



Full wwPDB NMR Structure Validation Report ⓘ

Mar 1, 2026 – 11:47 AM UTC

PDB ID : 9IA7 / pdb_00009ia7
BMRB ID : 34979
Title : NMR solution structure of RPRD2 CTD-interacting domain and pT4 RNAPII CTD peptide.
Authors : Linhartova, K.; Kubicek, K.; Stefl, R.
Deposited on : 2025-02-07

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with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
BMRB Restraints Analysis : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

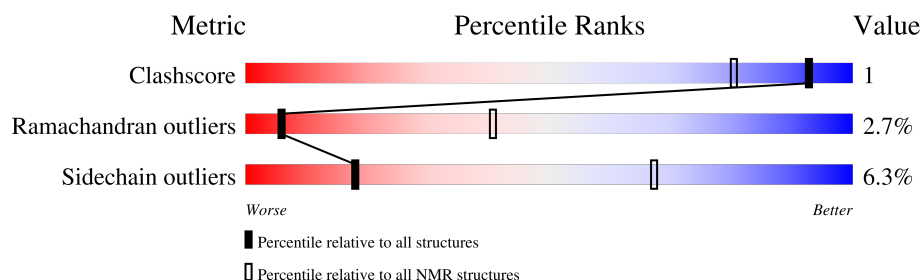
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 63%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	148	
2	B	12	

2 Ensemble composition and analysis

This entry contains 20 models. Model 11 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:24-A:146, B:151-B:153, B:155-B:155 (127)	1.15	11

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 3 clusters and 5 single-model clusters were found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2278 atoms, of which 1131 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Regulation of nuclear pre-mRNA domain-containing protein 2.

Mol	Chain	Residues	Atoms						Trace
1	A	129	Total	C	H	N	O	S	0
			2108	671	1054	187	191	5	

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	15	MET	-	initiating methionine	UNP Q5VT52
A	156	GLU	-	expression tag	UNP Q5VT52
A	157	HIS	-	expression tag	UNP Q5VT52
A	158	HIS	-	expression tag	UNP Q5VT52
A	159	HIS	-	expression tag	UNP Q5VT52
A	160	HIS	-	expression tag	UNP Q5VT52
A	161	HIS	-	expression tag	UNP Q5VT52
A	162	HIS	-	expression tag	UNP Q5VT52

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB1.

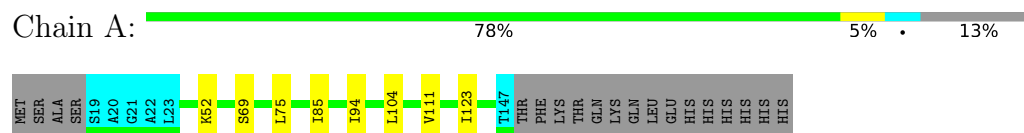
Mol	Chain	Residues	Atoms						Trace
2	B	12	Total	C	H	N	O	P	0
			170	55	77	12	25	1	

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Regulation of nuclear pre-mRNA domain-containing protein 2



- Molecule 2: DNA-directed RNA polymerase II subunit RPB1

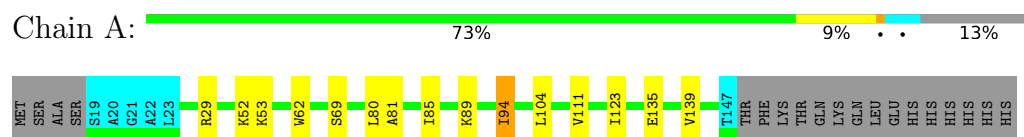


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Regulation of nuclear pre-mRNA domain-containing protein 2

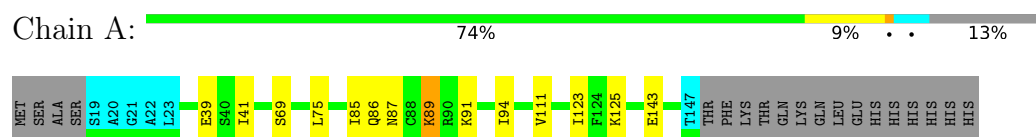


- Molecule 2: DNA-directed RNA polymerase II subunit RPB1



4.2.2 Score per residue for model 2

- Molecule 1: Regulation of nuclear pre-mRNA domain-containing protein 2

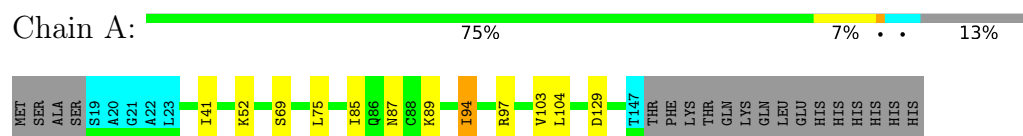


- Molecule 2: DNA-directed RNA polymerase II subunit RPB1



4.2.3 Score per residue for model 3

- Molecule 1: Regulation of nuclear pre-mRNA domain-containing protein 2

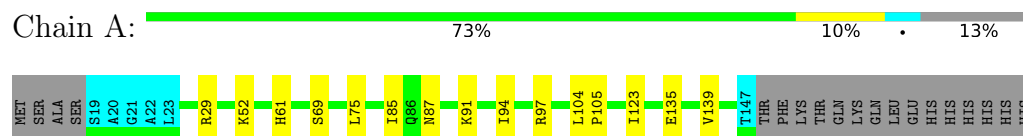


- Molecule 2: DNA-directed RNA polymerase II subunit RPB1



4.2.4 Score per residue for model 4

- Molecule 1: Regulation of nuclear pre-mRNA domain-containing protein 2



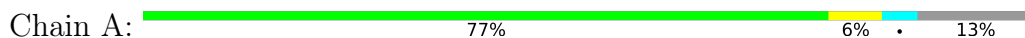
- Molecule 2: DNA-directed RNA polymerase II subunit RPB1





4.2.17 Score per residue for model 17

- Molecule 1: Regulation of nuclear pre-mRNA domain-containing protein 2

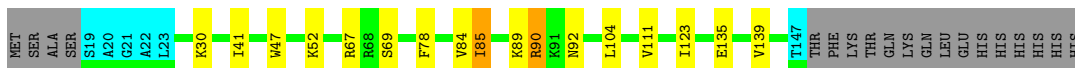


- Molecule 2: DNA-directed RNA polymerase II subunit RPB1

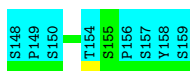


4.2.18 Score per residue for model 18

- Molecule 1: Regulation of nuclear pre-mRNA domain-containing protein 2



- Molecule 2: DNA-directed RNA polymerase II subunit RPB1



4.2.19 Score per residue for model 19

- Molecule 1: Regulation of nuclear pre-mRNA domain-containing protein 2

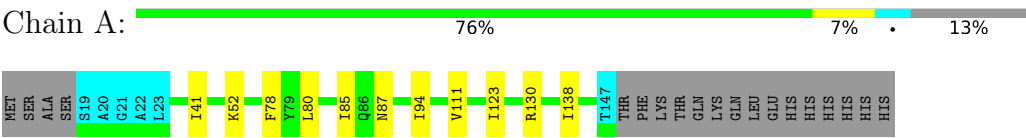


- Molecule 2: DNA-directed RNA polymerase II subunit RPB1



4.2.20 Score per residue for model 20

- Molecule 1: Regulation of nuclear pre-mRNA domain-containing protein 2



- Molecule 2: DNA-directed RNA polymerase II subunit RPB1



5 Refinement protocol and experimental data overview

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

Of the 50 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	
Amber	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	1161
Number of shifts mapped to atoms	1161
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	63%

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: TPO

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.55±0.00	0±0/1044 (0.0± 0.0%)	1.04±0.01	0±0/1412 (0.0± 0.0%)
2	B	0.61±0.02	0±0/32 (0.0± 0.0%)	1.07±0.08	0±0/44 (0.0± 0.0%)
All	All	0.55	0/21520 (0.0%)	1.05	6/29120 (0.0%)

There are no bond-length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	61	HIS	CB-CG-CD2	-5.94	123.48	131.20	19	5
1	A	129	ASP	CA-CB-CG	5.00	117.60	112.60	3	1

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	1019	1018	1018	3±2
2	B	31	26	26	0±0
All	All	21000	20880	20880	60

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 1.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:135:GLU:O	1:A:139:VAL:HG12	0.58	1.98	14	8
1:A:61:HIS:CE1	1:A:65:TRP:HE1	0.55	2.20	19	1
1:A:104:LEU:HD13	1:A:104:LEU:C	0.51	2.30	3	11
1:A:97:ARG:HE	1:A:98:GLU:CD	0.51	2.13	7	2
1:A:62:TRP:CZ2	1:A:81:ALA:HB2	0.51	2.39	1	1
1:A:39:GLU:CD	1:A:39:GLU:H	0.49	2.15	11	2
1:A:118:LYS:HE2	1:A:118:LYS:CA	0.48	2.38	11	1
1:A:97:ARG:HG3	1:A:133:TYR:CE2	0.47	2.45	14	1
1:A:75:LEU:C	1:A:75:LEU:HD13	0.47	2.35	9	10
1:A:62:TRP:CZ3	1:A:63:MET:HE2	0.47	2.44	6	1
1:A:66:LEU:HD13	1:A:66:LEU:C	0.46	2.36	7	1
1:A:92:ASN:C	1:A:94:ILE:H	0.45	2.20	15	1
1:A:30:LYS:HE2	1:A:47:TRP:CD1	0.44	2.47	8	1
1:A:30:LYS:HE2	1:A:47:TRP:CE3	0.44	2.48	18	1
1:A:118:LYS:HE2	1:A:118:LYS:N	0.43	2.28	11	1
1:A:104:LEU:HD12	1:A:141:LEU:HD22	0.43	1.91	5	1
1:A:118:LYS:HE2	1:A:118:LYS:HA	0.43	1.90	11	1
1:A:94:ILE:HG23	1:A:94:ILE:O	0.42	2.15	3	3
1:A:122:ARG:CZ	1:A:122:ARG:HA	0.42	2.45	14	1
2:B:151:TYR:CD2	2:B:151:TYR:C	0.42	2.96	17	1
1:A:123:ILE:HD11	1:A:127:TRP:CZ2	0.42	2.50	8	1
1:A:111:VAL:CG2	1:A:120:VAL:HG21	0.41	2.45	12	1
1:A:38:MET:SD	1:A:38:MET:C	0.41	3.04	11	1
1:A:94:ILE:O	1:A:94:ILE:CG2	0.41	2.68	9	1
1:A:104:LEU:N	1:A:105:PRO:HD2	0.41	2.31	4	1
1:A:39:GLU:N	1:A:39:GLU:CD	0.41	2.78	15	1
1:A:39:GLU:CD	1:A:39:GLU:N	0.41	2.79	19	1
1:A:125:LYS:HZ1	1:A:125:LYS:HA	0.40	1.76	8	1
1:A:85:ILE:HD13	1:A:85:ILE:H	0.40	1.76	18	1
1:A:85:ILE:HG13	1:A:127:TRP:CZ2	0.40	2.52	5	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	123/148 (83%)	108±3 (88±2%)	12±3 (10±2%)	3±1 (3±1%)	6	42
2	B	4/12 (33%)	4±1 (90±15%)	0±0 (5±10%)	0±0 (5±10%)	3	24
All	All	2540/3200 (79%)	2230 (88%)	242 (10%)	68 (3%)	6	41

All 17 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	52	LYS	16
1	A	69	SER	11
1	A	87	ASN	8
1	A	89	LYS	5
1	A	91	LYS	4
1	A	146	SER	4
2	B	155	SER	3
1	A	90	ARG	3
1	A	53	LYS	3
1	A	92	ASN	3
1	A	145	LEU	2
1	A	35	THR	1
1	A	93	ALA	1
2	B	153	PRO	1
1	A	56	SER	1
1	A	84	VAL	1
1	A	39	GLU	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	113/134 (84%)	105±3 (93±3%)	7±2 (6±2%)	18	67
2	B	4/11 (36%)	4±0 (96±9%)	0±0 (4±9%)	30	81
All	All	2327/2900 (80%)	2180 (94%)	147 (6%)	18	67

All 34 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	85	ILE	19
1	A	94	ILE	18
1	A	123	ILE	18
1	A	111	VAL	15
1	A	29	ARG	7
1	A	97	ARG	7
1	A	78	PHE	7
1	A	41	ILE	6
1	A	80	LEU	5
1	A	89	LYS	5
1	A	125	LYS	4
1	A	53	LYS	3
1	A	143	GLU	3
2	B	151	TYR	3
1	A	52	LYS	2
1	A	131	ASN	2
1	A	91	LYS	2
1	A	82	ASN	2
1	A	122	ARG	2
1	A	90	ARG	2
1	A	130	ARG	2
1	A	86	GLN	1
1	A	103	VAL	1
1	A	141	LEU	1
1	A	75	LEU	1
1	A	112	LYS	1
1	A	118	LYS	1
1	A	120	VAL	1
1	A	126	ILE	1
1	A	71	TYR	1
1	A	121	GLU	1
1	A	67	ARG	1
1	A	74	ARG	1
1	A	138	ILE	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	TPO	B	154	2	8,10,11	1.07±0.03	0±0 (0±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	TPO	B	154	2	10,14,16	1.39±0.13	1±1 (11±7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TPO	B	154	2	-	0±0,9,11,13	-

There are no bond-length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	B	154	TPO	CG2-CB-CA	4.02	105.44	113.26	14	15
2	B	154	TPO	O-C-CA	2.25	118.98	124.77	10	2
2	B	154	TPO	O3P-P-O2P	2.09	115.63	107.80	8	4
2	B	154	TPO	OG1-P-O1P	2.08	101.92	109.33	11	1

There are no chirality outliers.

All unique torsion outliers are listed below.

Mol	Chain	Res	Type	Atoms	Models (Total)
2	B	154	TPO	N-CA-CB-OG1	2

There are no ring outliers.

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

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 63% for the well-defined parts and 60% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chemical_shifts_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	1161
Number of shifts mapped to atoms	1161
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	4

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	118	2.09 ± 0.25	Should be checked
$^{13}\text{C}_\beta$	112	3.14 ± 0.09	Should be checked
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	112	1.05 ± 0.37	Should be applied

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 63%, i.e. 1136 atoms were assigned a chemical shift out of a possible 1816. 0 out of 19 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	448/626 (72%)	221/250 (88%)	116/254 (46%)	111/122 (91%)
Sidechain	647/1019 (63%)	428/661 (65%)	219/312 (70%)	0/46 (0%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	41/171 (24%)	37/85 (44%)	0/78 (0%)	4/8 (50%)
Overall	1136/1816 (63%)	686/996 (69%)	335/644 (52%)	115/176 (65%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 60%, i.e. 1161 atoms were assigned a chemical shift out of a possible 1950. 0 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	456/688 (66%)	226/275 (82%)	118/280 (42%)	112/133 (84%)
Sidechain	664/1082 (61%)	442/704 (63%)	222/332 (67%)	0/46 (0%)
Aromatic	41/180 (23%)	37/89 (42%)	0/83 (0%)	4/8 (50%)
Overall	1161/1950 (60%)	705/1068 (66%)	340/695 (49%)	116/187 (62%)

7.1.4 Statistically unusual chemical shifts ⓘ

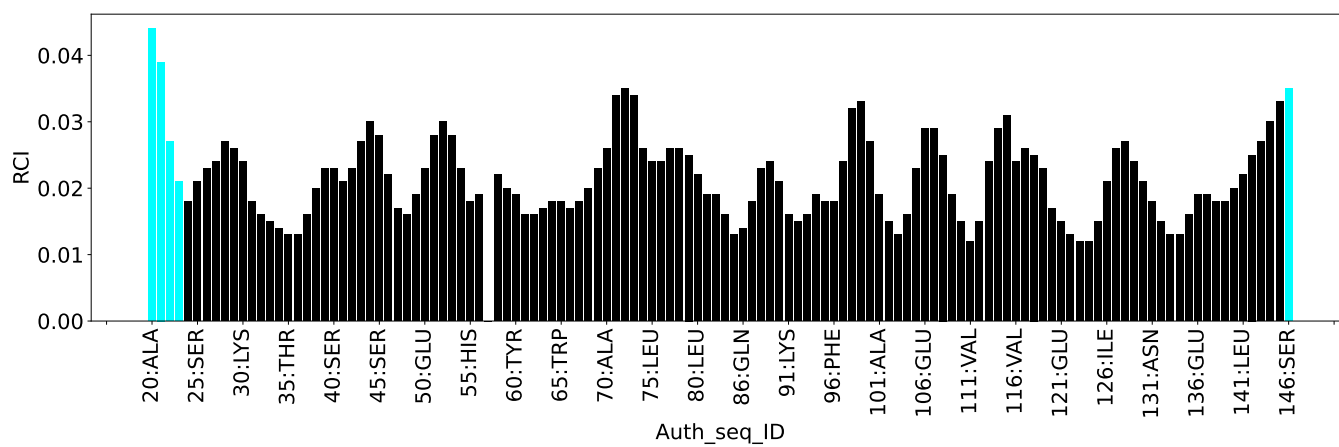
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	113	ASP	HB2	1.16	1.41 – 4.01	-6.0
1	A	120	VAL	HG21	-0.61	-0.58 – 2.19	-5.1
1	A	120	VAL	HG22	-0.61	-0.58 – 2.19	-5.1
1	A	120	VAL	HG23	-0.61	-0.58 – 2.19	-5.1

7.1.5 Random Coil Index (RCI) plots ⓘ

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	1548
Intra-residue ($ i-j =0$)	303
Sequential ($ i-j =1$)	414
Medium range ($ i-j >1$ and $ i-j <5$)	466
Long range ($ i-j \geq 5$)	344
Inter-chain	19
Hydrogen bond restraints	2
Disulfide bond restraints	0
Total dihedral-angle restraints	195
Number of unmapped restraints	0
Number of restraints per residue	10.9
Number of long range restraints per residue ¹	2.1

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)	19.9	0.2
0.2-0.5 (Medium)	17.8	0.5
>0.5 (Large)	16.8	2.22

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)	50.5	10.0
10.0-20.0 (Medium)	11.0	19.99
>20.0 (Large)	3.1	97.45

9 Distance violation analysis ⓘ

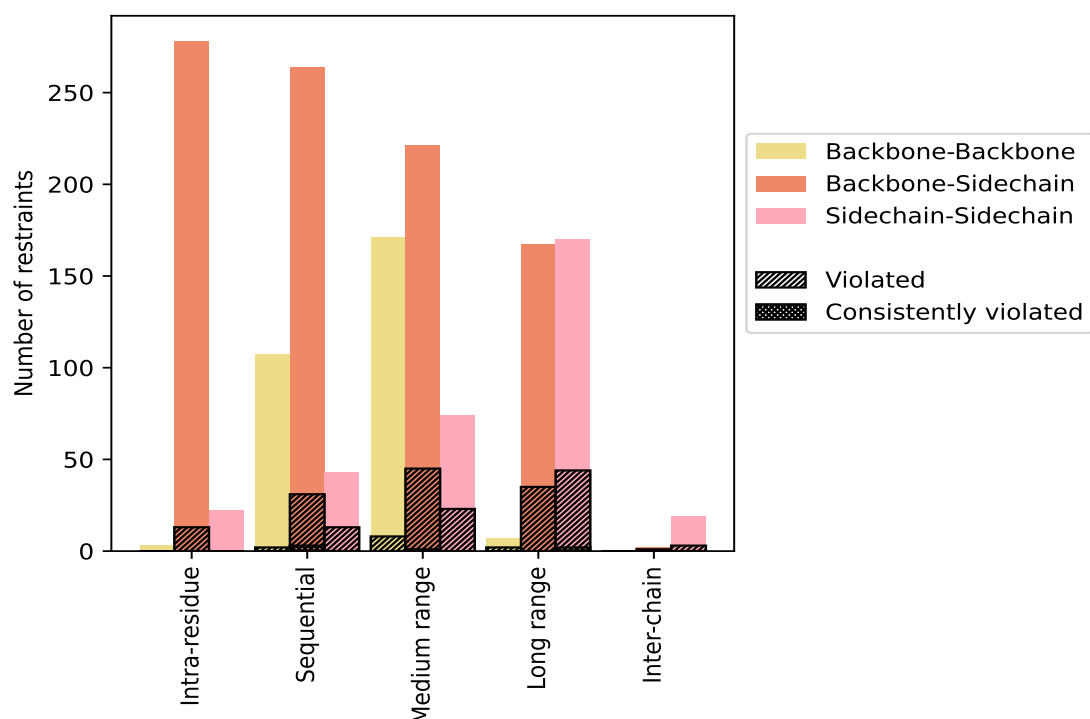
9.1 Summary of distance violations ⓘ

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 ($i-j =0$)	303	19.6	13	4.3	0.8	0	0.0	0.0
Backbone-Backbone	3	0.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	278	18.0	13	4.7	0.8	0	0.0	0.0
Sidechain-Sidechain	22	1.4	0	0.0	0.0	0	0.0	0.0
Sequential ($i-j =1$)	414	26.7	46	11.1	3.0	3	0.7	0.2
Backbone-Backbone	107	6.9	2	1.9	0.1	0	0.0	0.0
Backbone-Sidechain	264	17.1	31	11.7	2.0	3	1.1	0.2
Sidechain-Sidechain	43	2.8	13	30.2	0.8	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	466	30.1	76	16.3	4.9	1	0.2	0.1
Backbone-Backbone	171	11.0	8	4.7	0.5	0	0.0	0.0
Backbone-Sidechain	221	14.3	45	20.4	2.9	1	0.5	0.1
Sidechain-Sidechain	74	4.8	23	31.1	1.5	0	0.0	0.0
Long range ($i-j \geq 5$)	344	22.2	81	23.5	5.2	2	0.6	0.1
Backbone-Backbone	7	0.5	2	28.6	0.1	0	0.0	0.0
Backbone-Sidechain	167	10.8	35	21.0	2.3	0	0.0	0.0
Sidechain-Sidechain	170	11.0	44	25.9	2.8	2	1.2	0.1
Inter-chain	19	1.2	3	15.8	0.2	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	2	0.1	1	50.0	0.1	0	0.0	0.0
Sidechain-Sidechain	17	1.1	2	11.8	0.1	0	0.0	0.0
Hydrogen bond	2	0.1	1	50.0	0.1	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1548	100.0	220	14.2	14.2	6	0.4	0.4
Backbone-Backbone	288	18.6	12	4.2	0.8	0	0.0	0.0
Backbone-Sidechain	932	60.2	125	13.4	8.1	4	0.4	0.3
Sidechain-Sidechain	328	21.2	83	25.3	5.4	2	0.6	0.1

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	0	15	17	23	1	56	0.37	1.78	0.34	0.22
2	2	14	16	13	4	49	0.44	1.44	0.35	0.29
3	1	16	20	32	1	70	0.51	1.9	0.47	0.3
4	1	11	19	20	4	55	0.44	1.41	0.34	0.31
5	2	13	13	28	1	57	0.47	1.81	0.44	0.29
6	1	14	15	19	1	50	0.44	2.22	0.46	0.24
7	2	17	23	21	2	65	0.45	1.86	0.42	0.28
8	1	16	18	12	2	49	0.36	1.41	0.26	0.28
9	3	14	15	29	1	62	0.38	1.53	0.33	0.23
10	0	16	24	14	1	55	0.36	1.43	0.35	0.21

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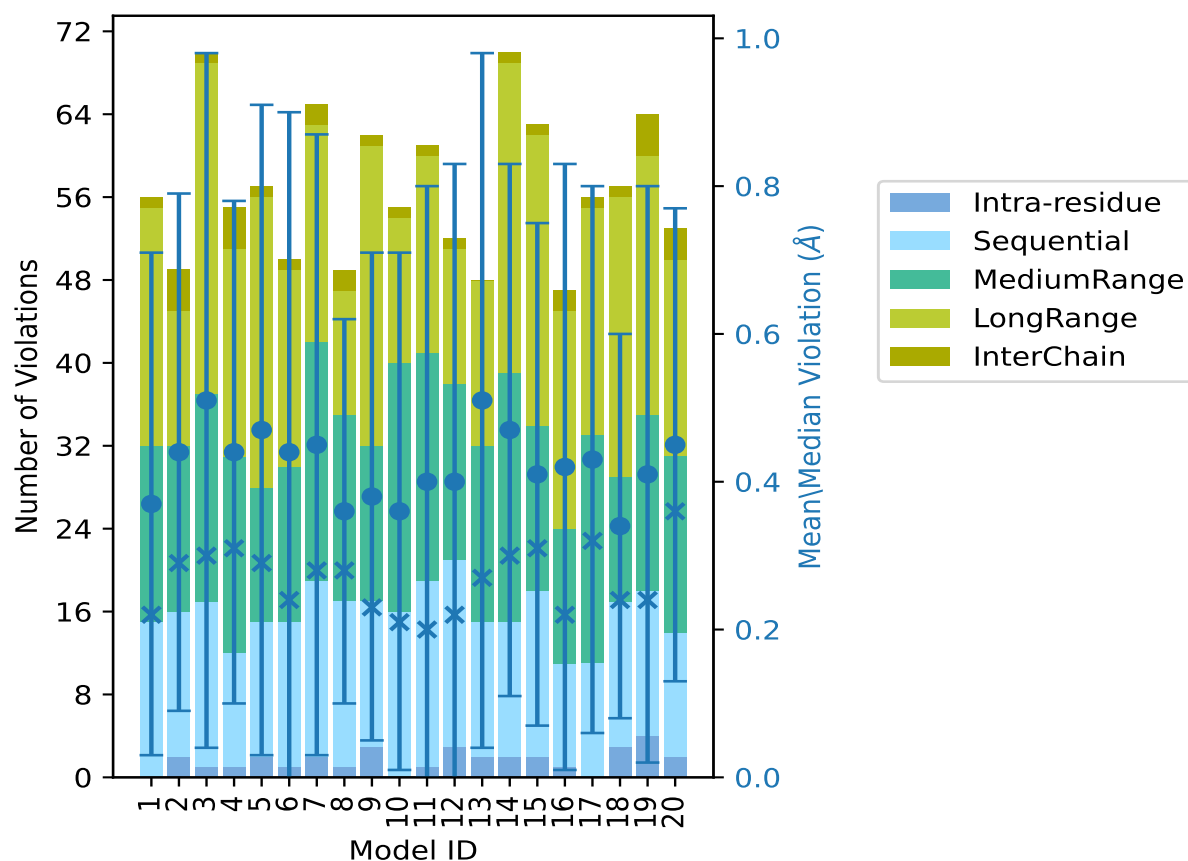
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	1	18	22	19	1	61	0.4	1.83	0.4	0.2
12	3	18	17	13	1	52	0.4	2.2	0.43	0.22
13	2	13	17	16	0	48	0.51	2.07	0.47	0.27
14	2	13	24	30	1	70	0.47	1.57	0.36	0.3
15	2	16	16	28	1	63	0.41	2.16	0.34	0.31
16	1	10	13	21	2	47	0.42	1.83	0.41	0.22
17	0	11	22	22	1	56	0.43	2.09	0.37	0.32
18	3	14	12	27	1	57	0.34	1.27	0.26	0.24
19	4	14	17	25	4	64	0.41	1.67	0.39	0.24
20	2	12	17	19	3	53	0.45	1.45	0.32	0.36

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

⁵Inter-chain restraints, ⁶Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



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

9.3 Distance violation statistics for the ensemble

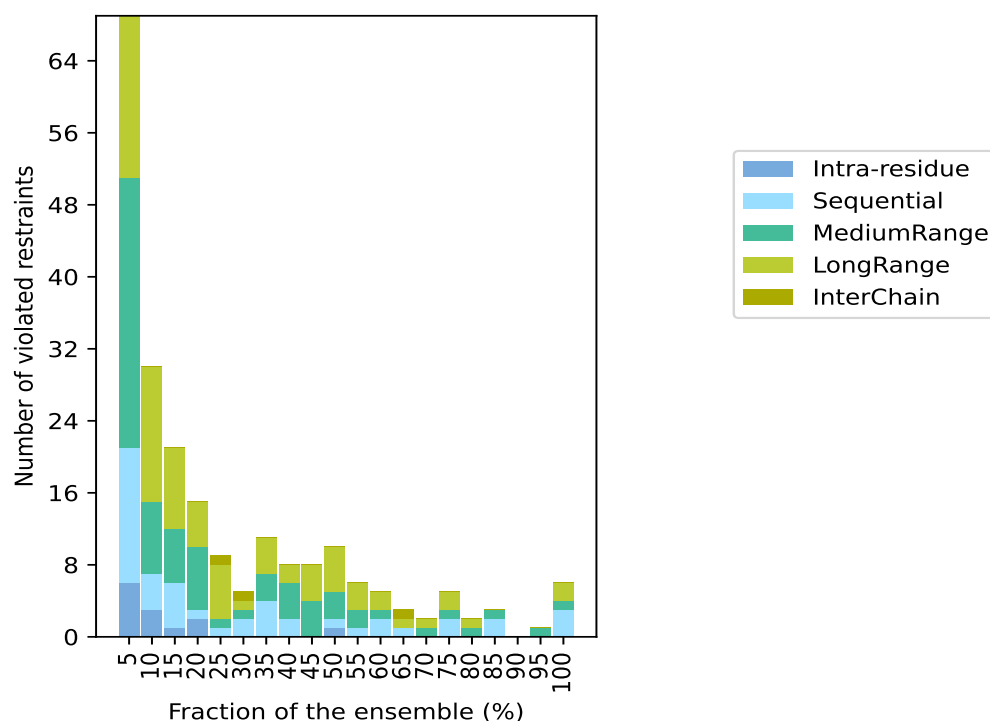
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1327(IR:290, SQ:368, MR:390, LR:263, IC:16) restraints are 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	%
6	15	30	18	0	69	1	5.0
3	4	8	15	0	30	2	10.0
1	5	6	9	0	21	3	15.0
2	1	7	5	0	15	4	20.0
0	1	1	6	1	9	5	25.0
0	2	1	1	1	5	6	30.0
0	4	3	4	0	11	7	35.0
0	2	4	2	0	8	8	40.0
0	0	4	4	0	8	9	45.0
1	1	3	5	0	10	10	50.0
0	1	2	3	0	6	11	55.0
0	2	1	2	0	5	12	60.0
0	1	0	1	1	3	13	65.0
0	0	1	1	0	2	14	70.0
0	2	1	2	0	5	15	75.0
0	0	1	1	0	2	16	80.0
0	2	1	0	0	3	17	85.0
0	0	0	0	0	0	18	90.0
0	0	1	0	0	1	19	95.0
0	3	1	2	0	6	20	100.0

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

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

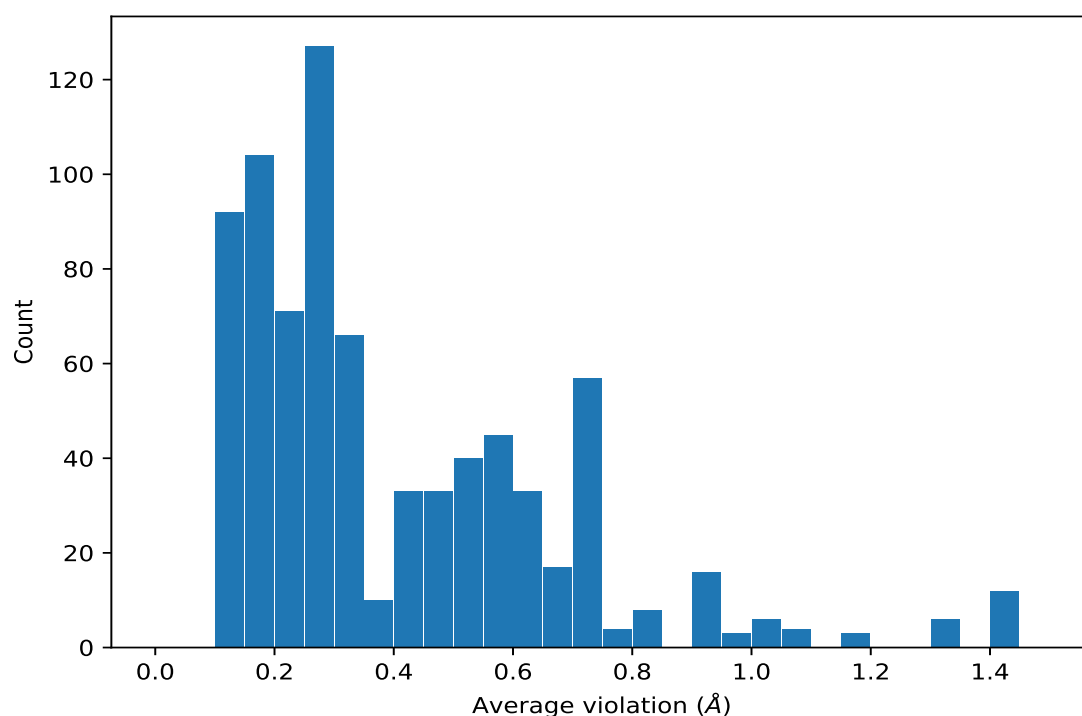
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(6,1)	2:148:B:SER:H1	2:149:B:PRO:HA	20	0.93	0.6	0.61
(1,1403)	1:104:A:LEU:HD11	1:141:A:LEU:HG	20	0.92	0.25	0.94
(1,1403)	1:104:A:LEU:HD12	1:141:A:LEU:HG	20	0.92	0.25	0.94
(1,1403)	1:104:A:LEU:HD13	1:141:A:LEU:HG	20	0.92	0.25	0.94
(1,1403)	1:104:A:LEU:HD21	1:141:A:LEU:HG	20	0.92	0.25	0.94
(1,1403)	1:104:A:LEU:HD22	1:141:A:LEU:HG	20	0.92	0.25	0.94
(1,1403)	1:104:A:LEU:HD23	1:141:A:LEU:HG	20	0.92	0.25	0.94
(1,478)	1:77:A:LEU:HD21	1:78:A:PHE:HA	20	0.5	0.11	0.52
(1,478)	1:77:A:LEU:HD22	1:78:A:PHE:HA	20	0.5	0.11	0.52
(1,478)	1:77:A:LEU:HD23	1:78:A:PHE:HA	20	0.5	0.11	0.52
(1,857)	1:111:A:VAL:HG11	1:112:A:LYS:H	20	0.25	0.09	0.24
(1,857)	1:111:A:VAL:HG12	1:112:A:LYS:H	20	0.25	0.09	0.24
(1,857)	1:111:A:VAL:HG13	1:112:A:LYS:H	20	0.25	0.09	0.24
(1,259)	1:111:A:VAL:HG21	1:124:A:PHE:HB2	20	0.23	0.03	0.23
(1,259)	1:111:A:VAL:HG21	1:124:A:PHE:HB3	20	0.23	0.03	0.23
(1,259)	1:111:A:VAL:HG22	1:124:A:PHE:HB2	20	0.23	0.03	0.23

