:H	1:68:A:ILE:HD11	4	0.44
(1,1353)	1:55:A:LEU:H	1:68:A:ILE:HD12	4	0.44
(1,1353)	1:55:A:LEU:H	1:68:A:ILE:HD13	4	0.44
(1,980)	1:54:A:ILE:HD11	1:42:A:ASP:H	15	0.44
(1,980)	1:54:A:ILE:HD12	1:42:A:ASP:H	15	0.44
(1,980)	1:54:A:ILE:HD13	1:42:A:ASP:H	15	0.44
(1,971)	1:60:A:LEU:HD21	1:62:A:LYS:H	10	0.44
(1,971)	1:60:A:LEU:HD22	1:62:A:LYS:H	10	0.44
(1,971)	1:60:A:LEU:HD23	1:62:A:LYS:H	10	0.44
(1,971)	1:60:A:LEU:HD21	1:62:A:LYS:H	15	0.44
(1,971)	1:60:A:LEU:HD22	1:62:A:LYS:H	15	0.44
(1,971)	1:60:A:LEU:HD23	1:62:A:LYS:H	15	0.44
(1,929)	1:3:A:VAL:HG11	1:34:A:LYS:H	9	0.44
(1,929)	1:3:A:VAL:HG12	1:34:A:LYS:H	9	0.44
(1,929)	1:3:A:VAL:HG13	1:34:A:LYS:H	9	0.44
(1,605)	1:90:A:TYR:HB2	1:93:A:ILE:H	15	0.44
(1,587)	1:9:A:ASP:HB3	1:11:A:ASN:H	4	0.44
(1,228)	1:19:A:TYR:HD1	1:57:A:MET:H	5	0.44
(1,228)	1:19:A:TYR:HD2	1:57:A:MET:H	5	0.44
(1,228)	1:19:A:TYR:HD1	1:57:A:MET:H	7	0.44
(1,228)	1:19:A:TYR:HD2	1:57:A:MET:H	7	0.44
(1,3943)	1:22:A:LEU:HD21	1:19:A:TYR:HD1	6	0.43
(1,3943)	1:22:A:LEU:HD21	1:19:A:TYR:HD2	6	0.43
(1,3943)	1:22:A:LEU:HD22	1:19:A:TYR:HD1	6	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3943)	1:22:A:LEU:HD22	1:19:A:TYR:HD2	6	0.43
(1,3943)	1:22:A:LEU:HD23	1:19:A:TYR:HD1	6	0.43
(1,3943)	1:22:A:LEU:HD23	1:19:A:TYR:HD2	6	0.43
(1,3805)	1:125:A:ILE:HG12	1:128:A:GLU:HG2	11	0.43
(1,3805)	1:125:A:ILE:HG12	1:128:A:GLU:HG3	11	0.43
(1,3791)	1:132:A:THR:H	1:134:A:ARG:HD2	6	0.43
(1,3791)	1:132:A:THR:H	1:134:A:ARG:HD3	6	0.43
(1,3457)	1:74:A:TYR:HB3	1:75:A:THR:HA	14	0.43
(1,3180)	1:127:A:ILE:HB	1:79:A:ILE:HD11	7	0.43
(1,3180)	1:127:A:ILE:HB	1:79:A:ILE:HD12	7	0.43
(1,3180)	1:127:A:ILE:HB	1:79:A:ILE:HD13	7	0.43
(1,2966)	1:94:A:CYS:HB3	1:97:A:ILE:HG21	11	0.43
(1,2966)	1:94:A:CYS:HB3	1:97:A:ILE:HG22	11	0.43
(1,2966)	1:94:A:CYS:HB3	1:97:A:ILE:HG23	11	0.43
(1,2962)	1:42:A:ASP:HB3	1:54:A:ILE:HG21	13	0.43
(1,2962)	1:42:A:ASP:HB3	1:54:A:ILE:HG22	13	0.43
(1,2962)	1:42:A:ASP:HB3	1:54:A:ILE:HG23	13	0.43
(1,2844)	1:58:A:TYR:H	1:68:A:ILE:HG21	12	0.43
(1,2844)	1:58:A:TYR:H	1:68:A:ILE:HG22	12	0.43
(1,2844)	1:58:A:TYR:H	1:68:A:ILE:HG23	12	0.43
(1,2765)	1:40:A:ASP:HB3	1:3:A:VAL:HG11	15	0.43
(1,2765)	1:40:A:ASP:HB3	1:3:A:VAL:HG12	15	0.43
(1,2765)	1:40:A:ASP:HB3	1:3:A:VAL:HG13	15	0.43
(1,2586)	1:39:A:ALA:HB1	1:36:A:LEU:HD11	7	0.43
(1,2586)	1:39:A:ALA:HB1	1:36:A:LEU:HD12	7	0.43
(1,2586)	1:39:A:ALA:HB1	1:36:A:LEU:HD13	7	0.43
(1,2586)	1:39:A:ALA:HB2	1:36:A:LEU:HD11	7	0.43
(1,2586)	1:39:A:ALA:HB2	1:36:A:LEU:HD12	7	0.43
(1,2586)	1:39:A:ALA:HB2	1:36:A:LEU:HD13	7	0.43
(1,2586)	1:39:A:ALA:HB3	1:36:A:LEU:HD11	7	0.43
(1,2586)	1:39:A:ALA:HB3	1:36:A:LEU:HD12	7	0.43
(1,2586)	1:39:A:ALA:HB3	1:36:A:LEU:HD13	7	0.43
(1,2546)	1:56:A:GLN:HB2	1:60:A:LEU:HD21	14	0.43
(1,2546)	1:56:A:GLN:HB2	1:60:A:LEU:HD22	14	0.43
(1,2546)	1:56:A:GLN:HB2	1:60:A:LEU:HD23	14	0.43
(1,2546)	1:56:A:GLN:HB3	1:60:A:LEU:HD21	14	0.43
(1,2546)	1:56:A:GLN:HB3	1:60:A:LEU:HD22	14	0.43
(1,2546)	1:56:A:GLN:HB3	1:60:A:LEU:HD23	14	0.43
(1,2484)	1:56:A:GLN:HE22	1:60:A:LEU:HD21	11	0.43
(1,2484)	1:56:A:GLN:HE22	1:60:A:LEU:HD22	11	0.43
(1,2484)	1:56:A:GLN:HE22	1:60:A:LEU:HD23	11	0.43
(1,2483)	1:56:A:GLN:HE21	1:60:A:LEU:HD21	6	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2483)	1:56:A:GLN:HE21	1:60:A:LEU:HD22	6	0.43
(1,2483)	1:56:A:GLN:HE21	1:60:A:LEU:HD23	6	0.43
(1,2466)	1:24:A:SER:H	1:23:A:LYS:HG2	5	0.43
(1,2339)	1:81:A:ASN:HD22	1:72:A:ARG:HG2	20	0.43
(1,1792)	1:132:A:THR:H	1:134:A:ARG:HD2	6	0.43
(1,1792)	1:132:A:THR:H	1:134:A:ARG:HD3	6	0.43
(1,1357)	1:123:A:ASP:H	1:93:A:ILE:HD11	6	0.43
(1,1357)	1:123:A:ASP:H	1:93:A:ILE:HD12	6	0.43
(1,1357)	1:123:A:ASP:H	1:93:A:ILE:HD13	6	0.43
(1,1225)	1:110:A:ALA:HA	1:76:A:TYR:H	20	0.43
(1,1162)	1:79:A:ILE:HG21	1:111:A:ALA:H	8	0.43
(1,1162)	1:79:A:ILE:HG22	1:111:A:ALA:H	8	0.43
(1,1162)	1:79:A:ILE:HG23	1:111:A:ALA:H	8	0.43
(1,1117)	1:96:A:HIS:HA	1:102:A:GLN:H	2	0.43
(1,1067)	1:68:A:ILE:HD11	1:63:A:GLY:H	15	0.43
(1,1067)	1:68:A:ILE:HD12	1:63:A:GLY:H	15	0.43
(1,1067)	1:68:A:ILE:HD13	1:63:A:GLY:H	15	0.43
(1,760)	1:97:A:ILE:HB	1:96:A:HIS:H	19	0.43
(1,605)	1:90:A:TYR:HB2	1:93:A:ILE:H	9	0.43
(1,605)	1:90:A:TYR:HB2	1:93:A:ILE:H	20	0.43
(1,572)	1:9:A:ASP:HB3	1:20:A:ALA:H	10	0.43
(1,3890)	1:4:A:LYS:H	1:2:A:SER:HB2	13	0.42
(1,3568)	1:89:A:ASP:HB2	1:88:A:ASN:HB2	2	0.42
(1,3568)	1:89:A:ASP:HB3	1:88:A:ASN:HB2	2	0.42
(1,3568)	1:86:A:ASP:HB2	1:88:A:ASN:HB2	5	0.42
(1,3457)	1:74:A:TYR:HB3	1:75:A:THR:HA	11	0.42
(1,3457)	1:74:A:TYR:HB3	1:75:A:THR:HA	20	0.42
(1,3238)	1:74:A:TYR:HB3	1:2:A:SER:HA	15	0.42
(1,2995)	1:70:A:LYS:HB3	1:5:A:ILE:HG21	13	0.42
(1,2995)	1:70:A:LYS:HB3	1:5:A:ILE:HG22	13	0.42
(1,2995)	1:70:A:LYS:HB3	1:5:A:ILE:HG23	13	0.42
(1,2970)	1:87:A:GLU:HG2	1:127:A:ILE:HG21	7	0.42
(1,2970)	1:87:A:GLU:HG2	1:127:A:ILE:HG22	7	0.42
(1,2970)	1:87:A:GLU:HG2	1:127:A:ILE:HG23	7	0.42
(1,2586)	1:39:A:ALA:HB1	1:36:A:LEU:HD11	20	0.42
(1,2586)	1:39:A:ALA:HB1	1:36:A:LEU:HD12	20	0.42
(1,2586)	1:39:A:ALA:HB1	1:36:A:LEU:HD13	20	0.42
(1,2586)	1:39:A:ALA:HB2	1:36:A:LEU:HD11	20	0.42
(1,2586)	1:39:A:ALA:HB2	1:36:A:LEU:HD12	20	0.42
(1,2586)	1:39:A:ALA:HB2	1:36:A:LEU:HD13	20	0.42
(1,2586)	1:39:A:ALA:HB3	1:36:A:LEU:HD11	20	0.42
(1,2586)	1:39:A:ALA:HB3	1:36:A:LEU:HD12	20	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2586)	1:39:A:ALA:HB3	1:36:A:LEU:HD13	20	0.42
(1,2546)	1:56:A:GLN:HB2	1:60:A:LEU:HD21	10	0.42
(1,2546)	1:56:A:GLN:HB2	1:60:A:LEU:HD22	10	0.42
(1,2546)	1:56:A:GLN:HB2	1:60:A:LEU:HD23	10	0.42
(1,2546)	1:56:A:GLN:HB3	1:60:A:LEU:HD21	10	0.42
(1,2546)	1:56:A:GLN:HB3	1:60:A:LEU:HD22	10	0.42
(1,2546)	1:56:A:GLN:HB3	1:60:A:LEU:HD23	10	0.42
(1,2537)	1:52:A:LEU:HA	1:55:A:LEU:HD11	1	0.42
(1,2537)	1:52:A:LEU:HA	1:55:A:LEU:HD12	1	0.42
(1,2537)	1:52:A:LEU:HA	1:55:A:LEU:HD13	1	0.42
(1,2537)	1:52:A:LEU:HA	1:55:A:LEU:HD11	13	0.42
(1,2537)	1:52:A:LEU:HA	1:55:A:LEU:HD12	13	0.42
(1,2537)	1:52:A:LEU:HA	1:55:A:LEU:HD13	13	0.42
(1,2537)	1:52:A:LEU:HA	1:55:A:LEU:HD11	20	0.42
(1,2537)	1:52:A:LEU:HA	1:55:A:LEU:HD12	20	0.42
(1,2537)	1:52:A:LEU:HA	1:55:A:LEU:HD13	20	0.42
(1,2483)	1:56:A:GLN:HE21	1:60:A:LEU:HD21	7	0.42
(1,2483)	1:56:A:GLN:HE21	1:60:A:LEU:HD22	7	0.42
(1,2483)	1:56:A:GLN:HE21	1:60:A:LEU:HD23	7	0.42
(1,2410)	1:102:A:GLN:HG3	1:108:A:LEU:HG	4	0.42
(1,2344)	1:19:A:TYR:HD1	1:59:A:LEU:HD21	7	0.42
(1,2344)	1:19:A:TYR:HD1	1:59:A:LEU:HD22	7	0.42
(1,2344)	1:19:A:TYR:HD1	1:59:A:LEU:HD23	7	0.42
(1,2344)	1:19:A:TYR:HD2	1:59:A:LEU:HD21	7	0.42
(1,2344)	1:19:A:TYR:HD2	1:59:A:LEU:HD22	7	0.42
(1,2344)	1:19:A:TYR:HD2	1:59:A:LEU:HD23	7	0.42
(1,2247)	1:70:A:LYS:HA	1:70:A:LYS:HD2	2	0.42
(1,2247)	1:70:A:LYS:HA	1:70:A:LYS:HD2	12	0.42
(1,1328)	1:97:A:ILE:HG21	1:121:A:GLN:H	14	0.42
(1,1328)	1:97:A:ILE:HG22	1:121:A:GLN:H	14	0.42
(1,1328)	1:97:A:ILE:HG23	1:121:A:GLN:H	14	0.42
(1,1162)	1:79:A:ILE:HG21	1:111:A:ALA:H	4	0.42
(1,1162)	1:79:A:ILE:HG22	1:111:A:ALA:H	4	0.42
(1,1162)	1:79:A:ILE:HG23	1:111:A:ALA:H	4	0.42
(1,1132)	1:131:A:ILE:HG12	1:130:A:TYR:H	19	0.42
(1,1091)	1:108:A:LEU:HD21	1:104:A:SER:H	4	0.42
(1,1091)	1:108:A:LEU:HD22	1:104:A:SER:H	4	0.42
(1,1091)	1:108:A:LEU:HD23	1:104:A:SER:H	4	0.42
(1,1043)	1:21:A:ILE:HG21	1:32:A:THR:H	20	0.42
(1,1043)	1:21:A:ILE:HG22	1:32:A:THR:H	20	0.42
(1,1043)	1:21:A:ILE:HG23	1:32:A:THR:H	20	0.42
(1,971)	1:60:A:LEU:HD21	1:62:A:LYS:H	13	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,971)	1:60:A:LEU:HD22	1:62:A:LYS:H	13	0.42
(1,971)	1:60:A:LEU:HD23	1:62:A:LYS:H	13	0.42
(1,743)	1:34:A:LYS:HD2	1:34:A:LYS:H	15	0.42
(1,605)	1:90:A:TYR:HB2	1:93:A:ILE:H	11	0.42
(1,587)	1:9:A:ASP:HB3	1:11:A:ASN:H	10	0.42
(1,3581)	1:56:A:GLN:H	1:68:A:ILE:HD11	20	0.41
(1,3581)	1:56:A:GLN:H	1:68:A:ILE:HD12	20	0.41
(1,3581)	1:56:A:GLN:H	1:68:A:ILE:HD13	20	0.41
(1,3568)	1:89:A:ASP:HB2	1:88:A:ASN:HB2	12	0.41
(1,3568)	1:89:A:ASP:HB3	1:88:A:ASN:HB2	12	0.41
(1,3568)	1:86:A:ASP:HB2	1:88:A:ASN:HB2	16	0.41
(1,3457)	1:74:A:TYR:HB3	1:75:A:THR:HA	1	0.41
(1,3274)	1:73:A:ILE:HA	1:72:A:ARG:HD2	13	0.41
(1,3238)	1:74:A:TYR:HB3	1:2:A:SER:HA	7	0.41
(1,3238)	1:74:A:TYR:HB3	1:2:A:SER:HA	12	0.41
(1,2995)	1:70:A:LYS:HB3	1:5:A:ILE:HG21	10	0.41
(1,2995)	1:70:A:LYS:HB3	1:5:A:ILE:HG22	10	0.41
(1,2995)	1:70:A:LYS:HB3	1:5:A:ILE:HG23	10	0.41
(1,2966)	1:94:A:CYS:HB3	1:97:A:ILE:HG21	7	0.41
(1,2966)	1:94:A:CYS:HB3	1:97:A:ILE:HG22	7	0.41
(1,2966)	1:94:A:CYS:HB3	1:97:A:ILE:HG23	7	0.41
(1,2942)	1:86:A:ASP:HB2	1:131:A:ILE:HG21	7	0.41
(1,2942)	1:86:A:ASP:HB2	1:131:A:ILE:HG22	7	0.41
(1,2942)	1:86:A:ASP:HB2	1:131:A:ILE:HG23	7	0.41
(1,2844)	1:58:A:TYR:H	1:68:A:ILE:HG21	19	0.41
(1,2844)	1:58:A:TYR:H	1:68:A:ILE:HG22	19	0.41
(1,2844)	1:58:A:TYR:H	1:68:A:ILE:HG23	19	0.41
(1,2484)	1:56:A:GLN:HE22	1:60:A:LEU:HD21	5	0.41
(1,2484)	1:56:A:GLN:HE22	1:60:A:LEU:HD22	5	0.41
(1,2484)	1:56:A:GLN:HE22	1:60:A:LEU:HD23	5	0.41
(1,2484)	1:56:A:GLN:HE22	1:60:A:LEU:HD21	7	0.41
(1,2484)	1:56:A:GLN:HE22	1:60:A:LEU:HD22	7	0.41
(1,2484)	1:56:A:GLN:HE22	1:60:A:LEU:HD23	7	0.41
(1,2484)	1:56:A:GLN:HE22	1:60:A:LEU:HD21	12	0.41
(1,2484)	1:56:A:GLN:HE22	1:60:A:LEU:HD22	12	0.41
(1,2484)	1:56:A:GLN:HE22	1:60:A:LEU:HD23	12	0.41
(1,2483)	1:56:A:GLN:HE21	1:60:A:LEU:HD21	5	0.41
(1,2483)	1:56:A:GLN:HE21	1:60:A:LEU:HD22	5	0.41
(1,2483)	1:56:A:GLN:HE21	1:60:A:LEU:HD23	5	0.41
(1,2247)	1:70:A:LYS:HA	1:70:A:LYS:HD2	1	0.41
(1,2247)	1:70:A:LYS:HA	1:70:A:LYS:HD2	4	0.41
(1,2247)	1:70:A:LYS:HA	1:70:A:LYS:HD2	9	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2247)	1:70:A:LYS:HA	1:70:A:LYS:HD2	11	0.41
(1,1353)	1:55:A:LEU:H	1:68:A:ILE:HD11	10	0.41
(1,1353)	1:55:A:LEU:H	1:68:A:ILE:HD12	10	0.41
(1,1353)	1:55:A:LEU:H	1:68:A:ILE:HD13	10	0.41
(1,1221)	1:62:A:LYS:HB3	1:63:A:GLY:H	17	0.41
(1,1220)	1:131:A:ILE:HG21	1:133:A:GLY:H	14	0.41
(1,1220)	1:131:A:ILE:HG22	1:133:A:GLY:H	14	0.41
(1,1220)	1:131:A:ILE:HG23	1:133:A:GLY:H	14	0.41
(1,1162)	1:79:A:ILE:HG21	1:111:A:ALA:H	10	0.41
(1,1162)	1:79:A:ILE:HG22	1:111:A:ALA:H	10	0.41
(1,1162)	1:79:A:ILE:HG23	1:111:A:ALA:H	10	0.41
(1,1162)	1:79:A:ILE:HG21	1:111:A:ALA:H	14	0.41
(1,1162)	1:79:A:ILE:HG22	1:111:A:ALA:H	14	0.41
(1,1162)	1:79:A:ILE:HG23	1:111:A:ALA:H	14	0.41
(1,1150)	1:134:A:ARG:HG2	1:129:A:LYS:H	18	0.41
(1,1150)	1:134:A:ARG:HG3	1:129:A:LYS:H	18	0.41
(1,1150)	1:134:A:ARG:HG2	1:129:A:LYS:H	19	0.41
(1,1150)	1:134:A:ARG:HG3	1:129:A:LYS:H	19	0.41
(1,1043)	1:8:A:ILE:HG21	1:32:A:THR:H	7	0.41
(1,1043)	1:8:A:ILE:HG22	1:32:A:THR:H	7	0.41
(1,1043)	1:8:A:ILE:HG23	1:32:A:THR:H	7	0.41
(1,1043)	1:8:A:ILE:HG21	1:32:A:THR:H	17	0.41
(1,1043)	1:8:A:ILE:HG22	1:32:A:THR:H	17	0.41
(1,1043)	1:8:A:ILE:HG23	1:32:A:THR:H	17	0.41
(1,962)	1:5:A:ILE:HD11	1:71:A:ASN:H	4	0.41
(1,962)	1:5:A:ILE:HD12	1:71:A:ASN:H	4	0.41
(1,962)	1:5:A:ILE:HD13	1:71:A:ASN:H	4	0.41
(1,929)	1:3:A:VAL:HG21	1:34:A:LYS:H	18	0.41
(1,929)	1:3:A:VAL:HG22	1:34:A:LYS:H	18	0.41
(1,929)	1:3:A:VAL:HG23	1:34:A:LYS:H	18	0.41
(1,925)	1:59:A:LEU:HD11	1:59:A:LEU:H	5	0.41
(1,925)	1:59:A:LEU:HD12	1:59:A:LEU:H	5	0.41
(1,925)	1:59:A:LEU:HD13	1:59:A:LEU:H	5	0.41
(1,866)	1:20:A:ALA:HB1	1:24:A:SER:H	19	0.41
(1,866)	1:20:A:ALA:HB2	1:24:A:SER:H	19	0.41
(1,866)	1:20:A:ALA:HB3	1:24:A:SER:H	19	0.41
(1,587)	1:9:A:ASP:HB3	1:11:A:ASN:H	3	0.41
(1,587)	1:9:A:ASP:HB3	1:11:A:ASN:H	5	0.41
(1,97)	1:144:A:LEU:H	1:143:A:GLN:H	3	0.41
(1,3568)	1:86:A:ASP:HB2	1:88:A:ASN:HB2	14	0.4
(1,3238)	1:74:A:TYR:HB3	1:2:A:SER:HA	2	0.4
(1,3171)	1:20:A:ALA:HB1	1:21:A:ILE:HA	15	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3171)	1:20:A:ALA:HB2	1:21:A:ILE:HA	15	0.4
(1,3171)	1:20:A:ALA:HB3	1:21:A:ILE:HA	15	0.4
(1,3040)	1:18:A:ASP:HB2	1:14:A:ILE:HG21	3	0.4
(1,3040)	1:18:A:ASP:HB2	1:14:A:ILE:HG22	3	0.4
(1,3040)	1:18:A:ASP:HB2	1:14:A:ILE:HG23	3	0.4
(1,3019)	1:63:A:GLY:HA2	1:65:A:THR:HB	20	0.4
(1,2966)	1:95:A:ASN:HB3	1:91:A:ILE:HG21	15	0.4
(1,2966)	1:95:A:ASN:HB3	1:91:A:ILE:HG22	15	0.4
(1,2966)	1:95:A:ASN:HB3	1:91:A:ILE:HG23	15	0.4
(1,2962)	1:42:A:ASP:HB3	1:50:A:ILE:HG21	3	0.4
(1,2962)	1:42:A:ASP:HB3	1:50:A:ILE:HG22	3	0.4
(1,2962)	1:42:A:ASP:HB3	1:50:A:ILE:HG23	3	0.4
(1,2962)	1:42:A:ASP:HB3	1:50:A:ILE:HG21	8	0.4
(1,2962)	1:42:A:ASP:HB3	1:50:A:ILE:HG22	8	0.4
(1,2962)	1:42:A:ASP:HB3	1:50:A:ILE:HG23	8	0.4
(1,2954)	1:9:A:ASP:HB3	1:20:A:ALA:HB1	15	0.4
(1,2954)	1:9:A:ASP:HB3	1:20:A:ALA:HB2	15	0.4
(1,2954)	1:9:A:ASP:HB3	1:20:A:ALA:HB3	15	0.4
(1,2546)	1:56:A:GLN:HB2	1:60:A:LEU:HD21	12	0.4
(1,2546)	1:56:A:GLN:HB2	1:60:A:LEU:HD22	12	0.4
(1,2546)	1:56:A:GLN:HB2	1:60:A:LEU:HD23	12	0.4
(1,2546)	1:56:A:GLN:HB3	1:60:A:LEU:HD21	12	0.4
(1,2546)	1:56:A:GLN:HB3	1:60:A:LEU:HD22	12	0.4
(1,2546)	1:56:A:GLN:HB3	1:60:A:LEU:HD23	12	0.4
(1,2484)	1:56:A:GLN:HE22	1:60:A:LEU:HD21	16	0.4
(1,2484)	1:56:A:GLN:HE22	1:60:A:LEU:HD22	16	0.4
(1,2484)	1:56:A:GLN:HE22	1:60:A:LEU:HD23	16	0.4
(1,2466)	1:24:A:SER:H	1:23:A:LYS:HG2	14	0.4
(1,2466)	1:24:A:SER:H	1:23:A:LYS:HG2	18	0.4
(1,2410)	1:102:A:GLN:HG3	1:108:A:LEU:HG	3	0.4
(1,2410)	1:102:A:GLN:HG3	1:108:A:LEU:HG	13	0.4
(1,2247)	1:70:A:LYS:HA	1:70:A:LYS:HD2	6	0.4
(1,1813)	1:35:A:GLN:HE21	1:34:A:LYS:HE2	2	0.4
(1,1505)	1:72:A:ARG:HA	1:73:A:ILE:HD11	16	0.4
(1,1505)	1:72:A:ARG:HA	1:73:A:ILE:HD12	16	0.4
(1,1505)	1:72:A:ARG:HA	1:73:A:ILE:HD13	16	0.4
(1,1357)	1:123:A:ASP:H	1:93:A:ILE:HD11	1	0.4
(1,1357)	1:123:A:ASP:H	1:93:A:ILE:HD12	1	0.4
(1,1357)	1:123:A:ASP:H	1:93:A:ILE:HD13	1	0.4
(1,1162)	1:79:A:ILE:HG21	1:111:A:ALA:H	11	0.4
(1,1162)	1:79:A:ILE:HG22	1:111:A:ALA:H	11	0.4
(1,1162)	1:79:A:ILE:HG23	1:111:A:ALA:H	11	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1150)	1:134:A:ARG:HG2	1:129:A:LYS:H	1	0.4
(1,1150)	1:134:A:ARG:HG3	1:129:A:LYS:H	1	0.4
(1,1150)	1:134:A:ARG:HG2	1:129:A:LYS:H	11	0.4
(1,1150)	1:134:A:ARG:HG3	1:129:A:LYS:H	11	0.4
(1,1022)	1:79:A:ILE:HG21	1:81:A:ASN:H	13	0.4
(1,1022)	1:79:A:ILE:HG22	1:81:A:ASN:H	13	0.4
(1,1022)	1:79:A:ILE:HG23	1:81:A:ASN:H	13	0.4
(1,1019)	1:22:A:LEU:HD21	1:52:A:LEU:H	1	0.4
(1,1019)	1:22:A:LEU:HD22	1:52:A:LEU:H	1	0.4
(1,1019)	1:22:A:LEU:HD23	1:52:A:LEU:H	1	0.4
(1,971)	1:60:A:LEU:HD21	1:62:A:LYS:H	8	0.4
(1,971)	1:60:A:LEU:HD22	1:62:A:LYS:H	8	0.4
(1,971)	1:60:A:LEU:HD23	1:62:A:LYS:H	8	0.4
(1,971)	1:60:A:LEU:HD21	1:62:A:LYS:H	17	0.4
(1,971)	1:60:A:LEU:HD22	1:62:A:LYS:H	17	0.4
(1,971)	1:60:A:LEU:HD23	1:62:A:LYS:H	17	0.4
(1,971)	1:60:A:LEU:HD21	1:62:A:LYS:H	20	0.4
(1,971)	1:60:A:LEU:HD22	1:62:A:LYS:H	20	0.4
(1,971)	1:60:A:LEU:HD23	1:62:A:LYS:H	20	0.4
(1,962)	1:5:A:ILE:HD11	1:71:A:ASN:H	8	0.4
(1,962)	1:5:A:ILE:HD12	1:71:A:ASN:H	8	0.4
(1,962)	1:5:A:ILE:HD13	1:71:A:ASN:H	8	0.4
(1,925)	1:59:A:LEU:HD11	1:59:A:LEU:H	3	0.4
(1,925)	1:59:A:LEU:HD12	1:59:A:LEU:H	3	0.4
(1,925)	1:59:A:LEU:HD13	1:59:A:LEU:H	3	0.4
(1,743)	1:34:A:LYS:HD2	1:34:A:LYS:H	5	0.4
(1,605)	1:90:A:TYR:HB2	1:93:A:ILE:H	6	0.4
(1,587)	1:7:A:ASP:HB3	1:11:A:ASN:H	17	0.4
(1,579)	1:142:A:ASN:HB3	1:143:A:GLN:H	20	0.4
(1,396)	1:39:A:ALA:HA	1:8:A:ILE:H	4	0.4
(1,3943)	1:22:A:LEU:HD21	1:19:A:TYR:HD1	9	0.39
(1,3943)	1:22:A:LEU:HD21	1:19:A:TYR:HD2	9	0.39
(1,3943)	1:22:A:LEU:HD22	1:19:A:TYR:HD1	9	0.39
(1,3943)	1:22:A:LEU:HD22	1:19:A:TYR:HD2	9	0.39
(1,3943)	1:22:A:LEU:HD23	1:19:A:TYR:HD1	9	0.39
(1,3943)	1:22:A:LEU:HD23	1:19:A:TYR:HD2	9	0.39
(1,3938)	1:14:A:ILE:HB	1:58:A:TYR:HD1	16	0.39
(1,3938)	1:14:A:ILE:HB	1:58:A:TYR:HD2	16	0.39
(1,3890)	1:4:A:LYS:H	1:2:A:SER:HB2	10	0.39
(1,3875)	1:55:A:LEU:HB3	1:8:A:ILE:HG12	9	0.39
(1,3875)	1:55:A:LEU:HB3	1:8:A:ILE:HG13	9	0.39
(1,3840)	1:123:A:ASP:HB2	1:111:A:ALA:HB1	7	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3840)	1:123:A:ASP:HB2	1:111:A:ALA:HB2	7	0.39
(1,3840)	1:123:A:ASP:HB2	1:111:A:ALA:HB3	7	0.39
(1,3724)	1:71:A:ASN:HB3	1:5:A:ILE:HG13	1	0.39
(1,3238)	1:74:A:TYR:HB3	1:2:A:SER:HA	1	0.39
(1,3183)	1:90:A:TYR:HB2	1:79:A:ILE:HD11	12	0.39
(1,3183)	1:90:A:TYR:HB2	1:79:A:ILE:HD12	12	0.39
(1,3183)	1:90:A:TYR:HB2	1:79:A:ILE:HD13	12	0.39
(1,3180)	1:127:A:ILE:HB	1:79:A:ILE:HD11	14	0.39
(1,3180)	1:127:A:ILE:HB	1:79:A:ILE:HD12	14	0.39
(1,3180)	1:127:A:ILE:HB	1:79:A:ILE:HD13	14	0.39
(1,3180)	1:127:A:ILE:HB	1:79:A:ILE:HD11	15	0.39
(1,3180)	1:127:A:ILE:HB	1:79:A:ILE:HD12	15	0.39
(1,3180)	1:127:A:ILE:HB	1:79:A:ILE:HD13	15	0.39
(1,3171)	1:53:A:ALA:HB1	1:54:A:ILE:HA	4	0.39
(1,3171)	1:53:A:ALA:HB2	1:54:A:ILE:HA	4	0.39
(1,3171)	1:53:A:ALA:HB3	1:54:A:ILE:HA	4	0.39
(1,3171)	1:20:A:ALA:HB1	1:21:A:ILE:HA	18	0.39
(1,3171)	1:20:A:ALA:HB2	1:21:A:ILE:HA	18	0.39
(1,3171)	1:20:A:ALA:HB3	1:21:A:ILE:HA	18	0.39
(1,3040)	1:6:A:GLY:HA2	1:14:A:ILE:HG21	18	0.39
(1,3040)	1:6:A:GLY:HA2	1:14:A:ILE:HG22	18	0.39
(1,3040)	1:6:A:GLY:HA2	1:14:A:ILE:HG23	18	0.39
(1,2962)	1:42:A:ASP:HB3	1:50:A:ILE:HG21	4	0.39
(1,2962)	1:42:A:ASP:HB3	1:50:A:ILE:HG22	4	0.39
(1,2962)	1:42:A:ASP:HB3	1:50:A:ILE:HG23	4	0.39
(1,2954)	1:23:A:LYS:HE2	1:20:A:ALA:HB1	2	0.39
(1,2954)	1:23:A:LYS:HE2	1:20:A:ALA:HB2	2	0.39
(1,2954)	1:23:A:LYS:HE2	1:20:A:ALA:HB3	2	0.39
(1,2874)	1:19:A:TYR:HD1	1:20:A:ALA:HB1	13	0.39
(1,2874)	1:19:A:TYR:HD1	1:20:A:ALA:HB2	13	0.39
(1,2874)	1:19:A:TYR:HD1	1:20:A:ALA:HB3	13	0.39
(1,2874)	1:19:A:TYR:HD2	1:20:A:ALA:HB1	13	0.39
(1,2874)	1:19:A:TYR:HD2	1:20:A:ALA:HB2	13	0.39
(1,2874)	1:19:A:TYR:HD2	1:20:A:ALA:HB3	13	0.39
(1,2844)	1:59:A:LEU:H	1:68:A:ILE:HG21	10	0.39
(1,2844)	1:59:A:LEU:H	1:68:A:ILE:HG22	10	0.39
(1,2844)	1:59:A:LEU:H	1:68:A:ILE:HG23	10	0.39
(1,2844)	1:58:A:TYR:H	1:68:A:ILE:HG21	18	0.39
(1,2844)	1:58:A:TYR:H	1:68:A:ILE:HG22	18	0.39
(1,2844)	1:58:A:TYR:H	1:68:A:ILE:HG23	18	0.39
(1,2586)	1:39:A:ALA:HB1	1:36:A:LEU:HD11	16	0.39
(1,2586)	1:39:A:ALA:HB1	1:36:A:LEU:HD12	16	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2586)	1:39:A:ALA:HB1	1:36:A:LEU:HD13	16	0.39
(1,2586)	1:39:A:ALA:HB2	1:36:A:LEU:HD11	16	0.39
(1,2586)	1:39:A:ALA:HB2	1:36:A:LEU:HD12	16	0.39
(1,2586)	1:39:A:ALA:HB2	1:36:A:LEU:HD13	16	0.39
(1,2586)	1:39:A:ALA:HB3	1:36:A:LEU:HD11	16	0.39
(1,2586)	1:39:A:ALA:HB3	1:36:A:LEU:HD12	16	0.39
(1,2586)	1:39:A:ALA:HB3	1:36:A:LEU:HD13	16	0.39
(1,2546)	1:56:A:GLN:HB2	1:60:A:LEU:HD21	1	0.39
(1,2546)	1:56:A:GLN:HB2	1:60:A:LEU:HD22	1	0.39
(1,2546)	1:56:A:GLN:HB2	1:60:A:LEU:HD23	1	0.39
(1,2546)	1:56:A:GLN:HB3	1:60:A:LEU:HD21	1	0.39
(1,2546)	1:56:A:GLN:HB3	1:60:A:LEU:HD22	1	0.39
(1,2546)	1:56:A:GLN:HB3	1:60:A:LEU:HD23	1	0.39
(1,2537)	1:52:A:LEU:HA	1:55:A:LEU:HD11	17	0.39
(1,2537)	1:52:A:LEU:HA	1:55:A:LEU:HD12	17	0.39
(1,2537)	1:52:A:LEU:HA	1:55:A:LEU:HD13	17	0.39
(1,2523)	1:8:A:ILE:HA	1:22:A:LEU:HD21	9	0.39
(1,2523)	1:8:A:ILE:HA	1:22:A:LEU:HD22	9	0.39
(1,2523)	1:8:A:ILE:HA	1:22:A:LEU:HD23	9	0.39
(1,2523)	1:8:A:ILE:HA	1:22:A:LEU:HD21	13	0.39
(1,2523)	1:8:A:ILE:HA	1:22:A:LEU:HD22	13	0.39
(1,2523)	1:8:A:ILE:HA	1:22:A:LEU:HD23	13	0.39
(1,2483)	1:56:A:GLN:HE21	1:60:A:LEU:HD21	4	0.39
(1,2483)	1:56:A:GLN:HE21	1:60:A:LEU:HD22	4	0.39
(1,2483)	1:56:A:GLN:HE21	1:60:A:LEU:HD23	4	0.39
(1,2466)	1:24:A:SER:H	1:23:A:LYS:HG2	3	0.39
(1,2466)	1:24:A:SER:H	1:23:A:LYS:HG2	13	0.39
(1,2456)	1:23:A:LYS:H	1:52:A:LEU:HD11	8	0.39
(1,2456)	1:23:A:LYS:H	1:52:A:LEU:HD12	8	0.39
(1,2456)	1:23:A:LYS:H	1:52:A:LEU:HD13	8	0.39
(1,2410)	1:102:A:GLN:HG3	1:108:A:LEU:HG	2	0.39
(1,2350)	1:52:A:LEU:H	1:52:A:LEU:HD21	11	0.39
(1,2350)	1:52:A:LEU:H	1:52:A:LEU:HD22	11	0.39
(1,2350)	1:52:A:LEU:H	1:52:A:LEU:HD23	11	0.39
(1,2344)	1:19:A:TYR:H	1:59:A:LEU:HD21	17	0.39
(1,2344)	1:19:A:TYR:H	1:59:A:LEU:HD22	17	0.39
(1,2344)	1:19:A:TYR:H	1:59:A:LEU:HD23	17	0.39
(1,2247)	1:70:A:LYS:HA	1:70:A:LYS:HD2	5	0.39
(1,2247)	1:70:A:LYS:HA	1:70:A:LYS:HD2	7	0.39
(1,2247)	1:70:A:LYS:HA	1:70:A:LYS:HD2	18	0.39
(1,2170)	1:124:A:ARG:HB2	1:128:A:GLU:HG2	13	0.39
(1,2170)	1:124:A:ARG:HB2	1:128:A:GLU:HG3	13	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2170)	1:124:A:ARG:HB3	1:128:A:GLU:HG2	13	0.39
(1,2170)	1:124:A:ARG:HB3	1:128:A:GLU:HG3	13	0.39
(1,2145)	1:37:A:ALA:HA	1:3:A:VAL:HB	14	0.39
(1,2145)	1:37:A:ALA:HA	1:3:A:VAL:HB	17	0.39
(1,1817)	1:132:A:THR:HB	1:134:A:ARG:HD2	14	0.39
(1,1817)	1:132:A:THR:HB	1:134:A:ARG:HD3	14	0.39
(1,1511)	1:3:A:VAL:HA	1:5:A:ILE:HD11	16	0.39
(1,1511)	1:3:A:VAL:HA	1:5:A:ILE:HD12	16	0.39
(1,1511)	1:3:A:VAL:HA	1:5:A:ILE:HD13	16	0.39
(1,1357)	1:90:A:TYR:H	1:93:A:ILE:HD11	3	0.39
(1,1357)	1:90:A:TYR:H	1:93:A:ILE:HD12	3	0.39
(1,1357)	1:90:A:TYR:H	1:93:A:ILE:HD13	3	0.39
(1,1357)	1:90:A:TYR:H	1:93:A:ILE:HD11	5	0.39
(1,1357)	1:90:A:TYR:H	1:93:A:ILE:HD12	5	0.39
(1,1357)	1:90:A:TYR:H	1:93:A:ILE:HD13	5	0.39
(1,1353)	1:66:A:SER:H	1:68:A:ILE:HD11	12	0.39
(1,1353)	1:66:A:SER:H	1:68:A:ILE:HD12	12	0.39
(1,1353)	1:66:A:SER:H	1:68:A:ILE:HD13	12	0.39
(1,1328)	1:97:A:ILE:HG21	1:121:A:GLN:H	9	0.39
(1,1328)	1:97:A:ILE:HG22	1:121:A:GLN:H	9	0.39
(1,1328)	1:97:A:ILE:HG23	1:121:A:GLN:H	9	0.39
(1,1162)	1:79:A:ILE:HG21	1:111:A:ALA:H	16	0.39
(1,1162)	1:79:A:ILE:HG22	1:111:A:ALA:H	16	0.39
(1,1162)	1:79:A:ILE:HG23	1:111:A:ALA:H	16	0.39
(1,1022)	1:79:A:ILE:HG21	1:81:A:ASN:H	9	0.39
(1,1022)	1:79:A:ILE:HG22	1:81:A:ASN:H	9	0.39
(1,1022)	1:79:A:ILE:HG23	1:81:A:ASN:H	9	0.39
(1,971)	1:60:A:LEU:HD21	1:62:A:LYS:H	11	0.39
(1,971)	1:60:A:LEU:HD22	1:62:A:LYS:H	11	0.39
(1,971)	1:60:A:LEU:HD23	1:62:A:LYS:H	11	0.39
(1,971)	1:60:A:LEU:HD21	1:62:A:LYS:H	16	0.39
(1,971)	1:60:A:LEU:HD22	1:62:A:LYS:H	16	0.39
(1,971)	1:60:A:LEU:HD23	1:62:A:LYS:H	16	0.39
(1,743)	1:34:A:LYS:HD2	1:34:A:LYS:H	7	0.39
(1,743)	1:34:A:LYS:HD2	1:34:A:LYS:H	17	0.39
(1,605)	1:90:A:TYR:HB2	1:93:A:ILE:H	1	0.39
(1,228)	1:19:A:TYR:HD1	1:57:A:MET:H	12	0.39
(1,228)	1:19:A:TYR:HD2	1:57:A:MET:H	12	0.39
(1,97)	1:144:A:LEU:H	1:143:A:GLN:H	8	0.39
(1,3938)	1:14:A:ILE:HB	1:58:A:TYR:HD1	7	0.38
(1,3938)	1:14:A:ILE:HB	1:58:A:TYR:HD2	7	0.38
(1,3871)	1:79:A:ILE:H	1:80:A:ASP:HB3	5	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3840)	1:123:A:ASP:HB2	1:111:A:ALA:HB1	4	0.38
(1,3840)	1:123:A:ASP:HB2	1:111:A:ALA:HB2	4	0.38
(1,3840)	1:123:A:ASP:HB2	1:111:A:ALA:HB3	4	0.38
(1,3581)	1:56:A:GLN:H	1:68:A:ILE:HD11	12	0.38
(1,3581)	1:56:A:GLN:H	1:68:A:ILE:HD12	12	0.38
(1,3581)	1:56:A:GLN:H	1:68:A:ILE:HD13	12	0.38
(1,3568)	1:86:A:ASP:HB2	1:88:A:ASN:HB2	10	0.38
(1,3568)	1:86:A:ASP:HB2	1:88:A:ASN:HB2	18	0.38
(1,3183)	1:90:A:TYR:HB2	1:79:A:ILE:HD11	19	0.38
(1,3183)	1:90:A:TYR:HB2	1:79:A:ILE:HD12	19	0.38
(1,3183)	1:90:A:TYR:HB2	1:79:A:ILE:HD13	19	0.38
(1,3180)	1:127:A:ILE:HB	1:79:A:ILE:HD11	20	0.38
(1,3180)	1:127:A:ILE:HB	1:79:A:ILE:HD12	20	0.38
(1,3180)	1:127:A:ILE:HB	1:79:A:ILE:HD13	20	0.38
(1,3171)	1:20:A:ALA:HB1	1:21:A:ILE:HA	5	0.38
(1,3171)	1:20:A:ALA:HB2	1:21:A:ILE:HA	5	0.38
(1,3171)	1:20:A:ALA:HB3	1:21:A:ILE:HA	5	0.38
(1,3171)	1:53:A:ALA:HB1	1:54:A:ILE:HA	11	0.38
(1,3171)	1:53:A:ALA:HB2	1:54:A:ILE:HA	11	0.38
(1,3171)	1:53:A:ALA:HB3	1:54:A:ILE:HA	11	0.38
(1,3040)	1:6:A:GLY:HA2	1:14:A:ILE:HG21	15	0.38
(1,3040)	1:6:A:GLY:HA2	1:14:A:ILE:HG22	15	0.38
(1,3040)	1:6:A:GLY:HA2	1:14:A:ILE:HG23	15	0.38
(1,2970)	1:87:A:GLU:HG2	1:127:A:ILE:HG21	19	0.38
(1,2970)	1:87:A:GLU:HG2	1:127:A:ILE:HG22	19	0.38
(1,2970)	1:87:A:GLU:HG2	1:127:A:ILE:HG23	19	0.38
(1,2966)	1:94:A:CYS:HB3	1:91:A:ILE:HG21	17	0.38
(1,2966)	1:94:A:CYS:HB3	1:91:A:ILE:HG22	17	0.38
(1,2966)	1:94:A:CYS:HB3	1:91:A:ILE:HG23	17	0.38
(1,2586)	1:39:A:ALA:HB1	1:36:A:LEU:HD11	9	0.38
(1,2586)	1:39:A:ALA:HB1	1:36:A:LEU:HD12	9	0.38
(1,2586)	1:39:A:ALA:HB1	1:36:A:LEU:HD13	9	0.38
(1,2586)	1:39:A:ALA:HB2	1:36:A:LEU:HD11	9	0.38
(1,2586)	1:39:A:ALA:HB2	1:36:A:LEU:HD12	9	0.38
(1,2586)	1:39:A:ALA:HB2	1:36:A:LEU:HD13	9	0.38
(1,2586)	1:39:A:ALA:HB3	1:36:A:LEU:HD11	9	0.38
(1,2586)	1:39:A:ALA:HB3	1:36:A:LEU:HD12	9	0.38
(1,2586)	1:39:A:ALA:HB3	1:36:A:LEU:HD13	9	0.38
(1,2546)	1:56:A:GLN:HB2	1:60:A:LEU:HD21	5	0.38
(1,2546)	1:56:A:GLN:HB2	1:60:A:LEU:HD22	5	0.38
(1,2546)	1:56:A:GLN:HB2	1:60:A:LEU:HD23	5	0.38
(1,2546)	1:56:A:GLN:HB3	1:60:A:LEU:HD21	5	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2546)	1:56:A:GLN:HB3	1:60:A:LEU:HD22	5	0.38
(1,2546)	1:56:A:GLN:HB3	1:60:A:LEU:HD23	5	0.38
(1,2367)	1:2:A:SER:HA	1:73:A:ILE:HG12	10	0.38
(1,2306)	1:71:A:ASN:H	1:5:A:ILE:HG13	4	0.38
(1,2247)	1:70:A:LYS:HA	1:70:A:LYS:HD2	13	0.38
(1,1505)	1:72:A:ARG:HA	1:73:A:ILE:HD11	6	0.38
(1,1505)	1:72:A:ARG:HA	1:73:A:ILE:HD12	6	0.38
(1,1505)	1:72:A:ARG:HA	1:73:A:ILE:HD13	6	0.38
(1,1357)	1:90:A:TYR:H	1:93:A:ILE:HD11	8	0.38
(1,1357)	1:90:A:TYR:H	1:93:A:ILE:HD12	8	0.38
(1,1357)	1:90:A:TYR:H	1:93:A:ILE:HD13	8	0.38
(1,1225)	1:110:A:ALA:HA	1:76:A:TYR:H	1	0.38
(1,1137)	1:79:A:ILE:HD11	1:96:A:HIS:H	9	0.38
(1,1137)	1:79:A:ILE:HD12	1:96:A:HIS:H	9	0.38
(1,1137)	1:79:A:ILE:HD13	1:96:A:HIS:H	9	0.38
(1,1042)	1:50:A:ILE:HD11	1:49:A:SER:H	13	0.38
(1,1042)	1:50:A:ILE:HD12	1:49:A:SER:H	13	0.38
(1,1042)	1:50:A:ILE:HD13	1:49:A:SER:H	13	0.38
(1,925)	1:59:A:LEU:HD11	1:59:A:LEU:H	4	0.38
(1,925)	1:59:A:LEU:HD12	1:59:A:LEU:H	4	0.38
(1,925)	1:59:A:LEU:HD13	1:59:A:LEU:H	4	0.38
(1,909)	1:73:A:ILE:HG21	1:73:A:ILE:H	7	0.38
(1,909)	1:73:A:ILE:HG22	1:73:A:ILE:H	7	0.38
(1,909)	1:73:A:ILE:HG23	1:73:A:ILE:H	7	0.38
(1,909)	1:73:A:ILE:HG21	1:73:A:ILE:H	19	0.38
(1,909)	1:73:A:ILE:HG22	1:73:A:ILE:H	19	0.38
(1,909)	1:73:A:ILE:HG23	1:73:A:ILE:H	19	0.38
(1,903)	1:41:A:VAL:HG21	1:48:A:ASN:H	11	0.38
(1,903)	1:41:A:VAL:HG22	1:48:A:ASN:H	11	0.38
(1,903)	1:41:A:VAL:HG23	1:48:A:ASN:H	11	0.38
(1,743)	1:34:A:LYS:HD2	1:34:A:LYS:H	4	0.38
(1,605)	1:90:A:TYR:HB2	1:93:A:ILE:H	3	0.38
(1,605)	1:90:A:TYR:HB2	1:93:A:ILE:H	10	0.38
(1,605)	1:90:A:TYR:HB2	1:93:A:ILE:H	18	0.38
(1,386)	1:117:A:ASN:HA	1:119:A:ILE:H	15	0.38
(1,386)	1:117:A:ASN:HA	1:119:A:ILE:H	19	0.38
(1,228)	1:19:A:TYR:HD1	1:57:A:MET:H	1	0.38
(1,228)	1:19:A:TYR:HD2	1:57:A:MET:H	1	0.38
(1,3938)	1:14:A:ILE:HB	1:58:A:TYR:HD1	1	0.37
(1,3938)	1:14:A:ILE:HB	1:58:A:TYR:HD2	1	0.37
(1,3812)	1:12:A:GLY:HA3	1:4:A:LYS:HD2	19	0.37
(1,3758)	1:102:A:GLN:HG3	1:108:A:LEU:HD11	11	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3758)	1:102:A:GLN:HG3	1:108:A:LEU:HD12	11	0.37
(1,3758)	1:102:A:GLN:HG3	1:108:A:LEU:HD13	11	0.37
(1,3724)	1:71:A:ASN:HB3	1:5:A:ILE:HG13	15	0.37
(1,3696)	1:108:A:LEU:HD11	1:102:A:GLN:HG3	11	0.37
(1,3696)	1:108:A:LEU:HD12	1:102:A:GLN:HG3	11	0.37
(1,3696)	1:108:A:LEU:HD13	1:102:A:GLN:HG3	11	0.37
(1,3457)	1:74:A:TYR:HB3	1:75:A:THR:HA	2	0.37
(1,3457)	1:74:A:TYR:HB3	1:75:A:THR:HA	3	0.37
(1,3457)	1:74:A:TYR:HB3	1:75:A:THR:HA	12	0.37
(1,3238)	1:74:A:TYR:HB3	1:2:A:SER:HA	3	0.37
(1,3238)	1:74:A:TYR:HB3	1:2:A:SER:HA	10	0.37
(1,3238)	1:74:A:TYR:HB3	1:2:A:SER:HA	14	0.37
(1,3171)	1:20:A:ALA:HB1	1:21:A:ILE:HA	7	0.37
(1,3171)	1:20:A:ALA:HB2	1:21:A:ILE:HA	7	0.37
(1,3171)	1:20:A:ALA:HB3	1:21:A:ILE:HA	7	0.37
(1,3171)	1:53:A:ALA:HB1	1:54:A:ILE:HA	17	0.37
(1,3171)	1:53:A:ALA:HB2	1:54:A:ILE:HA	17	0.37
(1,3171)	1:53:A:ALA:HB3	1:54:A:ILE:HA	17	0.37
(1,3049)	1:12:A:GLY:HA2	1:13:A:GLU:HG2	19	0.37
(1,3049)	1:12:A:GLY:HA2	1:13:A:GLU:HG3	19	0.37
(1,2844)	1:58:A:TYR:H	1:68:A:ILE:HG21	15	0.37
(1,2844)	1:58:A:TYR:H	1:68:A:ILE:HG22	15	0.37
(1,2844)	1:58:A:TYR:H	1:68:A:ILE:HG23	15	0.37
(1,2830)	1:65:A:THR:H	1:54:A:ILE:HG21	10	0.37
(1,2830)	1:65:A:THR:H	1:54:A:ILE:HG22	10	0.37
(1,2830)	1:65:A:THR:H	1:54:A:ILE:HG23	10	0.37
(1,2586)	1:39:A:ALA:HB1	1:36:A:LEU:HD11	14	0.37
(1,2586)	1:39:A:ALA:HB1	1:36:A:LEU:HD12	14	0.37
(1,2586)	1:39:A:ALA:HB1	1:36:A:LEU:HD13	14	0.37
(1,2586)	1:39:A:ALA:HB2	1:36:A:LEU:HD11	14	0.37
(1,2586)	1:39:A:ALA:HB2	1:36:A:LEU:HD12	14	0.37
(1,2586)	1:39:A:ALA:HB2	1:36:A:LEU:HD13	14	0.37
(1,2586)	1:39:A:ALA:HB3	1:36:A:LEU:HD11	14	0.37
(1,2586)	1:39:A:ALA:HB3	1:36:A:LEU:HD12	14	0.37
(1,2586)	1:39:A:ALA:HB3	1:36:A:LEU:HD13	14	0.37
(1,2586)	1:39:A:ALA:HB1	1:36:A:LEU:HD11	17	0.37
(1,2586)	1:39:A:ALA:HB1	1:36:A:LEU:HD12	17	0.37
(1,2586)	1:39:A:ALA:HB1	1:36:A:LEU:HD13	17	0.37
(1,2586)	1:39:A:ALA:HB2	1:36:A:LEU:HD11	17	0.37
(1,2586)	1:39:A:ALA:HB2	1:36:A:LEU:HD12	17	0.37
(1,2586)	1:39:A:ALA:HB2	1:36:A:LEU:HD13	17	0.37
(1,2586)	1:39:A:ALA:HB3	1:36:A:LEU:HD11	17	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2586)	1:39:A:ALA:HB3	1:36:A:LEU:HD12	17	0.37
(1,2586)	1:39:A:ALA:HB3	1:36:A:LEU:HD13	17	0.37
(1,2546)	1:56:A:GLN:HB2	1:60:A:LEU:HD21	11	0.37
(1,2546)	1:56:A:GLN:HB2	1:60:A:LEU:HD22	11	0.37
(1,2546)	1:56:A:GLN:HB2	1:60:A:LEU:HD23	11	0.37
(1,2546)	1:56:A:GLN:HB3	1:60:A:LEU:HD21	11	0.37
(1,2546)	1:56:A:GLN:HB3	1:60:A:LEU:HD22	11	0.37
(1,2546)	1:56:A:GLN:HB3	1:60:A:LEU:HD23	11	0.37
(1,2546)	1:56:A:GLN:HB2	1:60:A:LEU:HD21	18	0.37
(1,2546)	1:56:A:GLN:HB2	1:60:A:LEU:HD22	18	0.37
(1,2546)	1:56:A:GLN:HB2	1:60:A:LEU:HD23	18	0.37
(1,2546)	1:56:A:GLN:HB3	1:60:A:LEU:HD21	18	0.37
(1,2546)	1:56:A:GLN:HB3	1:60:A:LEU:HD22	18	0.37
(1,2546)	1:56:A:GLN:HB3	1:60:A:LEU:HD23	18	0.37
(1,2483)	1:56:A:GLN:HE21	1:52:A:LEU:HD21	18	0.37
(1,2483)	1:56:A:GLN:HE21	1:52:A:LEU:HD22	18	0.37
(1,2483)	1:56:A:GLN:HE21	1:52:A:LEU:HD23	18	0.37
(1,2483)	1:56:A:GLN:HE21	1:60:A:LEU:HD21	19	0.37
(1,2483)	1:56:A:GLN:HE21	1:60:A:LEU:HD22	19	0.37
(1,2483)	1:56:A:GLN:HE21	1:60:A:LEU:HD23	19	0.37
(1,2483)	1:56:A:GLN:HE21	1:60:A:LEU:HD21	20	0.37
(1,2483)	1:56:A:GLN:HE21	1:60:A:LEU:HD22	20	0.37
(1,2483)	1:56:A:GLN:HE21	1:60:A:LEU:HD23	20	0.37
(1,2373)	1:55:A:LEU:HA	1:59:A:LEU:HD21	20	0.37
(1,2373)	1:55:A:LEU:HA	1:59:A:LEU:HD22	20	0.37
(1,2373)	1:55:A:LEU:HA	1:59:A:LEU:HD23	20	0.37
(1,2344)	1:19:A:TYR:H	1:59:A:LEU:HD21	12	0.37
(1,2344)	1:19:A:TYR:H	1:59:A:LEU:HD22	12	0.37
(1,2344)	1:19:A:TYR:H	1:59:A:LEU:HD23	12	0.37
(1,2306)	1:71:A:ASN:H	1:5:A:ILE:HG13	5	0.37
(1,2277)	1:93:A:ILE:HB	1:127:A:ILE:HG12	18	0.37
(1,2277)	1:93:A:ILE:HB	1:127:A:ILE:HG13	18	0.37
(1,2247)	1:70:A:LYS:HA	1:70:A:LYS:HD2	8	0.37
(1,2247)	1:70:A:LYS:HA	1:70:A:LYS:HD2	20	0.37
(1,1949)	1:136:A:THR:HG21	1:135:A:ILE:HB	2	0.37
(1,1949)	1:136:A:THR:HG22	1:135:A:ILE:HB	2	0.37
(1,1949)	1:136:A:THR:HG23	1:135:A:ILE:HB	2	0.37
(1,1780)	1:129:A:LYS:H	1:134:A:ARG:HD2	13	0.37
(1,1780)	1:129:A:LYS:H	1:134:A:ARG:HD3	13	0.37
(1,1549)	1:70:A:LYS:HB2	1:5:A:ILE:HD11	2	0.37
(1,1549)	1:70:A:LYS:HB2	1:5:A:ILE:HD12	2	0.37
(1,1549)	1:70:A:LYS:HB2	1:5:A:ILE:HD13	2	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1358)	1:96:A:HIS:H	1:97:A:ILE:HD11	9	0.37
(1,1358)	1:96:A:HIS:H	1:97:A:ILE:HD12	9	0.37
(1,1358)	1:96:A:HIS:H	1:97:A:ILE:HD13	9	0.37
(1,1357)	1:90:A:TYR:H	1:93:A:ILE:HD11	9	0.37
(1,1357)	1:90:A:TYR:H	1:93:A:ILE:HD12	9	0.37
(1,1357)	1:90:A:TYR:H	1:93:A:ILE:HD13	9	0.37
(1,1357)	1:90:A:TYR:H	1:93:A:ILE:HD11	15	0.37
(1,1357)	1:90:A:TYR:H	1:93:A:ILE:HD12	15	0.37
(1,1357)	1:90:A:TYR:H	1:93:A:ILE:HD13	15	0.37
(1,1221)	1:62:A:LYS:HB3	1:63:A:GLY:H	11	0.37
(1,1221)	1:57:A:MET:HB2	1:63:A:GLY:H	20	0.37
(1,1137)	1:97:A:ILE:HG21	1:96:A:HIS:H	19	0.37
(1,1137)	1:97:A:ILE:HG22	1:96:A:HIS:H	19	0.37
(1,1137)	1:97:A:ILE:HG23	1:96:A:HIS:H	19	0.37
(1,1097)	1:108:A:LEU:HD21	1:112:A:ASP:H	9	0.37
(1,1097)	1:108:A:LEU:HD22	1:112:A:ASP:H	9	0.37
(1,1097)	1:108:A:LEU:HD23	1:112:A:ASP:H	9	0.37
(1,980)	1:54:A:ILE:HD11	1:42:A:ASP:H	16	0.37
(1,980)	1:54:A:ILE:HD12	1:42:A:ASP:H	16	0.37
(1,980)	1:54:A:ILE:HD13	1:42:A:ASP:H	16	0.37
(1,971)	1:60:A:LEU:HD21	1:62:A:LYS:H	9	0.37
(1,971)	1:60:A:LEU:HD22	1:62:A:LYS:H	9	0.37
(1,971)	1:60:A:LEU:HD23	1:62:A:LYS:H	9	0.37
(1,970)	1:4:A:LYS:HB2	1:71:A:ASN:H	9	0.37
(1,694)	1:9:A:ASP:HB3	1:35:A:GLN:HE22	9	0.37
(1,605)	1:90:A:TYR:HB2	1:93:A:ILE:H	19	0.37
(1,587)	1:9:A:ASP:HB3	1:11:A:ASN:H	20	0.37
(1,554)	1:4:A:LYS:HE2	1:4:A:LYS:H	8	0.37
(1,554)	1:4:A:LYS:HE3	1:4:A:LYS:H	8	0.37
(1,386)	1:117:A:ASN:HA	1:119:A:ILE:H	20	0.37
(1,228)	1:19:A:TYR:HD1	1:57:A:MET:H	4	0.37
(1,228)	1:19:A:TYR:HD2	1:57:A:MET:H	4	0.37
(1,3938)	1:14:A:ILE:HB	1:58:A:TYR:HD1	10	0.36
(1,3938)	1:14:A:ILE:HB	1:58:A:TYR:HD2	10	0.36
(1,3938)	1:14:A:ILE:HB	1:58:A:TYR:HD1	13	0.36
(1,3938)	1:14:A:ILE:HB	1:58:A:TYR:HD2	13	0.36
(1,3871)	1:79:A:ILE:H	1:80:A:ASP:HB3	1	0.36
(1,3832)	1:116:A:ASN:H	1:140:A:VAL:HG21	1	0.36
(1,3832)	1:116:A:ASN:H	1:140:A:VAL:HG22	1	0.36
(1,3832)	1:116:A:ASN:H	1:140:A:VAL:HG23	1	0.36
(1,3180)	1:127:A:ILE:HB	1:79:A:ILE:HD11	17	0.36
(1,3180)	1:127:A:ILE:HB	1:79:A:ILE:HD12	17	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3180)	1:127:A:ILE:HB	1:79:A:ILE:HD13	17	0.36
(1,3171)	1:53:A:ALA:HB1	1:54:A:ILE:HA	1	0.36
(1,3171)	1:53:A:ALA:HB2	1:54:A:ILE:HA	1	0.36
(1,3171)	1:53:A:ALA:HB3	1:54:A:ILE:HA	1	0.36
(1,3171)	1:53:A:ALA:HB1	1:54:A:ILE:HA	10	0.36
(1,3171)	1:53:A:ALA:HB2	1:54:A:ILE:HA	10	0.36
(1,3171)	1:53:A:ALA:HB3	1:54:A:ILE:HA	10	0.36
(1,3171)	1:53:A:ALA:HB1	1:54:A:ILE:HA	12	0.36
(1,3171)	1:53:A:ALA:HB2	1:54:A:ILE:HA	12	0.36
(1,3171)	1:53:A:ALA:HB3	1:54:A:ILE:HA	12	0.36
(1,3040)	1:6:A:GLY:HA2	1:14:A:ILE:HG21	16	0.36
(1,3040)	1:6:A:GLY:HA2	1:14:A:ILE:HG22	16	0.36
(1,3040)	1:6:A:GLY:HA2	1:14:A:ILE:HG23	16	0.36
(1,2999)	1:50:A:ILE:HG12	1:53:A:ALA:HB1	6	0.36
(1,2999)	1:50:A:ILE:HG12	1:53:A:ALA:HB2	6	0.36
(1,2999)	1:50:A:ILE:HG12	1:53:A:ALA:HB3	6	0.36
(1,2970)	1:87:A:GLU:HG2	1:127:A:ILE:HG21	8	0.36
(1,2970)	1:87:A:GLU:HG2	1:127:A:ILE:HG22	8	0.36
(1,2970)	1:87:A:GLU:HG2	1:127:A:ILE:HG23	8	0.36
(1,2962)	1:42:A:ASP:HB3	1:50:A:ILE:HG21	2	0.36
(1,2962)	1:42:A:ASP:HB3	1:50:A:ILE:HG22	2	0.36
(1,2962)	1:42:A:ASP:HB3	1:50:A:ILE:HG23	2	0.36
(1,2962)	1:42:A:ASP:HB3	1:50:A:ILE:HG21	12	0.36
(1,2962)	1:42:A:ASP:HB3	1:50:A:ILE:HG22	12	0.36
(1,2962)	1:42:A:ASP:HB3	1:50:A:ILE:HG23	12	0.36
(1,2954)	1:23:A:LYS:HE2	1:20:A:ALA:HB1	7	0.36
(1,2954)	1:23:A:LYS:HE2	1:20:A:ALA:HB2	7	0.36
(1,2954)	1:23:A:LYS:HE2	1:20:A:ALA:HB3	7	0.36
(1,2765)	1:40:A:ASP:HB3	1:3:A:VAL:HG11	1	0.36
(1,2765)	1:40:A:ASP:HB3	1:3:A:VAL:HG12	1	0.36
(1,2765)	1:40:A:ASP:HB3	1:3:A:VAL:HG13	1	0.36
(1,2765)	1:40:A:ASP:HB3	1:3:A:VAL:HG11	9	0.36
(1,2765)	1:40:A:ASP:HB3	1:3:A:VAL:HG12	9	0.36
(1,2765)	1:40:A:ASP:HB3	1:3:A:VAL:HG13	9	0.36
(1,2586)	1:39:A:ALA:HB1	1:36:A:LEU:HD11	4	0.36
(1,2586)	1:39:A:ALA:HB1	1:36:A:LEU:HD12	4	0.36
(1,2586)	1:39:A:ALA:HB1	1:36:A:LEU:HD13	4	0.36
(1,2586)	1:39:A:ALA:HB2	1:36:A:LEU:HD11	4	0.36
(1,2586)	1:39:A:ALA:HB2	1:36:A:LEU:HD12	4	0.36
(1,2586)	1:39:A:ALA:HB2	1:36:A:LEU:HD13	4	0.36
(1,2586)	1:39:A:ALA:HB3	1:36:A:LEU:HD11	4	0.36
(1,2586)	1:39:A:ALA:HB3	1:36:A:LEU:HD12	4	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2586)	1:39:A:ALA:HB3	1:36:A:LEU:HD13	4	0.36
(1,2546)	1:56:A:GLN:HB2	1:60:A:LEU:HD21	6	0.36
(1,2546)	1:56:A:GLN:HB2	1:60:A:LEU:HD22	6	0.36
(1,2546)	1:56:A:GLN:HB2	1:60:A:LEU:HD23	6	0.36
(1,2546)	1:56:A:GLN:HB3	1:60:A:LEU:HD21	6	0.36
(1,2546)	1:56:A:GLN:HB3	1:60:A:LEU:HD22	6	0.36
(1,2546)	1:56:A:GLN:HB3	1:60:A:LEU:HD23	6	0.36
(1,2537)	1:52:A:LEU:HA	1:55:A:LEU:HD11	8	0.36
(1,2537)	1:52:A:LEU:HA	1:55:A:LEU:HD12	8	0.36
(1,2537)	1:52:A:LEU:HA	1:55:A:LEU:HD13	8	0.36
(1,2247)	1:70:A:LYS:HA	1:70:A:LYS:HD2	3	0.36
(1,2145)	1:37:A:ALA:HA	1:3:A:VAL:HB	3	0.36
(1,2120)	1:74:A:TYR:HE1	1:72:A:ARG:HB2	17	0.36
(1,2120)	1:74:A:TYR:HE2	1:72:A:ARG:HB2	17	0.36
(1,1813)	1:35:A:GLN:HE21	1:34:A:LYS:HE2	13	0.36
(1,1505)	1:72:A:ARG:HA	1:73:A:ILE:HD11	12	0.36
(1,1505)	1:72:A:ARG:HA	1:73:A:ILE:HD12	12	0.36
(1,1505)	1:72:A:ARG:HA	1:73:A:ILE:HD13	12	0.36
(1,1388)	1:103:A:LEU:HA	1:107:A:SER:HB3	13	0.36
(1,1328)	1:97:A:ILE:HG21	1:121:A:GLN:H	15	0.36
(1,1328)	1:97:A:ILE:HG22	1:121:A:GLN:H	15	0.36
(1,1328)	1:97:A:ILE:HG23	1:121:A:GLN:H	15	0.36
(1,1328)	1:97:A:ILE:HG21	1:121:A:GLN:H	17	0.36
(1,1328)	1:97:A:ILE:HG22	1:121:A:GLN:H	17	0.36
(1,1328)	1:97:A:ILE:HG23	1:121:A:GLN:H	17	0.36
(1,1117)	1:96:A:HIS:HA	1:102:A:GLN:H	10	0.36
(1,980)	1:54:A:ILE:HD11	1:42:A:ASP:H	3	0.36
(1,980)	1:54:A:ILE:HD12	1:42:A:ASP:H	3	0.36
(1,980)	1:54:A:ILE:HD13	1:42:A:ASP:H	3	0.36
(1,909)	1:73:A:ILE:HG21	1:73:A:ILE:H	5	0.36
(1,909)	1:73:A:ILE:HG22	1:73:A:ILE:H	5	0.36
(1,909)	1:73:A:ILE:HG23	1:73:A:ILE:H	5	0.36
(1,909)	1:73:A:ILE:HG21	1:73:A:ILE:H	11	0.36
(1,909)	1:73:A:ILE:HG22	1:73:A:ILE:H	11	0.36
(1,909)	1:73:A:ILE:HG23	1:73:A:ILE:H	11	0.36
(1,909)	1:73:A:ILE:HG21	1:73:A:ILE:H	12	0.36
(1,909)	1:73:A:ILE:HG22	1:73:A:ILE:H	12	0.36
(1,909)	1:73:A:ILE:HG23	1:73:A:ILE:H	12	0.36
(1,743)	1:34:A:LYS:HD2	1:34:A:LYS:H	8	0.36
(1,694)	1:9:A:ASP:HB3	1:35:A:GLN:HE22	5	0.36
(1,396)	1:39:A:ALA:HA	1:8:A:ILE:H	8	0.36
(1,228)	1:19:A:TYR:HD1	1:57:A:MET:H	3	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,228)	1:19:A:TYR:HD2	1:57:A:MET:H	3	0.36
(1,81)	1:58:A:TYR:H	1:61:A:GLY:H	10	0.36
(1,3724)	1:71:A:ASN:HB3	1:5:A:ILE:HG13	16	0.35
(1,3568)	1:86:A:ASP:HB2	1:88:A:ASN:HB2	3	0.35
(1,3568)	1:86:A:ASP:HB2	1:88:A:ASN:HB2	20	0.35
(1,3171)	1:53:A:ALA:HB1	1:54:A:ILE:HA	19	0.35
(1,3171)	1:53:A:ALA:HB2	1:54:A:ILE:HA	19	0.35
(1,3171)	1:53:A:ALA:HB3	1:54:A:ILE:HA	19	0.35
(1,3171)	1:20:A:ALA:HB1	1:21:A:ILE:HA	20	0.35
(1,3171)	1:20:A:ALA:HB2	1:21:A:ILE:HA	20	0.35
(1,3171)	1:20:A:ALA:HB3	1:21:A:ILE:HA	20	0.35
(1,3074)	1:72:A:ARG:HB2	1:71:A:ASN:HA	16	0.35
(1,3040)	1:6:A:GLY:HA2	1:14:A:ILE:HG21	1	0.35
(1,3040)	1:6:A:GLY:HA2	1:14:A:ILE:HG22	1	0.35
(1,3040)	1:6:A:GLY:HA2	1:14:A:ILE:HG23	1	0.35
(1,3040)	1:6:A:GLY:HA2	1:14:A:ILE:HG21	5	0.35
(1,3040)	1:6:A:GLY:HA2	1:14:A:ILE:HG22	5	0.35
(1,3040)	1:6:A:GLY:HA2	1:14:A:ILE:HG23	5	0.35
(1,3019)	1:54:A:ILE:HA	1:65:A:THR:HB	3	0.35
(1,2966)	1:95:A:ASN:HB3	1:91:A:ILE:HG21	8	0.35
(1,2966)	1:95:A:ASN:HB3	1:91:A:ILE:HG22	8	0.35
(1,2966)	1:95:A:ASN:HB3	1:91:A:ILE:HG23	8	0.35
(1,2830)	1:66:A:SER:H	1:54:A:ILE:HG21	8	0.35
(1,2830)	1:66:A:SER:H	1:54:A:ILE:HG22	8	0.35
(1,2830)	1:66:A:SER:H	1:54:A:ILE:HG23	8	0.35
(1,2697)	1:128:A:GLU:HG2	1:132:A:THR:HG21	8	0.35
(1,2697)	1:128:A:GLU:HG2	1:132:A:THR:HG22	8	0.35
(1,2697)	1:128:A:GLU:HG2	1:132:A:THR:HG23	8	0.35
(1,2697)	1:128:A:GLU:HG3	1:132:A:THR:HG21	8	0.35
(1,2697)	1:128:A:GLU:HG3	1:132:A:THR:HG22	8	0.35
(1,2697)	1:128:A:GLU:HG3	1:132:A:THR:HG23	8	0.35
(1,2586)	1:39:A:ALA:HB1	1:36:A:LEU:HD11	13	0.35
(1,2586)	1:39:A:ALA:HB1	1:36:A:LEU:HD12	13	0.35
(1,2586)	1:39:A:ALA:HB1	1:36:A:LEU:HD13	13	0.35
(1,2586)	1:39:A:ALA:HB2	1:36:A:LEU:HD11	13	0.35
(1,2586)	1:39:A:ALA:HB2	1:36:A:LEU:HD12	13	0.35
(1,2586)	1:39:A:ALA:HB2	1:36:A:LEU:HD13	13	0.35
(1,2586)	1:39:A:ALA:HB3	1:36:A:LEU:HD11	13	0.35
(1,2586)	1:39:A:ALA:HB3	1:36:A:LEU:HD12	13	0.35
(1,2586)	1:39:A:ALA:HB3	1:36:A:LEU:HD13	13	0.35
(1,2546)	1:56:A:GLN:HB2	1:60:A:LEU:HD21	16	0.35
(1,2546)	1:56:A:GLN:HB2	1:60:A:LEU:HD22	16	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2546)	1:56:A:GLN:HB2	1:60:A:LEU:HD23	16	0.35
(1,2546)	1:56:A:GLN:HB3	1:60:A:LEU:HD21	16	0.35
(1,2546)	1:56:A:GLN:HB3	1:60:A:LEU:HD22	16	0.35
(1,2546)	1:56:A:GLN:HB3	1:60:A:LEU:HD23	16	0.35
(1,2546)	1:35:A:GLN:HB2	1:31:A:LEU:HD21	17	0.35
(1,2546)	1:35:A:GLN:HB2	1:31:A:LEU:HD22	17	0.35
(1,2546)	1:35:A:GLN:HB2	1:31:A:LEU:HD23	17	0.35
(1,2515)	1:93:A:ILE:HA	1:103:A:LEU:HD11	12	0.35
(1,2515)	1:93:A:ILE:HA	1:103:A:LEU:HD12	12	0.35
(1,2515)	1:93:A:ILE:HA	1:103:A:LEU:HD13	12	0.35
(1,2515)	1:92:A:LEU:HA	1:103:A:LEU:HD11	16	0.35
(1,2515)	1:92:A:LEU:HA	1:103:A:LEU:HD12	16	0.35
(1,2515)	1:92:A:LEU:HA	1:103:A:LEU:HD13	16	0.35
(1,2484)	1:56:A:GLN:HE22	1:60:A:LEU:HD21	18	0.35
(1,2484)	1:56:A:GLN:HE22	1:60:A:LEU:HD22	18	0.35
(1,2484)	1:56:A:GLN:HE22	1:60:A:LEU:HD23	18	0.35
(1,2483)	1:56:A:GLN:HE21	1:52:A:LEU:HD21	17	0.35
(1,2483)	1:56:A:GLN:HE21	1:52:A:LEU:HD22	17	0.35
(1,2483)	1:56:A:GLN:HE21	1:52:A:LEU:HD23	17	0.35
(1,2466)	1:24:A:SER:H	1:23:A:LYS:HG2	2	0.35
(1,2373)	1:55:A:LEU:HA	1:59:A:LEU:HD21	2	0.35
(1,2373)	1:55:A:LEU:HA	1:59:A:LEU:HD22	2	0.35
(1,2373)	1:55:A:LEU:HA	1:59:A:LEU:HD23	2	0.35
(1,2344)	1:58:A:TYR:HD1	1:59:A:LEU:HD21	19	0.35
(1,2344)	1:58:A:TYR:HD1	1:59:A:LEU:HD22	19	0.35
(1,2344)	1:58:A:TYR:HD1	1:59:A:LEU:HD23	19	0.35
(1,2344)	1:58:A:TYR:HD2	1:59:A:LEU:HD21	19	0.35
(1,2344)	1:58:A:TYR:HD2	1:59:A:LEU:HD22	19	0.35
(1,2344)	1:58:A:TYR:HD2	1:59:A:LEU:HD23	19	0.35
(1,2247)	1:70:A:LYS:HA	1:70:A:LYS:HD2	10	0.35
(1,2247)	1:70:A:LYS:HA	1:70:A:LYS:HD2	14	0.35
(1,1806)	1:81:A:ASN:HD22	1:72:A:ARG:HD3	17	0.35
(1,1549)	1:70:A:LYS:HB2	1:5:A:ILE:HD11	3	0.35
(1,1549)	1:70:A:LYS:HB2	1:5:A:ILE:HD12	3	0.35
(1,1549)	1:70:A:LYS:HB2	1:5:A:ILE:HD13	3	0.35
(1,1511)	1:3:A:VAL:HA	1:5:A:ILE:HD11	5	0.35
(1,1511)	1:3:A:VAL:HA	1:5:A:ILE:HD12	5	0.35
(1,1511)	1:3:A:VAL:HA	1:5:A:ILE:HD13	5	0.35
(1,1505)	1:72:A:ARG:HA	1:73:A:ILE:HD11	13	0.35
(1,1505)	1:72:A:ARG:HA	1:73:A:ILE:HD12	13	0.35
(1,1505)	1:72:A:ARG:HA	1:73:A:ILE:HD13	13	0.35
(1,1353)	1:66:A:SER:H	1:68:A:ILE:HD11	1	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1353)	1:66:A:SER:H	1:68:A:ILE:HD12	1	0.35
(1,1353)	1:66:A:SER:H	1:68:A:ILE:HD13	1	0.35
(1,1221)	1:62:A:LYS:HB3	1:63:A:GLY:H	6	0.35
(1,1221)	1:62:A:LYS:HB3	1:63:A:GLY:H	9	0.35
(1,1220)	1:131:A:ILE:HG21	1:133:A:GLY:H	8	0.35
(1,1220)	1:131:A:ILE:HG22	1:133:A:GLY:H	8	0.35
(1,1220)	1:131:A:ILE:HG23	1:133:A:GLY:H	8	0.35
(1,1117)	1:96:A:HIS:HA	1:102:A:GLN:H	12	0.35
(1,1115)	1:55:A:LEU:HD21	1:8:A:ILE:H	18	0.35
(1,1115)	1:55:A:LEU:HD22	1:8:A:ILE:H	18	0.35
(1,1115)	1:55:A:LEU:HD23	1:8:A:ILE:H	18	0.35
(1,1043)	1:8:A:ILE:HG21	1:32:A:THR:H	6	0.35
(1,1043)	1:8:A:ILE:HG22	1:32:A:THR:H	6	0.35
(1,1043)	1:8:A:ILE:HG23	1:32:A:THR:H	6	0.35
(1,1022)	1:79:A:ILE:HG21	1:81:A:ASN:H	16	0.35
(1,1022)	1:79:A:ILE:HG22	1:81:A:ASN:H	16	0.35
(1,1022)	1:79:A:ILE:HG23	1:81:A:ASN:H	16	0.35
(1,1019)	1:22:A:LEU:HD21	1:52:A:LEU:H	6	0.35
(1,1019)	1:22:A:LEU:HD22	1:52:A:LEU:H	6	0.35
(1,1019)	1:22:A:LEU:HD23	1:52:A:LEU:H	6	0.35
(1,962)	1:5:A:ILE:HD11	1:71:A:ASN:H	13	0.35
(1,962)	1:5:A:ILE:HD12	1:71:A:ASN:H	13	0.35
(1,962)	1:5:A:ILE:HD13	1:71:A:ASN:H	13	0.35
(1,962)	1:5:A:ILE:HD11	1:71:A:ASN:H	19	0.35
(1,962)	1:5:A:ILE:HD12	1:71:A:ASN:H	19	0.35
(1,962)	1:5:A:ILE:HD13	1:71:A:ASN:H	19	0.35
(1,909)	1:73:A:ILE:HG21	1:73:A:ILE:H	15	0.35
(1,909)	1:73:A:ILE:HG22	1:73:A:ILE:H	15	0.35
(1,909)	1:73:A:ILE:HG23	1:73:A:ILE:H	15	0.35
(1,903)	1:41:A:VAL:HG21	1:48:A:ASN:H	7	0.35
(1,903)	1:41:A:VAL:HG22	1:48:A:ASN:H	7	0.35
(1,903)	1:41:A:VAL:HG23	1:48:A:ASN:H	7	0.35
(1,870)	1:52:A:LEU:HG	1:56:A:GLN:HE21	15	0.35
(1,866)	1:20:A:ALA:HB1	1:24:A:SER:H	7	0.35
(1,866)	1:20:A:ALA:HB2	1:24:A:SER:H	7	0.35
(1,866)	1:20:A:ALA:HB3	1:24:A:SER:H	7	0.35
(1,743)	1:34:A:LYS:HD2	1:34:A:LYS:H	3	0.35
(1,694)	1:9:A:ASP:HB3	1:35:A:GLN:HE22	10	0.35
(1,572)	1:9:A:ASP:HB3	1:20:A:ALA:H	18	0.35
(1,396)	1:39:A:ALA:HA	1:8:A:ILE:H	13	0.35
(1,386)	1:117:A:ASN:HA	1:119:A:ILE:H	16	0.35
(1,228)	1:19:A:TYR:HD1	1:57:A:MET:H	10	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,228)	1:19:A:TYR:HD2	1:57:A:MET:H	10	0.35
(1,3943)	1:59:A:LEU:HD21	1:19:A:TYR:HD1	15	0.34
(1,3943)	1:59:A:LEU:HD21	1:19:A:TYR:HD2	15	0.34
(1,3943)	1:59:A:LEU:HD22	1:19:A:TYR:HD1	15	0.34
(1,3943)	1:59:A:LEU:HD22	1:19:A:TYR:HD2	15	0.34
(1,3943)	1:59:A:LEU:HD23	1:19:A:TYR:HD1	15	0.34
(1,3943)	1:59:A:LEU:HD23	1:19:A:TYR:HD2	15	0.34
(1,3871)	1:11:A:ASN:H	1:9:A:ASP:HB3	9	0.34
(1,3871)	1:79:A:ILE:H	1:80:A:ASP:HB3	11	0.34
(1,3797)	1:93:A:ILE:H	1:79:A:ILE:HB	17	0.34
(1,3797)	1:93:A:ILE:H	1:79:A:ILE:HB	20	0.34
(1,3712)	1:130:A:TYR:HE1	1:137:A:HIS:HB3	2	0.34
(1,3712)	1:130:A:TYR:HE2	1:137:A:HIS:HB3	2	0.34
(1,3581)	1:56:A:GLN:H	1:68:A:ILE:HD11	19	0.34
(1,3581)	1:56:A:GLN:H	1:68:A:ILE:HD12	19	0.34
(1,3581)	1:56:A:GLN:H	1:68:A:ILE:HD13	19	0.34
(1,3568)	1:86:A:ASP:HB2	1:88:A:ASN:HB2	1	0.34
(1,3568)	1:86:A:ASP:HB2	1:88:A:ASN:HB2	6	0.34
(1,3568)	1:86:A:ASP:HB2	1:88:A:ASN:HB2	15	0.34
(1,3404)	1:97:A:ILE:HA	1:119:A:ILE:HG21	8	0.34
(1,3404)	1:97:A:ILE:HA	1:119:A:ILE:HG22	8	0.34
(1,3404)	1:97:A:ILE:HA	1:119:A:ILE:HG23	8	0.34
(1,3274)	1:73:A:ILE:HA	1:72:A:ARG:HD2	12	0.34
(1,3238)	1:74:A:TYR:HB3	1:2:A:SER:HA	19	0.34
(1,3183)	1:90:A:TYR:HB2	1:79:A:ILE:HD11	5	0.34
(1,3183)	1:90:A:TYR:HB2	1:79:A:ILE:HD12	5	0.34
(1,3183)	1:90:A:TYR:HB2	1:79:A:ILE:HD13	5	0.34
(1,3171)	1:20:A:ALA:HB1	1:21:A:ILE:HA	2	0.34
(1,3171)	1:20:A:ALA:HB2	1:21:A:ILE:HA	2	0.34
(1,3171)	1:20:A:ALA:HB3	1:21:A:ILE:HA	2	0.34
(1,3171)	1:20:A:ALA:HB1	1:21:A:ILE:HA	3	0.34
(1,3171)	1:20:A:ALA:HB2	1:21:A:ILE:HA	3	0.34
(1,3171)	1:20:A:ALA:HB3	1:21:A:ILE:HA	3	0.34
(1,2966)	1:88:A:ASN:HB3	1:91:A:ILE:HG21	18	0.34
(1,2966)	1:88:A:ASN:HB3	1:91:A:ILE:HG22	18	0.34
(1,2966)	1:88:A:ASN:HB3	1:91:A:ILE:HG23	18	0.34
(1,2962)	1:42:A:ASP:HB3	1:50:A:ILE:HG21	1	0.34
(1,2962)	1:42:A:ASP:HB3	1:50:A:ILE:HG22	1	0.34
(1,2962)	1:42:A:ASP:HB3	1:50:A:ILE:HG23	1	0.34
(1,2904)	1:3:A:VAL:HA	1:38:A:ALA:HB1	8	0.34
(1,2904)	1:3:A:VAL:HA	1:38:A:ALA:HB2	8	0.34
(1,2904)	1:3:A:VAL:HA	1:38:A:ALA:HB3	8	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2844)	1:58:A:TYR:H	1:68:A:ILE:HG21	17	0.34
(1,2844)	1:58:A:TYR:H	1:68:A:ILE:HG22	17	0.34
(1,2844)	1:58:A:TYR:H	1:68:A:ILE:HG23	17	0.34
(1,2765)	1:40:A:ASP:HB3	1:3:A:VAL:HG11	3	0.34
(1,2765)	1:40:A:ASP:HB3	1:3:A:VAL:HG12	3	0.34
(1,2765)	1:40:A:ASP:HB3	1:3:A:VAL:HG13	3	0.34
(1,2546)	1:35:A:GLN:HB2	1:31:A:LEU:HD21	13	0.34
(1,2546)	1:35:A:GLN:HB2	1:31:A:LEU:HD22	13	0.34
(1,2546)	1:35:A:GLN:HB2	1:31:A:LEU:HD23	13	0.34
(1,2537)	1:52:A:LEU:HA	1:55:A:LEU:HD11	10	0.34
(1,2537)	1:52:A:LEU:HA	1:55:A:LEU:HD12	10	0.34
(1,2537)	1:52:A:LEU:HA	1:55:A:LEU:HD13	10	0.34
(1,2523)	1:8:A:ILE:HA	1:22:A:LEU:HD21	3	0.34
(1,2523)	1:8:A:ILE:HA	1:22:A:LEU:HD22	3	0.34
(1,2523)	1:8:A:ILE:HA	1:22:A:LEU:HD23	3	0.34
(1,2515)	1:92:A:LEU:HA	1:103:A:LEU:HD11	19	0.34
(1,2515)	1:92:A:LEU:HA	1:103:A:LEU:HD12	19	0.34
(1,2515)	1:92:A:LEU:HA	1:103:A:LEU:HD13	19	0.34
(1,2379)	1:107:A:SER:HA	1:108:A:LEU:HG	16	0.34
(1,2344)	1:19:A:TYR:HD1	1:59:A:LEU:HD21	18	0.34
(1,2344)	1:19:A:TYR:HD1	1:59:A:LEU:HD22	18	0.34
(1,2344)	1:19:A:TYR:HD1	1:59:A:LEU:HD23	18	0.34
(1,2344)	1:19:A:TYR:HD2	1:59:A:LEU:HD21	18	0.34
(1,2344)	1:19:A:TYR:HD2	1:59:A:LEU:HD22	18	0.34
(1,2344)	1:19:A:TYR:HD2	1:59:A:LEU:HD23	18	0.34
(1,2247)	1:70:A:LYS:HA	1:70:A:LYS:HD2	15	0.34
(1,1949)	1:138:A:LEU:HG	1:135:A:ILE:HB	11	0.34
(1,1806)	1:81:A:ASN:HD22	1:72:A:ARG:HD3	8	0.34
(1,1784)	1:125:A:ILE:H	1:129:A:LYS:HE2	9	0.34
(1,1784)	1:125:A:ILE:H	1:129:A:LYS:HE3	9	0.34
(1,1505)	1:72:A:ARG:HA	1:73:A:ILE:HD11	2	0.34
(1,1505)	1:72:A:ARG:HA	1:73:A:ILE:HD12	2	0.34
(1,1505)	1:72:A:ARG:HA	1:73:A:ILE:HD13	2	0.34
(1,1489)	1:70:A:LYS:H	1:5:A:ILE:HD11	20	0.34
(1,1489)	1:70:A:LYS:H	1:5:A:ILE:HD12	20	0.34
(1,1489)	1:70:A:LYS:H	1:5:A:ILE:HD13	20	0.34
(1,1357)	1:123:A:ASP:H	1:93:A:ILE:HD11	12	0.34
(1,1357)	1:123:A:ASP:H	1:93:A:ILE:HD12	12	0.34
(1,1357)	1:123:A:ASP:H	1:93:A:ILE:HD13	12	0.34
(1,1328)	1:97:A:ILE:HG21	1:121:A:GLN:H	12	0.34
(1,1328)	1:97:A:ILE:HG22	1:121:A:GLN:H	12	0.34
(1,1328)	1:97:A:ILE:HG23	1:121:A:GLN:H	12	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1326)	1:5:A:ILE:HD11	1:39:A:ALA:H	18	0.34
(1,1326)	1:5:A:ILE:HD12	1:39:A:ALA:H	18	0.34
(1,1326)	1:5:A:ILE:HD13	1:39:A:ALA:H	18	0.34
(1,1238)	1:59:A:LEU:HD21	1:20:A:ALA:H	7	0.34
(1,1238)	1:59:A:LEU:HD22	1:20:A:ALA:H	7	0.34
(1,1238)	1:59:A:LEU:HD23	1:20:A:ALA:H	7	0.34
(1,1238)	1:59:A:LEU:HD21	1:20:A:ALA:H	17	0.34
(1,1238)	1:59:A:LEU:HD22	1:20:A:ALA:H	17	0.34
(1,1238)	1:59:A:LEU:HD23	1:20:A:ALA:H	17	0.34
(1,1225)	1:110:A:ALA:HA	1:76:A:TYR:H	6	0.34
(1,1220)	1:131:A:ILE:HG21	1:133:A:GLY:H	19	0.34
(1,1220)	1:131:A:ILE:HG22	1:133:A:GLY:H	19	0.34
(1,1220)	1:131:A:ILE:HG23	1:133:A:GLY:H	19	0.34
(1,1162)	1:79:A:ILE:HG21	1:111:A:ALA:H	6	0.34
(1,1162)	1:79:A:ILE:HG22	1:111:A:ALA:H	6	0.34
(1,1162)	1:79:A:ILE:HG23	1:111:A:ALA:H	6	0.34
(1,1150)	1:134:A:ARG:HG2	1:129:A:LYS:H	4	0.34
(1,1150)	1:134:A:ARG:HG3	1:129:A:LYS:H	4	0.34
(1,1150)	1:134:A:ARG:HG2	1:129:A:LYS:H	9	0.34
(1,1150)	1:134:A:ARG:HG3	1:129:A:LYS:H	9	0.34
(1,1132)	1:131:A:ILE:HG12	1:130:A:TYR:H	8	0.34
(1,1056)	1:122:A:THR:HG21	1:114:A:ASP:H	4	0.34
(1,1056)	1:122:A:THR:HG22	1:114:A:ASP:H	4	0.34
(1,1056)	1:122:A:THR:HG23	1:114:A:ASP:H	4	0.34
(1,1019)	1:22:A:LEU:HD21	1:52:A:LEU:H	16	0.34
(1,1019)	1:22:A:LEU:HD22	1:52:A:LEU:H	16	0.34
(1,1019)	1:22:A:LEU:HD23	1:52:A:LEU:H	16	0.34
(1,1019)	1:22:A:LEU:HD21	1:52:A:LEU:H	20	0.34
(1,1019)	1:22:A:LEU:HD22	1:52:A:LEU:H	20	0.34
(1,1019)	1:22:A:LEU:HD23	1:52:A:LEU:H	20	0.34
(1,909)	1:73:A:ILE:HG21	1:73:A:ILE:H	4	0.34
(1,909)	1:73:A:ILE:HG22	1:73:A:ILE:H	4	0.34
(1,909)	1:73:A:ILE:HG23	1:73:A:ILE:H	4	0.34
(1,909)	1:73:A:ILE:HG21	1:73:A:ILE:H	18	0.34
(1,909)	1:73:A:ILE:HG22	1:73:A:ILE:H	18	0.34
(1,909)	1:73:A:ILE:HG23	1:73:A:ILE:H	18	0.34
(1,903)	1:41:A:VAL:HG21	1:48:A:ASN:H	17	0.34
(1,903)	1:41:A:VAL:HG22	1:48:A:ASN:H	17	0.34
(1,903)	1:41:A:VAL:HG23	1:48:A:ASN:H	17	0.34
(1,743)	1:34:A:LYS:HD2	1:34:A:LYS:H	1	0.34
(1,743)	1:34:A:LYS:HD2	1:34:A:LYS:H	13	0.34
(1,743)	1:34:A:LYS:HD2	1:34:A:LYS:H	18	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,587)	1:9:A:ASP:HB3	1:11:A:ASN:H	9	0.34
(1,579)	1:142:A:ASN:HB3	1:143:A:GLN:H	3	0.34
(1,579)	1:142:A:ASN:HB3	1:143:A:GLN:H	9	0.34
(1,228)	1:19:A:TYR:HD1	1:57:A:MET:H	8	0.34
(1,228)	1:19:A:TYR:HD2	1:57:A:MET:H	8	0.34
(1,81)	1:58:A:TYR:H	1:61:A:GLY:H	6	0.34
(1,3890)	1:4:A:LYS:H	1:2:A:SER:HB2	6	0.33
(1,3890)	1:4:A:LYS:H	1:2:A:SER:HB2	11	0.33
(1,3875)	1:55:A:LEU:HB3	1:8:A:ILE:HG12	20	0.33
(1,3875)	1:55:A:LEU:HB3	1:8:A:ILE:HG13	20	0.33
(1,3371)	1:36:A:LEU:HA	1:36:A:LEU:HD11	12	0.33
(1,3371)	1:36:A:LEU:HA	1:36:A:LEU:HD12	12	0.33
(1,3371)	1:36:A:LEU:HA	1:36:A:LEU:HD13	12	0.33
(1,3274)	1:43:A:GLY:HA2	1:72:A:ARG:HD2	15	0.33
(1,3238)	1:74:A:TYR:HB3	1:2:A:SER:HA	17	0.33
(1,3183)	1:90:A:TYR:HB2	1:79:A:ILE:HD11	15	0.33
(1,3183)	1:90:A:TYR:HB2	1:79:A:ILE:HD12	15	0.33
(1,3183)	1:90:A:TYR:HB2	1:79:A:ILE:HD13	15	0.33
(1,3180)	1:127:A:ILE:HB	1:79:A:ILE:HD11	3	0.33
(1,3180)	1:127:A:ILE:HB	1:79:A:ILE:HD12	3	0.33
(1,3180)	1:127:A:ILE:HB	1:79:A:ILE:HD13	3	0.33
(1,3171)	1:20:A:ALA:HB1	1:21:A:ILE:HA	6	0.33
(1,3171)	1:20:A:ALA:HB2	1:21:A:ILE:HA	6	0.33
(1,3171)	1:20:A:ALA:HB3	1:21:A:ILE:HA	6	0.33
(1,3171)	1:53:A:ALA:HB1	1:54:A:ILE:HA	8	0.33
(1,3171)	1:53:A:ALA:HB2	1:54:A:ILE:HA	8	0.33
(1,3171)	1:53:A:ALA:HB3	1:54:A:ILE:HA	8	0.33
(1,3040)	1:6:A:GLY:HA2	1:14:A:ILE:HG21	6	0.33
(1,3040)	1:6:A:GLY:HA2	1:14:A:ILE:HG22	6	0.33
(1,3040)	1:6:A:GLY:HA2	1:14:A:ILE:HG23	6	0.33
(1,2904)	1:6:A:GLY:HA3	1:38:A:ALA:HB1	2	0.33
(1,2904)	1:6:A:GLY:HA3	1:38:A:ALA:HB2	2	0.33
(1,2904)	1:6:A:GLY:HA3	1:38:A:ALA:HB3	2	0.33
(1,2874)	1:19:A:TYR:HD1	1:20:A:ALA:HB1	14	0.33
(1,2874)	1:19:A:TYR:HD1	1:20:A:ALA:HB2	14	0.33
(1,2874)	1:19:A:TYR:HD1	1:20:A:ALA:HB3	14	0.33
(1,2874)	1:19:A:TYR:HD2	1:20:A:ALA:HB1	14	0.33
(1,2874)	1:19:A:TYR:HD2	1:20:A:ALA:HB2	14	0.33
(1,2874)	1:19:A:TYR:HD2	1:20:A:ALA:HB3	14	0.33
(1,2761)	1:74:A:TYR:HB2	1:75:A:THR:HG21	2	0.33
(1,2761)	1:74:A:TYR:HB2	1:75:A:THR:HG22	2	0.33
(1,2761)	1:74:A:TYR:HB2	1:75:A:THR:HG23	2	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2752)	1:35:A:GLN:HB2	1:32:A:THR:HG21	2	0.33
(1,2752)	1:35:A:GLN:HB2	1:32:A:THR:HG22	2	0.33
(1,2752)	1:35:A:GLN:HB2	1:32:A:THR:HG23	2	0.33
(1,2546)	1:56:A:GLN:HB2	1:60:A:LEU:HD21	4	0.33
(1,2546)	1:56:A:GLN:HB2	1:60:A:LEU:HD22	4	0.33
(1,2546)	1:56:A:GLN:HB2	1:60:A:LEU:HD23	4	0.33
(1,2546)	1:56:A:GLN:HB3	1:60:A:LEU:HD21	4	0.33
(1,2546)	1:56:A:GLN:HB3	1:60:A:LEU:HD22	4	0.33
(1,2546)	1:56:A:GLN:HB3	1:60:A:LEU:HD23	4	0.33
(1,2537)	1:52:A:LEU:HA	1:55:A:LEU:HD11	14	0.33
(1,2537)	1:52:A:LEU:HA	1:55:A:LEU:HD12	14	0.33
(1,2537)	1:52:A:LEU:HA	1:55:A:LEU:HD13	14	0.33
(1,2379)	1:107:A:SER:HA	1:108:A:LEU:HG	10	0.33
(1,2367)	1:72:A:ARG:HA	1:73:A:ILE:HG12	5	0.33
(1,2350)	1:52:A:LEU:H	1:52:A:LEU:HD21	3	0.33
(1,2350)	1:52:A:LEU:H	1:52:A:LEU:HD22	3	0.33
(1,2350)	1:52:A:LEU:H	1:52:A:LEU:HD23	3	0.33
(1,2344)	1:19:A:TYR:H	1:59:A:LEU:HD21	20	0.33
(1,2344)	1:19:A:TYR:H	1:59:A:LEU:HD22	20	0.33
(1,2344)	1:19:A:TYR:H	1:59:A:LEU:HD23	20	0.33
(1,2120)	1:74:A:TYR:HE1	1:72:A:ARG:HB2	14	0.33
(1,2120)	1:74:A:TYR:HE2	1:72:A:ARG:HB2	14	0.33
(1,1949)	1:136:A:THR:HG21	1:135:A:ILE:HB	9	0.33
(1,1949)	1:136:A:THR:HG22	1:135:A:ILE:HB	9	0.33
(1,1949)	1:136:A:THR:HG23	1:135:A:ILE:HB	9	0.33
(1,1813)	1:35:A:GLN:HE21	1:34:A:LYS:HE2	9	0.33
(1,1357)	1:90:A:TYR:H	1:93:A:ILE:HD11	7	0.33
(1,1357)	1:90:A:TYR:H	1:93:A:ILE:HD12	7	0.33
(1,1357)	1:90:A:TYR:H	1:93:A:ILE:HD13	7	0.33
(1,1357)	1:123:A:ASP:H	1:93:A:ILE:HD11	11	0.33
(1,1357)	1:123:A:ASP:H	1:93:A:ILE:HD12	11	0.33
(1,1357)	1:123:A:ASP:H	1:93:A:ILE:HD13	11	0.33
(1,1357)	1:90:A:TYR:H	1:93:A:ILE:HD11	18	0.33
(1,1357)	1:90:A:TYR:H	1:93:A:ILE:HD12	18	0.33
(1,1357)	1:90:A:TYR:H	1:93:A:ILE:HD13	18	0.33
(1,1328)	1:97:A:ILE:HG21	1:121:A:GLN:H	20	0.33
(1,1328)	1:97:A:ILE:HG22	1:121:A:GLN:H	20	0.33
(1,1328)	1:97:A:ILE:HG23	1:121:A:GLN:H	20	0.33
(1,1326)	1:5:A:ILE:HD11	1:39:A:ALA:H	6	0.33
(1,1326)	1:5:A:ILE:HD12	1:39:A:ALA:H	6	0.33
(1,1326)	1:5:A:ILE:HD13	1:39:A:ALA:H	6	0.33
(1,1163)	1:27:A:ILE:HD11	1:27:A:ILE:H	5	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1163)	1:27:A:ILE:HD12	1:27:A:ILE:H	5	0.33
(1,1163)	1:27:A:ILE:HD13	1:27:A:ILE:H	5	0.33
(1,1137)	1:97:A:ILE:HG21	1:96:A:HIS:H	6	0.33
(1,1137)	1:97:A:ILE:HG22	1:96:A:HIS:H	6	0.33
(1,1137)	1:97:A:ILE:HG23	1:96:A:HIS:H	6	0.33
(1,1132)	1:134:A:ARG:HG2	1:130:A:TYR:H	11	0.33
(1,1132)	1:134:A:ARG:HG3	1:130:A:TYR:H	11	0.33
(1,1115)	1:55:A:LEU:HD21	1:8:A:ILE:H	7	0.33
(1,1115)	1:55:A:LEU:HD22	1:8:A:ILE:H	7	0.33
(1,1115)	1:55:A:LEU:HD23	1:8:A:ILE:H	7	0.33
(1,1022)	1:79:A:ILE:HG21	1:81:A:ASN:H	7	0.33
(1,1022)	1:79:A:ILE:HG22	1:81:A:ASN:H	7	0.33
(1,1022)	1:79:A:ILE:HG23	1:81:A:ASN:H	7	0.33
(1,1019)	1:22:A:LEU:HD21	1:52:A:LEU:H	7	0.33
(1,1019)	1:22:A:LEU:HD22	1:52:A:LEU:H	7	0.33
(1,1019)	1:22:A:LEU:HD23	1:52:A:LEU:H	7	0.33
(1,1019)	1:22:A:LEU:HD21	1:52:A:LEU:H	17	0.33
(1,1019)	1:22:A:LEU:HD22	1:52:A:LEU:H	17	0.33
(1,1019)	1:22:A:LEU:HD23	1:52:A:LEU:H	17	0.33
(1,980)	1:54:A:ILE:HD11	1:42:A:ASP:H	6	0.33
(1,980)	1:54:A:ILE:HD12	1:42:A:ASP:H	6	0.33
(1,980)	1:54:A:ILE:HD13	1:42:A:ASP:H	6	0.33
(1,962)	1:73:A:ILE:HD11	1:71:A:ASN:H	5	0.33
(1,962)	1:73:A:ILE:HD12	1:71:A:ASN:H	5	0.33
(1,962)	1:73:A:ILE:HD13	1:71:A:ASN:H	5	0.33
(1,929)	1:3:A:VAL:HG21	1:34:A:LYS:H	1	0.33
(1,929)	1:3:A:VAL:HG22	1:34:A:LYS:H	1	0.33
(1,929)	1:3:A:VAL:HG23	1:34:A:LYS:H	1	0.33
(1,909)	1:73:A:ILE:HD11	1:73:A:ILE:H	13	0.33
(1,909)	1:73:A:ILE:HD12	1:73:A:ILE:H	13	0.33
(1,909)	1:73:A:ILE:HD13	1:73:A:ILE:H	13	0.33
(1,909)	1:73:A:ILE:HG21	1:73:A:ILE:H	14	0.33
(1,909)	1:73:A:ILE:HG22	1:73:A:ILE:H	14	0.33
(1,909)	1:73:A:ILE:HG23	1:73:A:ILE:H	14	0.33
(1,866)	1:27:A:ILE:HG13	1:24:A:SER:H	16	0.33
(1,743)	1:34:A:LYS:HD2	1:34:A:LYS:H	12	0.33
(1,743)	1:34:A:LYS:HD2	1:34:A:LYS:H	19	0.33
(1,605)	1:90:A:TYR:HB2	1:93:A:ILE:H	4	0.33
(1,605)	1:90:A:TYR:HB2	1:93:A:ILE:H	16	0.33
(1,587)	1:9:A:ASP:HB3	1:11:A:ASN:H	15	0.33
(1,386)	1:117:A:ASN:HA	1:119:A:ILE:H	17	0.33
(1,386)	1:117:A:ASN:HA	1:119:A:ILE:H	18	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3871)	1:79:A:ILE:H	1:80:A:ASP:HB3	16	0.32
(1,3805)	1:125:A:ILE:HG12	1:128:A:GLU:HG2	2	0.32
(1,3805)	1:125:A:ILE:HG12	1:128:A:GLU:HG3	2	0.32
(1,3746)	1:57:A:MET:HA	1:62:A:LYS:HG2	9	0.32
(1,3635)	1:76:A:TYR:HB2	1:113:A:ALA:HA	14	0.32
(1,3571)	1:135:A:ILE:HG21	1:129:A:LYS:HD2	12	0.32
(1,3571)	1:135:A:ILE:HG21	1:129:A:LYS:HD3	12	0.32
(1,3571)	1:135:A:ILE:HG22	1:129:A:LYS:HD2	12	0.32
(1,3571)	1:135:A:ILE:HG22	1:129:A:LYS:HD3	12	0.32
(1,3571)	1:135:A:ILE:HG23	1:129:A:LYS:HD2	12	0.32
(1,3571)	1:135:A:ILE:HG23	1:129:A:LYS:HD3	12	0.32
(1,3457)	1:74:A:TYR:HB3	1:75:A:THR:HA	4	0.32
(1,3238)	1:74:A:TYR:HB3	1:2:A:SER:HA	13	0.32
(1,3183)	1:90:A:TYR:HB2	1:79:A:ILE:HD11	8	0.32
(1,3183)	1:90:A:TYR:HB2	1:79:A:ILE:HD12	8	0.32
(1,3183)	1:90:A:TYR:HB2	1:79:A:ILE:HD13	8	0.32
(1,3180)	1:127:A:ILE:HB	1:79:A:ILE:HD11	8	0.32
(1,3180)	1:127:A:ILE:HB	1:79:A:ILE:HD12	8	0.32
(1,3180)	1:127:A:ILE:HB	1:79:A:ILE:HD13	8	0.32
(1,3171)	1:103:A:LEU:HG	1:107:A:SER:HB3	9	0.32
(1,3171)	1:53:A:ALA:HB1	1:54:A:ILE:HA	13	0.32
(1,3171)	1:53:A:ALA:HB2	1:54:A:ILE:HA	13	0.32
(1,3171)	1:53:A:ALA:HB3	1:54:A:ILE:HA	13	0.32
(1,3171)	1:53:A:ALA:HB1	1:54:A:ILE:HA	14	0.32
(1,3171)	1:53:A:ALA:HB2	1:54:A:ILE:HA	14	0.32
(1,3171)	1:53:A:ALA:HB3	1:54:A:ILE:HA	14	0.32
(1,3040)	1:18:A:ASP:HB2	1:14:A:ILE:HG21	9	0.32
(1,3040)	1:18:A:ASP:HB2	1:14:A:ILE:HG22	9	0.32
(1,3040)	1:18:A:ASP:HB2	1:14:A:ILE:HG23	9	0.32
(1,2966)	1:94:A:CYS:HB3	1:97:A:ILE:HG21	12	0.32
(1,2966)	1:94:A:CYS:HB3	1:97:A:ILE:HG22	12	0.32
(1,2966)	1:94:A:CYS:HB3	1:97:A:ILE:HG23	12	0.32
(1,2942)	1:86:A:ASP:HB2	1:131:A:ILE:HG21	17	0.32
(1,2942)	1:86:A:ASP:HB2	1:131:A:ILE:HG22	17	0.32
(1,2942)	1:86:A:ASP:HB2	1:131:A:ILE:HG23	17	0.32
(1,2844)	1:59:A:LEU:H	1:68:A:ILE:HG21	2	0.32
(1,2844)	1:59:A:LEU:H	1:68:A:ILE:HG22	2	0.32
(1,2844)	1:59:A:LEU:H	1:68:A:ILE:HG23	2	0.32
(1,2844)	1:59:A:LEU:H	1:68:A:ILE:HG21	7	0.32
(1,2844)	1:59:A:LEU:H	1:68:A:ILE:HG22	7	0.32
(1,2844)	1:59:A:LEU:H	1:68:A:ILE:HG23	7	0.32
(1,2844)	1:59:A:LEU:H	1:68:A:ILE:HG21	9	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2844)	1:59:A:LEU:H	1:68:A:ILE:HG22	9	0.32
(1,2844)	1:59:A:LEU:H	1:68:A:ILE:HG23	9	0.32
(1,2697)	1:128:A:GLU:HG2	1:132:A:THR:HG21	16	0.32
(1,2697)	1:128:A:GLU:HG2	1:132:A:THR:HG22	16	0.32
(1,2697)	1:128:A:GLU:HG2	1:132:A:THR:HG23	16	0.32
(1,2697)	1:128:A:GLU:HG3	1:132:A:THR:HG21	16	0.32
(1,2697)	1:128:A:GLU:HG3	1:132:A:THR:HG22	16	0.32
(1,2697)	1:128:A:GLU:HG3	1:132:A:THR:HG23	16	0.32
(1,2586)	1:39:A:ALA:HB1	1:36:A:LEU:HD11	3	0.32
(1,2586)	1:39:A:ALA:HB1	1:36:A:LEU:HD12	3	0.32
(1,2586)	1:39:A:ALA:HB1	1:36:A:LEU:HD13	3	0.32
(1,2586)	1:39:A:ALA:HB2	1:36:A:LEU:HD11	3	0.32
(1,2586)	1:39:A:ALA:HB2	1:36:A:LEU:HD12	3	0.32
(1,2586)	1:39:A:ALA:HB2	1:36:A:LEU:HD13	3	0.32
(1,2586)	1:39:A:ALA:HB3	1:36:A:LEU:HD11	3	0.32
(1,2586)	1:39:A:ALA:HB3	1:36:A:LEU:HD12	3	0.32
(1,2586)	1:39:A:ALA:HB3	1:36:A:LEU:HD13	3	0.32
(1,2499)	1:62:A:LYS:HA	1:62:A:LYS:HG3	4	0.32
(1,2499)	1:135:A:ILE:HA	1:135:A:ILE:HG12	5	0.32
(1,2484)	1:56:A:GLN:HE22	1:60:A:LEU:HD21	14	0.32
(1,2484)	1:56:A:GLN:HE22	1:60:A:LEU:HD22	14	0.32
(1,2484)	1:56:A:GLN:HE22	1:60:A:LEU:HD23	14	0.32
(1,2482)	1:96:A:HIS:H	1:103:A:LEU:HD11	6	0.32
(1,2482)	1:96:A:HIS:H	1:103:A:LEU:HD12	6	0.32
(1,2482)	1:96:A:HIS:H	1:103:A:LEU:HD13	6	0.32
(1,2456)	1:23:A:LYS:H	1:52:A:LEU:HD11	17	0.32
(1,2456)	1:23:A:LYS:H	1:52:A:LEU:HD12	17	0.32
(1,2456)	1:23:A:LYS:H	1:52:A:LEU:HD13	17	0.32
(1,2356)	1:62:A:LYS:HA	1:62:A:LYS:HD3	9	0.32
(1,2344)	1:19:A:TYR:H	1:59:A:LEU:HD21	1	0.32
(1,2344)	1:19:A:TYR:H	1:59:A:LEU:HD22	1	0.32
(1,2344)	1:19:A:TYR:H	1:59:A:LEU:HD23	1	0.32
(1,2344)	1:58:A:TYR:HD1	1:59:A:LEU:HD21	11	0.32
(1,2344)	1:58:A:TYR:HD1	1:59:A:LEU:HD22	11	0.32
(1,2344)	1:58:A:TYR:HD1	1:59:A:LEU:HD23	11	0.32
(1,2344)	1:58:A:TYR:HD2	1:59:A:LEU:HD21	11	0.32
(1,2344)	1:58:A:TYR:HD2	1:59:A:LEU:HD22	11	0.32
(1,2344)	1:58:A:TYR:HD2	1:59:A:LEU:HD23	11	0.32
(1,2306)	1:71:A:ASN:H	1:5:A:ILE:HG13	18	0.32
(1,2260)	1:111:A:ALA:HA	1:127:A:ILE:HG12	18	0.32
(1,2260)	1:111:A:ALA:HA	1:127:A:ILE:HG13	18	0.32
(1,1813)	1:35:A:GLN:HE21	1:34:A:LYS:HE2	10	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1784)	1:125:A:ILE:H	1:129:A:LYS:HE2	14	0.32
(1,1784)	1:125:A:ILE:H	1:129:A:LYS:HE3	14	0.32
(1,1505)	1:72:A:ARG:HA	1:73:A:ILE:HD11	7	0.32
(1,1505)	1:72:A:ARG:HA	1:73:A:ILE:HD12	7	0.32
(1,1505)	1:72:A:ARG:HA	1:73:A:ILE:HD13	7	0.32
(1,1238)	1:59:A:LEU:HD21	1:20:A:ALA:H	1	0.32
(1,1238)	1:59:A:LEU:HD22	1:20:A:ALA:H	1	0.32
(1,1238)	1:59:A:LEU:HD23	1:20:A:ALA:H	1	0.32
(1,1221)	1:62:A:LYS:HB3	1:63:A:GLY:H	10	0.32
(1,1220)	1:131:A:ILE:HG21	1:133:A:GLY:H	18	0.32
(1,1220)	1:131:A:ILE:HG22	1:133:A:GLY:H	18	0.32
(1,1220)	1:131:A:ILE:HG23	1:133:A:GLY:H	18	0.32
(1,1132)	1:131:A:ILE:HG12	1:130:A:TYR:H	16	0.32
(1,1091)	1:103:A:LEU:HD21	1:104:A:SER:H	8	0.32
(1,1091)	1:103:A:LEU:HD22	1:104:A:SER:H	8	0.32
(1,1091)	1:103:A:LEU:HD23	1:104:A:SER:H	8	0.32
(1,1042)	1:50:A:ILE:HD11	1:49:A:SER:H	10	0.32
(1,1042)	1:50:A:ILE:HD12	1:49:A:SER:H	10	0.32
(1,1042)	1:50:A:ILE:HD13	1:49:A:SER:H	10	0.32
(1,1019)	1:22:A:LEU:HD21	1:52:A:LEU:H	12	0.32
(1,1019)	1:22:A:LEU:HD22	1:52:A:LEU:H	12	0.32
(1,1019)	1:22:A:LEU:HD23	1:52:A:LEU:H	12	0.32
(1,1019)	1:22:A:LEU:HD21	1:52:A:LEU:H	13	0.32
(1,1019)	1:22:A:LEU:HD22	1:52:A:LEU:H	13	0.32
(1,1019)	1:22:A:LEU:HD23	1:52:A:LEU:H	13	0.32
(1,925)	1:59:A:LEU:HD11	1:59:A:LEU:H	9	0.32
(1,925)	1:59:A:LEU:HD12	1:59:A:LEU:H	9	0.32
(1,925)	1:59:A:LEU:HD13	1:59:A:LEU:H	9	0.32
(1,925)	1:59:A:LEU:HD11	1:59:A:LEU:H	15	0.32
(1,925)	1:59:A:LEU:HD12	1:59:A:LEU:H	15	0.32
(1,925)	1:59:A:LEU:HD13	1:59:A:LEU:H	15	0.32
(1,909)	1:73:A:ILE:HG21	1:73:A:ILE:H	2	0.32
(1,909)	1:73:A:ILE:HG22	1:73:A:ILE:H	2	0.32
(1,909)	1:73:A:ILE:HG23	1:73:A:ILE:H	2	0.32
(1,909)	1:73:A:ILE:HG21	1:73:A:ILE:H	8	0.32
(1,909)	1:73:A:ILE:HG22	1:73:A:ILE:H	8	0.32
(1,909)	1:73:A:ILE:HG23	1:73:A:ILE:H	8	0.32
(1,903)	1:41:A:VAL:HG21	1:48:A:ASN:H	13	0.32
(1,903)	1:41:A:VAL:HG22	1:48:A:ASN:H	13	0.32
(1,903)	1:41:A:VAL:HG23	1:48:A:ASN:H	13	0.32
(1,870)	1:52:A:LEU:HG	1:56:A:GLN:HE21	4	0.32
(1,866)	1:27:A:ILE:HG13	1:24:A:SER:H	3	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,743)	1:34:A:LYS:HD2	1:34:A:LYS:H	10	0.32
(1,579)	1:142:A:ASN:HB3	1:143:A:GLN:H	8	0.32
(1,446)	1:43:A:GLY:HA2	1:44:A:ASN:H	9	0.32
(1,386)	1:117:A:ASN:HA	1:119:A:ILE:H	3	0.32
(1,97)	1:144:A:LEU:H	1:143:A:GLN:H	2	0.32
(1,3943)	1:59:A:LEU:HD21	1:19:A:TYR:HD1	11	0.31
(1,3943)	1:59:A:LEU:HD21	1:19:A:TYR:HD2	11	0.31
(1,3943)	1:59:A:LEU:HD22	1:19:A:TYR:HD1	11	0.31
(1,3943)	1:59:A:LEU:HD22	1:19:A:TYR:HD2	11	0.31
(1,3943)	1:59:A:LEU:HD23	1:19:A:TYR:HD1	11	0.31
(1,3943)	1:59:A:LEU:HD23	1:19:A:TYR:HD2	11	0.31
(1,3938)	1:14:A:ILE:HB	1:58:A:TYR:HD1	18	0.31
(1,3938)	1:14:A:ILE:HB	1:58:A:TYR:HD2	18	0.31
(1,3937)	1:20:A:ALA:HB1	1:19:A:TYR:HD1	17	0.31
(1,3937)	1:20:A:ALA:HB1	1:19:A:TYR:HD2	17	0.31
(1,3937)	1:20:A:ALA:HB2	1:19:A:TYR:HD1	17	0.31
(1,3937)	1:20:A:ALA:HB2	1:19:A:TYR:HD2	17	0.31
(1,3937)	1:20:A:ALA:HB3	1:19:A:TYR:HD1	17	0.31
(1,3937)	1:20:A:ALA:HB3	1:19:A:TYR:HD2	17	0.31
(1,3840)	1:112:A:ASP:HB3	1:111:A:ALA:HB1	11	0.31
(1,3840)	1:112:A:ASP:HB3	1:111:A:ALA:HB2	11	0.31
(1,3840)	1:112:A:ASP:HB3	1:111:A:ALA:HB3	11	0.31
(1,3797)	1:93:A:ILE:H	1:79:A:ILE:HB	8	0.31
(1,3791)	1:133:A:GLY:H	1:134:A:ARG:HD2	8	0.31
(1,3791)	1:133:A:GLY:H	1:134:A:ARG:HD3	8	0.31
(1,3791)	1:133:A:GLY:H	1:134:A:ARG:HD2	10	0.31
(1,3791)	1:133:A:GLY:H	1:134:A:ARG:HD3	10	0.31
(1,3238)	1:74:A:TYR:HB3	1:2:A:SER:HA	5	0.31
(1,3219)	1:93:A:ILE:HD11	1:119:A:ILE:HD11	18	0.31
(1,3219)	1:93:A:ILE:HD11	1:119:A:ILE:HD12	18	0.31
(1,3219)	1:93:A:ILE:HD11	1:119:A:ILE:HD13	18	0.31
(1,3219)	1:93:A:ILE:HD12	1:119:A:ILE:HD11	18	0.31
(1,3219)	1:93:A:ILE:HD12	1:119:A:ILE:HD12	18	0.31
(1,3219)	1:93:A:ILE:HD12	1:119:A:ILE:HD13	18	0.31
(1,3219)	1:93:A:ILE:HD13	1:119:A:ILE:HD11	18	0.31
(1,3219)	1:93:A:ILE:HD13	1:119:A:ILE:HD12	18	0.31
(1,3219)	1:93:A:ILE:HD13	1:119:A:ILE:HD13	18	0.31
(1,3183)	1:35:A:GLN:HG2	1:8:A:ILE:HD11	16	0.31
(1,3183)	1:35:A:GLN:HG2	1:8:A:ILE:HD12	16	0.31
(1,3183)	1:35:A:GLN:HG2	1:8:A:ILE:HD13	16	0.31
(1,3180)	1:127:A:ILE:HB	1:79:A:ILE:HD11	10	0.31
(1,3180)	1:127:A:ILE:HB	1:79:A:ILE:HD12	10	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3180)	1:127:A:ILE:HB	1:79:A:ILE:HD13	10	0.31
(1,3164)	1:123:A:ASP:HB2	1:93:A:ILE:HD11	4	0.31
(1,3164)	1:123:A:ASP:HB2	1:93:A:ILE:HD12	4	0.31
(1,3164)	1:123:A:ASP:HB2	1:93:A:ILE:HD13	4	0.31
(1,2966)	1:95:A:ASN:HB3	1:91:A:ILE:HG21	16	0.31
(1,2966)	1:95:A:ASN:HB3	1:91:A:ILE:HG22	16	0.31
(1,2966)	1:95:A:ASN:HB3	1:91:A:ILE:HG23	16	0.31
(1,2962)	1:42:A:ASP:HB3	1:50:A:ILE:HG21	11	0.31
(1,2962)	1:42:A:ASP:HB3	1:50:A:ILE:HG22	11	0.31
(1,2962)	1:42:A:ASP:HB3	1:50:A:ILE:HG23	11	0.31
(1,2874)	1:19:A:TYR:HD1	1:20:A:ALA:HB1	17	0.31
(1,2874)	1:19:A:TYR:HD1	1:20:A:ALA:HB2	17	0.31
(1,2874)	1:19:A:TYR:HD1	1:20:A:ALA:HB3	17	0.31
(1,2874)	1:19:A:TYR:HD2	1:20:A:ALA:HB1	17	0.31
(1,2874)	1:19:A:TYR:HD2	1:20:A:ALA:HB2	17	0.31
(1,2874)	1:19:A:TYR:HD2	1:20:A:ALA:HB3	17	0.31
(1,2844)	1:59:A:LEU:H	1:68:A:ILE:HG21	5	0.31
(1,2844)	1:59:A:LEU:H	1:68:A:ILE:HG22	5	0.31
(1,2844)	1:59:A:LEU:H	1:68:A:ILE:HG23	5	0.31
(1,2832)	1:91:A:ILE:H	1:91:A:ILE:HG21	5	0.31
(1,2832)	1:91:A:ILE:H	1:91:A:ILE:HG22	5	0.31
(1,2832)	1:91:A:ILE:H	1:91:A:ILE:HG23	5	0.31
(1,2830)	1:66:A:SER:H	1:54:A:ILE:HG21	20	0.31
(1,2830)	1:66:A:SER:H	1:54:A:ILE:HG22	20	0.31
(1,2830)	1:66:A:SER:H	1:54:A:ILE:HG23	20	0.31
(1,2583)	1:126:A:LEU:HB2	1:138:A:LEU:HD21	19	0.31
(1,2583)	1:126:A:LEU:HB2	1:138:A:LEU:HD22	19	0.31
(1,2583)	1:126:A:LEU:HB2	1:138:A:LEU:HD23	19	0.31
(1,2546)	1:35:A:GLN:HB2	1:31:A:LEU:HD21	2	0.31
(1,2546)	1:35:A:GLN:HB2	1:31:A:LEU:HD22	2	0.31
(1,2546)	1:35:A:GLN:HB2	1:31:A:LEU:HD23	2	0.31
(1,2546)	1:56:A:GLN:HB2	1:60:A:LEU:HD21	9	0.31
(1,2546)	1:56:A:GLN:HB2	1:60:A:LEU:HD22	9	0.31
(1,2546)	1:56:A:GLN:HB2	1:60:A:LEU:HD23	9	0.31
(1,2546)	1:56:A:GLN:HB3	1:60:A:LEU:HD21	9	0.31
(1,2546)	1:56:A:GLN:HB3	1:60:A:LEU:HD22	9	0.31
(1,2546)	1:56:A:GLN:HB3	1:60:A:LEU:HD23	9	0.31
(1,2546)	1:56:A:GLN:HB2	1:60:A:LEU:HD21	20	0.31
(1,2546)	1:56:A:GLN:HB2	1:60:A:LEU:HD22	20	0.31
(1,2546)	1:56:A:GLN:HB2	1:60:A:LEU:HD23	20	0.31
(1,2546)	1:56:A:GLN:HB3	1:60:A:LEU:HD21	20	0.31
(1,2546)	1:56:A:GLN:HB3	1:60:A:LEU:HD22	20	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2546)	1:56:A:GLN:HB3	1:60:A:LEU:HD23	20	0.31
(1,2537)	1:52:A:LEU:HA	1:55:A:LEU:HD11	12	0.31
(1,2537)	1:52:A:LEU:HA	1:55:A:LEU:HD12	12	0.31
(1,2537)	1:52:A:LEU:HA	1:55:A:LEU:HD13	12	0.31
(1,2499)	1:135:A:ILE:HA	1:135:A:ILE:HG12	10	0.31
(1,2484)	1:56:A:GLN:HE22	1:60:A:LEU:HD21	17	0.31
(1,2484)	1:56:A:GLN:HE22	1:60:A:LEU:HD22	17	0.31
(1,2484)	1:56:A:GLN:HE22	1:60:A:LEU:HD23	17	0.31
(1,2483)	1:56:A:GLN:HE21	1:60:A:LEU:HD21	3	0.31
(1,2483)	1:56:A:GLN:HE21	1:60:A:LEU:HD22	3	0.31
(1,2483)	1:56:A:GLN:HE21	1:60:A:LEU:HD23	3	0.31
(1,2483)	1:56:A:GLN:HE21	1:60:A:LEU:HD21	15	0.31
(1,2483)	1:56:A:GLN:HE21	1:60:A:LEU:HD22	15	0.31
(1,2483)	1:56:A:GLN:HE21	1:60:A:LEU:HD23	15	0.31
(1,2379)	1:107:A:SER:HA	1:108:A:LEU:HG	4	0.31
(1,2379)	1:107:A:SER:HA	1:108:A:LEU:HG	14	0.31
(1,2379)	1:107:A:SER:HA	1:108:A:LEU:HG	20	0.31
(1,2344)	1:19:A:TYR:H	1:59:A:LEU:HD21	16	0.31
(1,2344)	1:19:A:TYR:H	1:59:A:LEU:HD22	16	0.31
(1,2344)	1:19:A:TYR:H	1:59:A:LEU:HD23	16	0.31
(1,2306)	1:71:A:ASN:H	1:5:A:ILE:HG13	6	0.31
(1,2306)	1:71:A:ASN:H	1:5:A:ILE:HG13	13	0.31
(1,2306)	1:71:A:ASN:H	1:5:A:ILE:HG13	16	0.31
(1,1843)	1:24:A:SER:HB2	1:23:A:LYS:HE2	12	0.31
(1,1843)	1:24:A:SER:HB3	1:23:A:LYS:HE2	12	0.31
(1,1792)	1:133:A:GLY:H	1:134:A:ARG:HD2	8	0.31
(1,1792)	1:133:A:GLY:H	1:134:A:ARG:HD3	8	0.31
(1,1792)	1:133:A:GLY:H	1:134:A:ARG:HD2	10	0.31
(1,1792)	1:133:A:GLY:H	1:134:A:ARG:HD3	10	0.31
(1,1505)	1:72:A:ARG:HA	1:73:A:ILE:HD11	10	0.31
(1,1505)	1:72:A:ARG:HA	1:73:A:ILE:HD12	10	0.31
(1,1505)	1:72:A:ARG:HA	1:73:A:ILE:HD13	10	0.31
(1,1388)	1:103:A:LEU:HA	1:107:A:SER:HB3	5	0.31
(1,1357)	1:90:A:TYR:H	1:93:A:ILE:HD11	16	0.31
(1,1357)	1:90:A:TYR:H	1:93:A:ILE:HD12	16	0.31
(1,1357)	1:90:A:TYR:H	1:93:A:ILE:HD13	16	0.31
(1,1353)	1:66:A:SER:H	1:68:A:ILE:HD11	6	0.31
(1,1353)	1:66:A:SER:H	1:68:A:ILE:HD12	6	0.31
(1,1353)	1:66:A:SER:H	1:68:A:ILE:HD13	6	0.31
(1,1163)	1:27:A:ILE:HD11	1:27:A:ILE:H	20	0.31
(1,1163)	1:27:A:ILE:HD12	1:27:A:ILE:H	20	0.31
(1,1163)	1:27:A:ILE:HD13	1:27:A:ILE:H	20	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1137)	1:97:A:ILE:HG21	1:96:A:HIS:H	16	0.31
(1,1137)	1:97:A:ILE:HG22	1:96:A:HIS:H	16	0.31
(1,1137)	1:97:A:ILE:HG23	1:96:A:HIS:H	16	0.31
(1,1019)	1:22:A:LEU:HD21	1:52:A:LEU:H	2	0.31
(1,1019)	1:22:A:LEU:HD22	1:52:A:LEU:H	2	0.31
(1,1019)	1:22:A:LEU:HD23	1:52:A:LEU:H	2	0.31
(1,1019)	1:22:A:LEU:HD21	1:52:A:LEU:H	4	0.31
(1,1019)	1:22:A:LEU:HD22	1:52:A:LEU:H	4	0.31
(1,1019)	1:22:A:LEU:HD23	1:52:A:LEU:H	4	0.31
(1,980)	1:54:A:ILE:HD11	1:42:A:ASP:H	5	0.31
(1,980)	1:54:A:ILE:HD12	1:42:A:ASP:H	5	0.31
(1,980)	1:54:A:ILE:HD13	1:42:A:ASP:H	5	0.31
(1,929)	1:3:A:VAL:HG21	1:34:A:LYS:H	4	0.31
(1,929)	1:3:A:VAL:HG22	1:34:A:LYS:H	4	0.31
(1,929)	1:3:A:VAL:HG23	1:34:A:LYS:H	4	0.31
(1,909)	1:73:A:ILE:HG21	1:73:A:ILE:H	17	0.31
(1,909)	1:73:A:ILE:HG22	1:73:A:ILE:H	17	0.31
(1,909)	1:73:A:ILE:HG23	1:73:A:ILE:H	17	0.31
(1,866)	1:27:A:ILE:HG13	1:24:A:SER:H	8	0.31
(1,743)	1:34:A:LYS:HD2	1:34:A:LYS:H	6	0.31
(1,743)	1:34:A:LYS:HD2	1:34:A:LYS:H	14	0.31
(1,228)	1:19:A:TYR:HD1	1:57:A:MET:H	14	0.31
(1,228)	1:19:A:TYR:HD2	1:57:A:MET:H	14	0.31
(1,228)	1:19:A:TYR:HD1	1:57:A:MET:H	15	0.31
(1,228)	1:19:A:TYR:HD2	1:57:A:MET:H	15	0.31
(1,97)	1:144:A:LEU:H	1:143:A:GLN:H	9	0.31
(1,81)	1:58:A:TYR:H	1:61:A:GLY:H	18	0.31
(1,3937)	1:20:A:ALA:HB1	1:19:A:TYR:HD1	2	0.3
(1,3937)	1:20:A:ALA:HB1	1:19:A:TYR:HD2	2	0.3
(1,3937)	1:20:A:ALA:HB2	1:19:A:TYR:HD1	2	0.3
(1,3937)	1:20:A:ALA:HB2	1:19:A:TYR:HD2	2	0.3
(1,3937)	1:20:A:ALA:HB3	1:19:A:TYR:HD1	2	0.3
(1,3937)	1:20:A:ALA:HB3	1:19:A:TYR:HD2	2	0.3
(1,3871)	1:11:A:ASN:H	1:7:A:ASP:HB3	14	0.3
(1,3840)	1:123:A:ASP:HB2	1:111:A:ALA:HB1	13	0.3
(1,3840)	1:123:A:ASP:HB2	1:111:A:ALA:HB2	13	0.3
(1,3840)	1:123:A:ASP:HB2	1:111:A:ALA:HB3	13	0.3
(1,3758)	1:102:A:GLN:HG3	1:108:A:LEU:HD11	19	0.3
(1,3758)	1:102:A:GLN:HG3	1:108:A:LEU:HD12	19	0.3
(1,3758)	1:102:A:GLN:HG3	1:108:A:LEU:HD13	19	0.3
(1,3696)	1:108:A:LEU:HD11	1:102:A:GLN:HG3	19	0.3
(1,3696)	1:108:A:LEU:HD12	1:102:A:GLN:HG3	19	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3696)	1:108:A:LEU:HD13	1:102:A:GLN:HG3	19	0.3
(1,3581)	1:56:A:GLN:H	1:68:A:ILE:HD11	1	0.3
(1,3581)	1:56:A:GLN:H	1:68:A:ILE:HD12	1	0.3
(1,3581)	1:56:A:GLN:H	1:68:A:ILE:HD13	1	0.3
(1,3371)	1:36:A:LEU:HA	1:36:A:LEU:HD11	10	0.3
(1,3371)	1:36:A:LEU:HA	1:36:A:LEU:HD12	10	0.3
(1,3371)	1:36:A:LEU:HA	1:36:A:LEU:HD13	10	0.3
(1,3336)	1:126:A:LEU:HD11	1:139:A:PRO:HB3	6	0.3
(1,3336)	1:126:A:LEU:HD12	1:139:A:PRO:HB3	6	0.3
(1,3336)	1:126:A:LEU:HD13	1:139:A:PRO:HB3	6	0.3
(1,3238)	1:74:A:TYR:HB3	1:2:A:SER:HA	18	0.3
(1,3219)	1:93:A:ILE:HD11	1:119:A:ILE:HD11	6	0.3
(1,3219)	1:93:A:ILE:HD11	1:119:A:ILE:HD12	6	0.3
(1,3219)	1:93:A:ILE:HD11	1:119:A:ILE:HD13	6	0.3
(1,3219)	1:93:A:ILE:HD12	1:119:A:ILE:HD11	6	0.3
(1,3219)	1:93:A:ILE:HD12	1:119:A:ILE:HD12	6	0.3
(1,3219)	1:93:A:ILE:HD12	1:119:A:ILE:HD13	6	0.3
(1,3219)	1:93:A:ILE:HD13	1:119:A:ILE:HD11	6	0.3
(1,3219)	1:93:A:ILE:HD13	1:119:A:ILE:HD12	6	0.3
(1,3219)	1:93:A:ILE:HD13	1:119:A:ILE:HD13	6	0.3
(1,3177)	1:129:A:LYS:HE2	1:135:A:ILE:HD11	3	0.3
(1,3177)	1:129:A:LYS:HE2	1:135:A:ILE:HD12	3	0.3
(1,3177)	1:129:A:LYS:HE2	1:135:A:ILE:HD13	3	0.3
(1,3177)	1:129:A:LYS:HE3	1:135:A:ILE:HD11	3	0.3
(1,3177)	1:129:A:LYS:HE3	1:135:A:ILE:HD12	3	0.3
(1,3177)	1:129:A:LYS:HE3	1:135:A:ILE:HD13	3	0.3
(1,2966)	1:94:A:CYS:HB3	1:97:A:ILE:HG21	5	0.3
(1,2966)	1:94:A:CYS:HB3	1:97:A:ILE:HG22	5	0.3
(1,2966)	1:94:A:CYS:HB3	1:97:A:ILE:HG23	5	0.3
(1,2966)	1:94:A:CYS:HB3	1:91:A:ILE:HG21	9	0.3
(1,2966)	1:94:A:CYS:HB3	1:91:A:ILE:HG22	9	0.3
(1,2966)	1:94:A:CYS:HB3	1:91:A:ILE:HG23	9	0.3
(1,2966)	1:88:A:ASN:HB3	1:91:A:ILE:HG21	10	0.3
(1,2966)	1:88:A:ASN:HB3	1:91:A:ILE:HG22	10	0.3
(1,2966)	1:88:A:ASN:HB3	1:91:A:ILE:HG23	10	0.3
(1,2904)	1:3:A:VAL:HA	1:38:A:ALA:HB1	19	0.3
(1,2904)	1:3:A:VAL:HA	1:38:A:ALA:HB2	19	0.3
(1,2904)	1:3:A:VAL:HA	1:38:A:ALA:HB3	19	0.3
(1,2874)	1:19:A:TYR:HD1	1:20:A:ALA:HB1	2	0.3
(1,2874)	1:19:A:TYR:HD1	1:20:A:ALA:HB2	2	0.3
(1,2874)	1:19:A:TYR:HD1	1:20:A:ALA:HB3	2	0.3
(1,2874)	1:19:A:TYR:HD2	1:20:A:ALA:HB1	2	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2874)	1:19:A:TYR:HD2	1:20:A:ALA:HB2	2	0.3
(1,2874)	1:19:A:TYR:HD2	1:20:A:ALA:HB3	2	0.3
(1,2844)	1:59:A:LEU:H	1:68:A:ILE:HG21	3	0.3
(1,2844)	1:59:A:LEU:H	1:68:A:ILE:HG22	3	0.3
(1,2844)	1:59:A:LEU:H	1:68:A:ILE:HG23	3	0.3
(1,2844)	1:58:A:TYR:H	1:68:A:ILE:HG21	13	0.3
(1,2844)	1:58:A:TYR:H	1:68:A:ILE:HG22	13	0.3
(1,2844)	1:58:A:TYR:H	1:68:A:ILE:HG23	13	0.3
(1,2832)	1:131:A:ILE:H	1:131:A:ILE:HG21	3	0.3
(1,2832)	1:131:A:ILE:H	1:131:A:ILE:HG22	3	0.3
(1,2832)	1:131:A:ILE:H	1:131:A:ILE:HG23	3	0.3
(1,2832)	1:131:A:ILE:H	1:131:A:ILE:HG21	4	0.3
(1,2832)	1:131:A:ILE:H	1:131:A:ILE:HG22	4	0.3
(1,2832)	1:131:A:ILE:H	1:131:A:ILE:HG23	4	0.3
(1,2832)	1:131:A:ILE:H	1:131:A:ILE:HG21	6	0.3
(1,2832)	1:131:A:ILE:H	1:131:A:ILE:HG22	6	0.3
(1,2832)	1:131:A:ILE:H	1:131:A:ILE:HG23	6	0.3
(1,2832)	1:91:A:ILE:H	1:91:A:ILE:HG21	11	0.3
(1,2832)	1:91:A:ILE:H	1:91:A:ILE:HG22	11	0.3
(1,2832)	1:91:A:ILE:H	1:91:A:ILE:HG23	11	0.3
(1,2832)	1:91:A:ILE:H	1:91:A:ILE:HG21	12	0.3
(1,2832)	1:91:A:ILE:H	1:91:A:ILE:HG22	12	0.3
(1,2832)	1:91:A:ILE:H	1:91:A:ILE:HG23	12	0.3
(1,2765)	1:74:A:TYR:HB2	1:3:A:VAL:HG21	14	0.3
(1,2765)	1:74:A:TYR:HB2	1:3:A:VAL:HG22	14	0.3
(1,2765)	1:74:A:TYR:HB2	1:3:A:VAL:HG23	14	0.3
(1,2586)	1:39:A:ALA:HB1	1:36:A:LEU:HD11	8	0.3
(1,2586)	1:39:A:ALA:HB1	1:36:A:LEU:HD12	8	0.3
(1,2586)	1:39:A:ALA:HB1	1:36:A:LEU:HD13	8	0.3
(1,2586)	1:39:A:ALA:HB2	1:36:A:LEU:HD11	8	0.3
(1,2586)	1:39:A:ALA:HB2	1:36:A:LEU:HD12	8	0.3
(1,2586)	1:39:A:ALA:HB2	1:36:A:LEU:HD13	8	0.3
(1,2586)	1:39:A:ALA:HB3	1:36:A:LEU:HD11	8	0.3
(1,2586)	1:39:A:ALA:HB3	1:36:A:LEU:HD12	8	0.3
(1,2586)	1:39:A:ALA:HB3	1:36:A:LEU:HD13	8	0.3
(1,2583)	1:126:A:LEU:HB2	1:138:A:LEU:HD21	1	0.3
(1,2583)	1:126:A:LEU:HB2	1:138:A:LEU:HD22	1	0.3
(1,2583)	1:126:A:LEU:HB2	1:138:A:LEU:HD23	1	0.3
(1,2523)	1:8:A:ILE:HA	1:22:A:LEU:HD21	10	0.3
(1,2523)	1:8:A:ILE:HA	1:22:A:LEU:HD22	10	0.3
(1,2523)	1:8:A:ILE:HA	1:22:A:LEU:HD23	10	0.3
(1,2515)	1:92:A:LEU:HA	1:103:A:LEU:HD11	8	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2515)	1:92:A:LEU:HA	1:103:A:LEU:HD12	8	0.3
(1,2515)	1:92:A:LEU:HA	1:103:A:LEU:HD13	8	0.3
(1,2499)	1:135:A:ILE:HA	1:135:A:ILE:HG12	2	0.3
(1,2499)	1:135:A:ILE:HA	1:135:A:ILE:HG12	6	0.3
(1,2499)	1:135:A:ILE:HA	1:135:A:ILE:HG12	11	0.3
(1,2499)	1:135:A:ILE:HA	1:135:A:ILE:HG12	15	0.3
(1,2499)	1:135:A:ILE:HA	1:135:A:ILE:HG12	16	0.3
(1,2483)	1:56:A:GLN:HE21	1:60:A:LEU:HD21	9	0.3
(1,2483)	1:56:A:GLN:HE21	1:60:A:LEU:HD22	9	0.3
(1,2483)	1:56:A:GLN:HE21	1:60:A:LEU:HD23	9	0.3
(1,2379)	1:107:A:SER:HA	1:108:A:LEU:HG	17	0.3
(1,2300)	1:49:A:SER:H	1:50:A:ILE:HG13	13	0.3
(1,2247)	1:70:A:LYS:HA	1:70:A:LYS:HD2	16	0.3
(1,2120)	1:74:A:TYR:HE1	1:72:A:ARG:HB2	10	0.3
(1,2120)	1:74:A:TYR:HE2	1:72:A:ARG:HB2	10	0.3
(1,2001)	1:82:A:ASN:HD22	1:82:A:ASN:HB3	1	0.3
(1,2001)	1:82:A:ASN:HD22	1:82:A:ASN:HB3	3	0.3
(1,2001)	1:11:A:ASN:HD22	1:11:A:ASN:HB3	17	0.3
(1,1806)	1:81:A:ASN:HD22	1:72:A:ARG:HD3	14	0.3
(1,1388)	1:103:A:LEU:HA	1:107:A:SER:HB3	19	0.3
(1,1326)	1:5:A:ILE:HD11	1:39:A:ALA:H	13	0.3
(1,1326)	1:5:A:ILE:HD12	1:39:A:ALA:H	13	0.3
(1,1326)	1:5:A:ILE:HD13	1:39:A:ALA:H	13	0.3
(1,1238)	1:59:A:LEU:HD21	1:20:A:ALA:H	12	0.3
(1,1238)	1:59:A:LEU:HD22	1:20:A:ALA:H	12	0.3
(1,1238)	1:59:A:LEU:HD23	1:20:A:ALA:H	12	0.3
(1,1221)	1:62:A:LYS:HB3	1:63:A:GLY:H	15	0.3
(1,1221)	1:62:A:LYS:HB3	1:63:A:GLY:H	18	0.3
(1,1220)	1:131:A:ILE:HG21	1:133:A:GLY:H	17	0.3
(1,1220)	1:131:A:ILE:HG22	1:133:A:GLY:H	17	0.3
(1,1220)	1:131:A:ILE:HG23	1:133:A:GLY:H	17	0.3
(1,1137)	1:97:A:ILE:HG21	1:96:A:HIS:H	4	0.3
(1,1137)	1:97:A:ILE:HG22	1:96:A:HIS:H	4	0.3
(1,1137)	1:97:A:ILE:HG23	1:96:A:HIS:H	4	0.3
(1,1091)	1:103:A:LEU:HD21	1:104:A:SER:H	11	0.3
(1,1091)	1:103:A:LEU:HD22	1:104:A:SER:H	11	0.3
(1,1091)	1:103:A:LEU:HD23	1:104:A:SER:H	11	0.3
(1,1043)	1:21:A:ILE:HG21	1:32:A:THR:H	1	0.3
(1,1043)	1:21:A:ILE:HG22	1:32:A:THR:H	1	0.3
(1,1043)	1:21:A:ILE:HG23	1:32:A:THR:H	1	0.3
(1,1043)	1:8:A:ILE:HG21	1:32:A:THR:H	8	0.3
(1,1043)	1:8:A:ILE:HG22	1:32:A:THR:H	8	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1043)	1:8:A:ILE:HG23	1:32:A:THR:H	8	0.3
(1,980)	1:54:A:ILE:HD11	1:42:A:ASP:H	18	0.3
(1,980)	1:54:A:ILE:HD12	1:42:A:ASP:H	18	0.3
(1,980)	1:54:A:ILE:HD13	1:42:A:ASP:H	18	0.3
(1,971)	1:60:A:LEU:HD21	1:62:A:LYS:H	1	0.3
(1,971)	1:60:A:LEU:HD22	1:62:A:LYS:H	1	0.3
(1,971)	1:60:A:LEU:HD23	1:62:A:LYS:H	1	0.3
(1,929)	1:3:A:VAL:HG21	1:34:A:LYS:H	13	0.3
(1,929)	1:3:A:VAL:HG22	1:34:A:LYS:H	13	0.3
(1,929)	1:3:A:VAL:HG23	1:34:A:LYS:H	13	0.3
(1,909)	1:73:A:ILE:HD11	1:73:A:ILE:H	6	0.3
(1,909)	1:73:A:ILE:HD12	1:73:A:ILE:H	6	0.3
(1,909)	1:73:A:ILE:HD13	1:73:A:ILE:H	6	0.3
(1,909)	1:73:A:ILE:HG21	1:73:A:ILE:H	20	0.3
(1,909)	1:73:A:ILE:HG22	1:73:A:ILE:H	20	0.3
(1,909)	1:73:A:ILE:HG23	1:73:A:ILE:H	20	0.3
(1,903)	1:41:A:VAL:HG21	1:48:A:ASN:H	14	0.3
(1,903)	1:41:A:VAL:HG22	1:48:A:ASN:H	14	0.3
(1,903)	1:41:A:VAL:HG23	1:48:A:ASN:H	14	0.3
(1,903)	1:41:A:VAL:HG21	1:48:A:ASN:H	16	0.3
(1,903)	1:41:A:VAL:HG22	1:48:A:ASN:H	16	0.3
(1,903)	1:41:A:VAL:HG23	1:48:A:ASN:H	16	0.3
(1,866)	1:20:A:ALA:HB1	1:24:A:SER:H	17	0.3
(1,866)	1:20:A:ALA:HB2	1:24:A:SER:H	17	0.3
(1,866)	1:20:A:ALA:HB3	1:24:A:SER:H	17	0.3
(1,743)	1:34:A:LYS:HD2	1:34:A:LYS:H	20	0.3
(1,605)	1:90:A:TYR:HB2	1:93:A:ILE:H	7	0.3
(1,605)	1:90:A:TYR:HB2	1:93:A:ILE:H	13	0.3
(1,587)	1:7:A:ASP:HB3	1:11:A:ASN:H	14	0.3
(1,572)	1:9:A:ASP:HB3	1:20:A:ALA:H	9	0.3
(1,554)	1:4:A:LYS:HE2	1:4:A:LYS:H	13	0.3
(1,554)	1:4:A:LYS:HE3	1:4:A:LYS:H	13	0.3
(1,228)	1:19:A:TYR:HD1	1:57:A:MET:H	9	0.3
(1,228)	1:19:A:TYR:HD2	1:57:A:MET:H	9	0.3
(1,3890)	1:71:A:ASN:H	1:2:A:SER:HB2	15	0.29
(1,3890)	1:4:A:LYS:H	1:2:A:SER:HB2	20	0.29
(1,3871)	1:11:A:ASN:H	1:9:A:ASP:HB3	6	0.29
(1,3805)	1:125:A:ILE:HG12	1:128:A:GLU:HG2	5	0.29
(1,3805)	1:125:A:ILE:HG12	1:128:A:GLU:HG3	5	0.29
(1,3797)	1:93:A:ILE:H	1:79:A:ILE:HB	14	0.29
(1,3758)	1:102:A:GLN:HG3	1:108:A:LEU:HD21	8	0.29
(1,3758)	1:102:A:GLN:HG3	1:108:A:LEU:HD22	8	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3758)	1:102:A:GLN:HG3	1:108:A:LEU:HD23	8	0.29
(1,3758)	1:102:A:GLN:HG3	1:108:A:LEU:HD11	14	0.29
(1,3758)	1:102:A:GLN:HG3	1:108:A:LEU:HD12	14	0.29
(1,3758)	1:102:A:GLN:HG3	1:108:A:LEU:HD13	14	0.29
(1,3758)	1:102:A:GLN:HG3	1:108:A:LEU:HD11	15	0.29
(1,3758)	1:102:A:GLN:HG3	1:108:A:LEU:HD12	15	0.29
(1,3758)	1:102:A:GLN:HG3	1:108:A:LEU:HD13	15	0.29
(1,3696)	1:108:A:LEU:HD21	1:102:A:GLN:HG3	8	0.29
(1,3696)	1:108:A:LEU:HD22	1:102:A:GLN:HG3	8	0.29
(1,3696)	1:108:A:LEU:HD23	1:102:A:GLN:HG3	8	0.29
(1,3696)	1:108:A:LEU:HD11	1:102:A:GLN:HG3	14	0.29
(1,3696)	1:108:A:LEU:HD12	1:102:A:GLN:HG3	14	0.29
(1,3696)	1:108:A:LEU:HD13	1:102:A:GLN:HG3	14	0.29
(1,3696)	1:108:A:LEU:HD11	1:102:A:GLN:HG3	15	0.29
(1,3696)	1:108:A:LEU:HD12	1:102:A:GLN:HG3	15	0.29
(1,3696)	1:108:A:LEU:HD13	1:102:A:GLN:HG3	15	0.29
(1,3543)	1:17:A:ILE:HA	1:21:A:ILE:HD11	17	0.29
(1,3543)	1:17:A:ILE:HA	1:21:A:ILE:HD12	17	0.29
(1,3543)	1:17:A:ILE:HA	1:21:A:ILE:HD13	17	0.29
(1,3371)	1:36:A:LEU:HA	1:36:A:LEU:HD11	7	0.29
(1,3371)	1:36:A:LEU:HA	1:36:A:LEU:HD12	7	0.29
(1,3371)	1:36:A:LEU:HA	1:36:A:LEU:HD13	7	0.29
(1,3371)	1:36:A:LEU:HA	1:36:A:LEU:HD11	11	0.29
(1,3371)	1:36:A:LEU:HA	1:36:A:LEU:HD12	11	0.29
(1,3371)	1:36:A:LEU:HA	1:36:A:LEU:HD13	11	0.29
(1,3238)	1:74:A:TYR:HB3	1:2:A:SER:HA	8	0.29
(1,3183)	1:90:A:TYR:HB2	1:79:A:ILE:HD11	17	0.29
(1,3183)	1:90:A:TYR:HB2	1:79:A:ILE:HD12	17	0.29
(1,3183)	1:90:A:TYR:HB2	1:79:A:ILE:HD13	17	0.29
(1,3180)	1:127:A:ILE:HB	1:79:A:ILE:HD11	1	0.29
(1,3180)	1:127:A:ILE:HB	1:79:A:ILE:HD12	1	0.29
(1,3180)	1:127:A:ILE:HB	1:79:A:ILE:HD13	1	0.29
(1,3095)	1:57:A:MET:HE1	1:53:A:ALA:HA	17	0.29
(1,3095)	1:57:A:MET:HE2	1:53:A:ALA:HA	17	0.29
(1,3095)	1:57:A:MET:HE3	1:53:A:ALA:HA	17	0.29
(1,3074)	1:4:A:LYS:HB2	1:71:A:ASN:HA	6	0.29
(1,3074)	1:4:A:LYS:HB2	1:71:A:ASN:HA	19	0.29
(1,3019)	1:63:A:GLY:HA2	1:65:A:THR:HB	18	0.29
(1,2942)	1:86:A:ASP:HB2	1:131:A:ILE:HG21	6	0.29
(1,2942)	1:86:A:ASP:HB2	1:131:A:ILE:HG22	6	0.29
(1,2942)	1:86:A:ASP:HB2	1:131:A:ILE:HG23	6	0.29
(1,2844)	1:59:A:LEU:H	1:68:A:ILE:HG21	6	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2844)	1:59:A:LEU:H	1:68:A:ILE:HG22	6	0.29
(1,2844)	1:59:A:LEU:H	1:68:A:ILE:HG23	6	0.29
(1,2832)	1:91:A:ILE:H	1:91:A:ILE:HG21	1	0.29
(1,2832)	1:91:A:ILE:H	1:91:A:ILE:HG22	1	0.29
(1,2832)	1:91:A:ILE:H	1:91:A:ILE:HG23	1	0.29
(1,2832)	1:131:A:ILE:H	1:131:A:ILE:HG21	2	0.29
(1,2832)	1:131:A:ILE:H	1:131:A:ILE:HG22	2	0.29
(1,2832)	1:131:A:ILE:H	1:131:A:ILE:HG23	2	0.29
(1,2832)	1:91:A:ILE:H	1:91:A:ILE:HG21	8	0.29
(1,2832)	1:91:A:ILE:H	1:91:A:ILE:HG22	8	0.29
(1,2832)	1:91:A:ILE:H	1:91:A:ILE:HG23	8	0.29
(1,2832)	1:91:A:ILE:H	1:91:A:ILE:HG21	13	0.29
(1,2832)	1:91:A:ILE:H	1:91:A:ILE:HG22	13	0.29
(1,2832)	1:91:A:ILE:H	1:91:A:ILE:HG23	13	0.29
(1,2832)	1:131:A:ILE:H	1:131:A:ILE:HG21	17	0.29
(1,2832)	1:131:A:ILE:H	1:131:A:ILE:HG22	17	0.29
(1,2832)	1:131:A:ILE:H	1:131:A:ILE:HG23	17	0.29
(1,2832)	1:91:A:ILE:H	1:91:A:ILE:HG21	19	0.29
(1,2832)	1:91:A:ILE:H	1:91:A:ILE:HG22	19	0.29
(1,2832)	1:91:A:ILE:H	1:91:A:ILE:HG23	19	0.29
(1,2832)	1:91:A:ILE:H	1:91:A:ILE:HG21	20	0.29
(1,2832)	1:91:A:ILE:H	1:91:A:ILE:HG22	20	0.29
(1,2832)	1:91:A:ILE:H	1:91:A:ILE:HG23	20	0.29
(1,2586)	1:39:A:ALA:HB1	1:36:A:LEU:HD11	18	0.29
(1,2586)	1:39:A:ALA:HB1	1:36:A:LEU:HD12	18	0.29
(1,2586)	1:39:A:ALA:HB1	1:36:A:LEU:HD13	18	0.29
(1,2586)	1:39:A:ALA:HB2	1:36:A:LEU:HD11	18	0.29
(1,2586)	1:39:A:ALA:HB2	1:36:A:LEU:HD12	18	0.29
(1,2586)	1:39:A:ALA:HB2	1:36:A:LEU:HD13	18	0.29
(1,2586)	1:39:A:ALA:HB3	1:36:A:LEU:HD11	18	0.29
(1,2586)	1:39:A:ALA:HB3	1:36:A:LEU:HD12	18	0.29
(1,2586)	1:39:A:ALA:HB3	1:36:A:LEU:HD13	18	0.29
(1,2546)	1:56:A:GLN:HB2	1:60:A:LEU:HD21	3	0.29
(1,2546)	1:56:A:GLN:HB2	1:60:A:LEU:HD22	3	0.29
(1,2546)	1:56:A:GLN:HB2	1:60:A:LEU:HD23	3	0.29
(1,2546)	1:56:A:GLN:HB3	1:60:A:LEU:HD21	3	0.29
(1,2546)	1:56:A:GLN:HB3	1:60:A:LEU:HD22	3	0.29
(1,2546)	1:56:A:GLN:HB3	1:60:A:LEU:HD23	3	0.29
(1,2499)	1:135:A:ILE:HA	1:135:A:ILE:HG12	1	0.29
(1,2499)	1:135:A:ILE:HA	1:135:A:ILE:HG12	3	0.29
(1,2499)	1:62:A:LYS:HA	1:62:A:LYS:HG3	12	0.29
(1,2499)	1:135:A:ILE:HA	1:135:A:ILE:HG12	13	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2499)	1:135:A:ILE:HA	1:135:A:ILE:HG12	18	0.29
(1,2499)	1:135:A:ILE:HA	1:135:A:ILE:HG12	20	0.29
(1,2484)	1:56:A:GLN:HE22	1:60:A:LEU:HD21	19	0.29
(1,2484)	1:56:A:GLN:HE22	1:60:A:LEU:HD22	19	0.29
(1,2484)	1:56:A:GLN:HE22	1:60:A:LEU:HD23	19	0.29
(1,2484)	1:56:A:GLN:HE22	1:60:A:LEU:HD21	20	0.29
(1,2484)	1:56:A:GLN:HE22	1:60:A:LEU:HD22	20	0.29
(1,2484)	1:56:A:GLN:HE22	1:60:A:LEU:HD23	20	0.29
(1,2379)	1:107:A:SER:HA	1:108:A:LEU:HG	2	0.29
(1,2379)	1:107:A:SER:HA	1:108:A:LEU:HG	18	0.29
(1,2350)	1:52:A:LEU:H	1:52:A:LEU:HD21	15	0.29
(1,2350)	1:52:A:LEU:H	1:52:A:LEU:HD22	15	0.29
(1,2350)	1:52:A:LEU:H	1:52:A:LEU:HD23	15	0.29
(1,2344)	1:19:A:TYR:H	1:59:A:LEU:HD21	2	0.29
(1,2344)	1:19:A:TYR:H	1:59:A:LEU:HD22	2	0.29
(1,2344)	1:19:A:TYR:H	1:59:A:LEU:HD23	2	0.29
(1,2306)	1:71:A:ASN:H	1:5:A:ILE:HG13	15	0.29
(1,2145)	1:37:A:ALA:HA	1:3:A:VAL:HB	16	0.29
(1,2001)	1:82:A:ASN:HD22	1:82:A:ASN:HB3	18	0.29
(1,1859)	1:60:A:LEU:HD21	1:62:A:LYS:HE2	13	0.29
(1,1859)	1:60:A:LEU:HD22	1:62:A:LYS:HE2	13	0.29
(1,1859)	1:60:A:LEU:HD23	1:62:A:LYS:HE2	13	0.29
(1,1851)	1:125:A:ILE:HG12	1:124:A:ARG:HD2	16	0.29
(1,1851)	1:125:A:ILE:HG12	1:124:A:ARG:HD3	16	0.29
(1,1817)	1:132:A:THR:HB	1:134:A:ARG:HD2	10	0.29
(1,1817)	1:132:A:THR:HB	1:134:A:ARG:HD3	10	0.29
(1,1806)	1:74:A:TYR:HE1	1:72:A:ARG:HD3	11	0.29
(1,1511)	1:3:A:VAL:HA	1:5:A:ILE:HD11	11	0.29
(1,1511)	1:3:A:VAL:HA	1:5:A:ILE:HD12	11	0.29
(1,1511)	1:3:A:VAL:HA	1:5:A:ILE:HD13	11	0.29
(1,1505)	1:72:A:ARG:HA	1:73:A:ILE:HD11	5	0.29
(1,1505)	1:72:A:ARG:HA	1:73:A:ILE:HD12	5	0.29
(1,1505)	1:72:A:ARG:HA	1:73:A:ILE:HD13	5	0.29
(1,1328)	1:97:A:ILE:HG21	1:121:A:GLN:H	1	0.29