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,259)	1:111:A:VAL:HG22	1:124:A:PHE:HB3	20	0.23	0.03	0.23
(1,259)	1:111:A:VAL:HG23	1:124:A:PHE:HB2	20	0.23	0.03	0.23
(1,259)	1:111:A:VAL:HG23	1:124:A:PHE:HB3	20	0.23	0.03	0.23
(1,583)	1:48:A:CYS:H	1:51:A:ASN:HB2	20	0.17	0.04	0.18
(1,1203)	1:23:A:LEU:HD11	1:27:A:LEU:HB2	19	1.45	0.56	1.45
(1,1203)	1:23:A:LEU:HD11	1:27:A:LEU:HB3	19	1.45	0.56	1.45
(1,1203)	1:23:A:LEU:HD12	1:27:A:LEU:HB2	19	1.45	0.56	1.45
(1,1203)	1:23:A:LEU:HD12	1:27:A:LEU:HB3	19	1.45	0.56	1.45
(1,1203)	1:23:A:LEU:HD13	1:27:A:LEU:HB2	19	1.45	0.56	1.45
(1,1203)	1:23:A:LEU:HD13	1:27:A:LEU:HB3	19	1.45	0.56	1.45
(1,1203)	1:23:A:LEU:HD21	1:27:A:LEU:HB2	19	1.45	0.56	1.45
(1,1203)	1:23:A:LEU:HD21	1:27:A:LEU:HB3	19	1.45	0.56	1.45
(1,1203)	1:23:A:LEU:HD22	1:27:A:LEU:HB2	19	1.45	0.56	1.45
(1,1203)	1:23:A:LEU:HD22	1:27:A:LEU:HB3	19	1.45	0.56	1.45
(1,1203)	1:23:A:LEU:HD23	1:27:A:LEU:HB2	19	1.45	0.56	1.45
(1,1203)	1:23:A:LEU:HD23	1:27:A:LEU:HB3	19	1.45	0.56	1.45
(6,2)	2:148:B:SER:H1	2:149:B:PRO:HG2	17	0.82	0.39	0.91
(6,2)	2:148:B:SER:H1	2:149:B:PRO:HG3	17	0.82	0.39	0.91
(1,308)	1:103:A:VAL:HG21	1:107:A:ALA:HA	17	0.33	0.25	0.26
(1,308)	1:103:A:VAL:HG22	1:107:A:ALA:HA	17	0.33	0.25	0.26
(1,308)	1:103:A:VAL:HG23	1:107:A:ALA:HA	17	0.33	0.25	0.26
(1,981)	1:112:A:LYS:HB2	1:113:A:ASP:H	17	0.12	0.02	0.12
(1,981)	1:112:A:LYS:HB3	1:113:A:ASP:H	17	0.12	0.02	0.12
(1,1202)	1:23:A:LEU:HD11	1:27:A:LEU:HA	16	1.32	0.42	1.42
(1,1202)	1:23:A:LEU:HD12	1:27:A:LEU:HA	16	1.32	0.42	1.42
(1,1202)	1:23:A:LEU:HD13	1:27:A:LEU:HA	16	1.32	0.42	1.42
(1,1202)	1:23:A:LEU:HD21	1:27:A:LEU:HA	16	1.32	0.42	1.42
(1,1202)	1:23:A:LEU:HD22	1:27:A:LEU:HA	16	1.32	0.42	1.42
(1,1202)	1:23:A:LEU:HD23	1:27:A:LEU:HA	16	1.32	0.42	1.42
(1,648)	1:75:A:LEU:HD11	1:120:A:VAL:H	16	0.76	0.29	0.83
(1,648)	1:75:A:LEU:HD12	1:120:A:VAL:H	16	0.76	0.29	0.83
(1,648)	1:75:A:LEU:HD13	1:120:A:VAL:H	16	0.76	0.29	0.83
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD11	15	0.5	0.39	0.38
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD12	15	0.5	0.39	0.38
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD13	15	0.5	0.39	0.38
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD21	15	0.5	0.39	0.38
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD22	15	0.5	0.39	0.38
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD23	15	0.5	0.39	0.38
(1,574)	1:108:A:ALA:H	1:111:A:VAL:HG11	15	0.34	0.27	0.22
(1,574)	1:108:A:ALA:H	1:111:A:VAL:HG12	15	0.34	0.27	0.22
(1,574)	1:108:A:ALA:H	1:111:A:VAL:HG13	15	0.34	0.27	0.22
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD11	15	0.22	0.07	0.21

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD12	15	0.22	0.07	0.21
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD13	15	0.22	0.07	0.21
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD21	15	0.22	0.07	0.21
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD22	15	0.22	0.07	0.21
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD23	15	0.22	0.07	0.21
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD11	15	0.22	0.07	0.21
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD12	15	0.22	0.07	0.21
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD13	15	0.22	0.07	0.21
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD21	15	0.22	0.07	0.21
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD22	15	0.22	0.07	0.21
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD23	15	0.22	0.07	0.21
(1,252)	1:111:A:VAL:HG21	1:121:A:GLU:H	15	0.17	0.04	0.16
(1,252)	1:111:A:VAL:HG22	1:121:A:GLU:H	15	0.17	0.04	0.16
(1,252)	1:111:A:VAL:HG23	1:121:A:GLU:H	15	0.17	0.04	0.16
(1,656)	1:50:A:GLU:H	1:51:A:ASN:HD21	15	0.14	0.03	0.13
(1,359)	1:75:A:LEU:HD11	1:119:A:SER:HA	14	0.59	0.32	0.74
(1,359)	1:75:A:LEU:HD12	1:119:A:SER:HA	14	0.59	0.32	0.74
(1,359)	1:75:A:LEU:HD13	1:119:A:SER:HA	14	0.59	0.32	0.74
(1,771)	1:76:A:ASN:H	1:78:A:PHE:HB2	14	0.13	0.02	0.12
(2,12)	2:158:B:TYR:HD1	1:132:A:VAL:HG11	13	1.01	0.57	0.89
(2,12)	2:158:B:TYR:HD1	1:132:A:VAL:HG12	13	1.01	0.57	0.89
(2,12)	2:158:B:TYR:HD1	1:132:A:VAL:HG13	13	1.01	0.57	0.89
(2,12)	2:158:B:TYR:HD2	1:132:A:VAL:HG11	13	1.01	0.57	0.89
(2,12)	2:158:B:TYR:HD2	1:132:A:VAL:HG12	13	1.01	0.57	0.89
(2,12)	2:158:B:TYR:HD2	1:132:A:VAL:HG13	13	1.01	0.57	0.89
(1,83)	1:137:A:MET:HB3	1:138:A:ILE:HD11	13	0.43	0.18	0.42
(1,83)	1:137:A:MET:HB3	1:138:A:ILE:HD12	13	0.43	0.18	0.42
(1,83)	1:137:A:MET:HB3	1:138:A:ILE:HD13	13	0.43	0.18	0.42
(1,134)	1:59:A:VAL:HB	1:103:A:VAL:HG21	13	0.42	0.13	0.45
(1,134)	1:59:A:VAL:HB	1:103:A:VAL:HG22	13	0.42	0.13	0.45
(1,134)	1:59:A:VAL:HB	1:103:A:VAL:HG23	13	0.42	0.13	0.45
(1,1432)	1:113:A:ASP:H	1:145:A:LEU:HD11	12	0.72	0.37	0.8
(1,1432)	1:113:A:ASP:H	1:145:A:LEU:HD12	12	0.72	0.37	0.8
(1,1432)	1:113:A:ASP:H	1:145:A:LEU:HD13	12	0.72	0.37	0.8
(1,1432)	1:113:A:ASP:H	1:145:A:LEU:HD21	12	0.72	0.37	0.8
(1,1432)	1:113:A:ASP:H	1:145:A:LEU:HD22	12	0.72	0.37	0.8
(1,1432)	1:113:A:ASP:H	1:145:A:LEU:HD23	12	0.72	0.37	0.8
(6,3)	2:148:B:SER:H1	2:149:B:PRO:HB2	12	0.7	0.27	0.75
(6,3)	2:148:B:SER:H1	2:149:B:PRO:HB3	12	0.7	0.27	0.75
(1,438)	1:58:A:ILE:HG21	1:59:A:VAL:HG11	12	0.55	0.1	0.59
(1,438)	1:58:A:ILE:HG21	1:59:A:VAL:HG12	12	0.55	0.1	0.59
(1,438)	1:58:A:ILE:HG21	1:59:A:VAL:HG13	12	0.55	0.1	0.59

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,438)	1:58:A:ILE:HG22	1:59:A:VAL:HG11	12	0.55	0.1	0.59
(1,438)	1:58:A:ILE:HG22	1:59:A:VAL:HG12	12	0.55	0.1	0.59
(1,438)	1:58:A:ILE:HG22	1:59:A:VAL:HG13	12	0.55	0.1	0.59
(1,438)	1:58:A:ILE:HG23	1:59:A:VAL:HG11	12	0.55	0.1	0.59
(1,438)	1:58:A:ILE:HG23	1:59:A:VAL:HG12	12	0.55	0.1	0.59
(1,438)	1:58:A:ILE:HG23	1:59:A:VAL:HG13	12	0.55	0.1	0.59
(1,442)	1:75:A:LEU:HD11	1:78:A:PHE:HB3	12	0.34	0.17	0.31
(1,442)	1:75:A:LEU:HD12	1:78:A:PHE:HB3	12	0.34	0.17	0.31
(1,442)	1:75:A:LEU:HD13	1:78:A:PHE:HB3	12	0.34	0.17	0.31
(1,847)	1:49:A:ILE:H	1:84:A:VAL:HG11	12	0.17	0.06	0.17
(1,847)	1:49:A:ILE:H	1:84:A:VAL:HG12	12	0.17	0.06	0.17
(1,847)	1:49:A:ILE:H	1:84:A:VAL:HG13	12	0.17	0.06	0.17
(1,293)	1:31:A:PHE:HA	1:34:A:VAL:HG11	11	0.8	0.42	0.65
(1,293)	1:31:A:PHE:HA	1:34:A:VAL:HG12	11	0.8	0.42	0.65
(1,293)	1:31:A:PHE:HA	1:34:A:VAL:HG13	11	0.8	0.42	0.65
(1,1422)	1:112:A:LYS:H	1:145:A:LEU:HD11	11	0.74	0.37	0.82
(1,1422)	1:112:A:LYS:H	1:145:A:LEU:HD12	11	0.74	0.37	0.82
(1,1422)	1:112:A:LYS:H	1:145:A:LEU:HD13	11	0.74	0.37	0.82
(1,1422)	1:112:A:LYS:H	1:145:A:LEU:HD21	11	0.74	0.37	0.82
(1,1422)	1:112:A:LYS:H	1:145:A:LEU:HD22	11	0.74	0.37	0.82
(1,1422)	1:112:A:LYS:H	1:145:A:LEU:HD23	11	0.74	0.37	0.82
(1,1447)	1:116:A:VAL:HG11	1:118:A:LYS:HG2	11	0.59	0.16	0.65
(1,1447)	1:116:A:VAL:HG11	1:118:A:LYS:HG3	11	0.59	0.16	0.65
(1,1447)	1:116:A:VAL:HG12	1:118:A:LYS:HG2	11	0.59	0.16	0.65
(1,1447)	1:116:A:VAL:HG12	1:118:A:LYS:HG3	11	0.59	0.16	0.65
(1,1447)	1:116:A:VAL:HG13	1:118:A:LYS:HG2	11	0.59	0.16	0.65
(1,1447)	1:116:A:VAL:HG13	1:118:A:LYS:HG3	11	0.59	0.16	0.65
(1,1447)	1:116:A:VAL:HG21	1:118:A:LYS:HG2	11	0.59	0.16	0.65
(1,1447)	1:116:A:VAL:HG21	1:118:A:LYS:HG3	11	0.59	0.16	0.65
(1,1447)	1:116:A:VAL:HG22	1:118:A:LYS:HG2	11	0.59	0.16	0.65
(1,1447)	1:116:A:VAL:HG22	1:118:A:LYS:HG3	11	0.59	0.16	0.65
(1,1447)	1:116:A:VAL:HG23	1:118:A:LYS:HG2	11	0.59	0.16	0.65
(1,1447)	1:116:A:VAL:HG23	1:118:A:LYS:HG3	11	0.59	0.16	0.65
(1,461)	1:101:A:ALA:HB1	1:137:A:MET:HB2	11	0.41	0.17	0.42
(1,461)	1:101:A:ALA:HB2	1:137:A:MET:HB2	11	0.41	0.17	0.42
(1,461)	1:101:A:ALA:HB3	1:137:A:MET:HB2	11	0.41	0.17	0.42
(1,1320)	1:75:A:LEU:HD11	1:111:A:VAL:HG11	11	0.31	0.13	0.37
(1,1320)	1:75:A:LEU:HD11	1:111:A:VAL:HG12	11	0.31	0.13	0.37
(1,1320)	1:75:A:LEU:HD11	1:111:A:VAL:HG13	11	0.31	0.13	0.37
(1,1320)	1:75:A:LEU:HD12	1:111:A:VAL:HG11	11	0.31	0.13	0.37
(1,1320)	1:75:A:LEU:HD12	1:111:A:VAL:HG12	11	0.31	0.13	0.37
(1,1320)	1:75:A:LEU:HD12	1:111:A:VAL:HG13	11	0.31	0.13	0.37

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1320)	1:75:A:LEU:HD13	1:111:A:VAL:HG11	11	0.31	0.13	0.37
(1,1320)	1:75:A:LEU:HD13	1:111:A:VAL:HG12	11	0.31	0.13	0.37
(1,1320)	1:75:A:LEU:HD13	1:111:A:VAL:HG13	11	0.31	0.13	0.37
(1,1320)	1:75:A:LEU:HD21	1:111:A:VAL:HG11	11	0.31	0.13	0.37
(1,1320)	1:75:A:LEU:HD21	1:111:A:VAL:HG12	11	0.31	0.13	0.37
(1,1320)	1:75:A:LEU:HD21	1:111:A:VAL:HG13	11	0.31	0.13	0.37
(1,1320)	1:75:A:LEU:HD22	1:111:A:VAL:HG11	11	0.31	0.13	0.37
(1,1320)	1:75:A:LEU:HD22	1:111:A:VAL:HG12	11	0.31	0.13	0.37
(1,1320)	1:75:A:LEU:HD22	1:111:A:VAL:HG13	11	0.31	0.13	0.37
(1,1320)	1:75:A:LEU:HD23	1:111:A:VAL:HG11	11	0.31	0.13	0.37
(1,1320)	1:75:A:LEU:HD23	1:111:A:VAL:HG12	11	0.31	0.13	0.37
(1,1320)	1:75:A:LEU:HD23	1:111:A:VAL:HG13	11	0.31	0.13	0.37
(1,1511)	1:140:A:ALA:H	1:141:A:LEU:HD11	11	0.17	0.06	0.15
(1,1511)	1:140:A:ALA:H	1:141:A:LEU:HD12	11	0.17	0.06	0.15
(1,1511)	1:140:A:ALA:H	1:141:A:LEU:HD13	11	0.17	0.06	0.15
(1,1511)	1:140:A:ALA:H	1:141:A:LEU:HD21	11	0.17	0.06	0.15
(1,1511)	1:140:A:ALA:H	1:141:A:LEU:HD22	11	0.17	0.06	0.15
(1,1511)	1:140:A:ALA:H	1:141:A:LEU:HD23	11	0.17	0.06	0.15
(1,454)	1:116:A:VAL:HG11	1:118:A:LYS:HG2	10	0.73	0.07	0.72
(1,454)	1:116:A:VAL:HG11	1:118:A:LYS:HG3	10	0.73	0.07	0.72
(1,454)	1:116:A:VAL:HG12	1:118:A:LYS:HG2	10	0.73	0.07	0.72
(1,454)	1:116:A:VAL:HG12	1:118:A:LYS:HG3	10	0.73	0.07	0.72
(1,454)	1:116:A:VAL:HG13	1:118:A:LYS:HG2	10	0.73	0.07	0.72
(1,454)	1:116:A:VAL:HG13	1:118:A:LYS:HG3	10	0.73	0.07	0.72
(1,1229)	1:45:A:SER:HB2	1:80:A:LEU:HD11	10	0.64	0.34	0.48
(1,1229)	1:45:A:SER:HB2	1:80:A:LEU:HD12	10	0.64	0.34	0.48
(1,1229)	1:45:A:SER:HB2	1:80:A:LEU:HD13	10	0.64	0.34	0.48
(1,1229)	1:45:A:SER:HB2	1:80:A:LEU:HD21	10	0.64	0.34	0.48
(1,1229)	1:45:A:SER:HB2	1:80:A:LEU:HD22	10	0.64	0.34	0.48
(1,1229)	1:45:A:SER:HB2	1:80:A:LEU:HD23	10	0.64	0.34	0.48
(1,1229)	1:45:A:SER:HB3	1:80:A:LEU:HD11	10	0.64	0.34	0.48
(1,1229)	1:45:A:SER:HB3	1:80:A:LEU:HD12	10	0.64	0.34	0.48
(1,1229)	1:45:A:SER:HB3	1:80:A:LEU:HD13	10	0.64	0.34	0.48
(1,1229)	1:45:A:SER:HB3	1:80:A:LEU:HD21	10	0.64	0.34	0.48
(1,1229)	1:45:A:SER:HB3	1:80:A:LEU:HD22	10	0.64	0.34	0.48
(1,1229)	1:45:A:SER:HB3	1:80:A:LEU:HD23	10	0.64	0.34	0.48
(1,1427)	1:112:A:LYS:HB2	1:145:A:LEU:HD11	10	0.62	0.31	0.64
(1,1427)	1:112:A:LYS:HB2	1:145:A:LEU:HD12	10	0.62	0.31	0.64
(1,1427)	1:112:A:LYS:HB2	1:145:A:LEU:HD13	10	0.62	0.31	0.64
(1,1427)	1:112:A:LYS:HB2	1:145:A:LEU:HD21	10	0.62	0.31	0.64
(1,1427)	1:112:A:LYS:HB2	1:145:A:LEU:HD22	10	0.62	0.31	0.64
(1,1427)	1:112:A:LYS:HB2	1:145:A:LEU:HD23	10	0.62	0.31	0.64

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1427)	1:112:A:LYS:HB3	1:145:A:LEU:HD11	10	0.62	0.31	0.64
(1,1427)	1:112:A:LYS:HB3	1:145:A:LEU:HD12	10	0.62	0.31	0.64
(1,1427)	1:112:A:LYS:HB3	1:145:A:LEU:HD13	10	0.62	0.31	0.64
(1,1427)	1:112:A:LYS:HB3	1:145:A:LEU:HD21	10	0.62	0.31	0.64
(1,1427)	1:112:A:LYS:HB3	1:145:A:LEU:HD22	10	0.62	0.31	0.64
(1,1427)	1:112:A:LYS:HB3	1:145:A:LEU:HD23	10	0.62	0.31	0.64
(1,204)	1:59:A:VAL:HA	1:103:A:VAL:HG11	10	0.59	0.39	0.54
(1,204)	1:59:A:VAL:HA	1:103:A:VAL:HG12	10	0.59	0.39	0.54
(1,204)	1:59:A:VAL:HA	1:103:A:VAL:HG13	10	0.59	0.39	0.54
(1,14)	1:116:A:VAL:HG21	1:118:A:LYS:HG2	10	0.52	0.04	0.52
(1,14)	1:116:A:VAL:HG21	1:118:A:LYS:HG3	10	0.52	0.04	0.52
(1,14)	1:116:A:VAL:HG22	1:118:A:LYS:HG2	10	0.52	0.04	0.52
(1,14)	1:116:A:VAL:HG22	1:118:A:LYS:HG3	10	0.52	0.04	0.52
(1,14)	1:116:A:VAL:HG23	1:118:A:LYS:HG2	10	0.52	0.04	0.52
(1,14)	1:116:A:VAL:HG23	1:118:A:LYS:HG3	10	0.52	0.04	0.52
(1,1288)	1:63:A:MET:H	1:77:A:LEU:HD11	10	0.43	0.28	0.32
(1,1288)	1:63:A:MET:H	1:77:A:LEU:HD12	10	0.43	0.28	0.32
(1,1288)	1:63:A:MET:H	1:77:A:LEU:HD13	10	0.43	0.28	0.32
(1,1288)	1:63:A:MET:H	1:77:A:LEU:HD21	10	0.43	0.28	0.32
(1,1288)	1:63:A:MET:H	1:77:A:LEU:HD22	10	0.43	0.28	0.32
(1,1288)	1:63:A:MET:H	1:77:A:LEU:HD23	10	0.43	0.28	0.32
(1,1285)	1:62:A:TRP:HE1	1:77:A:LEU:HD11	10	0.28	0.09	0.28
(1,1285)	1:62:A:TRP:HE1	1:77:A:LEU:HD12	10	0.28	0.09	0.28
(1,1285)	1:62:A:TRP:HE1	1:77:A:LEU:HD13	10	0.28	0.09	0.28
(1,1285)	1:62:A:TRP:HE1	1:77:A:LEU:HD21	10	0.28	0.09	0.28
(1,1285)	1:62:A:TRP:HE1	1:77:A:LEU:HD22	10	0.28	0.09	0.28
(1,1285)	1:62:A:TRP:HE1	1:77:A:LEU:HD23	10	0.28	0.09	0.28
(1,1487)	1:132:A:VAL:HG11	1:133:A:TYR:H	10	0.18	0.04	0.18
(1,1487)	1:132:A:VAL:HG12	1:133:A:TYR:H	10	0.18	0.04	0.18
(1,1487)	1:132:A:VAL:HG13	1:133:A:TYR:H	10	0.18	0.04	0.18
(1,1487)	1:132:A:VAL:HG21	1:133:A:TYR:H	10	0.18	0.04	0.18
(1,1487)	1:132:A:VAL:HG22	1:133:A:TYR:H	10	0.18	0.04	0.18
(1,1487)	1:132:A:VAL:HG23	1:133:A:TYR:H	10	0.18	0.04	0.18
(1,719)	1:109:A:ALA:H	1:112:A:LYS:H	10	0.15	0.04	0.15
(1,537)	1:32:A:GLN:H	1:32:A:GLN:HB3	10	0.11	0.0	0.11
(4,1)	2:151:B:TYR:HH	1:82:A:ASN:ND2	9	0.76	0.33	0.96
(1,1410)	1:108:A:ALA:HB1	1:145:A:LEU:HD11	9	0.73	0.38	0.65
(1,1410)	1:108:A:ALA:HB1	1:145:A:LEU:HD12	9	0.73	0.38	0.65
(1,1410)	1:108:A:ALA:HB1	1:145:A:LEU:HD13	9	0.73	0.38	0.65
(1,1410)	1:108:A:ALA:HB1	1:145:A:LEU:HD21	9	0.73	0.38	0.65
(1,1410)	1:108:A:ALA:HB1	1:145:A:LEU:HD22	9	0.73	0.38	0.65
(1,1410)	1:108:A:ALA:HB1	1:145:A:LEU:HD23	9	0.73	0.38	0.65

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1410)	1:108:A:ALA:HB2	1:145:A:LEU:HD11	9	0.73	0.38	0.65
(1,1410)	1:108:A:ALA:HB2	1:145:A:LEU:HD12	9	0.73	0.38	0.65
(1,1410)	1:108:A:ALA:HB2	1:145:A:LEU:HD13	9	0.73	0.38	0.65
(1,1410)	1:108:A:ALA:HB2	1:145:A:LEU:HD21	9	0.73	0.38	0.65
(1,1410)	1:108:A:ALA:HB2	1:145:A:LEU:HD22	9	0.73	0.38	0.65
(1,1410)	1:108:A:ALA:HB2	1:145:A:LEU:HD23	9	0.73	0.38	0.65
(1,1410)	1:108:A:ALA:HB3	1:145:A:LEU:HD11	9	0.73	0.38	0.65
(1,1410)	1:108:A:ALA:HB3	1:145:A:LEU:HD12	9	0.73	0.38	0.65
(1,1410)	1:108:A:ALA:HB3	1:145:A:LEU:HD13	9	0.73	0.38	0.65
(1,1410)	1:108:A:ALA:HB3	1:145:A:LEU:HD21	9	0.73	0.38	0.65
(1,1410)	1:108:A:ALA:HB3	1:145:A:LEU:HD22	9	0.73	0.38	0.65
(1,1410)	1:108:A:ALA:HB3	1:145:A:LEU:HD23	9	0.73	0.38	0.65
(1,838)	1:31:A:PHE:H	1:34:A:VAL:HG21	9	0.57	0.14	0.58
(1,838)	1:31:A:PHE:H	1:34:A:VAL:HG22	9	0.57	0.14	0.58
(1,838)	1:31:A:PHE:H	1:34:A:VAL:HG23	9	0.57	0.14	0.58
(1,1276)	1:59:A:VAL:HG11	1:103:A:VAL:H	9	0.49	0.25	0.42
(1,1276)	1:59:A:VAL:HG12	1:103:A:VAL:H	9	0.49	0.25	0.42
(1,1276)	1:59:A:VAL:HG13	1:103:A:VAL:H	9	0.49	0.25	0.42
(1,1276)	1:59:A:VAL:HG21	1:103:A:VAL:H	9	0.49	0.25	0.42
(1,1276)	1:59:A:VAL:HG22	1:103:A:VAL:H	9	0.49	0.25	0.42
(1,1276)	1:59:A:VAL:HG23	1:103:A:VAL:H	9	0.49	0.25	0.42
(1,1275)	1:59:A:VAL:HG11	1:102:A:ASP:H	9	0.29	0.13	0.29
(1,1275)	1:59:A:VAL:HG12	1:102:A:ASP:H	9	0.29	0.13	0.29
(1,1275)	1:59:A:VAL:HG13	1:102:A:ASP:H	9	0.29	0.13	0.29
(1,1275)	1:59:A:VAL:HG21	1:102:A:ASP:H	9	0.29	0.13	0.29
(1,1275)	1:59:A:VAL:HG22	1:102:A:ASP:H	9	0.29	0.13	0.29
(1,1275)	1:59:A:VAL:HG23	1:102:A:ASP:H	9	0.29	0.13	0.29
(1,1450)	1:116:A:VAL:HG11	1:120:A:VAL:HG11	9	0.27	0.18	0.24
(1,1450)	1:116:A:VAL:HG11	1:120:A:VAL:HG12	9	0.27	0.18	0.24
(1,1450)	1:116:A:VAL:HG11	1:120:A:VAL:HG13	9	0.27	0.18	0.24
(1,1450)	1:116:A:VAL:HG11	1:120:A:VAL:HG21	9	0.27	0.18	0.24
(1,1450)	1:116:A:VAL:HG11	1:120:A:VAL:HG22	9	0.27	0.18	0.24
(1,1450)	1:116:A:VAL:HG11	1:120:A:VAL:HG23	9	0.27	0.18	0.24
(1,1450)	1:116:A:VAL:HG12	1:120:A:VAL:HG11	9	0.27	0.18	0.24
(1,1450)	1:116:A:VAL:HG12	1:120:A:VAL:HG12	9	0.27	0.18	0.24
(1,1450)	1:116:A:VAL:HG12	1:120:A:VAL:HG13	9	0.27	0.18	0.24
(1,1450)	1:116:A:VAL:HG12	1:120:A:VAL:HG21	9	0.27	0.18	0.24
(1,1450)	1:116:A:VAL:HG12	1:120:A:VAL:HG22	9	0.27	0.18	0.24
(1,1450)	1:116:A:VAL:HG12	1:120:A:VAL:HG23	9	0.27	0.18	0.24
(1,1450)	1:116:A:VAL:HG13	1:120:A:VAL:HG11	9	0.27	0.18	0.24
(1,1450)	1:116:A:VAL:HG13	1:120:A:VAL:HG12	9	0.27	0.18	0.24
(1,1450)	1:116:A:VAL:HG13	1:120:A:VAL:HG13	9	0.27	0.18	0.24

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1450)	1:116:A:VAL:HG13	1:120:A:VAL:HG21	9	0.27	0.18	0.24
(1,1450)	1:116:A:VAL:HG13	1:120:A:VAL:HG22	9	0.27	0.18	0.24
(1,1450)	1:116:A:VAL:HG13	1:120:A:VAL:HG23	9	0.27	0.18	0.24
(1,1450)	1:116:A:VAL:HG21	1:120:A:VAL:HG11	9	0.27	0.18	0.24
(1,1450)	1:116:A:VAL:HG21	1:120:A:VAL:HG12	9	0.27	0.18	0.24
(1,1450)	1:116:A:VAL:HG21	1:120:A:VAL:HG13	9	0.27	0.18	0.24
(1,1450)	1:116:A:VAL:HG21	1:120:A:VAL:HG21	9	0.27	0.18	0.24
(1,1450)	1:116:A:VAL:HG21	1:120:A:VAL:HG22	9	0.27	0.18	0.24
(1,1450)	1:116:A:VAL:HG21	1:120:A:VAL:HG23	9	0.27	0.18	0.24
(1,1450)	1:116:A:VAL:HG22	1:120:A:VAL:HG11	9	0.27	0.18	0.24
(1,1450)	1:116:A:VAL:HG22	1:120:A:VAL:HG12	9	0.27	0.18	0.24
(1,1450)	1:116:A:VAL:HG22	1:120:A:VAL:HG13	9	0.27	0.18	0.24
(1,1450)	1:116:A:VAL:HG22	1:120:A:VAL:HG21	9	0.27	0.18	0.24
(1,1450)	1:116:A:VAL:HG22	1:120:A:VAL:HG22	9	0.27	0.18	0.24
(1,1450)	1:116:A:VAL:HG22	1:120:A:VAL:HG23	9	0.27	0.18	0.24
(1,1450)	1:116:A:VAL:HG23	1:120:A:VAL:HG11	9	0.27	0.18	0.24
(1,1450)	1:116:A:VAL:HG23	1:120:A:VAL:HG12	9	0.27	0.18	0.24
(1,1450)	1:116:A:VAL:HG23	1:120:A:VAL:HG13	9	0.27	0.18	0.24
(1,1450)	1:116:A:VAL:HG23	1:120:A:VAL:HG21	9	0.27	0.18	0.24
(1,1450)	1:116:A:VAL:HG23	1:120:A:VAL:HG22	9	0.27	0.18	0.24
(1,1450)	1:116:A:VAL:HG23	1:120:A:VAL:HG23	9	0.27	0.18	0.24
(1,950)	1:103:A:VAL:HG21	1:107:A:ALA:H	9	0.26	0.29	0.16
(1,950)	1:103:A:VAL:HG22	1:107:A:ALA:H	9	0.26	0.29	0.16
(1,950)	1:103:A:VAL:HG23	1:107:A:ALA:H	9	0.26	0.29	0.16
(1,1189)	1:62:A:TRP:HE1	1:77:A:LEU:HD21	9	0.23	0.08	0.22
(1,1189)	1:62:A:TRP:HE1	1:77:A:LEU:HD22	9	0.23	0.08	0.22
(1,1189)	1:62:A:TRP:HE1	1:77:A:LEU:HD23	9	0.23	0.08	0.22
(1,296)	1:34:A:VAL:HG11	1:36:A:ASN:H	9	0.19	0.07	0.19
(1,296)	1:34:A:VAL:HG12	1:36:A:ASN:H	9	0.19	0.07	0.19
(1,296)	1:34:A:VAL:HG13	1:36:A:ASN:H	9	0.19	0.07	0.19
(1,1277)	1:59:A:VAL:HG11	1:103:A:VAL:HA	8	0.46	0.25	0.45
(1,1277)	1:59:A:VAL:HG12	1:103:A:VAL:HA	8	0.46	0.25	0.45
(1,1277)	1:59:A:VAL:HG13	1:103:A:VAL:HA	8	0.46	0.25	0.45
(1,1277)	1:59:A:VAL:HG21	1:103:A:VAL:HA	8	0.46	0.25	0.45
(1,1277)	1:59:A:VAL:HG22	1:103:A:VAL:HA	8	0.46	0.25	0.45
(1,1277)	1:59:A:VAL:HG23	1:103:A:VAL:HA	8	0.46	0.25	0.45
(1,313)	1:34:A:VAL:HG21	1:35:A:THR:HG21	8	0.45	0.1	0.43
(1,313)	1:34:A:VAL:HG21	1:35:A:THR:HG22	8	0.45	0.1	0.43
(1,313)	1:34:A:VAL:HG21	1:35:A:THR:HG23	8	0.45	0.1	0.43
(1,313)	1:34:A:VAL:HG22	1:35:A:THR:HG21	8	0.45	0.1	0.43
(1,313)	1:34:A:VAL:HG22	1:35:A:THR:HG22	8	0.45	0.1	0.43
(1,313)	1:34:A:VAL:HG22	1:35:A:THR:HG23	8	0.45	0.1	0.43