(1,1328)	1:97:A:ILE:HG22	1:121:A:GLN:H	1	0.29
(1,1328)	1:97:A:ILE:HG23	1:121:A:GLN:H	1	0.29
(1,1328)	1:97:A:ILE:HG21	1:121:A:GLN:H	8	0.29
(1,1328)	1:97:A:ILE:HG22	1:121:A:GLN:H	8	0.29
(1,1328)	1:97:A:ILE:HG23	1:121:A:GLN:H	8	0.29
(1,1163)	1:27:A:ILE:HD11	1:27:A:ILE:H	6	0.29
(1,1163)	1:27:A:ILE:HD12	1:27:A:ILE:H	6	0.29
(1,1163)	1:27:A:ILE:HD13	1:27:A:ILE:H	6	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1163)	1:27:A:ILE:HD11	1:27:A:ILE:H	13	0.29
(1,1163)	1:27:A:ILE:HD12	1:27:A:ILE:H	13	0.29
(1,1163)	1:27:A:ILE:HD13	1:27:A:ILE:H	13	0.29
(1,1163)	1:27:A:ILE:HD11	1:27:A:ILE:H	15	0.29
(1,1163)	1:27:A:ILE:HD12	1:27:A:ILE:H	15	0.29
(1,1163)	1:27:A:ILE:HD13	1:27:A:ILE:H	15	0.29
(1,1117)	1:96:A:HIS:HA	1:102:A:GLN:H	3	0.29
(1,1092)	1:103:A:LEU:HD21	1:111:A:ALA:H	4	0.29
(1,1092)	1:103:A:LEU:HD22	1:111:A:ALA:H	4	0.29
(1,1092)	1:103:A:LEU:HD23	1:111:A:ALA:H	4	0.29
(1,1043)	1:8:A:ILE:HG21	1:32:A:THR:H	13	0.29
(1,1043)	1:8:A:ILE:HG22	1:32:A:THR:H	13	0.29
(1,1043)	1:8:A:ILE:HG23	1:32:A:THR:H	13	0.29
(1,1024)	1:118:A:VAL:HG21	1:116:A:ASN:HD21	7	0.29
(1,1024)	1:118:A:VAL:HG22	1:116:A:ASN:HD21	7	0.29
(1,1024)	1:118:A:VAL:HG23	1:116:A:ASN:HD21	7	0.29
(1,1022)	1:79:A:ILE:HG21	1:81:A:ASN:H	1	0.29
(1,1022)	1:79:A:ILE:HG22	1:81:A:ASN:H	1	0.29
(1,1022)	1:79:A:ILE:HG23	1:81:A:ASN:H	1	0.29
(1,1022)	1:79:A:ILE:HG21	1:81:A:ASN:H	14	0.29
(1,1022)	1:79:A:ILE:HG22	1:81:A:ASN:H	14	0.29
(1,1022)	1:79:A:ILE:HG23	1:81:A:ASN:H	14	0.29
(1,1019)	1:22:A:LEU:HD21	1:52:A:LEU:H	9	0.29
(1,1019)	1:22:A:LEU:HD22	1:52:A:LEU:H	9	0.29
(1,1019)	1:22:A:LEU:HD23	1:52:A:LEU:H	9	0.29
(1,1019)	1:22:A:LEU:HD21	1:52:A:LEU:H	14	0.29
(1,1019)	1:22:A:LEU:HD22	1:52:A:LEU:H	14	0.29
(1,1019)	1:22:A:LEU:HD23	1:52:A:LEU:H	14	0.29
(1,1019)	1:22:A:LEU:HD21	1:52:A:LEU:H	19	0.29
(1,1019)	1:22:A:LEU:HD22	1:52:A:LEU:H	19	0.29
(1,1019)	1:22:A:LEU:HD23	1:52:A:LEU:H	19	0.29
(1,980)	1:54:A:ILE:HD11	1:42:A:ASP:H	12	0.29
(1,980)	1:54:A:ILE:HD12	1:42:A:ASP:H	12	0.29
(1,980)	1:54:A:ILE:HD13	1:42:A:ASP:H	12	0.29
(1,971)	1:60:A:LEU:HD21	1:62:A:LYS:H	4	0.29
(1,971)	1:60:A:LEU:HD22	1:62:A:LYS:H	4	0.29
(1,971)	1:60:A:LEU:HD23	1:62:A:LYS:H	4	0.29
(1,925)	1:59:A:LEU:HD11	1:59:A:LEU:H	11	0.29
(1,925)	1:59:A:LEU:HD12	1:59:A:LEU:H	11	0.29
(1,925)	1:59:A:LEU:HD13	1:59:A:LEU:H	11	0.29
(1,760)	1:97:A:ILE:HB	1:96:A:HIS:H	9	0.29
(1,743)	1:34:A:LYS:HD2	1:34:A:LYS:H	9	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,587)	1:9:A:ASP:HB3	1:11:A:ASN:H	6	0.29
(1,579)	1:142:A:ASN:HB3	1:143:A:GLN:H	2	0.29
(1,3871)	1:11:A:ASN:H	1:9:A:ASP:HB3	12	0.28
(1,3871)	1:79:A:ILE:H	1:80:A:ASP:HB3	20	0.28
(1,3832)	1:116:A:ASN:H	1:140:A:VAL:HG21	6	0.28
(1,3832)	1:116:A:ASN:H	1:140:A:VAL:HG22	6	0.28
(1,3832)	1:116:A:ASN:H	1:140:A:VAL:HG23	6	0.28
(1,3797)	1:93:A:ILE:H	1:79:A:ILE:HB	5	0.28
(1,3797)	1:93:A:ILE:H	1:79:A:ILE:HB	6	0.28
(1,3797)	1:93:A:ILE:H	1:79:A:ILE:HB	10	0.28
(1,3797)	1:93:A:ILE:H	1:79:A:ILE:HB	11	0.28
(1,3712)	1:130:A:TYR:HE1	1:137:A:HIS:HB3	8	0.28
(1,3712)	1:130:A:TYR:HE2	1:137:A:HIS:HB3	8	0.28
(1,3581)	1:67:A:ASP:H	1:68:A:ILE:HD11	14	0.28
(1,3581)	1:67:A:ASP:H	1:68:A:ILE:HD12	14	0.28
(1,3581)	1:67:A:ASP:H	1:68:A:ILE:HD13	14	0.28
(1,3568)	1:86:A:ASP:HB2	1:88:A:ASN:HB2	4	0.28
(1,3371)	1:36:A:LEU:HA	1:36:A:LEU:HD11	8	0.28
(1,3371)	1:36:A:LEU:HA	1:36:A:LEU:HD12	8	0.28
(1,3371)	1:36:A:LEU:HA	1:36:A:LEU:HD13	8	0.28
(1,3371)	1:36:A:LEU:HA	1:36:A:LEU:HD11	17	0.28
(1,3371)	1:36:A:LEU:HA	1:36:A:LEU:HD12	17	0.28
(1,3371)	1:36:A:LEU:HA	1:36:A:LEU:HD13	17	0.28
(1,3336)	1:126:A:LEU:HD11	1:139:A:PRO:HB3	1	0.28
(1,3336)	1:126:A:LEU:HD12	1:139:A:PRO:HB3	1	0.28
(1,3336)	1:126:A:LEU:HD13	1:139:A:PRO:HB3	1	0.28
(1,3219)	1:93:A:ILE:HD11	1:119:A:ILE:HD11	1	0.28
(1,3219)	1:93:A:ILE:HD11	1:119:A:ILE:HD12	1	0.28
(1,3219)	1:93:A:ILE:HD11	1:119:A:ILE:HD13	1	0.28
(1,3219)	1:93:A:ILE:HD12	1:119:A:ILE:HD11	1	0.28
(1,3219)	1:93:A:ILE:HD12	1:119:A:ILE:HD12	1	0.28
(1,3219)	1:93:A:ILE:HD12	1:119:A:ILE:HD13	1	0.28
(1,3219)	1:93:A:ILE:HD13	1:119:A:ILE:HD11	1	0.28
(1,3219)	1:93:A:ILE:HD13	1:119:A:ILE:HD12	1	0.28
(1,3219)	1:93:A:ILE:HD13	1:119:A:ILE:HD13	1	0.28
(1,3164)	1:123:A:ASP:HB2	1:93:A:ILE:HD11	19	0.28
(1,3164)	1:123:A:ASP:HB2	1:93:A:ILE:HD12	19	0.28
(1,3164)	1:123:A:ASP:HB2	1:93:A:ILE:HD13	19	0.28
(1,3095)	1:57:A:MET:HE1	1:53:A:ALA:HA	6	0.28
(1,3095)	1:57:A:MET:HE2	1:53:A:ALA:HA	6	0.28
(1,3095)	1:57:A:MET:HE3	1:53:A:ALA:HA	6	0.28
(1,3074)	1:4:A:LYS:HB2	1:71:A:ASN:HA	8	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2966)	1:94:A:CYS:HB3	1:97:A:ILE:HG21	2	0.28
(1,2966)	1:94:A:CYS:HB3	1:97:A:ILE:HG22	2	0.28
(1,2966)	1:94:A:CYS:HB3	1:97:A:ILE:HG23	2	0.28
(1,2966)	1:88:A:ASN:HB3	1:91:A:ILE:HG21	20	0.28
(1,2966)	1:88:A:ASN:HB3	1:91:A:ILE:HG22	20	0.28
(1,2966)	1:88:A:ASN:HB3	1:91:A:ILE:HG23	20	0.28
(1,2844)	1:58:A:TYR:H	1:68:A:ILE:HG21	20	0.28
(1,2844)	1:58:A:TYR:H	1:68:A:ILE:HG22	20	0.28
(1,2844)	1:58:A:TYR:H	1:68:A:ILE:HG23	20	0.28
(1,2761)	1:74:A:TYR:HB2	1:75:A:THR:HG21	9	0.28
(1,2761)	1:74:A:TYR:HB2	1:75:A:THR:HG22	9	0.28
(1,2761)	1:74:A:TYR:HB2	1:75:A:THR:HG23	9	0.28
(1,2747)	1:72:A:ARG:HD2	1:3:A:VAL:HG11	16	0.28
(1,2747)	1:72:A:ARG:HD2	1:3:A:VAL:HG12	16	0.28
(1,2747)	1:72:A:ARG:HD2	1:3:A:VAL:HG13	16	0.28
(1,2550)	1:40:A:ASP:HB3	1:47:A:VAL:HG11	7	0.28
(1,2550)	1:40:A:ASP:HB3	1:47:A:VAL:HG12	7	0.28
(1,2550)	1:40:A:ASP:HB3	1:47:A:VAL:HG13	7	0.28
(1,2546)	1:56:A:GLN:HB2	1:60:A:LEU:HD21	7	0.28
(1,2546)	1:56:A:GLN:HB2	1:60:A:LEU:HD22	7	0.28
(1,2546)	1:56:A:GLN:HB2	1:60:A:LEU:HD23	7	0.28
(1,2546)	1:56:A:GLN:HB3	1:60:A:LEU:HD21	7	0.28
(1,2546)	1:56:A:GLN:HB3	1:60:A:LEU:HD22	7	0.28
(1,2546)	1:56:A:GLN:HB3	1:60:A:LEU:HD23	7	0.28
(1,2499)	1:135:A:ILE:HA	1:135:A:ILE:HG12	14	0.28
(1,2499)	1:135:A:ILE:HA	1:135:A:ILE:HG12	17	0.28
(1,2499)	1:135:A:ILE:HA	1:135:A:ILE:HG12	19	0.28
(1,2482)	1:96:A:HIS:H	1:103:A:LEU:HD11	9	0.28
(1,2482)	1:96:A:HIS:H	1:103:A:LEU:HD12	9	0.28
(1,2482)	1:96:A:HIS:H	1:103:A:LEU:HD13	9	0.28
(1,2373)	1:55:A:LEU:HA	1:59:A:LEU:HD21	13	0.28
(1,2373)	1:55:A:LEU:HA	1:59:A:LEU:HD22	13	0.28
(1,2373)	1:55:A:LEU:HA	1:59:A:LEU:HD23	13	0.28
(1,2180)	1:23:A:LYS:HD2	1:23:A:LYS:HB2	9	0.28
(1,2001)	1:82:A:ASN:HD22	1:82:A:ASN:HB3	4	0.28
(1,2001)	1:82:A:ASN:HD22	1:82:A:ASN:HB3	5	0.28
(1,2001)	1:82:A:ASN:HD22	1:82:A:ASN:HB3	8	0.28
(1,2001)	1:82:A:ASN:HD22	1:82:A:ASN:HB3	9	0.28
(1,2001)	1:82:A:ASN:HD22	1:82:A:ASN:HB3	10	0.28
(1,2001)	1:11:A:ASN:HD22	1:11:A:ASN:HB3	11	0.28
(1,2001)	1:82:A:ASN:HD22	1:82:A:ASN:HB3	15	0.28
(1,1949)	1:138:A:LEU:HG	1:135:A:ILE:HB	18	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1827)	1:20:A:ALA:HA	1:23:A:LYS:HE2	9	0.28
(1,1505)	1:72:A:ARG:HA	1:73:A:ILE:HD11	20	0.28
(1,1505)	1:72:A:ARG:HA	1:73:A:ILE:HD12	20	0.28
(1,1505)	1:72:A:ARG:HA	1:73:A:ILE:HD13	20	0.28
(1,1388)	1:103:A:LEU:HA	1:107:A:SER:HB3	15	0.28
(1,1328)	1:97:A:ILE:HG21	1:121:A:GLN:H	16	0.28
(1,1328)	1:97:A:ILE:HG22	1:121:A:GLN:H	16	0.28
(1,1328)	1:97:A:ILE:HG23	1:121:A:GLN:H	16	0.28
(1,1221)	1:57:A:MET:HB2	1:63:A:GLY:H	12	0.28
(1,1091)	1:103:A:LEU:HD21	1:104:A:SER:H	20	0.28
(1,1091)	1:103:A:LEU:HD22	1:104:A:SER:H	20	0.28
(1,1091)	1:103:A:LEU:HD23	1:104:A:SER:H	20	0.28
(1,1043)	1:21:A:ILE:HG21	1:32:A:THR:H	15	0.28
(1,1043)	1:21:A:ILE:HG22	1:32:A:THR:H	15	0.28
(1,1043)	1:21:A:ILE:HG23	1:32:A:THR:H	15	0.28
(1,1042)	1:50:A:ILE:HD11	1:49:A:SER:H	20	0.28
(1,1042)	1:50:A:ILE:HD12	1:49:A:SER:H	20	0.28
(1,1042)	1:50:A:ILE:HD13	1:49:A:SER:H	20	0.28
(1,1022)	1:79:A:ILE:HG21	1:81:A:ASN:H	15	0.28
(1,1022)	1:79:A:ILE:HG22	1:81:A:ASN:H	15	0.28
(1,1022)	1:79:A:ILE:HG23	1:81:A:ASN:H	15	0.28
(1,929)	1:3:A:VAL:HG21	1:34:A:LYS:H	5	0.28
(1,929)	1:3:A:VAL:HG22	1:34:A:LYS:H	5	0.28
(1,929)	1:3:A:VAL:HG23	1:34:A:LYS:H	5	0.28
(1,925)	1:59:A:LEU:HD11	1:59:A:LEU:H	6	0.28
(1,925)	1:59:A:LEU:HD12	1:59:A:LEU:H	6	0.28
(1,925)	1:59:A:LEU:HD13	1:59:A:LEU:H	6	0.28
(1,870)	1:52:A:LEU:HG	1:56:A:GLN:HE21	9	0.28
(1,866)	1:20:A:ALA:HB1	1:24:A:SER:H	15	0.28
(1,866)	1:20:A:ALA:HB2	1:24:A:SER:H	15	0.28
(1,866)	1:20:A:ALA:HB3	1:24:A:SER:H	15	0.28
(1,587)	1:9:A:ASP:HB3	1:11:A:ASN:H	12	0.28
(1,554)	1:34:A:LYS:HE2	1:4:A:LYS:H	3	0.28
(1,3937)	1:23:A:LYS:HD2	1:19:A:TYR:HD1	13	0.27
(1,3937)	1:23:A:LYS:HD2	1:19:A:TYR:HD2	13	0.27
(1,3871)	1:11:A:ASN:H	1:9:A:ASP:HB3	7	0.27
(1,3871)	1:11:A:ASN:H	1:9:A:ASP:HB3	13	0.27
(1,3840)	1:123:A:ASP:HB2	1:111:A:ALA:HB1	8	0.27
(1,3840)	1:123:A:ASP:HB2	1:111:A:ALA:HB2	8	0.27
(1,3840)	1:123:A:ASP:HB2	1:111:A:ALA:HB3	8	0.27
(1,3805)	1:125:A:ILE:HG12	1:128:A:GLU:HG2	7	0.27
(1,3805)	1:125:A:ILE:HG12	1:128:A:GLU:HG3	7	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3797)	1:93:A:ILE:H	1:79:A:ILE:HB	4	0.27
(1,3581)	1:56:A:GLN:H	1:68:A:ILE:HD11	2	0.27
(1,3581)	1:56:A:GLN:H	1:68:A:ILE:HD12	2	0.27
(1,3581)	1:56:A:GLN:H	1:68:A:ILE:HD13	2	0.27
(1,3581)	1:56:A:GLN:H	1:68:A:ILE:HD11	6	0.27
(1,3581)	1:56:A:GLN:H	1:68:A:ILE:HD12	6	0.27
(1,3581)	1:56:A:GLN:H	1:68:A:ILE:HD13	6	0.27
(1,3581)	1:56:A:GLN:H	1:68:A:ILE:HD11	15	0.27
(1,3581)	1:56:A:GLN:H	1:68:A:ILE:HD12	15	0.27
(1,3581)	1:56:A:GLN:H	1:68:A:ILE:HD13	15	0.27
(1,3581)	1:56:A:GLN:H	1:68:A:ILE:HD11	17	0.27
(1,3581)	1:56:A:GLN:H	1:68:A:ILE:HD12	17	0.27
(1,3581)	1:56:A:GLN:H	1:68:A:ILE:HD13	17	0.27
(1,3581)	1:56:A:GLN:H	1:68:A:ILE:HD11	18	0.27
(1,3581)	1:56:A:GLN:H	1:68:A:ILE:HD12	18	0.27
(1,3581)	1:56:A:GLN:H	1:68:A:ILE:HD13	18	0.27
(1,3371)	1:36:A:LEU:HA	1:36:A:LEU:HD11	4	0.27
(1,3371)	1:36:A:LEU:HA	1:36:A:LEU:HD12	4	0.27
(1,3371)	1:36:A:LEU:HA	1:36:A:LEU:HD13	4	0.27
(1,3371)	1:36:A:LEU:HA	1:36:A:LEU:HD11	5	0.27
(1,3371)	1:36:A:LEU:HA	1:36:A:LEU:HD12	5	0.27
(1,3371)	1:36:A:LEU:HA	1:36:A:LEU:HD13	5	0.27
(1,3371)	1:36:A:LEU:HA	1:36:A:LEU:HD11	13	0.27
(1,3371)	1:36:A:LEU:HA	1:36:A:LEU:HD12	13	0.27
(1,3371)	1:36:A:LEU:HA	1:36:A:LEU:HD13	13	0.27
(1,3371)	1:36:A:LEU:HA	1:36:A:LEU:HD11	19	0.27
(1,3371)	1:36:A:LEU:HA	1:36:A:LEU:HD12	19	0.27
(1,3371)	1:36:A:LEU:HA	1:36:A:LEU:HD13	19	0.27
(1,3095)	1:57:A:MET:HE1	1:53:A:ALA:HA	12	0.27
(1,3095)	1:57:A:MET:HE2	1:53:A:ALA:HA	12	0.27
(1,3095)	1:57:A:MET:HE3	1:53:A:ALA:HA	12	0.27
(1,3040)	1:18:A:ASP:HB2	1:14:A:ILE:HG21	20	0.27
(1,3040)	1:18:A:ASP:HB2	1:14:A:ILE:HG22	20	0.27
(1,3040)	1:18:A:ASP:HB2	1:14:A:ILE:HG23	20	0.27
(1,2970)	1:87:A:GLU:HG2	1:127:A:ILE:HG21	4	0.27
(1,2970)	1:87:A:GLU:HG2	1:127:A:ILE:HG22	4	0.27
(1,2970)	1:87:A:GLU:HG2	1:127:A:ILE:HG23	4	0.27
(1,2966)	1:94:A:CYS:HB3	1:97:A:ILE:HG21	3	0.27
(1,2966)	1:94:A:CYS:HB3	1:97:A:ILE:HG22	3	0.27
(1,2966)	1:94:A:CYS:HB3	1:97:A:ILE:HG23	3	0.27
(1,2954)	1:23:A:LYS:HE2	1:20:A:ALA:HB1	4	0.27
(1,2954)	1:23:A:LYS:HE2	1:20:A:ALA:HB2	4	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2954)	1:23:A:LYS:HE2	1:20:A:ALA:HB3	4	0.27
(1,2954)	1:9:A:ASP:HB3	1:20:A:ALA:HB1	12	0.27
(1,2954)	1:9:A:ASP:HB3	1:20:A:ALA:HB2	12	0.27
(1,2954)	1:9:A:ASP:HB3	1:20:A:ALA:HB3	12	0.27
(1,2874)	1:19:A:TYR:HD1	1:20:A:ALA:HB1	3	0.27
(1,2874)	1:19:A:TYR:HD1	1:20:A:ALA:HB2	3	0.27
(1,2874)	1:19:A:TYR:HD1	1:20:A:ALA:HB3	3	0.27
(1,2874)	1:19:A:TYR:HD2	1:20:A:ALA:HB1	3	0.27
(1,2874)	1:19:A:TYR:HD2	1:20:A:ALA:HB2	3	0.27
(1,2874)	1:19:A:TYR:HD2	1:20:A:ALA:HB3	3	0.27
(1,2830)	1:66:A:SER:H	1:54:A:ILE:HG21	14	0.27
(1,2830)	1:66:A:SER:H	1:54:A:ILE:HG22	14	0.27
(1,2830)	1:66:A:SER:H	1:54:A:ILE:HG23	14	0.27
(1,2752)	1:57:A:MET:HB3	1:65:A:THR:HG21	11	0.27
(1,2752)	1:57:A:MET:HB3	1:65:A:THR:HG22	11	0.27
(1,2752)	1:57:A:MET:HB3	1:65:A:THR:HG23	11	0.27
(1,2747)	1:72:A:ARG:HD2	1:3:A:VAL:HG11	20	0.27
(1,2747)	1:72:A:ARG:HD2	1:3:A:VAL:HG12	20	0.27
(1,2747)	1:72:A:ARG:HD2	1:3:A:VAL:HG13	20	0.27
(1,2603)	1:26:A:LEU:HD11	1:22:A:LEU:HD21	3	0.27
(1,2603)	1:26:A:LEU:HD11	1:22:A:LEU:HD22	3	0.27
(1,2603)	1:26:A:LEU:HD11	1:22:A:LEU:HD23	3	0.27
(1,2603)	1:26:A:LEU:HD12	1:22:A:LEU:HD21	3	0.27
(1,2603)	1:26:A:LEU:HD12	1:22:A:LEU:HD22	3	0.27
(1,2603)	1:26:A:LEU:HD12	1:22:A:LEU:HD23	3	0.27
(1,2603)	1:26:A:LEU:HD13	1:22:A:LEU:HD21	3	0.27
(1,2603)	1:26:A:LEU:HD13	1:22:A:LEU:HD22	3	0.27
(1,2603)	1:26:A:LEU:HD13	1:22:A:LEU:HD23	3	0.27
(1,2586)	1:39:A:ALA:HB1	1:36:A:LEU:HD11	15	0.27
(1,2586)	1:39:A:ALA:HB1	1:36:A:LEU:HD12	15	0.27
(1,2586)	1:39:A:ALA:HB1	1:36:A:LEU:HD13	15	0.27
(1,2586)	1:39:A:ALA:HB2	1:36:A:LEU:HD11	15	0.27
(1,2586)	1:39:A:ALA:HB2	1:36:A:LEU:HD12	15	0.27
(1,2586)	1:39:A:ALA:HB2	1:36:A:LEU:HD13	15	0.27
(1,2586)	1:39:A:ALA:HB3	1:36:A:LEU:HD11	15	0.27
(1,2586)	1:39:A:ALA:HB3	1:36:A:LEU:HD12	15	0.27
(1,2586)	1:39:A:ALA:HB3	1:36:A:LEU:HD13	15	0.27
(1,2449)	1:59:A:LEU:H	1:60:A:LEU:HD21	9	0.27
(1,2449)	1:59:A:LEU:H	1:60:A:LEU:HD22	9	0.27
(1,2449)	1:59:A:LEU:H	1:60:A:LEU:HD23	9	0.27
(1,2379)	1:102:A:GLN:HA	1:108:A:LEU:HG	5	0.27
(1,2379)	1:107:A:SER:HA	1:108:A:LEU:HG	12	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2350)	1:52:A:LEU:H	1:52:A:LEU:HD21	7	0.27
(1,2350)	1:52:A:LEU:H	1:52:A:LEU:HD22	7	0.27
(1,2350)	1:52:A:LEU:H	1:52:A:LEU:HD23	7	0.27
(1,2350)	1:52:A:LEU:H	1:52:A:LEU:HD21	18	0.27
(1,2350)	1:52:A:LEU:H	1:52:A:LEU:HD22	18	0.27
(1,2350)	1:52:A:LEU:H	1:52:A:LEU:HD23	18	0.27
(1,2182)	1:131:A:ILE:HD11	1:87:A:GLU:HG3	6	0.27
(1,2182)	1:131:A:ILE:HD12	1:87:A:GLU:HG3	6	0.27
(1,2182)	1:131:A:ILE:HD13	1:87:A:GLU:HG3	6	0.27
(1,2001)	1:82:A:ASN:HD22	1:82:A:ASN:HB3	14	0.27
(1,2001)	1:82:A:ASN:HD22	1:82:A:ASN:HB3	16	0.27
(1,2001)	1:82:A:ASN:HD22	1:82:A:ASN:HB3	20	0.27
(1,1949)	1:138:A:LEU:HG	1:135:A:ILE:HB	15	0.27
(1,1949)	1:138:A:LEU:HG	1:135:A:ILE:HB	17	0.27
(1,1806)	1:74:A:TYR:HE2	1:72:A:ARG:HD3	19	0.27
(1,1511)	1:3:A:VAL:HA	1:5:A:ILE:HD11	1	0.27
(1,1511)	1:3:A:VAL:HA	1:5:A:ILE:HD12	1	0.27
(1,1511)	1:3:A:VAL:HA	1:5:A:ILE:HD13	1	0.27
(1,1511)	1:3:A:VAL:HA	1:5:A:ILE:HD11	3	0.27
(1,1511)	1:3:A:VAL:HA	1:5:A:ILE:HD12	3	0.27
(1,1511)	1:3:A:VAL:HA	1:5:A:ILE:HD13	3	0.27
(1,1489)	1:70:A:LYS:H	1:5:A:ILE:HD11	3	0.27
(1,1489)	1:70:A:LYS:H	1:5:A:ILE:HD12	3	0.27
(1,1489)	1:70:A:LYS:H	1:5:A:ILE:HD13	3	0.27
(1,1489)	1:70:A:LYS:H	1:5:A:ILE:HD11	15	0.27
(1,1489)	1:70:A:LYS:H	1:5:A:ILE:HD12	15	0.27
(1,1489)	1:70:A:LYS:H	1:5:A:ILE:HD13	15	0.27
(1,1444)	1:41:A:VAL:HB	1:68:A:ILE:HD11	3	0.27
(1,1444)	1:41:A:VAL:HB	1:68:A:ILE:HD12	3	0.27
(1,1444)	1:41:A:VAL:HB	1:68:A:ILE:HD13	3	0.27
(1,1388)	1:103:A:LEU:HA	1:107:A:SER:HB3	4	0.27
(1,1357)	1:90:A:TYR:H	1:93:A:ILE:HD11	13	0.27
(1,1357)	1:90:A:TYR:H	1:93:A:ILE:HD12	13	0.27
(1,1357)	1:90:A:TYR:H	1:93:A:ILE:HD13	13	0.27
(1,1357)	1:90:A:TYR:H	1:93:A:ILE:HD11	17	0.27
(1,1357)	1:90:A:TYR:H	1:93:A:ILE:HD12	17	0.27
(1,1357)	1:90:A:TYR:H	1:93:A:ILE:HD13	17	0.27
(1,1326)	1:5:A:ILE:HD11	1:39:A:ALA:H	11	0.27
(1,1326)	1:5:A:ILE:HD12	1:39:A:ALA:H	11	0.27
(1,1326)	1:5:A:ILE:HD13	1:39:A:ALA:H	11	0.27
(1,1221)	1:62:A:LYS:HB3	1:63:A:GLY:H	3	0.27
(1,1197)	1:126:A:LEU:HD11	1:122:A:THR:H	1	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1197)	1:126:A:LEU:HD12	1:122:A:THR:H	1	0.27
(1,1197)	1:126:A:LEU:HD13	1:122:A:THR:H	1	0.27
(1,1163)	1:27:A:ILE:HD11	1:27:A:ILE:H	12	0.27
(1,1163)	1:27:A:ILE:HD12	1:27:A:ILE:H	12	0.27
(1,1163)	1:27:A:ILE:HD13	1:27:A:ILE:H	12	0.27
(1,1132)	1:131:A:ILE:HG12	1:130:A:TYR:H	3	0.27
(1,1132)	1:131:A:ILE:HG12	1:130:A:TYR:H	6	0.27
(1,1024)	1:118:A:VAL:HG21	1:116:A:ASN:HD21	17	0.27
(1,1024)	1:118:A:VAL:HG22	1:116:A:ASN:HD21	17	0.27
(1,1024)	1:118:A:VAL:HG23	1:116:A:ASN:HD21	17	0.27
(1,1019)	1:22:A:LEU:HD21	1:52:A:LEU:H	10	0.27
(1,1019)	1:22:A:LEU:HD22	1:52:A:LEU:H	10	0.27
(1,1019)	1:22:A:LEU:HD23	1:52:A:LEU:H	10	0.27
(1,1004)	1:59:A:LEU:HD21	1:16:A:SER:H	1	0.27
(1,1004)	1:59:A:LEU:HD22	1:16:A:SER:H	1	0.27
(1,1004)	1:59:A:LEU:HD23	1:16:A:SER:H	1	0.27
(1,971)	1:60:A:LEU:HD21	1:62:A:LYS:H	3	0.27
(1,971)	1:60:A:LEU:HD22	1:62:A:LYS:H	3	0.27
(1,971)	1:60:A:LEU:HD23	1:62:A:LYS:H	3	0.27
(1,962)	1:73:A:ILE:HD11	1:71:A:ASN:H	15	0.27
(1,962)	1:73:A:ILE:HD12	1:71:A:ASN:H	15	0.27
(1,962)	1:73:A:ILE:HD13	1:71:A:ASN:H	15	0.27
(1,933)	1:52:A:LEU:HD21	1:26:A:LEU:H	17	0.27
(1,933)	1:52:A:LEU:HD22	1:26:A:LEU:H	17	0.27
(1,933)	1:52:A:LEU:HD23	1:26:A:LEU:H	17	0.27
(1,925)	1:59:A:LEU:HD11	1:59:A:LEU:H	19	0.27
(1,925)	1:59:A:LEU:HD12	1:59:A:LEU:H	19	0.27
(1,925)	1:59:A:LEU:HD13	1:59:A:LEU:H	19	0.27
(1,870)	1:52:A:LEU:HG	1:56:A:GLN:HE21	7	0.27
(1,870)	1:52:A:LEU:HG	1:56:A:GLN:HE21	14	0.27
(1,870)	1:52:A:LEU:HG	1:56:A:GLN:HE21	18	0.27
(1,866)	1:27:A:ILE:HG13	1:24:A:SER:H	6	0.27
(1,866)	1:27:A:ILE:HG13	1:24:A:SER:H	20	0.27
(1,743)	1:34:A:LYS:HD2	1:34:A:LYS:H	2	0.27
(1,587)	1:9:A:ASP:HB3	1:11:A:ASN:H	7	0.27
(1,587)	1:9:A:ASP:HB3	1:11:A:ASN:H	13	0.27
(1,500)	1:8:A:ILE:HA	1:35:A:GLN:H	18	0.27
(1,228)	1:19:A:TYR:HD1	1:57:A:MET:H	6	0.27
(1,228)	1:19:A:TYR:HD2	1:57:A:MET:H	6	0.27
(1,97)	1:144:A:LEU:H	1:143:A:GLN:H	6	0.27
(1,81)	1:58:A:TYR:H	1:61:A:GLY:H	9	0.27
(1,81)	1:58:A:TYR:H	1:61:A:GLY:H	19	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3938)	1:14:A:ILE:HB	1:58:A:TYR:HD1	9	0.26
(1,3938)	1:14:A:ILE:HB	1:58:A:TYR:HD2	9	0.26
(1,3937)	1:23:A:LYS:HD2	1:19:A:TYR:HD1	20	0.26
(1,3937)	1:23:A:LYS:HD2	1:19:A:TYR:HD2	20	0.26
(1,3890)	1:71:A:ASN:H	1:2:A:SER:HB2	17	0.26
(1,3840)	1:123:A:ASP:HB2	1:111:A:ALA:HB1	12	0.26
(1,3840)	1:123:A:ASP:HB2	1:111:A:ALA:HB2	12	0.26
(1,3840)	1:123:A:ASP:HB2	1:111:A:ALA:HB3	12	0.26
(1,3623)	1:135:A:ILE:HG12	1:134:A:ARG:HA	8	0.26
(1,3623)	1:135:A:ILE:HG12	1:134:A:ARG:HA	11	0.26
(1,3581)	1:56:A:GLN:H	1:68:A:ILE:HD11	9	0.26
(1,3581)	1:56:A:GLN:H	1:68:A:ILE:HD12	9	0.26
(1,3581)	1:56:A:GLN:H	1:68:A:ILE:HD13	9	0.26
(1,3581)	1:56:A:GLN:H	1:68:A:ILE:HD11	11	0.26
(1,3581)	1:56:A:GLN:H	1:68:A:ILE:HD12	11	0.26
(1,3581)	1:56:A:GLN:H	1:68:A:ILE:HD13	11	0.26
(1,3371)	1:36:A:LEU:HA	1:36:A:LEU:HD11	6	0.26
(1,3371)	1:36:A:LEU:HA	1:36:A:LEU:HD12	6	0.26
(1,3371)	1:36:A:LEU:HA	1:36:A:LEU:HD13	6	0.26
(1,3371)	1:36:A:LEU:HA	1:36:A:LEU:HD11	9	0.26
(1,3371)	1:36:A:LEU:HA	1:36:A:LEU:HD12	9	0.26
(1,3371)	1:36:A:LEU:HA	1:36:A:LEU:HD13	9	0.26
(1,3336)	1:126:A:LEU:HD11	1:139:A:PRO:HB3	5	0.26
(1,3336)	1:126:A:LEU:HD12	1:139:A:PRO:HB3	5	0.26
(1,3336)	1:126:A:LEU:HD13	1:139:A:PRO:HB3	5	0.26
(1,3238)	1:74:A:TYR:HB3	1:2:A:SER:HA	9	0.26
(1,3219)	1:93:A:ILE:HD11	1:119:A:ILE:HD11	11	0.26
(1,3219)	1:93:A:ILE:HD11	1:119:A:ILE:HD12	11	0.26
(1,3219)	1:93:A:ILE:HD11	1:119:A:ILE:HD13	11	0.26
(1,3219)	1:93:A:ILE:HD12	1:119:A:ILE:HD11	11	0.26
(1,3219)	1:93:A:ILE:HD12	1:119:A:ILE:HD12	11	0.26
(1,3219)	1:93:A:ILE:HD12	1:119:A:ILE:HD13	11	0.26
(1,3219)	1:93:A:ILE:HD13	1:119:A:ILE:HD11	11	0.26
(1,3219)	1:93:A:ILE:HD13	1:119:A:ILE:HD12	11	0.26
(1,3219)	1:93:A:ILE:HD13	1:119:A:ILE:HD13	11	0.26
(1,3212)	1:53:A:ALA:HB1	1:49:A:SER:HB2	8	0.26
(1,3212)	1:53:A:ALA:HB1	1:49:A:SER:HB3	8	0.26
(1,3212)	1:53:A:ALA:HB2	1:49:A:SER:HB2	8	0.26
(1,3212)	1:53:A:ALA:HB2	1:49:A:SER:HB3	8	0.26
(1,3212)	1:53:A:ALA:HB3	1:49:A:SER:HB2	8	0.26
(1,3212)	1:53:A:ALA:HB3	1:49:A:SER:HB3	8	0.26
(1,3180)	1:127:A:ILE:HB	1:79:A:ILE:HD11	9	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3180)	1:127:A:ILE:HB	1:79:A:ILE:HD12	9	0.26
(1,3180)	1:127:A:ILE:HB	1:79:A:ILE:HD13	9	0.26
(1,3171)	1:103:A:LEU:HG	1:107:A:SER:HB3	16	0.26
(1,3095)	1:57:A:MET:HE1	1:53:A:ALA:HA	4	0.26
(1,3095)	1:57:A:MET:HE2	1:53:A:ALA:HA	4	0.26
(1,3095)	1:57:A:MET:HE3	1:53:A:ALA:HA	4	0.26
(1,3095)	1:57:A:MET:HE1	1:53:A:ALA:HA	20	0.26
(1,3095)	1:57:A:MET:HE2	1:53:A:ALA:HA	20	0.26
(1,3095)	1:57:A:MET:HE3	1:53:A:ALA:HA	20	0.26
(1,3049)	1:12:A:GLY:HA2	1:13:A:GLU:HG2	20	0.26
(1,3049)	1:12:A:GLY:HA2	1:13:A:GLU:HG3	20	0.26
(1,2970)	1:87:A:GLU:HG2	1:127:A:ILE:HG21	2	0.26
(1,2970)	1:87:A:GLU:HG2	1:127:A:ILE:HG22	2	0.26
(1,2970)	1:87:A:GLU:HG2	1:127:A:ILE:HG23	2	0.26
(1,2904)	1:3:A:VAL:HA	1:38:A:ALA:HB1	3	0.26
(1,2904)	1:3:A:VAL:HA	1:38:A:ALA:HB2	3	0.26
(1,2904)	1:3:A:VAL:HA	1:38:A:ALA:HB3	3	0.26
(1,2904)	1:3:A:VAL:HA	1:38:A:ALA:HB1	9	0.26
(1,2904)	1:3:A:VAL:HA	1:38:A:ALA:HB2	9	0.26
(1,2904)	1:3:A:VAL:HA	1:38:A:ALA:HB3	9	0.26
(1,2904)	1:3:A:VAL:HA	1:38:A:ALA:HB1	16	0.26
(1,2904)	1:3:A:VAL:HA	1:38:A:ALA:HB2	16	0.26
(1,2904)	1:3:A:VAL:HA	1:38:A:ALA:HB3	16	0.26
(1,2844)	1:58:A:TYR:H	1:68:A:ILE:HG21	11	0.26
(1,2844)	1:58:A:TYR:H	1:68:A:ILE:HG22	11	0.26
(1,2844)	1:58:A:TYR:H	1:68:A:ILE:HG23	11	0.26
(1,2765)	1:74:A:TYR:HB2	1:3:A:VAL:HG21	5	0.26
(1,2765)	1:74:A:TYR:HB2	1:3:A:VAL:HG22	5	0.26
(1,2765)	1:74:A:TYR:HB2	1:3:A:VAL:HG23	5	0.26
(1,2697)	1:134:A:ARG:HB2	1:132:A:THR:HG21	6	0.26
(1,2697)	1:134:A:ARG:HB2	1:132:A:THR:HG22	6	0.26
(1,2697)	1:134:A:ARG:HB2	1:132:A:THR:HG23	6	0.26
(1,2537)	1:52:A:LEU:HA	1:55:A:LEU:HD11	19	0.26
(1,2537)	1:52:A:LEU:HA	1:55:A:LEU:HD12	19	0.26
(1,2537)	1:52:A:LEU:HA	1:55:A:LEU:HD13	19	0.26
(1,2515)	1:93:A:ILE:HA	1:103:A:LEU:HD11	5	0.26
(1,2515)	1:93:A:ILE:HA	1:103:A:LEU:HD12	5	0.26
(1,2515)	1:93:A:ILE:HA	1:103:A:LEU:HD13	5	0.26
(1,2499)	1:135:A:ILE:HA	1:135:A:ILE:HG12	7	0.26
(1,2379)	1:107:A:SER:HA	1:108:A:LEU:HG	7	0.26
(1,2356)	1:62:A:LYS:HA	1:62:A:LYS:HD2	8	0.26
(1,2350)	1:52:A:LEU:H	1:52:A:LEU:HD21	13	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2350)	1:52:A:LEU:H	1:52:A:LEU:HD22	13	0.26
(1,2350)	1:52:A:LEU:H	1:52:A:LEU:HD23	13	0.26
(1,2344)	1:58:A:TYR:HD1	1:59:A:LEU:HD21	4	0.26
(1,2344)	1:58:A:TYR:HD1	1:59:A:LEU:HD22	4	0.26
(1,2344)	1:58:A:TYR:HD1	1:59:A:LEU:HD23	4	0.26
(1,2344)	1:58:A:TYR:HD2	1:59:A:LEU:HD21	4	0.26
(1,2344)	1:58:A:TYR:HD2	1:59:A:LEU:HD22	4	0.26
(1,2344)	1:58:A:TYR:HD2	1:59:A:LEU:HD23	4	0.26
(1,2344)	1:58:A:TYR:HD1	1:59:A:LEU:HD21	15	0.26
(1,2344)	1:58:A:TYR:HD1	1:59:A:LEU:HD22	15	0.26
(1,2344)	1:58:A:TYR:HD1	1:59:A:LEU:HD23	15	0.26
(1,2344)	1:58:A:TYR:HD2	1:59:A:LEU:HD21	15	0.26
(1,2344)	1:58:A:TYR:HD2	1:59:A:LEU:HD22	15	0.26
(1,2344)	1:58:A:TYR:HD2	1:59:A:LEU:HD23	15	0.26
(1,2306)	1:71:A:ASN:H	1:5:A:ILE:HG13	8	0.26
(1,2180)	1:23:A:LYS:HD2	1:23:A:LYS:HB2	7	0.26
(1,2170)	1:124:A:ARG:HB2	1:128:A:GLU:HG2	7	0.26
(1,2170)	1:124:A:ARG:HB2	1:128:A:GLU:HG3	7	0.26
(1,2170)	1:124:A:ARG:HB3	1:128:A:GLU:HG2	7	0.26
(1,2170)	1:124:A:ARG:HB3	1:128:A:GLU:HG3	7	0.26
(1,2001)	1:82:A:ASN:HD22	1:82:A:ASN:HB3	2	0.26
(1,2001)	1:82:A:ASN:HD22	1:82:A:ASN:HB3	6	0.26
(1,2001)	1:82:A:ASN:HD22	1:82:A:ASN:HB3	7	0.26
(1,2001)	1:11:A:ASN:HD22	1:11:A:ASN:HB3	19	0.26
(1,1806)	1:74:A:TYR:HE2	1:72:A:ARG:HD3	5	0.26
(1,1806)	1:74:A:TYR:HE1	1:72:A:ARG:HD3	7	0.26
(1,1511)	1:3:A:VAL:HA	1:5:A:ILE:HD11	15	0.26
(1,1511)	1:3:A:VAL:HA	1:5:A:ILE:HD12	15	0.26
(1,1511)	1:3:A:VAL:HA	1:5:A:ILE:HD13	15	0.26
(1,1357)	1:90:A:TYR:H	1:93:A:ILE:HD11	14	0.26
(1,1357)	1:90:A:TYR:H	1:93:A:ILE:HD12	14	0.26
(1,1357)	1:90:A:TYR:H	1:93:A:ILE:HD13	14	0.26
(1,1357)	1:90:A:TYR:H	1:93:A:ILE:HD11	20	0.26
(1,1357)	1:90:A:TYR:H	1:93:A:ILE:HD12	20	0.26
(1,1357)	1:90:A:TYR:H	1:93:A:ILE:HD13	20	0.26
(1,1326)	1:5:A:ILE:HD11	1:39:A:ALA:H	14	0.26
(1,1326)	1:5:A:ILE:HD12	1:39:A:ALA:H	14	0.26
(1,1326)	1:5:A:ILE:HD13	1:39:A:ALA:H	14	0.26
(1,1326)	1:5:A:ILE:HD11	1:39:A:ALA:H	19	0.26
(1,1326)	1:5:A:ILE:HD12	1:39:A:ALA:H	19	0.26
(1,1326)	1:5:A:ILE:HD13	1:39:A:ALA:H	19	0.26
(1,1221)	1:62:A:LYS:HB3	1:63:A:GLY:H	2	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1163)	1:27:A:ILE:HD11	1:27:A:ILE:H	8	0.26
(1,1163)	1:27:A:ILE:HD12	1:27:A:ILE:H	8	0.26
(1,1163)	1:27:A:ILE:HD13	1:27:A:ILE:H	8	0.26
(1,1163)	1:27:A:ILE:HD11	1:27:A:ILE:H	9	0.26
(1,1163)	1:27:A:ILE:HD12	1:27:A:ILE:H	9	0.26
(1,1163)	1:27:A:ILE:HD13	1:27:A:ILE:H	9	0.26
(1,1163)	1:27:A:ILE:HD11	1:27:A:ILE:H	17	0.26
(1,1163)	1:27:A:ILE:HD12	1:27:A:ILE:H	17	0.26
(1,1163)	1:27:A:ILE:HD13	1:27:A:ILE:H	17	0.26
(1,1149)	1:135:A:ILE:HG12	1:129:A:LYS:H	7	0.26
(1,1149)	1:135:A:ILE:HG12	1:129:A:LYS:H	10	0.26
(1,1137)	1:97:A:ILE:HG21	1:96:A:HIS:H	8	0.26
(1,1137)	1:97:A:ILE:HG22	1:96:A:HIS:H	8	0.26
(1,1137)	1:97:A:ILE:HG23	1:96:A:HIS:H	8	0.26
(1,1137)	1:97:A:ILE:HG21	1:96:A:HIS:H	10	0.26
(1,1137)	1:97:A:ILE:HG22	1:96:A:HIS:H	10	0.26
(1,1137)	1:97:A:ILE:HG23	1:96:A:HIS:H	10	0.26
(1,1137)	1:97:A:ILE:HG21	1:96:A:HIS:H	15	0.26
(1,1137)	1:97:A:ILE:HG22	1:96:A:HIS:H	15	0.26
(1,1137)	1:97:A:ILE:HG23	1:96:A:HIS:H	15	0.26
(1,1132)	1:131:A:ILE:HG12	1:130:A:TYR:H	4	0.26
(1,1117)	1:96:A:HIS:HA	1:102:A:GLN:H	7	0.26
(1,1092)	1:103:A:LEU:HD21	1:111:A:ALA:H	9	0.26
(1,1092)	1:103:A:LEU:HD22	1:111:A:ALA:H	9	0.26
(1,1092)	1:103:A:LEU:HD23	1:111:A:ALA:H	9	0.26
(1,1091)	1:103:A:LEU:HD21	1:104:A:SER:H	16	0.26
(1,1091)	1:103:A:LEU:HD22	1:104:A:SER:H	16	0.26
(1,1091)	1:103:A:LEU:HD23	1:104:A:SER:H	16	0.26
(1,1042)	1:50:A:ILE:HD11	1:49:A:SER:H	18	0.26
(1,1042)	1:50:A:ILE:HD12	1:49:A:SER:H	18	0.26
(1,1042)	1:50:A:ILE:HD13	1:49:A:SER:H	18	0.26
(1,1022)	1:79:A:ILE:HG21	1:81:A:ASN:H	3	0.26
(1,1022)	1:79:A:ILE:HG22	1:81:A:ASN:H	3	0.26
(1,1022)	1:79:A:ILE:HG23	1:81:A:ASN:H	3	0.26
(1,1019)	1:22:A:LEU:HD21	1:52:A:LEU:H	5	0.26
(1,1019)	1:22:A:LEU:HD22	1:52:A:LEU:H	5	0.26
(1,1019)	1:22:A:LEU:HD23	1:52:A:LEU:H	5	0.26
(1,1019)	1:22:A:LEU:HD21	1:52:A:LEU:H	8	0.26
(1,1019)	1:22:A:LEU:HD22	1:52:A:LEU:H	8	0.26
(1,1019)	1:22:A:LEU:HD23	1:52:A:LEU:H	8	0.26
(1,962)	1:5:A:ILE:HD11	1:71:A:ASN:H	18	0.26
(1,962)	1:5:A:ILE:HD12	1:71:A:ASN:H	18	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,962)	1:5:A:ILE:HD13	1:71:A:ASN:H	18	0.26
(1,933)	1:47:A:VAL:HG11	1:26:A:LEU:H	8	0.26
(1,933)	1:47:A:VAL:HG12	1:26:A:LEU:H	8	0.26
(1,933)	1:47:A:VAL:HG13	1:26:A:LEU:H	8	0.26
(1,871)	1:52:A:LEU:HG	1:56:A:GLN:HE22	15	0.26
(1,870)	1:52:A:LEU:HG	1:56:A:GLN:HE21	11	0.26
(1,743)	1:34:A:LYS:HD2	1:34:A:LYS:H	11	0.26
(1,694)	1:9:A:ASP:HB3	1:35:A:GLN:HE22	13	0.26
(1,587)	1:9:A:ASP:HB3	1:11:A:ASN:H	19	0.26
(1,572)	1:9:A:ASP:HB3	1:20:A:ALA:H	2	0.26
(1,554)	1:34:A:LYS:HE2	1:4:A:LYS:H	5	0.26
(1,500)	1:83:A:GLY:HA2	1:82:A:ASN:HD22	8	0.26
(1,386)	1:117:A:ASN:HA	1:119:A:ILE:H	1	0.26
(1,228)	1:19:A:TYR:HD1	1:57:A:MET:H	11	0.26
(1,228)	1:19:A:TYR:HD2	1:57:A:MET:H	11	0.26
(1,3951)	1:135:A:ILE:HD11	1:130:A:TYR:HD1	14	0.25
(1,3951)	1:135:A:ILE:HD11	1:130:A:TYR:HD2	14	0.25
(1,3951)	1:135:A:ILE:HD12	1:130:A:TYR:HD1	14	0.25
(1,3951)	1:135:A:ILE:HD12	1:130:A:TYR:HD2	14	0.25
(1,3951)	1:135:A:ILE:HD13	1:130:A:TYR:HD1	14	0.25
(1,3951)	1:135:A:ILE:HD13	1:130:A:TYR:HD2	14	0.25
(1,3937)	1:20:A:ALA:HB1	1:19:A:TYR:HD1	8	0.25
(1,3937)	1:20:A:ALA:HB1	1:19:A:TYR:HD2	8	0.25
(1,3937)	1:20:A:ALA:HB2	1:19:A:TYR:HD1	8	0.25
(1,3937)	1:20:A:ALA:HB2	1:19:A:TYR:HD2	8	0.25
(1,3937)	1:20:A:ALA:HB3	1:19:A:TYR:HD1	8	0.25
(1,3937)	1:20:A:ALA:HB3	1:19:A:TYR:HD2	8	0.25
(1,3871)	1:79:A:ILE:H	1:80:A:ASP:HB3	15	0.25
(1,3840)	1:123:A:ASP:HB2	1:111:A:ALA:HB1	6	0.25
(1,3840)	1:123:A:ASP:HB2	1:111:A:ALA:HB2	6	0.25
(1,3840)	1:123:A:ASP:HB2	1:111:A:ALA:HB3	6	0.25
(1,3791)	1:132:A:THR:H	1:134:A:ARG:HD2	3	0.25
(1,3791)	1:132:A:THR:H	1:134:A:ARG:HD3	3	0.25
(1,3581)	1:56:A:GLN:H	1:68:A:ILE:HD11	16	0.25
(1,3581)	1:56:A:GLN:H	1:68:A:ILE:HD12	16	0.25
(1,3581)	1:56:A:GLN:H	1:68:A:ILE:HD13	16	0.25
(1,3543)	1:17:A:ILE:HA	1:21:A:ILE:HD11	1	0.25
(1,3543)	1:17:A:ILE:HA	1:21:A:ILE:HD12	1	0.25
(1,3543)	1:17:A:ILE:HA	1:21:A:ILE:HD13	1	0.25
(1,3459)	1:74:A:TYR:HB3	1:73:A:ILE:HA	5	0.25
(1,3431)	1:4:A:LYS:HG3	1:71:A:ASN:HA	16	0.25
(1,3371)	1:36:A:LEU:HA	1:36:A:LEU:HD11	14	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3371)	1:36:A:LEU:HA	1:36:A:LEU:HD12	14	0.25
(1,3371)	1:36:A:LEU:HA	1:36:A:LEU:HD13	14	0.25
(1,3371)	1:36:A:LEU:HA	1:36:A:LEU:HD11	16	0.25
(1,3371)	1:36:A:LEU:HA	1:36:A:LEU:HD12	16	0.25
(1,3371)	1:36:A:LEU:HA	1:36:A:LEU:HD13	16	0.25
(1,3238)	1:74:A:TYR:HB3	1:2:A:SER:HA	6	0.25
(1,3219)	1:93:A:ILE:HD11	1:119:A:ILE:HD11	2	0.25
(1,3219)	1:93:A:ILE:HD11	1:119:A:ILE:HD12	2	0.25
(1,3219)	1:93:A:ILE:HD11	1:119:A:ILE:HD13	2	0.25
(1,3219)	1:93:A:ILE:HD12	1:119:A:ILE:HD11	2	0.25
(1,3219)	1:93:A:ILE:HD12	1:119:A:ILE:HD12	2	0.25
(1,3219)	1:93:A:ILE:HD12	1:119:A:ILE:HD13	2	0.25
(1,3219)	1:93:A:ILE:HD13	1:119:A:ILE:HD11	2	0.25
(1,3219)	1:93:A:ILE:HD13	1:119:A:ILE:HD12	2	0.25
(1,3219)	1:93:A:ILE:HD13	1:119:A:ILE:HD13	2	0.25
(1,2942)	1:86:A:ASP:HB2	1:131:A:ILE:HG21	19	0.25
(1,2942)	1:86:A:ASP:HB2	1:131:A:ILE:HG22	19	0.25
(1,2942)	1:86:A:ASP:HB2	1:131:A:ILE:HG23	19	0.25
(1,2874)	1:19:A:TYR:HD1	1:20:A:ALA:HB1	8	0.25
(1,2874)	1:19:A:TYR:HD1	1:20:A:ALA:HB2	8	0.25
(1,2874)	1:19:A:TYR:HD1	1:20:A:ALA:HB3	8	0.25
(1,2874)	1:19:A:TYR:HD2	1:20:A:ALA:HB1	8	0.25
(1,2874)	1:19:A:TYR:HD2	1:20:A:ALA:HB2	8	0.25
(1,2874)	1:19:A:TYR:HD2	1:20:A:ALA:HB3	8	0.25
(1,2844)	1:58:A:TYR:H	1:68:A:ILE:HG21	14	0.25
(1,2844)	1:58:A:TYR:H	1:68:A:ILE:HG22	14	0.25
(1,2844)	1:58:A:TYR:H	1:68:A:ILE:HG23	14	0.25
(1,2844)	1:58:A:TYR:H	1:68:A:ILE:HG21	16	0.25
(1,2844)	1:58:A:TYR:H	1:68:A:ILE:HG22	16	0.25
(1,2844)	1:58:A:TYR:H	1:68:A:ILE:HG23	16	0.25
(1,2832)	1:136:A:THR:H	1:135:A:ILE:HG21	14	0.25
(1,2832)	1:136:A:THR:H	1:135:A:ILE:HG22	14	0.25
(1,2832)	1:136:A:THR:H	1:135:A:ILE:HG23	14	0.25
(1,2761)	1:74:A:TYR:HB2	1:75:A:THR:HG21	12	0.25
(1,2761)	1:74:A:TYR:HB2	1:75:A:THR:HG22	12	0.25
(1,2761)	1:74:A:TYR:HB2	1:75:A:THR:HG23	12	0.25
(1,2738)	1:127:A:ILE:HA	1:85:A:VAL:HG21	1	0.25
(1,2738)	1:127:A:ILE:HA	1:85:A:VAL:HG22	1	0.25
(1,2738)	1:127:A:ILE:HA	1:85:A:VAL:HG23	1	0.25
(1,2713)	1:80:A:ASP:HA	1:79:A:ILE:HG21	13	0.25
(1,2713)	1:80:A:ASP:HA	1:79:A:ILE:HG22	13	0.25
(1,2713)	1:80:A:ASP:HA	1:79:A:ILE:HG23	13	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2697)	1:128:A:GLU:HG2	1:132:A:THR:HG21	19	0.25
(1,2697)	1:128:A:GLU:HG2	1:132:A:THR:HG22	19	0.25
(1,2697)	1:128:A:GLU:HG2	1:132:A:THR:HG23	19	0.25
(1,2697)	1:128:A:GLU:HG3	1:132:A:THR:HG21	19	0.25
(1,2697)	1:128:A:GLU:HG3	1:132:A:THR:HG22	19	0.25
(1,2697)	1:128:A:GLU:HG3	1:132:A:THR:HG23	19	0.25
(1,2697)	1:128:A:GLU:HG2	1:132:A:THR:HG21	20	0.25
(1,2697)	1:128:A:GLU:HG2	1:132:A:THR:HG22	20	0.25
(1,2697)	1:128:A:GLU:HG2	1:132:A:THR:HG23	20	0.25
(1,2697)	1:128:A:GLU:HG3	1:132:A:THR:HG21	20	0.25
(1,2697)	1:128:A:GLU:HG3	1:132:A:THR:HG22	20	0.25
(1,2697)	1:128:A:GLU:HG3	1:132:A:THR:HG23	20	0.25
(1,2583)	1:126:A:LEU:HB2	1:138:A:LEU:HD21	12	0.25
(1,2583)	1:126:A:LEU:HB2	1:138:A:LEU:HD22	12	0.25
(1,2583)	1:126:A:LEU:HB2	1:138:A:LEU:HD23	12	0.25
(1,2484)	1:56:A:GLN:HE22	1:60:A:LEU:HD21	3	0.25
(1,2484)	1:56:A:GLN:HE22	1:60:A:LEU:HD22	3	0.25
(1,2484)	1:56:A:GLN:HE22	1:60:A:LEU:HD23	3	0.25
(1,2379)	1:107:A:SER:HA	1:108:A:LEU:HG	3	0.25
(1,2379)	1:107:A:SER:HA	1:108:A:LEU:HG	6	0.25
(1,2379)	1:107:A:SER:HA	1:108:A:LEU:HG	8	0.25
(1,2379)	1:107:A:SER:HA	1:108:A:LEU:HG	15	0.25
(1,2306)	1:71:A:ASN:H	1:5:A:ILE:HG13	19	0.25
(1,2180)	1:23:A:LYS:HD2	1:23:A:LYS:HB2	4	0.25
(1,2180)	1:23:A:LYS:HD2	1:23:A:LYS:HB2	15	0.25
(1,2145)	1:37:A:ALA:HA	1:3:A:VAL:HB	8	0.25
(1,1792)	1:132:A:THR:H	1:134:A:ARG:HD2	3	0.25
(1,1792)	1:132:A:THR:H	1:134:A:ARG:HD3	3	0.25
(1,1511)	1:3:A:VAL:HA	1:5:A:ILE:HD11	7	0.25
(1,1511)	1:3:A:VAL:HA	1:5:A:ILE:HD12	7	0.25
(1,1511)	1:3:A:VAL:HA	1:5:A:ILE:HD13	7	0.25
(1,1511)	1:3:A:VAL:HA	1:5:A:ILE:HD11	12	0.25
(1,1511)	1:3:A:VAL:HA	1:5:A:ILE:HD12	12	0.25
(1,1511)	1:3:A:VAL:HA	1:5:A:ILE:HD13	12	0.25
(1,1388)	1:103:A:LEU:HA	1:107:A:SER:HB3	6	0.25
(1,1379)	1:130:A:TYR:HD1	1:135:A:ILE:HD11	14	0.25
(1,1379)	1:130:A:TYR:HD1	1:135:A:ILE:HD12	14	0.25
(1,1379)	1:130:A:TYR:HD1	1:135:A:ILE:HD13	14	0.25
(1,1379)	1:130:A:TYR:HD2	1:135:A:ILE:HD11	14	0.25
(1,1379)	1:130:A:TYR:HD2	1:135:A:ILE:HD12	14	0.25
(1,1379)	1:130:A:TYR:HD2	1:135:A:ILE:HD13	14	0.25
(1,1326)	1:5:A:ILE:HD11	1:39:A:ALA:H	17	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1326)	1:5:A:ILE:HD12	1:39:A:ALA:H	17	0.25
(1,1326)	1:5:A:ILE:HD13	1:39:A:ALA:H	17	0.25
(1,1220)	1:131:A:ILE:HG21	1:133:A:GLY:H	16	0.25
(1,1220)	1:131:A:ILE:HG22	1:133:A:GLY:H	16	0.25
(1,1220)	1:131:A:ILE:HG23	1:133:A:GLY:H	16	0.25
(1,1195)	1:60:A:LEU:HD21	1:57:A:MET:H	12	0.25
(1,1195)	1:60:A:LEU:HD22	1:57:A:MET:H	12	0.25
(1,1195)	1:60:A:LEU:HD23	1:57:A:MET:H	12	0.25
(1,1137)	1:97:A:ILE:HG21	1:96:A:HIS:H	11	0.25
(1,1137)	1:97:A:ILE:HG22	1:96:A:HIS:H	11	0.25
(1,1137)	1:97:A:ILE:HG23	1:96:A:HIS:H	11	0.25
(1,1132)	1:131:A:ILE:HG12	1:130:A:TYR:H	18	0.25
(1,1042)	1:50:A:ILE:HD11	1:49:A:SER:H	7	0.25
(1,1042)	1:50:A:ILE:HD12	1:49:A:SER:H	7	0.25
(1,1042)	1:50:A:ILE:HD13	1:49:A:SER:H	7	0.25
(1,1024)	1:118:A:VAL:HG21	1:116:A:ASN:HD21	3	0.25
(1,1024)	1:118:A:VAL:HG22	1:116:A:ASN:HD21	3	0.25
(1,1024)	1:118:A:VAL:HG23	1:116:A:ASN:HD21	3	0.25
(1,1024)	1:118:A:VAL:HG21	1:116:A:ASN:HD21	11	0.25
(1,1024)	1:118:A:VAL:HG22	1:116:A:ASN:HD21	11	0.25
(1,1024)	1:118:A:VAL:HG23	1:116:A:ASN:HD21	11	0.25
(1,1022)	1:79:A:ILE:HG21	1:81:A:ASN:H	17	0.25
(1,1022)	1:79:A:ILE:HG22	1:81:A:ASN:H	17	0.25
(1,1022)	1:79:A:ILE:HG23	1:81:A:ASN:H	17	0.25
(1,1019)	1:22:A:LEU:HD21	1:52:A:LEU:H	18	0.25
(1,1019)	1:22:A:LEU:HD22	1:52:A:LEU:H	18	0.25
(1,1019)	1:22:A:LEU:HD23	1:52:A:LEU:H	18	0.25
(1,981)	1:84:A:ILE:HD11	1:82:A:ASN:H	2	0.25
(1,981)	1:84:A:ILE:HD12	1:82:A:ASN:H	2	0.25
(1,981)	1:84:A:ILE:HD13	1:82:A:ASN:H	2	0.25
(1,971)	1:60:A:LEU:HD21	1:62:A:LYS:H	2	0.25
(1,971)	1:60:A:LEU:HD22	1:62:A:LYS:H	2	0.25
(1,971)	1:60:A:LEU:HD23	1:62:A:LYS:H	2	0.25
(1,823)	1:70:A:LYS:HG2	1:69:A:GLY:H	8	0.25
(1,823)	1:70:A:LYS:HG3	1:69:A:GLY:H	8	0.25
(1,97)	1:144:A:LEU:H	1:143:A:GLN:H	12	0.25
(1,81)	1:58:A:TYR:H	1:61:A:GLY:H	7	0.25
(1,81)	1:58:A:TYR:H	1:61:A:GLY:H	14	0.25
(1,81)	1:58:A:TYR:H	1:61:A:GLY:H	17	0.25
(1,3871)	1:11:A:ASN:H	1:7:A:ASP:HB3	8	0.24
(1,3712)	1:130:A:TYR:HE1	1:137:A:HIS:HB3	20	0.24
(1,3712)	1:130:A:TYR:HE2	1:137:A:HIS:HB3	20	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3459)	1:74:A:TYR:HB3	1:73:A:ILE:HA	16	0.24
(1,3371)	1:36:A:LEU:HA	1:36:A:LEU:HD11	3	0.24
(1,3371)	1:36:A:LEU:HA	1:36:A:LEU:HD12	3	0.24
(1,3371)	1:36:A:LEU:HA	1:36:A:LEU:HD13	3	0.24
(1,3371)	1:36:A:LEU:HA	1:36:A:LEU:HD11	15	0.24
(1,3371)	1:36:A:LEU:HA	1:36:A:LEU:HD12	15	0.24
(1,3371)	1:36:A:LEU:HA	1:36:A:LEU:HD13	15	0.24
(1,3371)	1:36:A:LEU:HA	1:36:A:LEU:HD11	20	0.24
(1,3371)	1:36:A:LEU:HA	1:36:A:LEU:HD12	20	0.24
(1,3371)	1:36:A:LEU:HA	1:36:A:LEU:HD13	20	0.24
(1,3238)	1:74:A:TYR:HB3	1:2:A:SER:HA	16	0.24
(1,3219)	1:93:A:ILE:HD11	1:119:A:ILE:HD11	5	0.24
(1,3219)	1:93:A:ILE:HD11	1:119:A:ILE:HD12	5	0.24
(1,3219)	1:93:A:ILE:HD11	1:119:A:ILE:HD13	5	0.24
(1,3219)	1:93:A:ILE:HD12	1:119:A:ILE:HD11	5	0.24
(1,3219)	1:93:A:ILE:HD12	1:119:A:ILE:HD12	5	0.24
(1,3219)	1:93:A:ILE:HD12	1:119:A:ILE:HD13	5	0.24
(1,3219)	1:93:A:ILE:HD13	1:119:A:ILE:HD11	5	0.24
(1,3219)	1:93:A:ILE:HD13	1:119:A:ILE:HD12	5	0.24
(1,3219)	1:93:A:ILE:HD13	1:119:A:ILE:HD13	5	0.24
(1,3219)	1:93:A:ILE:HD11	1:119:A:ILE:HD11	7	0.24
(1,3219)	1:93:A:ILE:HD11	1:119:A:ILE:HD12	7	0.24
(1,3219)	1:93:A:ILE:HD11	1:119:A:ILE:HD13	7	0.24
(1,3219)	1:93:A:ILE:HD12	1:119:A:ILE:HD11	7	0.24
(1,3219)	1:93:A:ILE:HD12	1:119:A:ILE:HD12	7	0.24
(1,3219)	1:93:A:ILE:HD12	1:119:A:ILE:HD13	7	0.24
(1,3219)	1:93:A:ILE:HD13	1:119:A:ILE:HD11	7	0.24
(1,3219)	1:93:A:ILE:HD13	1:119:A:ILE:HD12	7	0.24
(1,3219)	1:93:A:ILE:HD13	1:119:A:ILE:HD13	7	0.24
(1,3219)	1:93:A:ILE:HD11	1:119:A:ILE:HD11	8	0.24
(1,3219)	1:93:A:ILE:HD11	1:119:A:ILE:HD12	8	0.24
(1,3219)	1:93:A:ILE:HD11	1:119:A:ILE:HD13	8	0.24
(1,3219)	1:93:A:ILE:HD12	1:119:A:ILE:HD11	8	0.24
(1,3219)	1:93:A:ILE:HD12	1:119:A:ILE:HD12	8	0.24
(1,3219)	1:93:A:ILE:HD12	1:119:A:ILE:HD13	8	0.24
(1,3219)	1:93:A:ILE:HD13	1:119:A:ILE:HD11	8	0.24
(1,3219)	1:93:A:ILE:HD13	1:119:A:ILE:HD12	8	0.24
(1,3219)	1:93:A:ILE:HD13	1:119:A:ILE:HD13	8	0.24
(1,3219)	1:93:A:ILE:HD11	1:119:A:ILE:HD11	16	0.24
(1,3219)	1:93:A:ILE:HD11	1:119:A:ILE:HD12	16	0.24
(1,3219)	1:93:A:ILE:HD11	1:119:A:ILE:HD13	16	0.24
(1,3219)	1:93:A:ILE:HD12	1:119:A:ILE:HD11	16	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3219)	1:93:A:ILE:HD12	1:119:A:ILE:HD12	16	0.24
(1,3219)	1:93:A:ILE:HD12	1:119:A:ILE:HD13	16	0.24
(1,3219)	1:93:A:ILE:HD13	1:119:A:ILE:HD11	16	0.24
(1,3219)	1:93:A:ILE:HD13	1:119:A:ILE:HD12	16	0.24
(1,3219)	1:93:A:ILE:HD13	1:119:A:ILE:HD13	16	0.24
(1,3183)	1:90:A:TYR:HB2	1:79:A:ILE:HD11	3	0.24
(1,3183)	1:90:A:TYR:HB2	1:79:A:ILE:HD12	3	0.24
(1,3183)	1:90:A:TYR:HB2	1:79:A:ILE:HD13	3	0.24
(1,3177)	1:129:A:LYS:HE2	1:135:A:ILE:HD11	20	0.24
(1,3177)	1:129:A:LYS:HE2	1:135:A:ILE:HD12	20	0.24
(1,3177)	1:129:A:LYS:HE2	1:135:A:ILE:HD13	20	0.24
(1,3177)	1:129:A:LYS:HE3	1:135:A:ILE:HD11	20	0.24
(1,3177)	1:129:A:LYS:HE3	1:135:A:ILE:HD12	20	0.24
(1,3177)	1:129:A:LYS:HE3	1:135:A:ILE:HD13	20	0.24
(1,3049)	1:12:A:GLY:HA2	1:13:A:GLU:HG2	17	0.24
(1,3049)	1:12:A:GLY:HA2	1:13:A:GLU:HG3	17	0.24
(1,3019)	1:63:A:GLY:HA2	1:65:A:THR:HB	13	0.24
(1,2962)	1:42:A:ASP:HB3	1:50:A:ILE:HG21	5	0.24
(1,2962)	1:42:A:ASP:HB3	1:50:A:ILE:HG22	5	0.24
(1,2962)	1:42:A:ASP:HB3	1:50:A:ILE:HG23	5	0.24
(1,2962)	1:42:A:ASP:HB3	1:50:A:ILE:HG21	17	0.24
(1,2962)	1:42:A:ASP:HB3	1:50:A:ILE:HG22	17	0.24
(1,2962)	1:42:A:ASP:HB3	1:50:A:ILE:HG23	17	0.24
(1,2904)	1:3:A:VAL:HA	1:38:A:ALA:HB1	14	0.24
(1,2904)	1:3:A:VAL:HA	1:38:A:ALA:HB2	14	0.24
(1,2904)	1:3:A:VAL:HA	1:38:A:ALA:HB3	14	0.24
(1,2761)	1:74:A:TYR:HB2	1:75:A:THR:HG21	4	0.24
(1,2761)	1:74:A:TYR:HB2	1:75:A:THR:HG22	4	0.24
(1,2761)	1:74:A:TYR:HB2	1:75:A:THR:HG23	4	0.24
(1,2619)	1:64:A:GLY:H	1:65:A:THR:HG21	15	0.24
(1,2619)	1:64:A:GLY:H	1:65:A:THR:HG22	15	0.24
(1,2619)	1:64:A:GLY:H	1:65:A:THR:HG23	15	0.24
(1,2583)	1:92:A:LEU:HG	1:103:A:LEU:HD11	11	0.24
(1,2583)	1:92:A:LEU:HG	1:103:A:LEU:HD12	11	0.24
(1,2583)	1:92:A:LEU:HG	1:103:A:LEU:HD13	11	0.24
(1,2515)	1:93:A:ILE:HA	1:103:A:LEU:HD11	20	0.24
(1,2515)	1:93:A:ILE:HA	1:103:A:LEU:HD12	20	0.24
(1,2515)	1:93:A:ILE:HA	1:103:A:LEU:HD13	20	0.24
(1,2180)	1:20:A:ALA:HB1	1:23:A:LYS:HB2	11	0.24
(1,2180)	1:20:A:ALA:HB2	1:23:A:LYS:HB2	11	0.24
(1,2180)	1:20:A:ALA:HB3	1:23:A:LYS:HB2	11	0.24
(1,2145)	1:37:A:ALA:HA	1:3:A:VAL:HB	10	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2001)	1:82:A:ASN:HD22	1:82:A:ASN:HB3	13	0.24
(1,1949)	1:138:A:LEU:HG	1:135:A:ILE:HB	8	0.24
(1,1859)	1:27:A:ILE:HD11	1:23:A:LYS:HE2	2	0.24
(1,1859)	1:27:A:ILE:HD12	1:23:A:LYS:HE2	2	0.24
(1,1859)	1:27:A:ILE:HD13	1:23:A:LYS:HE2	2	0.24
(1,1841)	1:62:A:LYS:HB3	1:62:A:LYS:HE3	3	0.24
(1,1822)	1:70:A:LYS:HA	1:70:A:LYS:HE2	1	0.24
(1,1822)	1:70:A:LYS:HA	1:70:A:LYS:HE3	1	0.24
(1,1806)	1:81:A:ASN:HD22	1:72:A:ARG:HD3	2	0.24
(1,1511)	1:3:A:VAL:HA	1:5:A:ILE:HD11	2	0.24
(1,1511)	1:3:A:VAL:HA	1:5:A:ILE:HD12	2	0.24
(1,1511)	1:3:A:VAL:HA	1:5:A:ILE:HD13	2	0.24
(1,1444)	1:41:A:VAL:HB	1:68:A:ILE:HD11	15	0.24
(1,1444)	1:41:A:VAL:HB	1:68:A:ILE:HD12	15	0.24
(1,1444)	1:41:A:VAL:HB	1:68:A:ILE:HD13	15	0.24
(1,1388)	1:103:A:LEU:HA	1:107:A:SER:HB3	9	0.24
(1,1328)	1:97:A:ILE:HG21	1:121:A:GLN:H	6	0.24
(1,1328)	1:97:A:ILE:HG22	1:121:A:GLN:H	6	0.24
(1,1328)	1:97:A:ILE:HG23	1:121:A:GLN:H	6	0.24
(1,1221)	1:62:A:LYS:HB3	1:63:A:GLY:H	16	0.24
(1,1195)	1:60:A:LEU:HD21	1:57:A:MET:H	16	0.24
(1,1195)	1:60:A:LEU:HD22	1:57:A:MET:H	16	0.24
(1,1195)	1:60:A:LEU:HD23	1:57:A:MET:H	16	0.24
(1,1195)	1:60:A:LEU:HD21	1:57:A:MET:H	18	0.24
(1,1195)	1:60:A:LEU:HD22	1:57:A:MET:H	18	0.24
(1,1195)	1:60:A:LEU:HD23	1:57:A:MET:H	18	0.24
(1,1163)	1:27:A:ILE:HD11	1:27:A:ILE:H	7	0.24
(1,1163)	1:27:A:ILE:HD12	1:27:A:ILE:H	7	0.24
(1,1163)	1:27:A:ILE:HD13	1:27:A:ILE:H	7	0.24
(1,1163)	1:27:A:ILE:HD11	1:27:A:ILE:H	10	0.24
(1,1163)	1:27:A:ILE:HD12	1:27:A:ILE:H	10	0.24
(1,1163)	1:27:A:ILE:HD13	1:27:A:ILE:H	10	0.24
(1,1163)	1:27:A:ILE:HD11	1:27:A:ILE:H	16	0.24
(1,1163)	1:27:A:ILE:HD12	1:27:A:ILE:H	16	0.24
(1,1163)	1:27:A:ILE:HD13	1:27:A:ILE:H	16	0.24
(1,1137)	1:97:A:ILE:HG21	1:96:A:HIS:H	1	0.24
(1,1137)	1:97:A:ILE:HG22	1:96:A:HIS:H	1	0.24
(1,1137)	1:97:A:ILE:HG23	1:96:A:HIS:H	1	0.24
(1,1137)	1:97:A:ILE:HG21	1:96:A:HIS:H	14	0.24
(1,1137)	1:97:A:ILE:HG22	1:96:A:HIS:H	14	0.24
(1,1137)	1:97:A:ILE:HG23	1:96:A:HIS:H	14	0.24
(1,1042)	1:50:A:ILE:HD11	1:49:A:SER:H	8	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1042)	1:50:A:ILE:HD12	1:49:A:SER:H	8	0.24
(1,1042)	1:50:A:ILE:HD13	1:49:A:SER:H	8	0.24
(1,1042)	1:50:A:ILE:HD11	1:49:A:SER:H	14	0.24
(1,1042)	1:50:A:ILE:HD12	1:49:A:SER:H	14	0.24
(1,1042)	1:50:A:ILE:HD13	1:49:A:SER:H	14	0.24
(1,1022)	1:79:A:ILE:HG21	1:81:A:ASN:H	2	0.24
(1,1022)	1:79:A:ILE:HG22	1:81:A:ASN:H	2	0.24
(1,1022)	1:79:A:ILE:HG23	1:81:A:ASN:H	2	0.24
(1,1022)	1:79:A:ILE:HG21	1:81:A:ASN:H	12	0.24
(1,1022)	1:79:A:ILE:HG22	1:81:A:ASN:H	12	0.24
(1,1022)	1:79:A:ILE:HG23	1:81:A:ASN:H	12	0.24
(1,1019)	1:22:A:LEU:HD21	1:52:A:LEU:H	3	0.24
(1,1019)	1:22:A:LEU:HD22	1:52:A:LEU:H	3	0.24
(1,1019)	1:22:A:LEU:HD23	1:52:A:LEU:H	3	0.24
(1,981)	1:84:A:ILE:HD11	1:82:A:ASN:H	5	0.24
(1,981)	1:84:A:ILE:HD12	1:82:A:ASN:H	5	0.24
(1,981)	1:84:A:ILE:HD13	1:82:A:ASN:H	5	0.24
(1,981)	1:84:A:ILE:HD11	1:82:A:ASN:H	8	0.24
(1,981)	1:84:A:ILE:HD12	1:82:A:ASN:H	8	0.24
(1,981)	1:84:A:ILE:HD13	1:82:A:ASN:H	8	0.24
(1,909)	1:73:A:ILE:HD11	1:73:A:ILE:H	9	0.24
(1,909)	1:73:A:ILE:HD12	1:73:A:ILE:H	9	0.24
(1,909)	1:73:A:ILE:HD13	1:73:A:ILE:H	9	0.24
(1,871)	1:52:A:LEU:HG	1:56:A:GLN:HE22	4	0.24
(1,871)	1:52:A:LEU:HG	1:56:A:GLN:HE22	9	0.24
(1,772)	1:20:A:ALA:HB1	1:23:A:LYS:H	17	0.24
(1,772)	1:20:A:ALA:HB2	1:23:A:LYS:H	17	0.24
(1,772)	1:20:A:ALA:HB3	1:23:A:LYS:H	17	0.24
(1,587)	1:7:A:ASP:HB3	1:11:A:ASN:H	8	0.24
(1,572)	1:9:A:ASP:HB3	1:20:A:ALA:H	20	0.24
(1,3943)	1:22:A:LEU:HD21	1:19:A:TYR:HD1	4	0.23
(1,3943)	1:22:A:LEU:HD21	1:19:A:TYR:HD2	4	0.23
(1,3943)	1:22:A:LEU:HD22	1:19:A:TYR:HD1	4	0.23
(1,3943)	1:22:A:LEU:HD22	1:19:A:TYR:HD2	4	0.23
(1,3943)	1:22:A:LEU:HD23	1:19:A:TYR:HD1	4	0.23
(1,3943)	1:22:A:LEU:HD23	1:19:A:TYR:HD2	4	0.23
(1,3871)	1:11:A:ASN:H	1:9:A:ASP:HB3	2	0.23
(1,3871)	1:79:A:ILE:H	1:80:A:ASP:HB3	4	0.23
(1,3843)	1:126:A:LEU:HA	1:113:A:ALA:HB1	1	0.23
(1,3843)	1:126:A:LEU:HA	1:113:A:ALA:HB2	1	0.23
(1,3843)	1:126:A:LEU:HA	1:113:A:ALA:HB3	1	0.23
(1,3724)	1:71:A:ASN:HB3	1:5:A:ILE:HG13	13	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3712)	1:130:A:TYR:HE1	1:137:A:HIS:HB3	11	0.23
(1,3712)	1:130:A:TYR:HE2	1:137:A:HIS:HB3	11	0.23
(1,3712)	1:130:A:TYR:HE1	1:137:A:HIS:HB3	18	0.23
(1,3712)	1:130:A:TYR:HE2	1:137:A:HIS:HB3	18	0.23
(1,3635)	1:76:A:TYR:HB2	1:113:A:ALA:HA	16	0.23
(1,3543)	1:17:A:ILE:HA	1:21:A:ILE:HD11	4	0.23
(1,3543)	1:17:A:ILE:HA	1:21:A:ILE:HD12	4	0.23
(1,3543)	1:17:A:ILE:HA	1:21:A:ILE:HD13	4	0.23
(1,3238)	1:74:A:TYR:HB3	1:2:A:SER:HA	20	0.23
(1,3219)	1:93:A:ILE:HD11	1:119:A:ILE:HD11	13	0.23
(1,3219)	1:93:A:ILE:HD11	1:119:A:ILE:HD12	13	0.23
(1,3219)	1:93:A:ILE:HD11	1:119:A:ILE:HD13	13	0.23
(1,3219)	1:93:A:ILE:HD12	1:119:A:ILE:HD11	13	0.23
(1,3219)	1:93:A:ILE:HD12	1:119:A:ILE:HD12	13	0.23
(1,3219)	1:93:A:ILE:HD12	1:119:A:ILE:HD13	13	0.23
(1,3219)	1:93:A:ILE:HD13	1:119:A:ILE:HD11	13	0.23
(1,3219)	1:93:A:ILE:HD13	1:119:A:ILE:HD12	13	0.23
(1,3219)	1:93:A:ILE:HD13	1:119:A:ILE:HD13	13	0.23
(1,3212)	1:53:A:ALA:HB1	1:49:A:SER:HB2	16	0.23
(1,3212)	1:53:A:ALA:HB1	1:49:A:SER:HB3	16	0.23
(1,3212)	1:53:A:ALA:HB2	1:49:A:SER:HB2	16	0.23
(1,3212)	1:53:A:ALA:HB2	1:49:A:SER:HB3	16	0.23
(1,3212)	1:53:A:ALA:HB3	1:49:A:SER:HB2	16	0.23
(1,3212)	1:53:A:ALA:HB3	1:49:A:SER:HB3	16	0.23
(1,3183)	1:90:A:TYR:HB2	1:79:A:ILE:HD11	1	0.23
(1,3183)	1:90:A:TYR:HB2	1:79:A:ILE:HD12	1	0.23
(1,3183)	1:90:A:TYR:HB2	1:79:A:ILE:HD13	1	0.23
(1,3164)	1:123:A:ASP:HB2	1:93:A:ILE:HD11	7	0.23
(1,3164)	1:123:A:ASP:HB2	1:93:A:ILE:HD12	7	0.23
(1,3164)	1:123:A:ASP:HB2	1:93:A:ILE:HD13	7	0.23
(1,3095)	1:57:A:MET:HE1	1:53:A:ALA:HA	2	0.23
(1,3095)	1:57:A:MET:HE2	1:53:A:ALA:HA	2	0.23
(1,3095)	1:57:A:MET:HE3	1:53:A:ALA:HA	2	0.23
(1,3095)	1:57:A:MET:HE1	1:53:A:ALA:HA	13	0.23
(1,3095)	1:57:A:MET:HE2	1:53:A:ALA:HA	13	0.23
(1,3095)	1:57:A:MET:HE3	1:53:A:ALA:HA	13	0.23
(1,3074)	1:4:A:LYS:HB2	1:71:A:ASN:HA	13	0.23
(1,2942)	1:86:A:ASP:HB2	1:131:A:ILE:HG21	3	0.23
(1,2942)	1:86:A:ASP:HB2	1:131:A:ILE:HG22	3	0.23
(1,2942)	1:86:A:ASP:HB2	1:131:A:ILE:HG23	3	0.23
(1,2904)	1:3:A:VAL:HA	1:38:A:ALA:HB1	1	0.23
(1,2904)	1:3:A:VAL:HA	1:38:A:ALA:HB2	1	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2904)	1:3:A:VAL:HA	1:38:A:ALA:HB3	1	0.23
(1,2844)	1:58:A:TYR:H	1:68:A:ILE:HG21	4	0.23
(1,2844)	1:58:A:TYR:H	1:68:A:ILE:HG22	4	0.23
(1,2844)	1:58:A:TYR:H	1:68:A:ILE:HG23	4	0.23
(1,2761)	1:74:A:TYR:HB2	1:75:A:THR:HG21	14	0.23
(1,2761)	1:74:A:TYR:HB2	1:75:A:THR:HG22	14	0.23
(1,2761)	1:74:A:TYR:HB2	1:75:A:THR:HG23	14	0.23
(1,2560)	1:62:A:LYS:HE3	1:62:A:LYS:HG2	8	0.23
(1,2546)	1:56:A:GLN:HB2	1:60:A:LEU:HD21	15	0.23
(1,2546)	1:56:A:GLN:HB2	1:60:A:LEU:HD22	15	0.23
(1,2546)	1:56:A:GLN:HB2	1:60:A:LEU:HD23	15	0.23
(1,2546)	1:56:A:GLN:HB3	1:60:A:LEU:HD21	15	0.23
(1,2546)	1:56:A:GLN:HB3	1:60:A:LEU:HD22	15	0.23
(1,2546)	1:56:A:GLN:HB3	1:60:A:LEU:HD23	15	0.23
(1,2515)	1:93:A:ILE:HA	1:103:A:LEU:HD11	3	0.23
(1,2515)	1:93:A:ILE:HA	1:103:A:LEU:HD12	3	0.23
(1,2515)	1:93:A:ILE:HA	1:103:A:LEU:HD13	3	0.23
(1,2456)	1:23:A:LYS:H	1:52:A:LEU:HD11	16	0.23
(1,2456)	1:23:A:LYS:H	1:52:A:LEU:HD12	16	0.23
(1,2456)	1:23:A:LYS:H	1:52:A:LEU:HD13	16	0.23
(1,2350)	1:52:A:LEU:H	1:52:A:LEU:HD21	20	0.23
(1,2350)	1:52:A:LEU:H	1:52:A:LEU:HD22	20	0.23
(1,2350)	1:52:A:LEU:H	1:52:A:LEU:HD23	20	0.23
(1,2344)	1:19:A:TYR:H	1:59:A:LEU:HD21	13	0.23
(1,2344)	1:19:A:TYR:H	1:59:A:LEU:HD22	13	0.23
(1,2344)	1:19:A:TYR:H	1:59:A:LEU:HD23	13	0.23
(1,2300)	1:49:A:SER:H	1:50:A:ILE:HG13	10	0.23
(1,2277)	1:93:A:ILE:HB	1:127:A:ILE:HG12	4	0.23
(1,2277)	1:93:A:ILE:HB	1:127:A:ILE:HG13	4	0.23
(1,2248)	1:70:A:LYS:HA	1:70:A:LYS:HD3	12	0.23
(1,2215)	1:9:A:ASP:H	1:8:A:ILE:HG12	14	0.23
(1,2215)	1:9:A:ASP:H	1:8:A:ILE:HG13	14	0.23
(1,2001)	1:82:A:ASN:HD22	1:82:A:ASN:HB3	12	0.23
(1,1949)	1:136:A:THR:HG21	1:135:A:ILE:HB	14	0.23
(1,1949)	1:136:A:THR:HG22	1:135:A:ILE:HB	14	0.23
(1,1949)	1:136:A:THR:HG23	1:135:A:ILE:HB	14	0.23
(1,1859)	1:27:A:ILE:HD11	1:23:A:LYS:HE2	17	0.23
(1,1859)	1:27:A:ILE:HD12	1:23:A:LYS:HE2	17	0.23
(1,1859)	1:27:A:ILE:HD13	1:23:A:LYS:HE2	17	0.23
(1,1841)	1:62:A:LYS:HB3	1:62:A:LYS:HE3	10	0.23
(1,1813)	1:35:A:GLN:HE21	1:34:A:LYS:HE2	3	0.23
(1,1813)	1:19:A:TYR:HD1	1:23:A:LYS:HE2	11	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1813)	1:19:A:TYR:HD2	1:23:A:LYS:HE2	11	0.23
(1,1768)	1:57:A:MET:HB2	1:64:A:GLY:HA2	16	0.23
(1,1768)	1:57:A:MET:HB2	1:64:A:GLY:HA3	16	0.23
(1,1534)	1:17:A:ILE:HB	1:17:A:ILE:HA	10	0.23
(1,1511)	1:3:A:VAL:HA	1:5:A:ILE:HD11	6	0.23
(1,1511)	1:3:A:VAL:HA	1:5:A:ILE:HD12	6	0.23
(1,1511)	1:3:A:VAL:HA	1:5:A:ILE:HD13	6	0.23
(1,1511)	1:3:A:VAL:HA	1:5:A:ILE:HD11	18	0.23
(1,1511)	1:3:A:VAL:HA	1:5:A:ILE:HD12	18	0.23
(1,1511)	1:3:A:VAL:HA	1:5:A:ILE:HD13	18	0.23
(1,1511)	1:3:A:VAL:HA	1:5:A:ILE:HD11	19	0.23
(1,1511)	1:3:A:VAL:HA	1:5:A:ILE:HD12	19	0.23
(1,1511)	1:3:A:VAL:HA	1:5:A:ILE:HD13	19	0.23
(1,1388)	1:103:A:LEU:HA	1:107:A:SER:HB3	12	0.23
(1,1388)	1:103:A:LEU:HA	1:107:A:SER:HB3	14	0.23
(1,1328)	1:97:A:ILE:HG21	1:121:A:GLN:H	13	0.23
(1,1328)	1:97:A:ILE:HG22	1:121:A:GLN:H	13	0.23
(1,1328)	1:97:A:ILE:HG23	1:121:A:GLN:H	13	0.23
(1,1326)	1:5:A:ILE:HD11	1:39:A:ALA:H	8	0.23
(1,1326)	1:5:A:ILE:HD12	1:39:A:ALA:H	8	0.23
(1,1326)	1:5:A:ILE:HD13	1:39:A:ALA:H	8	0.23
(1,1221)	1:62:A:LYS:HB3	1:63:A:GLY:H	5	0.23
(1,1220)	1:131:A:ILE:HG21	1:133:A:GLY:H	2	0.23
(1,1220)	1:131:A:ILE:HG22	1:133:A:GLY:H	2	0.23
(1,1220)	1:131:A:ILE:HG23	1:133:A:GLY:H	2	0.23
(1,1163)	1:27:A:ILE:HD11	1:27:A:ILE:H	4	0.23
(1,1163)	1:27:A:ILE:HD12	1:27:A:ILE:H	4	0.23
(1,1163)	1:27:A:ILE:HD13	1:27:A:ILE:H	4	0.23
(1,1117)	1:96:A:HIS:HA	1:102:A:GLN:H	5	0.23
(1,1042)	1:50:A:ILE:HD11	1:49:A:SER:H	4	0.23
(1,1042)	1:50:A:ILE:HD12	1:49:A:SER:H	4	0.23
(1,1042)	1:50:A:ILE:HD13	1:49:A:SER:H	4	0.23
(1,1022)	1:79:A:ILE:HG21	1:81:A:ASN:H	8	0.23
(1,1022)	1:79:A:ILE:HG22	1:81:A:ASN:H	8	0.23
(1,1022)	1:79:A:ILE:HG23	1:81:A:ASN:H	8	0.23
(1,1019)	1:22:A:LEU:HD21	1:52:A:LEU:H	11	0.23
(1,1019)	1:22:A:LEU:HD22	1:52:A:LEU:H	11	0.23
(1,1019)	1:22:A:LEU:HD23	1:52:A:LEU:H	11	0.23
(1,981)	1:84:A:ILE:HD11	1:82:A:ASN:H	6	0.23
(1,981)	1:84:A:ILE:HD12	1:82:A:ASN:H	6	0.23
(1,981)	1:84:A:ILE:HD13	1:82:A:ASN:H	6	0.23
(1,981)	1:84:A:ILE:HD11	1:82:A:ASN:H	14	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,981)	1:84:A:ILE:HD12	1:82:A:ASN:H	14	0.23
(1,981)	1:84:A:ILE:HD13	1:82:A:ASN:H	14	0.23
(1,980)	1:54:A:ILE:HD11	1:42:A:ASP:H	1	0.23
(1,980)	1:54:A:ILE:HD12	1:42:A:ASP:H	1	0.23
(1,980)	1:54:A:ILE:HD13	1:42:A:ASP:H	1	0.23
(1,971)	1:60:A:LEU:HD21	1:62:A:LYS:H	5	0.23
(1,971)	1:60:A:LEU:HD22	1:62:A:LYS:H	5	0.23
(1,971)	1:60:A:LEU:HD23	1:62:A:LYS:H	5	0.23
(1,971)	1:60:A:LEU:HD21	1:62:A:LYS:H	7	0.23
(1,971)	1:60:A:LEU:HD22	1:62:A:LYS:H	7	0.23
(1,971)	1:60:A:LEU:HD23	1:62:A:LYS:H	7	0.23
(1,933)	1:52:A:LEU:HD21	1:26:A:LEU:H	19	0.23
(1,933)	1:52:A:LEU:HD22	1:26:A:LEU:H	19	0.23
(1,933)	1:52:A:LEU:HD23	1:26:A:LEU:H	19	0.23
(1,931)	1:8:A:ILE:HG21	1:22:A:LEU:H	15	0.23
(1,931)	1:8:A:ILE:HG22	1:22:A:LEU:H	15	0.23
(1,931)	1:8:A:ILE:HG23	1:22:A:LEU:H	15	0.23
(1,909)	1:73:A:ILE:HD11	1:73:A:ILE:H	1	0.23
(1,909)	1:73:A:ILE:HD12	1:73:A:ILE:H	1	0.23
(1,909)	1:73:A:ILE:HD13	1:73:A:ILE:H	1	0.23
(1,870)	1:52:A:LEU:HG	1:56:A:GLN:HE21	3	0.23
(1,870)	1:52:A:LEU:HG	1:56:A:GLN:HE21	13	0.23
(1,823)	1:70:A:LYS:HG2	1:69:A:GLY:H	4	0.23
(1,823)	1:70:A:LYS:HG3	1:69:A:GLY:H	4	0.23
(1,823)	1:70:A:LYS:HG2	1:69:A:GLY:H	10	0.23
(1,823)	1:70:A:LYS:HG3	1:69:A:GLY:H	10	0.23
(1,806)	1:53:A:ALA:HB1	1:57:A:MET:H	4	0.23
(1,806)	1:53:A:ALA:HB2	1:57:A:MET:H	4	0.23
(1,806)	1:53:A:ALA:HB3	1:57:A:MET:H	4	0.23
(1,760)	1:97:A:ILE:HB	1:96:A:HIS:H	10	0.23
(1,746)	1:144:A:LEU:HG	1:144:A:LEU:H	14	0.23
(1,587)	1:9:A:ASP:HB3	1:11:A:ASN:H	2	0.23
(1,582)	1:57:A:MET:HB3	1:58:A:TYR:H	6	0.23
(1,228)	1:19:A:TYR:HD1	1:57:A:MET:H	19	0.23
(1,228)	1:19:A:TYR:HD2	1:57:A:MET:H	19	0.23
(1,3937)	1:20:A:ALA:HB1	1:19:A:TYR:HD1	5	0.22
(1,3937)	1:20:A:ALA:HB1	1:19:A:TYR:HD2	5	0.22
(1,3937)	1:20:A:ALA:HB2	1:19:A:TYR:HD1	5	0.22
(1,3937)	1:20:A:ALA:HB2	1:19:A:TYR:HD2	5	0.22
(1,3937)	1:20:A:ALA:HB3	1:19:A:TYR:HD1	5	0.22
(1,3937)	1:20:A:ALA:HB3	1:19:A:TYR:HD2	5	0.22
(1,3843)	1:126:A:LEU:HA	1:113:A:ALA:HB1	13	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3843)	1:126:A:LEU:HA	1:113:A:ALA:HB2	13	0.22
(1,3843)	1:126:A:LEU:HA	1:113:A:ALA:HB3	13	0.22
(1,3840)	1:123:A:ASP:HB2	1:111:A:ALA:HB1	10	0.22
(1,3840)	1:123:A:ASP:HB2	1:111:A:ALA:HB2	10	0.22
(1,3840)	1:123:A:ASP:HB2	1:111:A:ALA:HB3	10	0.22
(1,3581)	1:67:A:ASP:H	1:68:A:ILE:HD11	13	0.22
(1,3581)	1:67:A:ASP:H	1:68:A:ILE:HD12	13	0.22
(1,3581)	1:67:A:ASP:H	1:68:A:ILE:HD13	13	0.22
(1,3543)	1:17:A:ILE:HA	1:21:A:ILE:HD11	3	0.22
(1,3543)	1:17:A:ILE:HA	1:21:A:ILE:HD12	3	0.22
(1,3543)	1:17:A:ILE:HA	1:21:A:ILE:HD13	3	0.22
(1,3543)	1:17:A:ILE:HA	1:21:A:ILE:HD11	8	0.22
(1,3543)	1:17:A:ILE:HA	1:21:A:ILE:HD12	8	0.22
(1,3543)	1:17:A:ILE:HA	1:21:A:ILE:HD13	8	0.22
(1,3459)	1:74:A:TYR:HB3	1:73:A:ILE:HA	1	0.22
(1,3459)	1:74:A:TYR:HB3	1:73:A:ILE:HA	2	0.22
(1,3459)	1:74:A:TYR:HB3	1:73:A:ILE:HA	6	0.22
(1,3459)	1:74:A:TYR:HB3	1:73:A:ILE:HA	11	0.22
(1,3459)	1:74:A:TYR:HB3	1:73:A:ILE:HA	13	0.22
(1,3459)	1:74:A:TYR:HB3	1:73:A:ILE:HA	19	0.22
(1,3371)	1:36:A:LEU:HA	1:36:A:LEU:HD11	1	0.22
(1,3371)	1:36:A:LEU:HA	1:36:A:LEU:HD12	1	0.22
(1,3371)	1:36:A:LEU:HA	1:36:A:LEU:HD13	1	0.22
(1,3095)	1:57:A:MET:HE1	1:53:A:ALA:HA	9	0.22
(1,3095)	1:57:A:MET:HE2	1:53:A:ALA:HA	9	0.22
(1,3095)	1:57:A:MET:HE3	1:53:A:ALA:HA	9	0.22
(1,3095)	1:57:A:MET:HE1	1:53:A:ALA:HA	18	0.22
(1,3095)	1:57:A:MET:HE2	1:53:A:ALA:HA	18	0.22
(1,3095)	1:57:A:MET:HE3	1:53:A:ALA:HA	18	0.22
(1,3049)	1:12:A:GLY:HA2	1:13:A:GLU:HG2	4	0.22
(1,3049)	1:12:A:GLY:HA2	1:13:A:GLU:HG3	4	0.22
(1,3049)	1:12:A:GLY:HA2	1:13:A:GLU:HG2	8	0.22
(1,3049)	1:12:A:GLY:HA2	1:13:A:GLU:HG3	8	0.22
(1,3040)	1:18:A:ASP:HB2	1:14:A:ILE:HG21	4	0.22
(1,3040)	1:18:A:ASP:HB2	1:14:A:ILE:HG22	4	0.22
(1,3040)	1:18:A:ASP:HB2	1:14:A:ILE:HG23	4	0.22
(1,2999)	1:50:A:ILE:HG12	1:53:A:ALA:HB1	16	0.22
(1,2999)	1:50:A:ILE:HG12	1:53:A:ALA:HB2	16	0.22
(1,2999)	1:50:A:ILE:HG12	1:53:A:ALA:HB3	16	0.22
(1,2954)	1:23:A:LYS:HE2	1:20:A:ALA:HB1	13	0.22
(1,2954)	1:23:A:LYS:HE2	1:20:A:ALA:HB2	13	0.22
(1,2954)	1:23:A:LYS:HE2	1:20:A:ALA:HB3	13	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2942)	1:86:A:ASP:HB2	1:131:A:ILE:HG21	8	0.22
(1,2942)	1:86:A:ASP:HB2	1:131:A:ILE:HG22	8	0.22
(1,2942)	1:86:A:ASP:HB2	1:131:A:ILE:HG23	8	0.22
(1,2904)	1:3:A:VAL:HA	1:38:A:ALA:HB1	5	0.22
(1,2904)	1:3:A:VAL:HA	1:38:A:ALA:HB2	5	0.22
(1,2904)	1:3:A:VAL:HA	1:38:A:ALA:HB3	5	0.22
(1,2874)	1:19:A:TYR:HD1	1:20:A:ALA:HB1	5	0.22
(1,2874)	1:19:A:TYR:HD1	1:20:A:ALA:HB2	5	0.22
(1,2874)	1:19:A:TYR:HD1	1:20:A:ALA:HB3	5	0.22
(1,2874)	1:19:A:TYR:HD2	1:20:A:ALA:HB1	5	0.22
(1,2874)	1:19:A:TYR:HD2	1:20:A:ALA:HB2	5	0.22
(1,2874)	1:19:A:TYR:HD2	1:20:A:ALA:HB3	5	0.22
(1,2830)	1:66:A:SER:H	1:54:A:ILE:HG21	13	0.22
(1,2830)	1:66:A:SER:H	1:54:A:ILE:HG22	13	0.22
(1,2830)	1:66:A:SER:H	1:54:A:ILE:HG23	13	0.22
(1,2761)	1:74:A:TYR:HB2	1:75:A:THR:HG21	15	0.22
(1,2761)	1:74:A:TYR:HB2	1:75:A:THR:HG22	15	0.22
(1,2761)	1:74:A:TYR:HB2	1:75:A:THR:HG23	15	0.22
(1,2652)	1:80:A:ASP:H	1:79:A:ILE:HG21	13	0.22
(1,2652)	1:80:A:ASP:H	1:79:A:ILE:HG22	13	0.22
(1,2652)	1:80:A:ASP:H	1:79:A:ILE:HG23	13	0.22
(1,2641)	1:115:A:GLY:H	1:113:A:ALA:HB1	11	0.22
(1,2641)	1:115:A:GLY:H	1:113:A:ALA:HB2	11	0.22
(1,2641)	1:115:A:GLY:H	1:113:A:ALA:HB3	11	0.22
(1,2537)	1:52:A:LEU:HA	1:55:A:LEU:HD11	4	0.22
(1,2537)	1:52:A:LEU:HA	1:55:A:LEU:HD12	4	0.22
(1,2537)	1:52:A:LEU:HA	1:55:A:LEU:HD13	4	0.22
(1,2537)	1:52:A:LEU:HA	1:55:A:LEU:HD11	6	0.22
(1,2537)	1:52:A:LEU:HA	1:55:A:LEU:HD12	6	0.22
(1,2537)	1:52:A:LEU:HA	1:55:A:LEU:HD13	6	0.22
(1,2515)	1:92:A:LEU:HA	1:103:A:LEU:HD11	6	0.22
(1,2515)	1:92:A:LEU:HA	1:103:A:LEU:HD12	6	0.22
(1,2515)	1:92:A:LEU:HA	1:103:A:LEU:HD13	6	0.22
(1,2472)	1:144:A:LEU:H	1:144:A:LEU:HD21	19	0.22
(1,2472)	1:144:A:LEU:H	1:144:A:LEU:HD22	19	0.22
(1,2472)	1:144:A:LEU:H	1:144:A:LEU:HD23	19	0.22
(1,2466)	1:24:A:SER:H	1:23:A:LYS:HG2	12	0.22
(1,2455)	1:143:A:GLN:H	1:144:A:LEU:HD21	20	0.22
(1,2455)	1:143:A:GLN:H	1:144:A:LEU:HD22	20	0.22
(1,2455)	1:143:A:GLN:H	1:144:A:LEU:HD23	20	0.22
(1,2373)	1:55:A:LEU:HA	1:59:A:LEU:HD21	14	0.22
(1,2373)	1:55:A:LEU:HA	1:59:A:LEU:HD22	14	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2373)	1:55:A:LEU:HA	1:59:A:LEU:HD23	14	0.22
(1,2287)	1:119:A:ILE:HG21	1:93:A:ILE:HG13	13	0.22
(1,2287)	1:119:A:ILE:HG22	1:93:A:ILE:HG13	13	0.22
(1,2287)	1:119:A:ILE:HG23	1:93:A:ILE:HG13	13	0.22
(1,2180)	1:23:A:LYS:HD2	1:23:A:LYS:HB2	2	0.22
(1,2180)	1:23:A:LYS:HD2	1:23:A:LYS:HB2	5	0.22
(1,2180)	1:23:A:LYS:HD2	1:23:A:LYS:HB2	12	0.22
(1,2180)	1:23:A:LYS:HD2	1:23:A:LYS:HB2	19	0.22
(1,1949)	1:138:A:LEU:HG	1:135:A:ILE:HB	16	0.22
(1,1841)	1:62:A:LYS:HB3	1:62:A:LYS:HE3	18	0.22
(1,1813)	1:35:A:GLN:HE21	1:34:A:LYS:HE2	5	0.22
(1,1813)	1:19:A:TYR:HD1	1:23:A:LYS:HE2	7	0.22
(1,1813)	1:19:A:TYR:HD2	1:23:A:LYS:HE2	7	0.22
(1,1534)	1:20:A:ALA:HB1	1:17:A:ILE:HA	18	0.22
(1,1534)	1:20:A:ALA:HB2	1:17:A:ILE:HA	18	0.22
(1,1534)	1:20:A:ALA:HB3	1:17:A:ILE:HA	18	0.22
(1,1505)	1:72:A:ARG:HA	1:73:A:ILE:HD11	11	0.22
(1,1505)	1:72:A:ARG:HA	1:73:A:ILE:HD12	11	0.22
(1,1505)	1:72:A:ARG:HA	1:73:A:ILE:HD13	11	0.22
(1,1326)	1:5:A:ILE:HD11	1:39:A:ALA:H	4	0.22
(1,1326)	1:5:A:ILE:HD12	1:39:A:ALA:H	4	0.22
(1,1326)	1:5:A:ILE:HD13	1:39:A:ALA:H	4	0.22
(1,1220)	1:131:A:ILE:HG21	1:133:A:GLY:H	7	0.22
(1,1220)	1:131:A:ILE:HG22	1:133:A:GLY:H	7	0.22
(1,1220)	1:131:A:ILE:HG23	1:133:A:GLY:H	7	0.22
(1,1197)	1:126:A:LEU:HD11	1:122:A:THR:H	11	0.22
(1,1197)	1:126:A:LEU:HD12	1:122:A:THR:H	11	0.22
(1,1197)	1:126:A:LEU:HD13	1:122:A:THR:H	11	0.22
(1,1162)	1:79:A:ILE:HG21	1:111:A:ALA:H	5	0.22
(1,1162)	1:79:A:ILE:HG22	1:111:A:ALA:H	5	0.22
(1,1162)	1:79:A:ILE:HG23	1:111:A:ALA:H	5	0.22
(1,1150)	1:134:A:ARG:HG2	1:129:A:LYS:H	7	0.22
(1,1150)	1:134:A:ARG:HG3	1:129:A:LYS:H	7	0.22
(1,1149)	1:135:A:ILE:HG12	1:129:A:LYS:H	14	0.22
(1,1141)	1:144:A:LEU:HG	1:143:A:GLN:H	3	0.22
(1,1140)	1:144:A:LEU:HD21	1:143:A:GLN:H	20	0.22
(1,1140)	1:144:A:LEU:HD22	1:143:A:GLN:H	20	0.22
(1,1140)	1:144:A:LEU:HD23	1:143:A:GLN:H	20	0.22
(1,1137)	1:97:A:ILE:HG21	1:96:A:HIS:H	5	0.22
(1,1137)	1:97:A:ILE:HG22	1:96:A:HIS:H	5	0.22
(1,1137)	1:97:A:ILE:HG23	1:96:A:HIS:H	5	0.22
(1,1022)	1:79:A:ILE:HG21	1:81:A:ASN:H	5	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1022)	1:79:A:ILE:HG22	1:81:A:ASN:H	5	0.22
(1,1022)	1:79:A:ILE:HG23	1:81:A:ASN:H	5	0.22
(1,1022)	1:79:A:ILE:HG21	1:81:A:ASN:H	19	0.22
(1,1022)	1:79:A:ILE:HG22	1:81:A:ASN:H	19	0.22
(1,1022)	1:79:A:ILE:HG23	1:81:A:ASN:H	19	0.22
(1,1022)	1:79:A:ILE:HG21	1:81:A:ASN:H	20	0.22
(1,1022)	1:79:A:ILE:HG22	1:81:A:ASN:H	20	0.22
(1,1022)	1:79:A:ILE:HG23	1:81:A:ASN:H	20	0.22
(1,988)	1:85:A:VAL:HG21	1:78:A:ASP:H	13	0.22
(1,988)	1:85:A:VAL:HG22	1:78:A:ASP:H	13	0.22
(1,988)	1:85:A:VAL:HG23	1:78:A:ASP:H	13	0.22
(1,981)	1:84:A:ILE:HD11	1:82:A:ASN:H	4	0.22
(1,981)	1:84:A:ILE:HD12	1:82:A:ASN:H	4	0.22
(1,981)	1:84:A:ILE:HD13	1:82:A:ASN:H	4	0.22
(1,981)	1:84:A:ILE:HD11	1:82:A:ASN:H	18	0.22
(1,981)	1:84:A:ILE:HD12	1:82:A:ASN:H	18	0.22
(1,981)	1:84:A:ILE:HD13	1:82:A:ASN:H	18	0.22
(1,978)	1:131:A:ILE:HD11	1:131:A:ILE:H	1	0.22
(1,978)	1:131:A:ILE:HD12	1:131:A:ILE:H	1	0.22
(1,978)	1:131:A:ILE:HD13	1:131:A:ILE:H	1	0.22
(1,909)	1:73:A:ILE:HD11	1:73:A:ILE:H	16	0.22
(1,909)	1:73:A:ILE:HD12	1:73:A:ILE:H	16	0.22
(1,909)	1:73:A:ILE:HD13	1:73:A:ILE:H	16	0.22
(1,870)	1:52:A:LEU:HG	1:56:A:GLN:HE21	8	0.22
(1,806)	1:53:A:ALA:HB1	1:57:A:MET:H	3	0.22
(1,806)	1:53:A:ALA:HB2	1:57:A:MET:H	3	0.22
(1,806)	1:53:A:ALA:HB3	1:57:A:MET:H	3	0.22
(1,806)	1:53:A:ALA:HB1	1:57:A:MET:H	16	0.22
(1,806)	1:53:A:ALA:HB2	1:57:A:MET:H	16	0.22
(1,806)	1:53:A:ALA:HB3	1:57:A:MET:H	16	0.22
(1,743)	1:34:A:LYS:HD2	1:34:A:LYS:H	16	0.22
(1,554)	1:34:A:LYS:HE2	1:4:A:LYS:H	11	0.22
(1,554)	1:34:A:LYS:HE2	1:4:A:LYS:H	20	0.22
(1,386)	1:117:A:ASN:HA	1:119:A:ILE:H	13	0.22
(1,97)	1:144:A:LEU:H	1:143:A:GLN:H	20	0.22
(1,3875)	1:55:A:LEU:HB3	1:8:A:ILE:HG12	1	0.21
(1,3875)	1:55:A:LEU:HB3	1:8:A:ILE:HG13	1	0.21
(1,3871)	1:79:A:ILE:H	1:80:A:ASP:HB3	3	0.21
(1,3843)	1:126:A:LEU:HA	1:113:A:ALA:HB1	2	0.21
(1,3843)	1:126:A:LEU:HA	1:113:A:ALA:HB2	2	0.21
(1,3843)	1:126:A:LEU:HA	1:113:A:ALA:HB3	2	0.21
(1,3843)	1:126:A:LEU:HA	1:113:A:ALA:HB1	11	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3843)	1:126:A:LEU:HA	1:113:A:ALA:HB2	11	0.21
(1,3843)	1:126:A:LEU:HA	1:113:A:ALA:HB3	11	0.21
(1,3758)	1:102:A:GLN:HG3	1:108:A:LEU:HD21	17	0.21
(1,3758)	1:102:A:GLN:HG3	1:108:A:LEU:HD22	17	0.21
(1,3758)	1:102:A:GLN:HG3	1:108:A:LEU:HD23	17	0.21
(1,3697)	1:101:A:GLY:HA2	1:102:A:GLN:HG3	9	0.21
(1,3697)	1:101:A:GLY:HA2	1:102:A:GLN:HG3	11	0.21
(1,3696)	1:108:A:LEU:HD21	1:102:A:GLN:HG3	17	0.21
(1,3696)	1:108:A:LEU:HD22	1:102:A:GLN:HG3	17	0.21
(1,3696)	1:108:A:LEU:HD23	1:102:A:GLN:HG3	17	0.21
(1,3623)	1:135:A:ILE:HG12	1:134:A:ARG:HA	9	0.21
(1,3408)	1:59:A:LEU:HD11	1:15:A:SER:HB3	9	0.21
(1,3408)	1:59:A:LEU:HD12	1:15:A:SER:HB3	9	0.21
(1,3408)	1:59:A:LEU:HD13	1:15:A:SER:HB3	9	0.21
(1,3371)	1:36:A:LEU:HA	1:36:A:LEU:HD11	18	0.21
(1,3371)	1:36:A:LEU:HA	1:36:A:LEU:HD12	18	0.21
(1,3371)	1:36:A:LEU:HA	1:36:A:LEU:HD13	18	0.21
(1,3336)	1:126:A:LEU:HD11	1:139:A:PRO:HB3	4	0.21
(1,3336)	1:126:A:LEU:HD12	1:139:A:PRO:HB3	4	0.21
(1,3336)	1:126:A:LEU:HD13	1:139:A:PRO:HB3	4	0.21
(1,3219)	1:93:A:ILE:HD11	1:119:A:ILE:HD11	10	0.21
(1,3219)	1:93:A:ILE:HD11	1:119:A:ILE:HD12	10	0.21
(1,3219)	1:93:A:ILE:HD11	1:119:A:ILE:HD13	10	0.21
(1,3219)	1:93:A:ILE:HD12	1:119:A:ILE:HD11	10	0.21
(1,3219)	1:93:A:ILE:HD12	1:119:A:ILE:HD12	10	0.21
(1,3219)	1:93:A:ILE:HD12	1:119:A:ILE:HD13	10	0.21
(1,3219)	1:93:A:ILE:HD13	1:119:A:ILE:HD11	10	0.21
(1,3219)	1:93:A:ILE:HD13	1:119:A:ILE:HD12	10	0.21
(1,3219)	1:93:A:ILE:HD13	1:119:A:ILE:HD13	10	0.21
(1,3219)	1:93:A:ILE:HD11	1:119:A:ILE:HD11	12	0.21
(1,3219)	1:93:A:ILE:HD11	1:119:A:ILE:HD12	12	0.21
(1,3219)	1:93:A:ILE:HD11	1:119:A:ILE:HD13	12	0.21
(1,3219)	1:93:A:ILE:HD12	1:119:A:ILE:HD11	12	0.21
(1,3219)	1:93:A:ILE:HD12	1:119:A:ILE:HD12	12	0.21
(1,3219)	1:93:A:ILE:HD12	1:119:A:ILE:HD13	12	0.21
(1,3219)	1:93:A:ILE:HD13	1:119:A:ILE:HD11	12	0.21
(1,3219)	1:93:A:ILE:HD13	1:119:A:ILE:HD12	12	0.21
(1,3219)	1:93:A:ILE:HD13	1:119:A:ILE:HD13	12	0.21
(1,3177)	1:129:A:LYS:HE2	1:135:A:ILE:HD11	16	0.21
(1,3177)	1:129:A:LYS:HE2	1:135:A:ILE:HD12	16	0.21
(1,3177)	1:129:A:LYS:HE2	1:135:A:ILE:HD13	16	0.21
(1,3177)	1:129:A:LYS:HE3	1:135:A:ILE:HD11	16	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3177)	1:129:A:LYS:HE3	1:135:A:ILE:HD12	16	0.21
(1,3177)	1:129:A:LYS:HE3	1:135:A:ILE:HD13	16	0.21
(1,3095)	1:57:A:MET:HE1	1:53:A:ALA:HA	5	0.21
(1,3095)	1:57:A:MET:HE2	1:53:A:ALA:HA	5	0.21
(1,3095)	1:57:A:MET:HE3	1:53:A:ALA:HA	5	0.21
(1,3095)	1:57:A:MET:HE1	1:53:A:ALA:HA	11	0.21
(1,3095)	1:57:A:MET:HE2	1:53:A:ALA:HA	11	0.21
(1,3095)	1:57:A:MET:HE3	1:53:A:ALA:HA	11	0.21
(1,3074)	1:4:A:LYS:HB2	1:71:A:ASN:HA	4	0.21
(1,3049)	1:12:A:GLY:HA2	1:13:A:GLU:HG2	5	0.21
(1,3049)	1:12:A:GLY:HA2	1:13:A:GLU:HG3	5	0.21
(1,3049)	1:12:A:GLY:HA2	1:13:A:GLU:HG2	13	0.21
(1,3049)	1:12:A:GLY:HA2	1:13:A:GLU:HG3	13	0.21
(1,2904)	1:3:A:VAL:HA	1:38:A:ALA:HB1	12	0.21
(1,2904)	1:3:A:VAL:HA	1:38:A:ALA:HB2	12	0.21
(1,2904)	1:3:A:VAL:HA	1:38:A:ALA:HB3	12	0.21
(1,2904)	1:3:A:VAL:HA	1:38:A:ALA:HB1	15	0.21
(1,2904)	1:3:A:VAL:HA	1:38:A:ALA:HB2	15	0.21
(1,2904)	1:3:A:VAL:HA	1:38:A:ALA:HB3	15	0.21
(1,2858)	1:95:A:ASN:HD21	1:91:A:ILE:HG21	8	0.21
(1,2858)	1:95:A:ASN:HD21	1:91:A:ILE:HG22	8	0.21
(1,2858)	1:95:A:ASN:HD21	1:91:A:ILE:HG23	8	0.21
(1,2832)	1:136:A:THR:H	1:135:A:ILE:HG21	7	0.21
(1,2832)	1:136:A:THR:H	1:135:A:ILE:HG22	7	0.21
(1,2832)	1:136:A:THR:H	1:135:A:ILE:HG23	7	0.21
(1,2829)	1:59:A:LEU:H	1:14:A:ILE:HG21	10	0.21
(1,2829)	1:59:A:LEU:H	1:14:A:ILE:HG22	10	0.21
(1,2829)	1:59:A:LEU:H	1:14:A:ILE:HG23	10	0.21
(1,2761)	1:74:A:TYR:HB2	1:75:A:THR:HG21	5	0.21
(1,2761)	1:74:A:TYR:HB2	1:75:A:THR:HG22	5	0.21
(1,2761)	1:74:A:TYR:HB2	1:75:A:THR:HG23	5	0.21
(1,2641)	1:115:A:GLY:H	1:113:A:ALA:HB1	19	0.21
(1,2641)	1:115:A:GLY:H	1:113:A:ALA:HB2	19	0.21
(1,2641)	1:115:A:GLY:H	1:113:A:ALA:HB3	19	0.21
(1,2586)	1:39:A:ALA:HB1	1:36:A:LEU:HD11	19	0.21
(1,2586)	1:39:A:ALA:HB1	1:36:A:LEU:HD12	19	0.21
(1,2586)	1:39:A:ALA:HB1	1:36:A:LEU:HD13	19	0.21
(1,2586)	1:39:A:ALA:HB2	1:36:A:LEU:HD11	19	0.21
(1,2586)	1:39:A:ALA:HB2	1:36:A:LEU:HD12	19	0.21
(1,2586)	1:39:A:ALA:HB2	1:36:A:LEU:HD13	19	0.21
(1,2586)	1:39:A:ALA:HB3	1:36:A:LEU:HD11	19	0.21
(1,2586)	1:39:A:ALA:HB3	1:36:A:LEU:HD12	19	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2586)	1:39:A:ALA:HB3	1:36:A:LEU:HD13	19	0.21
(1,2550)	1:40:A:ASP:HB3	1:47:A:VAL:HG11	14	0.21
(1,2550)	1:40:A:ASP:HB3	1:47:A:VAL:HG12	14	0.21
(1,2550)	1:40:A:ASP:HB3	1:47:A:VAL:HG13	14	0.21
(1,2515)	1:93:A:ILE:HA	1:103:A:LEU:HD11	2	0.21
(1,2515)	1:93:A:ILE:HA	1:103:A:LEU:HD12	2	0.21
(1,2515)	1:93:A:ILE:HA	1:103:A:LEU:HD13	2	0.21
(1,2482)	1:96:A:HIS:H	1:103:A:LEU:HD11	4	0.21
(1,2482)	1:96:A:HIS:H	1:103:A:LEU:HD12	4	0.21
(1,2482)	1:96:A:HIS:H	1:103:A:LEU:HD13	4	0.21
(1,2472)	1:145:A:GLU:H	1:144:A:LEU:HD21	6	0.21
(1,2472)	1:145:A:GLU:H	1:144:A:LEU:HD22	6	0.21
(1,2472)	1:145:A:GLU:H	1:144:A:LEU:HD23	6	0.21
(1,2456)	1:23:A:LYS:H	1:52:A:LEU:HD11	20	0.21
(1,2456)	1:23:A:LYS:H	1:52:A:LEU:HD12	20	0.21
(1,2456)	1:23:A:LYS:H	1:52:A:LEU:HD13	20	0.21
(1,2379)	1:107:A:SER:HA	1:108:A:LEU:HG	13	0.21
(1,2350)	1:52:A:LEU:H	1:52:A:LEU:HD21	17	0.21
(1,2350)	1:52:A:LEU:H	1:52:A:LEU:HD22	17	0.21
(1,2350)	1:52:A:LEU:H	1:52:A:LEU:HD23	17	0.21
(1,2344)	1:19:A:TYR:H	1:59:A:LEU:HD21	10	0.21
(1,2344)	1:19:A:TYR:H	1:59:A:LEU:HD22	10	0.21
(1,2344)	1:19:A:TYR:H	1:59:A:LEU:HD23	10	0.21
(1,2287)	1:119:A:ILE:HG21	1:93:A:ILE:HG13	16	0.21
(1,2287)	1:119:A:ILE:HG22	1:93:A:ILE:HG13	16	0.21
(1,2287)	1:119:A:ILE:HG23	1:93:A:ILE:HG13	16	0.21
(1,2277)	1:93:A:ILE:HB	1:127:A:ILE:HG12	16	0.21
(1,2277)	1:93:A:ILE:HB	1:127:A:ILE:HG13	16	0.21
(1,2248)	1:70:A:LYS:HA	1:70:A:LYS:HD3	19	0.21
(1,2215)	1:9:A:ASP:H	1:8:A:ILE:HG12	17	0.21
(1,2215)	1:9:A:ASP:H	1:8:A:ILE:HG13	17	0.21
(1,2180)	1:23:A:LYS:HD2	1:23:A:LYS:HB2	17	0.21
(1,1949)	1:136:A:THR:HG21	1:135:A:ILE:HB	7	0.21
(1,1949)	1:136:A:THR:HG22	1:135:A:ILE:HB	7	0.21
(1,1949)	1:136:A:THR:HG23	1:135:A:ILE:HB	7	0.21
(1,1859)	1:27:A:ILE:HD11	1:23:A:LYS:HE2	14	0.21
(1,1859)	1:27:A:ILE:HD12	1:23:A:LYS:HE2	14	0.21
(1,1859)	1:27:A:ILE:HD13	1:23:A:LYS:HE2	14	0.21
(1,1534)	1:20:A:ALA:HB1	1:17:A:ILE:HA	13	0.21
(1,1534)	1:20:A:ALA:HB2	1:17:A:ILE:HA	13	0.21
(1,1534)	1:20:A:ALA:HB3	1:17:A:ILE:HA	13	0.21
(1,1511)	1:3:A:VAL:HA	1:5:A:ILE:HD11	14	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1511)	1:3:A:VAL:HA	1:5:A:ILE:HD12	14	0.21
(1,1511)	1:3:A:VAL:HA	1:5:A:ILE:HD13	14	0.21
(1,1326)	1:5:A:ILE:HD11	1:39:A:ALA:H	7	0.21
(1,1326)	1:5:A:ILE:HD12	1:39:A:ALA:H	7	0.21
(1,1326)	1:5:A:ILE:HD13	1:39:A:ALA:H	7	0.21
(1,1238)	1:59:A:LEU:HD21	1:20:A:ALA:H	16	0.21
(1,1238)	1:59:A:LEU:HD22	1:20:A:ALA:H	16	0.21
(1,1238)	1:59:A:LEU:HD23	1:20:A:ALA:H	16	0.21
(1,1221)	1:62:A:LYS:HB3	1:63:A:GLY:H	4	0.21
(1,1221)	1:57:A:MET:HB2	1:63:A:GLY:H	8	0.21
(1,1220)	1:131:A:ILE:HG21	1:133:A:GLY:H	1	0.21
(1,1220)	1:131:A:ILE:HG22	1:133:A:GLY:H	1	0.21
(1,1220)	1:131:A:ILE:HG23	1:133:A:GLY:H	1	0.21
(1,1220)	1:131:A:ILE:HG21	1:133:A:GLY:H	4	0.21
(1,1220)	1:131:A:ILE:HG22	1:133:A:GLY:H	4	0.21
(1,1220)	1:131:A:ILE:HG23	1:133:A:GLY:H	4	0.21
(1,1220)	1:131:A:ILE:HG21	1:133:A:GLY:H	5	0.21
(1,1220)	1:131:A:ILE:HG22	1:133:A:GLY:H	5	0.21
(1,1220)	1:131:A:ILE:HG23	1:133:A:GLY:H	5	0.21
(1,1197)	1:126:A:LEU:HD11	1:122:A:THR:H	6	0.21
(1,1197)	1:126:A:LEU:HD12	1:122:A:THR:H	6	0.21
(1,1197)	1:126:A:LEU:HD13	1:122:A:THR:H	6	0.21
(1,1195)	1:60:A:LEU:HD21	1:57:A:MET:H	1	0.21
(1,1195)	1:60:A:LEU:HD22	1:57:A:MET:H	1	0.21
(1,1195)	1:60:A:LEU:HD23	1:57:A:MET:H	1	0.21
(1,1195)	1:60:A:LEU:HD21	1:57:A:MET:H	10	0.21
(1,1195)	1:60:A:LEU:HD22	1:57:A:MET:H	10	0.21
(1,1195)	1:60:A:LEU:HD23	1:57:A:MET:H	10	0.21
(1,1163)	1:27:A:ILE:HD11	1:27:A:ILE:H	2	0.21
(1,1163)	1:27:A:ILE:HD12	1:27:A:ILE:H	2	0.21
(1,1163)	1:27:A:ILE:HD13	1:27:A:ILE:H	2	0.21
(1,1163)	1:27:A:ILE:HD11	1:27:A:ILE:H	19	0.21
(1,1163)	1:27:A:ILE:HD12	1:27:A:ILE:H	19	0.21
(1,1163)	1:27:A:ILE:HD13	1:27:A:ILE:H	19	0.21
(1,1149)	1:135:A:ILE:HG12	1:129:A:LYS:H	3	0.21
(1,1141)	1:144:A:LEU:HG	1:143:A:GLN:H	9	0.21
(1,1137)	1:97:A:ILE:HG21	1:96:A:HIS:H	7	0.21
(1,1137)	1:97:A:ILE:HG22	1:96:A:HIS:H	7	0.21
(1,1137)	1:97:A:ILE:HG23	1:96:A:HIS:H	7	0.21
(1,1137)	1:97:A:ILE:HG21	1:96:A:HIS:H	17	0.21
(1,1137)	1:97:A:ILE:HG22	1:96:A:HIS:H	17	0.21
(1,1137)	1:97:A:ILE:HG23	1:96:A:HIS:H	17	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1132)	1:131:A:ILE:HG12	1:130:A:TYR:H	15	0.21
(1,1043)	1:8:A:ILE:HG21	1:32:A:THR:H	10	0.21
(1,1043)	1:8:A:ILE:HG22	1:32:A:THR:H	10	0.21
(1,1043)	1:8:A:ILE:HG23	1:32:A:THR:H	10	0.21
(1,1042)	1:52:A:LEU:HD21	1:49:A:SER:H	6	0.21
(1,1042)	1:52:A:LEU:HD22	1:49:A:SER:H	6	0.21
(1,1042)	1:52:A:LEU:HD23	1:49:A:SER:H	6	0.21
(1,1042)	1:50:A:ILE:HD11	1:49:A:SER:H	12	0.21
(1,1042)	1:50:A:ILE:HD12	1:49:A:SER:H	12	0.21
(1,1042)	1:50:A:ILE:HD13	1:49:A:SER:H	12	0.21
(1,1004)	1:59:A:LEU:HD21	1:16:A:SER:H	7	0.21
(1,1004)	1:59:A:LEU:HD22	1:16:A:SER:H	7	0.21
(1,1004)	1:59:A:LEU:HD23	1:16:A:SER:H	7	0.21
(1,1004)	1:59:A:LEU:HD21	1:16:A:SER:H	16	0.21
(1,1004)	1:59:A:LEU:HD22	1:16:A:SER:H	16	0.21
(1,1004)	1:59:A:LEU:HD23	1:16:A:SER:H	16	0.21
(1,981)	1:84:A:ILE:HD11	1:82:A:ASN:H	3	0.21
(1,981)	1:84:A:ILE:HD12	1:82:A:ASN:H	3	0.21
(1,981)	1:84:A:ILE:HD13	1:82:A:ASN:H	3	0.21
(1,981)	1:84:A:ILE:HD11	1:82:A:ASN:H	7	0.21
(1,981)	1:84:A:ILE:HD12	1:82:A:ASN:H	7	0.21
(1,981)	1:84:A:ILE:HD13	1:82:A:ASN:H	7	0.21
(1,981)	1:84:A:ILE:HD11	1:82:A:ASN:H	13	0.21
(1,981)	1:84:A:ILE:HD12	1:82:A:ASN:H	13	0.21
(1,981)	1:84:A:ILE:HD13	1:82:A:ASN:H	13	0.21
(1,981)	1:84:A:ILE:HD11	1:82:A:ASN:H	19	0.21
(1,981)	1:84:A:ILE:HD12	1:82:A:ASN:H	19	0.21
(1,981)	1:84:A:ILE:HD13	1:82:A:ASN:H	19	0.21
(1,980)	1:54:A:ILE:HD11	1:42:A:ASP:H	10	0.21
(1,980)	1:54:A:ILE:HD12	1:42:A:ASP:H	10	0.21
(1,980)	1:54:A:ILE:HD13	1:42:A:ASP:H	10	0.21
(1,980)	1:54:A:ILE:HD11	1:42:A:ASP:H	13	0.21
(1,980)	1:54:A:ILE:HD12	1:42:A:ASP:H	13	0.21
(1,980)	1:54:A:ILE:HD13	1:42:A:ASP:H	13	0.21
(1,962)	1:73:A:ILE:HD11	1:71:A:ASN:H	17	0.21
(1,962)	1:73:A:ILE:HD12	1:71:A:ASN:H	17	0.21
(1,962)	1:73:A:ILE:HD13	1:71:A:ASN:H	17	0.21
(1,903)	1:41:A:VAL:HG21	1:48:A:ASN:H	20	0.21
(1,903)	1:41:A:VAL:HG22	1:48:A:ASN:H	20	0.21
(1,903)	1:41:A:VAL:HG23	1:48:A:ASN:H	20	0.21
(1,870)	1:52:A:LEU:HG	1:56:A:GLN:HE21	20	0.21
(1,774)	1:72:A:ARG:HB2	1:3:A:VAL:H	20	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,760)	1:97:A:ILE:HB	1:96:A:HIS:H	16	0.21
(1,3871)	1:79:A:ILE:H	1:80:A:ASP:HB3	10	0.2
(1,3843)	1:126:A:LEU:HA	1:113:A:ALA:HB1	5	0.2
(1,3843)	1:126:A:LEU:HA	1:113:A:ALA:HB2	5	0.2
(1,3843)	1:126:A:LEU:HA	1:113:A:ALA:HB3	5	0.2
(1,3843)	1:126:A:LEU:HA	1:113:A:ALA:HB1	6	0.2
(1,3843)	1:126:A:LEU:HA	1:113:A:ALA:HB2	6	0.2
(1,3843)	1:126:A:LEU:HA	1:113:A:ALA:HB3	6	0.2
(1,3843)	1:126:A:LEU:HA	1:113:A:ALA:HB1	15	0.2
(1,3843)	1:126:A:LEU:HA	1:113:A:ALA:HB2	15	0.2
(1,3843)	1:126:A:LEU:HA	1:113:A:ALA:HB3	15	0.2
(1,3724)	1:71:A:ASN:HB3	1:5:A:ILE:HG13	18	0.2
(1,3712)	1:130:A:TYR:HE1	1:137:A:HIS:HB3	12	0.2
(1,3712)	1:130:A:TYR:HE2	1:137:A:HIS:HB3	12	0.2
(1,3695)	1:108:A:LEU:HD21	1:102:A:GLN:HG2	9	0.2
(1,3695)	1:108:A:LEU:HD22	1:102:A:GLN:HG2	9	0.2
(1,3695)	1:108:A:LEU:HD23	1:102:A:GLN:HG2	9	0.2
(1,3543)	1:17:A:ILE:HA	1:21:A:ILE:HD11	6	0.2
(1,3543)	1:17:A:ILE:HA	1:21:A:ILE:HD12	6	0.2
(1,3543)	1:17:A:ILE:HA	1:21:A:ILE:HD13	6	0.2
(1,3459)	1:74:A:TYR:HB3	1:73:A:ILE:HA	9	0.2
(1,3219)	1:93:A:ILE:HD11	1:119:A:ILE:HD11	20	0.2
(1,3219)	1:93:A:ILE:HD11	1:119:A:ILE:HD12	20	0.2
(1,3219)	1:93:A:ILE:HD11	1:119:A:ILE:HD13	20	0.2
(1,3219)	1:93:A:ILE:HD12	1:119:A:ILE:HD11	20	0.2
(1,3219)	1:93:A:ILE:HD12	1:119:A:ILE:HD12	20	0.2
(1,3219)	1:93:A:ILE:HD12	1:119:A:ILE:HD13	20	0.2
(1,3219)	1:93:A:ILE:HD13	1:119:A:ILE:HD11	20	0.2
(1,3219)	1:93:A:ILE:HD13	1:119:A:ILE:HD12	20	0.2
(1,3219)	1:93:A:ILE:HD13	1:119:A:ILE:HD13	20	0.2
(1,3164)	1:123:A:ASP:HB2	1:93:A:ILE:HD11	13	0.2
(1,3164)	1:123:A:ASP:HB2	1:93:A:ILE:HD12	13	0.2
(1,3164)	1:123:A:ASP:HB2	1:93:A:ILE:HD13	13	0.2
(1,3019)	1:54:A:ILE:HA	1:65:A:THR:HB	15	0.2
(1,2995)	1:70:A:LYS:HB3	1:5:A:ILE:HG21	15	0.2
(1,2995)	1:70:A:LYS:HB3	1:5:A:ILE:HG22	15	0.2
(1,2995)	1:70:A:LYS:HB3	1:5:A:ILE:HG23	15	0.2
(1,2980)	1:54:A:ILE:HB	1:53:A:ALA:HB1	17	0.2
(1,2980)	1:54:A:ILE:HB	1:53:A:ALA:HB2	17	0.2
(1,2980)	1:54:A:ILE:HB	1:53:A:ALA:HB3	17	0.2
(1,2970)	1:87:A:GLU:HG2	1:127:A:ILE:HG21	3	0.2
(1,2970)	1:87:A:GLU:HG2	1:127:A:ILE:HG22	3	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2970)	1:87:A:GLU:HG2	1:127:A:ILE:HG23	3	0.2
(1,2829)	1:59:A:LEU:H	1:14:A:ILE:HG21	17	0.2
(1,2829)	1:59:A:LEU:H	1:14:A:ILE:HG22	17	0.2
(1,2829)	1:59:A:LEU:H	1:14:A:ILE:HG23	17	0.2
(1,2761)	1:74:A:TYR:HB2	1:75:A:THR:HG21	6	0.2
(1,2761)	1:74:A:TYR:HB2	1:75:A:THR:HG22	6	0.2
(1,2761)	1:74:A:TYR:HB2	1:75:A:THR:HG23	6	0.2
(1,2761)	1:74:A:TYR:HB2	1:75:A:THR:HG21	18	0.2
(1,2761)	1:74:A:TYR:HB2	1:75:A:THR:HG22	18	0.2
(1,2761)	1:74:A:TYR:HB2	1:75:A:THR:HG23	18	0.2
(1,2752)	1:35:A:GLN:HB2	1:32:A:THR:HG21	19	0.2
(1,2752)	1:35:A:GLN:HB2	1:32:A:THR:HG22	19	0.2
(1,2752)	1:35:A:GLN:HB2	1:32:A:THR:HG23	19	0.2
(1,2713)	1:80:A:ASP:HA	1:79:A:ILE:HG21	9	0.2
(1,2713)	1:80:A:ASP:HA	1:79:A:ILE:HG22	9	0.2
(1,2713)	1:80:A:ASP:HA	1:79:A:ILE:HG23	9	0.2
(1,2713)	1:80:A:ASP:HA	1:79:A:ILE:HG21	19	0.2
(1,2713)	1:80:A:ASP:HA	1:79:A:ILE:HG22	19	0.2
(1,2713)	1:80:A:ASP:HA	1:79:A:ILE:HG23	19	0.2
(1,2652)	1:80:A:ASP:H	1:79:A:ILE:HG21	9	0.2
(1,2652)	1:80:A:ASP:H	1:79:A:ILE:HG22	9	0.2
(1,2652)	1:80:A:ASP:H	1:79:A:ILE:HG23	9	0.2
(1,2583)	1:126:A:LEU:HB2	1:138:A:LEU:HD21	8	0.2
(1,2583)	1:126:A:LEU:HB2	1:138:A:LEU:HD22	8	0.2
(1,2583)	1:126:A:LEU:HB2	1:138:A:LEU:HD23	8	0.2
(1,2583)	1:126:A:LEU:HB2	1:138:A:LEU:HD21	18	0.2
(1,2583)	1:126:A:LEU:HB2	1:138:A:LEU:HD22	18	0.2
(1,2583)	1:126:A:LEU:HB2	1:138:A:LEU:HD23	18	0.2
(1,2515)	1:92:A:LEU:HA	1:103:A:LEU:HD11	1	0.2
(1,2515)	1:92:A:LEU:HA	1:103:A:LEU:HD12	1	0.2
(1,2515)	1:92:A:LEU:HA	1:103:A:LEU:HD13	1	0.2
(1,2515)	1:92:A:LEU:HA	1:103:A:LEU:HD11	10	0.2
(1,2515)	1:92:A:LEU:HA	1:103:A:LEU:HD12	10	0.2
(1,2515)	1:92:A:LEU:HA	1:103:A:LEU:HD13	10	0.2
(1,2515)	1:92:A:LEU:HA	1:103:A:LEU:HD11	11	0.2
(1,2515)	1:92:A:LEU:HA	1:103:A:LEU:HD12	11	0.2
(1,2515)	1:92:A:LEU:HA	1:103:A:LEU:HD13	11	0.2
(1,2483)	1:56:A:GLN:HE21	1:52:A:LEU:HD21	11	0.2
(1,2483)	1:56:A:GLN:HE21	1:52:A:LEU:HD22	11	0.2
(1,2483)	1:56:A:GLN:HE21	1:52:A:LEU:HD23	11	0.2
(1,2449)	1:130:A:TYR:H	1:126:A:LEU:HD21	3	0.2
(1,2449)	1:130:A:TYR:H	1:126:A:LEU:HD22	3	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2449)	1:130:A:TYR:H	1:126:A:LEU:HD23	3	0.2
(1,2379)	1:107:A:SER:HA	1:108:A:LEU:HG	9	0.2
(1,2379)	1:107:A:SER:HA	1:108:A:LEU:HG	11	0.2
(1,2379)	1:107:A:SER:HA	1:108:A:LEU:HG	19	0.2
(1,2300)	1:49:A:SER:H	1:50:A:ILE:HG13	8	0.2
(1,2248)	1:70:A:LYS:HA	1:70:A:LYS:HD3	2	0.2
(1,2215)	1:9:A:ASP:H	1:8:A:ILE:HG12	19	0.2
(1,2215)	1:9:A:ASP:H	1:8:A:ILE:HG13	19	0.2
(1,2180)	1:23:A:LYS:HD2	1:23:A:LYS:HB2	6	0.2
(1,2120)	1:81:A:ASN:HD22	1:72:A:ARG:HB2	20	0.2
(1,1949)	1:138:A:LEU:HG	1:135:A:ILE:HB	4	0.2
(1,1822)	1:70:A:LYS:HA	1:70:A:LYS:HE2	3	0.2
(1,1822)	1:70:A:LYS:HA	1:70:A:LYS:HE3	3	0.2
(1,1822)	1:70:A:LYS:HA	1:70:A:LYS:HE2	15	0.2
(1,1822)	1:70:A:LYS:HA	1:70:A:LYS:HE3	15	0.2
(1,1806)	1:74:A:TYR:HE1	1:72:A:ARG:HD3	12	0.2
(1,1534)	1:20:A:ALA:HB1	1:17:A:ILE:HA	5	0.2
(1,1534)	1:20:A:ALA:HB2	1:17:A:ILE:HA	5	0.2
(1,1534)	1:20:A:ALA:HB3	1:17:A:ILE:HA	5	0.2
(1,1357)	1:123:A:ASP:H	1:93:A:ILE:HD11	2	0.2
(1,1357)	1:123:A:ASP:H	1:93:A:ILE:HD12	2	0.2
(1,1357)	1:123:A:ASP:H	1:93:A:ILE:HD13	2	0.2
(1,1238)	1:59:A:LEU:HD21	1:20:A:ALA:H	2	0.2
(1,1238)	1:59:A:LEU:HD22	1:20:A:ALA:H	2	0.2
(1,1238)	1:59:A:LEU:HD23	1:20:A:ALA:H	2	0.2
(1,1221)	1:57:A:MET:HB2	1:63:A:GLY:H	14	0.2
(1,1197)	1:126:A:LEU:HD11	1:122:A:THR:H	5	0.2
(1,1197)	1:126:A:LEU:HD12	1:122:A:THR:H	5	0.2
(1,1197)	1:126:A:LEU:HD13	1:122:A:THR:H	5	0.2
(1,1197)	1:126:A:LEU:HD11	1:122:A:THR:H	15	0.2
(1,1197)	1:126:A:LEU:HD12	1:122:A:THR:H	15	0.2
(1,1197)	1:126:A:LEU:HD13	1:122:A:THR:H	15	0.2
(1,1195)	1:60:A:LEU:HD21	1:57:A:MET:H	5	0.2
(1,1195)	1:60:A:LEU:HD22	1:57:A:MET:H	5	0.2
(1,1195)	1:60:A:LEU:HD23	1:57:A:MET:H	5	0.2
(1,1195)	1:60:A:LEU:HD21	1:57:A:MET:H	8	0.2
(1,1195)	1:60:A:LEU:HD22	1:57:A:MET:H	8	0.2
(1,1195)	1:60:A:LEU:HD23	1:57:A:MET:H	8	0.2
(1,1182)	1:126:A:LEU:HD21	1:127:A:ILE:H	6	0.2
(1,1182)	1:126:A:LEU:HD22	1:127:A:ILE:H	6	0.2
(1,1182)	1:126:A:LEU:HD23	1:127:A:ILE:H	6	0.2
(1,1177)	1:92:A:LEU:HD11	1:89:A:ASP:H	19	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1177)	1:92:A:LEU:HD12	1:89:A:ASP:H	19	0.2
(1,1177)	1:92:A:LEU:HD13	1:89:A:ASP:H	19	0.2
(1,1149)	1:135:A:ILE:HG12	1:129:A:LYS:H	20	0.2
(1,1137)	1:97:A:ILE:HG21	1:96:A:HIS:H	2	0.2
(1,1137)	1:97:A:ILE:HG22	1:96:A:HIS:H	2	0.2
(1,1137)	1:97:A:ILE:HG23	1:96:A:HIS:H	2	0.2
(1,1042)	1:50:A:ILE:HD11	1:49:A:SER:H	16	0.2
(1,1042)	1:50:A:ILE:HD12	1:49:A:SER:H	16	0.2
(1,1042)	1:50:A:ILE:HD13	1:49:A:SER:H	16	0.2
(1,1022)	1:79:A:ILE:HG21	1:81:A:ASN:H	11	0.2
(1,1022)	1:79:A:ILE:HG22	1:81:A:ASN:H	11	0.2
(1,1022)	1:79:A:ILE:HG23	1:81:A:ASN:H	11	0.2
(1,983)	1:34:A:LYS:HD2	1:37:A:ALA:H	2	0.2
(1,981)	1:84:A:ILE:HD11	1:82:A:ASN:H	9	0.2
(1,981)	1:84:A:ILE:HD12	1:82:A:ASN:H	9	0.2
(1,981)	1:84:A:ILE:HD13	1:82:A:ASN:H	9	0.2
(1,981)	1:84:A:ILE:HD11	1:82:A:ASN:H	16	0.2
(1,981)	1:84:A:ILE:HD12	1:82:A:ASN:H	16	0.2
(1,981)	1:84:A:ILE:HD13	1:82:A:ASN:H	16	0.2
(1,981)	1:84:A:ILE:HD11	1:82:A:ASN:H	17	0.2
(1,981)	1:84:A:ILE:HD12	1:82:A:ASN:H	17	0.2
(1,981)	1:84:A:ILE:HD13	1:82:A:ASN:H	17	0.2
(1,980)	1:54:A:ILE:HD11	1:42:A:ASP:H	8	0.2
(1,980)	1:54:A:ILE:HD12	1:42:A:ASP:H	8	0.2
(1,980)	1:54:A:ILE:HD13	1:42:A:ASP:H	8	0.2
(1,933)	1:52:A:LEU:HD21	1:26:A:LEU:H	3	0.2
(1,933)	1:52:A:LEU:HD22	1:26:A:LEU:H	3	0.2
(1,933)	1:52:A:LEU:HD23	1:26:A:LEU:H	3	0.2
(1,931)	1:8:A:ILE:HG21	1:22:A:LEU:H	16	0.2
(1,931)	1:8:A:ILE:HG22	1:22:A:LEU:H	16	0.2
(1,931)	1:8:A:ILE:HG23	1:22:A:LEU:H	16	0.2
(1,929)	1:3:A:VAL:HG21	1:34:A:LYS:H	11	0.2
(1,929)	1:3:A:VAL:HG22	1:34:A:LYS:H	11	0.2
(1,929)	1:3:A:VAL:HG23	1:34:A:LYS:H	11	0.2
(1,903)	1:41:A:VAL:HG21	1:48:A:ASN:H	10	0.2
(1,903)	1:41:A:VAL:HG22	1:48:A:ASN:H	10	0.2
(1,903)	1:41:A:VAL:HG23	1:48:A:ASN:H	10	0.2
(1,823)	1:70:A:LYS:HG2	1:69:A:GLY:H	14	0.2
(1,823)	1:70:A:LYS:HG3	1:69:A:GLY:H	14	0.2
(1,823)	1:70:A:LYS:HG2	1:69:A:GLY:H	16	0.2
(1,823)	1:70:A:LYS:HG3	1:69:A:GLY:H	16	0.2
(1,772)	1:20:A:ALA:HB1	1:23:A:LYS:H	20	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,772)	1:20:A:ALA:HB2	1:23:A:LYS:H	20	0.2
(1,772)	1:20:A:ALA:HB3	1:23:A:LYS:H	20	0.2
(1,746)	1:144:A:LEU:HG	1:144:A:LEU:H	4	0.2
(1,746)	1:144:A:LEU:HG	1:144:A:LEU:H	11	0.2
(1,694)	1:9:A:ASP:HB3	1:35:A:GLN:HE22	16	0.2
(1,582)	1:57:A:MET:HB3	1:58:A:TYR:H	9	0.2
(1,386)	1:117:A:ASN:HA	1:119:A:ILE:H	8	0.2
(1,386)	1:117:A:ASN:HA	1:119:A:ILE:H	11	0.2
(1,3938)	1:14:A:ILE:HB	1:58:A:TYR:HD1	2	0.19
(1,3938)	1:14:A:ILE:HB	1:58:A:TYR:HD2	2	0.19
(1,3938)	1:14:A:ILE:HB	1:58:A:TYR:HD1	3	0.19
(1,3938)	1:14:A:ILE:HB	1:58:A:TYR:HD2	3	0.19
(1,3840)	1:123:A:ASP:HB2	1:111:A:ALA:HB1	5	0.19
(1,3840)	1:123:A:ASP:HB2	1:111:A:ALA:HB2	5	0.19
(1,3840)	1:123:A:ASP:HB2	1:111:A:ALA:HB3	5	0.19
(1,3840)	1:123:A:ASP:HB2	1:111:A:ALA:HB1	15	0.19
(1,3840)	1:123:A:ASP:HB2	1:111:A:ALA:HB2	15	0.19
(1,3840)	1:123:A:ASP:HB2	1:111:A:ALA:HB3	15	0.19
(1,3840)	1:123:A:ASP:HB2	1:111:A:ALA:HB1	16	0.19
(1,3840)	1:123:A:ASP:HB2	1:111:A:ALA:HB2	16	0.19
(1,3840)	1:123:A:ASP:HB2	1:111:A:ALA:HB3	16	0.19
(1,3805)	1:125:A:ILE:HG12	1:128:A:GLU:HG2	16	0.19
(1,3805)	1:125:A:ILE:HG12	1:128:A:GLU:HG3	16	0.19
(1,3797)	1:93:A:ILE:H	1:79:A:ILE:HB	7	0.19
(1,3797)	1:93:A:ILE:H	1:79:A:ILE:HB	15	0.19
(1,3724)	1:71:A:ASN:HB3	1:5:A:ILE:HG13	4	0.19
(1,3724)	1:71:A:ASN:HB3	1:5:A:ILE:HG13	12	0.19
(1,3581)	1:56:A:GLN:H	1:68:A:ILE:HD11	7	0.19
(1,3581)	1:56:A:GLN:H	1:68:A:ILE:HD12	7	0.19
(1,3581)	1:56:A:GLN:H	1:68:A:ILE:HD13	7	0.19
(1,3543)	1:17:A:ILE:HA	1:21:A:ILE:HD11	12	0.19
(1,3543)	1:17:A:ILE:HA	1:21:A:ILE:HD12	12	0.19
(1,3543)	1:17:A:ILE:HA	1:21:A:ILE:HD13	12	0.19
(1,3543)	1:17:A:ILE:HA	1:21:A:ILE:HD11	14	0.19
(1,3543)	1:17:A:ILE:HA	1:21:A:ILE:HD12	14	0.19
(1,3543)	1:17:A:ILE:HA	1:21:A:ILE:HD13	14	0.19
(1,3459)	1:74:A:TYR:HB3	1:73:A:ILE:HA	12	0.19
(1,3431)	1:4:A:LYS:HG3	1:71:A:ASN:HA	8	0.19
(1,3336)	1:126:A:LEU:HD11	1:139:A:PRO:HB3	13	0.19
(1,3336)	1:126:A:LEU:HD12	1:139:A:PRO:HB3	13	0.19
(1,3336)	1:126:A:LEU:HD13	1:139:A:PRO:HB3	13	0.19
(1,3274)	1:73:A:ILE:HA	1:72:A:ARG:HD2	5	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3274)	1:106:A:ALA:HA	1:72:A:ARG:HD2	8	0.19
(1,3180)	1:127:A:ILE:HB	1:79:A:ILE:HD11	4	0.19
(1,3180)	1:127:A:ILE:HB	1:79:A:ILE:HD12	4	0.19
(1,3180)	1:127:A:ILE:HB	1:79:A:ILE:HD13	4	0.19
(1,3095)	1:57:A:MET:HE1	1:53:A:ALA:HA	10	0.19
(1,3095)	1:57:A:MET:HE2	1:53:A:ALA:HA	10	0.19
(1,3095)	1:57:A:MET:HE3	1:53:A:ALA:HA	10	0.19
(1,3049)	1:12:A:GLY:HA2	1:13:A:GLU:HG2	9	0.19
(1,3049)	1:12:A:GLY:HA2	1:13:A:GLU:HG3	9	0.19
(1,3040)	1:6:A:GLY:HA2	1:14:A:ILE:HG21	10	0.19
(1,3040)	1:6:A:GLY:HA2	1:14:A:ILE:HG22	10	0.19
(1,3040)	1:6:A:GLY:HA2	1:14:A:ILE:HG23	10	0.19
(1,2980)	1:21:A:ILE:HB	1:20:A:ALA:HB1	1	0.19
(1,2980)	1:21:A:ILE:HB	1:20:A:ALA:HB2	1	0.19
(1,2980)	1:21:A:ILE:HB	1:20:A:ALA:HB3	1	0.19
(1,2980)	1:21:A:ILE:HB	1:20:A:ALA:HB1	2	0.19
(1,2980)	1:21:A:ILE:HB	1:20:A:ALA:HB2	2	0.19
(1,2980)	1:21:A:ILE:HB	1:20:A:ALA:HB3	2	0.19
(1,2970)	1:87:A:GLU:HG2	1:127:A:ILE:HG21	5	0.19
(1,2970)	1:87:A:GLU:HG2	1:127:A:ILE:HG22	5	0.19
(1,2970)	1:87:A:GLU:HG2	1:127:A:ILE:HG23	5	0.19
(1,2970)	1:87:A:GLU:HG2	1:127:A:ILE:HG21	14	0.19
(1,2970)	1:87:A:GLU:HG2	1:127:A:ILE:HG22	14	0.19
(1,2970)	1:87:A:GLU:HG2	1:127:A:ILE:HG23	14	0.19
(1,2954)	1:9:A:ASP:HB3	1:20:A:ALA:HB1	1	0.19
(1,2954)	1:9:A:ASP:HB3	1:20:A:ALA:HB2	1	0.19
(1,2954)	1:9:A:ASP:HB3	1:20:A:ALA:HB3	1	0.19
(1,2904)	1:3:A:VAL:HA	1:38:A:ALA:HB1	7	0.19
(1,2904)	1:3:A:VAL:HA	1:38:A:ALA:HB2	7	0.19
(1,2904)	1:3:A:VAL:HA	1:38:A:ALA:HB3	7	0.19
(1,2832)	1:87:A:GLU:H	1:131:A:ILE:HG21	16	0.19
(1,2832)	1:87:A:GLU:H	1:131:A:ILE:HG22	16	0.19
(1,2832)	1:87:A:GLU:H	1:131:A:ILE:HG23	16	0.19
(1,2829)	1:59:A:LEU:H	1:14:A:ILE:HG21	1	0.19
(1,2829)	1:59:A:LEU:H	1:14:A:ILE:HG22	1	0.19
(1,2829)	1:59:A:LEU:H	1:14:A:ILE:HG23	1	0.19
(1,2829)	1:59:A:LEU:H	1:14:A:ILE:HG21	12	0.19
(1,2829)	1:59:A:LEU:H	1:14:A:ILE:HG22	12	0.19
(1,2829)	1:59:A:LEU:H	1:14:A:ILE:HG23	12	0.19
(1,2641)	1:123:A:ASP:H	1:113:A:ALA:HB1	4	0.19
(1,2641)	1:123:A:ASP:H	1:113:A:ALA:HB2	4	0.19
(1,2641)	1:123:A:ASP:H	1:113:A:ALA:HB3	4	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2641)	1:115:A:GLY:H	1:113:A:ALA:HB1	9	0.19
(1,2641)	1:115:A:GLY:H	1:113:A:ALA:HB2	9	0.19
(1,2641)	1:115:A:GLY:H	1:113:A:ALA:HB3	9	0.19
(1,2641)	1:123:A:ASP:H	1:113:A:ALA:HB1	12	0.19
(1,2641)	1:123:A:ASP:H	1:113:A:ALA:HB2	12	0.19
(1,2641)	1:123:A:ASP:H	1:113:A:ALA:HB3	12	0.19
(1,2607)	1:47:A:VAL:H	1:39:A:ALA:HB1	17	0.19
(1,2607)	1:47:A:VAL:H	1:39:A:ALA:HB2	17	0.19
(1,2607)	1:47:A:VAL:H	1:39:A:ALA:HB3	17	0.19
(1,2603)	1:26:A:LEU:HD11	1:22:A:LEU:HD21	7	0.19
(1,2603)	1:26:A:LEU:HD11	1:22:A:LEU:HD22	7	0.19
(1,2603)	1:26:A:LEU:HD11	1:22:A:LEU:HD23	7	0.19
(1,2603)	1:26:A:LEU:HD12	1:22:A:LEU:HD21	7	0.19
(1,2603)	1:26:A:LEU:HD12	1:22:A:LEU:HD22	7	0.19
(1,2603)	1:26:A:LEU:HD12	1:22:A:LEU:HD23	7	0.19
(1,2603)	1:26:A:LEU:HD13	1:22:A:LEU:HD21	7	0.19
(1,2603)	1:26:A:LEU:HD13	1:22:A:LEU:HD22	7	0.19
(1,2603)	1:26:A:LEU:HD13	1:22:A:LEU:HD23	7	0.19
(1,2603)	1:26:A:LEU:HD11	1:22:A:LEU:HD21	15	0.19
(1,2603)	1:26:A:LEU:HD11	1:22:A:LEU:HD22	15	0.19
(1,2603)	1:26:A:LEU:HD11	1:22:A:LEU:HD23	15	0.19
(1,2603)	1:26:A:LEU:HD12	1:22:A:LEU:HD21	15	0.19
(1,2603)	1:26:A:LEU:HD12	1:22:A:LEU:HD22	15	0.19
(1,2603)	1:26:A:LEU:HD12	1:22:A:LEU:HD23	15	0.19
(1,2603)	1:26:A:LEU:HD13	1:22:A:LEU:HD21	15	0.19
(1,2603)	1:26:A:LEU:HD13	1:22:A:LEU:HD22	15	0.19
(1,2603)	1:26:A:LEU:HD13	1:22:A:LEU:HD23	15	0.19
(1,2603)	1:26:A:LEU:HD11	1:22:A:LEU:HD21	18	0.19
(1,2603)	1:26:A:LEU:HD11	1:22:A:LEU:HD22	18	0.19
(1,2603)	1:26:A:LEU:HD11	1:22:A:LEU:HD23	18	0.19
(1,2603)	1:26:A:LEU:HD12	1:22:A:LEU:HD21	18	0.19
(1,2603)	1:26:A:LEU:HD12	1:22:A:LEU:HD22	18	0.19
(1,2603)	1:26:A:LEU:HD12	1:22:A:LEU:HD23	18	0.19
(1,2603)	1:26:A:LEU:HD13	1:22:A:LEU:HD21	18	0.19
(1,2603)	1:26:A:LEU:HD13	1:22:A:LEU:HD22	18	0.19
(1,2603)	1:26:A:LEU:HD13	1:22:A:LEU:HD23	18	0.19
(1,2583)	1:126:A:LEU:HB2	1:138:A:LEU:HD21	15	0.19
(1,2583)	1:126:A:LEU:HB2	1:138:A:LEU:HD22	15	0.19
(1,2583)	1:126:A:LEU:HB2	1:138:A:LEU:HD23	15	0.19
(1,2550)	1:40:A:ASP:HB3	1:47:A:VAL:HG11	12	0.19
(1,2550)	1:40:A:ASP:HB3	1:47:A:VAL:HG12	12	0.19
(1,2550)	1:40:A:ASP:HB3	1:47:A:VAL:HG13	12	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2537)	1:52:A:LEU:HA	1:55:A:LEU:HD11	5	0.19