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,313)	1:34:A:VAL:HG23	1:35:A:THR:HG21	8	0.45	0.1	0.43
(1,313)	1:34:A:VAL:HG23	1:35:A:THR:HG22	8	0.45	0.1	0.43
(1,313)	1:34:A:VAL:HG23	1:35:A:THR:HG23	8	0.45	0.1	0.43
(1,279)	1:77:A:LEU:HD21	1:107:A:ALA:HB1	8	0.31	0.14	0.3
(1,279)	1:77:A:LEU:HD21	1:107:A:ALA:HB2	8	0.31	0.14	0.3
(1,279)	1:77:A:LEU:HD21	1:107:A:ALA:HB3	8	0.31	0.14	0.3
(1,279)	1:77:A:LEU:HD22	1:107:A:ALA:HB1	8	0.31	0.14	0.3
(1,279)	1:77:A:LEU:HD22	1:107:A:ALA:HB2	8	0.31	0.14	0.3
(1,279)	1:77:A:LEU:HD22	1:107:A:ALA:HB3	8	0.31	0.14	0.3
(1,279)	1:77:A:LEU:HD23	1:107:A:ALA:HB1	8	0.31	0.14	0.3
(1,279)	1:77:A:LEU:HD23	1:107:A:ALA:HB2	8	0.31	0.14	0.3
(1,279)	1:77:A:LEU:HD23	1:107:A:ALA:HB3	8	0.31	0.14	0.3
(1,371)	1:100:A:PHE:HA	1:103:A:VAL:HG11	8	0.29	0.27	0.2
(1,371)	1:100:A:PHE:HA	1:103:A:VAL:HG12	8	0.29	0.27	0.2
(1,371)	1:100:A:PHE:HA	1:103:A:VAL:HG13	8	0.29	0.27	0.2
(1,952)	1:104:A:LEU:HD21	1:106:A:GLU:H	8	0.28	0.12	0.28
(1,952)	1:104:A:LEU:HD22	1:106:A:GLU:H	8	0.28	0.12	0.28
(1,952)	1:104:A:LEU:HD23	1:106:A:GLU:H	8	0.28	0.12	0.28
(1,1169)	1:34:A:VAL:HG21	1:35:A:THR:H	8	0.26	0.11	0.25
(1,1169)	1:34:A:VAL:HG22	1:35:A:THR:H	8	0.26	0.11	0.25
(1,1169)	1:34:A:VAL:HG23	1:35:A:THR:H	8	0.26	0.11	0.25
(1,1494)	1:135:A:GLU:HA	1:139:A:VAL:HG11	8	0.24	0.03	0.24
(1,1494)	1:135:A:GLU:HA	1:139:A:VAL:HG12	8	0.24	0.03	0.24
(1,1494)	1:135:A:GLU:HA	1:139:A:VAL:HG13	8	0.24	0.03	0.24
(1,1494)	1:135:A:GLU:HA	1:139:A:VAL:HG21	8	0.24	0.03	0.24
(1,1494)	1:135:A:GLU:HA	1:139:A:VAL:HG22	8	0.24	0.03	0.24
(1,1494)	1:135:A:GLU:HA	1:139:A:VAL:HG23	8	0.24	0.03	0.24
(1,1259)	1:59:A:VAL:HG11	1:61:A:HIS:H	8	0.18	0.04	0.18
(1,1259)	1:59:A:VAL:HG12	1:61:A:HIS:H	8	0.18	0.04	0.18
(1,1259)	1:59:A:VAL:HG13	1:61:A:HIS:H	8	0.18	0.04	0.18
(1,1259)	1:59:A:VAL:HG21	1:61:A:HIS:H	8	0.18	0.04	0.18
(1,1259)	1:59:A:VAL:HG22	1:61:A:HIS:H	8	0.18	0.04	0.18
(1,1259)	1:59:A:VAL:HG23	1:61:A:HIS:H	8	0.18	0.04	0.18
(1,1425)	1:112:A:LYS:HA	1:145:A:LEU:HD11	7	0.54	0.15	0.59
(1,1425)	1:112:A:LYS:HA	1:145:A:LEU:HD12	7	0.54	0.15	0.59
(1,1425)	1:112:A:LYS:HA	1:145:A:LEU:HD13	7	0.54	0.15	0.59
(1,1425)	1:112:A:LYS:HA	1:145:A:LEU:HD21	7	0.54	0.15	0.59
(1,1425)	1:112:A:LYS:HA	1:145:A:LEU:HD22	7	0.54	0.15	0.59
(1,1425)	1:112:A:LYS:HA	1:145:A:LEU:HD23	7	0.54	0.15	0.59
(1,722)	1:34:A:VAL:HG21	1:40:A:SER:H	7	0.54	0.24	0.49
(1,722)	1:34:A:VAL:HG22	1:40:A:SER:H	7	0.54	0.24	0.49
(1,722)	1:34:A:VAL:HG23	1:40:A:SER:H	7	0.54	0.24	0.49

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1500)	1:137:A:MET:HB2	1:141:A:LEU:HD11	7	0.4	0.19	0.37
(1,1500)	1:137:A:MET:HB2	1:141:A:LEU:HD12	7	0.4	0.19	0.37
(1,1500)	1:137:A:MET:HB2	1:141:A:LEU:HD13	7	0.4	0.19	0.37
(1,1500)	1:137:A:MET:HB2	1:141:A:LEU:HD21	7	0.4	0.19	0.37
(1,1500)	1:137:A:MET:HB2	1:141:A:LEU:HD22	7	0.4	0.19	0.37
(1,1500)	1:137:A:MET:HB2	1:141:A:LEU:HD23	7	0.4	0.19	0.37
(1,53)	1:58:A:ILE:HG21	1:59:A:VAL:HG21	7	0.29	0.08	0.25
(1,53)	1:58:A:ILE:HG21	1:59:A:VAL:HG22	7	0.29	0.08	0.25
(1,53)	1:58:A:ILE:HG21	1:59:A:VAL:HG23	7	0.29	0.08	0.25
(1,53)	1:58:A:ILE:HG22	1:59:A:VAL:HG21	7	0.29	0.08	0.25
(1,53)	1:58:A:ILE:HG22	1:59:A:VAL:HG22	7	0.29	0.08	0.25
(1,53)	1:58:A:ILE:HG22	1:59:A:VAL:HG23	7	0.29	0.08	0.25
(1,53)	1:58:A:ILE:HG23	1:59:A:VAL:HG21	7	0.29	0.08	0.25
(1,53)	1:58:A:ILE:HG23	1:59:A:VAL:HG22	7	0.29	0.08	0.25
(1,53)	1:58:A:ILE:HG23	1:59:A:VAL:HG23	7	0.29	0.08	0.25
(1,424)	1:84:A:VAL:HG11	1:88:A:CYS:HB2	7	0.18	0.01	0.19
(1,424)	1:84:A:VAL:HG11	1:88:A:CYS:HB3	7	0.18	0.01	0.19
(1,424)	1:84:A:VAL:HG12	1:88:A:CYS:HB2	7	0.18	0.01	0.19
(1,424)	1:84:A:VAL:HG12	1:88:A:CYS:HB3	7	0.18	0.01	0.19
(1,424)	1:84:A:VAL:HG13	1:88:A:CYS:HB2	7	0.18	0.01	0.19
(1,424)	1:84:A:VAL:HG13	1:88:A:CYS:HB3	7	0.18	0.01	0.19
(1,1347)	1:84:A:VAL:HG11	1:85:A:ILE:HG12	7	0.15	0.06	0.13
(1,1347)	1:84:A:VAL:HG11	1:85:A:ILE:HG13	7	0.15	0.06	0.13
(1,1347)	1:84:A:VAL:HG12	1:85:A:ILE:HG12	7	0.15	0.06	0.13
(1,1347)	1:84:A:VAL:HG12	1:85:A:ILE:HG13	7	0.15	0.06	0.13
(1,1347)	1:84:A:VAL:HG13	1:85:A:ILE:HG12	7	0.15	0.06	0.13
(1,1347)	1:84:A:VAL:HG13	1:85:A:ILE:HG13	7	0.15	0.06	0.13
(1,496)	1:85:A:ILE:HD11	1:86:A:GLN:H	7	0.13	0.01	0.13
(1,496)	1:85:A:ILE:HD12	1:86:A:GLN:H	7	0.13	0.01	0.13
(1,496)	1:85:A:ILE:HD13	1:86:A:GLN:H	7	0.13	0.01	0.13
(1,1073)	1:139:A:VAL:HB	1:140:A:ALA:H	7	0.13	0.01	0.13
(1,804)	1:84:A:VAL:HB	1:87:A:ASN:H	7	0.12	0.01	0.11
(1,74)	1:49:A:ILE:HD11	1:84:A:VAL:HG11	7	0.11	0.01	0.11
(1,74)	1:49:A:ILE:HD11	1:84:A:VAL:HG12	7	0.11	0.01	0.11
(1,74)	1:49:A:ILE:HD11	1:84:A:VAL:HG13	7	0.11	0.01	0.11
(1,74)	1:49:A:ILE:HD12	1:84:A:VAL:HG11	7	0.11	0.01	0.11
(1,74)	1:49:A:ILE:HD12	1:84:A:VAL:HG12	7	0.11	0.01	0.11
(1,74)	1:49:A:ILE:HD12	1:84:A:VAL:HG13	7	0.11	0.01	0.11
(1,74)	1:49:A:ILE:HD13	1:84:A:VAL:HG11	7	0.11	0.01	0.11
(1,74)	1:49:A:ILE:HD13	1:84:A:VAL:HG12	7	0.11	0.01	0.11
(1,74)	1:49:A:ILE:HD13	1:84:A:VAL:HG13	7	0.11	0.01	0.11
(1,227)	1:85:A:ILE:HD11	1:101:A:ALA:H	7	0.11	0.01	0.1

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,227)	1:85:A:ILE:HD12	1:101:A:ALA:H	7	0.11	0.01	0.1
(1,227)	1:85:A:ILE:HD13	1:101:A:ALA:H	7	0.11	0.01	0.1
(5,1)	2:155:B:SER:H	1:130:A:ARG:NH2	6	0.53	0.24	0.52
(1,1085)	1:141:A:LEU:HG	1:142:A:ARG:H	6	0.25	0.03	0.26
(1,579)	1:48:A:CYS:H	1:84:A:VAL:HG21	6	0.19	0.11	0.16
(1,579)	1:48:A:CYS:H	1:84:A:VAL:HG22	6	0.19	0.11	0.16
(1,579)	1:48:A:CYS:H	1:84:A:VAL:HG23	6	0.19	0.11	0.16
(1,297)	1:37:A:THR:HG21	1:38:A:MET:HB2	6	0.14	0.02	0.14
(1,297)	1:37:A:THR:HG21	1:38:A:MET:HB3	6	0.14	0.02	0.14
(1,297)	1:37:A:THR:HG22	1:38:A:MET:HB2	6	0.14	0.02	0.14
(1,297)	1:37:A:THR:HG22	1:38:A:MET:HB3	6	0.14	0.02	0.14
(1,297)	1:37:A:THR:HG23	1:38:A:MET:HB2	6	0.14	0.02	0.14
(1,297)	1:37:A:THR:HG23	1:38:A:MET:HB3	6	0.14	0.02	0.14
(1,1108)	1:58:A:ILE:HG21	1:60:A:TYR:H	6	0.11	0.0	0.11
(1,1108)	1:58:A:ILE:HG22	1:60:A:TYR:H	6	0.11	0.0	0.11
(1,1108)	1:58:A:ILE:HG23	1:60:A:TYR:H	6	0.11	0.0	0.11
(1,1279)	1:59:A:VAL:HG11	1:103:A:VAL:HG11	5	0.74	0.61	0.61
(1,1279)	1:59:A:VAL:HG11	1:103:A:VAL:HG12	5	0.74	0.61	0.61
(1,1279)	1:59:A:VAL:HG11	1:103:A:VAL:HG13	5	0.74	0.61	0.61
(1,1279)	1:59:A:VAL:HG12	1:103:A:VAL:HG11	5	0.74	0.61	0.61
(1,1279)	1:59:A:VAL:HG12	1:103:A:VAL:HG12	5	0.74	0.61	0.61
(1,1279)	1:59:A:VAL:HG12	1:103:A:VAL:HG13	5	0.74	0.61	0.61
(1,1279)	1:59:A:VAL:HG13	1:103:A:VAL:HG11	5	0.74	0.61	0.61
(1,1279)	1:59:A:VAL:HG13	1:103:A:VAL:HG12	5	0.74	0.61	0.61
(1,1279)	1:59:A:VAL:HG13	1:103:A:VAL:HG13	5	0.74	0.61	0.61
(1,1279)	1:59:A:VAL:HG21	1:103:A:VAL:HG11	5	0.74	0.61	0.61
(1,1279)	1:59:A:VAL:HG21	1:103:A:VAL:HG12	5	0.74	0.61	0.61
(1,1279)	1:59:A:VAL:HG21	1:103:A:VAL:HG13	5	0.74	0.61	0.61
(1,1279)	1:59:A:VAL:HG22	1:103:A:VAL:HG11	5	0.74	0.61	0.61
(1,1279)	1:59:A:VAL:HG22	1:103:A:VAL:HG12	5	0.74	0.61	0.61
(1,1279)	1:59:A:VAL:HG22	1:103:A:VAL:HG13	5	0.74	0.61	0.61
(1,1279)	1:59:A:VAL:HG23	1:103:A:VAL:HG11	5	0.74	0.61	0.61
(1,1279)	1:59:A:VAL:HG23	1:103:A:VAL:HG12	5	0.74	0.61	0.61
(1,1279)	1:59:A:VAL:HG23	1:103:A:VAL:HG13	5	0.74	0.61	0.61
(2,2)	2:149:B:PRO:HG2	1:38:A:MET:HE2	5	0.47	0.21	0.44
(2,2)	2:149:B:PRO:HB2	1:38:A:MET:HE3	5	0.47	0.21	0.44
(2,2)	2:149:B:PRO:HG2	1:38:A:MET:HE1	5	0.47	0.21	0.44
(1,963)	1:109:A:ALA:H	1:111:A:VAL:HG11	5	0.37	0.26	0.26
(1,963)	1:109:A:ALA:H	1:111:A:VAL:HG12	5	0.37	0.26	0.26
(1,963)	1:109:A:ALA:H	1:111:A:VAL:HG13	5	0.37	0.26	0.26
(1,1294)	1:63:A:MET:HG2	1:103:A:VAL:HG11	5	0.37	0.34	0.21
(1,1294)	1:63:A:MET:HG2	1:103:A:VAL:HG12	5	0.37	0.34	0.21

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1294)	1:63:A:MET:HG2	1:103:A:VAL:HG13	5	0.37	0.34	0.21
(1,1294)	1:63:A:MET:HG3	1:103:A:VAL:HG11	5	0.37	0.34	0.21
(1,1294)	1:63:A:MET:HG3	1:103:A:VAL:HG12	5	0.37	0.34	0.21
(1,1294)	1:63:A:MET:HG3	1:103:A:VAL:HG13	5	0.37	0.34	0.21
(1,369)	1:63:A:MET:HG3	1:103:A:VAL:HG11	5	0.34	0.25	0.27
(1,369)	1:63:A:MET:HG3	1:103:A:VAL:HG12	5	0.34	0.25	0.27
(1,369)	1:63:A:MET:HG3	1:103:A:VAL:HG13	5	0.34	0.25	0.27
(1,1340)	1:78:A:PHE:HE1	1:104:A:LEU:HD11	5	0.26	0.11	0.28
(1,1340)	1:78:A:PHE:HE1	1:104:A:LEU:HD12	5	0.26	0.11	0.28
(1,1340)	1:78:A:PHE:HE1	1:104:A:LEU:HD13	5	0.26	0.11	0.28
(1,1340)	1:78:A:PHE:HE1	1:104:A:LEU:HD21	5	0.26	0.11	0.28
(1,1340)	1:78:A:PHE:HE1	1:104:A:LEU:HD22	5	0.26	0.11	0.28
(1,1340)	1:78:A:PHE:HE1	1:104:A:LEU:HD23	5	0.26	0.11	0.28
(1,1340)	1:78:A:PHE:HE2	1:104:A:LEU:HD11	5	0.26	0.11	0.28
(1,1340)	1:78:A:PHE:HE2	1:104:A:LEU:HD12	5	0.26	0.11	0.28
(1,1340)	1:78:A:PHE:HE2	1:104:A:LEU:HD13	5	0.26	0.11	0.28
(1,1340)	1:78:A:PHE:HE2	1:104:A:LEU:HD21	5	0.26	0.11	0.28
(1,1340)	1:78:A:PHE:HE2	1:104:A:LEU:HD22	5	0.26	0.11	0.28
(1,1340)	1:78:A:PHE:HE2	1:104:A:LEU:HD23	5	0.26	0.11	0.28
(1,20)	1:132:A:VAL:HG21	1:138:A:ILE:HD11	5	0.25	0.14	0.22
(1,20)	1:132:A:VAL:HG21	1:138:A:ILE:HD12	5	0.25	0.14	0.22
(1,20)	1:132:A:VAL:HG21	1:138:A:ILE:HD13	5	0.25	0.14	0.22
(1,20)	1:132:A:VAL:HG22	1:138:A:ILE:HD11	5	0.25	0.14	0.22
(1,20)	1:132:A:VAL:HG22	1:138:A:ILE:HD12	5	0.25	0.14	0.22
(1,20)	1:132:A:VAL:HG22	1:138:A:ILE:HD13	5	0.25	0.14	0.22
(1,20)	1:132:A:VAL:HG23	1:138:A:ILE:HD11	5	0.25	0.14	0.22
(1,20)	1:132:A:VAL:HG23	1:138:A:ILE:HD12	5	0.25	0.14	0.22
(1,20)	1:132:A:VAL:HG23	1:138:A:ILE:HD13	5	0.25	0.14	0.22
(1,1238)	1:48:A:CYS:HB2	1:84:A:VAL:HG21	5	0.24	0.08	0.27
(1,1238)	1:48:A:CYS:HB2	1:84:A:VAL:HG22	5	0.24	0.08	0.27
(1,1238)	1:48:A:CYS:HB2	1:84:A:VAL:HG23	5	0.24	0.08	0.27
(1,1238)	1:48:A:CYS:HB3	1:84:A:VAL:HG21	5	0.24	0.08	0.27
(1,1238)	1:48:A:CYS:HB3	1:84:A:VAL:HG22	5	0.24	0.08	0.27
(1,1238)	1:48:A:CYS:HB3	1:84:A:VAL:HG23	5	0.24	0.08	0.27
(1,1508)	1:139:A:VAL:HG11	1:140:A:ALA:HB1	5	0.16	0.04	0.13
(1,1508)	1:139:A:VAL:HG11	1:140:A:ALA:HB2	5	0.16	0.04	0.13
(1,1508)	1:139:A:VAL:HG11	1:140:A:ALA:HB3	5	0.16	0.04	0.13
(1,1508)	1:139:A:VAL:HG12	1:140:A:ALA:HB1	5	0.16	0.04	0.13
(1,1508)	1:139:A:VAL:HG12	1:140:A:ALA:HB2	5	0.16	0.04	0.13
(1,1508)	1:139:A:VAL:HG12	1:140:A:ALA:HB3	5	0.16	0.04	0.13
(1,1508)	1:139:A:VAL:HG13	1:140:A:ALA:HB1	5	0.16	0.04	0.13
(1,1508)	1:139:A:VAL:HG13	1:140:A:ALA:HB2	5	0.16	0.04	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1508)	1:139:A:VAL:HG13	1:140:A:ALA:HB3	5	0.16	0.04	0.13
(1,1508)	1:139:A:VAL:HG21	1:140:A:ALA:HB1	5	0.16	0.04	0.13
(1,1508)	1:139:A:VAL:HG21	1:140:A:ALA:HB2	5	0.16	0.04	0.13
(1,1508)	1:139:A:VAL:HG21	1:140:A:ALA:HB3	5	0.16	0.04	0.13
(1,1508)	1:139:A:VAL:HG22	1:140:A:ALA:HB1	5	0.16	0.04	0.13
(1,1508)	1:139:A:VAL:HG22	1:140:A:ALA:HB2	5	0.16	0.04	0.13
(1,1508)	1:139:A:VAL:HG22	1:140:A:ALA:HB3	5	0.16	0.04	0.13
(1,1508)	1:139:A:VAL:HG23	1:140:A:ALA:HB1	5	0.16	0.04	0.13
(1,1508)	1:139:A:VAL:HG23	1:140:A:ALA:HB2	5	0.16	0.04	0.13
(1,1508)	1:139:A:VAL:HG23	1:140:A:ALA:HB3	5	0.16	0.04	0.13
(1,954)	1:104:A:LEU:HD11	1:106:A:GLU:H	4	1.08	0.04	1.08
(1,954)	1:104:A:LEU:HD12	1:106:A:GLU:H	4	1.08	0.04	1.08
(1,954)	1:104:A:LEU:HD13	1:106:A:GLU:H	4	1.08	0.04	1.08
(1,575)	1:104:A:LEU:HD11	1:108:A:ALA:H	4	0.92	0.11	0.88
(1,575)	1:104:A:LEU:HD12	1:108:A:ALA:H	4	0.92	0.11	0.88
(1,575)	1:104:A:LEU:HD13	1:108:A:ALA:H	4	0.92	0.11	0.88
(1,1455)	1:120:A:VAL:HB	1:145:A:LEU:HD11	4	0.92	0.21	0.94
(1,1455)	1:120:A:VAL:HB	1:145:A:LEU:HD12	4	0.92	0.21	0.94
(1,1455)	1:120:A:VAL:HB	1:145:A:LEU:HD13	4	0.92	0.21	0.94
(1,1455)	1:120:A:VAL:HB	1:145:A:LEU:HD21	4	0.92	0.21	0.94
(1,1455)	1:120:A:VAL:HB	1:145:A:LEU:HD22	4	0.92	0.21	0.94
(1,1455)	1:120:A:VAL:HB	1:145:A:LEU:HD23	4	0.92	0.21	0.94
(1,153)	1:63:A:MET:HG2	1:103:A:VAL:HG11	4	0.74	0.17	0.75
(1,153)	1:63:A:MET:HG2	1:103:A:VAL:HG12	4	0.74	0.17	0.75
(1,153)	1:63:A:MET:HG2	1:103:A:VAL:HG13	4	0.74	0.17	0.75
(1,347)	1:104:A:LEU:HD11	1:108:A:ALA:HB1	4	0.62	0.18	0.54
(1,347)	1:104:A:LEU:HD11	1:108:A:ALA:HB2	4	0.62	0.18	0.54
(1,347)	1:104:A:LEU:HD11	1:108:A:ALA:HB3	4	0.62	0.18	0.54
(1,347)	1:104:A:LEU:HD12	1:108:A:ALA:HB1	4	0.62	0.18	0.54
(1,347)	1:104:A:LEU:HD12	1:108:A:ALA:HB2	4	0.62	0.18	0.54
(1,347)	1:104:A:LEU:HD12	1:108:A:ALA:HB3	4	0.62	0.18	0.54
(1,347)	1:104:A:LEU:HD13	1:108:A:ALA:HB1	4	0.62	0.18	0.54
(1,347)	1:104:A:LEU:HD13	1:108:A:ALA:HB2	4	0.62	0.18	0.54
(1,347)	1:104:A:LEU:HD13	1:108:A:ALA:HB3	4	0.62	0.18	0.54
(1,1281)	1:59:A:VAL:HG11	1:104:A:LEU:H	4	0.55	0.2	0.48
(1,1281)	1:59:A:VAL:HG12	1:104:A:LEU:H	4	0.55	0.2	0.48
(1,1281)	1:59:A:VAL:HG13	1:104:A:LEU:H	4	0.55	0.2	0.48
(1,1281)	1:59:A:VAL:HG21	1:104:A:LEU:H	4	0.55	0.2	0.48
(1,1281)	1:59:A:VAL:HG22	1:104:A:LEU:H	4	0.55	0.2	0.48
(1,1281)	1:59:A:VAL:HG23	1:104:A:LEU:H	4	0.55	0.2	0.48
(1,336)	1:108:A:ALA:HB1	1:111:A:VAL:HG11	4	0.51	0.28	0.5
(1,336)	1:108:A:ALA:HB1	1:111:A:VAL:HG12	4	0.51	0.28	0.5

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,336)	1:108:A:ALA:HB1	1:111:A:VAL:HG13	4	0.51	0.28	0.5
(1,336)	1:108:A:ALA:HB2	1:111:A:VAL:HG11	4	0.51	0.28	0.5
(1,336)	1:108:A:ALA:HB2	1:111:A:VAL:HG12	4	0.51	0.28	0.5
(1,336)	1:108:A:ALA:HB2	1:111:A:VAL:HG13	4	0.51	0.28	0.5
(1,336)	1:108:A:ALA:HB3	1:111:A:VAL:HG11	4	0.51	0.28	0.5
(1,336)	1:108:A:ALA:HB3	1:111:A:VAL:HG12	4	0.51	0.28	0.5
(1,336)	1:108:A:ALA:HB3	1:111:A:VAL:HG13	4	0.51	0.28	0.5
(1,69)	1:34:A:VAL:HG11	1:41:A:ILE:HD11	4	0.47	0.25	0.37
(1,69)	1:34:A:VAL:HG11	1:41:A:ILE:HD12	4	0.47	0.25	0.37
(1,69)	1:34:A:VAL:HG11	1:41:A:ILE:HD13	4	0.47	0.25	0.37
(1,69)	1:34:A:VAL:HG12	1:41:A:ILE:HD11	4	0.47	0.25	0.37
(1,69)	1:34:A:VAL:HG12	1:41:A:ILE:HD12	4	0.47	0.25	0.37
(1,69)	1:34:A:VAL:HG12	1:41:A:ILE:HD13	4	0.47	0.25	0.37
(1,69)	1:34:A:VAL:HG13	1:41:A:ILE:HD11	4	0.47	0.25	0.37
(1,69)	1:34:A:VAL:HG13	1:41:A:ILE:HD12	4	0.47	0.25	0.37
(1,69)	1:34:A:VAL:HG13	1:41:A:ILE:HD13	4	0.47	0.25	0.37
(1,379)	1:139:A:VAL:HG21	1:143:A:GLU:HG2	4	0.34	0.27	0.22
(1,379)	1:139:A:VAL:HG21	1:143:A:GLU:HG3	4	0.34	0.27	0.22
(1,379)	1:139:A:VAL:HG22	1:143:A:GLU:HG2	4	0.34	0.27	0.22
(1,379)	1:139:A:VAL:HG22	1:143:A:GLU:HG3	4	0.34	0.27	0.22
(1,379)	1:139:A:VAL:HG23	1:143:A:GLU:HG2	4	0.34	0.27	0.22
(1,379)	1:139:A:VAL:HG23	1:143:A:GLU:HG3	4	0.34	0.27	0.22
(1,61)	1:59:A:VAL:HG21	1:62:A:TRP:HE3	4	0.2	0.06	0.22
(1,61)	1:59:A:VAL:HG22	1:62:A:TRP:HE3	4	0.2	0.06	0.22
(1,61)	1:59:A:VAL:HG23	1:62:A:TRP:HE3	4	0.2	0.06	0.22
(1,1280)	1:59:A:VAL:HG11	1:103:A:VAL:HG21	4	0.19	0.08	0.16
(1,1280)	1:59:A:VAL:HG11	1:103:A:VAL:HG22	4	0.19	0.08	0.16
(1,1280)	1:59:A:VAL:HG11	1:103:A:VAL:HG23	4	0.19	0.08	0.16
(1,1280)	1:59:A:VAL:HG12	1:103:A:VAL:HG21	4	0.19	0.08	0.16
(1,1280)	1:59:A:VAL:HG12	1:103:A:VAL:HG22	4	0.19	0.08	0.16
(1,1280)	1:59:A:VAL:HG12	1:103:A:VAL:HG23	4	0.19	0.08	0.16
(1,1280)	1:59:A:VAL:HG13	1:103:A:VAL:HG21	4	0.19	0.08	0.16
(1,1280)	1:59:A:VAL:HG13	1:103:A:VAL:HG22	4	0.19	0.08	0.16
(1,1280)	1:59:A:VAL:HG13	1:103:A:VAL:HG23	4	0.19	0.08	0.16
(1,1280)	1:59:A:VAL:HG21	1:103:A:VAL:HG21	4	0.19	0.08	0.16
(1,1280)	1:59:A:VAL:HG21	1:103:A:VAL:HG22	4	0.19	0.08	0.16
(1,1280)	1:59:A:VAL:HG21	1:103:A:VAL:HG23	4	0.19	0.08	0.16
(1,1280)	1:59:A:VAL:HG22	1:103:A:VAL:HG21	4	0.19	0.08	0.16
(1,1280)	1:59:A:VAL:HG22	1:103:A:VAL:HG22	4	0.19	0.08	0.16
(1,1280)	1:59:A:VAL:HG22	1:103:A:VAL:HG23	4	0.19	0.08	0.16
(1,1280)	1:59:A:VAL:HG23	1:103:A:VAL:HG21	4	0.19	0.08	0.16
(1,1280)	1:59:A:VAL:HG23	1:103:A:VAL:HG22	4	0.19	0.08	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1280)	1:59:A:VAL:HG23	1:103:A:VAL:HG23	4	0.19	0.08	0.16
(1,1112)	1:61:A:HIS:H	1:61:A:HIS:HD2	4	0.18	0.05	0.2
(1,536)	1:122:A:ARG:H	1:122:A:ARG:HD2	4	0.17	0.02	0.18
(1,536)	1:122:A:ARG:H	1:122:A:ARG:HD3	4	0.17	0.02	0.18
(1,1366)	1:91:A:LYS:H	1:92:A:ASN:HB2	4	0.12	0.01	0.12
(1,1366)	1:91:A:LYS:H	1:92:A:ASN:HB3	4	0.12	0.01	0.12
(1,826)	1:82:A:ASN:H	1:84:A:VAL:HB	4	0.11	0.01	0.11
(1,56)	1:78:A:PHE:HB3	1:120:A:VAL:HG11	3	0.82	0.15	0.76
(1,56)	1:78:A:PHE:HB3	1:120:A:VAL:HG12	3	0.82	0.15	0.76
(1,56)	1:78:A:PHE:HB3	1:120:A:VAL:HG13	3	0.82	0.15	0.76
(1,1290)	1:63:A:MET:HB2	1:77:A:LEU:HD11	3	0.41	0.05	0.43
(1,1290)	1:63:A:MET:HB2	1:77:A:LEU:HD12	3	0.41	0.05	0.43
(1,1290)	1:63:A:MET:HB2	1:77:A:LEU:HD13	3	0.41	0.05	0.43
(1,1290)	1:63:A:MET:HB2	1:77:A:LEU:HD21	3	0.41	0.05	0.43
(1,1290)	1:63:A:MET:HB2	1:77:A:LEU:HD22	3	0.41	0.05	0.43
(1,1290)	1:63:A:MET:HB2	1:77:A:LEU:HD23	3	0.41	0.05	0.43
(1,1290)	1:63:A:MET:HB3	1:77:A:LEU:HD11	3	0.41	0.05	0.43
(1,1290)	1:63:A:MET:HB3	1:77:A:LEU:HD12	3	0.41	0.05	0.43
(1,1290)	1:63:A:MET:HB3	1:77:A:LEU:HD13	3	0.41	0.05	0.43
(1,1290)	1:63:A:MET:HB3	1:77:A:LEU:HD21	3	0.41	0.05	0.43
(1,1290)	1:63:A:MET:HB3	1:77:A:LEU:HD22	3	0.41	0.05	0.43
(1,1290)	1:63:A:MET:HB3	1:77:A:LEU:HD23	3	0.41	0.05	0.43
(1,1077)	1:137:A:MET:HB3	1:141:A:LEU:H	3	0.37	0.16	0.48
(1,1273)	1:59:A:VAL:HG11	1:100:A:PHE:HD1	3	0.34	0.11	0.35
(1,1273)	1:59:A:VAL:HG11	1:100:A:PHE:HD2	3	0.34	0.11	0.35
(1,1273)	1:59:A:VAL:HG12	1:100:A:PHE:HD1	3	0.34	0.11	0.35
(1,1273)	1:59:A:VAL:HG12	1:100:A:PHE:HD2	3	0.34	0.11	0.35
(1,1273)	1:59:A:VAL:HG13	1:100:A:PHE:HD1	3	0.34	0.11	0.35
(1,1273)	1:59:A:VAL:HG13	1:100:A:PHE:HD2	3	0.34	0.11	0.35
(1,1273)	1:59:A:VAL:HG21	1:100:A:PHE:HD1	3	0.34	0.11	0.35
(1,1273)	1:59:A:VAL:HG21	1:100:A:PHE:HD2	3	0.34	0.11	0.35
(1,1273)	1:59:A:VAL:HG22	1:100:A:PHE:HD1	3	0.34	0.11	0.35
(1,1273)	1:59:A:VAL:HG22	1:100:A:PHE:HD2	3	0.34	0.11	0.35
(1,1273)	1:59:A:VAL:HG23	1:100:A:PHE:HD1	3	0.34	0.11	0.35
(1,1273)	1:59:A:VAL:HG23	1:100:A:PHE:HD2	3	0.34	0.11	0.35
(1,1443)	1:116:A:VAL:HA	1:120:A:VAL:HG11	3	0.32	0.22	0.18
(1,1443)	1:116:A:VAL:HA	1:120:A:VAL:HG12	3	0.32	0.22	0.18
(1,1443)	1:116:A:VAL:HA	1:120:A:VAL:HG13	3	0.32	0.22	0.18
(1,1443)	1:116:A:VAL:HA	1:120:A:VAL:HG21	3	0.32	0.22	0.18
(1,1443)	1:116:A:VAL:HA	1:120:A:VAL:HG22	3	0.32	0.22	0.18
(1,1443)	1:116:A:VAL:HA	1:120:A:VAL:HG23	3	0.32	0.22	0.18
(1,62)	1:59:A:VAL:HG21	1:100:A:PHE:HD1	3	0.3	0.17	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,62)	1:59:A:VAL:HG21	1:100:A:PHE:HD2	3	0.3	0.17	0.2
(1,62)	1:59:A:VAL:HG22	1:100:A:PHE:HD1	3	0.3	0.17	0.2
(1,62)	1:59:A:VAL:HG22	1:100:A:PHE:HD2	3	0.3	0.17	0.2
(1,62)	1:59:A:VAL:HG23	1:100:A:PHE:HD1	3	0.3	0.17	0.2
(1,62)	1:59:A:VAL:HG23	1:100:A:PHE:HD2	3	0.3	0.17	0.2
(1,1402)	1:104:A:LEU:HD11	1:141:A:LEU:HB2	3	0.29	0.09	0.27
(1,1402)	1:104:A:LEU:HD11	1:141:A:LEU:HB3	3	0.29	0.09	0.27
(1,1402)	1:104:A:LEU:HD12	1:141:A:LEU:HB2	3	0.29	0.09	0.27
(1,1402)	1:104:A:LEU:HD12	1:141:A:LEU:HB3	3	0.29	0.09	0.27
(1,1402)	1:104:A:LEU:HD13	1:141:A:LEU:HB2	3	0.29	0.09	0.27
(1,1402)	1:104:A:LEU:HD13	1:141:A:LEU:HB3	3	0.29	0.09	0.27
(1,1402)	1:104:A:LEU:HD21	1:141:A:LEU:HB2	3	0.29	0.09	0.27
(1,1402)	1:104:A:LEU:HD21	1:141:A:LEU:HB3	3	0.29	0.09	0.27
(1,1402)	1:104:A:LEU:HD22	1:141:A:LEU:HB2	3	0.29	0.09	0.27
(1,1402)	1:104:A:LEU:HD22	1:141:A:LEU:HB3	3	0.29	0.09	0.27
(1,1402)	1:104:A:LEU:HD23	1:141:A:LEU:HB2	3	0.29	0.09	0.27
(1,1402)	1:104:A:LEU:HD23	1:141:A:LEU:HB3	3	0.29	0.09	0.27
(1,1295)	1:66:A:LEU:H	1:66:A:LEU:HD11	3	0.26	0.03	0.25
(1,1295)	1:66:A:LEU:H	1:66:A:LEU:HD12	3	0.26	0.03	0.25
(1,1295)	1:66:A:LEU:H	1:66:A:LEU:HD13	3	0.26	0.03	0.25
(1,1295)	1:66:A:LEU:H	1:66:A:LEU:HD21	3	0.26	0.03	0.25
(1,1295)	1:66:A:LEU:H	1:66:A:LEU:HD22	3	0.26	0.03	0.25
(1,1295)	1:66:A:LEU:H	1:66:A:LEU:HD23	3	0.26	0.03	0.25
(1,818)	1:110:A:LEU:H	1:111:A:VAL:HG11	3	0.24	0.13	0.17
(1,818)	1:110:A:LEU:H	1:111:A:VAL:HG12	3	0.24	0.13	0.17
(1,818)	1:110:A:LEU:H	1:111:A:VAL:HG13	3	0.24	0.13	0.17
(1,1381)	1:97:A:ARG:HB2	1:101:A:ALA:H	3	0.2	0.01	0.2
(1,1381)	1:97:A:ARG:HB3	1:101:A:ALA:H	3	0.2	0.01	0.2
(1,1505)	1:139:A:VAL:H	1:141:A:LEU:HD11	3	0.18	0.02	0.17
(1,1505)	1:139:A:VAL:H	1:141:A:LEU:HD12	3	0.18	0.02	0.17
(1,1505)	1:139:A:VAL:H	1:141:A:LEU:HD13	3	0.18	0.02	0.17
(1,1505)	1:139:A:VAL:H	1:141:A:LEU:HD21	3	0.18	0.02	0.17
(1,1505)	1:139:A:VAL:H	1:141:A:LEU:HD22	3	0.18	0.02	0.17
(1,1505)	1:139:A:VAL:H	1:141:A:LEU:HD23	3	0.18	0.02	0.17
(1,457)	1:95:A:ILE:HA	1:97:A:ARG:HG2	3	0.15	0.0	0.15
(1,457)	1:95:A:ILE:HA	1:97:A:ARG:HG3	3	0.15	0.0	0.15
(1,171)	1:34:A:VAL:H	1:36:A:ASN:HA	3	0.14	0.01	0.15
(1,604)	1:132:A:VAL:HG21	1:133:A:TYR:H	3	0.13	0.01	0.13
(1,604)	1:132:A:VAL:HG22	1:133:A:TYR:H	3	0.13	0.01	0.13
(1,604)	1:132:A:VAL:HG23	1:133:A:TYR:H	3	0.13	0.01	0.13
(1,846)	1:45:A:SER:HA	1:85:A:ILE:H	3	0.12	0.01	0.13
(1,1362)	1:88:A:CYS:H	1:89:A:LYS:HB2	3	0.12	0.01	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1362)	1:88:A:CYS:H	1:89:A:LYS:HB3	3	0.12	0.01	0.12
(1,1243)	1:53:A:LYS:HB2	1:54:A:HIS:HB2	3	0.12	0.0	0.12
(1,1243)	1:53:A:LYS:HB2	1:54:A:HIS:HB3	3	0.12	0.0	0.12
(1,1243)	1:53:A:LYS:HB3	1:54:A:HIS:HB2	3	0.12	0.0	0.12
(1,1243)	1:53:A:LYS:HB3	1:54:A:HIS:HB3	3	0.12	0.0	0.12
(1,1033)	1:128:A:GLU:H	1:138:A:ILE:HG12	3	0.11	0.01	0.11
(1,1033)	1:128:A:GLU:H	1:138:A:ILE:HG13	3	0.11	0.01	0.11
(6,6)	2:154:B:TPO:HG21	2:153:B:PRO:HB2	3	0.11	0.0	0.11
(6,6)	2:154:B:TPO:HG21	2:153:B:PRO:HB3	3	0.11	0.0	0.11
(1,66)	1:49:A:ILE:HA	1:84:A:VAL:HG11	3	0.11	0.0	0.11
(1,66)	1:49:A:ILE:HA	1:84:A:VAL:HG12	3	0.11	0.0	0.11
(1,66)	1:49:A:ILE:HA	1:84:A:VAL:HG13	3	0.11	0.0	0.11
(1,1147)	1:75:A:LEU:H	1:111:A:VAL:HG11	3	0.11	0.0	0.11
(1,1147)	1:75:A:LEU:H	1:111:A:VAL:HG12	3	0.11	0.0	0.11
(1,1147)	1:75:A:LEU:H	1:111:A:VAL:HG13	3	0.11	0.0	0.11
(1,271)	1:75:A:LEU:HD21	1:78:A:PHE:HB3	2	1.2	0.34	1.2
(1,271)	1:75:A:LEU:HD22	1:78:A:PHE:HB3	2	1.2	0.34	1.2
(1,271)	1:75:A:LEU:HD23	1:78:A:PHE:HB3	2	1.2	0.34	1.2
(1,290)	1:101:A:ALA:HA	1:137:A:MET:HB3	2	1.06	0.12	1.06
(1,267)	1:104:A:LEU:HD21	1:108:A:ALA:H	2	0.99	0.04	0.99
(1,267)	1:104:A:LEU:HD22	1:108:A:ALA:H	2	0.99	0.04	0.99
(1,267)	1:104:A:LEU:HD23	1:108:A:ALA:H	2	0.99	0.04	0.99
(1,289)	1:101:A:ALA:HB1	1:137:A:MET:HB3	2	0.68	0.36	0.68
(1,289)	1:101:A:ALA:HB2	1:137:A:MET:HB3	2	0.68	0.36	0.68
(1,289)	1:101:A:ALA:HB3	1:137:A:MET:HB3	2	0.68	0.36	0.68
(1,1293)	1:63:A:MET:HG2	1:77:A:LEU:HD11	2	0.68	0.46	0.68
(1,1293)	1:63:A:MET:HG2	1:77:A:LEU:HD12	2	0.68	0.46	0.68
(1,1293)	1:63:A:MET:HG2	1:77:A:LEU:HD13	2	0.68	0.46	0.68
(1,1293)	1:63:A:MET:HG2	1:77:A:LEU:HD21	2	0.68	0.46	0.68
(1,1293)	1:63:A:MET:HG2	1:77:A:LEU:HD22	2	0.68	0.46	0.68
(1,1293)	1:63:A:MET:HG2	1:77:A:LEU:HD23	2	0.68	0.46	0.68
(1,1293)	1:63:A:MET:HG3	1:77:A:LEU:HD11	2	0.68	0.46	0.68
(1,1293)	1:63:A:MET:HG3	1:77:A:LEU:HD12	2	0.68	0.46	0.68
(1,1293)	1:63:A:MET:HG3	1:77:A:LEU:HD13	2	0.68	0.46	0.68
(1,1293)	1:63:A:MET:HG3	1:77:A:LEU:HD21	2	0.68	0.46	0.68
(1,1293)	1:63:A:MET:HG3	1:77:A:LEU:HD22	2	0.68	0.46	0.68
(1,1293)	1:63:A:MET:HG3	1:77:A:LEU:HD23	2	0.68	0.46	0.68
(1,269)	1:104:A:LEU:HD21	1:108:A:ALA:HB1	2	0.57	0.11	0.57
(1,269)	1:104:A:LEU:HD21	1:108:A:ALA:HB2	2	0.57	0.11	0.57
(1,269)	1:104:A:LEU:HD21	1:108:A:ALA:HB3	2	0.57	0.11	0.57
(1,269)	1:104:A:LEU:HD22	1:108:A:ALA:HB1	2	0.57	0.11	0.57
(1,269)	1:104:A:LEU:HD22	1:108:A:ALA:HB2	2	0.57	0.11	0.57