(1,2537)	1:52:A:LEU:HA	1:55:A:LEU:HD12	5	0.19
(1,2537)	1:52:A:LEU:HA	1:55:A:LEU:HD13	5	0.19
(1,2515)	1:93:A:ILE:HA	1:103:A:LEU:HD11	13	0.19
(1,2515)	1:93:A:ILE:HA	1:103:A:LEU:HD12	13	0.19
(1,2515)	1:93:A:ILE:HA	1:103:A:LEU:HD13	13	0.19
(1,2515)	1:93:A:ILE:HA	1:103:A:LEU:HD11	18	0.19
(1,2515)	1:93:A:ILE:HA	1:103:A:LEU:HD12	18	0.19
(1,2515)	1:93:A:ILE:HA	1:103:A:LEU:HD13	18	0.19
(1,2484)	1:56:A:GLN:HE22	1:60:A:LEU:HD21	4	0.19
(1,2484)	1:56:A:GLN:HE22	1:60:A:LEU:HD22	4	0.19
(1,2484)	1:56:A:GLN:HE22	1:60:A:LEU:HD23	4	0.19
(1,2484)	1:56:A:GLN:HE22	1:60:A:LEU:HD21	10	0.19
(1,2484)	1:56:A:GLN:HE22	1:60:A:LEU:HD22	10	0.19
(1,2484)	1:56:A:GLN:HE22	1:60:A:LEU:HD23	10	0.19
(1,2379)	1:107:A:SER:HA	1:108:A:LEU:HG	1	0.19
(1,2367)	1:72:A:ARG:HA	1:73:A:ILE:HG12	11	0.19
(1,2350)	1:52:A:LEU:H	1:52:A:LEU:HD21	2	0.19
(1,2350)	1:52:A:LEU:H	1:52:A:LEU:HD22	2	0.19
(1,2350)	1:52:A:LEU:H	1:52:A:LEU:HD23	2	0.19
(1,2350)	1:52:A:LEU:H	1:52:A:LEU:HD21	14	0.19
(1,2350)	1:52:A:LEU:H	1:52:A:LEU:HD22	14	0.19
(1,2350)	1:52:A:LEU:H	1:52:A:LEU:HD23	14	0.19
(1,2350)	1:52:A:LEU:H	1:52:A:LEU:HD21	16	0.19
(1,2350)	1:52:A:LEU:H	1:52:A:LEU:HD22	16	0.19
(1,2350)	1:52:A:LEU:H	1:52:A:LEU:HD23	16	0.19
(1,2300)	1:49:A:SER:H	1:50:A:ILE:HG13	19	0.19
(1,2300)	1:49:A:SER:H	1:50:A:ILE:HG13	20	0.19
(1,2248)	1:70:A:LYS:HA	1:70:A:LYS:HD3	17	0.19
(1,2248)	1:70:A:LYS:HA	1:70:A:LYS:HD3	20	0.19
(1,2145)	1:2:A:SER:HB2	1:3:A:VAL:HB	9	0.19
(1,1939)	1:92:A:LEU:HD21	1:80:A:ASP:HB3	3	0.19
(1,1939)	1:92:A:LEU:HD22	1:80:A:ASP:HB3	3	0.19
(1,1939)	1:92:A:LEU:HD23	1:80:A:ASP:HB3	3	0.19
(1,1859)	1:27:A:ILE:HD11	1:23:A:LYS:HE2	18	0.19
(1,1859)	1:27:A:ILE:HD12	1:23:A:LYS:HE2	18	0.19
(1,1859)	1:27:A:ILE:HD13	1:23:A:LYS:HE2	18	0.19
(1,1843)	1:24:A:SER:HB2	1:23:A:LYS:HE2	9	0.19
(1,1843)	1:24:A:SER:HB3	1:23:A:LYS:HE2	9	0.19
(1,1780)	1:129:A:LYS:H	1:134:A:ARG:HD2	8	0.19
(1,1780)	1:129:A:LYS:H	1:134:A:ARG:HD3	8	0.19
(1,1549)	1:70:A:LYS:HB2	1:5:A:ILE:HD11	1	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1549)	1:70:A:LYS:HB2	1:5:A:ILE:HD12	1	0.19
(1,1549)	1:70:A:LYS:HB2	1:5:A:ILE:HD13	1	0.19
(1,1489)	1:70:A:LYS:H	1:5:A:ILE:HD11	8	0.19
(1,1489)	1:70:A:LYS:H	1:5:A:ILE:HD12	8	0.19
(1,1489)	1:70:A:LYS:H	1:5:A:ILE:HD13	8	0.19
(1,1489)	1:70:A:LYS:H	1:5:A:ILE:HD11	9	0.19
(1,1489)	1:70:A:LYS:H	1:5:A:ILE:HD12	9	0.19
(1,1489)	1:70:A:LYS:H	1:5:A:ILE:HD13	9	0.19
(1,1451)	1:119:A:ILE:HG21	1:93:A:ILE:HD11	9	0.19
(1,1451)	1:119:A:ILE:HG21	1:93:A:ILE:HD12	9	0.19
(1,1451)	1:119:A:ILE:HG21	1:93:A:ILE:HD13	9	0.19
(1,1451)	1:119:A:ILE:HG22	1:93:A:ILE:HD11	9	0.19
(1,1451)	1:119:A:ILE:HG22	1:93:A:ILE:HD12	9	0.19
(1,1451)	1:119:A:ILE:HG22	1:93:A:ILE:HD13	9	0.19
(1,1451)	1:119:A:ILE:HG23	1:93:A:ILE:HD11	9	0.19
(1,1451)	1:119:A:ILE:HG23	1:93:A:ILE:HD12	9	0.19
(1,1451)	1:119:A:ILE:HG23	1:93:A:ILE:HD13	9	0.19
(1,1444)	1:41:A:VAL:HB	1:68:A:ILE:HD11	5	0.19
(1,1444)	1:41:A:VAL:HB	1:68:A:ILE:HD12	5	0.19
(1,1444)	1:41:A:VAL:HB	1:68:A:ILE:HD13	5	0.19
(1,1326)	1:5:A:ILE:HD11	1:39:A:ALA:H	15	0.19
(1,1326)	1:5:A:ILE:HD12	1:39:A:ALA:H	15	0.19
(1,1326)	1:5:A:ILE:HD13	1:39:A:ALA:H	15	0.19
(1,1306)	1:50:A:ILE:HG21	1:53:A:ALA:H	6	0.19
(1,1306)	1:50:A:ILE:HG22	1:53:A:ALA:H	6	0.19
(1,1306)	1:50:A:ILE:HG23	1:53:A:ALA:H	6	0.19
(1,1225)	1:110:A:ALA:HA	1:76:A:TYR:H	17	0.19
(1,1220)	1:131:A:ILE:HG21	1:133:A:GLY:H	6	0.19
(1,1220)	1:131:A:ILE:HG22	1:133:A:GLY:H	6	0.19
(1,1220)	1:131:A:ILE:HG23	1:133:A:GLY:H	6	0.19
(1,1220)	1:131:A:ILE:HG21	1:133:A:GLY:H	11	0.19
(1,1220)	1:131:A:ILE:HG22	1:133:A:GLY:H	11	0.19
(1,1220)	1:131:A:ILE:HG23	1:133:A:GLY:H	11	0.19
(1,1220)	1:131:A:ILE:HG21	1:133:A:GLY:H	12	0.19
(1,1220)	1:131:A:ILE:HG22	1:133:A:GLY:H	12	0.19
(1,1220)	1:131:A:ILE:HG23	1:133:A:GLY:H	12	0.19
(1,1163)	1:27:A:ILE:HD11	1:27:A:ILE:H	1	0.19
(1,1163)	1:27:A:ILE:HD12	1:27:A:ILE:H	1	0.19
(1,1163)	1:27:A:ILE:HD13	1:27:A:ILE:H	1	0.19
(1,1163)	1:27:A:ILE:HD11	1:27:A:ILE:H	14	0.19
(1,1163)	1:27:A:ILE:HD12	1:27:A:ILE:H	14	0.19
(1,1163)	1:27:A:ILE:HD13	1:27:A:ILE:H	14	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1132)	1:131:A:ILE:HG12	1:130:A:TYR:H	20	0.19
(1,1122)	1:93:A:ILE:HD11	1:94:A:CYS:H	20	0.19
(1,1122)	1:93:A:ILE:HD12	1:94:A:CYS:H	20	0.19
(1,1122)	1:93:A:ILE:HD13	1:94:A:CYS:H	20	0.19
(1,1091)	1:103:A:LEU:HD21	1:104:A:SER:H	3	0.19
(1,1091)	1:103:A:LEU:HD22	1:104:A:SER:H	3	0.19
(1,1091)	1:103:A:LEU:HD23	1:104:A:SER:H	3	0.19
(1,1067)	1:68:A:ILE:HD11	1:63:A:GLY:H	20	0.19
(1,1067)	1:68:A:ILE:HD12	1:63:A:GLY:H	20	0.19
(1,1067)	1:68:A:ILE:HD13	1:63:A:GLY:H	20	0.19
(1,1042)	1:50:A:ILE:HD11	1:49:A:SER:H	19	0.19
(1,1042)	1:50:A:ILE:HD12	1:49:A:SER:H	19	0.19
(1,1042)	1:50:A:ILE:HD13	1:49:A:SER:H	19	0.19
(1,981)	1:84:A:ILE:HD11	1:82:A:ASN:H	10	0.19
(1,981)	1:84:A:ILE:HD12	1:82:A:ASN:H	10	0.19
(1,981)	1:84:A:ILE:HD13	1:82:A:ASN:H	10	0.19
(1,981)	1:84:A:ILE:HD11	1:82:A:ASN:H	11	0.19
(1,981)	1:84:A:ILE:HD12	1:82:A:ASN:H	11	0.19
(1,981)	1:84:A:ILE:HD13	1:82:A:ASN:H	11	0.19
(1,933)	1:52:A:LEU:HD21	1:26:A:LEU:H	18	0.19
(1,933)	1:52:A:LEU:HD22	1:26:A:LEU:H	18	0.19
(1,933)	1:52:A:LEU:HD23	1:26:A:LEU:H	18	0.19
(1,866)	1:27:A:ILE:HG13	1:24:A:SER:H	13	0.19
(1,866)	1:20:A:ALA:HB1	1:24:A:SER:H	18	0.19
(1,866)	1:20:A:ALA:HB2	1:24:A:SER:H	18	0.19
(1,866)	1:20:A:ALA:HB3	1:24:A:SER:H	18	0.19
(1,823)	1:70:A:LYS:HG2	1:69:A:GLY:H	15	0.19
(1,823)	1:70:A:LYS:HG3	1:69:A:GLY:H	15	0.19
(1,806)	1:53:A:ALA:HB1	1:57:A:MET:H	8	0.19
(1,806)	1:53:A:ALA:HB2	1:57:A:MET:H	8	0.19
(1,806)	1:53:A:ALA:HB3	1:57:A:MET:H	8	0.19
(1,806)	1:53:A:ALA:HB1	1:57:A:MET:H	11	0.19
(1,806)	1:53:A:ALA:HB2	1:57:A:MET:H	11	0.19
(1,806)	1:53:A:ALA:HB3	1:57:A:MET:H	11	0.19
(1,772)	1:20:A:ALA:HB1	1:23:A:LYS:H	5	0.19
(1,772)	1:20:A:ALA:HB2	1:23:A:LYS:H	5	0.19
(1,772)	1:20:A:ALA:HB3	1:23:A:LYS:H	5	0.19
(1,772)	1:20:A:ALA:HB1	1:23:A:LYS:H	6	0.19
(1,772)	1:20:A:ALA:HB2	1:23:A:LYS:H	6	0.19
(1,772)	1:20:A:ALA:HB3	1:23:A:LYS:H	6	0.19
(1,582)	1:57:A:MET:HB3	1:58:A:TYR:H	3	0.19
(1,81)	1:58:A:TYR:H	1:61:A:GLY:H	2	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3875)	1:35:A:GLN:HB2	1:8:A:ILE:HG12	15	0.18
(1,3875)	1:35:A:GLN:HB2	1:8:A:ILE:HG13	15	0.18
(1,3871)	1:79:A:ILE:H	1:80:A:ASP:HB3	17	0.18
(1,3834)	1:74:A:TYR:H	1:3:A:VAL:HG11	7	0.18
(1,3834)	1:74:A:TYR:H	1:3:A:VAL:HG12	7	0.18
(1,3834)	1:74:A:TYR:H	1:3:A:VAL:HG13	7	0.18
(1,3834)	1:74:A:TYR:H	1:3:A:VAL:HG11	19	0.18
(1,3834)	1:74:A:TYR:H	1:3:A:VAL:HG12	19	0.18
(1,3834)	1:74:A:TYR:H	1:3:A:VAL:HG13	19	0.18
(1,3828)	1:109:A:PHE:HD1	1:3:A:VAL:HG21	8	0.18
(1,3828)	1:109:A:PHE:HD1	1:3:A:VAL:HG22	8	0.18
(1,3828)	1:109:A:PHE:HD1	1:3:A:VAL:HG23	8	0.18
(1,3828)	1:109:A:PHE:HD2	1:3:A:VAL:HG21	8	0.18
(1,3828)	1:109:A:PHE:HD2	1:3:A:VAL:HG22	8	0.18
(1,3828)	1:109:A:PHE:HD2	1:3:A:VAL:HG23	8	0.18
(1,3791)	1:133:A:GLY:H	1:134:A:ARG:HD2	14	0.18
(1,3791)	1:133:A:GLY:H	1:134:A:ARG:HD3	14	0.18
(1,3724)	1:71:A:ASN:HB3	1:5:A:ILE:HG13	2	0.18
(1,3724)	1:71:A:ASN:HB3	1:5:A:ILE:HG13	5	0.18
(1,3712)	1:130:A:TYR:HE1	1:137:A:HIS:HB3	9	0.18
(1,3712)	1:130:A:TYR:HE2	1:137:A:HIS:HB3	9	0.18
(1,3623)	1:135:A:ILE:HG12	1:134:A:ARG:HA	18	0.18
(1,3581)	1:56:A:GLN:H	1:68:A:ILE:HD11	5	0.18
(1,3581)	1:56:A:GLN:H	1:68:A:ILE:HD12	5	0.18
(1,3581)	1:56:A:GLN:H	1:68:A:ILE:HD13	5	0.18
(1,3543)	1:17:A:ILE:HA	1:21:A:ILE:HD11	16	0.18
(1,3543)	1:17:A:ILE:HA	1:21:A:ILE:HD12	16	0.18
(1,3543)	1:17:A:ILE:HA	1:21:A:ILE:HD13	16	0.18
(1,3543)	1:17:A:ILE:HA	1:21:A:ILE:HD11	18	0.18
(1,3543)	1:17:A:ILE:HA	1:21:A:ILE:HD12	18	0.18
(1,3543)	1:17:A:ILE:HA	1:21:A:ILE:HD13	18	0.18
(1,3543)	1:17:A:ILE:HA	1:21:A:ILE:HD11	19	0.18
(1,3543)	1:17:A:ILE:HA	1:21:A:ILE:HD12	19	0.18
(1,3543)	1:17:A:ILE:HA	1:21:A:ILE:HD13	19	0.18
(1,3219)	1:93:A:ILE:HD11	1:119:A:ILE:HD11	4	0.18
(1,3219)	1:93:A:ILE:HD11	1:119:A:ILE:HD12	4	0.18
(1,3219)	1:93:A:ILE:HD11	1:119:A:ILE:HD13	4	0.18
(1,3219)	1:93:A:ILE:HD12	1:119:A:ILE:HD11	4	0.18
(1,3219)	1:93:A:ILE:HD12	1:119:A:ILE:HD12	4	0.18
(1,3219)	1:93:A:ILE:HD12	1:119:A:ILE:HD13	4	0.18
(1,3219)	1:93:A:ILE:HD13	1:119:A:ILE:HD11	4	0.18
(1,3219)	1:93:A:ILE:HD13	1:119:A:ILE:HD12	4	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3219)	1:93:A:ILE:HD13	1:119:A:ILE:HD13	4	0.18
(1,3095)	1:57:A:MET:HE1	1:53:A:ALA:HA	19	0.18
(1,3095)	1:57:A:MET:HE2	1:53:A:ALA:HA	19	0.18
(1,3095)	1:57:A:MET:HE3	1:53:A:ALA:HA	19	0.18
(1,3074)	1:4:A:LYS:HB2	1:71:A:ASN:HA	5	0.18
(1,3074)	1:4:A:LYS:HB2	1:71:A:ASN:HA	20	0.18
(1,3049)	1:12:A:GLY:HA2	1:13:A:GLU:HG2	10	0.18
(1,3049)	1:12:A:GLY:HA2	1:13:A:GLU:HG3	10	0.18
(1,2980)	1:54:A:ILE:HB	1:53:A:ALA:HB1	18	0.18
(1,2980)	1:54:A:ILE:HB	1:53:A:ALA:HB2	18	0.18
(1,2980)	1:54:A:ILE:HB	1:53:A:ALA:HB3	18	0.18
(1,2904)	1:3:A:VAL:HA	1:38:A:ALA:HB1	4	0.18
(1,2904)	1:3:A:VAL:HA	1:38:A:ALA:HB2	4	0.18
(1,2904)	1:3:A:VAL:HA	1:38:A:ALA:HB3	4	0.18
(1,2904)	1:3:A:VAL:HA	1:38:A:ALA:HB1	6	0.18
(1,2904)	1:3:A:VAL:HA	1:38:A:ALA:HB2	6	0.18
(1,2904)	1:3:A:VAL:HA	1:38:A:ALA:HB3	6	0.18
(1,2829)	1:59:A:LEU:H	1:14:A:ILE:HG21	13	0.18
(1,2829)	1:59:A:LEU:H	1:14:A:ILE:HG22	13	0.18
(1,2829)	1:59:A:LEU:H	1:14:A:ILE:HG23	13	0.18
(1,2752)	1:35:A:GLN:HB2	1:32:A:THR:HG21	7	0.18
(1,2752)	1:35:A:GLN:HB2	1:32:A:THR:HG22	7	0.18
(1,2752)	1:35:A:GLN:HB2	1:32:A:THR:HG23	7	0.18
(1,2743)	1:18:A:ASP:HB2	1:8:A:ILE:HG21	8	0.18
(1,2743)	1:18:A:ASP:HB2	1:8:A:ILE:HG22	8	0.18
(1,2743)	1:18:A:ASP:HB2	1:8:A:ILE:HG23	8	0.18
(1,2697)	1:57:A:MET:HB2	1:65:A:THR:HG21	3	0.18
(1,2697)	1:57:A:MET:HB2	1:65:A:THR:HG22	3	0.18
(1,2697)	1:57:A:MET:HB2	1:65:A:THR:HG23	3	0.18
(1,2664)	1:52:A:LEU:H	1:41:A:VAL:HG21	17	0.18
(1,2664)	1:52:A:LEU:H	1:41:A:VAL:HG22	17	0.18
(1,2664)	1:52:A:LEU:H	1:41:A:VAL:HG23	17	0.18
(1,2583)	1:126:A:LEU:HB2	1:138:A:LEU:HD21	16	0.18
(1,2583)	1:126:A:LEU:HB2	1:138:A:LEU:HD22	16	0.18
(1,2583)	1:126:A:LEU:HB2	1:138:A:LEU:HD23	16	0.18
(1,2550)	1:40:A:ASP:HB3	1:47:A:VAL:HG11	1	0.18
(1,2550)	1:40:A:ASP:HB3	1:47:A:VAL:HG12	1	0.18
(1,2550)	1:40:A:ASP:HB3	1:47:A:VAL:HG13	1	0.18
(1,2515)	1:93:A:ILE:HA	1:103:A:LEU:HD11	15	0.18
(1,2515)	1:93:A:ILE:HA	1:103:A:LEU:HD12	15	0.18
(1,2515)	1:93:A:ILE:HA	1:103:A:LEU:HD13	15	0.18
(1,2472)	1:145:A:GLU:H	1:144:A:LEU:HD21	2	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2472)	1:145:A:GLU:H	1:144:A:LEU:HD22	2	0.18
(1,2472)	1:145:A:GLU:H	1:144:A:LEU:HD23	2	0.18
(1,2455)	1:143:A:GLN:H	1:144:A:LEU:HD21	9	0.18
(1,2455)	1:143:A:GLN:H	1:144:A:LEU:HD22	9	0.18
(1,2455)	1:143:A:GLN:H	1:144:A:LEU:HD23	9	0.18
(1,2373)	1:55:A:LEU:HA	1:59:A:LEU:HD21	12	0.18
(1,2373)	1:55:A:LEU:HA	1:59:A:LEU:HD22	12	0.18
(1,2373)	1:55:A:LEU:HA	1:59:A:LEU:HD23	12	0.18
(1,2373)	1:55:A:LEU:HA	1:59:A:LEU:HD21	16	0.18
(1,2373)	1:55:A:LEU:HA	1:59:A:LEU:HD22	16	0.18
(1,2373)	1:55:A:LEU:HA	1:59:A:LEU:HD23	16	0.18
(1,2352)	1:85:A:VAL:HA	1:84:A:ILE:HG13	6	0.18
(1,2352)	1:85:A:VAL:HA	1:84:A:ILE:HG13	9	0.18
(1,2316)	1:121:A:GLN:H	1:121:A:GLN:HB3	18	0.18
(1,2300)	1:49:A:SER:H	1:50:A:ILE:HG13	16	0.18
(1,2273)	1:70:A:LYS:HB2	1:70:A:LYS:HD2	2	0.18
(1,2273)	1:70:A:LYS:HB2	1:70:A:LYS:HD2	13	0.18
(1,2248)	1:70:A:LYS:HA	1:70:A:LYS:HD3	1	0.18
(1,2248)	1:70:A:LYS:HA	1:70:A:LYS:HD3	14	0.18
(1,2180)	1:23:A:LYS:HD2	1:23:A:LYS:HB2	18	0.18
(1,1939)	1:92:A:LEU:HD21	1:80:A:ASP:HB3	15	0.18
(1,1939)	1:92:A:LEU:HD22	1:80:A:ASP:HB3	15	0.18
(1,1939)	1:92:A:LEU:HD23	1:80:A:ASP:HB3	15	0.18
(1,1841)	1:62:A:LYS:HB3	1:62:A:LYS:HE3	12	0.18
(1,1813)	1:35:A:GLN:HE21	1:34:A:LYS:HE2	17	0.18
(1,1806)	1:81:A:ASN:HD22	1:72:A:ARG:HD3	13	0.18
(1,1792)	1:133:A:GLY:H	1:134:A:ARG:HD2	14	0.18
(1,1792)	1:133:A:GLY:H	1:134:A:ARG:HD3	14	0.18
(1,1768)	1:57:A:MET:HB2	1:64:A:GLY:HA2	4	0.18
(1,1768)	1:57:A:MET:HB2	1:64:A:GLY:HA3	4	0.18
(1,1502)	1:26:A:LEU:HA	1:27:A:ILE:HA	11	0.18
(1,1489)	1:70:A:LYS:H	1:5:A:ILE:HD11	7	0.18
(1,1489)	1:70:A:LYS:H	1:5:A:ILE:HD12	7	0.18
(1,1489)	1:70:A:LYS:H	1:5:A:ILE:HD13	7	0.18
(1,1489)	1:70:A:LYS:H	1:5:A:ILE:HD11	12	0.18
(1,1489)	1:70:A:LYS:H	1:5:A:ILE:HD12	12	0.18
(1,1489)	1:70:A:LYS:H	1:5:A:ILE:HD13	12	0.18
(1,1451)	1:119:A:ILE:HG21	1:93:A:ILE:HD11	13	0.18
(1,1451)	1:119:A:ILE:HG21	1:93:A:ILE:HD12	13	0.18
(1,1451)	1:119:A:ILE:HG21	1:93:A:ILE:HD13	13	0.18
(1,1451)	1:119:A:ILE:HG22	1:93:A:ILE:HD11	13	0.18
(1,1451)	1:119:A:ILE:HG22	1:93:A:ILE:HD12	13	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1451)	1:119:A:ILE:HG22	1:93:A:ILE:HD13	13	0.18
(1,1451)	1:119:A:ILE:HG23	1:93:A:ILE:HD11	13	0.18
(1,1451)	1:119:A:ILE:HG23	1:93:A:ILE:HD12	13	0.18
(1,1451)	1:119:A:ILE:HG23	1:93:A:ILE:HD13	13	0.18
(1,1451)	1:119:A:ILE:HG21	1:93:A:ILE:HD11	17	0.18
(1,1451)	1:119:A:ILE:HG21	1:93:A:ILE:HD12	17	0.18
(1,1451)	1:119:A:ILE:HG21	1:93:A:ILE:HD13	17	0.18
(1,1451)	1:119:A:ILE:HG22	1:93:A:ILE:HD11	17	0.18
(1,1451)	1:119:A:ILE:HG22	1:93:A:ILE:HD12	17	0.18
(1,1451)	1:119:A:ILE:HG22	1:93:A:ILE:HD13	17	0.18
(1,1451)	1:119:A:ILE:HG23	1:93:A:ILE:HD11	17	0.18
(1,1451)	1:119:A:ILE:HG23	1:93:A:ILE:HD12	17	0.18
(1,1451)	1:119:A:ILE:HG23	1:93:A:ILE:HD13	17	0.18
(1,1328)	1:97:A:ILE:HG21	1:121:A:GLN:H	3	0.18
(1,1328)	1:97:A:ILE:HG22	1:121:A:GLN:H	3	0.18
(1,1328)	1:97:A:ILE:HG23	1:121:A:GLN:H	3	0.18
(1,1238)	1:59:A:LEU:HD21	1:20:A:ALA:H	10	0.18
(1,1238)	1:59:A:LEU:HD22	1:20:A:ALA:H	10	0.18
(1,1238)	1:59:A:LEU:HD23	1:20:A:ALA:H	10	0.18
(1,1238)	1:59:A:LEU:HD21	1:20:A:ALA:H	20	0.18
(1,1238)	1:59:A:LEU:HD22	1:20:A:ALA:H	20	0.18
(1,1238)	1:59:A:LEU:HD23	1:20:A:ALA:H	20	0.18
(1,1197)	1:126:A:LEU:HD11	1:122:A:THR:H	13	0.18
(1,1197)	1:126:A:LEU:HD12	1:122:A:THR:H	13	0.18
(1,1197)	1:126:A:LEU:HD13	1:122:A:THR:H	13	0.18
(1,1197)	1:126:A:LEU:HD11	1:122:A:THR:H	16	0.18
(1,1197)	1:126:A:LEU:HD12	1:122:A:THR:H	16	0.18
(1,1197)	1:126:A:LEU:HD13	1:122:A:THR:H	16	0.18
(1,1197)	1:126:A:LEU:HD11	1:122:A:THR:H	19	0.18
(1,1197)	1:126:A:LEU:HD12	1:122:A:THR:H	19	0.18
(1,1197)	1:126:A:LEU:HD13	1:122:A:THR:H	19	0.18
(1,1195)	1:60:A:LEU:HD21	1:57:A:MET:H	9	0.18
(1,1195)	1:60:A:LEU:HD22	1:57:A:MET:H	9	0.18
(1,1195)	1:60:A:LEU:HD23	1:57:A:MET:H	9	0.18
(1,1177)	1:92:A:LEU:HD11	1:89:A:ASP:H	10	0.18
(1,1177)	1:92:A:LEU:HD12	1:89:A:ASP:H	10	0.18
(1,1177)	1:92:A:LEU:HD13	1:89:A:ASP:H	10	0.18
(1,1163)	1:27:A:ILE:HD11	1:27:A:ILE:H	18	0.18
(1,1163)	1:27:A:ILE:HD12	1:27:A:ILE:H	18	0.18
(1,1163)	1:27:A:ILE:HD13	1:27:A:ILE:H	18	0.18
(1,1141)	1:144:A:LEU:HG	1:143:A:GLN:H	20	0.18
(1,1140)	1:144:A:LEU:HD21	1:143:A:GLN:H	9	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1140)	1:144:A:LEU:HD22	1:143:A:GLN:H	9	0.18
(1,1140)	1:144:A:LEU:HD23	1:143:A:GLN:H	9	0.18
(1,1137)	1:97:A:ILE:HG21	1:96:A:HIS:H	12	0.18
(1,1137)	1:97:A:ILE:HG22	1:96:A:HIS:H	12	0.18
(1,1137)	1:97:A:ILE:HG23	1:96:A:HIS:H	12	0.18
(1,1122)	1:93:A:ILE:HD11	1:94:A:CYS:H	11	0.18
(1,1122)	1:93:A:ILE:HD12	1:94:A:CYS:H	11	0.18
(1,1122)	1:93:A:ILE:HD13	1:94:A:CYS:H	11	0.18
(1,1122)	1:93:A:ILE:HD11	1:94:A:CYS:H	15	0.18
(1,1122)	1:93:A:ILE:HD12	1:94:A:CYS:H	15	0.18
(1,1122)	1:93:A:ILE:HD13	1:94:A:CYS:H	15	0.18
(1,1122)	1:93:A:ILE:HD11	1:94:A:CYS:H	19	0.18
(1,1122)	1:93:A:ILE:HD12	1:94:A:CYS:H	19	0.18
(1,1122)	1:93:A:ILE:HD13	1:94:A:CYS:H	19	0.18
(1,1117)	1:96:A:HIS:HA	1:102:A:GLN:H	13	0.18
(1,1117)	1:96:A:HIS:HA	1:102:A:GLN:H	16	0.18
(1,1091)	1:103:A:LEU:HD21	1:104:A:SER:H	1	0.18
(1,1091)	1:103:A:LEU:HD22	1:104:A:SER:H	1	0.18
(1,1091)	1:103:A:LEU:HD23	1:104:A:SER:H	1	0.18
(1,1091)	1:103:A:LEU:HD21	1:104:A:SER:H	7	0.18
(1,1091)	1:103:A:LEU:HD22	1:104:A:SER:H	7	0.18
(1,1091)	1:103:A:LEU:HD23	1:104:A:SER:H	7	0.18
(1,1056)	1:122:A:THR:HG21	1:114:A:ASP:H	19	0.18
(1,1056)	1:122:A:THR:HG22	1:114:A:ASP:H	19	0.18
(1,1056)	1:122:A:THR:HG23	1:114:A:ASP:H	19	0.18
(1,1043)	1:8:A:ILE:HG21	1:32:A:THR:H	14	0.18
(1,1043)	1:8:A:ILE:HG22	1:32:A:THR:H	14	0.18
(1,1043)	1:8:A:ILE:HG23	1:32:A:THR:H	14	0.18
(1,1042)	1:50:A:ILE:HD11	1:49:A:SER:H	1	0.18
(1,1042)	1:50:A:ILE:HD12	1:49:A:SER:H	1	0.18
(1,1042)	1:50:A:ILE:HD13	1:49:A:SER:H	1	0.18
(1,1042)	1:50:A:ILE:HD11	1:49:A:SER:H	11	0.18
(1,1042)	1:50:A:ILE:HD12	1:49:A:SER:H	11	0.18
(1,1042)	1:50:A:ILE:HD13	1:49:A:SER:H	11	0.18
(1,1022)	1:79:A:ILE:HG21	1:81:A:ASN:H	10	0.18
(1,1022)	1:79:A:ILE:HG22	1:81:A:ASN:H	10	0.18
(1,1022)	1:79:A:ILE:HG23	1:81:A:ASN:H	10	0.18
(1,1021)	1:92:A:LEU:HD11	1:88:A:ASN:HD22	1	0.18
(1,1021)	1:92:A:LEU:HD12	1:88:A:ASN:HD22	1	0.18
(1,1021)	1:92:A:LEU:HD13	1:88:A:ASN:HD22	1	0.18
(1,980)	1:54:A:ILE:HD11	1:42:A:ASP:H	17	0.18
(1,980)	1:54:A:ILE:HD12	1:42:A:ASP:H	17	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,980)	1:54:A:ILE:HD13	1:42:A:ASP:H	17	0.18
(1,948)	1:5:A:ILE:HG21	1:70:A:LYS:H	2	0.18
(1,948)	1:5:A:ILE:HG22	1:70:A:LYS:H	2	0.18
(1,948)	1:5:A:ILE:HG23	1:70:A:LYS:H	2	0.18
(1,909)	1:73:A:ILE:HD11	1:73:A:ILE:H	3	0.18
(1,909)	1:73:A:ILE:HD12	1:73:A:ILE:H	3	0.18
(1,909)	1:73:A:ILE:HD13	1:73:A:ILE:H	3	0.18
(1,903)	1:41:A:VAL:HG21	1:48:A:ASN:H	6	0.18
(1,903)	1:41:A:VAL:HG22	1:48:A:ASN:H	6	0.18
(1,903)	1:41:A:VAL:HG23	1:48:A:ASN:H	6	0.18
(1,903)	1:41:A:VAL:HG21	1:48:A:ASN:H	12	0.18
(1,903)	1:41:A:VAL:HG22	1:48:A:ASN:H	12	0.18
(1,903)	1:41:A:VAL:HG23	1:48:A:ASN:H	12	0.18
(1,874)	1:139:A:PRO:HG2	1:115:A:GLY:H	3	0.18
(1,874)	1:139:A:PRO:HG3	1:115:A:GLY:H	3	0.18
(1,870)	1:52:A:LEU:HG	1:56:A:GLN:HE21	19	0.18
(1,779)	1:62:A:LYS:HB3	1:62:A:LYS:H	8	0.18
(1,772)	1:23:A:LYS:HD2	1:23:A:LYS:H	13	0.18
(1,386)	1:96:A:HIS:HB3	1:119:A:ILE:H	5	0.18
(1,386)	1:96:A:HIS:HB3	1:119:A:ILE:H	6	0.18
(1,386)	1:117:A:ASN:HA	1:119:A:ILE:H	9	0.18
(1,81)	1:58:A:TYR:H	1:61:A:GLY:H	15	0.18
(1,3843)	1:126:A:LEU:HA	1:113:A:ALA:HB1	8	0.17
(1,3843)	1:126:A:LEU:HA	1:113:A:ALA:HB2	8	0.17
(1,3843)	1:126:A:LEU:HA	1:113:A:ALA:HB3	8	0.17
(1,3840)	1:123:A:ASP:HB2	1:111:A:ALA:HB1	2	0.17
(1,3840)	1:123:A:ASP:HB2	1:111:A:ALA:HB2	2	0.17
(1,3840)	1:123:A:ASP:HB2	1:111:A:ALA:HB3	2	0.17
(1,3834)	1:74:A:TYR:H	1:3:A:VAL:HG11	1	0.17
(1,3834)	1:74:A:TYR:H	1:3:A:VAL:HG12	1	0.17
(1,3834)	1:74:A:TYR:H	1:3:A:VAL:HG13	1	0.17
(1,3834)	1:74:A:TYR:H	1:3:A:VAL:HG11	8	0.17
(1,3834)	1:74:A:TYR:H	1:3:A:VAL:HG12	8	0.17
(1,3834)	1:74:A:TYR:H	1:3:A:VAL:HG13	8	0.17
(1,3812)	1:70:A:LYS:HA	1:4:A:LYS:HD2	2	0.17
(1,3791)	1:132:A:THR:H	1:134:A:ARG:HD2	13	0.17
(1,3791)	1:132:A:THR:H	1:134:A:ARG:HD3	13	0.17
(1,3697)	1:101:A:GLY:HA2	1:102:A:GLN:HG3	6	0.17
(1,3623)	1:135:A:ILE:HG12	1:134:A:ARG:HA	2	0.17
(1,3581)	1:67:A:ASP:H	1:68:A:ILE:HD11	8	0.17
(1,3581)	1:67:A:ASP:H	1:68:A:ILE:HD12	8	0.17
(1,3581)	1:67:A:ASP:H	1:68:A:ILE:HD13	8	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3543)	1:17:A:ILE:HA	1:21:A:ILE:HD11	9	0.17
(1,3543)	1:17:A:ILE:HA	1:21:A:ILE:HD12	9	0.17
(1,3543)	1:17:A:ILE:HA	1:21:A:ILE:HD13	9	0.17
(1,3543)	1:17:A:ILE:HA	1:21:A:ILE:HD11	11	0.17
(1,3543)	1:17:A:ILE:HA	1:21:A:ILE:HD12	11	0.17
(1,3543)	1:17:A:ILE:HA	1:21:A:ILE:HD13	11	0.17
(1,3543)	1:17:A:ILE:HA	1:21:A:ILE:HD11	15	0.17
(1,3543)	1:17:A:ILE:HA	1:21:A:ILE:HD12	15	0.17
(1,3543)	1:17:A:ILE:HA	1:21:A:ILE:HD13	15	0.17
(1,3274)	1:73:A:ILE:HA	1:72:A:ARG:HD2	19	0.17
(1,3219)	1:93:A:ILE:HD11	1:119:A:ILE:HD11	9	0.17
(1,3219)	1:93:A:ILE:HD11	1:119:A:ILE:HD12	9	0.17
(1,3219)	1:93:A:ILE:HD11	1:119:A:ILE:HD13	9	0.17
(1,3219)	1:93:A:ILE:HD12	1:119:A:ILE:HD11	9	0.17
(1,3219)	1:93:A:ILE:HD12	1:119:A:ILE:HD12	9	0.17
(1,3219)	1:93:A:ILE:HD12	1:119:A:ILE:HD13	9	0.17
(1,3219)	1:93:A:ILE:HD13	1:119:A:ILE:HD11	9	0.17
(1,3219)	1:93:A:ILE:HD13	1:119:A:ILE:HD12	9	0.17
(1,3219)	1:93:A:ILE:HD13	1:119:A:ILE:HD13	9	0.17
(1,3219)	1:93:A:ILE:HD11	1:119:A:ILE:HD11	14	0.17
(1,3219)	1:93:A:ILE:HD11	1:119:A:ILE:HD12	14	0.17
(1,3219)	1:93:A:ILE:HD11	1:119:A:ILE:HD13	14	0.17
(1,3219)	1:93:A:ILE:HD12	1:119:A:ILE:HD11	14	0.17
(1,3219)	1:93:A:ILE:HD12	1:119:A:ILE:HD12	14	0.17
(1,3219)	1:93:A:ILE:HD12	1:119:A:ILE:HD13	14	0.17
(1,3219)	1:93:A:ILE:HD13	1:119:A:ILE:HD11	14	0.17
(1,3219)	1:93:A:ILE:HD13	1:119:A:ILE:HD12	14	0.17
(1,3219)	1:93:A:ILE:HD13	1:119:A:ILE:HD13	14	0.17
(1,3183)	1:35:A:GLN:HG2	1:8:A:ILE:HD11	7	0.17
(1,3183)	1:35:A:GLN:HG2	1:8:A:ILE:HD12	7	0.17
(1,3183)	1:35:A:GLN:HG2	1:8:A:ILE:HD13	7	0.17
(1,3183)	1:88:A:ASN:HB3	1:79:A:ILE:HD11	11	0.17
(1,3183)	1:88:A:ASN:HB3	1:79:A:ILE:HD12	11	0.17
(1,3183)	1:88:A:ASN:HB3	1:79:A:ILE:HD13	11	0.17
(1,3183)	1:90:A:TYR:HB2	1:79:A:ILE:HD11	18	0.17
(1,3183)	1:90:A:TYR:HB2	1:79:A:ILE:HD12	18	0.17
(1,3183)	1:90:A:TYR:HB2	1:79:A:ILE:HD13	18	0.17
(1,3177)	1:129:A:LYS:HE2	1:135:A:ILE:HD11	17	0.17
(1,3177)	1:129:A:LYS:HE2	1:135:A:ILE:HD12	17	0.17
(1,3177)	1:129:A:LYS:HE2	1:135:A:ILE:HD13	17	0.17
(1,3177)	1:129:A:LYS:HE3	1:135:A:ILE:HD11	17	0.17
(1,3177)	1:129:A:LYS:HE3	1:135:A:ILE:HD12	17	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3177)	1:129:A:LYS:HE3	1:135:A:ILE:HD13	17	0.17
(1,3128)	1:24:A:SER:H	1:22:A:LEU:HA	4	0.17
(1,3049)	1:12:A:GLY:HA2	1:13:A:GLU:HG2	12	0.17
(1,3049)	1:12:A:GLY:HA2	1:13:A:GLU:HG3	12	0.17
(1,3040)	1:18:A:ASP:HB2	1:14:A:ILE:HG21	2	0.17
(1,3040)	1:18:A:ASP:HB2	1:14:A:ILE:HG22	2	0.17
(1,3040)	1:18:A:ASP:HB2	1:14:A:ILE:HG23	2	0.17
(1,2980)	1:21:A:ILE:HB	1:20:A:ALA:HB1	7	0.17
(1,2980)	1:21:A:ILE:HB	1:20:A:ALA:HB2	7	0.17
(1,2980)	1:21:A:ILE:HB	1:20:A:ALA:HB3	7	0.17
(1,2721)	1:134:A:ARG:HD2	1:132:A:THR:HG21	14	0.17
(1,2721)	1:134:A:ARG:HD2	1:132:A:THR:HG22	14	0.17
(1,2721)	1:134:A:ARG:HD2	1:132:A:THR:HG23	14	0.17
(1,2721)	1:134:A:ARG:HD3	1:132:A:THR:HG21	14	0.17
(1,2721)	1:134:A:ARG:HD3	1:132:A:THR:HG22	14	0.17
(1,2721)	1:134:A:ARG:HD3	1:132:A:THR:HG23	14	0.17
(1,2713)	1:80:A:ASP:HA	1:79:A:ILE:HG21	14	0.17
(1,2713)	1:80:A:ASP:HA	1:79:A:ILE:HG22	14	0.17
(1,2713)	1:80:A:ASP:HA	1:79:A:ILE:HG23	14	0.17
(1,2641)	1:115:A:GLY:H	1:113:A:ALA:HB1	17	0.17
(1,2641)	1:115:A:GLY:H	1:113:A:ALA:HB2	17	0.17
(1,2641)	1:115:A:GLY:H	1:113:A:ALA:HB3	17	0.17
(1,2583)	1:126:A:LEU:HB2	1:138:A:LEU:HD21	20	0.17
(1,2583)	1:126:A:LEU:HB2	1:138:A:LEU:HD22	20	0.17
(1,2583)	1:126:A:LEU:HB2	1:138:A:LEU:HD23	20	0.17
(1,2509)	1:52:A:LEU:HA	1:52:A:LEU:HD11	16	0.17
(1,2509)	1:52:A:LEU:HA	1:52:A:LEU:HD12	16	0.17
(1,2509)	1:52:A:LEU:HA	1:52:A:LEU:HD13	16	0.17
(1,2449)	1:59:A:LEU:H	1:60:A:LEU:HD21	15	0.17
(1,2449)	1:59:A:LEU:H	1:60:A:LEU:HD22	15	0.17
(1,2449)	1:59:A:LEU:H	1:60:A:LEU:HD23	15	0.17
(1,2350)	1:52:A:LEU:H	1:52:A:LEU:HD21	6	0.17
(1,2350)	1:52:A:LEU:H	1:52:A:LEU:HD22	6	0.17
(1,2350)	1:52:A:LEU:H	1:52:A:LEU:HD23	6	0.17
(1,2273)	1:70:A:LYS:HB2	1:70:A:LYS:HD2	12	0.17
(1,2273)	1:70:A:LYS:HB2	1:70:A:LYS:HD2	16	0.17
(1,2248)	1:70:A:LYS:HA	1:70:A:LYS:HD3	7	0.17
(1,2248)	1:70:A:LYS:HA	1:70:A:LYS:HD3	11	0.17
(1,2224)	1:39:A:ALA:H	1:35:A:GLN:HB3	2	0.17
(1,2180)	1:23:A:LYS:HD2	1:23:A:LYS:HB2	14	0.17
(1,2170)	1:124:A:ARG:HB2	1:128:A:GLU:HG2	5	0.17
(1,2170)	1:124:A:ARG:HB2	1:128:A:GLU:HG3	5	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2170)	1:124:A:ARG:HB3	1:128:A:GLU:HG2	5	0.17
(1,2170)	1:124:A:ARG:HB3	1:128:A:GLU:HG3	5	0.17
(1,2145)	1:37:A:ALA:HA	1:3:A:VAL:HB	15	0.17
(1,1853)	1:132:A:THR:HG21	1:134:A:ARG:HD2	14	0.17
(1,1853)	1:132:A:THR:HG21	1:134:A:ARG:HD3	14	0.17
(1,1853)	1:132:A:THR:HG22	1:134:A:ARG:HD2	14	0.17
(1,1853)	1:132:A:THR:HG22	1:134:A:ARG:HD3	14	0.17
(1,1853)	1:132:A:THR:HG23	1:134:A:ARG:HD2	14	0.17
(1,1853)	1:132:A:THR:HG23	1:134:A:ARG:HD3	14	0.17
(1,1843)	1:24:A:SER:HB2	1:23:A:LYS:HE2	20	0.17
(1,1843)	1:24:A:SER:HB3	1:23:A:LYS:HE2	20	0.17
(1,1840)	1:62:A:LYS:HB3	1:62:A:LYS:HE2	17	0.17
(1,1792)	1:132:A:THR:H	1:134:A:ARG:HD2	13	0.17
(1,1792)	1:132:A:THR:H	1:134:A:ARG:HD3	13	0.17
(1,1651)	1:60:A:LEU:HD11	1:56:A:GLN:HA	3	0.17
(1,1651)	1:60:A:LEU:HD12	1:56:A:GLN:HA	3	0.17
(1,1651)	1:60:A:LEU:HD13	1:56:A:GLN:HA	3	0.17
(1,1549)	1:70:A:LYS:HB2	1:5:A:ILE:HD11	11	0.17
(1,1549)	1:70:A:LYS:HB2	1:5:A:ILE:HD12	11	0.17
(1,1549)	1:70:A:LYS:HB2	1:5:A:ILE:HD13	11	0.17
(1,1511)	1:3:A:VAL:HA	1:5:A:ILE:HD11	4	0.17
(1,1511)	1:3:A:VAL:HA	1:5:A:ILE:HD12	4	0.17
(1,1511)	1:3:A:VAL:HA	1:5:A:ILE:HD13	4	0.17
(1,1489)	1:70:A:LYS:H	1:5:A:ILE:HD11	11	0.17
(1,1489)	1:70:A:LYS:H	1:5:A:ILE:HD12	11	0.17
(1,1489)	1:70:A:LYS:H	1:5:A:ILE:HD13	11	0.17
(1,1489)	1:70:A:LYS:H	1:5:A:ILE:HD11	17	0.17
(1,1489)	1:70:A:LYS:H	1:5:A:ILE:HD12	17	0.17
(1,1489)	1:70:A:LYS:H	1:5:A:ILE:HD13	17	0.17
(1,1358)	1:96:A:HIS:H	1:97:A:ILE:HD11	14	0.17
(1,1358)	1:96:A:HIS:H	1:97:A:ILE:HD12	14	0.17
(1,1358)	1:96:A:HIS:H	1:97:A:ILE:HD13	14	0.17
(1,1328)	1:97:A:ILE:HG21	1:121:A:GLN:H	18	0.17
(1,1328)	1:97:A:ILE:HG22	1:121:A:GLN:H	18	0.17
(1,1328)	1:97:A:ILE:HG23	1:121:A:GLN:H	18	0.17
(1,1260)	1:51:A:ASP:H	1:41:A:VAL:H	9	0.17
(1,1197)	1:126:A:LEU:HD11	1:122:A:THR:H	10	0.17
(1,1197)	1:126:A:LEU:HD12	1:122:A:THR:H	10	0.17
(1,1197)	1:126:A:LEU:HD13	1:122:A:THR:H	10	0.17
(1,1197)	1:126:A:LEU:HD11	1:122:A:THR:H	17	0.17
(1,1197)	1:126:A:LEU:HD12	1:122:A:THR:H	17	0.17
(1,1197)	1:126:A:LEU:HD13	1:122:A:THR:H	17	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1195)	1:60:A:LEU:HD21	1:57:A:MET:H	3	0.17
(1,1195)	1:60:A:LEU:HD22	1:57:A:MET:H	3	0.17
(1,1195)	1:60:A:LEU:HD23	1:57:A:MET:H	3	0.17
(1,1195)	1:60:A:LEU:HD21	1:57:A:MET:H	11	0.17
(1,1195)	1:60:A:LEU:HD22	1:57:A:MET:H	11	0.17
(1,1195)	1:60:A:LEU:HD23	1:57:A:MET:H	11	0.17
(1,1177)	1:92:A:LEU:HD11	1:89:A:ASP:H	15	0.17
(1,1177)	1:92:A:LEU:HD12	1:89:A:ASP:H	15	0.17
(1,1177)	1:92:A:LEU:HD13	1:89:A:ASP:H	15	0.17
(1,1163)	1:27:A:ILE:HD11	1:27:A:ILE:H	11	0.17
(1,1163)	1:27:A:ILE:HD12	1:27:A:ILE:H	11	0.17
(1,1163)	1:27:A:ILE:HD13	1:27:A:ILE:H	11	0.17
(1,1149)	1:135:A:ILE:HG12	1:129:A:LYS:H	17	0.17
(1,1122)	1:93:A:ILE:HD11	1:94:A:CYS:H	12	0.17
(1,1122)	1:93:A:ILE:HD12	1:94:A:CYS:H	12	0.17
(1,1122)	1:93:A:ILE:HD13	1:94:A:CYS:H	12	0.17
(1,1022)	1:79:A:ILE:HG21	1:81:A:ASN:H	4	0.17
(1,1022)	1:79:A:ILE:HG22	1:81:A:ASN:H	4	0.17
(1,1022)	1:79:A:ILE:HG23	1:81:A:ASN:H	4	0.17
(1,1021)	1:92:A:LEU:HD11	1:88:A:ASN:HD22	15	0.17
(1,1021)	1:92:A:LEU:HD12	1:88:A:ASN:HD22	15	0.17
(1,1021)	1:92:A:LEU:HD13	1:88:A:ASN:HD22	15	0.17
(1,1004)	1:59:A:LEU:HD11	1:16:A:SER:H	8	0.17
(1,1004)	1:59:A:LEU:HD12	1:16:A:SER:H	8	0.17
(1,1004)	1:59:A:LEU:HD13	1:16:A:SER:H	8	0.17
(1,988)	1:85:A:VAL:HG21	1:78:A:ASP:H	15	0.17
(1,988)	1:85:A:VAL:HG22	1:78:A:ASP:H	15	0.17
(1,988)	1:85:A:VAL:HG23	1:78:A:ASP:H	15	0.17
(1,980)	1:54:A:ILE:HD11	1:42:A:ASP:H	7	0.17
(1,980)	1:54:A:ILE:HD12	1:42:A:ASP:H	7	0.17
(1,980)	1:54:A:ILE:HD13	1:42:A:ASP:H	7	0.17
(1,980)	1:54:A:ILE:HD11	1:42:A:ASP:H	19	0.17
(1,980)	1:54:A:ILE:HD12	1:42:A:ASP:H	19	0.17
(1,980)	1:54:A:ILE:HD13	1:42:A:ASP:H	19	0.17
(1,978)	1:131:A:ILE:HD11	1:131:A:ILE:H	13	0.17
(1,978)	1:131:A:ILE:HD12	1:131:A:ILE:H	13	0.17
(1,978)	1:131:A:ILE:HD13	1:131:A:ILE:H	13	0.17
(1,939)	1:91:A:ILE:HD11	1:91:A:ILE:H	16	0.17
(1,939)	1:91:A:ILE:HD12	1:91:A:ILE:H	16	0.17
(1,939)	1:91:A:ILE:HD13	1:91:A:ILE:H	16	0.17
(1,933)	1:52:A:LEU:HD21	1:26:A:LEU:H	4	0.17
(1,933)	1:52:A:LEU:HD22	1:26:A:LEU:H	4	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,933)	1:52:A:LEU:HD23	1:26:A:LEU:H	4	0.17
(1,931)	1:8:A:ILE:HG21	1:22:A:LEU:H	11	0.17
(1,931)	1:8:A:ILE:HG22	1:22:A:LEU:H	11	0.17
(1,931)	1:8:A:ILE:HG23	1:22:A:LEU:H	11	0.17
(1,866)	1:27:A:ILE:HG13	1:24:A:SER:H	10	0.17
(1,823)	1:70:A:LYS:HG2	1:69:A:GLY:H	20	0.17
(1,823)	1:70:A:LYS:HG3	1:69:A:GLY:H	20	0.17
(1,779)	1:62:A:LYS:HB3	1:62:A:LYS:H	11	0.17
(1,760)	1:97:A:ILE:HB	1:96:A:HIS:H	6	0.17
(1,741)	1:59:A:LEU:HB3	1:59:A:LEU:H	11	0.17
(1,582)	1:57:A:MET:HB3	1:58:A:TYR:H	11	0.17
(1,582)	1:57:A:MET:HB3	1:58:A:TYR:H	19	0.17
(1,572)	1:9:A:ASP:HB3	1:20:A:ALA:H	6	0.17
(1,528)	1:48:A:ASN:HB2	1:49:A:SER:H	2	0.17
(1,446)	1:43:A:GLY:HA2	1:44:A:ASN:H	10	0.17
(1,386)	1:117:A:ASN:HA	1:119:A:ILE:H	12	0.17
(1,81)	1:58:A:TYR:H	1:61:A:GLY:H	3	0.17
(1,81)	1:58:A:TYR:H	1:61:A:GLY:H	12	0.17
(3,61)	1:109:A:PHE:H	1:105:A:ASP:O	13	0.16
(1,3938)	1:14:A:ILE:HB	1:58:A:TYR:HD1	19	0.16
(1,3938)	1:14:A:ILE:HB	1:58:A:TYR:HD2	19	0.16
(1,3937)	1:23:A:LYS:HD2	1:19:A:TYR:HD1	3	0.16
(1,3937)	1:23:A:LYS:HD2	1:19:A:TYR:HD2	3	0.16
(1,3920)	1:19:A:TYR:HA	1:19:A:TYR:HD1	1	0.16
(1,3920)	1:19:A:TYR:HA	1:19:A:TYR:HD2	1	0.16
(1,3875)	1:55:A:LEU:HB3	1:8:A:ILE:HG12	2	0.16
(1,3875)	1:55:A:LEU:HB3	1:8:A:ILE:HG13	2	0.16
(1,3843)	1:126:A:LEU:HA	1:113:A:ALA:HB1	17	0.16
(1,3843)	1:126:A:LEU:HA	1:113:A:ALA:HB2	17	0.16
(1,3843)	1:126:A:LEU:HA	1:113:A:ALA:HB3	17	0.16
(1,3834)	1:74:A:TYR:H	1:3:A:VAL:HG11	6	0.16
(1,3834)	1:74:A:TYR:H	1:3:A:VAL:HG12	6	0.16
(1,3834)	1:74:A:TYR:H	1:3:A:VAL:HG13	6	0.16
(1,3797)	1:93:A:ILE:H	1:79:A:ILE:HB	3	0.16
(1,3663)	1:68:A:ILE:HG21	1:4:A:LYS:HE2	14	0.16
(1,3663)	1:68:A:ILE:HG21	1:4:A:LYS:HE3	14	0.16
(1,3663)	1:68:A:ILE:HG22	1:4:A:LYS:HE2	14	0.16
(1,3663)	1:68:A:ILE:HG22	1:4:A:LYS:HE3	14	0.16
(1,3663)	1:68:A:ILE:HG23	1:4:A:LYS:HE2	14	0.16
(1,3663)	1:68:A:ILE:HG23	1:4:A:LYS:HE3	14	0.16
(1,3543)	1:17:A:ILE:HA	1:21:A:ILE:HD11	7	0.16
(1,3543)	1:17:A:ILE:HA	1:21:A:ILE:HD12	7	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3543)	1:17:A:ILE:HA	1:21:A:ILE:HD13	7	0.16
(1,3405)	1:121:A:GLN:HE22	1:97:A:ILE:HG21	14	0.16
(1,3405)	1:121:A:GLN:HE22	1:97:A:ILE:HG22	14	0.16
(1,3405)	1:121:A:GLN:HE22	1:97:A:ILE:HG23	14	0.16
(1,3287)	1:14:A:ILE:HG13	1:4:A:LYS:HE2	10	0.16
(1,3287)	1:14:A:ILE:HG13	1:4:A:LYS:HE3	10	0.16
(1,3219)	1:93:A:ILE:HD11	1:119:A:ILE:HD11	3	0.16
(1,3219)	1:93:A:ILE:HD11	1:119:A:ILE:HD12	3	0.16
(1,3219)	1:93:A:ILE:HD11	1:119:A:ILE:HD13	3	0.16
(1,3219)	1:93:A:ILE:HD12	1:119:A:ILE:HD11	3	0.16
(1,3219)	1:93:A:ILE:HD12	1:119:A:ILE:HD12	3	0.16
(1,3219)	1:93:A:ILE:HD12	1:119:A:ILE:HD13	3	0.16
(1,3219)	1:93:A:ILE:HD13	1:119:A:ILE:HD11	3	0.16
(1,3219)	1:93:A:ILE:HD13	1:119:A:ILE:HD12	3	0.16
(1,3219)	1:93:A:ILE:HD13	1:119:A:ILE:HD13	3	0.16
(1,3212)	1:53:A:ALA:HB1	1:49:A:SER:HB2	19	0.16
(1,3212)	1:53:A:ALA:HB1	1:49:A:SER:HB3	19	0.16
(1,3212)	1:53:A:ALA:HB2	1:49:A:SER:HB2	19	0.16
(1,3212)	1:53:A:ALA:HB2	1:49:A:SER:HB3	19	0.16
(1,3212)	1:53:A:ALA:HB3	1:49:A:SER:HB2	19	0.16
(1,3212)	1:53:A:ALA:HB3	1:49:A:SER:HB3	19	0.16
(1,3177)	1:129:A:LYS:HE2	1:135:A:ILE:HD11	12	0.16
(1,3177)	1:129:A:LYS:HE2	1:135:A:ILE:HD12	12	0.16
(1,3177)	1:129:A:LYS:HE2	1:135:A:ILE:HD13	12	0.16
(1,3177)	1:129:A:LYS:HE3	1:135:A:ILE:HD11	12	0.16
(1,3177)	1:129:A:LYS:HE3	1:135:A:ILE:HD12	12	0.16
(1,3177)	1:129:A:LYS:HE3	1:135:A:ILE:HD13	12	0.16
(1,3096)	1:79:A:ILE:HG21	1:80:A:ASP:HA	1	0.16
(1,3096)	1:79:A:ILE:HG22	1:80:A:ASP:HA	1	0.16
(1,3096)	1:79:A:ILE:HG23	1:80:A:ASP:HA	1	0.16
(1,3095)	1:57:A:MET:HE1	1:53:A:ALA:HA	14	0.16
(1,3095)	1:57:A:MET:HE2	1:53:A:ALA:HA	14	0.16
(1,3095)	1:57:A:MET:HE3	1:53:A:ALA:HA	14	0.16
(1,3019)	1:63:A:GLY:HA2	1:65:A:THR:HB	10	0.16
(1,2980)	1:54:A:ILE:HB	1:53:A:ALA:HB1	6	0.16
(1,2980)	1:54:A:ILE:HB	1:53:A:ALA:HB2	6	0.16
(1,2980)	1:54:A:ILE:HB	1:53:A:ALA:HB3	6	0.16
(1,2980)	1:54:A:ILE:HB	1:53:A:ALA:HB1	13	0.16
(1,2980)	1:54:A:ILE:HB	1:53:A:ALA:HB2	13	0.16
(1,2980)	1:54:A:ILE:HB	1:53:A:ALA:HB3	13	0.16
(1,2966)	1:94:A:CYS:HB3	1:91:A:ILE:HG21	6	0.16
(1,2966)	1:94:A:CYS:HB3	1:91:A:ILE:HG22	6	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2966)	1:94:A:CYS:HB3	1:91:A:ILE:HG23	6	0.16
(1,2904)	1:3:A:VAL:HA	1:38:A:ALA:HB1	11	0.16
(1,2904)	1:3:A:VAL:HA	1:38:A:ALA:HB2	11	0.16
(1,2904)	1:3:A:VAL:HA	1:38:A:ALA:HB3	11	0.16
(1,2904)	1:3:A:VAL:HA	1:38:A:ALA:HB1	18	0.16
(1,2904)	1:3:A:VAL:HA	1:38:A:ALA:HB2	18	0.16
(1,2904)	1:3:A:VAL:HA	1:38:A:ALA:HB3	18	0.16
(1,2761)	1:74:A:TYR:HB2	1:75:A:THR:HG21	10	0.16
(1,2761)	1:74:A:TYR:HB2	1:75:A:THR:HG22	10	0.16
(1,2761)	1:74:A:TYR:HB2	1:75:A:THR:HG23	10	0.16
(1,2752)	1:35:A:GLN:HB2	1:32:A:THR:HG21	12	0.16
(1,2752)	1:35:A:GLN:HB2	1:32:A:THR:HG22	12	0.16
(1,2752)	1:35:A:GLN:HB2	1:32:A:THR:HG23	12	0.16
(1,2713)	1:80:A:ASP:HA	1:79:A:ILE:HG21	1	0.16
(1,2713)	1:80:A:ASP:HA	1:79:A:ILE:HG22	1	0.16
(1,2713)	1:80:A:ASP:HA	1:79:A:ILE:HG23	1	0.16
(1,2682)	1:38:A:ALA:H	1:3:A:VAL:HG11	2	0.16
(1,2682)	1:38:A:ALA:H	1:3:A:VAL:HG12	2	0.16
(1,2682)	1:38:A:ALA:H	1:3:A:VAL:HG13	2	0.16
(1,2652)	1:80:A:ASP:H	1:79:A:ILE:HG21	19	0.16
(1,2652)	1:80:A:ASP:H	1:79:A:ILE:HG22	19	0.16
(1,2652)	1:80:A:ASP:H	1:79:A:ILE:HG23	19	0.16
(1,2630)	1:75:A:THR:H	1:75:A:THR:HG21	2	0.16
(1,2630)	1:75:A:THR:H	1:75:A:THR:HG22	2	0.16
(1,2630)	1:75:A:THR:H	1:75:A:THR:HG23	2	0.16
(1,2630)	1:75:A:THR:H	1:75:A:THR:HG21	18	0.16
(1,2630)	1:75:A:THR:H	1:75:A:THR:HG22	18	0.16
(1,2630)	1:75:A:THR:H	1:75:A:THR:HG23	18	0.16
(1,2603)	1:26:A:LEU:HD11	1:22:A:LEU:HD21	11	0.16
(1,2603)	1:26:A:LEU:HD11	1:22:A:LEU:HD22	11	0.16
(1,2603)	1:26:A:LEU:HD11	1:22:A:LEU:HD23	11	0.16
(1,2603)	1:26:A:LEU:HD12	1:22:A:LEU:HD21	11	0.16
(1,2603)	1:26:A:LEU:HD12	1:22:A:LEU:HD22	11	0.16
(1,2603)	1:26:A:LEU:HD12	1:22:A:LEU:HD23	11	0.16
(1,2603)	1:26:A:LEU:HD13	1:22:A:LEU:HD21	11	0.16
(1,2603)	1:26:A:LEU:HD13	1:22:A:LEU:HD22	11	0.16
(1,2603)	1:26:A:LEU:HD13	1:22:A:LEU:HD23	11	0.16
(1,2537)	1:52:A:LEU:HA	1:55:A:LEU:HD11	3	0.16
(1,2537)	1:52:A:LEU:HA	1:55:A:LEU:HD12	3	0.16
(1,2537)	1:52:A:LEU:HA	1:55:A:LEU:HD13	3	0.16
(1,2509)	1:52:A:LEU:HA	1:52:A:LEU:HD11	14	0.16
(1,2509)	1:52:A:LEU:HA	1:52:A:LEU:HD12	14	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2509)	1:52:A:LEU:HA	1:52:A:LEU:HD13	14	0.16
(1,2509)	1:52:A:LEU:HA	1:52:A:LEU:HD11	17	0.16
(1,2509)	1:52:A:LEU:HA	1:52:A:LEU:HD12	17	0.16
(1,2509)	1:52:A:LEU:HA	1:52:A:LEU:HD13	17	0.16
(1,2466)	1:24:A:SER:H	1:23:A:LYS:HG2	1	0.16
(1,2456)	1:23:A:LYS:H	1:52:A:LEU:HD11	2	0.16
(1,2456)	1:23:A:LYS:H	1:52:A:LEU:HD12	2	0.16
(1,2456)	1:23:A:LYS:H	1:52:A:LEU:HD13	2	0.16
(1,2373)	1:55:A:LEU:HA	1:59:A:LEU:HD21	1	0.16
(1,2373)	1:55:A:LEU:HA	1:59:A:LEU:HD22	1	0.16
(1,2373)	1:55:A:LEU:HA	1:59:A:LEU:HD23	1	0.16
(1,2352)	1:85:A:VAL:HA	1:84:A:ILE:HG13	1	0.16
(1,2352)	1:85:A:VAL:HA	1:84:A:ILE:HG13	2	0.16
(1,2352)	1:85:A:VAL:HA	1:84:A:ILE:HG13	8	0.16
(1,2352)	1:85:A:VAL:HA	1:84:A:ILE:HG13	17	0.16
(1,2316)	1:121:A:GLN:H	1:121:A:GLN:HB3	6	0.16
(1,2316)	1:121:A:GLN:H	1:121:A:GLN:HB3	13	0.16
(1,2316)	1:121:A:GLN:H	1:121:A:GLN:HB3	16	0.16
(1,2287)	1:119:A:ILE:HG21	1:93:A:ILE:HG13	20	0.16
(1,2287)	1:119:A:ILE:HG22	1:93:A:ILE:HG13	20	0.16
(1,2287)	1:119:A:ILE:HG23	1:93:A:ILE:HG13	20	0.16
(1,2278)	1:57:A:MET:HB2	1:54:A:ILE:HG12	4	0.16
(1,2278)	1:57:A:MET:HB2	1:54:A:ILE:HG13	4	0.16
(1,2273)	1:70:A:LYS:HB2	1:70:A:LYS:HD2	10	0.16
(1,2273)	1:70:A:LYS:HB2	1:70:A:LYS:HD2	14	0.16
(1,2273)	1:70:A:LYS:HB2	1:70:A:LYS:HD2	20	0.16
(1,2248)	1:70:A:LYS:HA	1:70:A:LYS:HD3	9	0.16
(1,2248)	1:70:A:LYS:HA	1:70:A:LYS:HD3	18	0.16
(1,2182)	1:131:A:ILE:HG21	1:87:A:GLU:HG3	12	0.16
(1,2182)	1:131:A:ILE:HG22	1:87:A:GLU:HG3	12	0.16
(1,2182)	1:131:A:ILE:HG23	1:87:A:GLU:HG3	12	0.16
(1,2180)	1:23:A:LYS:HD2	1:23:A:LYS:HB2	10	0.16
(1,1939)	1:92:A:LEU:HD21	1:80:A:ASP:HB3	5	0.16
(1,1939)	1:92:A:LEU:HD22	1:80:A:ASP:HB3	5	0.16
(1,1939)	1:92:A:LEU:HD23	1:80:A:ASP:HB3	5	0.16
(1,1841)	1:62:A:LYS:HB3	1:62:A:LYS:HE3	20	0.16
(1,1840)	1:62:A:LYS:HB3	1:62:A:LYS:HE2	6	0.16
(1,1651)	1:59:A:LEU:HD21	1:56:A:GLN:HA	9	0.16
(1,1651)	1:59:A:LEU:HD22	1:56:A:GLN:HA	9	0.16
(1,1651)	1:59:A:LEU:HD23	1:56:A:GLN:HA	9	0.16
(1,1534)	1:20:A:ALA:HB1	1:17:A:ILE:HA	8	0.16
(1,1534)	1:20:A:ALA:HB2	1:17:A:ILE:HA	8	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1534)	1:20:A:ALA:HB3	1:17:A:ILE:HA	8	0.16
(1,1502)	1:26:A:LEU:HA	1:27:A:ILE:HA	3	0.16
(1,1489)	1:70:A:LYS:H	1:5:A:ILE:HD11	1	0.16
(1,1489)	1:70:A:LYS:H	1:5:A:ILE:HD12	1	0.16
(1,1489)	1:70:A:LYS:H	1:5:A:ILE:HD13	1	0.16
(1,1417)	1:94:A:CYS:HB3	1:91:A:ILE:HA	14	0.16
(1,1358)	1:96:A:HIS:H	1:97:A:ILE:HD11	16	0.16
(1,1358)	1:96:A:HIS:H	1:97:A:ILE:HD12	16	0.16
(1,1358)	1:96:A:HIS:H	1:97:A:ILE:HD13	16	0.16
(1,1326)	1:5:A:ILE:HD11	1:39:A:ALA:H	20	0.16
(1,1326)	1:5:A:ILE:HD12	1:39:A:ALA:H	20	0.16
(1,1326)	1:5:A:ILE:HD13	1:39:A:ALA:H	20	0.16
(1,1322)	1:112:A:ASP:HB3	1:116:A:ASN:H	4	0.16
(1,1288)	1:121:A:GLN:HG2	1:122:A:THR:H	10	0.16
(1,1238)	1:59:A:LEU:HD21	1:20:A:ALA:H	13	0.16
(1,1238)	1:59:A:LEU:HD22	1:20:A:ALA:H	13	0.16
(1,1238)	1:59:A:LEU:HD23	1:20:A:ALA:H	13	0.16
(1,1197)	1:126:A:LEU:HD11	1:122:A:THR:H	7	0.16
(1,1197)	1:126:A:LEU:HD12	1:122:A:THR:H	7	0.16
(1,1197)	1:126:A:LEU:HD13	1:122:A:THR:H	7	0.16
(1,1197)	1:126:A:LEU:HD11	1:122:A:THR:H	9	0.16
(1,1197)	1:126:A:LEU:HD12	1:122:A:THR:H	9	0.16
(1,1197)	1:126:A:LEU:HD13	1:122:A:THR:H	9	0.16
(1,1195)	1:60:A:LEU:HD21	1:57:A:MET:H	7	0.16
(1,1195)	1:60:A:LEU:HD22	1:57:A:MET:H	7	0.16
(1,1195)	1:60:A:LEU:HD23	1:57:A:MET:H	7	0.16
(1,1177)	1:79:A:ILE:HD11	1:89:A:ASP:H	12	0.16
(1,1177)	1:79:A:ILE:HD12	1:89:A:ASP:H	12	0.16
(1,1177)	1:79:A:ILE:HD13	1:89:A:ASP:H	12	0.16
(1,1141)	1:144:A:LEU:HG	1:143:A:GLN:H	8	0.16
(1,1132)	1:134:A:ARG:HG2	1:130:A:TYR:H	7	0.16
(1,1132)	1:134:A:ARG:HG3	1:130:A:TYR:H	7	0.16
(1,1122)	1:93:A:ILE:HD11	1:94:A:CYS:H	2	0.16
(1,1122)	1:93:A:ILE:HD12	1:94:A:CYS:H	2	0.16
(1,1122)	1:93:A:ILE:HD13	1:94:A:CYS:H	2	0.16
(1,1117)	1:96:A:HIS:HA	1:102:A:GLN:H	11	0.16
(1,1115)	1:55:A:LEU:HD21	1:8:A:ILE:H	9	0.16
(1,1115)	1:55:A:LEU:HD22	1:8:A:ILE:H	9	0.16
(1,1115)	1:55:A:LEU:HD23	1:8:A:ILE:H	9	0.16
(1,1091)	1:108:A:LEU:HD21	1:104:A:SER:H	9	0.16
(1,1091)	1:108:A:LEU:HD22	1:104:A:SER:H	9	0.16
(1,1091)	1:108:A:LEU:HD23	1:104:A:SER:H	9	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1091)	1:103:A:LEU:HD21	1:104:A:SER:H	12	0.16
(1,1091)	1:103:A:LEU:HD22	1:104:A:SER:H	12	0.16
(1,1091)	1:103:A:LEU:HD23	1:104:A:SER:H	12	0.16
(1,1024)	1:118:A:VAL:HG21	1:116:A:ASN:HD21	2	0.16
(1,1024)	1:118:A:VAL:HG22	1:116:A:ASN:HD21	2	0.16
(1,1024)	1:118:A:VAL:HG23	1:116:A:ASN:HD21	2	0.16
(1,1022)	1:79:A:ILE:HG21	1:81:A:ASN:H	18	0.16
(1,1022)	1:79:A:ILE:HG22	1:81:A:ASN:H	18	0.16
(1,1022)	1:79:A:ILE:HG23	1:81:A:ASN:H	18	0.16
(1,1019)	1:22:A:LEU:HD21	1:52:A:LEU:H	15	0.16
(1,1019)	1:22:A:LEU:HD22	1:52:A:LEU:H	15	0.16
(1,1019)	1:22:A:LEU:HD23	1:52:A:LEU:H	15	0.16
(1,988)	1:85:A:VAL:HG21	1:78:A:ASP:H	8	0.16
(1,988)	1:85:A:VAL:HG22	1:78:A:ASP:H	8	0.16
(1,988)	1:85:A:VAL:HG23	1:78:A:ASP:H	8	0.16
(1,978)	1:131:A:ILE:HD11	1:131:A:ILE:H	2	0.16
(1,978)	1:131:A:ILE:HD12	1:131:A:ILE:H	2	0.16
(1,978)	1:131:A:ILE:HD13	1:131:A:ILE:H	2	0.16
(1,948)	1:5:A:ILE:HG21	1:70:A:LYS:H	9	0.16
(1,948)	1:5:A:ILE:HG22	1:70:A:LYS:H	9	0.16
(1,948)	1:5:A:ILE:HG23	1:70:A:LYS:H	9	0.16
(1,948)	1:5:A:ILE:HG21	1:70:A:LYS:H	14	0.16
(1,948)	1:5:A:ILE:HG22	1:70:A:LYS:H	14	0.16
(1,948)	1:5:A:ILE:HG23	1:70:A:LYS:H	14	0.16
(1,931)	1:8:A:ILE:HG21	1:22:A:LEU:H	5	0.16
(1,931)	1:8:A:ILE:HG22	1:22:A:LEU:H	5	0.16
(1,931)	1:8:A:ILE:HG23	1:22:A:LEU:H	5	0.16
(1,931)	1:8:A:ILE:HG21	1:22:A:LEU:H	12	0.16
(1,931)	1:8:A:ILE:HG22	1:22:A:LEU:H	12	0.16
(1,931)	1:8:A:ILE:HG23	1:22:A:LEU:H	12	0.16
(1,931)	1:8:A:ILE:HG21	1:22:A:LEU:H	17	0.16
(1,931)	1:8:A:ILE:HG22	1:22:A:LEU:H	17	0.16
(1,931)	1:8:A:ILE:HG23	1:22:A:LEU:H	17	0.16
(1,931)	1:8:A:ILE:HG21	1:22:A:LEU:H	20	0.16
(1,931)	1:8:A:ILE:HG22	1:22:A:LEU:H	20	0.16
(1,931)	1:8:A:ILE:HG23	1:22:A:LEU:H	20	0.16
(1,925)	1:59:A:LEU:HD11	1:59:A:LEU:H	8	0.16
(1,925)	1:59:A:LEU:HD12	1:59:A:LEU:H	8	0.16
(1,925)	1:59:A:LEU:HD13	1:59:A:LEU:H	8	0.16
(1,874)	1:139:A:PRO:HG2	1:115:A:GLY:H	8	0.16
(1,874)	1:139:A:PRO:HG3	1:115:A:GLY:H	8	0.16
(1,874)	1:139:A:PRO:HG2	1:115:A:GLY:H	14	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,874)	1:139:A:PRO:HG3	1:115:A:GLY:H	14	0.16
(1,874)	1:139:A:PRO:HG2	1:115:A:GLY:H	15	0.16
(1,874)	1:139:A:PRO:HG3	1:115:A:GLY:H	15	0.16
(1,874)	1:139:A:PRO:HG2	1:115:A:GLY:H	19	0.16
(1,874)	1:139:A:PRO:HG3	1:115:A:GLY:H	19	0.16
(1,806)	1:53:A:ALA:HB1	1:57:A:MET:H	7	0.16
(1,806)	1:53:A:ALA:HB2	1:57:A:MET:H	7	0.16
(1,806)	1:53:A:ALA:HB3	1:57:A:MET:H	7	0.16
(1,774)	1:72:A:ARG:HB2	1:3:A:VAL:H	2	0.16
(1,741)	1:59:A:LEU:HB3	1:59:A:LEU:H	3	0.16
(1,741)	1:59:A:LEU:HB3	1:59:A:LEU:H	9	0.16
(1,596)	1:95:A:ASN:HB3	1:95:A:ASN:H	5	0.16
(1,596)	1:95:A:ASN:HB3	1:95:A:ASN:H	11	0.16
(1,582)	1:57:A:MET:HB3	1:58:A:TYR:H	4	0.16
(1,582)	1:57:A:MET:HB3	1:58:A:TYR:H	15	0.16
(1,391)	1:72:A:ARG:HD2	1:73:A:ILE:H	7	0.16
(1,97)	1:144:A:LEU:H	1:143:A:GLN:H	7	0.16
(1,81)	1:58:A:TYR:H	1:61:A:GLY:H	11	0.16
(3,61)	1:109:A:PHE:H	1:105:A:ASP:O	1	0.15
(3,61)	1:109:A:PHE:H	1:105:A:ASP:O	15	0.15
(1,3843)	1:126:A:LEU:HA	1:113:A:ALA:HB1	10	0.15
(1,3843)	1:126:A:LEU:HA	1:113:A:ALA:HB2	10	0.15
(1,3843)	1:126:A:LEU:HA	1:113:A:ALA:HB3	10	0.15
(1,3840)	1:123:A:ASP:HB2	1:111:A:ALA:HB1	1	0.15
(1,3840)	1:123:A:ASP:HB2	1:111:A:ALA:HB2	1	0.15
(1,3840)	1:123:A:ASP:HB2	1:111:A:ALA:HB3	1	0.15
(1,3834)	1:74:A:TYR:H	1:3:A:VAL:HG11	2	0.15
(1,3834)	1:74:A:TYR:H	1:3:A:VAL:HG12	2	0.15
(1,3834)	1:74:A:TYR:H	1:3:A:VAL:HG13	2	0.15
(1,3834)	1:74:A:TYR:H	1:3:A:VAL:HG11	3	0.15
(1,3834)	1:74:A:TYR:H	1:3:A:VAL:HG12	3	0.15
(1,3834)	1:74:A:TYR:H	1:3:A:VAL:HG13	3	0.15
(1,3834)	1:74:A:TYR:H	1:3:A:VAL:HG11	10	0.15
(1,3834)	1:74:A:TYR:H	1:3:A:VAL:HG12	10	0.15
(1,3834)	1:74:A:TYR:H	1:3:A:VAL:HG13	10	0.15
(1,3797)	1:93:A:ILE:H	1:79:A:ILE:HB	12	0.15
(1,3724)	1:71:A:ASN:HB3	1:5:A:ILE:HG13	19	0.15
(1,3712)	1:130:A:TYR:HE1	1:137:A:HIS:HB3	17	0.15
(1,3712)	1:130:A:TYR:HE2	1:137:A:HIS:HB3	17	0.15
(1,3628)	1:72:A:ARG:HE	1:72:A:ARG:HA	20	0.15
(1,3623)	1:135:A:ILE:HG12	1:134:A:ARG:HA	4	0.15
(1,3623)	1:135:A:ILE:HG12	1:134:A:ARG:HA	15	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3581)	1:56:A:GLN:H	1:68:A:ILE:HD11	4	0.15
(1,3581)	1:56:A:GLN:H	1:68:A:ILE:HD12	4	0.15
(1,3581)	1:56:A:GLN:H	1:68:A:ILE:HD13	4	0.15
(1,3543)	1:17:A:ILE:HA	1:21:A:ILE:HD11	5	0.15
(1,3543)	1:17:A:ILE:HA	1:21:A:ILE:HD12	5	0.15
(1,3543)	1:17:A:ILE:HA	1:21:A:ILE:HD13	5	0.15
(1,3263)	1:5:A:ILE:HG21	1:6:A:GLY:HA2	14	0.15