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,269)	1:104:A:LEU:HD22	1:108:A:ALA:HB3	2	0.57	0.11	0.57
(1,269)	1:104:A:LEU:HD23	1:108:A:ALA:HB1	2	0.57	0.11	0.57
(1,269)	1:104:A:LEU:HD23	1:108:A:ALA:HB2	2	0.57	0.11	0.57
(1,269)	1:104:A:LEU:HD23	1:108:A:ALA:HB3	2	0.57	0.11	0.57
(1,154)	1:139:A:VAL:HG11	1:143:A:GLU:HG2	2	0.52	0.2	0.52
(1,154)	1:139:A:VAL:HG11	1:143:A:GLU:HG3	2	0.52	0.2	0.52
(1,154)	1:139:A:VAL:HG12	1:143:A:GLU:HG2	2	0.52	0.2	0.52
(1,154)	1:139:A:VAL:HG12	1:143:A:GLU:HG3	2	0.52	0.2	0.52
(1,154)	1:139:A:VAL:HG13	1:143:A:GLU:HG2	2	0.52	0.2	0.52
(1,154)	1:139:A:VAL:HG13	1:143:A:GLU:HG3	2	0.52	0.2	0.52
(1,273)	1:75:A:LEU:HA	1:75:A:LEU:HD21	2	0.35	0.01	0.35
(1,273)	1:75:A:LEU:HA	1:75:A:LEU:HD22	2	0.35	0.01	0.35
(1,273)	1:75:A:LEU:HA	1:75:A:LEU:HD23	2	0.35	0.01	0.35
(1,1218)	1:44:A:LEU:HB2	1:80:A:LEU:HD11	2	0.29	0.12	0.29
(1,1218)	1:44:A:LEU:HB2	1:80:A:LEU:HD12	2	0.29	0.12	0.29
(1,1218)	1:44:A:LEU:HB2	1:80:A:LEU:HD13	2	0.29	0.12	0.29
(1,1218)	1:44:A:LEU:HB2	1:80:A:LEU:HD21	2	0.29	0.12	0.29
(1,1218)	1:44:A:LEU:HB2	1:80:A:LEU:HD22	2	0.29	0.12	0.29
(1,1218)	1:44:A:LEU:HB2	1:80:A:LEU:HD23	2	0.29	0.12	0.29
(1,377)	1:62:A:TRP:HZ3	1:103:A:VAL:HG11	2	0.27	0.14	0.27
(1,377)	1:62:A:TRP:HZ3	1:103:A:VAL:HG12	2	0.27	0.14	0.27
(1,377)	1:62:A:TRP:HZ3	1:103:A:VAL:HG13	2	0.27	0.14	0.27
(1,1278)	1:59:A:VAL:HG11	1:103:A:VAL:HB	2	0.22	0.02	0.22
(1,1278)	1:59:A:VAL:HG12	1:103:A:VAL:HB	2	0.22	0.02	0.22
(1,1278)	1:59:A:VAL:HG13	1:103:A:VAL:HB	2	0.22	0.02	0.22
(1,1278)	1:59:A:VAL:HG21	1:103:A:VAL:HB	2	0.22	0.02	0.22
(1,1278)	1:59:A:VAL:HG22	1:103:A:VAL:HB	2	0.22	0.02	0.22
(1,1278)	1:59:A:VAL:HG23	1:103:A:VAL:HB	2	0.22	0.02	0.22
(1,1490)	1:132:A:VAL:HG11	1:138:A:ILE:HD11	2	0.21	0.08	0.21
(1,1490)	1:132:A:VAL:HG11	1:138:A:ILE:HD12	2	0.21	0.08	0.21
(1,1490)	1:132:A:VAL:HG11	1:138:A:ILE:HD13	2	0.21	0.08	0.21
(1,1490)	1:132:A:VAL:HG12	1:138:A:ILE:HD11	2	0.21	0.08	0.21
(1,1490)	1:132:A:VAL:HG12	1:138:A:ILE:HD12	2	0.21	0.08	0.21
(1,1490)	1:132:A:VAL:HG12	1:138:A:ILE:HD13	2	0.21	0.08	0.21
(1,1490)	1:132:A:VAL:HG13	1:138:A:ILE:HD11	2	0.21	0.08	0.21
(1,1490)	1:132:A:VAL:HG13	1:138:A:ILE:HD12	2	0.21	0.08	0.21
(1,1490)	1:132:A:VAL:HG13	1:138:A:ILE:HD13	2	0.21	0.08	0.21
(1,1490)	1:132:A:VAL:HG21	1:138:A:ILE:HD11	2	0.21	0.08	0.21
(1,1490)	1:132:A:VAL:HG21	1:138:A:ILE:HD12	2	0.21	0.08	0.21
(1,1490)	1:132:A:VAL:HG21	1:138:A:ILE:HD13	2	0.21	0.08	0.21
(1,1490)	1:132:A:VAL:HG22	1:138:A:ILE:HD11	2	0.21	0.08	0.21
(1,1490)	1:132:A:VAL:HG22	1:138:A:ILE:HD12	2	0.21	0.08	0.21

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1490)	1:132:A:VAL:HG22	1:138:A:ILE:HD13	2	0.21	0.08	0.21
(1,1490)	1:132:A:VAL:HG23	1:138:A:ILE:HD11	2	0.21	0.08	0.21
(1,1490)	1:132:A:VAL:HG23	1:138:A:ILE:HD12	2	0.21	0.08	0.21
(1,1490)	1:132:A:VAL:HG23	1:138:A:ILE:HD13	2	0.21	0.08	0.21
(1,1262)	1:59:A:VAL:HG11	1:62:A:TRP:HE3	2	0.2	0.1	0.2
(1,1262)	1:59:A:VAL:HG12	1:62:A:TRP:HE3	2	0.2	0.1	0.2
(1,1262)	1:59:A:VAL:HG13	1:62:A:TRP:HE3	2	0.2	0.1	0.2
(1,1262)	1:59:A:VAL:HG21	1:62:A:TRP:HE3	2	0.2	0.1	0.2
(1,1262)	1:59:A:VAL:HG22	1:62:A:TRP:HE3	2	0.2	0.1	0.2
(1,1262)	1:59:A:VAL:HG23	1:62:A:TRP:HE3	2	0.2	0.1	0.2
(1,471)	1:47:A:TRP:HA	1:47:A:TRP:HD1	2	0.18	0.01	0.18
(1,625)	1:100:A:PHE:HD1	1:102:A:ASP:H	2	0.18	0.01	0.18
(1,625)	1:100:A:PHE:HD2	1:102:A:ASP:H	2	0.18	0.01	0.18
(1,344)	1:49:A:ILE:H	1:84:A:VAL:HG21	2	0.18	0.04	0.18
(1,344)	1:49:A:ILE:H	1:84:A:VAL:HG22	2	0.18	0.04	0.18
(1,344)	1:49:A:ILE:H	1:84:A:VAL:HG23	2	0.18	0.04	0.18
(1,82)	1:132:A:VAL:HG11	1:138:A:ILE:HD11	2	0.18	0.03	0.18
(1,82)	1:132:A:VAL:HG11	1:138:A:ILE:HD12	2	0.18	0.03	0.18
(1,82)	1:132:A:VAL:HG11	1:138:A:ILE:HD13	2	0.18	0.03	0.18
(1,82)	1:132:A:VAL:HG12	1:138:A:ILE:HD11	2	0.18	0.03	0.18
(1,82)	1:132:A:VAL:HG12	1:138:A:ILE:HD12	2	0.18	0.03	0.18
(1,82)	1:132:A:VAL:HG12	1:138:A:ILE:HD13	2	0.18	0.03	0.18
(1,82)	1:132:A:VAL:HG13	1:138:A:ILE:HD11	2	0.18	0.03	0.18
(1,82)	1:132:A:VAL:HG13	1:138:A:ILE:HD12	2	0.18	0.03	0.18
(1,82)	1:132:A:VAL:HG13	1:138:A:ILE:HD13	2	0.18	0.03	0.18
(1,1078)	1:141:A:LEU:H	1:142:A:ARG:HG2	2	0.18	0.0	0.18
(1,1078)	1:141:A:LEU:H	1:142:A:ARG:HG3	2	0.18	0.0	0.18
(1,388)	1:78:A:PHE:HB3	1:111:A:VAL:HG11	2	0.16	0.01	0.16
(1,388)	1:78:A:PHE:HB3	1:111:A:VAL:HG12	2	0.16	0.01	0.16
(1,388)	1:78:A:PHE:HB3	1:111:A:VAL:HG13	2	0.16	0.01	0.16
(1,824)	1:98:A:GLU:H	1:133:A:TYR:HD1	2	0.16	0.02	0.16
(1,824)	1:98:A:GLU:H	1:133:A:TYR:HD2	2	0.16	0.02	0.16
(1,1196)	1:82:A:ASN:H	1:127:A:TRP:HE1	2	0.15	0.01	0.15
(1,433)	1:84:A:VAL:HG11	1:96:A:PHE:HE1	2	0.14	0.02	0.14
(1,433)	1:84:A:VAL:HG11	1:96:A:PHE:HE2	2	0.14	0.02	0.14
(1,433)	1:84:A:VAL:HG12	1:96:A:PHE:HE1	2	0.14	0.02	0.14
(1,433)	1:84:A:VAL:HG12	1:96:A:PHE:HE2	2	0.14	0.02	0.14
(1,433)	1:84:A:VAL:HG13	1:96:A:PHE:HE1	2	0.14	0.02	0.14
(1,433)	1:84:A:VAL:HG13	1:96:A:PHE:HE2	2	0.14	0.02	0.14
(1,1072)	1:139:A:VAL:HG21	1:140:A:ALA:H	2	0.14	0.02	0.14
(1,1072)	1:139:A:VAL:HG22	1:140:A:ALA:H	2	0.14	0.02	0.14
(1,1072)	1:139:A:VAL:HG23	1:140:A:ALA:H	2	0.14	0.02	0.14

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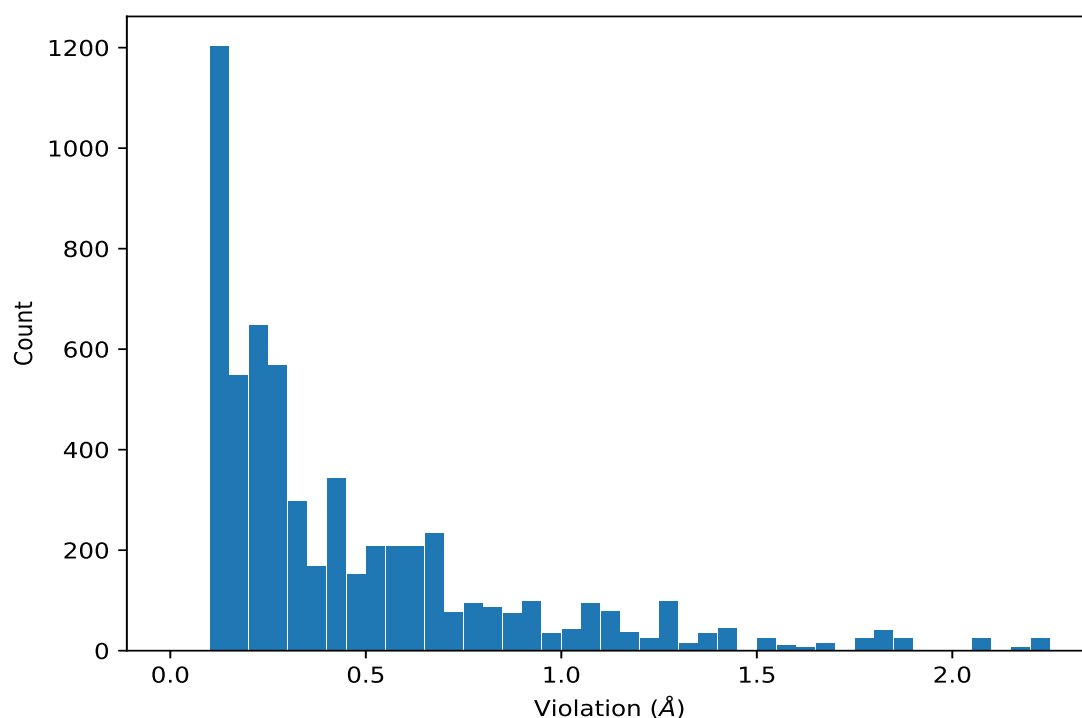
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1502)	1:138:A:ILE:H	1:141:A:LEU:HD11	2	0.14	0.0	0.14
(1,1502)	1:138:A:ILE:H	1:141:A:LEU:HD12	2	0.14	0.0	0.14
(1,1502)	1:138:A:ILE:H	1:141:A:LEU:HD13	2	0.14	0.0	0.14
(1,1502)	1:138:A:ILE:H	1:141:A:LEU:HD21	2	0.14	0.0	0.14
(1,1502)	1:138:A:ILE:H	1:141:A:LEU:HD22	2	0.14	0.0	0.14
(1,1502)	1:138:A:ILE:H	1:141:A:LEU:HD23	2	0.14	0.0	0.14
(1,596)	1:101:A:ALA:H	1:133:A:TYR:HD1	2	0.13	0.0	0.13
(1,596)	1:101:A:ALA:H	1:133:A:TYR:HD2	2	0.13	0.0	0.13
(1,162)	1:93:A:ALA:HA	1:94:A:ILE:HG21	2	0.12	0.01	0.12
(1,162)	1:93:A:ALA:HA	1:94:A:ILE:HG22	2	0.12	0.01	0.12
(1,162)	1:93:A:ALA:HA	1:94:A:ILE:HG23	2	0.12	0.01	0.12
(1,322)	1:142:A:ARG:HA	1:142:A:ARG:HD2	2	0.12	0.0	0.12
(1,322)	1:142:A:ARG:HA	1:142:A:ARG:HD3	2	0.12	0.0	0.12
(1,155)	1:90:A:ARG:HD2	1:91:A:LYS:HA	2	0.11	0.01	0.11
(1,155)	1:90:A:ARG:HD3	1:91:A:LYS:HA	2	0.11	0.01	0.11
(1,819)	1:100:A:PHE:HD1	1:104:A:LEU:H	2	0.11	0.0	0.11
(1,819)	1:100:A:PHE:HD2	1:104:A:LEU:H	2	0.11	0.0	0.11
(1,185)	1:75:A:LEU:H	1:111:A:VAL:HA	2	0.1	0.0	0.1

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1203)	1:23:A:LEU:HD11	1:27:A:LEU:HB2	6	2.22
(1,1203)	1:23:A:LEU:HD11	1:27:A:LEU:HB3	6	2.22
(1,1203)	1:23:A:LEU:HD12	1:27:A:LEU:HB2	6	2.22
(1,1203)	1:23:A:LEU:HD12	1:27:A:LEU:HB3	6	2.22
(1,1203)	1:23:A:LEU:HD13	1:27:A:LEU:HB2	6	2.22
(1,1203)	1:23:A:LEU:HD13	1:27:A:LEU:HB3	6	2.22
(1,1203)	1:23:A:LEU:HD21	1:27:A:LEU:HB2	6	2.22
(1,1203)	1:23:A:LEU:HD21	1:27:A:LEU:HB3	6	2.22
(1,1203)	1:23:A:LEU:HD22	1:27:A:LEU:HB2	6	2.22
(1,1203)	1:23:A:LEU:HD22	1:27:A:LEU:HB3	6	2.22
(1,1203)	1:23:A:LEU:HD23	1:27:A:LEU:HB2	6	2.22
(1,1203)	1:23:A:LEU:HD23	1:27:A:LEU:HB3	6	2.22
(1,1203)	1:23:A:LEU:HD11	1:27:A:LEU:HB2	12	2.2
(1,1203)	1:23:A:LEU:HD11	1:27:A:LEU:HB3	12	2.2
(1,1203)	1:23:A:LEU:HD12	1:27:A:LEU:HB2	12	2.2
(1,1203)	1:23:A:LEU:HD12	1:27:A:LEU:HB3	12	2.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1203)	1:23:A:LEU:HD13	1:27:A:LEU:HB2	12	2.2
(1,1203)	1:23:A:LEU:HD13	1:27:A:LEU:HB3	12	2.2
(1,1203)	1:23:A:LEU:HD21	1:27:A:LEU:HB2	12	2.2
(1,1203)	1:23:A:LEU:HD21	1:27:A:LEU:HB3	12	2.2
(1,1203)	1:23:A:LEU:HD22	1:27:A:LEU:HB2	12	2.2
(1,1203)	1:23:A:LEU:HD22	1:27:A:LEU:HB3	12	2.2
(1,1203)	1:23:A:LEU:HD23	1:27:A:LEU:HB2	12	2.2
(1,1203)	1:23:A:LEU:HD23	1:27:A:LEU:HB3	12	2.2
(2,12)	2:158:B:TYR:HD1	1:132:A:VAL:HG11	15	2.16
(2,12)	2:158:B:TYR:HD1	1:132:A:VAL:HG12	15	2.16
(2,12)	2:158:B:TYR:HD1	1:132:A:VAL:HG13	15	2.16
(2,12)	2:158:B:TYR:HD2	1:132:A:VAL:HG11	15	2.16
(2,12)	2:158:B:TYR:HD2	1:132:A:VAL:HG12	15	2.16
(2,12)	2:158:B:TYR:HD2	1:132:A:VAL:HG13	15	2.16
(1,1203)	1:23:A:LEU:HD11	1:27:A:LEU:HB2	17	2.09
(1,1203)	1:23:A:LEU:HD11	1:27:A:LEU:HB3	17	2.09
(1,1203)	1:23:A:LEU:HD12	1:27:A:LEU:HB2	17	2.09
(1,1203)	1:23:A:LEU:HD12	1:27:A:LEU:HB3	17	2.09
(1,1203)	1:23:A:LEU:HD13	1:27:A:LEU:HB2	17	2.09
(1,1203)	1:23:A:LEU:HD13	1:27:A:LEU:HB3	17	2.09
(1,1203)	1:23:A:LEU:HD21	1:27:A:LEU:HB2	17	2.09
(1,1203)	1:23:A:LEU:HD21	1:27:A:LEU:HB3	17	2.09
(1,1203)	1:23:A:LEU:HD22	1:27:A:LEU:HB2	17	2.09
(1,1203)	1:23:A:LEU:HD22	1:27:A:LEU:HB3	17	2.09
(1,1203)	1:23:A:LEU:HD23	1:27:A:LEU:HB2	17	2.09
(1,1203)	1:23:A:LEU:HD23	1:27:A:LEU:HB3	17	2.09
(1,1203)	1:23:A:LEU:HD11	1:27:A:LEU:HB2	13	2.07
(1,1203)	1:23:A:LEU:HD11	1:27:A:LEU:HB3	13	2.07
(1,1203)	1:23:A:LEU:HD12	1:27:A:LEU:HB2	13	2.07
(1,1203)	1:23:A:LEU:HD12	1:27:A:LEU:HB3	13	2.07
(1,1203)	1:23:A:LEU:HD13	1:27:A:LEU:HB2	13	2.07
(1,1203)	1:23:A:LEU:HD13	1:27:A:LEU:HB3	13	2.07
(1,1203)	1:23:A:LEU:HD21	1:27:A:LEU:HB2	13	2.07
(1,1203)	1:23:A:LEU:HD21	1:27:A:LEU:HB3	13	2.07
(1,1203)	1:23:A:LEU:HD22	1:27:A:LEU:HB2	13	2.07
(1,1203)	1:23:A:LEU:HD22	1:27:A:LEU:HB3	13	2.07
(1,1203)	1:23:A:LEU:HD23	1:27:A:LEU:HB2	13	2.07
(1,1203)	1:23:A:LEU:HD23	1:27:A:LEU:HB3	13	2.07
(1,1279)	1:59:A:VAL:HG11	1:103:A:VAL:HG11	3	1.9
(1,1279)	1:59:A:VAL:HG11	1:103:A:VAL:HG12	3	1.9
(1,1279)	1:59:A:VAL:HG11	1:103:A:VAL:HG13	3	1.9
(1,1279)	1:59:A:VAL:HG12	1:103:A:VAL:HG11	3	1.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1279)	1:59:A:VAL:HG12	1:103:A:VAL:HG12	3	1.9
(1,1279)	1:59:A:VAL:HG12	1:103:A:VAL:HG13	3	1.9
(1,1279)	1:59:A:VAL:HG13	1:103:A:VAL:HG11	3	1.9
(1,1279)	1:59:A:VAL:HG13	1:103:A:VAL:HG12	3	1.9
(1,1279)	1:59:A:VAL:HG13	1:103:A:VAL:HG13	3	1.9
(1,1279)	1:59:A:VAL:HG21	1:103:A:VAL:HG11	3	1.9
(1,1279)	1:59:A:VAL:HG21	1:103:A:VAL:HG12	3	1.9
(1,1279)	1:59:A:VAL:HG21	1:103:A:VAL:HG13	3	1.9
(1,1279)	1:59:A:VAL:HG22	1:103:A:VAL:HG11	3	1.9
(1,1279)	1:59:A:VAL:HG22	1:103:A:VAL:HG12	3	1.9
(1,1279)	1:59:A:VAL:HG22	1:103:A:VAL:HG13	3	1.9
(1,1279)	1:59:A:VAL:HG23	1:103:A:VAL:HG11	3	1.9
(1,1279)	1:59:A:VAL:HG23	1:103:A:VAL:HG12	3	1.9
(1,1279)	1:59:A:VAL:HG23	1:103:A:VAL:HG13	3	1.9
(6,1)	2:148:B:SER:H1	2:149:B:PRO:HA	7	1.86
(1,1202)	1:23:A:LEU:HD11	1:27:A:LEU:HA	6	1.86
(1,1202)	1:23:A:LEU:HD12	1:27:A:LEU:HA	6	1.86
(1,1202)	1:23:A:LEU:HD13	1:27:A:LEU:HA	6	1.86
(1,1202)	1:23:A:LEU:HD21	1:27:A:LEU:HA	6	1.86
(1,1202)	1:23:A:LEU:HD22	1:27:A:LEU:HA	6	1.86
(1,1202)	1:23:A:LEU:HD23	1:27:A:LEU:HA	6	1.86
(6,1)	2:148:B:SER:H1	2:149:B:PRO:HA	11	1.83
(1,1203)	1:23:A:LEU:HD11	1:27:A:LEU:HB2	16	1.83
(1,1203)	1:23:A:LEU:HD11	1:27:A:LEU:HB3	16	1.83
(1,1203)	1:23:A:LEU:HD12	1:27:A:LEU:HB2	16	1.83
(1,1203)	1:23:A:LEU:HD12	1:27:A:LEU:HB3	16	1.83
(1,1203)	1:23:A:LEU:HD13	1:27:A:LEU:HB2	16	1.83
(1,1203)	1:23:A:LEU:HD13	1:27:A:LEU:HB3	16	1.83
(1,1203)	1:23:A:LEU:HD21	1:27:A:LEU:HB2	16	1.83
(1,1203)	1:23:A:LEU:HD21	1:27:A:LEU:HB3	16	1.83
(1,1203)	1:23:A:LEU:HD22	1:27:A:LEU:HB2	16	1.83
(1,1203)	1:23:A:LEU:HD22	1:27:A:LEU:HB3	16	1.83
(1,1203)	1:23:A:LEU:HD23	1:27:A:LEU:HB2	16	1.83
(1,1203)	1:23:A:LEU:HD23	1:27:A:LEU:HB3	16	1.83
(1,1202)	1:23:A:LEU:HD11	1:27:A:LEU:HA	12	1.83
(1,1202)	1:23:A:LEU:HD12	1:27:A:LEU:HA	12	1.83
(1,1202)	1:23:A:LEU:HD13	1:27:A:LEU:HA	12	1.83
(1,1202)	1:23:A:LEU:HD21	1:27:A:LEU:HA	12	1.83
(1,1202)	1:23:A:LEU:HD22	1:27:A:LEU:HA	12	1.83
(1,1202)	1:23:A:LEU:HD23	1:27:A:LEU:HA	12	1.83
(1,1203)	1:23:A:LEU:HD11	1:27:A:LEU:HB2	3	1.82
(1,1203)	1:23:A:LEU:HD11	1:27:A:LEU:HB3	3	1.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1203)	1:23:A:LEU:HD12	1:27:A:LEU:HB2	3	1.82
(1,1203)	1:23:A:LEU:HD12	1:27:A:LEU:HB3	3	1.82
(1,1203)	1:23:A:LEU:HD13	1:27:A:LEU:HB2	3	1.82
(1,1203)	1:23:A:LEU:HD13	1:27:A:LEU:HB3	3	1.82
(1,1203)	1:23:A:LEU:HD21	1:27:A:LEU:HB2	3	1.82
(1,1203)	1:23:A:LEU:HD21	1:27:A:LEU:HB3	3	1.82
(1,1203)	1:23:A:LEU:HD22	1:27:A:LEU:HB2	3	1.82
(1,1203)	1:23:A:LEU:HD22	1:27:A:LEU:HB3	3	1.82
(1,1203)	1:23:A:LEU:HD23	1:27:A:LEU:HB2	3	1.82
(1,1203)	1:23:A:LEU:HD23	1:27:A:LEU:HB3	3	1.82
(6,1)	2:148:B:SER:H1	2:149:B:PRO:HA	5	1.81
(1,293)	1:31:A:PHE:HA	1:34:A:VAL:HG11	5	1.81
(1,293)	1:31:A:PHE:HA	1:34:A:VAL:HG12	5	1.81
(1,293)	1:31:A:PHE:HA	1:34:A:VAL:HG13	5	1.81
(1,1202)	1:23:A:LEU:HD11	1:27:A:LEU:HA	3	1.8
(1,1202)	1:23:A:LEU:HD12	1:27:A:LEU:HA	3	1.8
(1,1202)	1:23:A:LEU:HD13	1:27:A:LEU:HA	3	1.8
(1,1202)	1:23:A:LEU:HD21	1:27:A:LEU:HA	3	1.8
(1,1202)	1:23:A:LEU:HD22	1:27:A:LEU:HA	3	1.8
(1,1202)	1:23:A:LEU:HD23	1:27:A:LEU:HA	3	1.8
(1,1203)	1:23:A:LEU:HD11	1:27:A:LEU:HB2	7	1.79
(1,1203)	1:23:A:LEU:HD11	1:27:A:LEU:HB3	7	1.79
(1,1203)	1:23:A:LEU:HD12	1:27:A:LEU:HB2	7	1.79
(1,1203)	1:23:A:LEU:HD12	1:27:A:LEU:HB3	7	1.79
(1,1203)	1:23:A:LEU:HD13	1:27:A:LEU:HB2	7	1.79
(1,1203)	1:23:A:LEU:HD13	1:27:A:LEU:HB3	7	1.79
(1,1203)	1:23:A:LEU:HD21	1:27:A:LEU:HB2	7	1.79
(1,1203)	1:23:A:LEU:HD21	1:27:A:LEU:HB3	7	1.79
(1,1203)	1:23:A:LEU:HD22	1:27:A:LEU:HB2	7	1.79
(1,1203)	1:23:A:LEU:HD22	1:27:A:LEU:HB3	7	1.79
(1,1203)	1:23:A:LEU:HD23	1:27:A:LEU:HB2	7	1.79
(1,1203)	1:23:A:LEU:HD23	1:27:A:LEU:HB3	7	1.79
(2,12)	2:158:B:TYR:HD1	1:132:A:VAL:HG11	1	1.78
(2,12)	2:158:B:TYR:HD1	1:132:A:VAL:HG12	1	1.78
(2,12)	2:158:B:TYR:HD1	1:132:A:VAL:HG13	1	1.78
(2,12)	2:158:B:TYR:HD2	1:132:A:VAL:HG11	1	1.78
(2,12)	2:158:B:TYR:HD2	1:132:A:VAL:HG12	1	1.78
(2,12)	2:158:B:TYR:HD2	1:132:A:VAL:HG13	1	1.78
(1,1202)	1:23:A:LEU:HD11	1:27:A:LEU:HA	7	1.77
(1,1202)	1:23:A:LEU:HD12	1:27:A:LEU:HA	7	1.77
(1,1202)	1:23:A:LEU:HD13	1:27:A:LEU:HA	7	1.77
(1,1202)	1:23:A:LEU:HD21	1:27:A:LEU:HA	7	1.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1202)	1:23:A:LEU:HD22	1:27:A:LEU:HA	7	1.77
(1,1202)	1:23:A:LEU:HD23	1:27:A:LEU:HA	7	1.77
(6,1)	2:148:B:SER:H1	2:149:B:PRO:HA	13	1.7
(1,1203)	1:23:A:LEU:HD11	1:27:A:LEU:HB2	5	1.7
(1,1203)	1:23:A:LEU:HD11	1:27:A:LEU:HB3	5	1.7
(1,1203)	1:23:A:LEU:HD12	1:27:A:LEU:HB2	5	1.7
(1,1203)	1:23:A:LEU:HD12	1:27:A:LEU:HB3	5	1.7
(1,1203)	1:23:A:LEU:HD13	1:27:A:LEU:HB2	5	1.7
(1,1203)	1:23:A:LEU:HD13	1:27:A:LEU:HB3	5	1.7
(1,1203)	1:23:A:LEU:HD21	1:27:A:LEU:HB2	5	1.7
(1,1203)	1:23:A:LEU:HD21	1:27:A:LEU:HB3	5	1.7
(1,1203)	1:23:A:LEU:HD22	1:27:A:LEU:HB2	5	1.7
(1,1203)	1:23:A:LEU:HD22	1:27:A:LEU:HB3	5	1.7
(1,1203)	1:23:A:LEU:HD23	1:27:A:LEU:HB2	5	1.7
(1,1203)	1:23:A:LEU:HD23	1:27:A:LEU:HB3	5	1.7
(6,1)	2:148:B:SER:H1	2:149:B:PRO:HA	19	1.67
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD11	11	1.63
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD12	11	1.63
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD13	11	1.63
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD21	11	1.63
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD22	11	1.63
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD23	11	1.63
(6,1)	2:148:B:SER:H1	2:149:B:PRO:HA	6	1.61
(6,1)	2:148:B:SER:H1	2:149:B:PRO:HA	14	1.57
(1,610)	1:34:A:VAL:HG21	1:37:A:THR:H	19	1.56
(1,610)	1:34:A:VAL:HG22	1:37:A:THR:H	19	1.56
(1,610)	1:34:A:VAL:HG23	1:37:A:THR:H	19	1.56
(1,271)	1:75:A:LEU:HD21	1:78:A:PHE:HB3	13	1.55
(1,271)	1:75:A:LEU:HD22	1:78:A:PHE:HB3	13	1.55
(1,271)	1:75:A:LEU:HD23	1:78:A:PHE:HB3	13	1.55
(1,204)	1:59:A:VAL:HA	1:103:A:VAL:HG11	3	1.55
(1,204)	1:59:A:VAL:HA	1:103:A:VAL:HG12	3	1.55
(1,204)	1:59:A:VAL:HA	1:103:A:VAL:HG13	3	1.55
(2,12)	2:158:B:TYR:HD1	1:132:A:VAL:HG11	11	1.53
(2,12)	2:158:B:TYR:HD1	1:132:A:VAL:HG12	11	1.53
(2,12)	2:158:B:TYR:HD1	1:132:A:VAL:HG13	11	1.53
(2,12)	2:158:B:TYR:HD2	1:132:A:VAL:HG11	11	1.53
(2,12)	2:158:B:TYR:HD2	1:132:A:VAL:HG12	11	1.53
(2,12)	2:158:B:TYR:HD2	1:132:A:VAL:HG13	11	1.53
(1,1203)	1:23:A:LEU:HD11	1:27:A:LEU:HB2	9	1.53
(1,1203)	1:23:A:LEU:HD11	1:27:A:LEU:HB3	9	1.53
(1,1203)	1:23:A:LEU:HD12	1:27:A:LEU:HB2	9	1.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1203)	1:23:A:LEU:HD12	1:27:A:LEU:HB3	9	1.53
(1,1203)	1:23:A:LEU:HD13	1:27:A:LEU:HB2	9	1.53
(1,1203)	1:23:A:LEU:HD13	1:27:A:LEU:HB3	9	1.53
(1,1203)	1:23:A:LEU:HD21	1:27:A:LEU:HB2	9	1.53
(1,1203)	1:23:A:LEU:HD21	1:27:A:LEU:HB3	9	1.53
(1,1203)	1:23:A:LEU:HD22	1:27:A:LEU:HB2	9	1.53
(1,1203)	1:23:A:LEU:HD22	1:27:A:LEU:HB3	9	1.53
(1,1203)	1:23:A:LEU:HD23	1:27:A:LEU:HB2	9	1.53
(1,1203)	1:23:A:LEU:HD23	1:27:A:LEU:HB3	9	1.53
(1,1202)	1:23:A:LEU:HD11	1:27:A:LEU:HA	17	1.53
(1,1202)	1:23:A:LEU:HD12	1:27:A:LEU:HA	17	1.53
(1,1202)	1:23:A:LEU:HD13	1:27:A:LEU:HA	17	1.53
(1,1202)	1:23:A:LEU:HD21	1:27:A:LEU:HA	17	1.53
(1,1202)	1:23:A:LEU:HD22	1:27:A:LEU:HA	17	1.53
(1,1202)	1:23:A:LEU:HD23	1:27:A:LEU:HA	17	1.53
(1,1203)	1:23:A:LEU:HD11	1:27:A:LEU:HB2	20	1.45
(1,1203)	1:23:A:LEU:HD11	1:27:A:LEU:HB3	20	1.45
(1,1203)	1:23:A:LEU:HD12	1:27:A:LEU:HB2	20	1.45
(1,1203)	1:23:A:LEU:HD12	1:27:A:LEU:HB3	20	1.45
(1,1203)	1:23:A:LEU:HD13	1:27:A:LEU:HB2	20	1.45
(1,1203)	1:23:A:LEU:HD13	1:27:A:LEU:HB3	20	1.45
(1,1203)	1:23:A:LEU:HD21	1:27:A:LEU:HB2	20	1.45
(1,1203)	1:23:A:LEU:HD21	1:27:A:LEU:HB3	20	1.45
(1,1203)	1:23:A:LEU:HD22	1:27:A:LEU:HB2	20	1.45
(1,1203)	1:23:A:LEU:HD22	1:27:A:LEU:HB3	20	1.45
(1,1203)	1:23:A:LEU:HD23	1:27:A:LEU:HB2	20	1.45
(1,1203)	1:23:A:LEU:HD23	1:27:A:LEU:HB3	20	1.45
(1,1202)	1:23:A:LEU:HD11	1:27:A:LEU:HA	2	1.44
(1,1202)	1:23:A:LEU:HD12	1:27:A:LEU:HA	2	1.44
(1,1202)	1:23:A:LEU:HD13	1:27:A:LEU:HA	2	1.44
(1,1202)	1:23:A:LEU:HD21	1:27:A:LEU:HA	2	1.44
(1,1202)	1:23:A:LEU:HD22	1:27:A:LEU:HA	2	1.44
(1,1202)	1:23:A:LEU:HD23	1:27:A:LEU:HA	2	1.44
(1,1202)	1:23:A:LEU:HD11	1:27:A:LEU:HA	5	1.43
(1,1202)	1:23:A:LEU:HD12	1:27:A:LEU:HA	5	1.43
(1,1202)	1:23:A:LEU:HD13	1:27:A:LEU:HA	5	1.43
(1,1202)	1:23:A:LEU:HD21	1:27:A:LEU:HA	5	1.43
(1,1202)	1:23:A:LEU:HD22	1:27:A:LEU:HA	5	1.43
(1,1202)	1:23:A:LEU:HD23	1:27:A:LEU:HA	5	1.43
(1,1202)	1:23:A:LEU:HD11	1:27:A:LEU:HA	10	1.43
(1,1202)	1:23:A:LEU:HD12	1:27:A:LEU:HA	10	1.43
(1,1202)	1:23:A:LEU:HD13	1:27:A:LEU:HA	10	1.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1202)	1:23:A:LEU:HD21	1:27:A:LEU:HA	10	1.43
(1,1202)	1:23:A:LEU:HD22	1:27:A:LEU:HA	10	1.43
(1,1202)	1:23:A:LEU:HD23	1:27:A:LEU:HA	10	1.43
(6,2)	2:148:B:SER:H1	2:149:B:PRO:HG2	8	1.41
(6,2)	2:148:B:SER:H1	2:149:B:PRO:HG3	8	1.41
(2,12)	2:158:B:TYR:HD1	1:132:A:VAL:HG11	4	1.41
(2,12)	2:158:B:TYR:HD1	1:132:A:VAL:HG12	4	1.41
(2,12)	2:158:B:TYR:HD1	1:132:A:VAL:HG13	4	1.41
(2,12)	2:158:B:TYR:HD2	1:132:A:VAL:HG11	4	1.41
(2,12)	2:158:B:TYR:HD2	1:132:A:VAL:HG12	4	1.41
(2,12)	2:158:B:TYR:HD2	1:132:A:VAL:HG13	4	1.41
(1,1202)	1:23:A:LEU:HD11	1:27:A:LEU:HA	16	1.41
(1,1202)	1:23:A:LEU:HD12	1:27:A:LEU:HA	16	1.41
(1,1202)	1:23:A:LEU:HD13	1:27:A:LEU:HA	16	1.41
(1,1202)	1:23:A:LEU:HD21	1:27:A:LEU:HA	16	1.41
(1,1202)	1:23:A:LEU:HD22	1:27:A:LEU:HA	16	1.41
(1,1202)	1:23:A:LEU:HD23	1:27:A:LEU:HA	16	1.41
(6,2)	2:148:B:SER:H1	2:149:B:PRO:HG2	12	1.4
(6,2)	2:148:B:SER:H1	2:149:B:PRO:HG3	12	1.4
(1,1202)	1:23:A:LEU:HD11	1:27:A:LEU:HA	13	1.4
(1,1202)	1:23:A:LEU:HD12	1:27:A:LEU:HA	13	1.4
(1,1202)	1:23:A:LEU:HD13	1:27:A:LEU:HA	13	1.4
(1,1202)	1:23:A:LEU:HD21	1:27:A:LEU:HA	13	1.4
(1,1202)	1:23:A:LEU:HD22	1:27:A:LEU:HA	13	1.4
(1,1202)	1:23:A:LEU:HD23	1:27:A:LEU:HA	13	1.4
(6,2)	2:148:B:SER:H1	2:149:B:PRO:HG2	13	1.38
(6,2)	2:148:B:SER:H1	2:149:B:PRO:HG3	13	1.38
(1,1203)	1:23:A:LEU:HD11	1:27:A:LEU:HB2	1	1.36
(1,1203)	1:23:A:LEU:HD11	1:27:A:LEU:HB3	1	1.36
(1,1203)	1:23:A:LEU:HD12	1:27:A:LEU:HB2	1	1.36
(1,1203)	1:23:A:LEU:HD12	1:27:A:LEU:HB3	1	1.36
(1,1203)	1:23:A:LEU:HD13	1:27:A:LEU:HB2	1	1.36
(1,1203)	1:23:A:LEU:HD13	1:27:A:LEU:HB3	1	1.36
(1,1203)	1:23:A:LEU:HD21	1:27:A:LEU:HB2	1	1.36
(1,1203)	1:23:A:LEU:HD21	1:27:A:LEU:HB3	1	1.36
(1,1203)	1:23:A:LEU:HD22	1:27:A:LEU:HB2	1	1.36
(1,1203)	1:23:A:LEU:HD22	1:27:A:LEU:HB3	1	1.36
(1,1203)	1:23:A:LEU:HD23	1:27:A:LEU:HB2	1	1.36
(1,1203)	1:23:A:LEU:HD23	1:27:A:LEU:HB3	1	1.36
(1,1203)	1:23:A:LEU:HD11	1:27:A:LEU:HB2	4	1.35
(1,1203)	1:23:A:LEU:HD11	1:27:A:LEU:HB3	4	1.35
(1,1203)	1:23:A:LEU:HD12	1:27:A:LEU:HB2	4	1.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1203)	1:23:A:LEU:HD12	1:27:A:LEU:HB3	4	1.35
(1,1203)	1:23:A:LEU:HD13	1:27:A:LEU:HB2	4	1.35
(1,1203)	1:23:A:LEU:HD13	1:27:A:LEU:HB3	4	1.35
(1,1203)	1:23:A:LEU:HD21	1:27:A:LEU:HB2	4	1.35
(1,1203)	1:23:A:LEU:HD21	1:27:A:LEU:HB3	4	1.35
(1,1203)	1:23:A:LEU:HD22	1:27:A:LEU:HB2	4	1.35
(1,1203)	1:23:A:LEU:HD22	1:27:A:LEU:HB3	4	1.35
(1,1203)	1:23:A:LEU:HD23	1:27:A:LEU:HB2	4	1.35
(1,1203)	1:23:A:LEU:HD23	1:27:A:LEU:HB3	4	1.35
(1,1203)	1:23:A:LEU:HD11	1:27:A:LEU:HB2	10	1.33
(1,1203)	1:23:A:LEU:HD11	1:27:A:LEU:HB3	10	1.33
(1,1203)	1:23:A:LEU:HD12	1:27:A:LEU:HB2	10	1.33
(1,1203)	1:23:A:LEU:HD12	1:27:A:LEU:HB3	10	1.33
(1,1203)	1:23:A:LEU:HD13	1:27:A:LEU:HB2	10	1.33
(1,1203)	1:23:A:LEU:HD13	1:27:A:LEU:HB3	10	1.33
(1,1203)	1:23:A:LEU:HD21	1:27:A:LEU:HB2	10	1.33
(1,1203)	1:23:A:LEU:HD21	1:27:A:LEU:HB3	10	1.33
(1,1203)	1:23:A:LEU:HD22	1:27:A:LEU:HB2	10	1.33
(1,1203)	1:23:A:LEU:HD22	1:27:A:LEU:HB3	10	1.33
(1,1203)	1:23:A:LEU:HD23	1:27:A:LEU:HB2	10	1.33
(1,1203)	1:23:A:LEU:HD23	1:27:A:LEU:HB3	10	1.33
(1,308)	1:103:A:VAL:HG21	1:107:A:ALA:HA	3	1.33
(1,308)	1:103:A:VAL:HG22	1:107:A:ALA:HA	3	1.33
(1,308)	1:103:A:VAL:HG23	1:107:A:ALA:HA	3	1.33
(1,1203)	1:23:A:LEU:HD11	1:27:A:LEU:HB2	2	1.29
(1,1203)	1:23:A:LEU:HD11	1:27:A:LEU:HB3	2	1.29
(1,1203)	1:23:A:LEU:HD12	1:27:A:LEU:HB2	2	1.29
(1,1203)	1:23:A:LEU:HD12	1:27:A:LEU:HB3	2	1.29
(1,1203)	1:23:A:LEU:HD13	1:27:A:LEU:HB2	2	1.29
(1,1203)	1:23:A:LEU:HD13	1:27:A:LEU:HB3	2	1.29
(1,1203)	1:23:A:LEU:HD21	1:27:A:LEU:HB2	2	1.29
(1,1203)	1:23:A:LEU:HD21	1:27:A:LEU:HB3	2	1.29
(1,1203)	1:23:A:LEU:HD22	1:27:A:LEU:HB2	2	1.29
(1,1203)	1:23:A:LEU:HD22	1:27:A:LEU:HB3	2	1.29
(1,1203)	1:23:A:LEU:HD23	1:27:A:LEU:HB2	2	1.29
(1,1203)	1:23:A:LEU:HD23	1:27:A:LEU:HB3	2	1.29
(1,293)	1:31:A:PHE:HA	1:34:A:VAL:HG11	3	1.29
(1,293)	1:31:A:PHE:HA	1:34:A:VAL:HG12	3	1.29
(1,293)	1:31:A:PHE:HA	1:34:A:VAL:HG13	3	1.29
(2,12)	2:158:B:TYR:HD1	1:132:A:VAL:HG11	19	1.28
(2,12)	2:158:B:TYR:HD1	1:132:A:VAL:HG12	19	1.28
(2,12)	2:158:B:TYR:HD1	1:132:A:VAL:HG13	19	1.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,12)	2:158:B:TYR:HD2	1:132:A:VAL:HG11	19	1.28
(2,12)	2:158:B:TYR:HD2	1:132:A:VAL:HG12	19	1.28
(2,12)	2:158:B:TYR:HD2	1:132:A:VAL:HG13	19	1.28
(1,1422)	1:112:A:LYS:H	1:145:A:LEU:HD11	10	1.28
(1,1422)	1:112:A:LYS:H	1:145:A:LEU:HD12	10	1.28
(1,1422)	1:112:A:LYS:H	1:145:A:LEU:HD13	10	1.28
(1,1422)	1:112:A:LYS:H	1:145:A:LEU:HD21	10	1.28
(1,1422)	1:112:A:LYS:H	1:145:A:LEU:HD22	10	1.28
(1,1422)	1:112:A:LYS:H	1:145:A:LEU:HD23	10	1.28
(1,1168)	1:33:A:SER:H	1:34:A:VAL:HG11	19	1.28
(1,1168)	1:33:A:SER:H	1:34:A:VAL:HG12	19	1.28
(1,1168)	1:33:A:SER:H	1:34:A:VAL:HG13	19	1.28
(1,1410)	1:108:A:ALA:HB1	1:145:A:LEU:HD11	10	1.27
(1,1410)	1:108:A:ALA:HB1	1:145:A:LEU:HD12	10	1.27
(1,1410)	1:108:A:ALA:HB1	1:145:A:LEU:HD13	10	1.27
(1,1410)	1:108:A:ALA:HB1	1:145:A:LEU:HD21	10	1.27
(1,1410)	1:108:A:ALA:HB1	1:145:A:LEU:HD22	10	1.27
(1,1410)	1:108:A:ALA:HB1	1:145:A:LEU:HD23	10	1.27
(1,1410)	1:108:A:ALA:HB2	1:145:A:LEU:HD11	10	1.27
(1,1410)	1:108:A:ALA:HB2	1:145:A:LEU:HD12	10	1.27
(1,1410)	1:108:A:ALA:HB2	1:145:A:LEU:HD13	10	1.27
(1,1410)	1:108:A:ALA:HB2	1:145:A:LEU:HD21	10	1.27
(1,1410)	1:108:A:ALA:HB2	1:145:A:LEU:HD22	10	1.27
(1,1410)	1:108:A:ALA:HB2	1:145:A:LEU:HD23	10	1.27
(1,1410)	1:108:A:ALA:HB3	1:145:A:LEU:HD11	10	1.27
(1,1410)	1:108:A:ALA:HB3	1:145:A:LEU:HD12	10	1.27
(1,1410)	1:108:A:ALA:HB3	1:145:A:LEU:HD13	10	1.27
(1,1410)	1:108:A:ALA:HB3	1:145:A:LEU:HD21	10	1.27
(1,1410)	1:108:A:ALA:HB3	1:145:A:LEU:HD22	10	1.27
(1,1410)	1:108:A:ALA:HB3	1:145:A:LEU:HD23	10	1.27
(1,1403)	1:104:A:LEU:HD11	1:141:A:LEU:HG	18	1.27
(1,1403)	1:104:A:LEU:HD12	1:141:A:LEU:HG	18	1.27
(1,1403)	1:104:A:LEU:HD13	1:141:A:LEU:HG	18	1.27
(1,1403)	1:104:A:LEU:HD21	1:141:A:LEU:HG	18	1.27
(1,1403)	1:104:A:LEU:HD22	1:141:A:LEU:HG	18	1.27
(1,1403)	1:104:A:LEU:HD23	1:141:A:LEU:HG	18	1.27
(1,1229)	1:45:A:SER:HB2	1:80:A:LEU:HD11	11	1.27
(1,1229)	1:45:A:SER:HB2	1:80:A:LEU:HD12	11	1.27
(1,1229)	1:45:A:SER:HB2	1:80:A:LEU:HD13	11	1.27
(1,1229)	1:45:A:SER:HB2	1:80:A:LEU:HD21	11	1.27
(1,1229)	1:45:A:SER:HB2	1:80:A:LEU:HD22	11	1.27
(1,1229)	1:45:A:SER:HB2	1:80:A:LEU:HD23	11	1.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1229)	1:45:A:SER:HB3	1:80:A:LEU:HD11	11	1.27
(1,1229)	1:45:A:SER:HB3	1:80:A:LEU:HD12	11	1.27
(1,1229)	1:45:A:SER:HB3	1:80:A:LEU:HD13	11	1.27
(1,1229)	1:45:A:SER:HB3	1:80:A:LEU:HD21	11	1.27
(1,1229)	1:45:A:SER:HB3	1:80:A:LEU:HD22	11	1.27
(1,1229)	1:45:A:SER:HB3	1:80:A:LEU:HD23	11	1.27
(1,1202)	1:23:A:LEU:HD11	1:27:A:LEU:HA	4	1.27
(1,1202)	1:23:A:LEU:HD12	1:27:A:LEU:HA	4	1.27
(1,1202)	1:23:A:LEU:HD13	1:27:A:LEU:HA	4	1.27
(1,1202)	1:23:A:LEU:HD21	1:27:A:LEU:HA	4	1.27
(1,1202)	1:23:A:LEU:HD22	1:27:A:LEU:HA	4	1.27
(1,1202)	1:23:A:LEU:HD23	1:27:A:LEU:HA	4	1.27
(1,1403)	1:104:A:LEU:HD11	1:141:A:LEU:HG	19	1.26
(1,1403)	1:104:A:LEU:HD12	1:141:A:LEU:HG	19	1.26
(1,1403)	1:104:A:LEU:HD13	1:141:A:LEU:HG	19	1.26
(1,1403)	1:104:A:LEU:HD21	1:141:A:LEU:HG	19	1.26
(1,1403)	1:104:A:LEU:HD22	1:141:A:LEU:HG	19	1.26
(1,1403)	1:104:A:LEU:HD23	1:141:A:LEU:HG	19	1.26
(1,1203)	1:23:A:LEU:HD11	1:27:A:LEU:HB2	11	1.25
(1,1203)	1:23:A:LEU:HD11	1:27:A:LEU:HB3	11	1.25
(1,1203)	1:23:A:LEU:HD12	1:27:A:LEU:HB2	11	1.25
(1,1203)	1:23:A:LEU:HD12	1:27:A:LEU:HB3	11	1.25
(1,1203)	1:23:A:LEU:HD13	1:27:A:LEU:HB2	11	1.25
(1,1203)	1:23:A:LEU:HD13	1:27:A:LEU:HB3	11	1.25
(1,1203)	1:23:A:LEU:HD21	1:27:A:LEU:HB2	11	1.25
(1,1203)	1:23:A:LEU:HD21	1:27:A:LEU:HB3	11	1.25
(1,1203)	1:23:A:LEU:HD22	1:27:A:LEU:HB2	11	1.25
(1,1203)	1:23:A:LEU:HD22	1:27:A:LEU:HB3	11	1.25
(1,1203)	1:23:A:LEU:HD23	1:27:A:LEU:HB2	11	1.25
(1,1203)	1:23:A:LEU:HD23	1:27:A:LEU:HB3	11	1.25
(1,278)	1:103:A:VAL:HG21	1:107:A:ALA:HB1	3	1.25
(1,278)	1:103:A:VAL:HG21	1:107:A:ALA:HB2	3	1.25
(1,278)	1:103:A:VAL:HG21	1:107:A:ALA:HB3	3	1.25
(1,278)	1:103:A:VAL:HG22	1:107:A:ALA:HB1	3	1.25
(1,278)	1:103:A:VAL:HG22	1:107:A:ALA:HB2	3	1.25
(1,278)	1:103:A:VAL:HG22	1:107:A:ALA:HB3	3	1.25
(1,278)	1:103:A:VAL:HG23	1:107:A:ALA:HB1	3	1.25
(1,278)	1:103:A:VAL:HG23	1:107:A:ALA:HB2	3	1.25
(1,278)	1:103:A:VAL:HG23	1:107:A:ALA:HB3	3	1.25
(1,1410)	1:108:A:ALA:HB1	1:145:A:LEU:HD11	16	1.22
(1,1410)	1:108:A:ALA:HB1	1:145:A:LEU:HD12	16	1.22
(1,1410)	1:108:A:ALA:HB1	1:145:A:LEU:HD13	16	1.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1410)	1:108:A:ALA:HB1	1:145:A:LEU:HD21	16	1.22
(1,1410)	1:108:A:ALA:HB1	1:145:A:LEU:HD22	16	1.22
(1,1410)	1:108:A:ALA:HB1	1:145:A:LEU:HD23	16	1.22
(1,1410)	1:108:A:ALA:HB2	1:145:A:LEU:HD11	16	1.22
(1,1410)	1:108:A:ALA:HB2	1:145:A:LEU:HD12	16	1.22
(1,1410)	1:108:A:ALA:HB2	1:145:A:LEU:HD13	16	1.22