(1,3263)	1:5:A:ILE:HG22	1:6:A:GLY:HA2	14	0.15
(1,3263)	1:5:A:ILE:HG23	1:6:A:GLY:HA2	14	0.15
(1,3183)	1:35:A:GLN:HG2	1:8:A:ILE:HD11	6	0.15
(1,3183)	1:35:A:GLN:HG2	1:8:A:ILE:HD12	6	0.15
(1,3183)	1:35:A:GLN:HG2	1:8:A:ILE:HD13	6	0.15
(1,3164)	1:123:A:ASP:HB2	1:93:A:ILE:HD11	3	0.15
(1,3164)	1:123:A:ASP:HB2	1:93:A:ILE:HD12	3	0.15
(1,3164)	1:123:A:ASP:HB2	1:93:A:ILE:HD13	3	0.15
(1,3095)	1:57:A:MET:HE1	1:53:A:ALA:HA	7	0.15
(1,3095)	1:57:A:MET:HE2	1:53:A:ALA:HA	7	0.15
(1,3095)	1:57:A:MET:HE3	1:53:A:ALA:HA	7	0.15
(1,3040)	1:6:A:GLY:HA2	1:14:A:ILE:HG21	13	0.15
(1,3040)	1:6:A:GLY:HA2	1:14:A:ILE:HG22	13	0.15
(1,3040)	1:6:A:GLY:HA2	1:14:A:ILE:HG23	13	0.15
(1,3030)	1:58:A:TYR:H	1:57:A:MET:HE1	13	0.15
(1,3030)	1:58:A:TYR:H	1:57:A:MET:HE2	13	0.15
(1,3030)	1:58:A:TYR:H	1:57:A:MET:HE3	13	0.15
(1,3030)	1:58:A:TYR:H	1:57:A:MET:HE1	14	0.15
(1,3030)	1:58:A:TYR:H	1:57:A:MET:HE2	14	0.15
(1,3030)	1:58:A:TYR:H	1:57:A:MET:HE3	14	0.15
(1,2906)	1:59:A:LEU:HA	1:14:A:ILE:HG21	10	0.15
(1,2906)	1:59:A:LEU:HA	1:14:A:ILE:HG22	10	0.15
(1,2906)	1:59:A:LEU:HA	1:14:A:ILE:HG23	10	0.15
(1,2878)	1:40:A:ASP:H	1:38:A:ALA:HB1	15	0.15
(1,2878)	1:40:A:ASP:H	1:38:A:ALA:HB2	15	0.15
(1,2878)	1:40:A:ASP:H	1:38:A:ALA:HB3	15	0.15
(1,2832)	1:87:A:GLU:H	1:131:A:ILE:HG21	10	0.15
(1,2832)	1:87:A:GLU:H	1:131:A:ILE:HG22	10	0.15
(1,2832)	1:87:A:GLU:H	1:131:A:ILE:HG23	10	0.15
(1,2761)	1:74:A:TYR:HB2	1:75:A:THR:HG21	19	0.15
(1,2761)	1:74:A:TYR:HB2	1:75:A:THR:HG22	19	0.15
(1,2761)	1:74:A:TYR:HB2	1:75:A:THR:HG23	19	0.15
(1,2760)	1:120:A:ASP:HB2	1:118:A:VAL:HG11	3	0.15
(1,2760)	1:120:A:ASP:HB2	1:118:A:VAL:HG12	3	0.15
(1,2760)	1:120:A:ASP:HB2	1:118:A:VAL:HG13	3	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2752)	1:35:A:GLN:HB2	1:32:A:THR:HG21	1	0.15
(1,2752)	1:35:A:GLN:HB2	1:32:A:THR:HG22	1	0.15
(1,2752)	1:35:A:GLN:HB2	1:32:A:THR:HG23	1	0.15
(1,2713)	1:80:A:ASP:HA	1:79:A:ILE:HG21	3	0.15
(1,2713)	1:80:A:ASP:HA	1:79:A:ILE:HG22	3	0.15
(1,2713)	1:80:A:ASP:HA	1:79:A:ILE:HG23	3	0.15
(1,2713)	1:80:A:ASP:HA	1:79:A:ILE:HG21	7	0.15
(1,2713)	1:80:A:ASP:HA	1:79:A:ILE:HG22	7	0.15
(1,2713)	1:80:A:ASP:HA	1:79:A:ILE:HG23	7	0.15
(1,2682)	1:38:A:ALA:H	1:3:A:VAL:HG11	8	0.15
(1,2682)	1:38:A:ALA:H	1:3:A:VAL:HG12	8	0.15
(1,2682)	1:38:A:ALA:H	1:3:A:VAL:HG13	8	0.15
(1,2682)	1:38:A:ALA:H	1:3:A:VAL:HG11	19	0.15
(1,2682)	1:38:A:ALA:H	1:3:A:VAL:HG12	19	0.15
(1,2682)	1:38:A:ALA:H	1:3:A:VAL:HG13	19	0.15
(1,2641)	1:123:A:ASP:H	1:113:A:ALA:HB1	7	0.15
(1,2641)	1:123:A:ASP:H	1:113:A:ALA:HB2	7	0.15
(1,2641)	1:123:A:ASP:H	1:113:A:ALA:HB3	7	0.15
(1,2630)	1:75:A:THR:H	1:75:A:THR:HG21	12	0.15
(1,2630)	1:75:A:THR:H	1:75:A:THR:HG22	12	0.15
(1,2630)	1:75:A:THR:H	1:75:A:THR:HG23	12	0.15
(1,2583)	1:126:A:LEU:HB2	1:138:A:LEU:HD21	2	0.15
(1,2583)	1:126:A:LEU:HB2	1:138:A:LEU:HD22	2	0.15
(1,2583)	1:126:A:LEU:HB2	1:138:A:LEU:HD23	2	0.15
(1,2583)	1:126:A:LEU:HB2	1:138:A:LEU:HD21	3	0.15
(1,2583)	1:126:A:LEU:HB2	1:138:A:LEU:HD22	3	0.15
(1,2583)	1:126:A:LEU:HB2	1:138:A:LEU:HD23	3	0.15
(1,2515)	1:93:A:ILE:HA	1:103:A:LEU:HD11	14	0.15
(1,2515)	1:93:A:ILE:HA	1:103:A:LEU:HD12	14	0.15
(1,2515)	1:93:A:ILE:HA	1:103:A:LEU:HD13	14	0.15
(1,2484)	1:56:A:GLN:HE22	1:60:A:LEU:HD21	15	0.15
(1,2484)	1:56:A:GLN:HE22	1:60:A:LEU:HD22	15	0.15
(1,2484)	1:56:A:GLN:HE22	1:60:A:LEU:HD23	15	0.15
(1,2456)	1:23:A:LYS:H	1:52:A:LEU:HD11	13	0.15
(1,2456)	1:23:A:LYS:H	1:52:A:LEU:HD12	13	0.15
(1,2456)	1:23:A:LYS:H	1:52:A:LEU:HD13	13	0.15
(1,2449)	1:59:A:LEU:H	1:60:A:LEU:HD21	8	0.15
(1,2449)	1:59:A:LEU:H	1:60:A:LEU:HD22	8	0.15
(1,2449)	1:59:A:LEU:H	1:60:A:LEU:HD23	8	0.15
(1,2373)	1:55:A:LEU:HA	1:59:A:LEU:HD21	18	0.15
(1,2373)	1:55:A:LEU:HA	1:59:A:LEU:HD22	18	0.15
(1,2373)	1:55:A:LEU:HA	1:59:A:LEU:HD23	18	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2367)	1:2:A:SER:HA	1:73:A:ILE:HG12	2	0.15
(1,2352)	1:85:A:VAL:HA	1:84:A:ILE:HG13	3	0.15
(1,2352)	1:85:A:VAL:HA	1:84:A:ILE:HG13	7	0.15
(1,2352)	1:85:A:VAL:HA	1:84:A:ILE:HG13	11	0.15
(1,2352)	1:85:A:VAL:HA	1:84:A:ILE:HG13	15	0.15
(1,2352)	1:85:A:VAL:HA	1:84:A:ILE:HG13	16	0.15
(1,2316)	1:121:A:GLN:H	1:121:A:GLN:HB3	12	0.15
(1,2316)	1:121:A:GLN:H	1:121:A:GLN:HB3	17	0.15
(1,2273)	1:70:A:LYS:HB2	1:70:A:LYS:HD2	8	0.15
(1,2273)	1:70:A:LYS:HB2	1:70:A:LYS:HD2	19	0.15
(1,2248)	1:70:A:LYS:HA	1:70:A:LYS:HD3	4	0.15
(1,2182)	1:131:A:ILE:HD11	1:87:A:GLU:HG3	17	0.15
(1,2182)	1:131:A:ILE:HD12	1:87:A:GLU:HG3	17	0.15
(1,2182)	1:131:A:ILE:HD13	1:87:A:GLU:HG3	17	0.15
(1,2180)	1:23:A:LYS:HD2	1:23:A:LYS:HB2	3	0.15
(1,2180)	1:23:A:LYS:HD2	1:23:A:LYS:HB2	8	0.15
(1,2180)	1:23:A:LYS:HD2	1:23:A:LYS:HB2	13	0.15
(1,2180)	1:23:A:LYS:HD2	1:23:A:LYS:HB2	20	0.15
(1,2145)	1:37:A:ALA:HA	1:3:A:VAL:HB	7	0.15
(1,1939)	1:92:A:LEU:HD21	1:80:A:ASP:HB3	1	0.15
(1,1939)	1:92:A:LEU:HD22	1:80:A:ASP:HB3	1	0.15
(1,1939)	1:92:A:LEU:HD23	1:80:A:ASP:HB3	1	0.15
(1,1939)	1:92:A:LEU:HD21	1:80:A:ASP:HB3	16	0.15
(1,1939)	1:92:A:LEU:HD22	1:80:A:ASP:HB3	16	0.15
(1,1939)	1:92:A:LEU:HD23	1:80:A:ASP:HB3	16	0.15
(1,1651)	1:59:A:LEU:HD21	1:56:A:GLN:HA	4	0.15
(1,1651)	1:59:A:LEU:HD22	1:56:A:GLN:HA	4	0.15
(1,1651)	1:59:A:LEU:HD23	1:56:A:GLN:HA	4	0.15
(1,1510)	1:72:A:ARG:HA	1:5:A:ILE:HD11	7	0.15
(1,1510)	1:72:A:ARG:HA	1:5:A:ILE:HD12	7	0.15
(1,1510)	1:72:A:ARG:HA	1:5:A:ILE:HD13	7	0.15
(1,1451)	1:119:A:ILE:HG21	1:93:A:ILE:HD11	16	0.15
(1,1451)	1:119:A:ILE:HG21	1:93:A:ILE:HD12	16	0.15
(1,1451)	1:119:A:ILE:HG21	1:93:A:ILE:HD13	16	0.15
(1,1451)	1:119:A:ILE:HG22	1:93:A:ILE:HD11	16	0.15
(1,1451)	1:119:A:ILE:HG22	1:93:A:ILE:HD12	16	0.15
(1,1451)	1:119:A:ILE:HG22	1:93:A:ILE:HD13	16	0.15
(1,1451)	1:119:A:ILE:HG23	1:93:A:ILE:HD11	16	0.15
(1,1451)	1:119:A:ILE:HG23	1:93:A:ILE:HD12	16	0.15
(1,1451)	1:119:A:ILE:HG23	1:93:A:ILE:HD13	16	0.15
(1,1388)	1:103:A:LEU:HA	1:107:A:SER:HB3	18	0.15
(1,1328)	1:97:A:ILE:HG21	1:121:A:GLN:H	5	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1328)	1:97:A:ILE:HG22	1:121:A:GLN:H	5	0.15
(1,1328)	1:97:A:ILE:HG23	1:121:A:GLN:H	5	0.15
(1,1260)	1:51:A:ASP:H	1:41:A:VAL:H	13	0.15
(1,1222)	1:63:A:GLY:HA3	1:63:A:GLY:H	15	0.15
(1,1220)	1:131:A:ILE:HG21	1:133:A:GLY:H	15	0.15
(1,1220)	1:131:A:ILE:HG22	1:133:A:GLY:H	15	0.15
(1,1220)	1:131:A:ILE:HG23	1:133:A:GLY:H	15	0.15
(1,1205)	1:97:A:ILE:HD11	1:98:A:ASN:H	6	0.15
(1,1205)	1:97:A:ILE:HD12	1:98:A:ASN:H	6	0.15
(1,1205)	1:97:A:ILE:HD13	1:98:A:ASN:H	6	0.15
(1,1195)	1:60:A:LEU:HD21	1:57:A:MET:H	6	0.15
(1,1195)	1:60:A:LEU:HD22	1:57:A:MET:H	6	0.15
(1,1195)	1:60:A:LEU:HD23	1:57:A:MET:H	6	0.15
(1,1182)	1:126:A:LEU:HD11	1:127:A:ILE:H	13	0.15
(1,1182)	1:126:A:LEU:HD12	1:127:A:ILE:H	13	0.15
(1,1182)	1:126:A:LEU:HD13	1:127:A:ILE:H	13	0.15
(1,1137)	1:97:A:ILE:HG21	1:96:A:HIS:H	3	0.15
(1,1137)	1:97:A:ILE:HG22	1:96:A:HIS:H	3	0.15
(1,1137)	1:97:A:ILE:HG23	1:96:A:HIS:H	3	0.15
(1,1132)	1:134:A:ARG:HG2	1:130:A:TYR:H	5	0.15
(1,1132)	1:134:A:ARG:HG3	1:130:A:TYR:H	5	0.15
(1,1132)	1:131:A:ILE:HG12	1:130:A:TYR:H	12	0.15
(1,1122)	1:91:A:ILE:HG21	1:94:A:CYS:H	6	0.15
(1,1122)	1:91:A:ILE:HG22	1:94:A:CYS:H	6	0.15
(1,1122)	1:91:A:ILE:HG23	1:94:A:CYS:H	6	0.15
(1,1097)	1:103:A:LEU:HD21	1:112:A:ASP:H	19	0.15
(1,1097)	1:103:A:LEU:HD22	1:112:A:ASP:H	19	0.15
(1,1097)	1:103:A:LEU:HD23	1:112:A:ASP:H	19	0.15
(1,1056)	1:122:A:THR:HG21	1:114:A:ASP:H	13	0.15
(1,1056)	1:122:A:THR:HG22	1:114:A:ASP:H	13	0.15
(1,1056)	1:122:A:THR:HG23	1:114:A:ASP:H	13	0.15
(1,1024)	1:118:A:VAL:HG21	1:116:A:ASN:HD21	12	0.15
(1,1024)	1:118:A:VAL:HG22	1:116:A:ASN:HD21	12	0.15
(1,1024)	1:118:A:VAL:HG23	1:116:A:ASN:HD21	12	0.15
(1,1023)	1:65:A:THR:HG21	1:65:A:THR:H	10	0.15
(1,1023)	1:65:A:THR:HG22	1:65:A:THR:H	10	0.15
(1,1023)	1:65:A:THR:HG23	1:65:A:THR:H	10	0.15
(1,1022)	1:79:A:ILE:HG21	1:81:A:ASN:H	6	0.15
(1,1022)	1:79:A:ILE:HG22	1:81:A:ASN:H	6	0.15
(1,1022)	1:79:A:ILE:HG23	1:81:A:ASN:H	6	0.15
(1,1004)	1:59:A:LEU:HD11	1:16:A:SER:H	9	0.15
(1,1004)	1:59:A:LEU:HD12	1:16:A:SER:H	9	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1004)	1:59:A:LEU:HD13	1:16:A:SER:H	9	0.15
(1,981)	1:84:A:ILE:HD11	1:82:A:ASN:H	12	0.15
(1,981)	1:84:A:ILE:HD12	1:82:A:ASN:H	12	0.15
(1,981)	1:84:A:ILE:HD13	1:82:A:ASN:H	12	0.15
(1,980)	1:54:A:ILE:HD11	1:42:A:ASP:H	11	0.15
(1,980)	1:54:A:ILE:HD12	1:42:A:ASP:H	11	0.15
(1,980)	1:54:A:ILE:HD13	1:42:A:ASP:H	11	0.15
(1,978)	1:131:A:ILE:HD11	1:131:A:ILE:H	19	0.15
(1,978)	1:131:A:ILE:HD12	1:131:A:ILE:H	19	0.15
(1,978)	1:131:A:ILE:HD13	1:131:A:ILE:H	19	0.15
(1,962)	1:73:A:ILE:HD11	1:71:A:ASN:H	6	0.15
(1,962)	1:73:A:ILE:HD12	1:71:A:ASN:H	6	0.15
(1,962)	1:73:A:ILE:HD13	1:71:A:ASN:H	6	0.15
(1,874)	1:139:A:PRO:HG2	1:115:A:GLY:H	18	0.15
(1,874)	1:139:A:PRO:HG3	1:115:A:GLY:H	18	0.15
(1,874)	1:139:A:PRO:HG2	1:115:A:GLY:H	20	0.15
(1,874)	1:139:A:PRO:HG3	1:115:A:GLY:H	20	0.15
(1,823)	1:70:A:LYS:HG2	1:69:A:GLY:H	11	0.15
(1,823)	1:70:A:LYS:HG3	1:69:A:GLY:H	11	0.15
(1,806)	1:53:A:ALA:HB1	1:57:A:MET:H	9	0.15
(1,806)	1:53:A:ALA:HB2	1:57:A:MET:H	9	0.15
(1,806)	1:53:A:ALA:HB3	1:57:A:MET:H	9	0.15
(1,779)	1:62:A:LYS:HB3	1:62:A:LYS:H	9	0.15
(1,779)	1:62:A:LYS:HB3	1:62:A:LYS:H	17	0.15
(1,772)	1:23:A:LYS:HD2	1:23:A:LYS:H	14	0.15
(1,753)	1:129:A:LYS:HD2	1:128:A:GLU:H	8	0.15
(1,753)	1:129:A:LYS:HD3	1:128:A:GLU:H	8	0.15
(1,741)	1:59:A:LEU:HB3	1:59:A:LEU:H	5	0.15
(1,741)	1:59:A:LEU:HB3	1:59:A:LEU:H	8	0.15
(1,596)	1:95:A:ASN:HB3	1:95:A:ASN:H	1	0.15
(1,596)	1:95:A:ASN:HB3	1:95:A:ASN:H	2	0.15
(1,596)	1:95:A:ASN:HB3	1:95:A:ASN:H	4	0.15
(1,596)	1:95:A:ASN:HB3	1:95:A:ASN:H	15	0.15
(1,582)	1:57:A:MET:HB3	1:58:A:TYR:H	5	0.15
(1,486)	1:123:A:ASP:HB3	1:124:A:ARG:H	2	0.15
(3,61)	1:109:A:PHE:H	1:105:A:ASP:O	4	0.14
(3,61)	1:109:A:PHE:H	1:105:A:ASP:O	5	0.14
(3,61)	1:109:A:PHE:H	1:105:A:ASP:O	6	0.14
(3,61)	1:109:A:PHE:H	1:105:A:ASP:O	14	0.14
(1,3875)	1:55:A:LEU:HB3	1:8:A:ILE:HG12	10	0.14
(1,3875)	1:55:A:LEU:HB3	1:8:A:ILE:HG13	10	0.14
(1,3871)	1:21:A:ILE:H	1:9:A:ASP:HB3	19	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3843)	1:126:A:LEU:HA	1:113:A:ALA:HB1	3	0.14
(1,3843)	1:126:A:LEU:HA	1:113:A:ALA:HB2	3	0.14
(1,3843)	1:126:A:LEU:HA	1:113:A:ALA:HB3	3	0.14
(1,3843)	1:126:A:LEU:HA	1:113:A:ALA:HB1	7	0.14
(1,3843)	1:126:A:LEU:HA	1:113:A:ALA:HB2	7	0.14
(1,3843)	1:126:A:LEU:HA	1:113:A:ALA:HB3	7	0.14
(1,3843)	1:126:A:LEU:HA	1:113:A:ALA:HB1	9	0.14
(1,3843)	1:126:A:LEU:HA	1:113:A:ALA:HB2	9	0.14
(1,3843)	1:126:A:LEU:HA	1:113:A:ALA:HB3	9	0.14
(1,3843)	1:126:A:LEU:HA	1:113:A:ALA:HB1	16	0.14
(1,3843)	1:126:A:LEU:HA	1:113:A:ALA:HB2	16	0.14
(1,3843)	1:126:A:LEU:HA	1:113:A:ALA:HB3	16	0.14
(1,3840)	1:123:A:ASP:HB2	1:111:A:ALA:HB1	18	0.14
(1,3840)	1:123:A:ASP:HB2	1:111:A:ALA:HB2	18	0.14
(1,3840)	1:123:A:ASP:HB2	1:111:A:ALA:HB3	18	0.14
(1,3834)	1:74:A:TYR:H	1:3:A:VAL:HG11	5	0.14
(1,3834)	1:74:A:TYR:H	1:3:A:VAL:HG12	5	0.14
(1,3834)	1:74:A:TYR:H	1:3:A:VAL:HG13	5	0.14
(1,3834)	1:74:A:TYR:H	1:3:A:VAL:HG11	12	0.14
(1,3834)	1:74:A:TYR:H	1:3:A:VAL:HG12	12	0.14
(1,3834)	1:74:A:TYR:H	1:3:A:VAL:HG13	12	0.14
(1,3834)	1:74:A:TYR:H	1:3:A:VAL:HG11	15	0.14
(1,3834)	1:74:A:TYR:H	1:3:A:VAL:HG12	15	0.14
(1,3834)	1:74:A:TYR:H	1:3:A:VAL:HG13	15	0.14
(1,3834)	1:74:A:TYR:H	1:3:A:VAL:HG11	18	0.14
(1,3834)	1:74:A:TYR:H	1:3:A:VAL:HG12	18	0.14
(1,3834)	1:74:A:TYR:H	1:3:A:VAL:HG13	18	0.14
(1,3805)	1:125:A:ILE:HG12	1:128:A:GLU:HG2	19	0.14
(1,3805)	1:125:A:ILE:HG12	1:128:A:GLU:HG3	19	0.14
(1,3797)	1:93:A:ILE:H	1:79:A:ILE:HB	1	0.14
(1,3758)	1:102:A:GLN:HG3	1:108:A:LEU:HD21	9	0.14
(1,3758)	1:102:A:GLN:HG3	1:108:A:LEU:HD22	9	0.14
(1,3758)	1:102:A:GLN:HG3	1:108:A:LEU:HD23	9	0.14
(1,3724)	1:71:A:ASN:HB3	1:5:A:ILE:HG13	17	0.14
(1,3697)	1:101:A:GLY:HA2	1:102:A:GLN:HG3	7	0.14
(1,3697)	1:101:A:GLY:HA2	1:102:A:GLN:HG3	13	0.14
(1,3697)	1:101:A:GLY:HA2	1:102:A:GLN:HG3	17	0.14
(1,3697)	1:101:A:GLY:HA2	1:102:A:GLN:HG3	19	0.14
(1,3697)	1:101:A:GLY:HA2	1:102:A:GLN:HG3	20	0.14
(1,3696)	1:108:A:LEU:HD21	1:102:A:GLN:HG3	9	0.14
(1,3696)	1:108:A:LEU:HD22	1:102:A:GLN:HG3	9	0.14
(1,3696)	1:108:A:LEU:HD23	1:102:A:GLN:HG3	9	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3675)	1:19:A:TYR:HA	1:8:A:ILE:HB	20	0.14
(1,3581)	1:56:A:GLN:H	1:68:A:ILE:HD11	3	0.14
(1,3581)	1:56:A:GLN:H	1:68:A:ILE:HD12	3	0.14
(1,3581)	1:56:A:GLN:H	1:68:A:ILE:HD13	3	0.14
(1,3520)	1:127:A:ILE:HD11	1:126:A:LEU:HB2	10	0.14
(1,3520)	1:127:A:ILE:HD12	1:126:A:LEU:HB2	10	0.14
(1,3520)	1:127:A:ILE:HD13	1:126:A:LEU:HB2	10	0.14
(1,3459)	1:74:A:TYR:HB3	1:73:A:ILE:HA	7	0.14
(1,3459)	1:74:A:TYR:HB3	1:73:A:ILE:HA	18	0.14
(1,3457)	1:74:A:TYR:HB3	1:75:A:THR:HA	16	0.14
(1,3404)	1:97:A:ILE:HA	1:119:A:ILE:HG21	4	0.14
(1,3404)	1:97:A:ILE:HA	1:119:A:ILE:HG22	4	0.14
(1,3404)	1:97:A:ILE:HA	1:119:A:ILE:HG23	4	0.14
(1,3337)	1:5:A:ILE:HG21	1:41:A:VAL:HB	3	0.14
(1,3337)	1:5:A:ILE:HG22	1:41:A:VAL:HB	3	0.14
(1,3337)	1:5:A:ILE:HG23	1:41:A:VAL:HB	3	0.14
(1,3263)	1:5:A:ILE:HG21	1:6:A:GLY:HA2	7	0.14
(1,3263)	1:5:A:ILE:HG22	1:6:A:GLY:HA2	7	0.14
(1,3263)	1:5:A:ILE:HG23	1:6:A:GLY:HA2	7	0.14
(1,3242)	1:144:A:LEU:H	1:144:A:LEU:HA	19	0.14
(1,3177)	1:129:A:LYS:HE2	1:135:A:ILE:HD11	10	0.14
(1,3177)	1:129:A:LYS:HE2	1:135:A:ILE:HD12	10	0.14
(1,3177)	1:129:A:LYS:HE2	1:135:A:ILE:HD13	10	0.14
(1,3177)	1:129:A:LYS:HE3	1:135:A:ILE:HD11	10	0.14
(1,3177)	1:129:A:LYS:HE3	1:135:A:ILE:HD12	10	0.14
(1,3177)	1:129:A:LYS:HE3	1:135:A:ILE:HD13	10	0.14
(1,3096)	1:92:A:LEU:HD21	1:80:A:ASP:HA	3	0.14
(1,3096)	1:92:A:LEU:HD22	1:80:A:ASP:HA	3	0.14
(1,3096)	1:92:A:LEU:HD23	1:80:A:ASP:HA	3	0.14
(1,3096)	1:92:A:LEU:HD21	1:80:A:ASP:HA	14	0.14
(1,3096)	1:92:A:LEU:HD22	1:80:A:ASP:HA	14	0.14
(1,3096)	1:92:A:LEU:HD23	1:80:A:ASP:HA	14	0.14
(1,3095)	1:57:A:MET:HE1	1:53:A:ALA:HA	3	0.14
(1,3095)	1:57:A:MET:HE2	1:53:A:ALA:HA	3	0.14
(1,3095)	1:57:A:MET:HE3	1:53:A:ALA:HA	3	0.14
(1,3095)	1:57:A:MET:HE1	1:53:A:ALA:HA	15	0.14
(1,3095)	1:57:A:MET:HE2	1:53:A:ALA:HA	15	0.14
(1,3095)	1:57:A:MET:HE3	1:53:A:ALA:HA	15	0.14
(1,3049)	1:12:A:GLY:HA2	1:13:A:GLU:HG2	15	0.14
(1,3049)	1:12:A:GLY:HA2	1:13:A:GLU:HG3	15	0.14
(1,3040)	1:6:A:GLY:HA2	1:14:A:ILE:HG21	17	0.14
(1,3040)	1:6:A:GLY:HA2	1:14:A:ILE:HG22	17	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3040)	1:6:A:GLY:HA2	1:14:A:ILE:HG23	17	0.14
(1,2980)	1:21:A:ILE:HB	1:20:A:ALA:HB1	9	0.14
(1,2980)	1:21:A:ILE:HB	1:20:A:ALA:HB2	9	0.14
(1,2980)	1:21:A:ILE:HB	1:20:A:ALA:HB3	9	0.14
(1,2980)	1:54:A:ILE:HB	1:53:A:ALA:HB1	15	0.14
(1,2980)	1:54:A:ILE:HB	1:53:A:ALA:HB2	15	0.14
(1,2980)	1:54:A:ILE:HB	1:53:A:ALA:HB3	15	0.14
(1,2979)	1:57:A:MET:HE1	1:53:A:ALA:HB1	8	0.14
(1,2979)	1:57:A:MET:HE1	1:53:A:ALA:HB2	8	0.14
(1,2979)	1:57:A:MET:HE1	1:53:A:ALA:HB3	8	0.14
(1,2979)	1:57:A:MET:HE2	1:53:A:ALA:HB1	8	0.14
(1,2979)	1:57:A:MET:HE2	1:53:A:ALA:HB2	8	0.14
(1,2979)	1:57:A:MET:HE2	1:53:A:ALA:HB3	8	0.14
(1,2979)	1:57:A:MET:HE3	1:53:A:ALA:HB1	8	0.14
(1,2979)	1:57:A:MET:HE3	1:53:A:ALA:HB2	8	0.14
(1,2979)	1:57:A:MET:HE3	1:53:A:ALA:HB3	8	0.14
(1,2979)	1:57:A:MET:HE1	1:53:A:ALA:HB1	19	0.14
(1,2979)	1:57:A:MET:HE1	1:53:A:ALA:HB2	19	0.14
(1,2979)	1:57:A:MET:HE1	1:53:A:ALA:HB3	19	0.14
(1,2979)	1:57:A:MET:HE2	1:53:A:ALA:HB1	19	0.14
(1,2979)	1:57:A:MET:HE2	1:53:A:ALA:HB2	19	0.14
(1,2979)	1:57:A:MET:HE2	1:53:A:ALA:HB3	19	0.14
(1,2979)	1:57:A:MET:HE3	1:53:A:ALA:HB1	19	0.14
(1,2979)	1:57:A:MET:HE3	1:53:A:ALA:HB2	19	0.14
(1,2979)	1:57:A:MET:HE3	1:53:A:ALA:HB3	19	0.14
(1,2978)	1:53:A:ALA:HB1	1:57:A:MET:HE1	8	0.14
(1,2978)	1:53:A:ALA:HB1	1:57:A:MET:HE2	8	0.14
(1,2978)	1:53:A:ALA:HB1	1:57:A:MET:HE3	8	0.14
(1,2978)	1:53:A:ALA:HB2	1:57:A:MET:HE1	8	0.14
(1,2978)	1:53:A:ALA:HB2	1:57:A:MET:HE2	8	0.14
(1,2978)	1:53:A:ALA:HB2	1:57:A:MET:HE3	8	0.14
(1,2978)	1:53:A:ALA:HB3	1:57:A:MET:HE1	8	0.14
(1,2978)	1:53:A:ALA:HB3	1:57:A:MET:HE2	8	0.14
(1,2978)	1:53:A:ALA:HB3	1:57:A:MET:HE3	8	0.14
(1,2978)	1:53:A:ALA:HB1	1:57:A:MET:HE1	19	0.14
(1,2978)	1:53:A:ALA:HB1	1:57:A:MET:HE2	19	0.14
(1,2978)	1:53:A:ALA:HB1	1:57:A:MET:HE3	19	0.14
(1,2978)	1:53:A:ALA:HB2	1:57:A:MET:HE1	19	0.14
(1,2978)	1:53:A:ALA:HB2	1:57:A:MET:HE2	19	0.14
(1,2978)	1:53:A:ALA:HB2	1:57:A:MET:HE3	19	0.14
(1,2978)	1:53:A:ALA:HB3	1:57:A:MET:HE1	19	0.14
(1,2978)	1:53:A:ALA:HB3	1:57:A:MET:HE2	19	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2978)	1:53:A:ALA:HB3	1:57:A:MET:HE3	19	0.14
(1,2878)	1:40:A:ASP:H	1:38:A:ALA:HB1	19	0.14
(1,2878)	1:40:A:ASP:H	1:38:A:ALA:HB2	19	0.14
(1,2878)	1:40:A:ASP:H	1:38:A:ALA:HB3	19	0.14
(1,2830)	1:66:A:SER:H	1:54:A:ILE:HG21	7	0.14
(1,2830)	1:66:A:SER:H	1:54:A:ILE:HG22	7	0.14
(1,2830)	1:66:A:SER:H	1:54:A:ILE:HG23	7	0.14
(1,2789)	1:39:A:ALA:HB1	1:31:A:LEU:HD11	8	0.14
(1,2789)	1:39:A:ALA:HB1	1:31:A:LEU:HD12	8	0.14
(1,2789)	1:39:A:ALA:HB1	1:31:A:LEU:HD13	8	0.14
(1,2789)	1:39:A:ALA:HB2	1:31:A:LEU:HD11	8	0.14
(1,2789)	1:39:A:ALA:HB2	1:31:A:LEU:HD12	8	0.14
(1,2789)	1:39:A:ALA:HB2	1:31:A:LEU:HD13	8	0.14
(1,2789)	1:39:A:ALA:HB3	1:31:A:LEU:HD11	8	0.14
(1,2789)	1:39:A:ALA:HB3	1:31:A:LEU:HD12	8	0.14
(1,2789)	1:39:A:ALA:HB3	1:31:A:LEU:HD13	8	0.14
(1,2765)	1:40:A:ASP:HB3	1:3:A:VAL:HG11	16	0.14
(1,2765)	1:40:A:ASP:HB3	1:3:A:VAL:HG12	16	0.14
(1,2765)	1:40:A:ASP:HB3	1:3:A:VAL:HG13	16	0.14
(1,2763)	1:34:A:LYS:HE3	1:3:A:VAL:HG11	7	0.14
(1,2763)	1:34:A:LYS:HE3	1:3:A:VAL:HG12	7	0.14
(1,2763)	1:34:A:LYS:HE3	1:3:A:VAL:HG13	7	0.14
(1,2763)	1:34:A:LYS:HE3	1:3:A:VAL:HG11	18	0.14
(1,2763)	1:34:A:LYS:HE3	1:3:A:VAL:HG12	18	0.14
(1,2763)	1:34:A:LYS:HE3	1:3:A:VAL:HG13	18	0.14
(1,2682)	1:38:A:ALA:H	1:3:A:VAL:HG11	6	0.14
(1,2682)	1:38:A:ALA:H	1:3:A:VAL:HG12	6	0.14
(1,2682)	1:38:A:ALA:H	1:3:A:VAL:HG13	6	0.14
(1,2664)	1:52:A:LEU:H	1:41:A:VAL:HG21	16	0.14
(1,2664)	1:52:A:LEU:H	1:41:A:VAL:HG22	16	0.14
(1,2664)	1:52:A:LEU:H	1:41:A:VAL:HG23	16	0.14
(1,2664)	1:52:A:LEU:H	1:41:A:VAL:HG21	20	0.14
(1,2664)	1:52:A:LEU:H	1:41:A:VAL:HG22	20	0.14
(1,2664)	1:52:A:LEU:H	1:41:A:VAL:HG23	20	0.14
(1,2652)	1:80:A:ASP:H	1:79:A:ILE:HG21	7	0.14
(1,2652)	1:80:A:ASP:H	1:79:A:ILE:HG22	7	0.14
(1,2652)	1:80:A:ASP:H	1:79:A:ILE:HG23	7	0.14
(1,2641)	1:115:A:GLY:H	1:113:A:ALA:HB1	8	0.14
(1,2641)	1:115:A:GLY:H	1:113:A:ALA:HB2	8	0.14
(1,2641)	1:115:A:GLY:H	1:113:A:ALA:HB3	8	0.14
(1,2630)	1:75:A:THR:H	1:75:A:THR:HG21	4	0.14
(1,2630)	1:75:A:THR:H	1:75:A:THR:HG22	4	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2630)	1:75:A:THR:H	1:75:A:THR:HG23	4	0.14
(1,2630)	1:75:A:THR:H	1:75:A:THR:HG21	14	0.14
(1,2630)	1:75:A:THR:H	1:75:A:THR:HG22	14	0.14
(1,2630)	1:75:A:THR:H	1:75:A:THR:HG23	14	0.14
(1,2630)	1:75:A:THR:H	1:75:A:THR:HG21	16	0.14
(1,2630)	1:75:A:THR:H	1:75:A:THR:HG22	16	0.14
(1,2630)	1:75:A:THR:H	1:75:A:THR:HG23	16	0.14
(1,2630)	1:75:A:THR:H	1:75:A:THR:HG21	19	0.14
(1,2630)	1:75:A:THR:H	1:75:A:THR:HG22	19	0.14
(1,2630)	1:75:A:THR:H	1:75:A:THR:HG23	19	0.14
(1,2560)	1:62:A:LYS:HE2	1:62:A:LYS:HG2	2	0.14
(1,2544)	1:62:A:LYS:HE2	1:60:A:LEU:HD21	5	0.14
(1,2544)	1:62:A:LYS:HE2	1:60:A:LEU:HD22	5	0.14
(1,2544)	1:62:A:LYS:HE2	1:60:A:LEU:HD23	5	0.14
(1,2509)	1:49:A:SER:HB2	1:52:A:LEU:HD11	8	0.14
(1,2509)	1:49:A:SER:HB2	1:52:A:LEU:HD12	8	0.14
(1,2509)	1:49:A:SER:HB2	1:52:A:LEU:HD13	8	0.14
(1,2509)	1:49:A:SER:HB3	1:52:A:LEU:HD11	8	0.14
(1,2509)	1:49:A:SER:HB3	1:52:A:LEU:HD12	8	0.14
(1,2509)	1:49:A:SER:HB3	1:52:A:LEU:HD13	8	0.14
(1,2484)	1:56:A:GLN:HE22	1:60:A:LEU:HD21	9	0.14
(1,2484)	1:56:A:GLN:HE22	1:60:A:LEU:HD22	9	0.14
(1,2484)	1:56:A:GLN:HE22	1:60:A:LEU:HD23	9	0.14
(1,2455)	1:143:A:GLN:H	1:144:A:LEU:HD21	3	0.14
(1,2455)	1:143:A:GLN:H	1:144:A:LEU:HD22	3	0.14
(1,2455)	1:143:A:GLN:H	1:144:A:LEU:HD23	3	0.14
(1,2455)	1:143:A:GLN:H	1:144:A:LEU:HD21	8	0.14
(1,2455)	1:143:A:GLN:H	1:144:A:LEU:HD22	8	0.14
(1,2455)	1:143:A:GLN:H	1:144:A:LEU:HD23	8	0.14
(1,2449)	1:130:A:TYR:H	1:126:A:LEU:HD21	4	0.14
(1,2449)	1:130:A:TYR:H	1:126:A:LEU:HD22	4	0.14
(1,2449)	1:130:A:TYR:H	1:126:A:LEU:HD23	4	0.14
(1,2373)	1:55:A:LEU:HA	1:59:A:LEU:HD21	10	0.14
(1,2373)	1:55:A:LEU:HA	1:59:A:LEU:HD22	10	0.14
(1,2373)	1:55:A:LEU:HA	1:59:A:LEU:HD23	10	0.14
(1,2352)	1:85:A:VAL:HA	1:84:A:ILE:HG13	19	0.14
(1,2344)	1:58:A:TYR:HD1	1:59:A:LEU:HD21	5	0.14
(1,2344)	1:58:A:TYR:HD1	1:59:A:LEU:HD22	5	0.14
(1,2344)	1:58:A:TYR:HD1	1:59:A:LEU:HD23	5	0.14
(1,2344)	1:58:A:TYR:HD2	1:59:A:LEU:HD21	5	0.14
(1,2344)	1:58:A:TYR:HD2	1:59:A:LEU:HD22	5	0.14
(1,2344)	1:58:A:TYR:HD2	1:59:A:LEU:HD23	5	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2316)	1:121:A:GLN:H	1:121:A:GLN:HB3	3	0.14
(1,2300)	1:49:A:SER:H	1:50:A:ILE:HG13	7	0.14
(1,2278)	1:57:A:MET:HB2	1:54:A:ILE:HG12	3	0.14
(1,2278)	1:57:A:MET:HB2	1:54:A:ILE:HG13	3	0.14
(1,2273)	1:70:A:LYS:HB2	1:70:A:LYS:HD2	5	0.14
(1,2273)	1:70:A:LYS:HB2	1:70:A:LYS:HD2	6	0.14
(1,2273)	1:70:A:LYS:HB2	1:70:A:LYS:HD2	17	0.14
(1,2260)	1:124:A:ARG:HA	1:127:A:ILE:HG12	10	0.14
(1,2260)	1:124:A:ARG:HA	1:127:A:ILE:HG13	10	0.14
(1,2248)	1:70:A:LYS:HA	1:70:A:LYS:HD3	16	0.14
(1,2215)	1:9:A:ASP:H	1:8:A:ILE:HG12	16	0.14
(1,2215)	1:9:A:ASP:H	1:8:A:ILE:HG13	16	0.14
(1,2180)	1:23:A:LYS:HD2	1:23:A:LYS:HB2	1	0.14
(1,1939)	1:92:A:LEU:HD21	1:80:A:ASP:HB3	7	0.14
(1,1939)	1:92:A:LEU:HD22	1:80:A:ASP:HB3	7	0.14
(1,1939)	1:92:A:LEU:HD23	1:80:A:ASP:HB3	7	0.14
(1,1939)	1:92:A:LEU:HD21	1:80:A:ASP:HB3	18	0.14
(1,1939)	1:92:A:LEU:HD22	1:80:A:ASP:HB3	18	0.14
(1,1939)	1:92:A:LEU:HD23	1:80:A:ASP:HB3	18	0.14
(1,1859)	1:60:A:LEU:HD21	1:62:A:LYS:HE2	7	0.14
(1,1859)	1:60:A:LEU:HD22	1:62:A:LYS:HE2	7	0.14
(1,1859)	1:60:A:LEU:HD23	1:62:A:LYS:HE2	7	0.14
(1,1843)	1:57:A:MET:HA	1:62:A:LYS:HE2	17	0.14
(1,1725)	1:47:A:VAL:HG21	1:39:A:ALA:HA	11	0.14
(1,1725)	1:47:A:VAL:HG22	1:39:A:ALA:HA	11	0.14
(1,1725)	1:47:A:VAL:HG23	1:39:A:ALA:HA	11	0.14
(1,1510)	1:72:A:ARG:HA	1:5:A:ILE:HD11	2	0.14
(1,1510)	1:72:A:ARG:HA	1:5:A:ILE:HD12	2	0.14
(1,1510)	1:72:A:ARG:HA	1:5:A:ILE:HD13	2	0.14
(1,1489)	1:70:A:LYS:H	1:5:A:ILE:HD11	4	0.14
(1,1489)	1:70:A:LYS:H	1:5:A:ILE:HD12	4	0.14
(1,1489)	1:70:A:LYS:H	1:5:A:ILE:HD13	4	0.14
(1,1489)	1:70:A:LYS:H	1:5:A:ILE:HD11	14	0.14
(1,1489)	1:70:A:LYS:H	1:5:A:ILE:HD12	14	0.14
(1,1489)	1:70:A:LYS:H	1:5:A:ILE:HD13	14	0.14
(1,1489)	1:70:A:LYS:H	1:5:A:ILE:HD11	16	0.14
(1,1489)	1:70:A:LYS:H	1:5:A:ILE:HD12	16	0.14
(1,1489)	1:70:A:LYS:H	1:5:A:ILE:HD13	16	0.14
(1,1417)	1:94:A:CYS:HB3	1:91:A:ILE:HA	1	0.14
(1,1417)	1:94:A:CYS:HB3	1:91:A:ILE:HA	19	0.14
(1,1408)	1:82:A:ASN:HB3	1:84:A:ILE:HD11	7	0.14
(1,1408)	1:82:A:ASN:HB3	1:84:A:ILE:HD12	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1408)	1:82:A:ASN:HB3	1:84:A:ILE:HD13	7	0.14
(1,1357)	1:90:A:TYR:H	1:93:A:ILE:HD11	10	0.14
(1,1357)	1:90:A:TYR:H	1:93:A:ILE:HD12	10	0.14
(1,1357)	1:90:A:TYR:H	1:93:A:ILE:HD13	10	0.14
(1,1326)	1:5:A:ILE:HD11	1:39:A:ALA:H	12	0.14
(1,1326)	1:5:A:ILE:HD12	1:39:A:ALA:H	12	0.14
(1,1326)	1:5:A:ILE:HD13	1:39:A:ALA:H	12	0.14
(1,1226)	1:68:A:ILE:HD11	1:58:A:TYR:H	12	0.14
(1,1226)	1:68:A:ILE:HD12	1:58:A:TYR:H	12	0.14
(1,1226)	1:68:A:ILE:HD13	1:58:A:TYR:H	12	0.14
(1,1222)	1:63:A:GLY:HA3	1:63:A:GLY:H	17	0.14
(1,1220)	1:131:A:ILE:HG21	1:133:A:GLY:H	20	0.14
(1,1220)	1:131:A:ILE:HG22	1:133:A:GLY:H	20	0.14
(1,1220)	1:131:A:ILE:HG23	1:133:A:GLY:H	20	0.14
(1,1205)	1:97:A:ILE:HD11	1:98:A:ASN:H	17	0.14
(1,1205)	1:97:A:ILE:HD12	1:98:A:ASN:H	17	0.14
(1,1205)	1:97:A:ILE:HD13	1:98:A:ASN:H	17	0.14
(1,1197)	1:126:A:LEU:HD11	1:122:A:THR:H	20	0.14
(1,1197)	1:126:A:LEU:HD12	1:122:A:THR:H	20	0.14
(1,1197)	1:126:A:LEU:HD13	1:122:A:THR:H	20	0.14
(1,1195)	1:60:A:LEU:HD21	1:57:A:MET:H	19	0.14
(1,1195)	1:60:A:LEU:HD22	1:57:A:MET:H	19	0.14
(1,1195)	1:60:A:LEU:HD23	1:57:A:MET:H	19	0.14
(1,1182)	1:126:A:LEU:HD11	1:127:A:ILE:H	17	0.14
(1,1182)	1:126:A:LEU:HD12	1:127:A:ILE:H	17	0.14
(1,1182)	1:126:A:LEU:HD13	1:127:A:ILE:H	17	0.14
(1,1177)	1:92:A:LEU:HD11	1:89:A:ASP:H	20	0.14
(1,1177)	1:92:A:LEU:HD12	1:89:A:ASP:H	20	0.14
(1,1177)	1:92:A:LEU:HD13	1:89:A:ASP:H	20	0.14
(1,1140)	1:144:A:LEU:HD21	1:143:A:GLN:H	3	0.14
(1,1140)	1:144:A:LEU:HD22	1:143:A:GLN:H	3	0.14
(1,1140)	1:144:A:LEU:HD23	1:143:A:GLN:H	3	0.14
(1,1140)	1:144:A:LEU:HD21	1:143:A:GLN:H	8	0.14
(1,1140)	1:144:A:LEU:HD22	1:143:A:GLN:H	8	0.14
(1,1140)	1:144:A:LEU:HD23	1:143:A:GLN:H	8	0.14
(1,1122)	1:93:A:ILE:HD11	1:94:A:CYS:H	3	0.14
(1,1122)	1:93:A:ILE:HD12	1:94:A:CYS:H	3	0.14
(1,1122)	1:93:A:ILE:HD13	1:94:A:CYS:H	3	0.14
(1,1042)	1:50:A:ILE:HD11	1:49:A:SER:H	17	0.14
(1,1042)	1:50:A:ILE:HD12	1:49:A:SER:H	17	0.14
(1,1042)	1:50:A:ILE:HD13	1:49:A:SER:H	17	0.14
(1,1004)	1:59:A:LEU:HD21	1:16:A:SER:H	13	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1004)	1:59:A:LEU:HD22	1:16:A:SER:H	13	0.14
(1,1004)	1:59:A:LEU:HD23	1:16:A:SER:H	13	0.14
(1,970)	1:70:A:LYS:HD3	1:71:A:ASN:H	7	0.14
(1,948)	1:5:A:ILE:HG21	1:70:A:LYS:H	17	0.14
(1,948)	1:5:A:ILE:HG22	1:70:A:LYS:H	17	0.14
(1,948)	1:5:A:ILE:HG23	1:70:A:LYS:H	17	0.14
(1,931)	1:8:A:ILE:HG21	1:22:A:LEU:H	6	0.14
(1,931)	1:8:A:ILE:HG22	1:22:A:LEU:H	6	0.14
(1,931)	1:8:A:ILE:HG23	1:22:A:LEU:H	6	0.14
(1,931)	1:8:A:ILE:HG21	1:22:A:LEU:H	7	0.14
(1,931)	1:8:A:ILE:HG22	1:22:A:LEU:H	7	0.14
(1,931)	1:8:A:ILE:HG23	1:22:A:LEU:H	7	0.14
(1,931)	1:8:A:ILE:HG21	1:22:A:LEU:H	18	0.14
(1,931)	1:8:A:ILE:HG22	1:22:A:LEU:H	18	0.14
(1,931)	1:8:A:ILE:HG23	1:22:A:LEU:H	18	0.14
(1,903)	1:41:A:VAL:HG21	1:48:A:ASN:H	19	0.14
(1,903)	1:41:A:VAL:HG22	1:48:A:ASN:H	19	0.14
(1,903)	1:41:A:VAL:HG23	1:48:A:ASN:H	19	0.14
(1,874)	1:139:A:PRO:HG2	1:115:A:GLY:H	4	0.14
(1,874)	1:139:A:PRO:HG3	1:115:A:GLY:H	4	0.14
(1,874)	1:139:A:PRO:HG2	1:115:A:GLY:H	12	0.14
(1,874)	1:139:A:PRO:HG3	1:115:A:GLY:H	12	0.14
(1,806)	1:53:A:ALA:HB1	1:57:A:MET:H	5	0.14
(1,806)	1:53:A:ALA:HB2	1:57:A:MET:H	5	0.14
(1,806)	1:53:A:ALA:HB3	1:57:A:MET:H	5	0.14
(1,779)	1:62:A:LYS:HB3	1:62:A:LYS:H	12	0.14
(1,779)	1:62:A:LYS:HB3	1:62:A:LYS:H	14	0.14
(1,779)	1:62:A:LYS:HB3	1:62:A:LYS:H	19	0.14
(1,772)	1:20:A:ALA:HB1	1:23:A:LYS:H	18	0.14
(1,772)	1:20:A:ALA:HB2	1:23:A:LYS:H	18	0.14
(1,772)	1:20:A:ALA:HB3	1:23:A:LYS:H	18	0.14
(1,760)	1:97:A:ILE:HB	1:96:A:HIS:H	8	0.14
(1,753)	1:124:A:ARG:HB2	1:128:A:GLU:H	13	0.14
(1,753)	1:124:A:ARG:HB3	1:128:A:GLU:H	13	0.14
(1,753)	1:129:A:LYS:HD2	1:128:A:GLU:H	15	0.14
(1,753)	1:129:A:LYS:HD3	1:128:A:GLU:H	15	0.14
(1,746)	1:144:A:LEU:HG	1:144:A:LEU:H	15	0.14
(1,741)	1:59:A:LEU:HB3	1:59:A:LEU:H	4	0.14
(1,741)	1:59:A:LEU:HB3	1:59:A:LEU:H	15	0.14
(1,596)	1:95:A:ASN:HB3	1:95:A:ASN:H	16	0.14
(1,596)	1:95:A:ASN:HB3	1:95:A:ASN:H	17	0.14
(1,582)	1:57:A:MET:HB3	1:58:A:TYR:H	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,582)	1:57:A:MET:HB3	1:58:A:TYR:H	10	0.14
(1,581)	1:94:A:CYS:HB2	1:91:A:ILE:H	4	0.14
(1,358)	1:24:A:SER:HB2	1:28:A:ASN:HD22	14	0.14
(1,358)	1:24:A:SER:HB3	1:28:A:ASN:HD22	14	0.14
(3,61)	1:109:A:PHE:H	1:105:A:ASP:O	3	0.13
(3,61)	1:109:A:PHE:H	1:105:A:ASP:O	9	0.13
(1,3943)	1:22:A:LEU:HD21	1:19:A:TYR:HD1	19	0.13
(1,3943)	1:22:A:LEU:HD21	1:19:A:TYR:HD2	19	0.13
(1,3943)	1:22:A:LEU:HD22	1:19:A:TYR:HD1	19	0.13
(1,3943)	1:22:A:LEU:HD22	1:19:A:TYR:HD2	19	0.13
(1,3943)	1:22:A:LEU:HD23	1:19:A:TYR:HD1	19	0.13
(1,3943)	1:22:A:LEU:HD23	1:19:A:TYR:HD2	19	0.13
(1,3834)	1:74:A:TYR:H	1:3:A:VAL:HG11	11	0.13
(1,3834)	1:74:A:TYR:H	1:3:A:VAL:HG12	11	0.13
(1,3834)	1:74:A:TYR:H	1:3:A:VAL:HG13	11	0.13
(1,3834)	1:74:A:TYR:H	1:3:A:VAL:HG11	13	0.13
(1,3834)	1:74:A:TYR:H	1:3:A:VAL:HG12	13	0.13
(1,3834)	1:74:A:TYR:H	1:3:A:VAL:HG13	13	0.13
(1,3834)	1:74:A:TYR:H	1:3:A:VAL:HG11	14	0.13
(1,3834)	1:74:A:TYR:H	1:3:A:VAL:HG12	14	0.13
(1,3834)	1:74:A:TYR:H	1:3:A:VAL:HG13	14	0.13
(1,3834)	1:74:A:TYR:H	1:3:A:VAL:HG11	16	0.13
(1,3834)	1:74:A:TYR:H	1:3:A:VAL:HG12	16	0.13
(1,3834)	1:74:A:TYR:H	1:3:A:VAL:HG13	16	0.13
(1,3834)	1:74:A:TYR:H	1:3:A:VAL:HG11	20	0.13
(1,3834)	1:74:A:TYR:H	1:3:A:VAL:HG12	20	0.13
(1,3834)	1:74:A:TYR:H	1:3:A:VAL:HG13	20	0.13
(1,3797)	1:93:A:ILE:H	1:79:A:ILE:HB	16	0.13
(1,3753)	1:109:A:PHE:HB2	1:108:A:LEU:HD11	16	0.13
(1,3753)	1:109:A:PHE:HB2	1:108:A:LEU:HD12	16	0.13
(1,3753)	1:109:A:PHE:HB2	1:108:A:LEU:HD13	16	0.13
(1,3753)	1:109:A:PHE:HB3	1:108:A:LEU:HD11	16	0.13
(1,3753)	1:109:A:PHE:HB3	1:108:A:LEU:HD12	16	0.13
(1,3753)	1:109:A:PHE:HB3	1:108:A:LEU:HD13	16	0.13
(1,3697)	1:101:A:GLY:HA2	1:102:A:GLN:HG3	16	0.13
(1,3520)	1:127:A:ILE:HD11	1:126:A:LEU:HB2	7	0.13
(1,3520)	1:127:A:ILE:HD12	1:126:A:LEU:HB2	7	0.13
(1,3520)	1:127:A:ILE:HD13	1:126:A:LEU:HB2	7	0.13
(1,3337)	1:5:A:ILE:HG21	1:41:A:VAL:HB	5	0.13
(1,3337)	1:5:A:ILE:HG22	1:41:A:VAL:HB	5	0.13
(1,3337)	1:5:A:ILE:HG23	1:41:A:VAL:HB	5	0.13
(1,3274)	1:73:A:ILE:HA	1:72:A:ARG:HD2	18	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3212)	1:53:A:ALA:HB1	1:49:A:SER:HB2	17	0.13
(1,3212)	1:53:A:ALA:HB1	1:49:A:SER:HB3	17	0.13
(1,3212)	1:53:A:ALA:HB2	1:49:A:SER:HB2	17	0.13
(1,3212)	1:53:A:ALA:HB2	1:49:A:SER:HB3	17	0.13
(1,3212)	1:53:A:ALA:HB3	1:49:A:SER:HB2	17	0.13
(1,3212)	1:53:A:ALA:HB3	1:49:A:SER:HB3	17	0.13
(1,3205)	1:51:A:ASP:H	1:50:A:ILE:HD11	20	0.13
(1,3205)	1:51:A:ASP:H	1:50:A:ILE:HD12	20	0.13
(1,3205)	1:51:A:ASP:H	1:50:A:ILE:HD13	20	0.13
(1,3096)	1:79:A:ILE:HG21	1:80:A:ASP:HA	15	0.13
(1,3096)	1:79:A:ILE:HG22	1:80:A:ASP:HA	15	0.13
(1,3096)	1:79:A:ILE:HG23	1:80:A:ASP:HA	15	0.13
(1,2999)	1:50:A:ILE:HG12	1:53:A:ALA:HB1	14	0.13
(1,2999)	1:50:A:ILE:HG12	1:53:A:ALA:HB2	14	0.13
(1,2999)	1:50:A:ILE:HG12	1:53:A:ALA:HB3	14	0.13
(1,2954)	1:23:A:LYS:HE2	1:20:A:ALA:HB1	17	0.13
(1,2954)	1:23:A:LYS:HE2	1:20:A:ALA:HB2	17	0.13
(1,2954)	1:23:A:LYS:HE2	1:20:A:ALA:HB3	17	0.13
(1,2942)	1:86:A:ASP:HB2	1:131:A:ILE:HG21	16	0.13
(1,2942)	1:86:A:ASP:HB2	1:131:A:ILE:HG22	16	0.13
(1,2942)	1:86:A:ASP:HB2	1:131:A:ILE:HG23	16	0.13
(1,2830)	1:66:A:SER:H	1:54:A:ILE:HG21	11	0.13
(1,2830)	1:66:A:SER:H	1:54:A:ILE:HG22	11	0.13
(1,2830)	1:66:A:SER:H	1:54:A:ILE:HG23	11	0.13
(1,2829)	1:59:A:LEU:H	1:14:A:ILE:HG21	14	0.13
(1,2829)	1:59:A:LEU:H	1:14:A:ILE:HG22	14	0.13
(1,2829)	1:59:A:LEU:H	1:14:A:ILE:HG23	14	0.13
(1,2763)	1:34:A:LYS:HE3	1:3:A:VAL:HG11	15	0.13
(1,2763)	1:34:A:LYS:HE3	1:3:A:VAL:HG12	15	0.13
(1,2763)	1:34:A:LYS:HE3	1:3:A:VAL:HG13	15	0.13
(1,2761)	1:74:A:TYR:HB2	1:75:A:THR:HG21	17	0.13
(1,2761)	1:74:A:TYR:HB2	1:75:A:THR:HG22	17	0.13
(1,2761)	1:74:A:TYR:HB2	1:75:A:THR:HG23	17	0.13
(1,2752)	1:35:A:GLN:HB2	1:32:A:THR:HG21	14	0.13
(1,2752)	1:35:A:GLN:HB2	1:32:A:THR:HG22	14	0.13
(1,2752)	1:35:A:GLN:HB2	1:32:A:THR:HG23	14	0.13
(1,2713)	1:80:A:ASP:HA	1:79:A:ILE:HG21	15	0.13
(1,2713)	1:80:A:ASP:HA	1:79:A:ILE:HG22	15	0.13
(1,2713)	1:80:A:ASP:HA	1:79:A:ILE:HG23	15	0.13
(1,2682)	1:38:A:ALA:H	1:3:A:VAL:HG11	17	0.13
(1,2682)	1:38:A:ALA:H	1:3:A:VAL:HG12	17	0.13
(1,2682)	1:38:A:ALA:H	1:3:A:VAL:HG13	17	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2652)	1:80:A:ASP:H	1:79:A:ILE:HG21	15	0.13
(1,2652)	1:80:A:ASP:H	1:79:A:ILE:HG22	15	0.13
(1,2652)	1:80:A:ASP:H	1:79:A:ILE:HG23	15	0.13
(1,2641)	1:123:A:ASP:H	1:113:A:ALA:HB1	13	0.13
(1,2641)	1:123:A:ASP:H	1:113:A:ALA:HB2	13	0.13
(1,2641)	1:123:A:ASP:H	1:113:A:ALA:HB3	13	0.13
(1,2618)	1:131:A:ILE:H	1:132:A:THR:HG21	3	0.13
(1,2618)	1:131:A:ILE:H	1:132:A:THR:HG22	3	0.13
(1,2618)	1:131:A:ILE:H	1:132:A:THR:HG23	3	0.13
(1,2583)	1:126:A:LEU:HB2	1:138:A:LEU:HD21	17	0.13
(1,2583)	1:126:A:LEU:HB2	1:138:A:LEU:HD22	17	0.13
(1,2583)	1:126:A:LEU:HB2	1:138:A:LEU:HD23	17	0.13
(1,2560)	1:62:A:LYS:HE2	1:62:A:LYS:HG2	5	0.13
(1,2550)	1:40:A:ASP:HB3	1:47:A:VAL:HG11	3	0.13
(1,2550)	1:40:A:ASP:HB3	1:47:A:VAL:HG12	3	0.13
(1,2550)	1:40:A:ASP:HB3	1:47:A:VAL:HG13	3	0.13
(1,2550)	1:40:A:ASP:HB3	1:47:A:VAL:HG11	20	0.13
(1,2550)	1:40:A:ASP:HB3	1:47:A:VAL:HG12	20	0.13
(1,2550)	1:40:A:ASP:HB3	1:47:A:VAL:HG13	20	0.13
(1,2537)	1:52:A:LEU:HA	1:55:A:LEU:HD11	18	0.13
(1,2537)	1:52:A:LEU:HA	1:55:A:LEU:HD12	18	0.13
(1,2537)	1:52:A:LEU:HA	1:55:A:LEU:HD13	18	0.13
(1,2456)	1:23:A:LYS:H	1:52:A:LEU:HD11	14	0.13
(1,2456)	1:23:A:LYS:H	1:52:A:LEU:HD12	14	0.13
(1,2456)	1:23:A:LYS:H	1:52:A:LEU:HD13	14	0.13
(1,2449)	1:59:A:LEU:H	1:60:A:LEU:HD21	18	0.13
(1,2449)	1:59:A:LEU:H	1:60:A:LEU:HD22	18	0.13
(1,2449)	1:59:A:LEU:H	1:60:A:LEU:HD23	18	0.13
(1,2400)	1:94:A:CYS:HB3	1:124:A:ARG:HG2	4	0.13
(1,2400)	1:94:A:CYS:HB3	1:124:A:ARG:HG2	12	0.13
(1,2352)	1:85:A:VAL:HA	1:84:A:ILE:HG13	4	0.13
(1,2352)	1:85:A:VAL:HA	1:84:A:ILE:HG13	5	0.13
(1,2352)	1:85:A:VAL:HA	1:84:A:ILE:HG13	10	0.13
(1,2352)	1:85:A:VAL:HA	1:84:A:ILE:HG13	12	0.13
(1,2350)	1:52:A:LEU:H	1:52:A:LEU:HD21	4	0.13
(1,2350)	1:52:A:LEU:H	1:52:A:LEU:HD22	4	0.13
(1,2350)	1:52:A:LEU:H	1:52:A:LEU:HD23	4	0.13
(1,2344)	1:58:A:TYR:HD1	1:59:A:LEU:HD21	3	0.13
(1,2344)	1:58:A:TYR:HD1	1:59:A:LEU:HD22	3	0.13
(1,2344)	1:58:A:TYR:HD1	1:59:A:LEU:HD23	3	0.13
(1,2344)	1:58:A:TYR:HD2	1:59:A:LEU:HD21	3	0.13
(1,2344)	1:58:A:TYR:HD2	1:59:A:LEU:HD22	3	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2344)	1:58:A:TYR:HD2	1:59:A:LEU:HD23	3	0.13
(1,2316)	1:121:A:GLN:H	1:121:A:GLN:HB3	7	0.13
(1,2316)	1:121:A:GLN:H	1:121:A:GLN:HB3	20	0.13
(1,2273)	1:70:A:LYS:HB2	1:70:A:LYS:HD2	1	0.13
(1,2273)	1:70:A:LYS:HB2	1:70:A:LYS:HD2	7	0.13
(1,2273)	1:70:A:LYS:HB2	1:70:A:LYS:HD2	9	0.13
(1,2273)	1:70:A:LYS:HB2	1:70:A:LYS:HD2	18	0.13
(1,2260)	1:124:A:ARG:HA	1:127:A:ILE:HG12	5	0.13
(1,2260)	1:124:A:ARG:HA	1:127:A:ILE:HG13	5	0.13
(1,2215)	1:9:A:ASP:H	1:8:A:ILE:HG12	12	0.13
(1,2215)	1:9:A:ASP:H	1:8:A:ILE:HG13	12	0.13
(1,2145)	1:37:A:ALA:HA	1:3:A:VAL:HB	5	0.13
(1,1939)	1:92:A:LEU:HD21	1:80:A:ASP:HB3	14	0.13
(1,1939)	1:92:A:LEU:HD22	1:80:A:ASP:HB3	14	0.13
(1,1939)	1:92:A:LEU:HD23	1:80:A:ASP:HB3	14	0.13
(1,1841)	1:62:A:LYS:HB3	1:62:A:LYS:HE3	14	0.13
(1,1840)	1:62:A:LYS:HB3	1:62:A:LYS:HE2	7	0.13
(1,1840)	1:62:A:LYS:HB3	1:62:A:LYS:HE2	13	0.13
(1,1797)	1:62:A:LYS:H	1:62:A:LYS:HE2	9	0.13
(1,1639)	1:23:A:LYS:HD2	1:23:A:LYS:HA	3	0.13
(1,1549)	1:70:A:LYS:HB2	1:5:A:ILE:HD11	9	0.13
(1,1549)	1:70:A:LYS:HB2	1:5:A:ILE:HD12	9	0.13
(1,1549)	1:70:A:LYS:HB2	1:5:A:ILE:HD13	9	0.13
(1,1482)	1:28:A:ASN:H	1:27:A:ILE:HA	10	0.13
(1,1451)	1:119:A:ILE:HG21	1:93:A:ILE:HD11	11	0.13
(1,1451)	1:119:A:ILE:HG21	1:93:A:ILE:HD12	11	0.13
(1,1451)	1:119:A:ILE:HG21	1:93:A:ILE:HD13	11	0.13
(1,1451)	1:119:A:ILE:HG22	1:93:A:ILE:HD11	11	0.13
(1,1451)	1:119:A:ILE:HG22	1:93:A:ILE:HD12	11	0.13
(1,1451)	1:119:A:ILE:HG22	1:93:A:ILE:HD13	11	0.13
(1,1451)	1:119:A:ILE:HG23	1:93:A:ILE:HD11	11	0.13
(1,1451)	1:119:A:ILE:HG23	1:93:A:ILE:HD12	11	0.13
(1,1451)	1:119:A:ILE:HG23	1:93:A:ILE:HD13	11	0.13
(1,1451)	1:119:A:ILE:HG21	1:93:A:ILE:HD11	20	0.13
(1,1451)	1:119:A:ILE:HG21	1:93:A:ILE:HD12	20	0.13
(1,1451)	1:119:A:ILE:HG21	1:93:A:ILE:HD13	20	0.13
(1,1451)	1:119:A:ILE:HG22	1:93:A:ILE:HD11	20	0.13
(1,1451)	1:119:A:ILE:HG22	1:93:A:ILE:HD12	20	0.13
(1,1451)	1:119:A:ILE:HG22	1:93:A:ILE:HD13	20	0.13
(1,1451)	1:119:A:ILE:HG23	1:93:A:ILE:HD11	20	0.13
(1,1451)	1:119:A:ILE:HG23	1:93:A:ILE:HD12	20	0.13
(1,1451)	1:119:A:ILE:HG23	1:93:A:ILE:HD13	20	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1417)	1:94:A:CYS:HB3	1:91:A:ILE:HA	2	0.13
(1,1388)	1:103:A:LEU:HA	1:107:A:SER:HB3	11	0.13
(1,1383)	1:58:A:TYR:HD1	1:68:A:ILE:HD11	10	0.13
(1,1383)	1:58:A:TYR:HD1	1:68:A:ILE:HD12	10	0.13
(1,1383)	1:58:A:TYR:HD1	1:68:A:ILE:HD13	10	0.13
(1,1383)	1:58:A:TYR:HD2	1:68:A:ILE:HD11	10	0.13
(1,1383)	1:58:A:TYR:HD2	1:68:A:ILE:HD12	10	0.13
(1,1383)	1:58:A:TYR:HD2	1:68:A:ILE:HD13	10	0.13
(1,1321)	1:23:A:LYS:HB3	1:23:A:LYS:H	15	0.13
(1,1288)	1:121:A:GLN:HG3	1:122:A:THR:H	3	0.13
(1,1288)	1:121:A:GLN:HG2	1:122:A:THR:H	11	0.13
(1,1260)	1:51:A:ASP:H	1:41:A:VAL:H	17	0.13
(1,1260)	1:51:A:ASP:H	1:41:A:VAL:H	18	0.13
(1,1222)	1:63:A:GLY:HA3	1:63:A:GLY:H	6	0.13
(1,1222)	1:63:A:GLY:HA3	1:63:A:GLY:H	9	0.13
(1,1222)	1:63:A:GLY:HA3	1:63:A:GLY:H	10	0.13
(1,1222)	1:63:A:GLY:HA3	1:63:A:GLY:H	18	0.13
(1,1195)	1:60:A:LEU:HD21	1:57:A:MET:H	2	0.13
(1,1195)	1:60:A:LEU:HD22	1:57:A:MET:H	2	0.13
(1,1195)	1:60:A:LEU:HD23	1:57:A:MET:H	2	0.13
(1,1182)	1:126:A:LEU:HD11	1:127:A:ILE:H	5	0.13
(1,1182)	1:126:A:LEU:HD12	1:127:A:ILE:H	5	0.13
(1,1182)	1:126:A:LEU:HD13	1:127:A:ILE:H	5	0.13
(1,1182)	1:126:A:LEU:HD11	1:127:A:ILE:H	11	0.13
(1,1182)	1:126:A:LEU:HD12	1:127:A:ILE:H	11	0.13
(1,1182)	1:126:A:LEU:HD13	1:127:A:ILE:H	11	0.13
(1,1182)	1:126:A:LEU:HD11	1:127:A:ILE:H	20	0.13
(1,1182)	1:126:A:LEU:HD12	1:127:A:ILE:H	20	0.13
(1,1182)	1:126:A:LEU:HD13	1:127:A:ILE:H	20	0.13
(1,1177)	1:92:A:LEU:HD11	1:89:A:ASP:H	11	0.13
(1,1177)	1:92:A:LEU:HD12	1:89:A:ASP:H	11	0.13
(1,1177)	1:92:A:LEU:HD13	1:89:A:ASP:H	11	0.13
(1,1141)	1:144:A:LEU:HG	1:143:A:GLN:H	10	0.13
(1,1137)	1:97:A:ILE:HG21	1:96:A:HIS:H	13	0.13
(1,1137)	1:97:A:ILE:HG22	1:96:A:HIS:H	13	0.13
(1,1137)	1:97:A:ILE:HG23	1:96:A:HIS:H	13	0.13
(1,1091)	1:103:A:LEU:HD21	1:104:A:SER:H	14	0.13
(1,1091)	1:103:A:LEU:HD22	1:104:A:SER:H	14	0.13
(1,1091)	1:103:A:LEU:HD23	1:104:A:SER:H	14	0.13
(1,1004)	1:59:A:LEU:HD21	1:16:A:SER:H	12	0.13
(1,1004)	1:59:A:LEU:HD22	1:16:A:SER:H	12	0.13
(1,1004)	1:59:A:LEU:HD23	1:16:A:SER:H	12	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1004)	1:59:A:LEU:HD11	1:16:A:SER:H	19	0.13
(1,1004)	1:59:A:LEU:HD12	1:16:A:SER:H	19	0.13
(1,1004)	1:59:A:LEU:HD13	1:16:A:SER:H	19	0.13
(1,981)	1:84:A:ILE:HD11	1:82:A:ASN:H	15	0.13
(1,981)	1:84:A:ILE:HD12	1:82:A:ASN:H	15	0.13
(1,981)	1:84:A:ILE:HD13	1:82:A:ASN:H	15	0.13
(1,981)	1:84:A:ILE:HD11	1:82:A:ASN:H	20	0.13
(1,981)	1:84:A:ILE:HD12	1:82:A:ASN:H	20	0.13
(1,981)	1:84:A:ILE:HD13	1:82:A:ASN:H	20	0.13
(1,978)	1:131:A:ILE:HD11	1:131:A:ILE:H	11	0.13
(1,978)	1:131:A:ILE:HD12	1:131:A:ILE:H	11	0.13
(1,978)	1:131:A:ILE:HD13	1:131:A:ILE:H	11	0.13
(1,977)	1:132:A:THR:HG21	1:131:A:ILE:H	3	0.13
(1,977)	1:132:A:THR:HG22	1:131:A:ILE:H	3	0.13
(1,977)	1:132:A:THR:HG23	1:131:A:ILE:H	3	0.13
(1,939)	1:91:A:ILE:HD11	1:91:A:ILE:H	5	0.13
(1,939)	1:91:A:ILE:HD12	1:91:A:ILE:H	5	0.13
(1,939)	1:91:A:ILE:HD13	1:91:A:ILE:H	5	0.13
(1,933)	1:52:A:LEU:HD21	1:26:A:LEU:H	10	0.13
(1,933)	1:52:A:LEU:HD22	1:26:A:LEU:H	10	0.13
(1,933)	1:52:A:LEU:HD23	1:26:A:LEU:H	10	0.13
(1,931)	1:8:A:ILE:HG21	1:22:A:LEU:H	9	0.13
(1,931)	1:8:A:ILE:HG22	1:22:A:LEU:H	9	0.13
(1,931)	1:8:A:ILE:HG23	1:22:A:LEU:H	9	0.13
(1,909)	1:73:A:ILE:HD11	1:73:A:ILE:H	10	0.13
(1,909)	1:73:A:ILE:HD12	1:73:A:ILE:H	10	0.13
(1,909)	1:73:A:ILE:HD13	1:73:A:ILE:H	10	0.13
(1,903)	1:41:A:VAL:HG21	1:48:A:ASN:H	15	0.13
(1,903)	1:41:A:VAL:HG22	1:48:A:ASN:H	15	0.13
(1,903)	1:41:A:VAL:HG23	1:48:A:ASN:H	15	0.13
(1,874)	1:139:A:PRO:HG2	1:115:A:GLY:H	10	0.13
(1,874)	1:139:A:PRO:HG3	1:115:A:GLY:H	10	0.13
(1,874)	1:139:A:PRO:HG2	1:115:A:GLY:H	13	0.13
(1,874)	1:139:A:PRO:HG3	1:115:A:GLY:H	13	0.13
(1,874)	1:139:A:PRO:HG2	1:115:A:GLY:H	16	0.13
(1,874)	1:139:A:PRO:HG3	1:115:A:GLY:H	16	0.13
(1,806)	1:53:A:ALA:HB1	1:57:A:MET:H	10	0.13
(1,806)	1:53:A:ALA:HB2	1:57:A:MET:H	10	0.13
(1,806)	1:53:A:ALA:HB3	1:57:A:MET:H	10	0.13
(1,806)	1:53:A:ALA:HB1	1:57:A:MET:H	15	0.13
(1,806)	1:53:A:ALA:HB2	1:57:A:MET:H	15	0.13
(1,806)	1:53:A:ALA:HB3	1:57:A:MET:H	15	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,806)	1:53:A:ALA:HB1	1:57:A:MET:H	19	0.13
(1,806)	1:53:A:ALA:HB2	1:57:A:MET:H	19	0.13
(1,806)	1:53:A:ALA:HB3	1:57:A:MET:H	19	0.13
(1,779)	1:62:A:LYS:HB3	1:62:A:LYS:H	2	0.13
(1,779)	1:62:A:LYS:HB3	1:62:A:LYS:H	6	0.13
(1,779)	1:62:A:LYS:HB3	1:62:A:LYS:H	15	0.13
(1,779)	1:62:A:LYS:HB3	1:62:A:LYS:H	20	0.13
(1,753)	1:124:A:ARG:HB2	1:128:A:GLU:H	17	0.13
(1,753)	1:124:A:ARG:HB3	1:128:A:GLU:H	17	0.13
(1,741)	1:59:A:LEU:HB3	1:59:A:LEU:H	6	0.13
(1,741)	1:59:A:LEU:HB3	1:59:A:LEU:H	19	0.13
(1,596)	1:95:A:ASN:HB3	1:95:A:ASN:H	9	0.13
(1,579)	1:142:A:ASN:HB3	1:143:A:GLN:H	12	0.13
(1,572)	1:9:A:ASP:HB3	1:20:A:ALA:H	7	0.13
(1,391)	1:72:A:ARG:HD2	1:73:A:ILE:H	12	0.13
(1,380)	1:61:A:GLY:HA3	1:61:A:GLY:H	4	0.13
(1,359)	1:83:A:GLY:HA3	1:83:A:GLY:H	13	0.13
(1,250)	1:102:A:GLN:HE22	1:101:A:GLY:H	4	0.13
(1,250)	1:102:A:GLN:HE22	1:101:A:GLY:H	19	0.13
(1,175)	1:48:A:ASN:HD22	1:48:A:ASN:H	2	0.13
(3,61)	1:109:A:PHE:H	1:105:A:ASP:O	7	0.12
(3,61)	1:109:A:PHE:H	1:105:A:ASP:O	10	0.12
(3,61)	1:109:A:PHE:H	1:105:A:ASP:O	11	0.12
(3,61)	1:109:A:PHE:H	1:105:A:ASP:O	17	0.12
(3,61)	1:109:A:PHE:H	1:105:A:ASP:O	18	0.12
(3,61)	1:109:A:PHE:H	1:105:A:ASP:O	19	0.12
(1,3875)	1:55:A:LEU:HB3	1:8:A:ILE:HG12	4	0.12
(1,3875)	1:55:A:LEU:HB3	1:8:A:ILE:HG13	4	0.12
(1,3843)	1:126:A:LEU:HA	1:113:A:ALA:HB1	12	0.12
(1,3843)	1:126:A:LEU:HA	1:113:A:ALA:HB2	12	0.12
(1,3843)	1:126:A:LEU:HA	1:113:A:ALA:HB3	12	0.12
(1,3834)	1:74:A:TYR:H	1:3:A:VAL:HG11	17	0.12
(1,3834)	1:74:A:TYR:H	1:3:A:VAL:HG12	17	0.12
(1,3834)	1:74:A:TYR:H	1:3:A:VAL:HG13	17	0.12
(1,3721)	1:7:A:ASP:H	1:4:A:LYS:HD2	12	0.12
(1,3707)	1:71:A:ASN:HA	1:72:A:ARG:HB2	6	0.12
(1,3697)	1:101:A:GLY:HA2	1:102:A:GLN:HG3	8	0.12
(1,3697)	1:101:A:GLY:HA2	1:102:A:GLN:HG3	18	0.12
(1,3623)	1:135:A:ILE:HG12	1:134:A:ARG:HA	12	0.12
(1,3620)	1:73:A:ILE:HG13	1:2:A:SER:HA	10	0.12
(1,3459)	1:74:A:TYR:HB3	1:73:A:ILE:HA	8	0.12
(1,3459)	1:74:A:TYR:HB3	1:73:A:ILE:HA	10	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3336)	1:126:A:LEU:HD11	1:139:A:PRO:HB3	7	0.12
(1,3336)	1:126:A:LEU:HD12	1:139:A:PRO:HB3	7	0.12
(1,3336)	1:126:A:LEU:HD13	1:139:A:PRO:HB3	7	0.12
(1,3299)	1:34:A:LYS:HG2	1:112:A:ASP:HB3	14	0.12
(1,3299)	1:34:A:LYS:HG3	1:112:A:ASP:HB3	14	0.12
(1,3263)	1:5:A:ILE:HG21	1:6:A:GLY:HA2	6	0.12
(1,3263)	1:5:A:ILE:HG22	1:6:A:GLY:HA2	6	0.12
(1,3263)	1:5:A:ILE:HG23	1:6:A:GLY:HA2	6	0.12
(1,3263)	1:5:A:ILE:HG21	1:6:A:GLY:HA2	18	0.12
(1,3263)	1:5:A:ILE:HG22	1:6:A:GLY:HA2	18	0.12
(1,3263)	1:5:A:ILE:HG23	1:6:A:GLY:HA2	18	0.12
(1,3242)	1:144:A:LEU:H	1:144:A:LEU:HA	10	0.12
(1,3230)	1:54:A:ILE:HD11	1:51:A:ASP:HA	8	0.12
(1,3230)	1:54:A:ILE:HD12	1:51:A:ASP:HA	8	0.12
(1,3230)	1:54:A:ILE:HD13	1:51:A:ASP:HA	8	0.12
(1,3164)	1:123:A:ASP:HB2	1:93:A:ILE:HD11	8	0.12
(1,3164)	1:123:A:ASP:HB2	1:93:A:ILE:HD12	8	0.12
(1,3164)	1:123:A:ASP:HB2	1:93:A:ILE:HD13	8	0.12
(1,3164)	1:123:A:ASP:HB2	1:93:A:ILE:HD11	20	0.12
(1,3164)	1:123:A:ASP:HB2	1:93:A:ILE:HD12	20	0.12
(1,3164)	1:123:A:ASP:HB2	1:93:A:ILE:HD13	20	0.12
(1,3095)	1:57:A:MET:HE1	1:53:A:ALA:HA	1	0.12
(1,3095)	1:57:A:MET:HE2	1:53:A:ALA:HA	1	0.12
(1,3095)	1:57:A:MET:HE3	1:53:A:ALA:HA	1	0.12
(1,3049)	1:12:A:GLY:HA2	1:13:A:GLU:HG2	18	0.12
(1,3049)	1:12:A:GLY:HA2	1:13:A:GLU:HG3	18	0.12
(1,3030)	1:58:A:TYR:H	1:57:A:MET:HE1	12	0.12
(1,3030)	1:58:A:TYR:H	1:57:A:MET:HE2	12	0.12
(1,3030)	1:58:A:TYR:H	1:57:A:MET:HE3	12	0.12
(1,2980)	1:54:A:ILE:HB	1:53:A:ALA:HB1	10	0.12
(1,2980)	1:54:A:ILE:HB	1:53:A:ALA:HB2	10	0.12
(1,2980)	1:54:A:ILE:HB	1:53:A:ALA:HB3	10	0.12
(1,2979)	1:57:A:MET:HE1	1:53:A:ALA:HB1	3	0.12
(1,2979)	1:57:A:MET:HE1	1:53:A:ALA:HB2	3	0.12
(1,2979)	1:57:A:MET:HE1	1:53:A:ALA:HB3	3	0.12
(1,2979)	1:57:A:MET:HE2	1:53:A:ALA:HB1	3	0.12
(1,2979)	1:57:A:MET:HE2	1:53:A:ALA:HB2	3	0.12
(1,2979)	1:57:A:MET:HE2	1:53:A:ALA:HB3	3	0.12
(1,2979)	1:57:A:MET:HE3	1:53:A:ALA:HB1	3	0.12
(1,2979)	1:57:A:MET:HE3	1:53:A:ALA:HB2	3	0.12
(1,2979)	1:57:A:MET:HE3	1:53:A:ALA:HB3	3	0.12
(1,2970)	1:87:A:GLU:HG2	1:127:A:ILE:HG21	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2970)	1:87:A:GLU:HG2	1:127:A:ILE:HG22	1	0.12
(1,2970)	1:87:A:GLU:HG2	1:127:A:ILE:HG23	1	0.12
(1,2966)	1:94:A:CYS:HB3	1:91:A:ILE:HG21	13	0.12
(1,2966)	1:94:A:CYS:HB3	1:91:A:ILE:HG22	13	0.12
(1,2966)	1:94:A:CYS:HB3	1:91:A:ILE:HG23	13	0.12
(1,2891)	1:58:A:TYR:HD1	1:54:A:ILE:HG21	4	0.12
(1,2891)	1:58:A:TYR:HD1	1:54:A:ILE:HG22	4	0.12
(1,2891)	1:58:A:TYR:HD1	1:54:A:ILE:HG23	4	0.12
(1,2891)	1:58:A:TYR:HD2	1:54:A:ILE:HG21	4	0.12
(1,2891)	1:58:A:TYR:HD2	1:54:A:ILE:HG22	4	0.12
(1,2891)	1:58:A:TYR:HD2	1:54:A:ILE:HG23	4	0.12
(1,2891)	1:58:A:TYR:HD1	1:54:A:ILE:HG21	15	0.12
(1,2891)	1:58:A:TYR:HD1	1:54:A:ILE:HG22	15	0.12
(1,2891)	1:58:A:TYR:HD1	1:54:A:ILE:HG23	15	0.12
(1,2891)	1:58:A:TYR:HD2	1:54:A:ILE:HG21	15	0.12
(1,2891)	1:58:A:TYR:HD2	1:54:A:ILE:HG22	15	0.12
(1,2891)	1:58:A:TYR:HD2	1:54:A:ILE:HG23	15	0.12
(1,2878)	1:40:A:ASP:H	1:38:A:ALA:HB1	20	0.12
(1,2878)	1:40:A:ASP:H	1:38:A:ALA:HB2	20	0.12
(1,2878)	1:40:A:ASP:H	1:38:A:ALA:HB3	20	0.12
(1,2830)	1:65:A:THR:H	1:54:A:ILE:HG21	2	0.12
(1,2830)	1:65:A:THR:H	1:54:A:ILE:HG22	2	0.12
(1,2830)	1:65:A:THR:H	1:54:A:ILE:HG23	2	0.12
(1,2829)	1:59:A:LEU:H	1:14:A:ILE:HG21	16	0.12
(1,2829)	1:59:A:LEU:H	1:14:A:ILE:HG22	16	0.12
(1,2829)	1:59:A:LEU:H	1:14:A:ILE:HG23	16	0.12
(1,2765)	1:40:A:ASP:HB3	1:3:A:VAL:HG11	13	0.12
(1,2765)	1:40:A:ASP:HB3	1:3:A:VAL:HG12	13	0.12
(1,2765)	1:40:A:ASP:HB3	1:3:A:VAL:HG13	13	0.12
(1,2763)	1:34:A:LYS:HE3	1:3:A:VAL:HG11	13	0.12
(1,2763)	1:34:A:LYS:HE3	1:3:A:VAL:HG12	13	0.12
(1,2763)	1:34:A:LYS:HE3	1:3:A:VAL:HG13	13	0.12
(1,2761)	1:74:A:TYR:HB2	1:75:A:THR:HG21	16	0.12
(1,2761)	1:74:A:TYR:HB2	1:75:A:THR:HG22	16	0.12
(1,2761)	1:74:A:TYR:HB2	1:75:A:THR:HG23	16	0.12
(1,2752)	1:35:A:GLN:HB2	1:32:A:THR:HG21	17	0.12
(1,2752)	1:35:A:GLN:HB2	1:32:A:THR:HG22	17	0.12
(1,2752)	1:35:A:GLN:HB2	1:32:A:THR:HG23	17	0.12
(1,2744)	1:35:A:GLN:HA	1:31:A:LEU:HD11	3	0.12
(1,2744)	1:35:A:GLN:HA	1:31:A:LEU:HD12	3	0.12
(1,2744)	1:35:A:GLN:HA	1:31:A:LEU:HD13	3	0.12
(1,2664)	1:52:A:LEU:H	1:41:A:VAL:HG21	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2664)	1:52:A:LEU:H	1:41:A:VAL:HG22	3	0.12
(1,2664)	1:52:A:LEU:H	1:41:A:VAL:HG23	3	0.12
(1,2652)	1:80:A:ASP:H	1:79:A:ILE:HG21	16	0.12
(1,2652)	1:80:A:ASP:H	1:79:A:ILE:HG22	16	0.12
(1,2652)	1:80:A:ASP:H	1:79:A:ILE:HG23	16	0.12
(1,2641)	1:123:A:ASP:H	1:113:A:ALA:HB1	2	0.12
(1,2641)	1:123:A:ASP:H	1:113:A:ALA:HB2	2	0.12
(1,2641)	1:123:A:ASP:H	1:113:A:ALA:HB3	2	0.12
(1,2630)	1:75:A:THR:H	1:75:A:THR:HG21	9	0.12
(1,2630)	1:75:A:THR:H	1:75:A:THR:HG22	9	0.12
(1,2630)	1:75:A:THR:H	1:75:A:THR:HG23	9	0.12
(1,2630)	1:75:A:THR:H	1:75:A:THR:HG21	17	0.12
(1,2630)	1:75:A:THR:H	1:75:A:THR:HG22	17	0.12
(1,2630)	1:75:A:THR:H	1:75:A:THR:HG23	17	0.12
(1,2630)	1:75:A:THR:H	1:75:A:THR:HG21	20	0.12
(1,2630)	1:75:A:THR:H	1:75:A:THR:HG22	20	0.12
(1,2630)	1:75:A:THR:H	1:75:A:THR:HG23	20	0.12
(1,2583)	1:126:A:LEU:HB2	1:138:A:LEU:HD21	13	0.12
(1,2583)	1:126:A:LEU:HB2	1:138:A:LEU:HD22	13	0.12
(1,2583)	1:126:A:LEU:HB2	1:138:A:LEU:HD23	13	0.12
(1,2549)	1:40:A:ASP:HB2	1:47:A:VAL:HG11	7	0.12
(1,2549)	1:40:A:ASP:HB2	1:47:A:VAL:HG12	7	0.12
(1,2549)	1:40:A:ASP:HB2	1:47:A:VAL:HG13	7	0.12
(1,2537)	1:52:A:LEU:HA	1:55:A:LEU:HD11	9	0.12
(1,2537)	1:52:A:LEU:HA	1:55:A:LEU:HD12	9	0.12
(1,2537)	1:52:A:LEU:HA	1:55:A:LEU:HD13	9	0.12
(1,2515)	1:92:A:LEU:HA	1:103:A:LEU:HD11	9	0.12
(1,2515)	1:92:A:LEU:HA	1:103:A:LEU:HD12	9	0.12
(1,2515)	1:92:A:LEU:HA	1:103:A:LEU:HD13	9	0.12
(1,2337)	1:84:A:ILE:H	1:84:A:ILE:HG12	1	0.12
(1,2316)	1:121:A:GLN:H	1:121:A:GLN:HB3	1	0.12
(1,2300)	1:49:A:SER:H	1:50:A:ILE:HG13	4	0.12
(1,2300)	1:49:A:SER:H	1:50:A:ILE:HG13	12	0.12
(1,2300)	1:49:A:SER:H	1:50:A:ILE:HG13	18	0.12
(1,2277)	1:93:A:ILE:HB	1:127:A:ILE:HG12	5	0.12
(1,2277)	1:93:A:ILE:HB	1:127:A:ILE:HG13	5	0.12
(1,2273)	1:70:A:LYS:HB2	1:70:A:LYS:HD2	4	0.12
(1,2273)	1:70:A:LYS:HB2	1:70:A:LYS:HD2	11	0.12
(1,2260)	1:124:A:ARG:HA	1:127:A:ILE:HG12	9	0.12
(1,2260)	1:124:A:ARG:HA	1:127:A:ILE:HG13	9	0.12
(1,2248)	1:70:A:LYS:HA	1:70:A:LYS:HD3	3	0.12
(1,2215)	1:9:A:ASP:H	1:8:A:ILE:HG12	5	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2215)	1:9:A:ASP:H	1:8:A:ILE:HG13	5	0.12
(1,2180)	1:23:A:LYS:HD2	1:23:A:LYS:HB2	16	0.12
(1,2157)	1:4:A:LYS:HE2	1:13:A:GLU:HB3	14	0.12
(1,2157)	1:4:A:LYS:HE3	1:13:A:GLU:HB3	14	0.12
(1,2154)	1:104:A:SER:HA	1:102:A:GLN:HG3	2	0.12
(1,1939)	1:92:A:LEU:HD21	1:80:A:ASP:HB3	10	0.12
(1,1939)	1:92:A:LEU:HD22	1:80:A:ASP:HB3	10	0.12
(1,1939)	1:92:A:LEU:HD23	1:80:A:ASP:HB3	10	0.12
(1,1939)	1:92:A:LEU:HD21	1:80:A:ASP:HB3	17	0.12
(1,1939)	1:92:A:LEU:HD22	1:80:A:ASP:HB3	17	0.12
(1,1939)	1:92:A:LEU:HD23	1:80:A:ASP:HB3	17	0.12
(1,1939)	1:92:A:LEU:HD21	1:80:A:ASP:HB3	19	0.12
(1,1939)	1:92:A:LEU:HD22	1:80:A:ASP:HB3	19	0.12
(1,1939)	1:92:A:LEU:HD23	1:80:A:ASP:HB3	19	0.12
(1,1840)	1:57:A:MET:HE1	1:62:A:LYS:HE2	15	0.12
(1,1840)	1:57:A:MET:HE2	1:62:A:LYS:HE2	15	0.12
(1,1840)	1:57:A:MET:HE3	1:62:A:LYS:HE2	15	0.12
(1,1651)	1:59:A:LEU:HD21	1:56:A:GLN:HA	11	0.12
(1,1651)	1:59:A:LEU:HD22	1:56:A:GLN:HA	11	0.12
(1,1651)	1:59:A:LEU:HD23	1:56:A:GLN:HA	11	0.12
(1,1639)	1:23:A:LYS:HD2	1:23:A:LYS:HA	8	0.12
(1,1639)	1:23:A:LYS:HD2	1:23:A:LYS:HA	16	0.12
(1,1534)	1:20:A:ALA:HB1	1:17:A:ILE:HA	1	0.12
(1,1534)	1:20:A:ALA:HB2	1:17:A:ILE:HA	1	0.12
(1,1534)	1:20:A:ALA:HB3	1:17:A:ILE:HA	1	0.12
(1,1534)	1:20:A:ALA:HB1	1:17:A:ILE:HA	15	0.12
(1,1534)	1:20:A:ALA:HB2	1:17:A:ILE:HA	15	0.12
(1,1534)	1:20:A:ALA:HB3	1:17:A:ILE:HA	15	0.12
(1,1482)	1:28:A:ASN:H	1:27:A:ILE:HA	1	0.12
(1,1482)	1:28:A:ASN:H	1:27:A:ILE:HA	2	0.12
(1,1482)	1:28:A:ASN:H	1:27:A:ILE:HA	7	0.12
(1,1451)	1:119:A:ILE:HG21	1:93:A:ILE:HD11	7	0.12
(1,1451)	1:119:A:ILE:HG21	1:93:A:ILE:HD12	7	0.12
(1,1451)	1:119:A:ILE:HG21	1:93:A:ILE:HD13	7	0.12
(1,1451)	1:119:A:ILE:HG22	1:93:A:ILE:HD11	7	0.12
(1,1451)	1:119:A:ILE:HG22	1:93:A:ILE:HD12	7	0.12
(1,1451)	1:119:A:ILE:HG22	1:93:A:ILE:HD13	7	0.12
(1,1451)	1:119:A:ILE:HG23	1:93:A:ILE:HD11	7	0.12
(1,1451)	1:119:A:ILE:HG23	1:93:A:ILE:HD12	7	0.12
(1,1451)	1:119:A:ILE:HG23	1:93:A:ILE:HD13	7	0.12
(1,1322)	1:117:A:ASN:HA	1:116:A:ASN:H	3	0.12
(1,1321)	1:23:A:LYS:HB3	1:23:A:LYS:H	2	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1321)	1:23:A:LYS:HB3	1:23:A:LYS:H	5	0.12
(1,1321)	1:23:A:LYS:HB3	1:23:A:LYS:H	11	0.12
(1,1260)	1:51:A:ASP:H	1:41:A:VAL:H	16	0.12
(1,1226)	1:68:A:ILE:HD11	1:58:A:TYR:H	1	0.12
(1,1226)	1:68:A:ILE:HD12	1:58:A:TYR:H	1	0.12
(1,1226)	1:68:A:ILE:HD13	1:58:A:TYR:H	1	0.12
(1,1222)	1:63:A:GLY:HA3	1:63:A:GLY:H	2	0.12
(1,1222)	1:63:A:GLY:HA3	1:63:A:GLY:H	7	0.12
(1,1222)	1:63:A:GLY:HA3	1:63:A:GLY:H	19	0.12
(1,1221)	1:62:A:LYS:HB3	1:63:A:GLY:H	19	0.12
(1,1220)	1:131:A:ILE:HG21	1:133:A:GLY:H	3	0.12
(1,1220)	1:131:A:ILE:HG22	1:133:A:GLY:H	3	0.12
(1,1220)	1:131:A:ILE:HG23	1:133:A:GLY:H	3	0.12
(1,1220)	1:131:A:ILE:HG21	1:133:A:GLY:H	13	0.12
(1,1220)	1:131:A:ILE:HG22	1:133:A:GLY:H	13	0.12
(1,1220)	1:131:A:ILE:HG23	1:133:A:GLY:H	13	0.12
(1,1205)	1:97:A:ILE:HD11	1:98:A:ASN:H	15	0.12
(1,1205)	1:97:A:ILE:HD12	1:98:A:ASN:H	15	0.12
(1,1205)	1:97:A:ILE:HD13	1:98:A:ASN:H	15	0.12
(1,1197)	1:126:A:LEU:HD11	1:122:A:THR:H	3	0.12
(1,1197)	1:126:A:LEU:HD12	1:122:A:THR:H	3	0.12
(1,1197)	1:126:A:LEU:HD13	1:122:A:THR:H	3	0.12
(1,1195)	1:60:A:LEU:HD21	1:57:A:MET:H	4	0.12
(1,1195)	1:60:A:LEU:HD22	1:57:A:MET:H	4	0.12
(1,1195)	1:60:A:LEU:HD23	1:57:A:MET:H	4	0.12
(1,1195)	1:60:A:LEU:HD21	1:57:A:MET:H	13	0.12
(1,1195)	1:60:A:LEU:HD22	1:57:A:MET:H	13	0.12
(1,1195)	1:60:A:LEU:HD23	1:57:A:MET:H	13	0.12
(1,1182)	1:126:A:LEU:HD11	1:127:A:ILE:H	1	0.12
(1,1182)	1:126:A:LEU:HD12	1:127:A:ILE:H	1	0.12
(1,1182)	1:126:A:LEU:HD13	1:127:A:ILE:H	1	0.12
(1,1182)	1:126:A:LEU:HD11	1:127:A:ILE:H	10	0.12
(1,1182)	1:126:A:LEU:HD12	1:127:A:ILE:H	10	0.12
(1,1182)	1:126:A:LEU:HD13	1:127:A:ILE:H	10	0.12
(1,1182)	1:126:A:LEU:HD11	1:127:A:ILE:H	15	0.12
(1,1182)	1:126:A:LEU:HD12	1:127:A:ILE:H	15	0.12
(1,1182)	1:126:A:LEU:HD13	1:127:A:ILE:H	15	0.12
(1,1149)	1:135:A:ILE:HG12	1:129:A:LYS:H	2	0.12
(1,1122)	1:91:A:ILE:HG21	1:94:A:CYS:H	4	0.12
(1,1122)	1:91:A:ILE:HG22	1:94:A:CYS:H	4	0.12
(1,1122)	1:91:A:ILE:HG23	1:94:A:CYS:H	4	0.12
(1,1117)	1:96:A:HIS:HA	1:102:A:GLN:H	4	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1091)	1:103:A:LEU:HD21	1:104:A:SER:H	18	0.12
(1,1091)	1:103:A:LEU:HD22	1:104:A:SER:H	18	0.12
(1,1091)	1:103:A:LEU:HD23	1:104:A:SER:H	18	0.12
(1,1043)	1:21:A:ILE:HG21	1:32:A:THR:H	19	0.12
(1,1043)	1:21:A:ILE:HG22	1:32:A:THR:H	19	0.12
(1,1043)	1:21:A:ILE:HG23	1:32:A:THR:H	19	0.12
(1,1042)	1:50:A:ILE:HD11	1:49:A:SER:H	3	0.12
(1,1042)	1:50:A:ILE:HD12	1:49:A:SER:H	3	0.12
(1,1042)	1:50:A:ILE:HD13	1:49:A:SER:H	3	0.12
(1,1042)	1:52:A:LEU:HD21	1:49:A:SER:H	9	0.12
(1,1042)	1:52:A:LEU:HD22	1:49:A:SER:H	9	0.12
(1,1042)	1:52:A:LEU:HD23	1:49:A:SER:H	9	0.12
(1,980)	1:54:A:ILE:HD11	1:42:A:ASP:H	9	0.12
(1,980)	1:54:A:ILE:HD12	1:42:A:ASP:H	9	0.12
(1,980)	1:54:A:ILE:HD13	1:42:A:ASP:H	9	0.12
(1,978)	1:131:A:ILE:HD11	1:131:A:ILE:H	7	0.12
(1,978)	1:131:A:ILE:HD12	1:131:A:ILE:H	7	0.12
(1,978)	1:131:A:ILE:HD13	1:131:A:ILE:H	7	0.12
(1,939)	1:91:A:ILE:HD11	1:91:A:ILE:H	10	0.12
(1,939)	1:91:A:ILE:HD12	1:91:A:ILE:H	10	0.12
(1,939)	1:91:A:ILE:HD13	1:91:A:ILE:H	10	0.12
(1,939)	1:91:A:ILE:HD11	1:91:A:ILE:H	20	0.12
(1,939)	1:91:A:ILE:HD12	1:91:A:ILE:H	20	0.12
(1,939)	1:91:A:ILE:HD13	1:91:A:ILE:H	20	0.12
(1,933)	1:52:A:LEU:HD21	1:26:A:LEU:H	5	0.12
(1,933)	1:52:A:LEU:HD22	1:26:A:LEU:H	5	0.12
(1,933)	1:52:A:LEU:HD23	1:26:A:LEU:H	5	0.12
(1,903)	1:41:A:VAL:HG21	1:48:A:ASN:H	4	0.12
(1,903)	1:41:A:VAL:HG22	1:48:A:ASN:H	4	0.12
(1,903)	1:41:A:VAL:HG23	1:48:A:ASN:H	4	0.12
(1,874)	1:139:A:PRO:HG2	1:115:A:GLY:H	7	0.12
(1,874)	1:139:A:PRO:HG3	1:115:A:GLY:H	7	0.12
(1,874)	1:139:A:PRO:HG2	1:115:A:GLY:H	9	0.12
(1,874)	1:139:A:PRO:HG3	1:115:A:GLY:H	9	0.12
(1,823)	1:70:A:LYS:HG2	1:69:A:GLY:H	5	0.12
(1,823)	1:70:A:LYS:HG3	1:69:A:GLY:H	5	0.12
(1,823)	1:70:A:LYS:HG2	1:69:A:GLY:H	18	0.12
(1,823)	1:70:A:LYS:HG3	1:69:A:GLY:H	18	0.12
(1,798)	1:13:A:GLU:HG2	1:13:A:GLU:H	16	0.12
(1,798)	1:13:A:GLU:HG3	1:13:A:GLU:H	16	0.12
(1,779)	1:62:A:LYS:HB3	1:62:A:LYS:H	1	0.12
(1,779)	1:62:A:LYS:HB3	1:62:A:LYS:H	13	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,760)	1:97:A:ILE:HB	1:96:A:HIS:H	4	0.12
(1,760)	1:97:A:ILE:HB	1:96:A:HIS:H	11	0.12
(1,760)	1:97:A:ILE:HB	1:96:A:HIS:H	15	0.12
(1,596)	1:95:A:ASN:HB3	1:95:A:ASN:H	6	0.12
(1,582)	1:57:A:MET:HB3	1:58:A:TYR:H	1	0.12
(1,582)	1:57:A:MET:HB3	1:58:A:TYR:H	12	0.12
(1,582)	1:57:A:MET:HB3	1:58:A:TYR:H	17	0.12
(1,582)	1:57:A:MET:HB3	1:58:A:TYR:H	18	0.12
(1,582)	1:57:A:MET:HB3	1:58:A:TYR:H	20	0.12
(1,387)	1:38:A:ALA:HA	1:4:A:LYS:H	2	0.12
(1,380)	1:61:A:GLY:HA3	1:61:A:GLY:H	1	0.12
(1,380)	1:61:A:GLY:HA3	1:61:A:GLY:H	16	0.12
(1,359)	1:45:A:GLY:HA3	1:45:A:GLY:H	5	0.12
(1,359)	1:45:A:GLY:HA3	1:45:A:GLY:H	6	0.12
(1,359)	1:45:A:GLY:HA3	1:45:A:GLY:H	8	0.12
(1,359)	1:45:A:GLY:HA3	1:45:A:GLY:H	11	0.12
(1,359)	1:83:A:GLY:HA3	1:83:A:GLY:H	12	0.12
(1,359)	1:45:A:GLY:HA3	1:45:A:GLY:H	17	0.12
(1,250)	1:102:A:GLN:HE22	1:101:A:GLY:H	2	0.12
(1,250)	1:102:A:GLN:HE22	1:101:A:GLY:H	12	0.12
(1,250)	1:102:A:GLN:HE22	1:101:A:GLY:H	20	0.12
(3,61)	1:109:A:PHE:H	1:105:A:ASP:O	12	0.11
(1,3875)	1:55:A:LEU:HB3	1:8:A:ILE:HG12	8	0.11
(1,3875)	1:55:A:LEU:HB3	1:8:A:ILE:HG13	8	0.11
(1,3840)	1:123:A:ASP:HB2	1:111:A:ALA:HB1	20	0.11
(1,3840)	1:123:A:ASP:HB2	1:111:A:ALA:HB2	20	0.11
(1,3840)	1:123:A:ASP:HB2	1:111:A:ALA:HB3	20	0.11
(1,3834)	1:74:A:TYR:H	1:3:A:VAL:HG11	4	0.11
(1,3834)	1:74:A:TYR:H	1:3:A:VAL:HG12	4	0.11
(1,3834)	1:74:A:TYR:H	1:3:A:VAL:HG13	4	0.11
(1,3724)	1:71:A:ASN:HB3	1:5:A:ILE:HG13	20	0.11
(1,3721)	1:7:A:ASP:H	1:4:A:LYS:HD2	2	0.11
(1,3707)	1:71:A:ASN:HA	1:72:A:ARG:HB2	2	0.11
(1,3707)	1:71:A:ASN:HA	1:72:A:ARG:HB2	8	0.11
(1,3707)	1:71:A:ASN:HA	1:72:A:ARG:HB2	14	0.11
(1,3697)	1:101:A:GLY:HA2	1:102:A:GLN:HG3	3	0.11
(1,3623)	1:135:A:ILE:HG12	1:134:A:ARG:HA	16	0.11
(1,3581)	1:56:A:GLN:H	1:68:A:ILE:HD11	10	0.11
(1,3581)	1:56:A:GLN:H	1:68:A:ILE:HD12	10	0.11
(1,3581)	1:56:A:GLN:H	1:68:A:ILE:HD13	10	0.11
(1,3520)	1:127:A:ILE:HD11	1:126:A:LEU:HB2	5	0.11
(1,3520)	1:127:A:ILE:HD12	1:126:A:LEU:HB2	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3520)	1:127:A:ILE:HD13	1:126:A:LEU:HB2	5	0.11
(1,3520)	1:127:A:ILE:HD11	1:126:A:LEU:HB2	11	0.11
(1,3520)	1:127:A:ILE:HD12	1:126:A:LEU:HB2	11	0.11
(1,3520)	1:127:A:ILE:HD13	1:126:A:LEU:HB2	11	0.11
(1,3520)	1:127:A:ILE:HD11	1:126:A:LEU:HB2	12	0.11
(1,3520)	1:127:A:ILE:HD12	1:126:A:LEU:HB2	12	0.11
(1,3520)	1:127:A:ILE:HD13	1:126:A:LEU:HB2	12	0.11
(1,3520)	1:127:A:ILE:HD11	1:126:A:LEU:HB2	17	0.11
(1,3520)	1:127:A:ILE:HD12	1:126:A:LEU:HB2	17	0.11
(1,3520)	1:127:A:ILE:HD13	1:126:A:LEU:HB2	17	0.11
(1,3520)	1:127:A:ILE:HD11	1:126:A:LEU:HB2	20	0.11
(1,3520)	1:127:A:ILE:HD12	1:126:A:LEU:HB2	20	0.11
(1,3520)	1:127:A:ILE:HD13	1:126:A:LEU:HB2	20	0.11
(1,3419)	1:80:A:ASP:H	1:81:A:ASN:HA	14	0.11
(1,3404)	1:2:A:SER:HB3	1:73:A:ILE:HG21	16	0.11
(1,3404)	1:2:A:SER:HB3	1:73:A:ILE:HG22	16	0.11
(1,3404)	1:2:A:SER:HB3	1:73:A:ILE:HG23	16	0.11
(1,3274)	1:73:A:ILE:HA	1:72:A:ARG:HD2	17	0.11
(1,3263)	1:5:A:ILE:HG21	1:6:A:GLY:HA2	10	0.11
(1,3263)	1:5:A:ILE:HG22	1:6:A:GLY:HA2	10	0.11
(1,3263)	1:5:A:ILE:HG23	1:6:A:GLY:HA2	10	0.11
(1,3263)	1:5:A:ILE:HG21	1:6:A:GLY:HA2	13	0.11
(1,3263)	1:5:A:ILE:HG22	1:6:A:GLY:HA2	13	0.11
(1,3263)	1:5:A:ILE:HG23	1:6:A:GLY:HA2	13	0.11
(1,3234)	1:95:A:ASN:H	1:92:A:LEU:HA	14	0.11
(1,3212)	1:53:A:ALA:HB1	1:49:A:SER:HB2	20	0.11
(1,3212)	1:53:A:ALA:HB1	1:49:A:SER:HB3	20	0.11
(1,3212)	1:53:A:ALA:HB2	1:49:A:SER:HB2	20	0.11
(1,3212)	1:53:A:ALA:HB2	1:49:A:SER:HB3	20	0.11
(1,3212)	1:53:A:ALA:HB3	1:49:A:SER:HB2	20	0.11
(1,3212)	1:53:A:ALA:HB3	1:49:A:SER:HB3	20	0.11
(1,3205)	1:51:A:ASP:H	1:50:A:ILE:HD11	8	0.11
(1,3205)	1:51:A:ASP:H	1:50:A:ILE:HD12	8	0.11
(1,3205)	1:51:A:ASP:H	1:50:A:ILE:HD13	8	0.11
(1,3180)	1:127:A:ILE:HB	1:79:A:ILE:HD11	5	0.11
(1,3180)	1:127:A:ILE:HB	1:79:A:ILE:HD12	5	0.11
(1,3180)	1:127:A:ILE:HB	1:79:A:ILE:HD13	5	0.11
(1,3169)	1:128:A:GLU:HA	1:125:A:ILE:HD11	17	0.11
(1,3169)	1:128:A:GLU:HA	1:125:A:ILE:HD12	17	0.11
(1,3169)	1:128:A:GLU:HA	1:125:A:ILE:HD13	17	0.11
(1,3164)	1:123:A:ASP:HB2	1:93:A:ILE:HD11	9	0.11
(1,3164)	1:123:A:ASP:HB2	1:93:A:ILE:HD12	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3164)	1:123:A:ASP:HB2	1:93:A:ILE:HD13	9	0.11
(1,3164)	1:123:A:ASP:HB2	1:93:A:ILE:HD11	18	0.11
(1,3164)	1:123:A:ASP:HB2	1:93:A:ILE:HD12	18	0.11
(1,3164)	1:123:A:ASP:HB2	1:93:A:ILE:HD13	18	0.11
(1,3133)	1:125:A:ILE:HD11	1:128:A:GLU:HA	17	0.11
(1,3133)	1:125:A:ILE:HD12	1:128:A:GLU:HA	17	0.11
(1,3133)	1:125:A:ILE:HD13	1:128:A:GLU:HA	17	0.11
(1,3095)	1:57:A:MET:HE1	1:53:A:ALA:HA	8	0.11
(1,3095)	1:57:A:MET:HE2	1:53:A:ALA:HA	8	0.11
(1,3095)	1:57:A:MET:HE3	1:53:A:ALA:HA	8	0.11
(1,3049)	1:12:A:GLY:HA2	1:13:A:GLU:HG2	2	0.11
(1,3049)	1:12:A:GLY:HA2	1:13:A:GLU:HG3	2	0.11
(1,3049)	1:12:A:GLY:HA2	1:13:A:GLU:HG2	16	0.11
(1,3049)	1:12:A:GLY:HA2	1:13:A:GLU:HG3	16	0.11
(1,3030)	1:58:A:TYR:H	1:57:A:MET:HE1	17	0.11
(1,3030)	1:58:A:TYR:H	1:57:A:MET:HE2	17	0.11
(1,3030)	1:58:A:TYR:H	1:57:A:MET:HE3	17	0.11
(1,2979)	1:57:A:MET:HE1	1:53:A:ALA:HB1	6	0.11
(1,2979)	1:57:A:MET:HE1	1:53:A:ALA:HB2	6	0.11
(1,2979)	1:57:A:MET:HE1	1:53:A:ALA:HB3	6	0.11
(1,2979)	1:57:A:MET:HE2	1:53:A:ALA:HB1	6	0.11
(1,2979)	1:57:A:MET:HE2	1:53:A:ALA:HB2	6	0.11
(1,2979)	1:57:A:MET:HE2	1:53:A:ALA:HB3	6	0.11
(1,2979)	1:57:A:MET:HE3	1:53:A:ALA:HB1	6	0.11
(1,2979)	1:57:A:MET:HE3	1:53:A:ALA:HB2	6	0.11
(1,2979)	1:57:A:MET:HE3	1:53:A:ALA:HB3	6	0.11
(1,2979)	1:57:A:MET:HE1	1:53:A:ALA:HB1	10	0.11
(1,2979)	1:57:A:MET:HE1	1:53:A:ALA:HB2	10	0.11
(1,2979)	1:57:A:MET:HE1	1:53:A:ALA:HB3	10	0.11
(1,2979)	1:57:A:MET:HE2	1:53:A:ALA:HB1	10	0.11
(1,2979)	1:57:A:MET:HE2	1:53:A:ALA:HB2	10	0.11
(1,2979)	1:57:A:MET:HE2	1:53:A:ALA:HB3	10	0.11
(1,2979)	1:57:A:MET:HE3	1:53:A:ALA:HB1	10	0.11
(1,2979)	1:57:A:MET:HE3	1:53:A:ALA:HB2	10	0.11
(1,2979)	1:57:A:MET:HE3	1:53:A:ALA:HB3	10	0.11
(1,2979)	1:57:A:MET:HE1	1:53:A:ALA:HB1	11	0.11
(1,2979)	1:57:A:MET:HE1	1:53:A:ALA:HB2	11	0.11
(1,2979)	1:57:A:MET:HE1	1:53:A:ALA:HB3	11	0.11
(1,2979)	1:57:A:MET:HE2	1:53:A:ALA:HB1	11	0.11
(1,2979)	1:57:A:MET:HE2	1:53:A:ALA:HB2	11	0.11
(1,2979)	1:57:A:MET:HE2	1:53:A:ALA:HB3	11	0.11
(1,2979)	1:57:A:MET:HE3	1:53:A:ALA:HB1	11	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2979)	1:57:A:MET:HE3	1:53:A:ALA:HB2	11	0.11
(1,2979)	1:57:A:MET:HE3	1:53:A:ALA:HB3	11	0.11
(1,2979)	1:57:A:MET:HE1	1:53:A:ALA:HB1	12	0.11
(1,2979)	1:57:A:MET:HE1	1:53:A:ALA:HB2	12	0.11
(1,2979)	1:57:A:MET:HE1	1:53:A:ALA:HB3	12	0.11
(1,2979)	1:57:A:MET:HE2	1:53:A:ALA:HB1	12	0.11
(1,2979)	1:57:A:MET:HE2	1:53:A:ALA:HB2	12	0.11
(1,2979)	1:57:A:MET:HE2	1:53:A:ALA:HB3	12	0.11
(1,2979)	1:57:A:MET:HE3	1:53:A:ALA:HB1	12	0.11
(1,2979)	1:57:A:MET:HE3	1:53:A:ALA:HB2	12	0.11
(1,2979)	1:57:A:MET:HE3	1:53:A:ALA:HB3	12	0.11
(1,2979)	1:57:A:MET:HE1	1:53:A:ALA:HB1	17	0.11
(1,2979)	1:57:A:MET:HE1	1:53:A:ALA:HB2	17	0.11
(1,2979)	1:57:A:MET:HE1	1:53:A:ALA:HB3	17	0.11
(1,2979)	1:57:A:MET:HE2	1:53:A:ALA:HB1	17	0.11
(1,2979)	1:57:A:MET:HE2	1:53:A:ALA:HB2	17	0.11
(1,2979)	1:57:A:MET:HE2	1:53:A:ALA:HB3	17	0.11
(1,2979)	1:57:A:MET:HE3	1:53:A:ALA:HB1	17	0.11
(1,2979)	1:57:A:MET:HE3	1:53:A:ALA:HB2	17	0.11
(1,2979)	1:57:A:MET:HE3	1:53:A:ALA:HB3	17	0.11
(1,2979)	1:57:A:MET:HE1	1:53:A:ALA:HB1	20	0.11
(1,2979)	1:57:A:MET:HE1	1:53:A:ALA:HB2	20	0.11
(1,2979)	1:57:A:MET:HE1	1:53:A:ALA:HB3	20	0.11
(1,2979)	1:57:A:MET:HE2	1:53:A:ALA:HB1	20	0.11
(1,2979)	1:57:A:MET:HE2	1:53:A:ALA:HB2	20	0.11
(1,2979)	1:57:A:MET:HE2	1:53:A:ALA:HB3	20	0.11
(1,2979)	1:57:A:MET:HE3	1:53:A:ALA:HB1	20	0.11
(1,2979)	1:57:A:MET:HE3	1:53:A:ALA:HB2	20	0.11
(1,2979)	1:57:A:MET:HE3	1:53:A:ALA:HB3	20	0.11
(1,2891)	1:58:A:TYR:HD1	1:54:A:ILE:HG21	18	0.11
(1,2891)	1:58:A:TYR:HD1	1:54:A:ILE:HG22	18	0.11
(1,2891)	1:58:A:TYR:HD1	1:54:A:ILE:HG23	18	0.11
(1,2891)	1:58:A:TYR:HD2	1:54:A:ILE:HG21	18	0.11
(1,2891)	1:58:A:TYR:HD2	1:54:A:ILE:HG22	18	0.11
(1,2891)	1:58:A:TYR:HD2	1:54:A:ILE:HG23	18	0.11
(1,2886)	1:18:A:ASP:H	1:17:A:ILE:HG21	19	0.11
(1,2886)	1:18:A:ASP:H	1:17:A:ILE:HG22	19	0.11
(1,2886)	1:18:A:ASP:H	1:17:A:ILE:HG23	19	0.11
(1,2854)	1:48:A:ASN:HD21	1:50:A:ILE:HG21	6	0.11
(1,2854)	1:48:A:ASN:HD21	1:50:A:ILE:HG22	6	0.11
(1,2854)	1:48:A:ASN:HD21	1:50:A:ILE:HG23	6	0.11
(1,2763)	1:34:A:LYS:HE3	1:3:A:VAL:HG11	12	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2763)	1:34:A:LYS:HE3	1:3:A:VAL:HG12	12	0.11
(1,2763)	1:34:A:LYS:HE3	1:3:A:VAL:HG13	12	0.11
(1,2743)	1:18:A:ASP:HB2	1:8:A:ILE:HG21	14	0.11
(1,2743)	1:18:A:ASP:HB2	1:8:A:ILE:HG22	14	0.11
(1,2743)	1:18:A:ASP:HB2	1:8:A:ILE:HG23	14	0.11
(1,2721)	1:134:A:ARG:HD2	1:132:A:THR:HG21	17	0.11
(1,2721)	1:134:A:ARG:HD2	1:132:A:THR:HG22	17	0.11
(1,2721)	1:134:A:ARG:HD2	1:132:A:THR:HG23	17	0.11
(1,2721)	1:134:A:ARG:HD3	1:132:A:THR:HG21	17	0.11
(1,2721)	1:134:A:ARG:HD3	1:132:A:THR:HG22	17	0.11
(1,2721)	1:134:A:ARG:HD3	1:132:A:THR:HG23	17	0.11
(1,2718)	1:114:A:ASP:HA	1:140:A:VAL:HG21	5	0.11
(1,2718)	1:114:A:ASP:HA	1:140:A:VAL:HG22	5	0.11
(1,2718)	1:114:A:ASP:HA	1:140:A:VAL:HG23	5	0.11
(1,2697)	1:128:A:GLU:HG2	1:132:A:THR:HG21	10	0.11
(1,2697)	1:128:A:GLU:HG2	1:132:A:THR:HG22	10	0.11
(1,2697)	1:128:A:GLU:HG2	1:132:A:THR:HG23	10	0.11
(1,2697)	1:128:A:GLU:HG3	1:132:A:THR:HG21	10	0.11
(1,2697)	1:128:A:GLU:HG3	1:132:A:THR:HG22	10	0.11
(1,2697)	1:128:A:GLU:HG3	1:132:A:THR:HG23	10	0.11
(1,2682)	1:38:A:ALA:H	1:3:A:VAL:HG11	5	0.11
(1,2682)	1:38:A:ALA:H	1:3:A:VAL:HG12	5	0.11
(1,2682)	1:38:A:ALA:H	1:3:A:VAL:HG13	5	0.11
(1,2682)	1:38:A:ALA:H	1:3:A:VAL:HG11	11	0.11
(1,2682)	1:38:A:ALA:H	1:3:A:VAL:HG12	11	0.11
(1,2682)	1:38:A:ALA:H	1:3:A:VAL:HG13	11	0.11
(1,2682)	1:38:A:ALA:H	1:3:A:VAL:HG11	14	0.11
(1,2682)	1:38:A:ALA:H	1:3:A:VAL:HG12	14	0.11
(1,2682)	1:38:A:ALA:H	1:3:A:VAL:HG13	14	0.11
(1,2664)	1:52:A:LEU:H	1:41:A:VAL:HG21	1	0.11
(1,2664)	1:52:A:LEU:H	1:41:A:VAL:HG22	1	0.11
(1,2664)	1:52:A:LEU:H	1:41:A:VAL:HG23	1	0.11
(1,2664)	1:52:A:LEU:H	1:41:A:VAL:HG21	4	0.11
(1,2664)	1:52:A:LEU:H	1:41:A:VAL:HG22	4	0.11
(1,2664)	1:52:A:LEU:H	1:41:A:VAL:HG23	4	0.11
(1,2630)	1:75:A:THR:H	1:75:A:THR:HG21	1	0.11
(1,2630)	1:75:A:THR:H	1:75:A:THR:HG22	1	0.11
(1,2630)	1:75:A:THR:H	1:75:A:THR:HG23	1	0.11
(1,2630)	1:75:A:THR:H	1:75:A:THR:HG21	10	0.11
(1,2630)	1:75:A:THR:H	1:75:A:THR:HG22	10	0.11
(1,2630)	1:75:A:THR:H	1:75:A:THR:HG23	10	0.11
(1,2618)	1:131:A:ILE:H	1:132:A:THR:HG21	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2618)	1:131:A:ILE:H	1:132:A:THR:HG22	9	0.11
(1,2618)	1:131:A:ILE:H	1:132:A:THR:HG23	9	0.11
(1,2618)	1:131:A:ILE:H	1:132:A:THR:HG21	20	0.11
(1,2618)	1:131:A:ILE:H	1:132:A:THR:HG22	20	0.11
(1,2618)	1:131:A:ILE:H	1:132:A:THR:HG23	20	0.11
(1,2603)	1:26:A:LEU:HD11	1:22:A:LEU:HD21	19	0.11
(1,2603)	1:26:A:LEU:HD11	1:22:A:LEU:HD22	19	0.11
(1,2603)	1:26:A:LEU:HD11	1:22:A:LEU:HD23	19	0.11
(1,2603)	1:26:A:LEU:HD12	1:22:A:LEU:HD21	19	0.11
(1,2603)	1:26:A:LEU:HD12	1:22:A:LEU:HD22	19	0.11
(1,2603)	1:26:A:LEU:HD12	1:22:A:LEU:HD23	19	0.11
(1,2603)	1:26:A:LEU:HD13	1:22:A:LEU:HD21	19	0.11
(1,2603)	1:26:A:LEU:HD13	1:22:A:LEU:HD22	19	0.11
(1,2603)	1:26:A:LEU:HD13	1:22:A:LEU:HD23	19	0.11
(1,2583)	1:126:A:LEU:HB2	1:138:A:LEU:HD21	5	0.11
(1,2583)	1:126:A:LEU:HB2	1:138:A:LEU:HD22	5	0.11
(1,2583)	1:126:A:LEU:HB2	1:138:A:LEU:HD23	5	0.11
(1,2583)	1:126:A:LEU:HB2	1:138:A:LEU:HD21	14	0.11
(1,2583)	1:126:A:LEU:HB2	1:138:A:LEU:HD22	14	0.11
(1,2583)	1:126:A:LEU:HB2	1:138:A:LEU:HD23	14	0.11
(1,2509)	1:49:A:SER:HB2	1:52:A:LEU:HD11	20	0.11
(1,2509)	1:49:A:SER:HB2	1:52:A:LEU:HD12	20	0.11
(1,2509)	1:49:A:SER:HB2	1:52:A:LEU:HD13	20	0.11
(1,2509)	1:49:A:SER:HB3	1:52:A:LEU:HD11	20	0.11
(1,2509)	1:49:A:SER:HB3	1:52:A:LEU:HD12	20	0.11
(1,2509)	1:49:A:SER:HB3	1:52:A:LEU:HD13	20	0.11
(1,2466)	1:24:A:SER:H	1:23:A:LYS:HG2	15	0.11
(1,2456)	1:23:A:LYS:H	1:52:A:LEU:HD11	18	0.11
(1,2456)	1:23:A:LYS:H	1:52:A:LEU:HD12	18	0.11
(1,2456)	1:23:A:LYS:H	1:52:A:LEU:HD13	18	0.11
(1,2414)	1:62:A:LYS:HB3	1:62:A:LYS:HD2	5	0.11
(1,2400)	1:94:A:CYS:HB3	1:124:A:ARG:HG2	1	0.11
(1,2352)	1:85:A:VAL:HA	1:84:A:ILE:HG13	13	0.11
(1,2350)	1:52:A:LEU:H	1:52:A:LEU:HD21	5	0.11
(1,2350)	1:52:A:LEU:H	1:52:A:LEU:HD22	5	0.11
(1,2350)	1:52:A:LEU:H	1:52:A:LEU:HD23	5	0.11
(1,2350)	1:52:A:LEU:H	1:52:A:LEU:HD21	19	0.11
(1,2350)	1:52:A:LEU:H	1:52:A:LEU:HD22	19	0.11
(1,2350)	1:52:A:LEU:H	1:52:A:LEU:HD23	19	0.11
(1,2344)	1:58:A:TYR:HD1	1:59:A:LEU:HD21	9	0.11
(1,2344)	1:58:A:TYR:HD1	1:59:A:LEU:HD22	9	0.11
(1,2344)	1:58:A:TYR:HD1	1:59:A:LEU:HD23	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2344)	1:58:A:TYR:HD2	1:59:A:LEU:HD21	9	0.11
(1,2344)	1:58:A:TYR:HD2	1:59:A:LEU:HD22	9	0.11
(1,2344)	1:58:A:TYR:HD2	1:59:A:LEU:HD23	9	0.11
(1,2316)	1:121:A:GLN:H	1:121:A:GLN:HB3	2	0.11
(1,2316)	1:121:A:GLN:H	1:121:A:GLN:HB3	14	0.11
(1,2300)	1:49:A:SER:H	1:50:A:ILE:HG13	17	0.11
(1,2278)	1:50:A:ILE:HB	1:54:A:ILE:HG12	17	0.11
(1,2278)	1:50:A:ILE:HB	1:54:A:ILE:HG13	17	0.11
(1,2273)	1:70:A:LYS:HB2	1:70:A:LYS:HD2	3	0.11
(1,2231)	1:35:A:GLN:H	1:34:A:LYS:HD2	14	0.11
(1,1859)	1:60:A:LEU:HD21	1:62:A:LYS:HE2	3	0.11
(1,1859)	1:60:A:LEU:HD22	1:62:A:LYS:HE2	3	0.11
(1,1859)	1:60:A:LEU:HD23	1:62:A:LYS:HE2	3	0.11
(1,1853)	1:132:A:THR:HG21	1:134:A:ARG:HD2	17	0.11
(1,1853)	1:132:A:THR:HG21	1:134:A:ARG:HD3	17	0.11
(1,1853)	1:132:A:THR:HG22	1:134:A:ARG:HD2	17	0.11
(1,1853)	1:132:A:THR:HG22	1:134:A:ARG:HD3	17	0.11
(1,1853)	1:132:A:THR:HG23	1:134:A:ARG:HD2	17	0.11
(1,1853)	1:132:A:THR:HG23	1:134:A:ARG:HD3	17	0.11
(1,1821)	1:67:A:ASP:HA	1:70:A:LYS:HE2	13	0.11
(1,1821)	1:67:A:ASP:HA	1:70:A:LYS:HE3	13	0.11
(1,1809)	1:74:A:TYR:HE1	1:72:A:ARG:HD2	1	0.11
(1,1809)	1:74:A:TYR:HE2	1:72:A:ARG:HD2	1	0.11
(1,1801)	1:144:A:LEU:H	1:144:A:LEU:HB2	15	0.11
(1,1768)	1:57:A:MET:HB2	1:64:A:GLY:HA2	11	0.11
(1,1768)	1:57:A:MET:HB2	1:64:A:GLY:HA3	11	0.11
(1,1639)	1:23:A:LYS:HD2	1:23:A:LYS:HA	5	0.11
(1,1639)	1:23:A:LYS:HD2	1:23:A:LYS:HA	13	0.11
(1,1639)	1:23:A:LYS:HD2	1:23:A:LYS:HA	18	0.11
(1,1534)	1:20:A:ALA:HB1	1:17:A:ILE:HA	14	0.11
(1,1534)	1:20:A:ALA:HB2	1:17:A:ILE:HA	14	0.11
(1,1534)	1:20:A:ALA:HB3	1:17:A:ILE:HA	14	0.11
(1,1507)	1:69:A:GLY:HA3	1:14:A:ILE:HD11	10	0.11
(1,1507)	1:69:A:GLY:HA3	1:14:A:ILE:HD12	10	0.11
(1,1507)	1:69:A:GLY:HA3	1:14:A:ILE:HD13	10	0.11
(1,1502)	1:26:A:LEU:HA	1:27:A:ILE:HA	4	0.11
(1,1502)	1:26:A:LEU:HA	1:27:A:ILE:HA	17	0.11
(1,1482)	1:28:A:ASN:H	1:27:A:ILE:HA	6	0.11
(1,1482)	1:28:A:ASN:H	1:27:A:ILE:HA	16	0.11
(1,1482)	1:28:A:ASN:H	1:27:A:ILE:HA	18	0.11
(1,1482)	1:28:A:ASN:H	1:27:A:ILE:HA	20	0.11
(1,1451)	1:119:A:ILE:HG21	1:93:A:ILE:HD11	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1451)	1:119:A:ILE:HG21	1:93:A:ILE:HD12	5	0.11
(1,1451)	1:119:A:ILE:HG21	1:93:A:ILE:HD13	5	0.11
(1,1451)	1:119:A:ILE:HG22	1:93:A:ILE:HD11	5	0.11
(1,1451)	1:119:A:ILE:HG22	1:93:A:ILE:HD12	5	0.11
(1,1451)	1:119:A:ILE:HG22	1:93:A:ILE:HD13	5	0.11
(1,1451)	1:119:A:ILE:HG23	1:93:A:ILE:HD11	5	0.11
(1,1451)	1:119:A:ILE:HG23	1:93:A:ILE:HD12	5	0.11
(1,1451)	1:119:A:ILE:HG23	1:93:A:ILE:HD13	5	0.11
(1,1379)	1:130:A:TYR:HD1	1:135:A:ILE:HD11	17	0.11
(1,1379)	1:130:A:TYR:HD1	1:135:A:ILE:HD12	17	0.11
(1,1379)	1:130:A:TYR:HD1	1:135:A:ILE:HD13	17	0.11
(1,1379)	1:130:A:TYR:HD2	1:135:A:ILE:HD11	17	0.11
(1,1379)	1:130:A:TYR:HD2	1:135:A:ILE:HD12	17	0.11
(1,1379)	1:130:A:TYR:HD2	1:135:A:ILE:HD13	17	0.11
(1,1326)	1:5:A:ILE:HD11	1:39:A:ALA:H	9	0.11
(1,1326)	1:5:A:ILE:HD12	1:39:A:ALA:H	9	0.11
(1,1326)	1:5:A:ILE:HD13	1:39:A:ALA:H	9	0.11
(1,1321)	1:23:A:LYS:HB3	1:23:A:LYS:H	18	0.11
(1,1260)	1:51:A:ASP:H	1:41:A:VAL:H	3	0.11
(1,1260)	1:51:A:ASP:H	1:41:A:VAL:H	7	0.11
(1,1260)	1:51:A:ASP:H	1:41:A:VAL:H	19	0.11
(1,1241)	1:127:A:ILE:HA	1:128:A:GLU:H	17	0.11
(1,1226)	1:68:A:ILE:HD11	1:58:A:TYR:H	5	0.11
(1,1226)	1:68:A:ILE:HD12	1:58:A:TYR:H	5	0.11
(1,1226)	1:68:A:ILE:HD13	1:58:A:TYR:H	5	0.11
(1,1222)	1:63:A:GLY:HA3	1:63:A:GLY:H	1	0.11
(1,1222)	1:63:A:GLY:HA3	1:63:A:GLY:H	11	0.11
(1,1205)	1:97:A:ILE:HD11	1:98:A:ASN:H	11	0.11
(1,1205)	1:97:A:ILE:HD12	1:98:A:ASN:H	11	0.11
(1,1205)	1:97:A:ILE:HD13	1:98:A:ASN:H	11	0.11
(1,1197)	1:126:A:LEU:HD11	1:122:A:THR:H	4	0.11
(1,1197)	1:126:A:LEU:HD12	1:122:A:THR:H	4	0.11
(1,1197)	1:126:A:LEU:HD13	1:122:A:THR:H	4	0.11
(1,1195)	1:60:A:LEU:HD21	1:57:A:MET:H	15	0.11
(1,1195)	1:60:A:LEU:HD22	1:57:A:MET:H	15	0.11
(1,1195)	1:60:A:LEU:HD23	1:57:A:MET:H	15	0.11
(1,1182)	1:126:A:LEU:HD11	1:127:A:ILE:H	7	0.11
(1,1182)	1:126:A:LEU:HD12	1:127:A:ILE:H	7	0.11
(1,1182)	1:126:A:LEU:HD13	1:127:A:ILE:H	7	0.11
(1,1182)	1:126:A:LEU:HD11	1:127:A:ILE:H	12	0.11
(1,1182)	1:126:A:LEU:HD12	1:127:A:ILE:H	12	0.11
(1,1182)	1:126:A:LEU:HD13	1:127:A:ILE:H	12	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1182)	1:126:A:LEU:HD11	1:127:A:ILE:H	16	0.11
(1,1182)	1:126:A:LEU:HD12	1:127:A:ILE:H	16	0.11
(1,1182)	1:126:A:LEU:HD13	1:127:A:ILE:H	16	0.11
(1,1177)	1:92:A:LEU:HD11	1:89:A:ASP:H	18	0.11
(1,1177)	1:92:A:LEU:HD12	1:89:A:ASP:H	18	0.11
(1,1177)	1:92:A:LEU:HD13	1:89:A:ASP:H	18	0.11
(1,1150)	1:134:A:ARG:HG2	1:129:A:LYS:H	5	0.11
(1,1150)	1:134:A:ARG:HG3	1:129:A:LYS:H	5	0.11
(1,1149)	1:135:A:ILE:HG12	1:129:A:LYS:H	13	0.11
(1,1122)	1:93:A:ILE:HD11	1:94:A:CYS:H	8	0.11
(1,1122)	1:93:A:ILE:HD12	1:94:A:CYS:H	8	0.11
(1,1122)	1:93:A:ILE:HD13	1:94:A:CYS:H	8	0.11
(1,1122)	1:93:A:ILE:HD11	1:94:A:CYS:H	10	0.11
(1,1122)	1:93:A:ILE:HD12	1:94:A:CYS:H	10	0.11
(1,1122)	1:93:A:ILE:HD13	1:94:A:CYS:H	10	0.11
(1,1117)	1:96:A:HIS:HA	1:102:A:GLN:H	20	0.11
(1,1092)	1:103:A:LEU:HD21	1:111:A:ALA:H	6	0.11
(1,1092)	1:103:A:LEU:HD22	1:111:A:ALA:H	6	0.11
(1,1092)	1:103:A:LEU:HD23	1:111:A:ALA:H	6	0.11
(1,1091)	1:108:A:LEU:HD21	1:104:A:SER:H	6	0.11
(1,1091)	1:108:A:LEU:HD22	1:104:A:SER:H	6	0.11
(1,1091)	1:108:A:LEU:HD23	1:104:A:SER:H	6	0.11
(1,1091)	1:103:A:LEU:HD21	1:104:A:SER:H	15	0.11
(1,1091)	1:103:A:LEU:HD22	1:104:A:SER:H	15	0.11
(1,1091)	1:103:A:LEU:HD23	1:104:A:SER:H	15	0.11
(1,1021)	1:92:A:LEU:HD11	1:88:A:ASN:HD22	10	0.11
(1,1021)	1:92:A:LEU:HD12	1:88:A:ASN:HD22	10	0.11
(1,1021)	1:92:A:LEU:HD13	1:88:A:ASN:HD22	10	0.11
(1,1009)	1:131:A:ILE:HG21	1:87:A:GLU:H	7	0.11
(1,1009)	1:131:A:ILE:HG22	1:87:A:GLU:H	7	0.11
(1,1009)	1:131:A:ILE:HG23	1:87:A:GLU:H	7	0.11
(1,1007)	1:14:A:ILE:HG12	1:69:A:GLY:H	20	0.11
(1,1004)	1:59:A:LEU:HD21	1:16:A:SER:H	10	0.11
(1,1004)	1:59:A:LEU:HD22	1:16:A:SER:H	10	0.11
(1,1004)	1:59:A:LEU:HD23	1:16:A:SER:H	10	0.11
(1,981)	1:84:A:ILE:HD11	1:82:A:ASN:H	1	0.11
(1,981)	1:84:A:ILE:HD12	1:82:A:ASN:H	1	0.11
(1,981)	1:84:A:ILE:HD13	1:82:A:ASN:H	1	0.11
(1,980)	1:54:A:ILE:HD11	1:42:A:ASP:H	4	0.11
(1,980)	1:54:A:ILE:HD12	1:42:A:ASP:H	4	0.11
(1,980)	1:54:A:ILE:HD13	1:42:A:ASP:H	4	0.11
(1,977)	1:132:A:THR:HG21	1:131:A:ILE:H	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,977)	1:132:A:THR:HG22	1:131:A:ILE:H	9	0.11
(1,977)	1:132:A:THR:HG23	1:131:A:ILE:H	9	0.11
(1,977)	1:132:A:THR:HG21	1:131:A:ILE:H	20	0.11
(1,977)	1:132:A:THR:HG22	1:131:A:ILE:H	20	0.11
(1,977)	1:132:A:THR:HG23	1:131:A:ILE:H	20	0.11
(1,974)	1:17:A:ILE:HG21	1:18:A:ASP:H	19	0.11
(1,974)	1:17:A:ILE:HG22	1:18:A:ASP:H	19	0.11
(1,974)	1:17:A:ILE:HG23	1:18:A:ASP:H	19	0.11
(1,939)	1:91:A:ILE:HD11	1:91:A:ILE:H	13	0.11
(1,939)	1:91:A:ILE:HD12	1:91:A:ILE:H	13	0.11
(1,939)	1:91:A:ILE:HD13	1:91:A:ILE:H	13	0.11
(1,931)	1:8:A:ILE:HG21	1:22:A:LEU:H	13	0.11
(1,931)	1:8:A:ILE:HG22	1:22:A:LEU:H	13	0.11
(1,931)	1:8:A:ILE:HG23	1:22:A:LEU:H	13	0.11
(1,874)	1:139:A:PRO:HG2	1:115:A:GLY:H	11	0.11
(1,874)	1:139:A:PRO:HG3	1:115:A:GLY:H	11	0.11
(1,871)	1:52:A:LEU:HG	1:56:A:GLN:HE22	14	0.11
(1,806)	1:53:A:ALA:HB1	1:57:A:MET:H	17	0.11
(1,806)	1:53:A:ALA:HB2	1:57:A:MET:H	17	0.11
(1,806)	1:53:A:ALA:HB3	1:57:A:MET:H	17	0.11
(1,798)	1:13:A:GLU:HG2	1:13:A:GLU:H	14	0.11
(1,798)	1:13:A:GLU:HG3	1:13:A:GLU:H	14	0.11
(1,779)	1:62:A:LYS:HB3	1:62:A:LYS:H	5	0.11
(1,779)	1:62:A:LYS:HB3	1:62:A:LYS:H	10	0.11
(1,596)	1:95:A:ASN:HB3	1:95:A:ASN:H	8	0.11
(1,596)	1:95:A:ASN:HB3	1:95:A:ASN:H	18	0.11
(1,582)	1:57:A:MET:HB3	1:58:A:TYR:H	2	0.11
(1,582)	1:57:A:MET:HB3	1:58:A:TYR:H	8	0.11
(1,579)	1:142:A:ASN:HB3	1:143:A:GLN:H	11	0.11
(1,391)	1:72:A:ARG:HD2	1:73:A:ILE:H	11	0.11
(1,380)	1:61:A:GLY:HA3	1:61:A:GLY:H	2	0.11
(1,380)	1:61:A:GLY:HA3	1:61:A:GLY:H	7	0.11
(1,380)	1:61:A:GLY:HA3	1:61:A:GLY:H	8	0.11
(1,380)	1:61:A:GLY:HA3	1:61:A:GLY:H	13	0.11
(1,359)	1:45:A:GLY:HA3	1:45:A:GLY:H	1	0.11
(1,359)	1:45:A:GLY:HA3	1:45:A:GLY:H	18	0.11
(1,359)	1:45:A:GLY:HA3	1:45:A:GLY:H	19	0.11
(1,333)	1:75:A:THR:HB	1:78:A:ASP:H	12	0.11
(1,250)	1:102:A:GLN:HE22	1:101:A:GLY:H	17	0.11
(1,250)	1:102:A:GLN:HE22	1:101:A:GLY:H	18	0.11
(1,81)	1:58:A:TYR:H	1:61:A:GLY:H	1	0.11
(1,81)	1:58:A:TYR:H	1:61:A:GLY:H	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,81)	1:58:A:TYR:H	1:61:A:GLY:H	8	0.11
(1,81)	1:58:A:TYR:H	1:61:A:GLY:H	13	0.11
(1,81)	1:58:A:TYR:H	1:61:A:GLY:H	20	0.11
(3,61)	1:109:A:PHE:H	1:105:A:ASP:O	20	0.1
(1,3943)	1:22:A:LEU:HD21	1:19:A:TYR:HD1	3	0.1
(1,3943)	1:22:A:LEU:HD21	1:19:A:TYR:HD2	3	0.1
(1,3943)	1:22:A:LEU:HD22	1:19:A:TYR:HD1	3	0.1
(1,3943)	1:22:A:LEU:HD22	1:19:A:TYR:HD2	3	0.1
(1,3943)	1:22:A:LEU:HD23	1:19:A:TYR:HD1	3	0.1
(1,3943)	1:22:A:LEU:HD23	1:19:A:TYR:HD2	3	0.1
(1,3938)	1:14:A:ILE:HB	1:58:A:TYR:HD1	6	0.1
(1,3938)	1:14:A:ILE:HB	1:58:A:TYR:HD2	6	0.1
(1,3716)	1:121:A:GLN:HE22	1:97:A:ILE:HG12	4	0.1
(1,3707)	1:71:A:ASN:HA	1:72:A:ARG:HB2	5	0.1
(1,3707)	1:71:A:ASN:HA	1:72:A:ARG:HB2	17	0.1
(1,3707)	1:71:A:ASN:HA	1:72:A:ARG:HB2	18	0.1
(1,3543)	1:17:A:ILE:HA	1:21:A:ILE:HD11	20	0.1
(1,3543)	1:17:A:ILE:HA	1:21:A:ILE:HD12	20	0.1
(1,3543)	1:17:A:ILE:HA	1:21:A:ILE:HD13	20	0.1
(1,3520)	1:127:A:ILE:HD11	1:126:A:LEU:HB2	19	0.1
(1,3520)	1:127:A:ILE:HD12	1:126:A:LEU:HB2	19	0.1
(1,3520)	1:127:A:ILE:HD13	1:126:A:LEU:HB2	19	0.1
(1,3459)	1:74:A:TYR:HB3	1:73:A:ILE:HA	20	0.1
(1,3242)	1:144:A:LEU:H	1:144:A:LEU:HA	1	0.1
(1,3177)	1:129:A:LYS:HE2	1:135:A:ILE:HD11	4	0.1
(1,3177)	1:129:A:LYS:HE2	1:135:A:ILE:HD12	4	0.1
(1,3177)	1:129:A:LYS:HE2	1:135:A:ILE:HD13	4	0.1
(1,3177)	1:129:A:LYS:HE3	1:135:A:ILE:HD11	4	0.1
(1,3177)	1:129:A:LYS:HE3	1:135:A:ILE:HD12	4	0.1
(1,3177)	1:129:A:LYS:HE3	1:135:A:ILE:HD13	4	0.1
(1,3140)	1:54:A:ILE:H	1:51:A:ASP:HA	3	0.1
(1,3096)	1:79:A:ILE:HG21	1:80:A:ASP:HA	16	0.1
(1,3096)	1:79:A:ILE:HG22	1:80:A:ASP:HA	16	0.1
(1,3096)	1:79:A:ILE:HG23	1:80:A:ASP:HA	16	0.1
(1,3030)	1:58:A:TYR:H	1:57:A:MET:HE1	20	0.1
(1,3030)	1:58:A:TYR:H	1:57:A:MET:HE2	20	0.1
(1,3030)	1:58:A:TYR:H	1:57:A:MET:HE3	20	0.1
(1,2995)	1:70:A:LYS:HB3	1:5:A:ILE:HG21	16	0.1
(1,2995)	1:70:A:LYS:HB3	1:5:A:ILE:HG22	16	0.1
(1,2995)	1:70:A:LYS:HB3	1:5:A:ILE:HG23	16	0.1
(1,2980)	1:54:A:ILE:HB	1:53:A:ALA:HB1	8	0.1
(1,2980)	1:54:A:ILE:HB	1:53:A:ALA:HB2	8	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2980)	1:54:A:ILE:HB	1:53:A:ALA:HB3	8	0.1
(1,2980)	1:54:A:ILE:HB	1:53:A:ALA:HB1	12	0.1
(1,2980)	1:54:A:ILE:HB	1:53:A:ALA:HB2	12	0.1
(1,2980)	1:54:A:ILE:HB	1:53:A:ALA:HB3	12	0.1
(1,2980)	1:54:A:ILE:HB	1:53:A:ALA:HB1	14	0.1
(1,2980)	1:54:A:ILE:HB	1:53:A:ALA:HB2	14	0.1
(1,2980)	1:54:A:ILE:HB	1:53:A:ALA:HB3	14	0.1
(1,2979)	1:57:A:MET:HE1	1:53:A:ALA:HB1	13	0.1
(1,2979)	1:57:A:MET:HE1	1:53:A:ALA:HB2	13	0.1
(1,2979)	1:57:A:MET:HE1	1:53:A:ALA:HB3	13	0.1
(1,2979)	1:57:A:MET:HE2	1:53:A:ALA:HB1	13	0.1
(1,2979)	1:57:A:MET:HE2	1:53:A:ALA:HB2	13	0.1
(1,2979)	1:57:A:MET:HE2	1:53:A:ALA:HB3	13	0.1
(1,2979)	1:57:A:MET:HE3	1:53:A:ALA:HB1	13	0.1
(1,2979)	1:57:A:MET:HE3	1:53:A:ALA:HB2	13	0.1
(1,2979)	1:57:A:MET:HE3	1:53:A:ALA:HB3	13	0.1
(1,2978)	1:53:A:ALA:HB1	1:57:A:MET:HE1	13	0.1
(1,2978)	1:53:A:ALA:HB1	1:57:A:MET:HE2	13	0.1
(1,2978)	1:53:A:ALA:HB1	1:57:A:MET:HE3	13	0.1
(1,2978)	1:53:A:ALA:HB2	1:57:A:MET:HE1	13	0.1
(1,2978)	1:53:A:ALA:HB2	1:57:A:MET:HE2	13	0.1
(1,2978)	1:53:A:ALA:HB2	1:57:A:MET:HE3	13	0.1
(1,2978)	1:53:A:ALA:HB3	1:57:A:MET:HE1	13	0.1
(1,2978)	1:53:A:ALA:HB3	1:57:A:MET:HE2	13	0.1
(1,2978)	1:53:A:ALA:HB3	1:57:A:MET:HE3	13	0.1
(1,2844)	1:58:A:TYR:H	1:68:A:ILE:HG21	8	0.1
(1,2844)	1:58:A:TYR:H	1:68:A:ILE:HG22	8	0.1
(1,2844)	1:58:A:TYR:H	1:68:A:ILE:HG23	8	0.1
(1,2765)	1:40:A:ASP:HB3	1:3:A:VAL:HG11	7	0.1
(1,2765)	1:40:A:ASP:HB3	1:3:A:VAL:HG12	7	0.1
(1,2765)	1:40:A:ASP:HB3	1:3:A:VAL:HG13	7	0.1
(1,2764)	1:74:A:TYR:HB3	1:3:A:VAL:HG21	3	0.1
(1,2764)	1:74:A:TYR:HB3	1:3:A:VAL:HG22	3	0.1
(1,2764)	1:74:A:TYR:HB3	1:3:A:VAL:HG23	3	0.1
(1,2713)	1:80:A:ASP:HA	1:79:A:ILE:HG21	16	0.1
(1,2713)	1:80:A:ASP:HA	1:79:A:ILE:HG22	16	0.1
(1,2713)	1:80:A:ASP:HA	1:79:A:ILE:HG23	16	0.1
(1,2682)	1:38:A:ALA:H	1:3:A:VAL:HG11	15	0.1
(1,2682)	1:38:A:ALA:H	1:3:A:VAL:HG12	15	0.1
(1,2682)	1:38:A:ALA:H	1:3:A:VAL:HG13	15	0.1
(1,2664)	1:52:A:LEU:H	1:41:A:VAL:HG21	12	0.1
(1,2664)	1:52:A:LEU:H	1:41:A:VAL:HG22	12	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2664)	1:52:A:LEU:H	1:41:A:VAL:HG23	12	0.1
(1,2652)	1:80:A:ASP:H	1:79:A:ILE:HG21	1	0.1
(1,2652)	1:80:A:ASP:H	1:79:A:ILE:HG22	1	0.1
(1,2652)	1:80:A:ASP:H	1:79:A:ILE:HG23	1	0.1
(1,2652)	1:80:A:ASP:H	1:79:A:ILE:HG21	3	0.1
(1,2652)	1:80:A:ASP:H	1:79:A:ILE:HG22	3	0.1
(1,2652)	1:80:A:ASP:H	1:79:A:ILE:HG23	3	0.1
(1,2652)	1:80:A:ASP:H	1:79:A:ILE:HG21	14	0.1
(1,2652)	1:80:A:ASP:H	1:79:A:ILE:HG22	14	0.1
(1,2652)	1:80:A:ASP:H	1:79:A:ILE:HG23	14	0.1
(1,2630)	1:75:A:THR:H	1:75:A:THR:HG21	6	0.1
(1,2630)	1:75:A:THR:H	1:75:A:THR:HG22	6	0.1
(1,2630)	1:75:A:THR:H	1:75:A:THR:HG23	6	0.1
(1,2630)	1:75:A:THR:H	1:75:A:THR:HG21	15	0.1
(1,2630)	1:75:A:THR:H	1:75:A:THR:HG22	15	0.1
(1,2630)	1:75:A:THR:H	1:75:A:THR:HG23	15	0.1
(1,2456)	1:23:A:LYS:H	1:52:A:LEU:HD11	19	0.1
(1,2456)	1:23:A:LYS:H	1:52:A:LEU:HD12	19	0.1
(1,2456)	1:23:A:LYS:H	1:52:A:LEU:HD13	19	0.1
(1,2373)	1:55:A:LEU:HA	1:59:A:LEU:HD21	7	0.1
(1,2373)	1:55:A:LEU:HA	1:59:A:LEU:HD22	7	0.1
(1,2373)	1:55:A:LEU:HA	1:59:A:LEU:HD23	7	0.1
(1,2352)	1:85:A:VAL:HA	1:84:A:ILE:HG13	14	0.1
(1,2337)	1:84:A:ILE:H	1:84:A:ILE:HG12	20	0.1
(1,2316)	1:121:A:GLN:H	1:121:A:GLN:HB3	9	0.1
(1,2300)	1:49:A:SER:H	1:50:A:ILE:HG13	11	0.1
(1,2277)	1:93:A:ILE:HB	1:127:A:ILE:HG12	3	0.1
(1,2277)	1:93:A:ILE:HB	1:127:A:ILE:HG13	3	0.1
(1,2273)	1:70:A:LYS:HB2	1:70:A:LYS:HD2	15	0.1
(1,1939)	1:92:A:LEU:HD21	1:80:A:ASP:HB3	11	0.1
(1,1939)	1:92:A:LEU:HD22	1:80:A:ASP:HB3	11	0.1
(1,1939)	1:92:A:LEU:HD23	1:80:A:ASP:HB3	11	0.1
(1,1939)	1:92:A:LEU:HD21	1:80:A:ASP:HB3	13	0.1
(1,1939)	1:92:A:LEU:HD22	1:80:A:ASP:HB3	13	0.1
(1,1939)	1:92:A:LEU:HD23	1:80:A:ASP:HB3	13	0.1
(1,1801)	1:144:A:LEU:H	1:144:A:LEU:HB2	4	0.1
(1,1609)	1:123:A:ASP:HA	1:121:A:GLN:HA	10	0.1
(1,1555)	1:52:A:LEU:HD21	1:49:A:SER:HB2	16	0.1
(1,1555)	1:52:A:LEU:HD21	1:49:A:SER:HB3	16	0.1
(1,1555)	1:52:A:LEU:HD22	1:49:A:SER:HB2	16	0.1
(1,1555)	1:52:A:LEU:HD22	1:49:A:SER:HB3	16	0.1
(1,1555)	1:52:A:LEU:HD23	1:49:A:SER:HB2	16	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1555)	1:52:A:LEU:HD23	1:49:A:SER:HB3	16	0.1
(1,1549)	1:70:A:LYS:HB2	1:5:A:ILE:HD11	20	0.1
(1,1549)	1:70:A:LYS:HB2	1:5:A:ILE:HD12	20	0.1
(1,1549)	1:70:A:LYS:HB2	1:5:A:ILE:HD13	20	0.1
(1,1502)	1:26:A:LEU:HA	1:27:A:ILE:HA	2	0.1
(1,1482)	1:28:A:ASN:H	1:27:A:ILE:HA	4	0.1
(1,1482)	1:28:A:ASN:H	1:27:A:ILE:HA	12	0.1
(1,1482)	1:28:A:ASN:H	1:27:A:ILE:HA	15	0.1
(1,1482)	1:28:A:ASN:H	1:27:A:ILE:HA	19	0.1
(1,1451)	1:119:A:ILE:HG21	1:93:A:ILE:HD11	1	0.1
(1,1451)	1:119:A:ILE:HG21	1:93:A:ILE:HD12	1	0.1
(1,1451)	1:119:A:ILE:HG21	1:93:A:ILE:HD13	1	0.1
(1,1451)	1:119:A:ILE:HG22	1:93:A:ILE:HD11	1	0.1
(1,1451)	1:119:A:ILE:HG22	1:93:A:ILE:HD12	1	0.1
(1,1451)	1:119:A:ILE:HG22	1:93:A:ILE:HD13	1	0.1
(1,1451)	1:119:A:ILE:HG23	1:93:A:ILE:HD11	1	0.1
(1,1451)	1:119:A:ILE:HG23	1:93:A:ILE:HD12	1	0.1
(1,1451)	1:119:A:ILE:HG23	1:93:A:ILE:HD13	1	0.1
(1,1401)	1:121:A:GLN:HA	1:97:A:ILE:HD11	14	0.1
(1,1401)	1:121:A:GLN:HA	1:97:A:ILE:HD12	14	0.1
(1,1401)	1:121:A:GLN:HA	1:97:A:ILE:HD13	14	0.1
(1,1321)	1:23:A:LYS:HB3	1:23:A:LYS:H	8	0.1
(1,1226)	1:68:A:ILE:HD11	1:58:A:TYR:H	19	0.1
(1,1226)	1:68:A:ILE:HD12	1:58:A:TYR:H	19	0.1
(1,1226)	1:68:A:ILE:HD13	1:58:A:TYR:H	19	0.1
(1,1177)	1:92:A:LEU:HD21	1:89:A:ASP:H	8	0.1
(1,1177)	1:92:A:LEU:HD22	1:89:A:ASP:H	8	0.1
(1,1177)	1:92:A:LEU:HD23	1:89:A:ASP:H	8	0.1
(1,1122)	1:93:A:ILE:HD11	1:94:A:CYS:H	18	0.1
(1,1122)	1:93:A:ILE:HD12	1:94:A:CYS:H	18	0.1
(1,1122)	1:93:A:ILE:HD13	1:94:A:CYS:H	18	0.1
(1,1115)	1:55:A:LEU:HD21	1:8:A:ILE:H	6	0.1
(1,1115)	1:55:A:LEU:HD22	1:8:A:ILE:H	6	0.1
(1,1115)	1:55:A:LEU:HD23	1:8:A:ILE:H	6	0.1
(1,1004)	1:59:A:LEU:HD21	1:16:A:SER:H	2	0.1
(1,1004)	1:59:A:LEU:HD22	1:16:A:SER:H	2	0.1
(1,1004)	1:59:A:LEU:HD23	1:16:A:SER:H	2	0.1
(1,939)	1:91:A:ILE:HD11	1:91:A:ILE:H	1	0.1
(1,939)	1:91:A:ILE:HD12	1:91:A:ILE:H	1	0.1
(1,939)	1:91:A:ILE:HD13	1:91:A:ILE:H	1	0.1
(1,939)	1:91:A:ILE:HD11	1:91:A:ILE:H	6	0.1
(1,939)	1:91:A:ILE:HD12	1:91:A:ILE:H	6	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,939)	1:91:A:ILE:HD13	1:91:A:ILE:H	6	0.1
(1,872)	1:63:A:GLY:HA2	1:63:A:GLY:H	14	0.1
(1,857)	1:97:A:ILE:HG12	1:121:A:GLN:HE22	4	0.1
(1,779)	1:62:A:LYS:HB3	1:62:A:LYS:H	4	0.1
(1,779)	1:62:A:LYS:HB3	1:62:A:LYS:H	7	0.1
(1,779)	1:62:A:LYS:HB3	1:62:A:LYS:H	18	0.1
(1,772)	1:20:A:ALA:HB1	1:23:A:LYS:H	2	0.1
(1,772)	1:20:A:ALA:HB2	1:23:A:LYS:H	2	0.1
(1,772)	1:20:A:ALA:HB3	1:23:A:LYS:H	2	0.1
(1,582)	1:57:A:MET:HB3	1:58:A:TYR:H	16	0.1
(1,391)	1:72:A:ARG:HD2	1:73:A:ILE:H	15	0.1
(1,391)	1:72:A:ARG:HD2	1:73:A:ILE:H	19	0.1
(1,380)	1:61:A:GLY:HA3	1:61:A:GLY:H	5	0.1
(1,380)	1:61:A:GLY:HA3	1:61:A:GLY:H	15	0.1
(1,359)	1:45:A:GLY:HA3	1:45:A:GLY:H	2	0.1
(1,359)	1:45:A:GLY:HA3	1:45:A:GLY:H	4	0.1
(1,359)	1:45:A:GLY:HA3	1:45:A:GLY:H	10	0.1
(1,359)	1:45:A:GLY:HA3	1:45:A:GLY:H	15	0.1
(1,359)	1:45:A:GLY:HA3	1:45:A:GLY:H	16	0.1
(1,282)	1:144:A:LEU:HA	1:144:A:LEU:H	1	0.1
(1,250)	1:102:A:GLN:HE22	1:101:A:GLY:H	6	0.1
(1,250)	1:102:A:GLN:HE22	1:101:A:GLY:H	8	0.1
(1,81)	1:58:A:TYR:H	1:61:A:GLY:H	5	0.1