(1,1410)	1:108:A:ALA:HB2	1:145:A:LEU:HD21	16	1.22
(1,1410)	1:108:A:ALA:HB2	1:145:A:LEU:HD22	16	1.22
(1,1410)	1:108:A:ALA:HB2	1:145:A:LEU:HD23	16	1.22
(1,1410)	1:108:A:ALA:HB3	1:145:A:LEU:HD11	16	1.22
(1,1410)	1:108:A:ALA:HB3	1:145:A:LEU:HD12	16	1.22
(1,1410)	1:108:A:ALA:HB3	1:145:A:LEU:HD13	16	1.22
(1,1410)	1:108:A:ALA:HB3	1:145:A:LEU:HD21	16	1.22
(1,1410)	1:108:A:ALA:HB3	1:145:A:LEU:HD22	16	1.22
(1,1410)	1:108:A:ALA:HB3	1:145:A:LEU:HD23	16	1.22
(1,1403)	1:104:A:LEU:HD11	1:141:A:LEU:HG	14	1.21
(1,1403)	1:104:A:LEU:HD12	1:141:A:LEU:HG	14	1.21
(1,1403)	1:104:A:LEU:HD13	1:141:A:LEU:HG	14	1.21
(1,1403)	1:104:A:LEU:HD21	1:141:A:LEU:HG	14	1.21
(1,1403)	1:104:A:LEU:HD22	1:141:A:LEU:HG	14	1.21
(1,1403)	1:104:A:LEU:HD23	1:141:A:LEU:HG	14	1.21
(1,1403)	1:104:A:LEU:HD11	1:141:A:LEU:HG	20	1.19
(1,1403)	1:104:A:LEU:HD12	1:141:A:LEU:HG	20	1.19
(1,1403)	1:104:A:LEU:HD13	1:141:A:LEU:HG	20	1.19
(1,1403)	1:104:A:LEU:HD21	1:141:A:LEU:HG	20	1.19
(1,1403)	1:104:A:LEU:HD22	1:141:A:LEU:HG	20	1.19
(1,1403)	1:104:A:LEU:HD23	1:141:A:LEU:HG	20	1.19
(1,1229)	1:45:A:SER:HB2	1:80:A:LEU:HD11	14	1.19
(1,1229)	1:45:A:SER:HB2	1:80:A:LEU:HD12	14	1.19
(1,1229)	1:45:A:SER:HB2	1:80:A:LEU:HD13	14	1.19
(1,1229)	1:45:A:SER:HB2	1:80:A:LEU:HD21	14	1.19
(1,1229)	1:45:A:SER:HB2	1:80:A:LEU:HD22	14	1.19
(1,1229)	1:45:A:SER:HB2	1:80:A:LEU:HD23	14	1.19
(1,1229)	1:45:A:SER:HB3	1:80:A:LEU:HD11	14	1.19
(1,1229)	1:45:A:SER:HB3	1:80:A:LEU:HD12	14	1.19
(1,1229)	1:45:A:SER:HB3	1:80:A:LEU:HD13	14	1.19
(1,1229)	1:45:A:SER:HB3	1:80:A:LEU:HD21	14	1.19
(1,1229)	1:45:A:SER:HB3	1:80:A:LEU:HD22	14	1.19
(1,1229)	1:45:A:SER:HB3	1:80:A:LEU:HD23	14	1.19
(1,290)	1:101:A:ALA:HA	1:137:A:MET:HB3	14	1.18
(1,1422)	1:112:A:LYS:H	1:145:A:LEU:HD11	14	1.17
(1,1422)	1:112:A:LYS:H	1:145:A:LEU:HD12	14	1.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1422)	1:112:A:LYS:H	1:145:A:LEU:HD13	14	1.17
(1,1422)	1:112:A:LYS:H	1:145:A:LEU:HD21	14	1.17
(1,1422)	1:112:A:LYS:H	1:145:A:LEU:HD22	14	1.17
(1,1422)	1:112:A:LYS:H	1:145:A:LEU:HD23	14	1.17
(1,1403)	1:104:A:LEU:HD11	1:141:A:LEU:HG	13	1.17
(1,1403)	1:104:A:LEU:HD12	1:141:A:LEU:HG	13	1.17
(1,1403)	1:104:A:LEU:HD13	1:141:A:LEU:HG	13	1.17
(1,1403)	1:104:A:LEU:HD21	1:141:A:LEU:HG	13	1.17
(1,1403)	1:104:A:LEU:HD22	1:141:A:LEU:HG	13	1.17
(1,1403)	1:104:A:LEU:HD23	1:141:A:LEU:HG	13	1.17
(1,1455)	1:120:A:VAL:HB	1:145:A:LEU:HD11	20	1.16
(1,1455)	1:120:A:VAL:HB	1:145:A:LEU:HD12	20	1.16
(1,1455)	1:120:A:VAL:HB	1:145:A:LEU:HD13	20	1.16
(1,1455)	1:120:A:VAL:HB	1:145:A:LEU:HD21	20	1.16
(1,1455)	1:120:A:VAL:HB	1:145:A:LEU:HD22	20	1.16
(1,1455)	1:120:A:VAL:HB	1:145:A:LEU:HD23	20	1.16
(1,1293)	1:63:A:MET:HG2	1:77:A:LEU:HD11	7	1.15
(1,1293)	1:63:A:MET:HG2	1:77:A:LEU:HD12	7	1.15
(1,1293)	1:63:A:MET:HG2	1:77:A:LEU:HD13	7	1.15
(1,1293)	1:63:A:MET:HG2	1:77:A:LEU:HD21	7	1.15
(1,1293)	1:63:A:MET:HG2	1:77:A:LEU:HD22	7	1.15
(1,1293)	1:63:A:MET:HG2	1:77:A:LEU:HD23	7	1.15
(1,1293)	1:63:A:MET:HG3	1:77:A:LEU:HD11	7	1.15
(1,1293)	1:63:A:MET:HG3	1:77:A:LEU:HD12	7	1.15
(1,1293)	1:63:A:MET:HG3	1:77:A:LEU:HD13	7	1.15
(1,1293)	1:63:A:MET:HG3	1:77:A:LEU:HD21	7	1.15
(1,1293)	1:63:A:MET:HG3	1:77:A:LEU:HD22	7	1.15
(1,1293)	1:63:A:MET:HG3	1:77:A:LEU:HD23	7	1.15
(1,370)	1:102:A:ASP:HA	1:103:A:VAL:HG11	3	1.15
(1,370)	1:102:A:ASP:HA	1:103:A:VAL:HG12	3	1.15
(1,370)	1:102:A:ASP:HA	1:103:A:VAL:HG13	3	1.15
(1,1432)	1:113:A:ASP:H	1:145:A:LEU:HD11	13	1.14
(1,1432)	1:113:A:ASP:H	1:145:A:LEU:HD12	13	1.14
(1,1432)	1:113:A:ASP:H	1:145:A:LEU:HD13	13	1.14
(1,1432)	1:113:A:ASP:H	1:145:A:LEU:HD21	13	1.14
(1,1432)	1:113:A:ASP:H	1:145:A:LEU:HD22	13	1.14
(1,1432)	1:113:A:ASP:H	1:145:A:LEU:HD23	13	1.14
(1,648)	1:75:A:LEU:HD11	1:120:A:VAL:H	18	1.14
(1,648)	1:75:A:LEU:HD12	1:120:A:VAL:H	18	1.14
(1,648)	1:75:A:LEU:HD13	1:120:A:VAL:H	18	1.14
(1,574)	1:108:A:ALA:H	1:111:A:VAL:HG11	17	1.14
(1,574)	1:108:A:ALA:H	1:111:A:VAL:HG12	17	1.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,574)	1:108:A:ALA:H	1:111:A:VAL:HG13	17	1.14
(1,17)	1:78:A:PHE:HB3	1:120:A:VAL:HG21	14	1.14
(1,17)	1:78:A:PHE:HB3	1:120:A:VAL:HG22	14	1.14
(1,17)	1:78:A:PHE:HB3	1:120:A:VAL:HG23	14	1.14
(1,1422)	1:112:A:LYS:H	1:145:A:LEU:HD11	16	1.13
(1,1422)	1:112:A:LYS:H	1:145:A:LEU:HD12	16	1.13
(1,1422)	1:112:A:LYS:H	1:145:A:LEU:HD13	16	1.13
(1,1422)	1:112:A:LYS:H	1:145:A:LEU:HD21	16	1.13
(1,1422)	1:112:A:LYS:H	1:145:A:LEU:HD22	16	1.13
(1,1422)	1:112:A:LYS:H	1:145:A:LEU:HD23	16	1.13
(1,1410)	1:108:A:ALA:HB1	1:145:A:LEU:HD11	14	1.13
(1,1410)	1:108:A:ALA:HB1	1:145:A:LEU:HD12	14	1.13
(1,1410)	1:108:A:ALA:HB1	1:145:A:LEU:HD13	14	1.13
(1,1410)	1:108:A:ALA:HB1	1:145:A:LEU:HD21	14	1.13
(1,1410)	1:108:A:ALA:HB1	1:145:A:LEU:HD22	14	1.13
(1,1410)	1:108:A:ALA:HB1	1:145:A:LEU:HD23	14	1.13
(1,1410)	1:108:A:ALA:HB2	1:145:A:LEU:HD11	14	1.13
(1,1410)	1:108:A:ALA:HB2	1:145:A:LEU:HD12	14	1.13
(1,1410)	1:108:A:ALA:HB2	1:145:A:LEU:HD13	14	1.13
(1,1410)	1:108:A:ALA:HB2	1:145:A:LEU:HD21	14	1.13
(1,1410)	1:108:A:ALA:HB2	1:145:A:LEU:HD22	14	1.13
(1,1410)	1:108:A:ALA:HB2	1:145:A:LEU:HD23	14	1.13
(1,1410)	1:108:A:ALA:HB3	1:145:A:LEU:HD11	14	1.13
(1,1410)	1:108:A:ALA:HB3	1:145:A:LEU:HD12	14	1.13
(1,1410)	1:108:A:ALA:HB3	1:145:A:LEU:HD13	14	1.13
(1,1410)	1:108:A:ALA:HB3	1:145:A:LEU:HD21	14	1.13
(1,1410)	1:108:A:ALA:HB3	1:145:A:LEU:HD22	14	1.13
(1,1410)	1:108:A:ALA:HB3	1:145:A:LEU:HD23	14	1.13
(4,1)	2:151:B:TYR:HH	1:82:A:ASN:ND2	20	1.12
(2,12)	2:158:B:TYR:HD1	1:132:A:VAL:HG11	2	1.12
(2,12)	2:158:B:TYR:HD1	1:132:A:VAL:HG12	2	1.12
(2,12)	2:158:B:TYR:HD1	1:132:A:VAL:HG13	2	1.12
(2,12)	2:158:B:TYR:HD2	1:132:A:VAL:HG11	2	1.12
(2,12)	2:158:B:TYR:HD2	1:132:A:VAL:HG12	2	1.12
(2,12)	2:158:B:TYR:HD2	1:132:A:VAL:HG13	2	1.12
(1,1403)	1:104:A:LEU:HD11	1:141:A:LEU:HG	16	1.12
(1,1403)	1:104:A:LEU:HD12	1:141:A:LEU:HG	16	1.12
(1,1403)	1:104:A:LEU:HD13	1:141:A:LEU:HG	16	1.12
(1,1403)	1:104:A:LEU:HD21	1:141:A:LEU:HG	16	1.12
(1,1403)	1:104:A:LEU:HD22	1:141:A:LEU:HG	16	1.12
(1,1403)	1:104:A:LEU:HD23	1:141:A:LEU:HG	16	1.12
(1,954)	1:104:A:LEU:HD11	1:106:A:GLU:H	4	1.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,954)	1:104:A:LEU:HD12	1:106:A:GLU:H	4	1.12
(1,954)	1:104:A:LEU:HD13	1:106:A:GLU:H	4	1.12
(1,1432)	1:113:A:ASP:H	1:145:A:LEU:HD11	14	1.1
(1,1432)	1:113:A:ASP:H	1:145:A:LEU:HD12	14	1.1
(1,1432)	1:113:A:ASP:H	1:145:A:LEU:HD13	14	1.1
(1,1432)	1:113:A:ASP:H	1:145:A:LEU:HD21	14	1.1
(1,1432)	1:113:A:ASP:H	1:145:A:LEU:HD22	14	1.1
(1,1432)	1:113:A:ASP:H	1:145:A:LEU:HD23	14	1.1
(1,954)	1:104:A:LEU:HD11	1:106:A:GLU:H	9	1.1
(1,954)	1:104:A:LEU:HD12	1:106:A:GLU:H	9	1.1
(1,954)	1:104:A:LEU:HD13	1:106:A:GLU:H	9	1.1
(1,1432)	1:113:A:ASP:H	1:145:A:LEU:HD11	10	1.09
(1,1432)	1:113:A:ASP:H	1:145:A:LEU:HD12	10	1.09
(1,1432)	1:113:A:ASP:H	1:145:A:LEU:HD13	10	1.09
(1,1432)	1:113:A:ASP:H	1:145:A:LEU:HD21	10	1.09
(1,1432)	1:113:A:ASP:H	1:145:A:LEU:HD22	10	1.09
(1,1432)	1:113:A:ASP:H	1:145:A:LEU:HD23	10	1.09
(1,575)	1:104:A:LEU:HD11	1:108:A:ALA:H	9	1.09
(1,575)	1:104:A:LEU:HD12	1:108:A:ALA:H	9	1.09
(1,575)	1:104:A:LEU:HD13	1:108:A:ALA:H	9	1.09
(1,293)	1:31:A:PHE:HA	1:34:A:VAL:HG11	19	1.09
(1,293)	1:31:A:PHE:HA	1:34:A:VAL:HG12	19	1.09
(1,293)	1:31:A:PHE:HA	1:34:A:VAL:HG13	19	1.09
(6,2)	2:148:B:SER:H1	2:149:B:PRO:HG2	19	1.08
(6,2)	2:148:B:SER:H1	2:149:B:PRO:HG3	19	1.08
(4,1)	2:151:B:TYR:HH	1:82:A:ASN:ND2	7	1.08
(1,1202)	1:23:A:LEU:HD11	1:27:A:LEU:HA	9	1.08
(1,1202)	1:23:A:LEU:HD12	1:27:A:LEU:HA	9	1.08
(1,1202)	1:23:A:LEU:HD13	1:27:A:LEU:HA	9	1.08
(1,1202)	1:23:A:LEU:HD21	1:27:A:LEU:HA	9	1.08
(1,1202)	1:23:A:LEU:HD22	1:27:A:LEU:HA	9	1.08
(1,1202)	1:23:A:LEU:HD23	1:27:A:LEU:HA	9	1.08
(1,950)	1:103:A:VAL:HG21	1:107:A:ALA:H	3	1.08
(1,950)	1:103:A:VAL:HG22	1:107:A:ALA:H	3	1.08
(1,950)	1:103:A:VAL:HG23	1:107:A:ALA:H	3	1.08
(1,648)	1:75:A:LEU:HD11	1:120:A:VAL:H	9	1.08
(1,648)	1:75:A:LEU:HD12	1:120:A:VAL:H	9	1.08
(1,648)	1:75:A:LEU:HD13	1:120:A:VAL:H	9	1.08
(6,3)	2:148:B:SER:H1	2:149:B:PRO:HB2	12	1.07
(6,3)	2:148:B:SER:H1	2:149:B:PRO:HB3	12	1.07
(1,1455)	1:120:A:VAL:HB	1:145:A:LEU:HD11	14	1.06
(1,1455)	1:120:A:VAL:HB	1:145:A:LEU:HD12	14	1.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1455)	1:120:A:VAL:HB	1:145:A:LEU:HD13	14	1.06
(1,1455)	1:120:A:VAL:HB	1:145:A:LEU:HD21	14	1.06
(1,1455)	1:120:A:VAL:HB	1:145:A:LEU:HD22	14	1.06
(1,1455)	1:120:A:VAL:HB	1:145:A:LEU:HD23	14	1.06
(1,1403)	1:104:A:LEU:HD11	1:141:A:LEU:HG	5	1.06
(1,1403)	1:104:A:LEU:HD12	1:141:A:LEU:HG	5	1.06
(1,1403)	1:104:A:LEU:HD13	1:141:A:LEU:HG	5	1.06
(1,1403)	1:104:A:LEU:HD21	1:141:A:LEU:HG	5	1.06
(1,1403)	1:104:A:LEU:HD22	1:141:A:LEU:HG	5	1.06
(1,1403)	1:104:A:LEU:HD23	1:141:A:LEU:HG	5	1.06
(1,1403)	1:104:A:LEU:HD11	1:141:A:LEU:HG	17	1.06
(1,1403)	1:104:A:LEU:HD12	1:141:A:LEU:HG	17	1.06
(1,1403)	1:104:A:LEU:HD13	1:141:A:LEU:HG	17	1.06
(1,1403)	1:104:A:LEU:HD21	1:141:A:LEU:HG	17	1.06
(1,1403)	1:104:A:LEU:HD22	1:141:A:LEU:HG	17	1.06
(1,1403)	1:104:A:LEU:HD23	1:141:A:LEU:HG	17	1.06
(1,1294)	1:63:A:MET:HG2	1:103:A:VAL:HG11	5	1.06
(1,1294)	1:63:A:MET:HG2	1:103:A:VAL:HG12	5	1.06
(1,1294)	1:63:A:MET:HG2	1:103:A:VAL:HG13	5	1.06
(1,1294)	1:63:A:MET:HG3	1:103:A:VAL:HG11	5	1.06
(1,1294)	1:63:A:MET:HG3	1:103:A:VAL:HG12	5	1.06
(1,1294)	1:63:A:MET:HG3	1:103:A:VAL:HG13	5	1.06
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD11	15	1.06
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD12	15	1.06
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD13	15	1.06
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD21	15	1.06
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD22	15	1.06
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD23	15	1.06
(1,954)	1:104:A:LEU:HD11	1:106:A:GLU:H	7	1.06
(1,954)	1:104:A:LEU:HD12	1:106:A:GLU:H	7	1.06
(1,954)	1:104:A:LEU:HD13	1:106:A:GLU:H	7	1.06
(1,1432)	1:113:A:ASP:H	1:145:A:LEU:HD11	3	1.05
(1,1432)	1:113:A:ASP:H	1:145:A:LEU:HD12	3	1.05
(1,1432)	1:113:A:ASP:H	1:145:A:LEU:HD13	3	1.05
(1,1432)	1:113:A:ASP:H	1:145:A:LEU:HD21	3	1.05
(1,1432)	1:113:A:ASP:H	1:145:A:LEU:HD22	3	1.05
(1,1432)	1:113:A:ASP:H	1:145:A:LEU:HD23	3	1.05
(1,1403)	1:104:A:LEU:HD11	1:141:A:LEU:HG	1	1.05
(1,1403)	1:104:A:LEU:HD12	1:141:A:LEU:HG	1	1.05
(1,1403)	1:104:A:LEU:HD13	1:141:A:LEU:HG	1	1.05
(1,1403)	1:104:A:LEU:HD21	1:141:A:LEU:HG	1	1.05
(1,1403)	1:104:A:LEU:HD22	1:141:A:LEU:HG	1	1.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1403)	1:104:A:LEU:HD23	1:141:A:LEU:HG	1	1.05
(1,1265)	1:59:A:VAL:HG11	1:63:A:MET:HG2	5	1.05
(1,1265)	1:59:A:VAL:HG11	1:63:A:MET:HG3	5	1.05
(1,1265)	1:59:A:VAL:HG12	1:63:A:MET:HG2	5	1.05
(1,1265)	1:59:A:VAL:HG12	1:63:A:MET:HG3	5	1.05
(1,1265)	1:59:A:VAL:HG13	1:63:A:MET:HG2	5	1.05
(1,1265)	1:59:A:VAL:HG13	1:63:A:MET:HG3	5	1.05
(1,1265)	1:59:A:VAL:HG21	1:63:A:MET:HG2	5	1.05
(1,1265)	1:59:A:VAL:HG21	1:63:A:MET:HG3	5	1.05
(1,1265)	1:59:A:VAL:HG22	1:63:A:MET:HG2	5	1.05
(1,1265)	1:59:A:VAL:HG22	1:63:A:MET:HG3	5	1.05
(1,1265)	1:59:A:VAL:HG23	1:63:A:MET:HG2	5	1.05
(1,1265)	1:59:A:VAL:HG23	1:63:A:MET:HG3	5	1.05
(1,648)	1:75:A:LEU:HD11	1:120:A:VAL:H	15	1.05
(1,648)	1:75:A:LEU:HD12	1:120:A:VAL:H	15	1.05
(1,648)	1:75:A:LEU:HD13	1:120:A:VAL:H	15	1.05
(1,359)	1:75:A:LEU:HD11	1:119:A:SER:HA	18	1.05
(1,359)	1:75:A:LEU:HD12	1:119:A:SER:HA	18	1.05
(1,359)	1:75:A:LEU:HD13	1:119:A:SER:HA	18	1.05
(1,289)	1:101:A:ALA:HB1	1:137:A:MET:HB3	14	1.05
(1,289)	1:101:A:ALA:HB2	1:137:A:MET:HB3	14	1.05
(1,289)	1:101:A:ALA:HB3	1:137:A:MET:HB3	14	1.05
(1,267)	1:104:A:LEU:HD21	1:108:A:ALA:H	15	1.03
(1,267)	1:104:A:LEU:HD22	1:108:A:ALA:H	15	1.03
(1,267)	1:104:A:LEU:HD23	1:108:A:ALA:H	15	1.03
(1,56)	1:78:A:PHE:HB3	1:120:A:VAL:HG11	20	1.03
(1,56)	1:78:A:PHE:HB3	1:120:A:VAL:HG12	20	1.03
(1,56)	1:78:A:PHE:HB3	1:120:A:VAL:HG13	20	1.03
(1,954)	1:104:A:LEU:HD11	1:106:A:GLU:H	2	1.02
(1,954)	1:104:A:LEU:HD12	1:106:A:GLU:H	2	1.02
(1,954)	1:104:A:LEU:HD13	1:106:A:GLU:H	2	1.02
(6,2)	2:148:B:SER:H1	2:149:B:PRO:HG2	9	1.01
(6,2)	2:148:B:SER:H1	2:149:B:PRO:HG3	9	1.01
(1,371)	1:100:A:PHE:HA	1:103:A:VAL:HG11	3	1.01
(1,371)	1:100:A:PHE:HA	1:103:A:VAL:HG12	3	1.01
(1,371)	1:100:A:PHE:HA	1:103:A:VAL:HG13	3	1.01
(6,2)	2:148:B:SER:H1	2:149:B:PRO:HG2	4	1.0
(6,2)	2:148:B:SER:H1	2:149:B:PRO:HG3	4	1.0
(6,2)	2:148:B:SER:H1	2:149:B:PRO:HG2	18	1.0
(6,2)	2:148:B:SER:H1	2:149:B:PRO:HG3	18	1.0
(4,1)	2:151:B:TYR:HH	1:82:A:ASN:ND2	19	1.0
(1,1432)	1:113:A:ASP:H	1:145:A:LEU:HD11	16	1.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1432)	1:113:A:ASP:H	1:145:A:LEU:HD12	16	1.0
(1,1432)	1:113:A:ASP:H	1:145:A:LEU:HD13	16	1.0
(1,1432)	1:113:A:ASP:H	1:145:A:LEU:HD21	16	1.0
(1,1432)	1:113:A:ASP:H	1:145:A:LEU:HD22	16	1.0
(1,1432)	1:113:A:ASP:H	1:145:A:LEU:HD23	16	1.0
(1,1427)	1:112:A:LYS:HB2	1:145:A:LEU:HD11	1	1.0
(1,1427)	1:112:A:LYS:HB2	1:145:A:LEU:HD12	1	1.0
(1,1427)	1:112:A:LYS:HB2	1:145:A:LEU:HD13	1	1.0
(1,1427)	1:112:A:LYS:HB2	1:145:A:LEU:HD21	1	1.0
(1,1427)	1:112:A:LYS:HB2	1:145:A:LEU:HD22	1	1.0
(1,1427)	1:112:A:LYS:HB2	1:145:A:LEU:HD23	1	1.0
(1,1427)	1:112:A:LYS:HB3	1:145:A:LEU:HD11	1	1.0
(1,1427)	1:112:A:LYS:HB3	1:145:A:LEU:HD12	1	1.0
(1,1427)	1:112:A:LYS:HB3	1:145:A:LEU:HD13	1	1.0
(1,1427)	1:112:A:LYS:HB3	1:145:A:LEU:HD21	1	1.0
(1,1427)	1:112:A:LYS:HB3	1:145:A:LEU:HD22	1	1.0
(1,1427)	1:112:A:LYS:HB3	1:145:A:LEU:HD23	1	1.0
(1,1202)	1:23:A:LEU:HD11	1:27:A:LEU:HA	1	1.0
(1,1202)	1:23:A:LEU:HD12	1:27:A:LEU:HA	1	1.0
(1,1202)	1:23:A:LEU:HD13	1:27:A:LEU:HA	1	1.0
(1,1202)	1:23:A:LEU:HD21	1:27:A:LEU:HA	1	1.0
(1,1202)	1:23:A:LEU:HD22	1:27:A:LEU:HA	1	1.0
(1,1202)	1:23:A:LEU:HD23	1:27:A:LEU:HA	1	1.0
(1,1427)	1:112:A:LYS:HB2	1:145:A:LEU:HD11	3	0.98
(1,1427)	1:112:A:LYS:HB2	1:145:A:LEU:HD12	3	0.98
(1,1427)	1:112:A:LYS:HB2	1:145:A:LEU:HD13	3	0.98
(1,1427)	1:112:A:LYS:HB2	1:145:A:LEU:HD21	3	0.98
(1,1427)	1:112:A:LYS:HB2	1:145:A:LEU:HD22	3	0.98
(1,1427)	1:112:A:LYS:HB2	1:145:A:LEU:HD23	3	0.98
(1,1427)	1:112:A:LYS:HB3	1:145:A:LEU:HD11	3	0.98
(1,1427)	1:112:A:LYS:HB3	1:145:A:LEU:HD12	3	0.98
(1,1427)	1:112:A:LYS:HB3	1:145:A:LEU:HD13	3	0.98
(1,1427)	1:112:A:LYS:HB3	1:145:A:LEU:HD21	3	0.98
(1,1427)	1:112:A:LYS:HB3	1:145:A:LEU:HD22	3	0.98
(1,1427)	1:112:A:LYS:HB3	1:145:A:LEU:HD23	3	0.98
(1,1403)	1:104:A:LEU:HD11	1:141:A:LEU:HG	12	0.98
(1,1403)	1:104:A:LEU:HD12	1:141:A:LEU:HG	12	0.98
(1,1403)	1:104:A:LEU:HD13	1:141:A:LEU:HG	12	0.98
(1,1403)	1:104:A:LEU:HD21	1:141:A:LEU:HG	12	0.98
(1,1403)	1:104:A:LEU:HD22	1:141:A:LEU:HG	12	0.98
(1,1403)	1:104:A:LEU:HD23	1:141:A:LEU:HG	12	0.98
(1,648)	1:75:A:LEU:HD11	1:120:A:VAL:H	3	0.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,648)	1:75:A:LEU:HD12	1:120:A:VAL:H	3	0.98
(1,648)	1:75:A:LEU:HD13	1:120:A:VAL:H	3	0.98
(6,3)	2:148:B:SER:H1	2:149:B:PRO:HB2	6	0.97
(6,3)	2:148:B:SER:H1	2:149:B:PRO:HB3	6	0.97
(1,1432)	1:113:A:ASP:H	1:145:A:LEU:HD11	1	0.97
(1,1432)	1:113:A:ASP:H	1:145:A:LEU:HD12	1	0.97
(1,1432)	1:113:A:ASP:H	1:145:A:LEU:HD13	1	0.97
(1,1432)	1:113:A:ASP:H	1:145:A:LEU:HD21	1	0.97
(1,1432)	1:113:A:ASP:H	1:145:A:LEU:HD22	1	0.97
(1,1432)	1:113:A:ASP:H	1:145:A:LEU:HD23	1	0.97
(1,648)	1:75:A:LEU:HD11	1:120:A:VAL:H	6	0.97
(1,648)	1:75:A:LEU:HD12	1:120:A:VAL:H	6	0.97
(1,648)	1:75:A:LEU:HD13	1:120:A:VAL:H	6	0.97
(5,1)	2:155:B:SER:H	1:130:A:ARG:NH2	5	0.96
(4,1)	2:151:B:TYR:HH	1:82:A:ASN:ND2	6	0.96
(4,1)	2:151:B:TYR:HH	1:82:A:ASN:ND2	16	0.96
(1,648)	1:75:A:LEU:HD11	1:120:A:VAL:H	7	0.95
(1,648)	1:75:A:LEU:HD12	1:120:A:VAL:H	7	0.95
(1,648)	1:75:A:LEU:HD13	1:120:A:VAL:H	7	0.95
(1,267)	1:104:A:LEU:HD21	1:108:A:ALA:H	8	0.95
(1,267)	1:104:A:LEU:HD22	1:108:A:ALA:H	8	0.95
(1,267)	1:104:A:LEU:HD23	1:108:A:ALA:H	8	0.95
(6,3)	2:148:B:SER:H1	2:149:B:PRO:HB2	7	0.94
(6,3)	2:148:B:SER:H1	2:149:B:PRO:HB3	7	0.94
(6,3)	2:148:B:SER:H1	2:149:B:PRO:HB2	14	0.94
(6,3)	2:148:B:SER:H1	2:149:B:PRO:HB3	14	0.94
(1,1203)	1:23:A:LEU:HD11	1:27:A:LEU:HB2	19	0.94
(1,1203)	1:23:A:LEU:HD11	1:27:A:LEU:HB3	19	0.94
(1,1203)	1:23:A:LEU:HD12	1:27:A:LEU:HB2	19	0.94
(1,1203)	1:23:A:LEU:HD12	1:27:A:LEU:HB3	19	0.94
(1,1203)	1:23:A:LEU:HD13	1:27:A:LEU:HB2	19	0.94
(1,1203)	1:23:A:LEU:HD13	1:27:A:LEU:HB3	19	0.94
(1,1203)	1:23:A:LEU:HD21	1:27:A:LEU:HB2	19	0.94
(1,1203)	1:23:A:LEU:HD21	1:27:A:LEU:HB3	19	0.94
(1,1203)	1:23:A:LEU:HD22	1:27:A:LEU:HB2	19	0.94
(1,1203)	1:23:A:LEU:HD22	1:27:A:LEU:HB3	19	0.94
(1,1203)	1:23:A:LEU:HD23	1:27:A:LEU:HB2	19	0.94
(1,1203)	1:23:A:LEU:HD23	1:27:A:LEU:HB3	19	0.94
(1,290)	1:101:A:ALA:HA	1:137:A:MET:HB3	4	0.94
(6,3)	2:148:B:SER:H1	2:149:B:PRO:HB2	11	0.93
(6,3)	2:148:B:SER:H1	2:149:B:PRO:HB3	11	0.93
(6,1)	2:148:B:SER:H1	2:149:B:PRO:HA	12	0.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1276)	1:59:A:VAL:HG11	1:103:A:VAL:H	3	0.93
(1,1276)	1:59:A:VAL:HG12	1:103:A:VAL:H	3	0.93
(1,1276)	1:59:A:VAL:HG13	1:103:A:VAL:H	3	0.93
(1,1276)	1:59:A:VAL:HG21	1:103:A:VAL:H	3	0.93
(1,1276)	1:59:A:VAL:HG22	1:103:A:VAL:H	3	0.93
(1,1276)	1:59:A:VAL:HG23	1:103:A:VAL:H	3	0.93
(1,204)	1:59:A:VAL:HA	1:103:A:VAL:HG11	14	0.93
(1,204)	1:59:A:VAL:HA	1:103:A:VAL:HG12	14	0.93
(1,204)	1:59:A:VAL:HA	1:103:A:VAL:HG13	14	0.93
(6,2)	2:148:B:SER:H1	2:149:B:PRO:HG2	5	0.92
(6,2)	2:148:B:SER:H1	2:149:B:PRO:HG3	5	0.92
(1,1427)	1:112:A:LYS:HB2	1:145:A:LEU:HD11	13	0.92
(1,1427)	1:112:A:LYS:HB2	1:145:A:LEU:HD12	13	0.92
(1,1427)	1:112:A:LYS:HB2	1:145:A:LEU:HD13	13	0.92
(1,1427)	1:112:A:LYS:HB2	1:145:A:LEU:HD21	13	0.92
(1,1427)	1:112:A:LYS:HB2	1:145:A:LEU:HD22	13	0.92
(1,1427)	1:112:A:LYS:HB2	1:145:A:LEU:HD23	13	0.92
(1,1427)	1:112:A:LYS:HB3	1:145:A:LEU:HD11	13	0.92
(1,1427)	1:112:A:LYS:HB3	1:145:A:LEU:HD12	13	0.92
(1,1427)	1:112:A:LYS:HB3	1:145:A:LEU:HD13	13	0.92
(1,1427)	1:112:A:LYS:HB3	1:145:A:LEU:HD21	13	0.92
(1,1427)	1:112:A:LYS:HB3	1:145:A:LEU:HD22	13	0.92
(1,1427)	1:112:A:LYS:HB3	1:145:A:LEU:HD23	13	0.92
(1,1288)	1:63:A:MET:H	1:77:A:LEU:HD11	7	0.92
(1,1288)	1:63:A:MET:H	1:77:A:LEU:HD12	7	0.92
(1,1288)	1:63:A:MET:H	1:77:A:LEU:HD13	7	0.92
(1,1288)	1:63:A:MET:H	1:77:A:LEU:HD21	7	0.92
(1,1288)	1:63:A:MET:H	1:77:A:LEU:HD22	7	0.92
(1,1288)	1:63:A:MET:H	1:77:A:LEU:HD23	7	0.92
(1,575)	1:104:A:LEU:HD11	1:108:A:ALA:H	2	0.92
(1,575)	1:104:A:LEU:HD12	1:108:A:ALA:H	2	0.92
(1,575)	1:104:A:LEU:HD13	1:108:A:ALA:H	2	0.92
(1,347)	1:104:A:LEU:HD11	1:108:A:ALA:HB1	9	0.92
(1,347)	1:104:A:LEU:HD11	1:108:A:ALA:HB2	9	0.92
(1,347)	1:104:A:LEU:HD11	1:108:A:ALA:HB3	9	0.92
(1,347)	1:104:A:LEU:HD12	1:108:A:ALA:HB1	9	0.92
(1,347)	1:104:A:LEU:HD12	1:108:A:ALA:HB2	9	0.92
(1,347)	1:104:A:LEU:HD12	1:108:A:ALA:HB3	9	0.92
(1,347)	1:104:A:LEU:HD13	1:108:A:ALA:HB1	9	0.92
(1,347)	1:104:A:LEU:HD13	1:108:A:ALA:HB2	9	0.92
(1,347)	1:104:A:LEU:HD13	1:108:A:ALA:HB3	9	0.92
(6,2)	2:148:B:SER:H1	2:149:B:PRO:HG2	11	0.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,2)	2:148:B:SER:H1	2:149:B:PRO:HG3	11	0.91
(1,1403)	1:104:A:LEU:HD11	1:141:A:LEU:HG	6	0.91
(1,1403)	1:104:A:LEU:HD12	1:141:A:LEU:HG	6	0.91
(1,1403)	1:104:A:LEU:HD13	1:141:A:LEU:HG	6	0.91
(1,1403)	1:104:A:LEU:HD21	1:141:A:LEU:HG	6	0.91
(1,1403)	1:104:A:LEU:HD22	1:141:A:LEU:HG	6	0.91
(1,1403)	1:104:A:LEU:HD23	1:141:A:LEU:HG	6	0.91
(1,1202)	1:23:A:LEU:HD11	1:27:A:LEU:HA	20	0.91
(1,1202)	1:23:A:LEU:HD12	1:27:A:LEU:HA	20	0.91
(1,1202)	1:23:A:LEU:HD13	1:27:A:LEU:HA	20	0.91
(1,1202)	1:23:A:LEU:HD21	1:27:A:LEU:HA	20	0.91
(1,1202)	1:23:A:LEU:HD22	1:27:A:LEU:HA	20	0.91
(1,1202)	1:23:A:LEU:HD23	1:27:A:LEU:HA	20	0.91
(1,722)	1:34:A:VAL:HG21	1:40:A:SER:H	19	0.91
(1,722)	1:34:A:VAL:HG22	1:40:A:SER:H	19	0.91
(1,722)	1:34:A:VAL:HG23	1:40:A:SER:H	19	0.91
(1,336)	1:108:A:ALA:HB1	1:111:A:VAL:HG11	17	0.91
(1,336)	1:108:A:ALA:HB1	1:111:A:VAL:HG12	17	0.91
(1,336)	1:108:A:ALA:HB1	1:111:A:VAL:HG13	17	0.91
(1,336)	1:108:A:ALA:HB2	1:111:A:VAL:HG11	17	0.91
(1,336)	1:108:A:ALA:HB2	1:111:A:VAL:HG12	17	0.91
(1,336)	1:108:A:ALA:HB2	1:111:A:VAL:HG13	17	0.91
(1,336)	1:108:A:ALA:HB3	1:111:A:VAL:HG11	17	0.91
(1,336)	1:108:A:ALA:HB3	1:111:A:VAL:HG12	17	0.91
(1,336)	1:108:A:ALA:HB3	1:111:A:VAL:HG13	17	0.91
(1,153)	1:63:A:MET:HG2	1:103:A:VAL:HG11	2	0.91
(1,153)	1:63:A:MET:HG2	1:103:A:VAL:HG12	2	0.91
(1,153)	1:63:A:MET:HG2	1:103:A:VAL:HG13	2	0.91
(1,153)	1:63:A:MET:HG2	1:103:A:VAL:HG11	5	0.91
(1,153)	1:63:A:MET:HG2	1:103:A:VAL:HG12	5	0.91
(1,153)	1:63:A:MET:HG2	1:103:A:VAL:HG13	5	0.91
(2,12)	2:158:B:TYR:HD1	1:132:A:VAL:HG11	16	0.89
(2,12)	2:158:B:TYR:HD1	1:132:A:VAL:HG12	16	0.89
(2,12)	2:158:B:TYR:HD1	1:132:A:VAL:HG13	16	0.89
(2,12)	2:158:B:TYR:HD2	1:132:A:VAL:HG11	16	0.89
(2,12)	2:158:B:TYR:HD2	1:132:A:VAL:HG12	16	0.89
(2,12)	2:158:B:TYR:HD2	1:132:A:VAL:HG13	16	0.89
(1,1422)	1:112:A:LYS:H	1:145:A:LEU:HD11	3	0.89
(1,1422)	1:112:A:LYS:H	1:145:A:LEU:HD12	3	0.89
(1,1422)	1:112:A:LYS:H	1:145:A:LEU:HD13	3	0.89
(1,1422)	1:112:A:LYS:H	1:145:A:LEU:HD21	3	0.89
(1,1422)	1:112:A:LYS:H	1:145:A:LEU:HD22	3	0.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1422)	1:112:A:LYS:H	1:145:A:LEU:HD23	3	0.89
(1,1403)	1:104:A:LEU:HD11	1:141:A:LEU:HG	2	0.89
(1,1403)	1:104:A:LEU:HD12	1:141:A:LEU:HG	2	0.89
(1,1403)	1:104:A:LEU:HD13	1:141:A:LEU:HG	2	0.89
(1,1403)	1:104:A:LEU:HD21	1:141:A:LEU:HG	2	0.89
(1,1403)	1:104:A:LEU:HD22	1:141:A:LEU:HG	2	0.89
(1,1403)	1:104:A:LEU:HD23	1:141:A:LEU:HG	2	0.89
(1,1288)	1:63:A:MET:H	1:77:A:LEU:HD11	15	0.89
(1,1288)	1:63:A:MET:H	1:77:A:LEU:HD12	15	0.89
(1,1288)	1:63:A:MET:H	1:77:A:LEU:HD13	15	0.89
(1,1288)	1:63:A:MET:H	1:77:A:LEU:HD21	15	0.89
(1,1288)	1:63:A:MET:H	1:77:A:LEU:HD22	15	0.89
(1,1288)	1:63:A:MET:H	1:77:A:LEU:HD23	15	0.89
(1,359)	1:75:A:LEU:HD11	1:119:A:SER:HA	2	0.89
(1,359)	1:75:A:LEU:HD12	1:119:A:SER:HA	2	0.89
(1,359)	1:75:A:LEU:HD13	1:119:A:SER:HA	2	0.89
(1,69)	1:34:A:VAL:HG11	1:41:A:ILE:HD11	4	0.89
(1,69)	1:34:A:VAL:HG11	1:41:A:ILE:HD12	4	0.89
(1,69)	1:34:A:VAL:HG11	1:41:A:ILE:HD13	4	0.89
(1,69)	1:34:A:VAL:HG12	1:41:A:ILE:HD11	4	0.89
(1,69)	1:34:A:VAL:HG12	1:41:A:ILE:HD12	4	0.89
(1,69)	1:34:A:VAL:HG12	1:41:A:ILE:HD13	4	0.89
(1,69)	1:34:A:VAL:HG13	1:41:A:ILE:HD11	4	0.89
(1,69)	1:34:A:VAL:HG13	1:41:A:ILE:HD12	4	0.89
(1,69)	1:34:A:VAL:HG13	1:41:A:ILE:HD13	4	0.89
(1,1427)	1:112:A:LYS:HB2	1:145:A:LEU:HD11	16	0.88
(1,1427)	1:112:A:LYS:HB2	1:145:A:LEU:HD12	16	0.88
(1,1427)	1:112:A:LYS:HB2	1:145:A:LEU:HD13	16	0.88
(1,1427)	1:112:A:LYS:HB2	1:145:A:LEU:HD21	16	0.88
(1,1427)	1:112:A:LYS:HB2	1:145:A:LEU:HD22	16	0.88
(1,1427)	1:112:A:LYS:HB2	1:145:A:LEU:HD23	16	0.88
(1,1427)	1:112:A:LYS:HB3	1:145:A:LEU:HD11	16	0.88
(1,1427)	1:112:A:LYS:HB3	1:145:A:LEU:HD12	16	0.88
(1,1427)	1:112:A:LYS:HB3	1:145:A:LEU:HD13	16	0.88
(1,1427)	1:112:A:LYS:HB3	1:145:A:LEU:HD21	16	0.88
(1,1427)	1:112:A:LYS:HB3	1:145:A:LEU:HD22	16	0.88
(1,1427)	1:112:A:LYS:HB3	1:145:A:LEU:HD23	16	0.88
(1,454)	1:116:A:VAL:HG11	1:118:A:LYS:HG2	2	0.88
(1,454)	1:116:A:VAL:HG11	1:118:A:LYS:HG3	2	0.88
(1,454)	1:116:A:VAL:HG12	1:118:A:LYS:HG2	2	0.88
(1,454)	1:116:A:VAL:HG12	1:118:A:LYS:HG3	2	0.88
(1,454)	1:116:A:VAL:HG13	1:118:A:LYS:HG2	2	0.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,454)	1:116:A:VAL:HG13	1:118:A:LYS:HG3	2	0.88
(1,359)	1:75:A:LEU:HD11	1:119:A:SER:HA	9	0.88
(1,359)	1:75:A:LEU:HD12	1:119:A:SER:HA	9	0.88
(1,359)	1:75:A:LEU:HD13	1:119:A:SER:HA	9	0.88
(1,648)	1:75:A:LEU:HD11	1:120:A:VAL:H	8	0.87
(1,648)	1:75:A:LEU:HD12	1:120:A:VAL:H	8	0.87
(1,648)	1:75:A:LEU:HD13	1:120:A:VAL:H	8	0.87
(1,1281)	1:59:A:VAL:HG11	1:104:A:LEU:H	3	0.86
(1,1281)	1:59:A:VAL:HG12	1:104:A:LEU:H	3	0.86
(1,1281)	1:59:A:VAL:HG13	1:104:A:LEU:H	3	0.86
(1,1281)	1:59:A:VAL:HG21	1:104:A:LEU:H	3	0.86
(1,1281)	1:59:A:VAL:HG22	1:104:A:LEU:H	3	0.86
(1,1281)	1:59:A:VAL:HG23	1:104:A:LEU:H	3	0.86
(1,963)	1:109:A:ALA:H	1:111:A:VAL:HG11	17	0.86
(1,963)	1:109:A:ALA:H	1:111:A:VAL:HG12	17	0.86
(1,963)	1:109:A:ALA:H	1:111:A:VAL:HG13	17	0.86
(1,359)	1:75:A:LEU:HD11	1:119:A:SER:HA	7	0.86
(1,359)	1:75:A:LEU:HD12	1:119:A:SER:HA	7	0.86
(1,359)	1:75:A:LEU:HD13	1:119:A:SER:HA	7	0.86
(1,271)	1:75:A:LEU:HD21	1:78:A:PHE:HB3	14	0.86
(1,271)	1:75:A:LEU:HD22	1:78:A:PHE:HB3	14	0.86
(1,271)	1:75:A:LEU:HD23	1:78:A:PHE:HB3	14	0.86
(2,2)	2:149:B:PRO:HG2	1:38:A:MET:HE1	19	0.85
(1,648)	1:75:A:LEU:HD11	1:120:A:VAL:H	2	0.85
(1,648)	1:75:A:LEU:HD12	1:120:A:VAL:H	2	0.85
(1,648)	1:75:A:LEU:HD13	1:120:A:VAL:H	2	0.85
(1,1422)	1:112:A:LYS:H	1:145:A:LEU:HD11	1	0.84
(1,1422)	1:112:A:LYS:H	1:145:A:LEU:HD12	1	0.84
(1,1422)	1:112:A:LYS:H	1:145:A:LEU:HD13	1	0.84
(1,1422)	1:112:A:LYS:H	1:145:A:LEU:HD21	1	0.84
(1,1422)	1:112:A:LYS:H	1:145:A:LEU:HD22	1	0.84
(1,1422)	1:112:A:LYS:H	1:145:A:LEU:HD23	1	0.84
(1,575)	1:104:A:LEU:HD11	1:108:A:ALA:H	7	0.84
(1,575)	1:104:A:LEU:HD12	1:108:A:ALA:H	7	0.84
(1,575)	1:104:A:LEU:HD13	1:108:A:ALA:H	7	0.84
(1,293)	1:31:A:PHE:HA	1:34:A:VAL:HG11	8	0.84
(1,293)	1:31:A:PHE:HA	1:34:A:VAL:HG12	8	0.84
(1,293)	1:31:A:PHE:HA	1:34:A:VAL:HG13	8	0.84
(1,1455)	1:120:A:VAL:HB	1:145:A:LEU:HD11	4	0.83
(1,1455)	1:120:A:VAL:HB	1:145:A:LEU:HD12	4	0.83
(1,1455)	1:120:A:VAL:HB	1:145:A:LEU:HD13	4	0.83
(1,1455)	1:120:A:VAL:HB	1:145:A:LEU:HD21	4	0.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1455)	1:120:A:VAL:HB	1:145:A:LEU:HD22	4	0.83
(1,1455)	1:120:A:VAL:HB	1:145:A:LEU:HD23	4	0.83
(1,1277)	1:59:A:VAL:HG11	1:103:A:VAL:HA	3	0.83
(1,1277)	1:59:A:VAL:HG12	1:103:A:VAL:HA	3	0.83
(1,1277)	1:59:A:VAL:HG13	1:103:A:VAL:HA	3	0.83
(1,1277)	1:59:A:VAL:HG21	1:103:A:VAL:HA	3	0.83
(1,1277)	1:59:A:VAL:HG22	1:103:A:VAL:HA	3	0.83
(1,1277)	1:59:A:VAL:HG23	1:103:A:VAL:HA	3	0.83
(1,369)	1:63:A:MET:HG3	1:103:A:VAL:HG11	5	0.83
(1,369)	1:63:A:MET:HG3	1:103:A:VAL:HG12	5	0.83
(1,369)	1:63:A:MET:HG3	1:103:A:VAL:HG13	5	0.83
(1,1422)	1:112:A:LYS:H	1:145:A:LEU:HD11	13	0.82
(1,1422)	1:112:A:LYS:H	1:145:A:LEU:HD12	13	0.82
(1,1422)	1:112:A:LYS:H	1:145:A:LEU:HD13	13	0.82
(1,1422)	1:112:A:LYS:H	1:145:A:LEU:HD21	13	0.82
(1,1422)	1:112:A:LYS:H	1:145:A:LEU:HD22	13	0.82
(1,1422)	1:112:A:LYS:H	1:145:A:LEU:HD23	13	0.82
(1,1403)	1:104:A:LEU:HD11	1:141:A:LEU:HG	11	0.82
(1,1403)	1:104:A:LEU:HD12	1:141:A:LEU:HG	11	0.82
(1,1403)	1:104:A:LEU:HD13	1:141:A:LEU:HG	11	0.82
(1,1403)	1:104:A:LEU:HD21	1:141:A:LEU:HG	11	0.82
(1,1403)	1:104:A:LEU:HD22	1:141:A:LEU:HG	11	0.82
(1,1403)	1:104:A:LEU:HD23	1:141:A:LEU:HG	11	0.82
(1,722)	1:34:A:VAL:HG21	1:40:A:SER:H	15	0.82
(1,722)	1:34:A:VAL:HG22	1:40:A:SER:H	15	0.82
(1,722)	1:34:A:VAL:HG23	1:40:A:SER:H	15	0.82
(1,359)	1:75:A:LEU:HD11	1:119:A:SER:HA	15	0.82
(1,359)	1:75:A:LEU:HD12	1:119:A:SER:HA	15	0.82
(1,359)	1:75:A:LEU:HD13	1:119:A:SER:HA	15	0.82
(6,3)	2:148:B:SER:H1	2:149:B:PRO:HB2	13	0.81
(6,3)	2:148:B:SER:H1	2:149:B:PRO:HB3	13	0.81
(1,1229)	1:45:A:SER:HB2	1:80:A:LEU:HD11	15	0.81
(1,1229)	1:45:A:SER:HB2	1:80:A:LEU:HD12	15	0.81
(1,1229)	1:45:A:SER:HB2	1:80:A:LEU:HD13	15	0.81
(1,1229)	1:45:A:SER:HB2	1:80:A:LEU:HD21	15	0.81
(1,1229)	1:45:A:SER:HB2	1:80:A:LEU:HD22	15	0.81
(1,1229)	1:45:A:SER:HB2	1:80:A:LEU:HD23	15	0.81
(1,1229)	1:45:A:SER:HB3	1:80:A:LEU:HD11	15	0.81
(1,1229)	1:45:A:SER:HB3	1:80:A:LEU:HD12	15	0.81
(1,1229)	1:45:A:SER:HB3	1:80:A:LEU:HD13	15	0.81
(1,1229)	1:45:A:SER:HB3	1:80:A:LEU:HD21	15	0.81
(1,1229)	1:45:A:SER:HB3	1:80:A:LEU:HD22	15	0.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1229)	1:45:A:SER:HB3	1:80:A:LEU:HD23	15	0.81
(1,648)	1:75:A:LEU:HD11	1:120:A:VAL:H	10	0.81
(1,648)	1:75:A:LEU:HD12	1:120:A:VAL:H	10	0.81
(1,648)	1:75:A:LEU:HD13	1:120:A:VAL:H	10	0.81
(1,575)	1:104:A:LEU:HD11	1:108:A:ALA:H	4	0.81
(1,575)	1:104:A:LEU:HD12	1:108:A:ALA:H	4	0.81
(1,575)	1:104:A:LEU:HD13	1:108:A:ALA:H	4	0.81
(1,378)	1:102:A:ASP:H	1:103:A:VAL:HG11	3	0.81
(1,378)	1:102:A:ASP:H	1:103:A:VAL:HG12	3	0.81
(1,378)	1:102:A:ASP:H	1:103:A:VAL:HG13	3	0.81
(1,359)	1:75:A:LEU:HD11	1:119:A:SER:HA	3	0.81
(1,359)	1:75:A:LEU:HD12	1:119:A:SER:HA	3	0.81
(1,359)	1:75:A:LEU:HD13	1:119:A:SER:HA	3	0.81
(1,359)	1:75:A:LEU:HD11	1:119:A:SER:HA	6	0.81
(1,359)	1:75:A:LEU:HD12	1:119:A:SER:HA	6	0.81
(1,359)	1:75:A:LEU:HD13	1:119:A:SER:HA	6	0.81
(6,2)	2:148:B:SER:H1	2:149:B:PRO:HG2	6	0.8
(6,2)	2:148:B:SER:H1	2:149:B:PRO:HG3	6	0.8
(1,379)	1:139:A:VAL:HG21	1:143:A:GLU:HG2	13	0.8
(1,379)	1:139:A:VAL:HG21	1:143:A:GLU:HG3	13	0.8
(1,379)	1:139:A:VAL:HG22	1:143:A:GLU:HG2	13	0.8
(1,379)	1:139:A:VAL:HG22	1:143:A:GLU:HG3	13	0.8
(1,379)	1:139:A:VAL:HG23	1:143:A:GLU:HG2	13	0.8
(1,379)	1:139:A:VAL:HG23	1:143:A:GLU:HG3	13	0.8
(6,2)	2:148:B:SER:H1	2:149:B:PRO:HG2	7	0.79
(6,2)	2:148:B:SER:H1	2:149:B:PRO:HG3	7	0.79
(1,1403)	1:104:A:LEU:HD11	1:141:A:LEU:HG	9	0.79
(1,1403)	1:104:A:LEU:HD12	1:141:A:LEU:HG	9	0.79
(1,1403)	1:104:A:LEU:HD13	1:141:A:LEU:HG	9	0.79
(1,1403)	1:104:A:LEU:HD21	1:141:A:LEU:HG	9	0.79
(1,1403)	1:104:A:LEU:HD22	1:141:A:LEU:HG	9	0.79
(1,1403)	1:104:A:LEU:HD23	1:141:A:LEU:HG	9	0.79
(1,1277)	1:59:A:VAL:HG11	1:103:A:VAL:HA	14	0.79
(1,1277)	1:59:A:VAL:HG12	1:103:A:VAL:HA	14	0.79
(1,1277)	1:59:A:VAL:HG13	1:103:A:VAL:HA	14	0.79
(1,1277)	1:59:A:VAL:HG21	1:103:A:VAL:HA	14	0.79
(1,1277)	1:59:A:VAL:HG22	1:103:A:VAL:HA	14	0.79
(1,1277)	1:59:A:VAL:HG23	1:103:A:VAL:HA	14	0.79
(1,454)	1:116:A:VAL:HG11	1:118:A:LYS:HG2	11	0.79
(1,454)	1:116:A:VAL:HG11	1:118:A:LYS:HG3	11	0.79
(1,454)	1:116:A:VAL:HG12	1:118:A:LYS:HG2	11	0.79
(1,454)	1:116:A:VAL:HG12	1:118:A:LYS:HG3	11	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,454)	1:116:A:VAL:HG13	1:118:A:LYS:HG2	11	0.79
(1,454)	1:116:A:VAL:HG13	1:118:A:LYS:HG3	11	0.79
(1,454)	1:116:A:VAL:HG11	1:118:A:LYS:HG2	9	0.78
(1,454)	1:116:A:VAL:HG11	1:118:A:LYS:HG3	9	0.78
(1,454)	1:116:A:VAL:HG12	1:118:A:LYS:HG2	9	0.78
(1,454)	1:116:A:VAL:HG12	1:118:A:LYS:HG3	9	0.78
(1,454)	1:116:A:VAL:HG13	1:118:A:LYS:HG2	9	0.78
(1,454)	1:116:A:VAL:HG13	1:118:A:LYS:HG3	9	0.78
(2,12)	2:158:B:TYR:HD1	1:132:A:VAL:HG11	20	0.77
(2,12)	2:158:B:TYR:HD1	1:132:A:VAL:HG12	20	0.77
(2,12)	2:158:B:TYR:HD1	1:132:A:VAL:HG13	20	0.77
(2,12)	2:158:B:TYR:HD2	1:132:A:VAL:HG11	20	0.77
(2,12)	2:158:B:TYR:HD2	1:132:A:VAL:HG12	20	0.77
(2,12)	2:158:B:TYR:HD2	1:132:A:VAL:HG13	20	0.77
(1,1276)	1:59:A:VAL:HG11	1:103:A:VAL:H	14	0.77
(1,1276)	1:59:A:VAL:HG12	1:103:A:VAL:H	14	0.77
(1,1276)	1:59:A:VAL:HG13	1:103:A:VAL:H	14	0.77
(1,1276)	1:59:A:VAL:HG21	1:103:A:VAL:H	14	0.77
(1,1276)	1:59:A:VAL:HG22	1:103:A:VAL:H	14	0.77
(1,1276)	1:59:A:VAL:HG23	1:103:A:VAL:H	14	0.77
(1,648)	1:75:A:LEU:HD11	1:120:A:VAL:H	11	0.77
(1,648)	1:75:A:LEU:HD12	1:120:A:VAL:H	11	0.77
(1,648)	1:75:A:LEU:HD13	1:120:A:VAL:H	11	0.77
(1,83)	1:137:A:MET:HB3	1:138:A:ILE:HD11	17	0.77
(1,83)	1:137:A:MET:HB3	1:138:A:ILE:HD12	17	0.77
(1,83)	1:137:A:MET:HB3	1:138:A:ILE:HD13	17	0.77
(1,838)	1:31:A:PHE:H	1:34:A:VAL:HG21	15	0.76
(1,838)	1:31:A:PHE:H	1:34:A:VAL:HG22	15	0.76
(1,838)	1:31:A:PHE:H	1:34:A:VAL:HG23	15	0.76
(1,648)	1:75:A:LEU:HD11	1:120:A:VAL:H	5	0.76
(1,648)	1:75:A:LEU:HD12	1:120:A:VAL:H	5	0.76
(1,648)	1:75:A:LEU:HD13	1:120:A:VAL:H	5	0.76
(1,574)	1:108:A:ALA:H	1:111:A:VAL:HG11	12	0.76
(1,574)	1:108:A:ALA:H	1:111:A:VAL:HG12	12	0.76
(1,574)	1:108:A:ALA:H	1:111:A:VAL:HG13	12	0.76
(1,56)	1:78:A:PHE:HB3	1:120:A:VAL:HG11	4	0.76
(1,56)	1:78:A:PHE:HB3	1:120:A:VAL:HG12	4	0.76
(1,56)	1:78:A:PHE:HB3	1:120:A:VAL:HG13	4	0.76
(1,1410)	1:108:A:ALA:HB1	1:145:A:LEU:HD11	20	0.75
(1,1410)	1:108:A:ALA:HB1	1:145:A:LEU:HD12	20	0.75
(1,1410)	1:108:A:ALA:HB1	1:145:A:LEU:HD13	20	0.75
(1,1410)	1:108:A:ALA:HB1	1:145:A:LEU:HD21	20	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1410)	1:108:A:ALA:HB1	1:145:A:LEU:HD22	20	0.75
(1,1410)	1:108:A:ALA:HB1	1:145:A:LEU:HD23	20	0.75
(1,1410)	1:108:A:ALA:HB2	1:145:A:LEU:HD11	20	0.75
(1,1410)	1:108:A:ALA:HB2	1:145:A:LEU:HD12	20	0.75
(1,1410)	1:108:A:ALA:HB2	1:145:A:LEU:HD13	20	0.75
(1,1410)	1:108:A:ALA:HB2	1:145:A:LEU:HD21	20	0.75
(1,1410)	1:108:A:ALA:HB2	1:145:A:LEU:HD22	20	0.75
(1,1410)	1:108:A:ALA:HB2	1:145:A:LEU:HD23	20	0.75
(1,1410)	1:108:A:ALA:HB3	1:145:A:LEU:HD11	20	0.75
(1,1410)	1:108:A:ALA:HB3	1:145:A:LEU:HD12	20	0.75
(1,1410)	1:108:A:ALA:HB3	1:145:A:LEU:HD13	20	0.75
(1,1410)	1:108:A:ALA:HB3	1:145:A:LEU:HD21	20	0.75
(1,1410)	1:108:A:ALA:HB3	1:145:A:LEU:HD22	20	0.75
(1,1410)	1:108:A:ALA:HB3	1:145:A:LEU:HD23	20	0.75
(1,1403)	1:104:A:LEU:HD11	1:141:A:LEU:HG	3	0.75
(1,1403)	1:104:A:LEU:HD12	1:141:A:LEU:HG	3	0.75
(1,1403)	1:104:A:LEU:HD13	1:141:A:LEU:HG	3	0.75
(1,1403)	1:104:A:LEU:HD21	1:141:A:LEU:HG	3	0.75
(1,1403)	1:104:A:LEU:HD22	1:141:A:LEU:HG	3	0.75
(1,1403)	1:104:A:LEU:HD23	1:141:A:LEU:HG	3	0.75
(1,1229)	1:45:A:SER:HB2	1:80:A:LEU:HD11	9	0.75
(1,1229)	1:45:A:SER:HB2	1:80:A:LEU:HD12	9	0.75
(1,1229)	1:45:A:SER:HB2	1:80:A:LEU:HD13	9	0.75
(1,1229)	1:45:A:SER:HB2	1:80:A:LEU:HD21	9	0.75
(1,1229)	1:45:A:SER:HB2	1:80:A:LEU:HD22	9	0.75
(1,1229)	1:45:A:SER:HB2	1:80:A:LEU:HD23	9	0.75
(1,1229)	1:45:A:SER:HB3	1:80:A:LEU:HD11	9	0.75
(1,1229)	1:45:A:SER:HB3	1:80:A:LEU:HD12	9	0.75
(1,1229)	1:45:A:SER:HB3	1:80:A:LEU:HD13	9	0.75
(1,1229)	1:45:A:SER:HB3	1:80:A:LEU:HD21	9	0.75
(1,1229)	1:45:A:SER:HB3	1:80:A:LEU:HD22	9	0.75
(1,1229)	1:45:A:SER:HB3	1:80:A:LEU:HD23	9	0.75
(1,83)	1:137:A:MET:HB3	1:138:A:ILE:HD11	9	0.75
(1,83)	1:137:A:MET:HB3	1:138:A:ILE:HD12	9	0.75
(1,83)	1:137:A:MET:HB3	1:138:A:ILE:HD13	9	0.75
(1,1427)	1:112:A:LYS:HB2	1:145:A:LEU:HD11	10	0.74
(1,1427)	1:112:A:LYS:HB2	1:145:A:LEU:HD12	10	0.74
(1,1427)	1:112:A:LYS:HB2	1:145:A:LEU:HD13	10	0.74
(1,1427)	1:112:A:LYS:HB2	1:145:A:LEU:HD21	10	0.74
(1,1427)	1:112:A:LYS:HB2	1:145:A:LEU:HD22	10	0.74
(1,1427)	1:112:A:LYS:HB2	1:145:A:LEU:HD23	10	0.74
(1,1427)	1:112:A:LYS:HB3	1:145:A:LEU:HD11	10	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1427)	1:112:A:LYS:HB3	1:145:A:LEU:HD12	10	0.74
(1,1427)	1:112:A:LYS:HB3	1:145:A:LEU:HD13	10	0.74
(1,1427)	1:112:A:LYS:HB3	1:145:A:LEU:HD21	10	0.74
(1,1427)	1:112:A:LYS:HB3	1:145:A:LEU:HD22	10	0.74
(1,1427)	1:112:A:LYS:HB3	1:145:A:LEU:HD23	10	0.74
(1,838)	1:31:A:PHE:H	1:34:A:VAL:HG21	20	0.74
(1,838)	1:31:A:PHE:H	1:34:A:VAL:HG22	20	0.74
(1,838)	1:31:A:PHE:H	1:34:A:VAL:HG23	20	0.74
(1,454)	1:116:A:VAL:HG11	1:118:A:LYS:HG2	14	0.74
(1,454)	1:116:A:VAL:HG11	1:118:A:LYS:HG3	14	0.74
(1,454)	1:116:A:VAL:HG12	1:118:A:LYS:HG2	14	0.74
(1,454)	1:116:A:VAL:HG12	1:118:A:LYS:HG3	14	0.74
(1,454)	1:116:A:VAL:HG13	1:118:A:LYS:HG2	14	0.74
(1,454)	1:116:A:VAL:HG13	1:118:A:LYS:HG3	14	0.74
(1,454)	1:116:A:VAL:HG11	1:118:A:LYS:HG2	6	0.73
(1,454)	1:116:A:VAL:HG11	1:118:A:LYS:HG3	6	0.73
(1,454)	1:116:A:VAL:HG12	1:118:A:LYS:HG2	6	0.73
(1,454)	1:116:A:VAL:HG12	1:118:A:LYS:HG3	6	0.73
(1,454)	1:116:A:VAL:HG13	1:118:A:LYS:HG2	6	0.73
(1,454)	1:116:A:VAL:HG13	1:118:A:LYS:HG3	6	0.73
(6,2)	2:148:B:SER:H1	2:149:B:PRO:HG2	14	0.72
(6,2)	2:148:B:SER:H1	2:149:B:PRO:HG3	14	0.72
(1,1288)	1:63:A:MET:H	1:77:A:LEU:HD11	18	0.72
(1,1288)	1:63:A:MET:H	1:77:A:LEU:HD12	18	0.72
(1,1288)	1:63:A:MET:H	1:77:A:LEU:HD13	18	0.72
(1,1288)	1:63:A:MET:H	1:77:A:LEU:HD21	18	0.72
(1,1288)	1:63:A:MET:H	1:77:A:LEU:HD22	18	0.72
(1,1288)	1:63:A:MET:H	1:77:A:LEU:HD23	18	0.72
(1,1279)	1:59:A:VAL:HG11	1:103:A:VAL:HG11	17	0.72
(1,1279)	1:59:A:VAL:HG11	1:103:A:VAL:HG12	17	0.72
(1,1279)	1:59:A:VAL:HG11	1:103:A:VAL:HG13	17	0.72
(1,1279)	1:59:A:VAL:HG12	1:103:A:VAL:HG11	17	0.72
(1,1279)	1:59:A:VAL:HG12	1:103:A:VAL:HG12	17	0.72
(1,1279)	1:59:A:VAL:HG12	1:103:A:VAL:HG13	17	0.72
(1,1279)	1:59:A:VAL:HG13	1:103:A:VAL:HG11	17	0.72
(1,1279)	1:59:A:VAL:HG13	1:103:A:VAL:HG12	17	0.72
(1,1279)	1:59:A:VAL:HG13	1:103:A:VAL:HG13	17	0.72
(1,1279)	1:59:A:VAL:HG21	1:103:A:VAL:HG11	17	0.72
(1,1279)	1:59:A:VAL:HG21	1:103:A:VAL:HG12	17	0.72
(1,1279)	1:59:A:VAL:HG21	1:103:A:VAL:HG13	17	0.72
(1,1279)	1:59:A:VAL:HG22	1:103:A:VAL:HG11	17	0.72
(1,1279)	1:59:A:VAL:HG22	1:103:A:VAL:HG12	17	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1279)	1:59:A:VAL:HG22	1:103:A:VAL:HG13	17	0.72
(1,1279)	1:59:A:VAL:HG23	1:103:A:VAL:HG11	17	0.72
(1,1279)	1:59:A:VAL:HG23	1:103:A:VAL:HG12	17	0.72
(1,1279)	1:59:A:VAL:HG23	1:103:A:VAL:HG13	17	0.72
(1,154)	1:139:A:VAL:HG11	1:143:A:GLU:HG2	8	0.72
(1,154)	1:139:A:VAL:HG11	1:143:A:GLU:HG3	8	0.72
(1,154)	1:139:A:VAL:HG12	1:143:A:GLU:HG2	8	0.72
(1,154)	1:139:A:VAL:HG12	1:143:A:GLU:HG3	8	0.72
(1,154)	1:139:A:VAL:HG13	1:143:A:GLU:HG2	8	0.72
(1,154)	1:139:A:VAL:HG13	1:143:A:GLU:HG3	8	0.72
(1,1425)	1:112:A:LYS:HA	1:145:A:LEU:HD11	13	0.71
(1,1425)	1:112:A:LYS:HA	1:145:A:LEU:HD12	13	0.71
(1,1425)	1:112:A:LYS:HA	1:145:A:LEU:HD13	13	0.71
(1,1425)	1:112:A:LYS:HA	1:145:A:LEU:HD21	13	0.71
(1,1425)	1:112:A:LYS:HA	1:145:A:LEU:HD22	13	0.71
(1,1425)	1:112:A:LYS:HA	1:145:A:LEU:HD23	13	0.71
(1,1403)	1:104:A:LEU:HD11	1:141:A:LEU:HG	15	0.71
(1,1403)	1:104:A:LEU:HD12	1:141:A:LEU:HG	15	0.71
(1,1403)	1:104:A:LEU:HD13	1:141:A:LEU:HG	15	0.71
(1,1403)	1:104:A:LEU:HD21	1:141:A:LEU:HG	15	0.71
(1,1403)	1:104:A:LEU:HD22	1:141:A:LEU:HG	15	0.71
(1,1403)	1:104:A:LEU:HD23	1:141:A:LEU:HG	15	0.71
(1,454)	1:116:A:VAL:HG11	1:118:A:LYS:HG2	20	0.71
(1,454)	1:116:A:VAL:HG11	1:118:A:LYS:HG3	20	0.71
(1,454)	1:116:A:VAL:HG12	1:118:A:LYS:HG2	20	0.71
(1,454)	1:116:A:VAL:HG12	1:118:A:LYS:HG3	20	0.71
(1,454)	1:116:A:VAL:HG13	1:118:A:LYS:HG2	20	0.71
(1,454)	1:116:A:VAL:HG13	1:118:A:LYS:HG3	20	0.71
(1,478)	1:77:A:LEU:HD21	1:78:A:PHE:HA	16	0.7
(1,478)	1:77:A:LEU:HD22	1:78:A:PHE:HA	16	0.7
(1,478)	1:77:A:LEU:HD23	1:78:A:PHE:HA	16	0.7
(1,454)	1:116:A:VAL:HG11	1:118:A:LYS:HG2	10	0.7
(1,454)	1:116:A:VAL:HG11	1:118:A:LYS:HG3	10	0.7
(1,454)	1:116:A:VAL:HG12	1:118:A:LYS:HG2	10	0.7
(1,454)	1:116:A:VAL:HG12	1:118:A:LYS:HG3	10	0.7
(1,454)	1:116:A:VAL:HG13	1:118:A:LYS:HG2	10	0.7
(1,454)	1:116:A:VAL:HG13	1:118:A:LYS:HG3	10	0.7
(6,3)	2:148:B:SER:H1	2:149:B:PRO:HB2	5	0.69
(6,3)	2:148:B:SER:H1	2:149:B:PRO:HB3	5	0.69
(1,1450)	1:116:A:VAL:HG11	1:120:A:VAL:HG11	20	0.69
(1,1450)	1:116:A:VAL:HG11	1:120:A:VAL:HG12	20	0.69
(1,1450)	1:116:A:VAL:HG11	1:120:A:VAL:HG13	20	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1450)	1:116:A:VAL:HG11	1:120:A:VAL:HG21	20	0.69
(1,1450)	1:116:A:VAL:HG11	1:120:A:VAL:HG22	20	0.69
(1,1450)	1:116:A:VAL:HG11	1:120:A:VAL:HG23	20	0.69
(1,1450)	1:116:A:VAL:HG12	1:120:A:VAL:HG11	20	0.69
(1,1450)	1:116:A:VAL:HG12	1:120:A:VAL:HG12	20	0.69
(1,1450)	1:116:A:VAL:HG12	1:120:A:VAL:HG13	20	0.69
(1,1450)	1:116:A:VAL:HG12	1:120:A:VAL:HG21	20	0.69
(1,1450)	1:116:A:VAL:HG12	1:120:A:VAL:HG22	20	0.69
(1,1450)	1:116:A:VAL:HG12	1:120:A:VAL:HG23	20	0.69
(1,1450)	1:116:A:VAL:HG13	1:120:A:VAL:HG11	20	0.69
(1,1450)	1:116:A:VAL:HG13	1:120:A:VAL:HG12	20	0.69
(1,1450)	1:116:A:VAL:HG13	1:120:A:VAL:HG13	20	0.69
(1,1450)	1:116:A:VAL:HG13	1:120:A:VAL:HG21	20	0.69
(1,1450)	1:116:A:VAL:HG13	1:120:A:VAL:HG22	20	0.69
(1,1450)	1:116:A:VAL:HG13	1:120:A:VAL:HG23	20	0.69
(1,1450)	1:116:A:VAL:HG21	1:120:A:VAL:HG11	20	0.69
(1,1450)	1:116:A:VAL:HG21	1:120:A:VAL:HG12	20	0.69
(1,1450)	1:116:A:VAL:HG21	1:120:A:VAL:HG13	20	0.69
(1,1450)	1:116:A:VAL:HG21	1:120:A:VAL:HG21	20	0.69
(1,1450)	1:116:A:VAL:HG21	1:120:A:VAL:HG22	20	0.69
(1,1450)	1:116:A:VAL:HG21	1:120:A:VAL:HG23	20	0.69
(1,1450)	1:116:A:VAL:HG22	1:120:A:VAL:HG11	20	0.69
(1,1450)	1:116:A:VAL:HG22	1:120:A:VAL:HG12	20	0.69
(1,1450)	1:116:A:VAL:HG22	1:120:A:VAL:HG13	20	0.69
(1,1450)	1:116:A:VAL:HG22	1:120:A:VAL:HG21	20	0.69
(1,1450)	1:116:A:VAL:HG22	1:120:A:VAL:HG22	20	0.69
(1,1450)	1:116:A:VAL:HG22	1:120:A:VAL:HG23	20	0.69
(1,1450)	1:116:A:VAL:HG23	1:120:A:VAL:HG11	20	0.69
(1,1450)	1:116:A:VAL:HG23	1:120:A:VAL:HG12	20	0.69
(1,1450)	1:116:A:VAL:HG23	1:120:A:VAL:HG13	20	0.69
(1,1450)	1:116:A:VAL:HG23	1:120:A:VAL:HG21	20	0.69
(1,1450)	1:116:A:VAL:HG23	1:120:A:VAL:HG22	20	0.69
(1,1450)	1:116:A:VAL:HG23	1:120:A:VAL:HG23	20	0.69
(1,1447)	1:116:A:VAL:HG11	1:118:A:LYS:HG2	11	0.69
(1,1447)	1:116:A:VAL:HG11	1:118:A:LYS:HG3	11	0.69
(1,1447)	1:116:A:VAL:HG12	1:118:A:LYS:HG2	11	0.69
(1,1447)	1:116:A:VAL:HG12	1:118:A:LYS:HG3	11	0.69
(1,1447)	1:116:A:VAL:HG13	1:118:A:LYS:HG2	11	0.69
(1,1447)	1:116:A:VAL:HG13	1:118:A:LYS:HG3	11	0.69
(1,1447)	1:116:A:VAL:HG21	1:118:A:LYS:HG2	11	0.69
(1,1447)	1:116:A:VAL:HG21	1:118:A:LYS:HG3	11	0.69
(1,1447)	1:116:A:VAL:HG22	1:118:A:LYS:HG2	11	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1447)	1:116:A:VAL:HG22	1:118:A:LYS:HG3	11	0.69
(1,1447)	1:116:A:VAL:HG23	1:118:A:LYS:HG2	11	0.69
(1,1447)	1:116:A:VAL:HG23	1:118:A:LYS:HG3	11	0.69
(1,1403)	1:104:A:LEU:HD11	1:141:A:LEU:HG	4	0.69
(1,1403)	1:104:A:LEU:HD12	1:141:A:LEU:HG	4	0.69
(1,1403)	1:104:A:LEU:HD13	1:141:A:LEU:HG	4	0.69
(1,1403)	1:104:A:LEU:HD21	1:141:A:LEU:HG	4	0.69
(1,1403)	1:104:A:LEU:HD22	1:141:A:LEU:HG	4	0.69