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

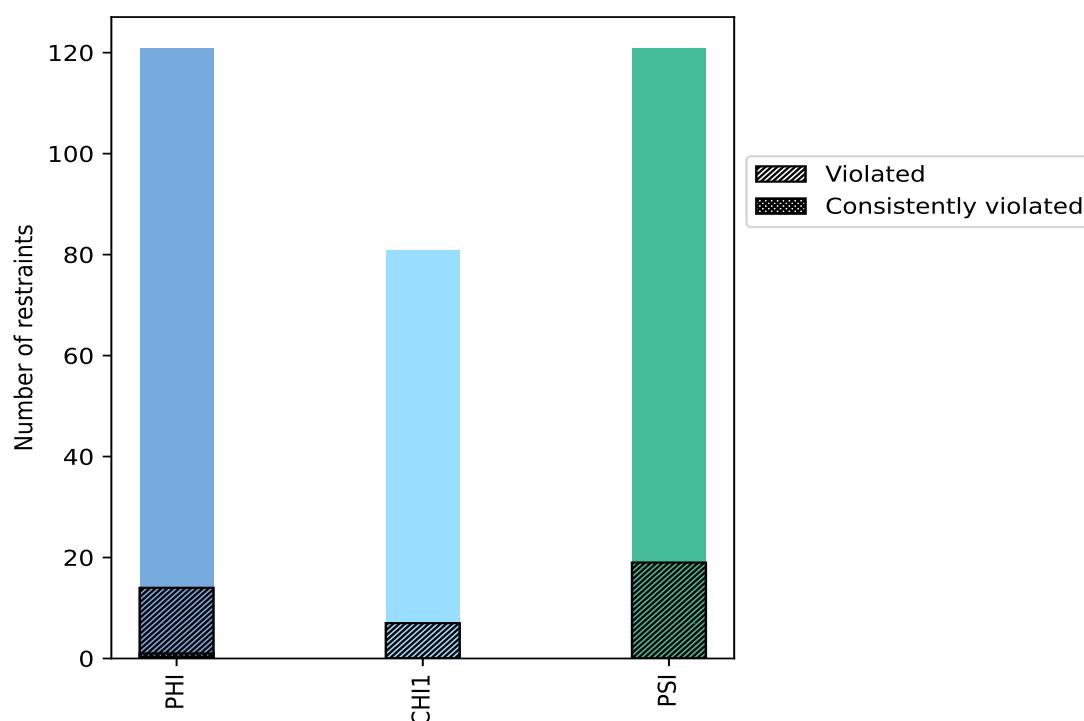
10.1 Summary of dihedral-angle violations [i](#)

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	121	37.5	14	11.6	4.3	1	0.8	0.3
CHI1	81	25.1	7	8.6	2.2	0	0.0	0.0
PSI	121	37.5	19	15.7	5.9	0	0.0	0.0
Total	323	100.0	40	12.4	12.4	1	0.3	0.3

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](#)



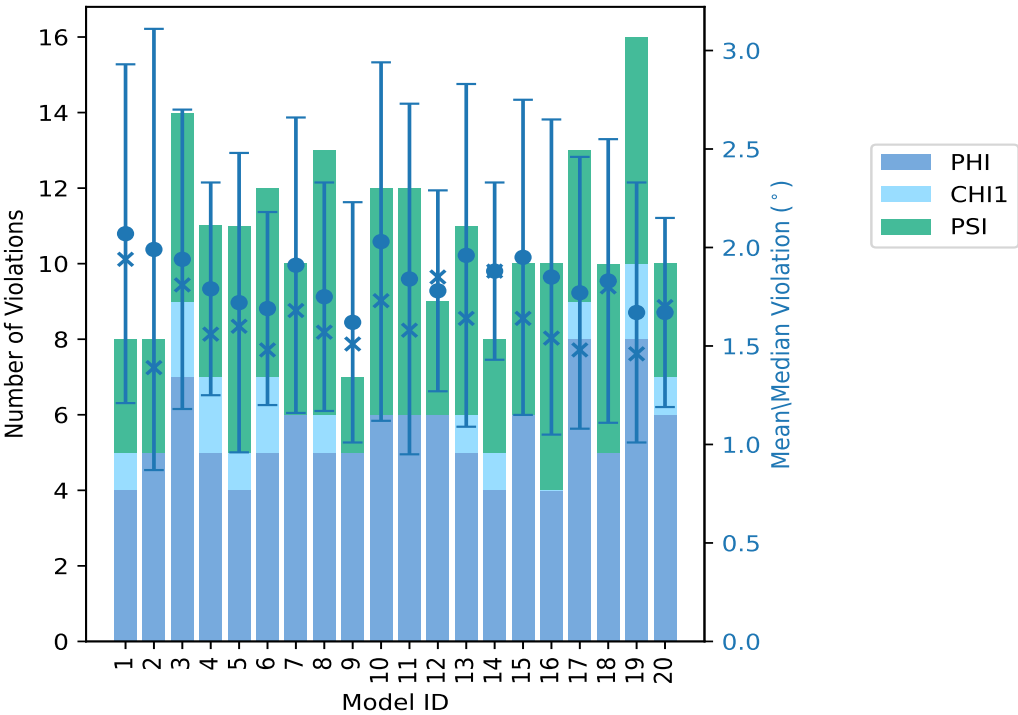
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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	CHI1	PSI	Total				
1	4	1	3	8	2.07	3.64	0.86	1.94
2	5	0	3	8	1.99	4.33	1.12	1.39
3	7	2	5	14	1.94	3.32	0.76	1.81
4	5	2	4	11	1.79	2.62	0.54	1.56
5	4	1	6	11	1.72	3.79	0.76	1.6
6	5	2	5	12	1.69	2.74	0.49	1.48
7	6	0	4	10	1.91	3.51	0.75	1.68
8	5	1	7	13	1.75	3.29	0.58	1.57
9	5	0	2	7	1.62	3.0	0.61	1.51
10	6	0	6	12	2.03	4.41	0.91	1.73
11	6	0	6	12	1.84	4.2	0.89	1.58
12	6	0	3	9	1.78	2.64	0.51	1.85
13	5	1	5	11	1.96	3.79	0.87	1.64
14	4	1	3	8	1.88	2.72	0.45	1.88
15	6	0	4	10	1.95	4.05	0.8	1.64
16	4	0	6	10	1.85	3.37	0.8	1.54
17	8	1	4	13	1.77	3.73	0.69	1.48
18	5	0	5	10	1.83	3.61	0.72	1.8
19	8	2	6	16	1.67	3.74	0.66	1.46
20	6	1	3	10	1.67	2.39	0.48	1.7

10.2.1 Bar graph : Dihedral violation statistics for each model ⓘ



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

10.3 Dihedral-angle violation statistics for the ensemble ⓘ

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

Number of violated restraints				Fraction of the ensemble	
PHI	CHI1	PSI	Total	Count ¹	%
2	5	6	13	1	5.0
3	1	4	8	2	10.0
1	0	3	4	3	15.0
0	0	0	0	4	20.0
2	0	0	2	5	25.0
0	0	3	3	6	30.0
0	0	0	0	7	35.0
0	1	0	1	8	40.0
1	0	0	1	9	45.0
0	0	0	0	10	50.0
1	0	0	1	11	55.0

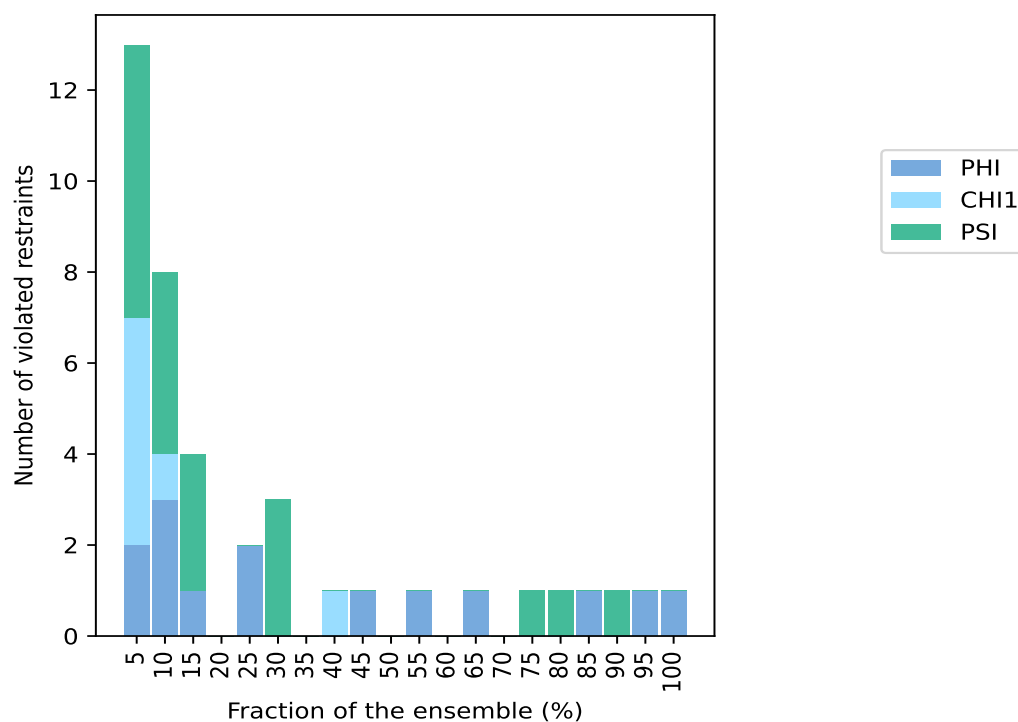
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Number of violated restraints				Fraction of the ensemble	
PHI	CHI1	PSI	Total	Count ¹	%
0	0	0	0	12	60.0
1	0	0	1	13	65.0
0	0	0	0	14	70.0
0	0	1	1	15	75.0
0	0	1	1	16	80.0
1	0	0	1	17	85.0
0	0	1	1	18	90.0
1	0	0	1	19	95.0
1	0	0	1	20	100.0

¹ Number of models with violations

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

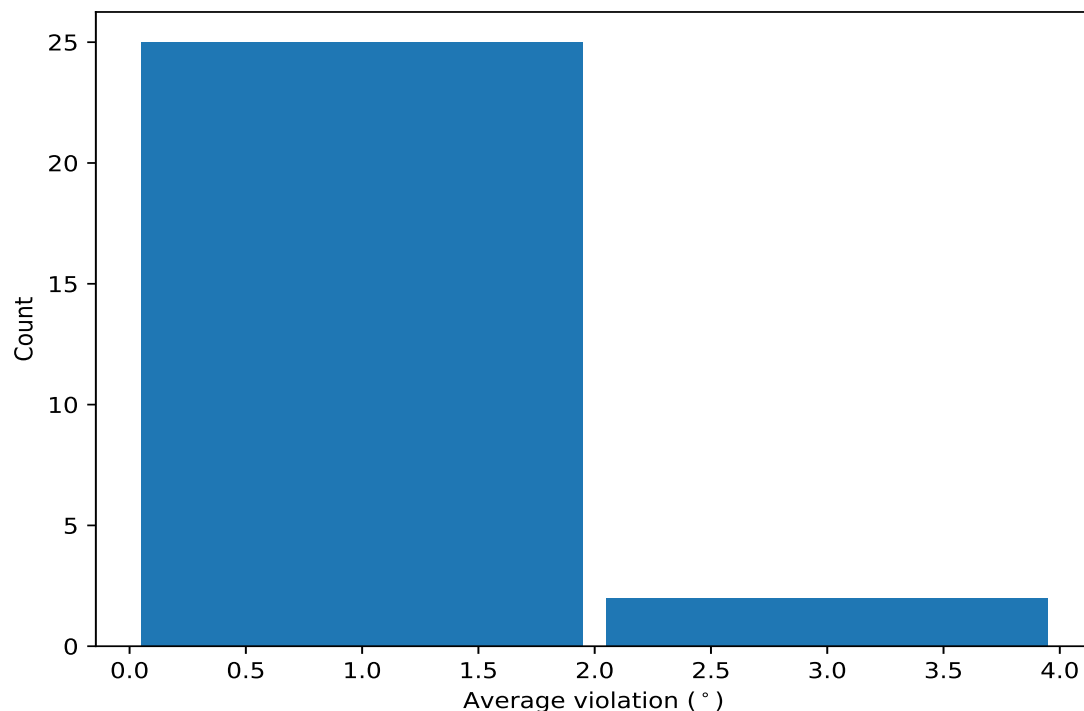


10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

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

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

in the ensemble



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,201)	1:119:A:ILE:C	1:120:A:ASP:N	1:120:A:ASP:CA	1:120:A:ASP:C	20	3.31	0.72	3.34
(1,43)	1:24:A:SER:C	1:25:A:HIS:N	1:25:A:HIS:CA	1:25:A:HIS:C	19	1.93	0.4	1.92
(1,74)	1:45:A:GLY:N	1:45:A:GLY:CA	1:45:A:GLY:C	1:46:A:TYR:N	18	1.62	0.33	1.6
(1,79)	1:47:A:VAL:C	1:48:A:ASN:N	1:48:A:ASN:CA	1:48:A:ASN:C	17	2.52	0.6	2.48
(1,200)	1:119:A:ILE:N	1:119:A:ILE:CA	1:119:A:ILE:C	1:120:A:ASP:N	16	1.89	0.6	1.9
(1,118)	1:73:A:ILE:N	1:73:A:ILE:CA	1:73:A:ILE:C	1:74:A:TYR:N	15	1.97	0.49	2.02
(1,125)	1:78:A:ASP:C	1:79:A:ILE:N	1:79:A:ILE:CA	1:79:A:ILE:C	13	1.5	0.37	1.5
(1,13)	1:9:A:ASP:C	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	11	1.4	0.26	1.32
(1,69)	1:42:A:ASP:C	1:43:A:GLY:N	1:43:A:GLY:CA	1:43:A:GLY:C	9	1.2	0.2	1.17
(1,301)	1:104:A:SER:N	1:104:A:SER:CA	1:104:A:SER:CB	1:104:A:SER:OG	8	1.92	0.64	1.84
(1,78)	1:47:A:VAL:N	1:47:A:VAL:CA	1:47:A:VAL:C	1:48:A:ASN:N	6	1.72	0.45	1.62
(1,44)	1:25:A:HIS:N	1:25:A:HIS:CA	1:25:A:HIS:C	1:26:A:LEU:N	6	1.59	0.33	1.6
(1,168)	1:102:A:GLN:N	1:102:A:GLN:CA	1:102:A:GLN:C	1:103:A:LEU:N	6	1.29	0.47	1.12
(1,1)	1:2:A:SER:C	1:3:A:VAL:N	1:3:A:VAL:CA	1:3:A:VAL:C	5	1.46	0.36	1.35
(1,9)	1:7:A:ASP:C	1:8:A:ILE:N	1:8:A:ILE:CA	1:8:A:ILE:C	5	1.34	0.17	1.34
(1,82)	1:49:A:SER:N	1:49:A:SER:CA	1:49:A:SER:C	1:50:A:ILE:N	3	1.56	0.03	1.56
(1,130)	1:81:A:ASN:N	1:81:A:ASN:CA	1:81:A:ASN:C	1:82:A:ASN:N	3	1.48	0.6	1.09
(1,167)	1:101:A:GLY:C	1:102:A:GLN:N	1:102:A:GLN:CA	1:102:A:GLN:C	3	1.33	0.26	1.24
(1,116)	1:72:A:ARG:N	1:72:A:ARG:CA	1:72:A:ARG:C	1:73:A:ILE:N	3	1.19	0.1	1.19
(1,111)	1:69:A:GLY:C	1:70:A:LYS:N	1:70:A:LYS:CA	1:70:A:LYS:C	2	1.51	0.03	1.51

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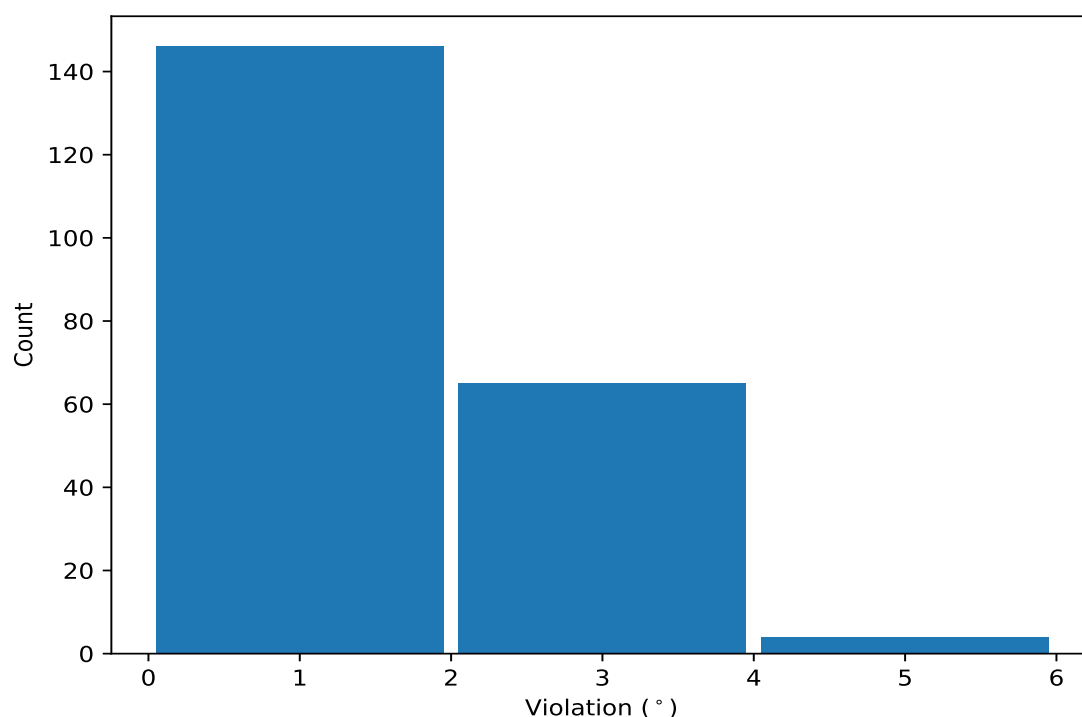
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,190)	1:114:A:ASP:N	1:114:A:ASP:CA	1:114:A:ASP:C	1:115:A:GLY:N	2	1.48	0.35	1.48
(1,112)	1:70:A:LYS:N	1:70:A:LYS:CA	1:70:A:LYS:C	1:71:A:ASN:N	2	1.45	0.03	1.45
(1,244)	1:4:A:LYS:N	1:4:A:LYS:CA	1:4:A:LYS:CB	1:4:A:LYS:CG	2	1.42	0.14	1.42
(1,117)	1:72:A:ARG:C	1:73:A:ILE:N	1:73:A:ILE:CA	1:73:A:ILE:C	2	1.42	0.39	1.42
(1,139)	1:85:A:VAL:C	1:86:A:ASP:N	1:86:A:ASP:CA	1:86:A:ASP:C	2	1.27	0.1	1.27
(1,186)	1:112:A:ASP:N	1:112:A:ASP:CA	1:112:A:ASP:C	1:113:A:ALA:N	2	1.24	0.14	1.24
(1,26)	1:16:A:SER:N	1:16:A:SER:CA	1:16:A:SER:C	1:17:A:ILE:N	2	1.06	0.06	1.06

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 (°)
(1,201)	1:119:A:ILE:C	1:120:A:ASP:N	1:120:A:ASP:CA	1:120:A:ASP:C	10	4.41

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,201)	1:119:A:ILE:C	1:120:A:ASP:N	1:120:A:ASP:CA	1:120:A:ASP:C	2	4.33
(1,201)	1:119:A:ILE:C	1:120:A:ASP:N	1:120:A:ASP:CA	1:120:A:ASP:C	11	4.2
(1,201)	1:119:A:ILE:C	1:120:A:ASP:N	1:120:A:ASP:CA	1:120:A:ASP:C	15	4.05
(1,201)	1:119:A:ILE:C	1:120:A:ASP:N	1:120:A:ASP:CA	1:120:A:ASP:C	5	3.79
(1,79)	1:47:A:VAL:C	1:48:A:ASN:N	1:48:A:ASN:CA	1:48:A:ASN:C	13	3.79
(1,201)	1:119:A:ILE:C	1:120:A:ASP:N	1:120:A:ASP:CA	1:120:A:ASP:C	19	3.74
(1,201)	1:119:A:ILE:C	1:120:A:ASP:N	1:120:A:ASP:CA	1:120:A:ASP:C	17	3.73
(1,201)	1:119:A:ILE:C	1:120:A:ASP:N	1:120:A:ASP:CA	1:120:A:ASP:C	1	3.64
(1,201)	1:119:A:ILE:C	1:120:A:ASP:N	1:120:A:ASP:CA	1:120:A:ASP:C	18	3.61
(1,79)	1:47:A:VAL:C	1:48:A:ASN:N	1:48:A:ASN:CA	1:48:A:ASN:C	7	3.51
(1,201)	1:119:A:ILE:C	1:120:A:ASP:N	1:120:A:ASP:CA	1:120:A:ASP:C	16	3.37
(1,201)	1:119:A:ILE:C	1:120:A:ASP:N	1:120:A:ASP:CA	1:120:A:ASP:C	3	3.32
(1,201)	1:119:A:ILE:C	1:120:A:ASP:N	1:120:A:ASP:CA	1:120:A:ASP:C	8	3.29
(1,201)	1:119:A:ILE:C	1:120:A:ASP:N	1:120:A:ASP:CA	1:120:A:ASP:C	13	3.29
(1,301)	1:104:A:SER:N	1:104:A:SER:CA	1:104:A:SER:CB	1:104:A:SER:OG	3	3.28
(1,79)	1:47:A:VAL:C	1:48:A:ASN:N	1:48:A:ASN:CA	1:48:A:ASN:C	16	3.2
(1,200)	1:119:A:ILE:N	1:119:A:ILE:CA	1:119:A:ILE:C	1:120:A:ASP:N	2	3.15
(1,201)	1:119:A:ILE:C	1:120:A:ASP:N	1:120:A:ASP:CA	1:120:A:ASP:C	9	3.0
(1,79)	1:47:A:VAL:C	1:48:A:ASN:N	1:48:A:ASN:CA	1:48:A:ASN:C	3	2.95
(1,200)	1:119:A:ILE:N	1:119:A:ILE:CA	1:119:A:ILE:C	1:120:A:ASP:N	10	2.93
(1,118)	1:73:A:ILE:N	1:73:A:ILE:CA	1:73:A:ILE:C	1:74:A:TYR:N	1	2.9
(1,79)	1:47:A:VAL:C	1:48:A:ASN:N	1:48:A:ASN:CA	1:48:A:ASN:C	11	2.78
(1,201)	1:119:A:ILE:C	1:120:A:ASP:N	1:120:A:ASP:CA	1:120:A:ASP:C	7	2.75
(1,201)	1:119:A:ILE:C	1:120:A:ASP:N	1:120:A:ASP:CA	1:120:A:ASP:C	6	2.74
(1,79)	1:47:A:VAL:C	1:48:A:ASN:N	1:48:A:ASN:CA	1:48:A:ASN:C	14	2.72
(1,201)	1:119:A:ILE:C	1:120:A:ASP:N	1:120:A:ASP:CA	1:120:A:ASP:C	12	2.64
(1,118)	1:73:A:ILE:N	1:73:A:ILE:CA	1:73:A:ILE:C	1:74:A:TYR:N	4	2.62
(1,125)	1:78:A:ASP:C	1:79:A:ILE:N	1:79:A:ILE:CA	1:79:A:ILE:C	13	2.59
(1,79)	1:47:A:VAL:C	1:48:A:ASN:N	1:48:A:ASN:CA	1:48:A:ASN:C	10	2.58
(1,79)	1:47:A:VAL:C	1:48:A:ASN:N	1:48:A:ASN:CA	1:48:A:ASN:C	4	2.51
(1,43)	1:24:A:SER:C	1:25:A:HIS:N	1:25:A:HIS:CA	1:25:A:HIS:C	12	2.5
(1,79)	1:47:A:VAL:C	1:48:A:ASN:N	1:48:A:ASN:CA	1:48:A:ASN:C	6	2.48
(1,43)	1:24:A:SER:C	1:25:A:HIS:N	1:25:A:HIS:CA	1:25:A:HIS:C	1	2.48
(1,79)	1:47:A:VAL:C	1:48:A:ASN:N	1:48:A:ASN:CA	1:48:A:ASN:C	8	2.47
(1,74)	1:45:A:GLY:N	1:45:A:GLY:CA	1:45:A:GLY:C	1:46:A:TYR:N	17	2.47
(1,201)	1:119:A:ILE:C	1:120:A:ASP:N	1:120:A:ASP:CA	1:120:A:ASP:C	4	2.45
(1,118)	1:73:A:ILE:N	1:73:A:ILE:CA	1:73:A:ILE:C	1:74:A:TYR:N	15	2.44
(1,43)	1:24:A:SER:C	1:25:A:HIS:N	1:25:A:HIS:CA	1:25:A:HIS:C	15	2.41
(1,79)	1:47:A:VAL:C	1:48:A:ASN:N	1:48:A:ASN:CA	1:48:A:ASN:C	20	2.39
(1,78)	1:47:A:VAL:N	1:47:A:VAL:CA	1:47:A:VAL:C	1:48:A:ASN:N	16	2.38
(1,200)	1:119:A:ILE:N	1:119:A:ILE:CA	1:119:A:ILE:C	1:120:A:ASP:N	1	2.37
(1,301)	1:104:A:SER:N	1:104:A:SER:CA	1:104:A:SER:CB	1:104:A:SER:OG	14	2.34
(1,200)	1:119:A:ILE:N	1:119:A:ILE:CA	1:119:A:ILE:C	1:120:A:ASP:N	5	2.34
(1,43)	1:24:A:SER:C	1:25:A:HIS:N	1:25:A:HIS:CA	1:25:A:HIS:C	2	2.34
(1,168)	1:102:A:GLN:N	1:102:A:GLN:CA	1:102:A:GLN:C	1:103:A:LEU:N	7	2.33
(1,130)	1:81:A:ASN:N	1:81:A:ASN:CA	1:81:A:ASN:C	1:82:A:ASN:N	3	2.32
(1,118)	1:73:A:ILE:N	1:73:A:ILE:CA	1:73:A:ILE:C	1:74:A:TYR:N	10	2.31
(1,43)	1:24:A:SER:C	1:25:A:HIS:N	1:25:A:HIS:CA	1:25:A:HIS:C	4	2.31
(1,79)	1:47:A:VAL:C	1:48:A:ASN:N	1:48:A:ASN:CA	1:48:A:ASN:C	18	2.29
(1,118)	1:73:A:ILE:N	1:73:A:ILE:CA	1:73:A:ILE:C	1:74:A:TYR:N	11	2.27
(1,200)	1:119:A:ILE:N	1:119:A:ILE:CA	1:119:A:ILE:C	1:120:A:ASP:N	11	2.26

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,78)	1:47:A:VAL:N	1:47:A:VAL:CA	1:47:A:VAL:C	1:48:A:ASN:N	7	2.24
(1,43)	1:24:A:SER:C	1:25:A:HIS:N	1:25:A:HIS:CA	1:25:A:HIS:C	20	2.23
(1,118)	1:73:A:ILE:N	1:73:A:ILE:CA	1:73:A:ILE:C	1:74:A:TYR:N	6	2.18
(1,79)	1:47:A:VAL:C	1:48:A:ASN:N	1:48:A:ASN:CA	1:48:A:ASN:C	17	2.16
(1,200)	1:119:A:ILE:N	1:119:A:ILE:CA	1:119:A:ILE:C	1:120:A:ASP:N	19	2.15
(1,1)	1:2:A:SER:C	1:3:A:VAL:N	1:3:A:VAL:CA	1:3:A:VAL:C	10	2.11
(1,301)	1:104:A:SER:N	1:104:A:SER:CA	1:104:A:SER:CB	1:104:A:SER:OG	13	2.1
(1,301)	1:104:A:SER:N	1:104:A:SER:CA	1:104:A:SER:CB	1:104:A:SER:OG	20	2.1
(1,74)	1:45:A:GLY:N	1:45:A:GLY:CA	1:45:A:GLY:C	1:46:A:TYR:N	3	2.08
(1,43)	1:24:A:SER:C	1:25:A:HIS:N	1:25:A:HIS:CA	1:25:A:HIS:C	3	2.07
(1,79)	1:47:A:VAL:C	1:48:A:ASN:N	1:48:A:ASN:CA	1:48:A:ASN:C	19	2.06
(1,44)	1:25:A:HIS:N	1:25:A:HIS:CA	1:25:A:HIS:C	1:26:A:LEU:N	19	2.06
(1,43)	1:24:A:SER:C	1:25:A:HIS:N	1:25:A:HIS:CA	1:25:A:HIS:C	8	2.06
(1,312)	1:130:A:TYR:N	1:130:A:TYR:CA	1:130:A:TYR:CB	1:130:A:TYR:CG	3	2.03
(1,118)	1:73:A:ILE:N	1:73:A:ILE:CA	1:73:A:ILE:C	1:74:A:TYR:N	19	2.03
(1,118)	1:73:A:ILE:N	1:73:A:ILE:CA	1:73:A:ILE:C	1:74:A:TYR:N	18	2.02
(1,13)	1:9:A:ASP:C	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	12	2.01
(1,200)	1:119:A:ILE:N	1:119:A:ILE:CA	1:119:A:ILE:C	1:120:A:ASP:N	8	1.99
(1,201)	1:119:A:ILE:C	1:120:A:ASP:N	1:120:A:ASP:CA	1:120:A:ASP:C	14	1.98
(1,74)	1:45:A:GLY:N	1:45:A:GLY:CA	1:45:A:GLY:C	1:46:A:TYR:N	20	1.98
(1,200)	1:119:A:ILE:N	1:119:A:ILE:CA	1:119:A:ILE:C	1:120:A:ASP:N	18	1.97
(1,43)	1:24:A:SER:C	1:25:A:HIS:N	1:25:A:HIS:CA	1:25:A:HIS:C	18	1.97
(1,264)	1:40:A:ASP:N	1:40:A:ASP:CA	1:40:A:ASP:CB	1:40:A:ASP:CG	17	1.94
(1,43)	1:24:A:SER:C	1:25:A:HIS:N	1:25:A:HIS:CA	1:25:A:HIS:C	5	1.92
(1,43)	1:24:A:SER:C	1:25:A:HIS:N	1:25:A:HIS:CA	1:25:A:HIS:C	14	1.92
(1,79)	1:47:A:VAL:C	1:48:A:ASN:N	1:48:A:ASN:CA	1:48:A:ASN:C	12	1.9
(1,74)	1:45:A:GLY:N	1:45:A:GLY:CA	1:45:A:GLY:C	1:46:A:TYR:N	7	1.87
(1,44)	1:25:A:HIS:N	1:25:A:HIS:CA	1:25:A:HIS:C	1:26:A:LEU:N	10	1.86
(1,118)	1:73:A:ILE:N	1:73:A:ILE:CA	1:73:A:ILE:C	1:74:A:TYR:N	12	1.85
(1,200)	1:119:A:ILE:N	1:119:A:ILE:CA	1:119:A:ILE:C	1:120:A:ASP:N	6	1.84
(1,118)	1:73:A:ILE:N	1:73:A:ILE:CA	1:73:A:ILE:C	1:74:A:TYR:N	14	1.84
(1,43)	1:24:A:SER:C	1:25:A:HIS:N	1:25:A:HIS:CA	1:25:A:HIS:C	17	1.83
(1,201)	1:119:A:ILE:C	1:120:A:ASP:N	1:120:A:ASP:CA	1:120:A:ASP:C	20	1.82
(1,190)	1:114:A:ASP:N	1:114:A:ASP:CA	1:114:A:ASP:C	1:115:A:GLY:N	8	1.82
(1,117)	1:72:A:ARG:C	1:73:A:ILE:N	1:73:A:ILE:CA	1:73:A:ILE:C	19	1.81
(1,43)	1:24:A:SER:C	1:25:A:HIS:N	1:25:A:HIS:CA	1:25:A:HIS:C	11	1.8
(1,74)	1:45:A:GLY:N	1:45:A:GLY:CA	1:45:A:GLY:C	1:46:A:TYR:N	15	1.78
(1,43)	1:24:A:SER:C	1:25:A:HIS:N	1:25:A:HIS:CA	1:25:A:HIS:C	9	1.74
(1,43)	1:24:A:SER:C	1:25:A:HIS:N	1:25:A:HIS:CA	1:25:A:HIS:C	13	1.73
(1,43)	1:24:A:SER:C	1:25:A:HIS:N	1:25:A:HIS:CA	1:25:A:HIS:C	16	1.71
(1,167)	1:101:A:GLY:C	1:102:A:GLN:N	1:102:A:GLN:CA	1:102:A:GLN:C	15	1.68
(1,125)	1:78:A:ASP:C	1:79:A:ILE:N	1:79:A:ILE:CA	1:79:A:ILE:C	11	1.67
(1,74)	1:45:A:GLY:N	1:45:A:GLY:CA	1:45:A:GLY:C	1:46:A:TYR:N	9	1.67
(1,74)	1:45:A:GLY:N	1:45:A:GLY:CA	1:45:A:GLY:C	1:46:A:TYR:N	5	1.66
(1,13)	1:9:A:ASP:C	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	5	1.65
(1,125)	1:78:A:ASP:C	1:79:A:ILE:N	1:79:A:ILE:CA	1:79:A:ILE:C	18	1.64
(1,78)	1:47:A:VAL:N	1:47:A:VAL:CA	1:47:A:VAL:C	1:48:A:ASN:N	13	1.64
(1,74)	1:45:A:GLY:N	1:45:A:GLY:CA	1:45:A:GLY:C	1:46:A:TYR:N	19	1.64
(1,9)	1:7:A:ASP:C	1:8:A:ILE:N	1:8:A:ILE:CA	1:8:A:ILE:C	8	1.63
(1,44)	1:25:A:HIS:N	1:25:A:HIS:CA	1:25:A:HIS:C	1:26:A:LEU:N	2	1.61
(1,193)	1:115:A:GLY:C	1:116:A:ASN:N	1:116:A:ASN:CA	1:116:A:ASN:C	15	1.6

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,118)	1:73:A:ILE:N	1:73:A:ILE:CA	1:73:A:ILE:C	1:74:A:TYR:N	5	1.6
(1,118)	1:73:A:ILE:N	1:73:A:ILE:CA	1:73:A:ILE:C	1:74:A:TYR:N	13	1.6
(1,74)	1:45:A:GLY:N	1:45:A:GLY:CA	1:45:A:GLY:C	1:46:A:TYR:N	10	1.6
(1,200)	1:119:A:ILE:N	1:119:A:ILE:CA	1:119:A:ILE:C	1:120:A:ASP:N	17	1.59
(1,125)	1:78:A:ASP:C	1:79:A:ILE:N	1:79:A:ILE:CA	1:79:A:ILE:C	14	1.59
(1,82)	1:49:A:SER:N	1:49:A:SER:CA	1:49:A:SER:C	1:50:A:ILE:N	10	1.59
(1,78)	1:47:A:VAL:N	1:47:A:VAL:CA	1:47:A:VAL:C	1:48:A:ASN:N	20	1.59
(1,74)	1:45:A:GLY:N	1:45:A:GLY:CA	1:45:A:GLY:C	1:46:A:TYR:N	16	1.59
(1,69)	1:42:A:ASP:C	1:43:A:GLY:N	1:43:A:GLY:CA	1:43:A:GLY:C	3	1.59
(1,301)	1:104:A:SER:N	1:104:A:SER:CA	1:104:A:SER:CB	1:104:A:SER:OG	4	1.58
(1,79)	1:47:A:VAL:C	1:48:A:ASN:N	1:48:A:ASN:CA	1:48:A:ASN:C	15	1.58
(1,44)	1:25:A:HIS:N	1:25:A:HIS:CA	1:25:A:HIS:C	1:26:A:LEU:N	6	1.58
(1,74)	1:45:A:GLY:N	1:45:A:GLY:CA	1:45:A:GLY:C	1:46:A:TYR:N	6	1.57
(1,13)	1:9:A:ASP:C	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	8	1.57
(1,244)	1:4:A:LYS:N	1:4:A:LYS:CA	1:4:A:LYS:CB	1:4:A:LYS:CG	4	1.56
(1,125)	1:78:A:ASP:C	1:79:A:ILE:N	1:79:A:ILE:CA	1:79:A:ILE:C	19	1.56
(1,82)	1:49:A:SER:N	1:49:A:SER:CA	1:49:A:SER:C	1:50:A:ILE:N	13	1.56
(1,125)	1:78:A:ASP:C	1:79:A:ILE:N	1:79:A:ILE:CA	1:79:A:ILE:C	15	1.54
(1,111)	1:69:A:GLY:C	1:70:A:LYS:N	1:70:A:LYS:CA	1:70:A:LYS:C	3	1.54
(1,13)	1:9:A:ASP:C	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	3	1.54
(1,82)	1:49:A:SER:N	1:49:A:SER:CA	1:49:A:SER:C	1:50:A:ILE:N	4	1.52
(1,200)	1:119:A:ILE:N	1:119:A:ILE:CA	1:119:A:ILE:C	1:120:A:ASP:N	12	1.51
(1,79)	1:47:A:VAL:C	1:48:A:ASN:N	1:48:A:ASN:CA	1:48:A:ASN:C	9	1.51
(1,74)	1:45:A:GLY:N	1:45:A:GLY:CA	1:45:A:GLY:C	1:46:A:TYR:N	8	1.51
(1,125)	1:78:A:ASP:C	1:79:A:ILE:N	1:79:A:ILE:CA	1:79:A:ILE:C	10	1.5
(1,74)	1:45:A:GLY:N	1:45:A:GLY:CA	1:45:A:GLY:C	1:46:A:TYR:N	4	1.5
(1,69)	1:42:A:ASP:C	1:43:A:GLY:N	1:43:A:GLY:CA	1:43:A:GLY:C	1	1.5
(1,301)	1:104:A:SER:N	1:104:A:SER:CA	1:104:A:SER:CB	1:104:A:SER:OG	5	1.48
(1,118)	1:73:A:ILE:N	1:73:A:ILE:CA	1:73:A:ILE:C	1:74:A:TYR:N	17	1.48
(1,112)	1:70:A:LYS:N	1:70:A:LYS:CA	1:70:A:LYS:C	1:71:A:ASN:N	11	1.48
(1,111)	1:69:A:GLY:C	1:70:A:LYS:N	1:70:A:LYS:CA	1:70:A:LYS:C	7	1.48
(1,18)	1:12:A:GLY:N	1:12:A:GLY:CA	1:12:A:GLY:C	1:13:A:GLU:N	16	1.48
(1,1)	1:2:A:SER:C	1:3:A:VAL:N	1:3:A:VAL:CA	1:3:A:VAL:C	17	1.48
(1,246)	1:7:A:ASP:N	1:7:A:ASP:CA	1:7:A:ASP:CB	1:7:A:ASP:CG	8	1.46
(1,112)	1:70:A:LYS:N	1:70:A:LYS:CA	1:70:A:LYS:C	1:71:A:ASN:N	5	1.42
(1,293)	1:92:A:LEU:N	1:92:A:LEU:CA	1:92:A:LEU:CB	1:92:A:LEU:CG	6	1.39
(1,74)	1:45:A:GLY:N	1:45:A:GLY:CA	1:45:A:GLY:C	1:46:A:TYR:N	18	1.39
(1,44)	1:25:A:HIS:N	1:25:A:HIS:CA	1:25:A:HIS:C	1:26:A:LEU:N	7	1.39
(1,200)	1:119:A:ILE:N	1:119:A:ILE:CA	1:119:A:ILE:C	1:120:A:ASP:N	15	1.37
(1,186)	1:112:A:ASP:N	1:112:A:ASP:CA	1:112:A:ASP:C	1:113:A:ALA:N	19	1.37
(1,10)	1:8:A:ILE:N	1:8:A:ILE:CA	1:8:A:ILE:C	1:9:A:ASP:N	8	1.37
(1,139)	1:85:A:VAL:C	1:86:A:ASP:N	1:86:A:ASP:CA	1:86:A:ASP:C	17	1.36
(1,125)	1:78:A:ASP:C	1:79:A:ILE:N	1:79:A:ILE:CA	1:79:A:ILE:C	17	1.36
(1,9)	1:7:A:ASP:C	1:8:A:ILE:N	1:8:A:ILE:CA	1:8:A:ILE:C	6	1.36
(1,78)	1:47:A:VAL:N	1:47:A:VAL:CA	1:47:A:VAL:C	1:48:A:ASN:N	17	1.35
(1,1)	1:2:A:SER:C	1:3:A:VAL:N	1:3:A:VAL:CA	1:3:A:VAL:C	4	1.35
(1,1)	1:2:A:SER:C	1:3:A:VAL:N	1:3:A:VAL:CA	1:3:A:VAL:C	7	1.35
(1,74)	1:45:A:GLY:N	1:45:A:GLY:CA	1:45:A:GLY:C	1:46:A:TYR:N	14	1.34
(1,13)	1:9:A:ASP:C	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	6	1.34
(1,9)	1:7:A:ASP:C	1:8:A:ILE:N	1:8:A:ILE:CA	1:8:A:ILE:C	19	1.34
(1,200)	1:119:A:ILE:N	1:119:A:ILE:CA	1:119:A:ILE:C	1:120:A:ASP:N	14	1.32

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,13)	1:9:A:ASP:C	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	19	1.32
(1,125)	1:78:A:ASP:C	1:79:A:ILE:N	1:79:A:ILE:CA	1:79:A:ILE:C	20	1.31
(1,116)	1:72:A:ARG:N	1:72:A:ARG:CA	1:72:A:ARG:C	1:73:A:ILE:N	12	1.31
(1,43)	1:24:A:SER:C	1:25:A:HIS:N	1:25:A:HIS:CA	1:25:A:HIS:C	6	1.31
(1,200)	1:119:A:ILE:N	1:119:A:ILE:CA	1:119:A:ILE:C	1:120:A:ASP:N	16	1.3
(1,13)	1:9:A:ASP:C	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	10	1.3
(1,244)	1:4:A:LYS:N	1:4:A:LYS:CA	1:4:A:LYS:CB	1:4:A:LYS:CG	19	1.29
(1,118)	1:73:A:ILE:N	1:73:A:ILE:CA	1:73:A:ILE:C	1:74:A:TYR:N	8	1.29
(1,74)	1:45:A:GLY:N	1:45:A:GLY:CA	1:45:A:GLY:C	1:46:A:TYR:N	1	1.29
(1,172)	1:105:A:ASP:N	1:105:A:ASP:CA	1:105:A:ASP:C	1:106:A:ALA:N	6	1.28
(1,301)	1:104:A:SER:N	1:104:A:SER:CA	1:104:A:SER:CB	1:104:A:SER:OG	1	1.27
(1,125)	1:78:A:ASP:C	1:79:A:ILE:N	1:79:A:ILE:CA	1:79:A:ILE:C	9	1.26
(1,13)	1:9:A:ASP:C	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	16	1.25
(1,301)	1:104:A:SER:N	1:104:A:SER:CA	1:104:A:SER:CB	1:104:A:SER:OG	6	1.24
(1,167)	1:101:A:GLY:C	1:102:A:GLN:N	1:102:A:GLN:CA	1:102:A:GLN:C	11	1.24
(1,125)	1:78:A:ASP:C	1:79:A:ILE:N	1:79:A:ILE:CA	1:79:A:ILE:C	12	1.22
(1,13)	1:9:A:ASP:C	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	20	1.22
(1,9)	1:7:A:ASP:C	1:8:A:ILE:N	1:8:A:ILE:CA	1:8:A:ILE:C	4	1.21
(1,116)	1:72:A:ARG:N	1:72:A:ARG:CA	1:72:A:ARG:C	1:73:A:ILE:N	8	1.19
(1,69)	1:42:A:ASP:C	1:43:A:GLY:N	1:43:A:GLY:CA	1:43:A:GLY:C	11	1.18
(1,69)	1:42:A:ASP:C	1:43:A:GLY:N	1:43:A:GLY:CA	1:43:A:GLY:C	18	1.18
(1,43)	1:24:A:SER:C	1:25:A:HIS:N	1:25:A:HIS:CA	1:25:A:HIS:C	7	1.18
(1,139)	1:85:A:VAL:C	1:86:A:ASP:N	1:86:A:ASP:CA	1:86:A:ASP:C	2	1.17
(1,69)	1:42:A:ASP:C	1:43:A:GLY:N	1:43:A:GLY:CA	1:43:A:GLY:C	17	1.17
(1,168)	1:102:A:GLN:N	1:102:A:GLN:CA	1:102:A:GLN:C	1:103:A:LEU:N	13	1.16
(1,125)	1:78:A:ASP:C	1:79:A:ILE:N	1:79:A:ILE:CA	1:79:A:ILE:C	2	1.16
(1,74)	1:45:A:GLY:N	1:45:A:GLY:CA	1:45:A:GLY:C	1:46:A:TYR:N	11	1.16
(1,43)	1:24:A:SER:C	1:25:A:HIS:N	1:25:A:HIS:CA	1:25:A:HIS:C	10	1.16
(1,76)	1:46:A:TYR:N	1:46:A:TYR:CA	1:46:A:TYR:C	1:47:A:VAL:N	3	1.15
(1,9)	1:7:A:ASP:C	1:8:A:ILE:N	1:8:A:ILE:CA	1:8:A:ILE:C	3	1.15
(1,236)	1:137:A:HIS:N	1:137:A:HIS:CA	1:137:A:HIS:C	1:138:A:LEU:N	16	1.13
(1,190)	1:114:A:ASP:N	1:114:A:ASP:CA	1:114:A:ASP:C	1:115:A:GLY:N	19	1.13
(1,168)	1:102:A:GLN:N	1:102:A:GLN:CA	1:102:A:GLN:C	1:103:A:LEU:N	16	1.13
(1,78)	1:47:A:VAL:N	1:47:A:VAL:CA	1:47:A:VAL:C	1:48:A:ASN:N	8	1.12
(1,26)	1:16:A:SER:N	1:16:A:SER:CA	1:16:A:SER:C	1:17:A:ILE:N	18	1.12
(1,203)	1:120:A:ASP:C	1:121:A:GLN:N	1:121:A:GLN:CA	1:121:A:GLN:C	12	1.11
(1,186)	1:112:A:ASP:N	1:112:A:ASP:CA	1:112:A:ASP:C	1:113:A:ALA:N	4	1.1
(1,168)	1:102:A:GLN:N	1:102:A:GLN:CA	1:102:A:GLN:C	1:103:A:LEU:N	3	1.1
(1,251)	1:15:A:SER:N	1:15:A:SER:CA	1:15:A:SER:CB	1:15:A:SER:OG	19	1.09
(1,130)	1:81:A:ASN:N	1:81:A:ASN:CA	1:81:A:ASN:C	1:82:A:ASN:N	15	1.09
(1,118)	1:73:A:ILE:N	1:73:A:ILE:CA	1:73:A:ILE:C	1:74:A:TYR:N	2	1.09
(1,69)	1:42:A:ASP:C	1:43:A:GLY:N	1:43:A:GLY:CA	1:43:A:GLY:C	9	1.09
(1,13)	1:9:A:ASP:C	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	1	1.09
(1,200)	1:119:A:ILE:N	1:119:A:ILE:CA	1:119:A:ILE:C	1:120:A:ASP:N	3	1.08
(1,200)	1:119:A:ILE:N	1:119:A:ILE:CA	1:119:A:ILE:C	1:120:A:ASP:N	9	1.08
(1,69)	1:42:A:ASP:C	1:43:A:GLY:N	1:43:A:GLY:CA	1:43:A:GLY:C	2	1.08
(1,13)	1:9:A:ASP:C	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	13	1.08
(1,167)	1:101:A:GLY:C	1:102:A:GLN:N	1:102:A:GLN:CA	1:102:A:GLN:C	19	1.07
(1,116)	1:72:A:ARG:N	1:72:A:ARG:CA	1:72:A:ARG:C	1:73:A:ILE:N	11	1.07
(1,64)	1:40:A:ASP:N	1:40:A:ASP:CA	1:40:A:ASP:C	1:41:A:VAL:N	18	1.07
(1,125)	1:78:A:ASP:C	1:79:A:ILE:N	1:79:A:ILE:CA	1:79:A:ILE:C	5	1.05

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,117)	1:72:A:ARG:C	1:73:A:ILE:N	1:73:A:ILE:CA	1:73:A:ILE:C	17	1.03
(1,168)	1:102:A:GLN:N	1:102:A:GLN:CA	1:102:A:GLN:C	1:103:A:LEU:N	5	1.02
(1,130)	1:81:A:ASN:N	1:81:A:ASN:CA	1:81:A:ASN:C	1:82:A:ASN:N	20	1.02
(1,74)	1:45:A:GLY:N	1:45:A:GLY:CA	1:45:A:GLY:C	1:46:A:TYR:N	13	1.02
(1,44)	1:25:A:HIS:N	1:25:A:HIS:CA	1:25:A:HIS:C	1:26:A:LEU:N	11	1.02
(1,168)	1:102:A:GLN:N	1:102:A:GLN:CA	1:102:A:GLN:C	1:103:A:LEU:N	10	1.01
(1,69)	1:42:A:ASP:C	1:43:A:GLY:N	1:43:A:GLY:CA	1:43:A:GLY:C	7	1.01
(1,69)	1:42:A:ASP:C	1:43:A:GLY:N	1:43:A:GLY:CA	1:43:A:GLY:C	20	1.01
(1,26)	1:16:A:SER:N	1:16:A:SER:CA	1:16:A:SER:C	1:17:A:ILE:N	5	1.01
(1,1)	1:2:A:SER:C	1:3:A:VAL:N	1:3:A:VAL:CA	1:3:A:VAL:C	19	1.0