(1,1403)	1:104:A:LEU:HD23	1:141:A:LEU:HG	4	0.69
(1,461)	1:101:A:ALA:HB1	1:137:A:MET:HB2	17	0.69
(1,461)	1:101:A:ALA:HB2	1:137:A:MET:HB2	17	0.69
(1,461)	1:101:A:ALA:HB3	1:137:A:MET:HB2	17	0.69
(2,12)	2:158:B:TYR:HD1	1:132:A:VAL:HG11	14	0.68
(2,12)	2:158:B:TYR:HD1	1:132:A:VAL:HG12	14	0.68
(2,12)	2:158:B:TYR:HD1	1:132:A:VAL:HG13	14	0.68
(2,12)	2:158:B:TYR:HD2	1:132:A:VAL:HG11	14	0.68
(2,12)	2:158:B:TYR:HD2	1:132:A:VAL:HG12	14	0.68
(2,12)	2:158:B:TYR:HD2	1:132:A:VAL:HG13	14	0.68
(1,1447)	1:116:A:VAL:HG11	1:118:A:LYS:HG2	2	0.68
(1,1447)	1:116:A:VAL:HG11	1:118:A:LYS:HG3	2	0.68
(1,1447)	1:116:A:VAL:HG12	1:118:A:LYS:HG2	2	0.68
(1,1447)	1:116:A:VAL:HG12	1:118:A:LYS:HG3	2	0.68
(1,1447)	1:116:A:VAL:HG13	1:118:A:LYS:HG2	2	0.68
(1,1447)	1:116:A:VAL:HG13	1:118:A:LYS:HG3	2	0.68
(1,1447)	1:116:A:VAL:HG21	1:118:A:LYS:HG2	2	0.68
(1,1447)	1:116:A:VAL:HG21	1:118:A:LYS:HG3	2	0.68
(1,1447)	1:116:A:VAL:HG22	1:118:A:LYS:HG2	2	0.68
(1,1447)	1:116:A:VAL:HG22	1:118:A:LYS:HG3	2	0.68
(1,1447)	1:116:A:VAL:HG23	1:118:A:LYS:HG2	2	0.68
(1,1447)	1:116:A:VAL:HG23	1:118:A:LYS:HG3	2	0.68
(1,454)	1:116:A:VAL:HG11	1:118:A:LYS:HG2	7	0.68
(1,454)	1:116:A:VAL:HG11	1:118:A:LYS:HG3	7	0.68
(1,454)	1:116:A:VAL:HG12	1:118:A:LYS:HG2	7	0.68
(1,454)	1:116:A:VAL:HG12	1:118:A:LYS:HG3	7	0.68
(1,454)	1:116:A:VAL:HG13	1:118:A:LYS:HG2	7	0.68
(1,454)	1:116:A:VAL:HG13	1:118:A:LYS:HG3	7	0.68
(1,204)	1:59:A:VAL:HA	1:103:A:VAL:HG11	18	0.68
(1,204)	1:59:A:VAL:HA	1:103:A:VAL:HG12	18	0.68
(1,204)	1:59:A:VAL:HA	1:103:A:VAL:HG13	18	0.68
(1,56)	1:78:A:PHE:HB3	1:120:A:VAL:HG11	17	0.68
(1,56)	1:78:A:PHE:HB3	1:120:A:VAL:HG12	17	0.68
(1,56)	1:78:A:PHE:HB3	1:120:A:VAL:HG13	17	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1422)	1:112:A:LYS:H	1:145:A:LEU:HD11	15	0.67
(1,1422)	1:112:A:LYS:H	1:145:A:LEU:HD12	15	0.67
(1,1422)	1:112:A:LYS:H	1:145:A:LEU:HD13	15	0.67
(1,1422)	1:112:A:LYS:H	1:145:A:LEU:HD21	15	0.67
(1,1422)	1:112:A:LYS:H	1:145:A:LEU:HD22	15	0.67
(1,1422)	1:112:A:LYS:H	1:145:A:LEU:HD23	15	0.67
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD11	3	0.67
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD12	3	0.67
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD13	3	0.67
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD21	3	0.67
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD22	3	0.67
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD23	3	0.67
(1,442)	1:75:A:LEU:HD11	1:78:A:PHE:HB3	3	0.67
(1,442)	1:75:A:LEU:HD12	1:78:A:PHE:HB3	3	0.67
(1,442)	1:75:A:LEU:HD13	1:78:A:PHE:HB3	3	0.67
(1,359)	1:75:A:LEU:HD11	1:119:A:SER:HA	4	0.67
(1,359)	1:75:A:LEU:HD12	1:119:A:SER:HA	4	0.67
(1,359)	1:75:A:LEU:HD13	1:119:A:SER:HA	4	0.67
(1,313)	1:34:A:VAL:HG21	1:35:A:THR:HG21	19	0.67
(1,313)	1:34:A:VAL:HG21	1:35:A:THR:HG22	19	0.67
(1,313)	1:34:A:VAL:HG21	1:35:A:THR:HG23	19	0.67
(1,313)	1:34:A:VAL:HG22	1:35:A:THR:HG21	19	0.67
(1,313)	1:34:A:VAL:HG22	1:35:A:THR:HG22	19	0.67
(1,313)	1:34:A:VAL:HG22	1:35:A:THR:HG23	19	0.67
(1,313)	1:34:A:VAL:HG23	1:35:A:THR:HG21	19	0.67
(1,313)	1:34:A:VAL:HG23	1:35:A:THR:HG22	19	0.67
(1,313)	1:34:A:VAL:HG23	1:35:A:THR:HG23	19	0.67
(1,293)	1:31:A:PHE:HA	1:34:A:VAL:HG11	16	0.67
(1,293)	1:31:A:PHE:HA	1:34:A:VAL:HG12	16	0.67
(1,293)	1:31:A:PHE:HA	1:34:A:VAL:HG13	16	0.67
(1,269)	1:104:A:LEU:HD21	1:108:A:ALA:HB1	15	0.67
(1,269)	1:104:A:LEU:HD21	1:108:A:ALA:HB2	15	0.67
(1,269)	1:104:A:LEU:HD21	1:108:A:ALA:HB3	15	0.67
(1,269)	1:104:A:LEU:HD22	1:108:A:ALA:HB1	15	0.67
(1,269)	1:104:A:LEU:HD22	1:108:A:ALA:HB2	15	0.67
(1,269)	1:104:A:LEU:HD22	1:108:A:ALA:HB3	15	0.67
(1,269)	1:104:A:LEU:HD23	1:108:A:ALA:HB1	15	0.67
(1,269)	1:104:A:LEU:HD23	1:108:A:ALA:HB2	15	0.67
(1,269)	1:104:A:LEU:HD23	1:108:A:ALA:HB3	15	0.67
(4,1)	2:151:B:TYR:HH	1:82:A:ASN:ND2	2	0.66
(4,1)	2:151:B:TYR:HH	1:82:A:ASN:ND2	8	0.66
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD11	4	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD12	4	0.66
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD13	4	0.66
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD21	4	0.66
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD22	4	0.66
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD23	4	0.66
(6,1)	2:148:B:SER:H1	2:149:B:PRO:HA	18	0.65
(1,1447)	1:116:A:VAL:HG11	1:118:A:LYS:HG2	6	0.65
(1,1447)	1:116:A:VAL:HG11	1:118:A:LYS:HG3	6	0.65
(1,1447)	1:116:A:VAL:HG12	1:118:A:LYS:HG2	6	0.65
(1,1447)	1:116:A:VAL:HG12	1:118:A:LYS:HG3	6	0.65
(1,1447)	1:116:A:VAL:HG13	1:118:A:LYS:HG2	6	0.65
(1,1447)	1:116:A:VAL:HG13	1:118:A:LYS:HG3	6	0.65
(1,1447)	1:116:A:VAL:HG21	1:118:A:LYS:HG2	6	0.65
(1,1447)	1:116:A:VAL:HG21	1:118:A:LYS:HG3	6	0.65
(1,1447)	1:116:A:VAL:HG22	1:118:A:LYS:HG2	6	0.65
(1,1447)	1:116:A:VAL:HG22	1:118:A:LYS:HG3	6	0.65
(1,1447)	1:116:A:VAL:HG23	1:118:A:LYS:HG2	6	0.65
(1,1447)	1:116:A:VAL:HG23	1:118:A:LYS:HG3	6	0.65
(1,1447)	1:116:A:VAL:HG11	1:118:A:LYS:HG2	7	0.65
(1,1447)	1:116:A:VAL:HG11	1:118:A:LYS:HG3	7	0.65
(1,1447)	1:116:A:VAL:HG12	1:118:A:LYS:HG2	7	0.65
(1,1447)	1:116:A:VAL:HG12	1:118:A:LYS:HG3	7	0.65
(1,1447)	1:116:A:VAL:HG13	1:118:A:LYS:HG2	7	0.65
(1,1447)	1:116:A:VAL:HG13	1:118:A:LYS:HG3	7	0.65
(1,1447)	1:116:A:VAL:HG21	1:118:A:LYS:HG2	7	0.65
(1,1447)	1:116:A:VAL:HG21	1:118:A:LYS:HG3	7	0.65
(1,1447)	1:116:A:VAL:HG22	1:118:A:LYS:HG2	7	0.65
(1,1447)	1:116:A:VAL:HG22	1:118:A:LYS:HG3	7	0.65
(1,1447)	1:116:A:VAL:HG23	1:118:A:LYS:HG2	7	0.65
(1,1447)	1:116:A:VAL:HG23	1:118:A:LYS:HG3	7	0.65
(1,1447)	1:116:A:VAL:HG11	1:118:A:LYS:HG2	9	0.65
(1,1447)	1:116:A:VAL:HG11	1:118:A:LYS:HG3	9	0.65
(1,1447)	1:116:A:VAL:HG12	1:118:A:LYS:HG2	9	0.65
(1,1447)	1:116:A:VAL:HG12	1:118:A:LYS:HG3	9	0.65
(1,1447)	1:116:A:VAL:HG13	1:118:A:LYS:HG2	9	0.65
(1,1447)	1:116:A:VAL:HG13	1:118:A:LYS:HG3	9	0.65
(1,1447)	1:116:A:VAL:HG21	1:118:A:LYS:HG2	9	0.65
(1,1447)	1:116:A:VAL:HG21	1:118:A:LYS:HG3	9	0.65
(1,1447)	1:116:A:VAL:HG22	1:118:A:LYS:HG2	9	0.65
(1,1447)	1:116:A:VAL:HG22	1:118:A:LYS:HG3	9	0.65
(1,1447)	1:116:A:VAL:HG23	1:118:A:LYS:HG2	9	0.65
(1,1447)	1:116:A:VAL:HG23	1:118:A:LYS:HG3	9	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1447)	1:116:A:VAL:HG11	1:118:A:LYS:HG2	20	0.65
(1,1447)	1:116:A:VAL:HG11	1:118:A:LYS:HG3	20	0.65
(1,1447)	1:116:A:VAL:HG12	1:118:A:LYS:HG2	20	0.65
(1,1447)	1:116:A:VAL:HG12	1:118:A:LYS:HG3	20	0.65
(1,1447)	1:116:A:VAL:HG13	1:118:A:LYS:HG2	20	0.65
(1,1447)	1:116:A:VAL:HG13	1:118:A:LYS:HG3	20	0.65
(1,1447)	1:116:A:VAL:HG21	1:118:A:LYS:HG2	20	0.65
(1,1447)	1:116:A:VAL:HG21	1:118:A:LYS:HG3	20	0.65
(1,1447)	1:116:A:VAL:HG22	1:118:A:LYS:HG2	20	0.65
(1,1447)	1:116:A:VAL:HG22	1:118:A:LYS:HG3	20	0.65
(1,1447)	1:116:A:VAL:HG23	1:118:A:LYS:HG2	20	0.65
(1,1447)	1:116:A:VAL:HG23	1:118:A:LYS:HG3	20	0.65
(1,1410)	1:108:A:ALA:HB1	1:145:A:LEU:HD11	15	0.65
(1,1410)	1:108:A:ALA:HB1	1:145:A:LEU:HD12	15	0.65
(1,1410)	1:108:A:ALA:HB1	1:145:A:LEU:HD13	15	0.65
(1,1410)	1:108:A:ALA:HB1	1:145:A:LEU:HD21	15	0.65
(1,1410)	1:108:A:ALA:HB1	1:145:A:LEU:HD22	15	0.65
(1,1410)	1:108:A:ALA:HB1	1:145:A:LEU:HD23	15	0.65
(1,1410)	1:108:A:ALA:HB2	1:145:A:LEU:HD11	15	0.65
(1,1410)	1:108:A:ALA:HB2	1:145:A:LEU:HD12	15	0.65
(1,1410)	1:108:A:ALA:HB2	1:145:A:LEU:HD13	15	0.65
(1,1410)	1:108:A:ALA:HB2	1:145:A:LEU:HD21	15	0.65
(1,1410)	1:108:A:ALA:HB2	1:145:A:LEU:HD22	15	0.65
(1,1410)	1:108:A:ALA:HB2	1:145:A:LEU:HD23	15	0.65
(1,1410)	1:108:A:ALA:HB3	1:145:A:LEU:HD11	15	0.65
(1,1410)	1:108:A:ALA:HB3	1:145:A:LEU:HD12	15	0.65
(1,1410)	1:108:A:ALA:HB3	1:145:A:LEU:HD13	15	0.65
(1,1410)	1:108:A:ALA:HB3	1:145:A:LEU:HD21	15	0.65
(1,1410)	1:108:A:ALA:HB3	1:145:A:LEU:HD22	15	0.65
(1,1410)	1:108:A:ALA:HB3	1:145:A:LEU:HD23	15	0.65
(1,1403)	1:104:A:LEU:HD11	1:141:A:LEU:HG	7	0.65
(1,1403)	1:104:A:LEU:HD12	1:141:A:LEU:HG	7	0.65
(1,1403)	1:104:A:LEU:HD13	1:141:A:LEU:HG	7	0.65
(1,1403)	1:104:A:LEU:HD21	1:141:A:LEU:HG	7	0.65
(1,1403)	1:104:A:LEU:HD22	1:141:A:LEU:HG	7	0.65
(1,1403)	1:104:A:LEU:HD23	1:141:A:LEU:HG	7	0.65
(1,722)	1:34:A:VAL:HG21	1:40:A:SER:H	7	0.65
(1,722)	1:34:A:VAL:HG22	1:40:A:SER:H	7	0.65
(1,722)	1:34:A:VAL:HG23	1:40:A:SER:H	7	0.65
(1,648)	1:75:A:LEU:HD11	1:120:A:VAL:H	19	0.65
(1,648)	1:75:A:LEU:HD12	1:120:A:VAL:H	19	0.65
(1,648)	1:75:A:LEU:HD13	1:120:A:VAL:H	19	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,442)	1:75:A:LEU:HD11	1:78:A:PHE:HB3	6	0.65
(1,442)	1:75:A:LEU:HD12	1:78:A:PHE:HB3	6	0.65
(1,442)	1:75:A:LEU:HD13	1:78:A:PHE:HB3	6	0.65
(1,293)	1:31:A:PHE:HA	1:34:A:VAL:HG11	11	0.65
(1,293)	1:31:A:PHE:HA	1:34:A:VAL:HG12	11	0.65
(1,293)	1:31:A:PHE:HA	1:34:A:VAL:HG13	11	0.65
(1,293)	1:31:A:PHE:HA	1:34:A:VAL:HG11	13	0.65
(1,293)	1:31:A:PHE:HA	1:34:A:VAL:HG12	13	0.65
(1,293)	1:31:A:PHE:HA	1:34:A:VAL:HG13	13	0.65
(1,1447)	1:116:A:VAL:HG11	1:118:A:LYS:HG2	10	0.64
(1,1447)	1:116:A:VAL:HG11	1:118:A:LYS:HG3	10	0.64
(1,1447)	1:116:A:VAL:HG12	1:118:A:LYS:HG2	10	0.64
(1,1447)	1:116:A:VAL:HG12	1:118:A:LYS:HG3	10	0.64
(1,1447)	1:116:A:VAL:HG13	1:118:A:LYS:HG2	10	0.64
(1,1447)	1:116:A:VAL:HG13	1:118:A:LYS:HG3	10	0.64
(1,1447)	1:116:A:VAL:HG21	1:118:A:LYS:HG2	10	0.64
(1,1447)	1:116:A:VAL:HG21	1:118:A:LYS:HG3	10	0.64
(1,1447)	1:116:A:VAL:HG22	1:118:A:LYS:HG2	10	0.64
(1,1447)	1:116:A:VAL:HG22	1:118:A:LYS:HG3	10	0.64
(1,1447)	1:116:A:VAL:HG23	1:118:A:LYS:HG2	10	0.64
(1,1447)	1:116:A:VAL:HG23	1:118:A:LYS:HG3	10	0.64
(1,1447)	1:116:A:VAL:HG11	1:118:A:LYS:HG2	14	0.64
(1,1447)	1:116:A:VAL:HG11	1:118:A:LYS:HG3	14	0.64
(1,1447)	1:116:A:VAL:HG12	1:118:A:LYS:HG2	14	0.64
(1,1447)	1:116:A:VAL:HG12	1:118:A:LYS:HG3	14	0.64
(1,1447)	1:116:A:VAL:HG13	1:118:A:LYS:HG2	14	0.64
(1,1447)	1:116:A:VAL:HG13	1:118:A:LYS:HG3	14	0.64
(1,1447)	1:116:A:VAL:HG21	1:118:A:LYS:HG2	14	0.64
(1,1447)	1:116:A:VAL:HG21	1:118:A:LYS:HG3	14	0.64
(1,1447)	1:116:A:VAL:HG22	1:118:A:LYS:HG2	14	0.64
(1,1447)	1:116:A:VAL:HG22	1:118:A:LYS:HG3	14	0.64
(1,1447)	1:116:A:VAL:HG23	1:118:A:LYS:HG2	14	0.64
(1,1447)	1:116:A:VAL:HG23	1:118:A:LYS:HG3	14	0.64
(1,1276)	1:59:A:VAL:HG11	1:103:A:VAL:H	5	0.64
(1,1276)	1:59:A:VAL:HG12	1:103:A:VAL:H	5	0.64
(1,1276)	1:59:A:VAL:HG13	1:103:A:VAL:H	5	0.64
(1,1276)	1:59:A:VAL:HG21	1:103:A:VAL:H	5	0.64
(1,1276)	1:59:A:VAL:HG22	1:103:A:VAL:H	5	0.64
(1,1276)	1:59:A:VAL:HG23	1:103:A:VAL:H	5	0.64
(1,1276)	1:59:A:VAL:HG11	1:103:A:VAL:H	17	0.64
(1,1276)	1:59:A:VAL:HG12	1:103:A:VAL:H	17	0.64
(1,1276)	1:59:A:VAL:HG13	1:103:A:VAL:H	17	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1276)	1:59:A:VAL:HG21	1:103:A:VAL:H	17	0.64
(1,1276)	1:59:A:VAL:HG22	1:103:A:VAL:H	17	0.64
(1,1276)	1:59:A:VAL:HG23	1:103:A:VAL:H	17	0.64
(1,478)	1:77:A:LEU:HD21	1:78:A:PHE:HA	12	0.64
(1,478)	1:77:A:LEU:HD22	1:78:A:PHE:HA	12	0.64
(1,478)	1:77:A:LEU:HD23	1:78:A:PHE:HA	12	0.64
(1,454)	1:116:A:VAL:HG11	1:118:A:LYS:HG2	13	0.64
(1,454)	1:116:A:VAL:HG11	1:118:A:LYS:HG3	13	0.64
(1,454)	1:116:A:VAL:HG12	1:118:A:LYS:HG2	13	0.64
(1,454)	1:116:A:VAL:HG12	1:118:A:LYS:HG3	13	0.64
(1,454)	1:116:A:VAL:HG13	1:118:A:LYS:HG2	13	0.64
(1,454)	1:116:A:VAL:HG13	1:118:A:LYS:HG3	13	0.64
(1,438)	1:58:A:ILE:HG21	1:59:A:VAL:HG11	7	0.64
(1,438)	1:58:A:ILE:HG21	1:59:A:VAL:HG12	7	0.64
(1,438)	1:58:A:ILE:HG21	1:59:A:VAL:HG13	7	0.64
(1,438)	1:58:A:ILE:HG22	1:59:A:VAL:HG11	7	0.64
(1,438)	1:58:A:ILE:HG22	1:59:A:VAL:HG12	7	0.64
(1,438)	1:58:A:ILE:HG22	1:59:A:VAL:HG13	7	0.64
(1,438)	1:58:A:ILE:HG23	1:59:A:VAL:HG11	7	0.64
(1,438)	1:58:A:ILE:HG23	1:59:A:VAL:HG12	7	0.64
(1,438)	1:58:A:ILE:HG23	1:59:A:VAL:HG13	7	0.64
(1,1443)	1:116:A:VAL:HA	1:120:A:VAL:HG11	20	0.63
(1,1443)	1:116:A:VAL:HA	1:120:A:VAL:HG12	20	0.63
(1,1443)	1:116:A:VAL:HA	1:120:A:VAL:HG13	20	0.63
(1,1443)	1:116:A:VAL:HA	1:120:A:VAL:HG21	20	0.63
(1,1443)	1:116:A:VAL:HA	1:120:A:VAL:HG22	20	0.63
(1,1443)	1:116:A:VAL:HA	1:120:A:VAL:HG23	20	0.63
(1,1432)	1:113:A:ASP:H	1:145:A:LEU:HD11	9	0.63
(1,1432)	1:113:A:ASP:H	1:145:A:LEU:HD12	9	0.63
(1,1432)	1:113:A:ASP:H	1:145:A:LEU:HD13	9	0.63
(1,1432)	1:113:A:ASP:H	1:145:A:LEU:HD21	9	0.63
(1,1432)	1:113:A:ASP:H	1:145:A:LEU:HD22	9	0.63
(1,1432)	1:113:A:ASP:H	1:145:A:LEU:HD23	9	0.63
(1,1425)	1:112:A:LYS:HA	1:145:A:LEU:HD11	10	0.63
(1,1425)	1:112:A:LYS:HA	1:145:A:LEU:HD12	10	0.63
(1,1425)	1:112:A:LYS:HA	1:145:A:LEU:HD13	10	0.63
(1,1425)	1:112:A:LYS:HA	1:145:A:LEU:HD21	10	0.63
(1,1425)	1:112:A:LYS:HA	1:145:A:LEU:HD22	10	0.63
(1,1425)	1:112:A:LYS:HA	1:145:A:LEU:HD23	10	0.63
(1,1203)	1:23:A:LEU:HD11	1:27:A:LEU:HB2	8	0.63
(1,1203)	1:23:A:LEU:HD11	1:27:A:LEU:HB3	8	0.63
(1,1203)	1:23:A:LEU:HD12	1:27:A:LEU:HB2	8	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1203)	1:23:A:LEU:HD12	1:27:A:LEU:HB3	8	0.63
(1,1203)	1:23:A:LEU:HD13	1:27:A:LEU:HB2	8	0.63
(1,1203)	1:23:A:LEU:HD13	1:27:A:LEU:HB3	8	0.63
(1,1203)	1:23:A:LEU:HD21	1:27:A:LEU:HB2	8	0.63
(1,1203)	1:23:A:LEU:HD21	1:27:A:LEU:HB3	8	0.63
(1,1203)	1:23:A:LEU:HD22	1:27:A:LEU:HB2	8	0.63
(1,1203)	1:23:A:LEU:HD22	1:27:A:LEU:HB3	8	0.63
(1,1203)	1:23:A:LEU:HD23	1:27:A:LEU:HB2	8	0.63
(1,1203)	1:23:A:LEU:HD23	1:27:A:LEU:HB3	8	0.63
(1,438)	1:58:A:ILE:HG21	1:59:A:VAL:HG11	12	0.63
(1,438)	1:58:A:ILE:HG21	1:59:A:VAL:HG12	12	0.63
(1,438)	1:58:A:ILE:HG21	1:59:A:VAL:HG13	12	0.63
(1,438)	1:58:A:ILE:HG22	1:59:A:VAL:HG11	12	0.63
(1,438)	1:58:A:ILE:HG22	1:59:A:VAL:HG12	12	0.63
(1,438)	1:58:A:ILE:HG22	1:59:A:VAL:HG13	12	0.63
(1,438)	1:58:A:ILE:HG23	1:59:A:VAL:HG11	12	0.63
(1,438)	1:58:A:ILE:HG23	1:59:A:VAL:HG12	12	0.63
(1,438)	1:58:A:ILE:HG23	1:59:A:VAL:HG13	12	0.63
(1,279)	1:77:A:LEU:HD21	1:107:A:ALA:HB1	20	0.63
(1,279)	1:77:A:LEU:HD21	1:107:A:ALA:HB2	20	0.63
(1,279)	1:77:A:LEU:HD21	1:107:A:ALA:HB3	20	0.63
(1,279)	1:77:A:LEU:HD22	1:107:A:ALA:HB1	20	0.63
(1,279)	1:77:A:LEU:HD22	1:107:A:ALA:HB2	20	0.63
(1,279)	1:77:A:LEU:HD22	1:107:A:ALA:HB3	20	0.63
(1,279)	1:77:A:LEU:HD23	1:107:A:ALA:HB1	20	0.63
(1,279)	1:77:A:LEU:HD23	1:107:A:ALA:HB2	20	0.63
(1,279)	1:77:A:LEU:HD23	1:107:A:ALA:HB3	20	0.63
(6,1)	2:148:B:SER:H1	2:149:B:PRO:HA	8	0.62
(1,1500)	1:137:A:MET:HB2	1:141:A:LEU:HD11	10	0.62
(1,1500)	1:137:A:MET:HB2	1:141:A:LEU:HD12	10	0.62
(1,1500)	1:137:A:MET:HB2	1:141:A:LEU:HD13	10	0.62
(1,1500)	1:137:A:MET:HB2	1:141:A:LEU:HD21	10	0.62
(1,1500)	1:137:A:MET:HB2	1:141:A:LEU:HD22	10	0.62
(1,1500)	1:137:A:MET:HB2	1:141:A:LEU:HD23	10	0.62
(1,1432)	1:113:A:ASP:H	1:145:A:LEU:HD11	15	0.62
(1,1432)	1:113:A:ASP:H	1:145:A:LEU:HD12	15	0.62
(1,1432)	1:113:A:ASP:H	1:145:A:LEU:HD13	15	0.62
(1,1432)	1:113:A:ASP:H	1:145:A:LEU:HD21	15	0.62
(1,1432)	1:113:A:ASP:H	1:145:A:LEU:HD22	15	0.62
(1,1432)	1:113:A:ASP:H	1:145:A:LEU:HD23	15	0.62
(1,478)	1:77:A:LEU:HD21	1:78:A:PHE:HA	4	0.62
(1,478)	1:77:A:LEU:HD22	1:78:A:PHE:HA	4	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,478)	1:77:A:LEU:HD23	1:78:A:PHE:HA	4	0.62
(1,466)	1:102:A:ASP:HB2	1:103:A:VAL:HG11	3	0.62
(1,466)	1:102:A:ASP:HB2	1:103:A:VAL:HG12	3	0.62
(1,466)	1:102:A:ASP:HB2	1:103:A:VAL:HG13	3	0.62
(1,466)	1:102:A:ASP:HB3	1:103:A:VAL:HG11	3	0.62
(1,466)	1:102:A:ASP:HB3	1:103:A:VAL:HG12	3	0.62
(1,466)	1:102:A:ASP:HB3	1:103:A:VAL:HG13	3	0.62
(1,454)	1:116:A:VAL:HG11	1:118:A:LYS:HG2	5	0.62
(1,454)	1:116:A:VAL:HG11	1:118:A:LYS:HG3	5	0.62
(1,454)	1:116:A:VAL:HG12	1:118:A:LYS:HG2	5	0.62
(1,454)	1:116:A:VAL:HG12	1:118:A:LYS:HG3	5	0.62
(1,454)	1:116:A:VAL:HG13	1:118:A:LYS:HG2	5	0.62
(1,454)	1:116:A:VAL:HG13	1:118:A:LYS:HG3	5	0.62
(1,438)	1:58:A:ILE:HG21	1:59:A:VAL:HG11	19	0.62
(1,438)	1:58:A:ILE:HG21	1:59:A:VAL:HG12	19	0.62
(1,438)	1:58:A:ILE:HG21	1:59:A:VAL:HG13	19	0.62
(1,438)	1:58:A:ILE:HG22	1:59:A:VAL:HG11	19	0.62
(1,438)	1:58:A:ILE:HG22	1:59:A:VAL:HG12	19	0.62
(1,438)	1:58:A:ILE:HG22	1:59:A:VAL:HG13	19	0.62
(1,438)	1:58:A:ILE:HG23	1:59:A:VAL:HG11	19	0.62
(1,438)	1:58:A:ILE:HG23	1:59:A:VAL:HG12	19	0.62
(1,438)	1:58:A:ILE:HG23	1:59:A:VAL:HG13	19	0.62
(1,1500)	1:137:A:MET:HB2	1:141:A:LEU:HD11	4	0.61
(1,1500)	1:137:A:MET:HB2	1:141:A:LEU:HD12	4	0.61
(1,1500)	1:137:A:MET:HB2	1:141:A:LEU:HD13	4	0.61
(1,1500)	1:137:A:MET:HB2	1:141:A:LEU:HD21	4	0.61
(1,1500)	1:137:A:MET:HB2	1:141:A:LEU:HD22	4	0.61
(1,1500)	1:137:A:MET:HB2	1:141:A:LEU:HD23	4	0.61
(1,1455)	1:120:A:VAL:HB	1:145:A:LEU:HD11	17	0.61
(1,1455)	1:120:A:VAL:HB	1:145:A:LEU:HD12	17	0.61
(1,1455)	1:120:A:VAL:HB	1:145:A:LEU:HD13	17	0.61
(1,1455)	1:120:A:VAL:HB	1:145:A:LEU:HD21	17	0.61
(1,1455)	1:120:A:VAL:HB	1:145:A:LEU:HD22	17	0.61
(1,1455)	1:120:A:VAL:HB	1:145:A:LEU:HD23	17	0.61
(1,1410)	1:108:A:ALA:HB1	1:145:A:LEU:HD11	3	0.61
(1,1410)	1:108:A:ALA:HB1	1:145:A:LEU:HD12	3	0.61
(1,1410)	1:108:A:ALA:HB1	1:145:A:LEU:HD13	3	0.61
(1,1410)	1:108:A:ALA:HB1	1:145:A:LEU:HD21	3	0.61
(1,1410)	1:108:A:ALA:HB1	1:145:A:LEU:HD22	3	0.61
(1,1410)	1:108:A:ALA:HB1	1:145:A:LEU:HD23	3	0.61
(1,1410)	1:108:A:ALA:HB2	1:145:A:LEU:HD11	3	0.61
(1,1410)	1:108:A:ALA:HB2	1:145:A:LEU:HD12	3	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1410)	1:108:A:ALA:HB2	1:145:A:LEU:HD13	3	0.61
(1,1410)	1:108:A:ALA:HB2	1:145:A:LEU:HD21	3	0.61
(1,1410)	1:108:A:ALA:HB2	1:145:A:LEU:HD22	3	0.61
(1,1410)	1:108:A:ALA:HB2	1:145:A:LEU:HD23	3	0.61
(1,1410)	1:108:A:ALA:HB3	1:145:A:LEU:HD11	3	0.61
(1,1410)	1:108:A:ALA:HB3	1:145:A:LEU:HD12	3	0.61
(1,1410)	1:108:A:ALA:HB3	1:145:A:LEU:HD13	3	0.61
(1,1410)	1:108:A:ALA:HB3	1:145:A:LEU:HD21	3	0.61
(1,1410)	1:108:A:ALA:HB3	1:145:A:LEU:HD22	3	0.61
(1,1410)	1:108:A:ALA:HB3	1:145:A:LEU:HD23	3	0.61
(1,1279)	1:59:A:VAL:HG11	1:103:A:VAL:HG11	14	0.61
(1,1279)	1:59:A:VAL:HG11	1:103:A:VAL:HG12	14	0.61
(1,1279)	1:59:A:VAL:HG11	1:103:A:VAL:HG13	14	0.61
(1,1279)	1:59:A:VAL:HG12	1:103:A:VAL:HG11	14	0.61
(1,1279)	1:59:A:VAL:HG12	1:103:A:VAL:HG12	14	0.61
(1,1279)	1:59:A:VAL:HG12	1:103:A:VAL:HG13	14	0.61
(1,1279)	1:59:A:VAL:HG13	1:103:A:VAL:HG11	14	0.61
(1,1279)	1:59:A:VAL:HG13	1:103:A:VAL:HG12	14	0.61
(1,1279)	1:59:A:VAL:HG13	1:103:A:VAL:HG13	14	0.61
(1,1279)	1:59:A:VAL:HG21	1:103:A:VAL:HG11	14	0.61
(1,1279)	1:59:A:VAL:HG21	1:103:A:VAL:HG12	14	0.61
(1,1279)	1:59:A:VAL:HG21	1:103:A:VAL:HG13	14	0.61
(1,1279)	1:59:A:VAL:HG22	1:103:A:VAL:HG11	14	0.61
(1,1279)	1:59:A:VAL:HG22	1:103:A:VAL:HG12	14	0.61
(1,1279)	1:59:A:VAL:HG22	1:103:A:VAL:HG13	14	0.61
(1,1279)	1:59:A:VAL:HG23	1:103:A:VAL:HG11	14	0.61
(1,1279)	1:59:A:VAL:HG23	1:103:A:VAL:HG12	14	0.61
(1,1279)	1:59:A:VAL:HG23	1:103:A:VAL:HG13	14	0.61
(1,838)	1:31:A:PHE:H	1:34:A:VAL:HG21	2	0.61
(1,838)	1:31:A:PHE:H	1:34:A:VAL:HG22	2	0.61
(1,838)	1:31:A:PHE:H	1:34:A:VAL:HG23	2	0.61
(1,438)	1:58:A:ILE:HG21	1:59:A:VAL:HG11	1	0.61
(1,438)	1:58:A:ILE:HG21	1:59:A:VAL:HG12	1	0.61
(1,438)	1:58:A:ILE:HG21	1:59:A:VAL:HG13	1	0.61
(1,438)	1:58:A:ILE:HG22	1:59:A:VAL:HG11	1	0.61
(1,438)	1:58:A:ILE:HG22	1:59:A:VAL:HG12	1	0.61
(1,438)	1:58:A:ILE:HG22	1:59:A:VAL:HG13	1	0.61
(1,438)	1:58:A:ILE:HG23	1:59:A:VAL:HG11	1	0.61
(1,438)	1:58:A:ILE:HG23	1:59:A:VAL:HG12	1	0.61
(1,438)	1:58:A:ILE:HG23	1:59:A:VAL:HG13	1	0.61
(1,438)	1:58:A:ILE:HG21	1:59:A:VAL:HG11	13	0.61
(1,438)	1:58:A:ILE:HG21	1:59:A:VAL:HG12	13	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,438)	1:58:A:ILE:HG21	1:59:A:VAL:HG13	13	0.61
(1,438)	1:58:A:ILE:HG22	1:59:A:VAL:HG11	13	0.61
(1,438)	1:58:A:ILE:HG22	1:59:A:VAL:HG12	13	0.61
(1,438)	1:58:A:ILE:HG22	1:59:A:VAL:HG13	13	0.61
(1,438)	1:58:A:ILE:HG23	1:59:A:VAL:HG11	13	0.61
(1,438)	1:58:A:ILE:HG23	1:59:A:VAL:HG12	13	0.61
(1,438)	1:58:A:ILE:HG23	1:59:A:VAL:HG13	13	0.61
(6,1)	2:148:B:SER:H1	2:149:B:PRO:HA	9	0.6
(1,1500)	1:137:A:MET:HB2	1:141:A:LEU:HD11	14	0.6
(1,1500)	1:137:A:MET:HB2	1:141:A:LEU:HD12	14	0.6
(1,1500)	1:137:A:MET:HB2	1:141:A:LEU:HD13	14	0.6
(1,1500)	1:137:A:MET:HB2	1:141:A:LEU:HD21	14	0.6
(1,1500)	1:137:A:MET:HB2	1:141:A:LEU:HD22	14	0.6
(1,1500)	1:137:A:MET:HB2	1:141:A:LEU:HD23	14	0.6
(1,1447)	1:116:A:VAL:HG11	1:118:A:LYS:HG2	13	0.6
(1,1447)	1:116:A:VAL:HG11	1:118:A:LYS:HG3	13	0.6
(1,1447)	1:116:A:VAL:HG12	1:118:A:LYS:HG2	13	0.6
(1,1447)	1:116:A:VAL:HG12	1:118:A:LYS:HG3	13	0.6
(1,1447)	1:116:A:VAL:HG13	1:118:A:LYS:HG2	13	0.6
(1,1447)	1:116:A:VAL:HG13	1:118:A:LYS:HG3	13	0.6
(1,1447)	1:116:A:VAL:HG21	1:118:A:LYS:HG2	13	0.6
(1,1447)	1:116:A:VAL:HG21	1:118:A:LYS:HG3	13	0.6
(1,1447)	1:116:A:VAL:HG22	1:118:A:LYS:HG2	13	0.6
(1,1447)	1:116:A:VAL:HG22	1:118:A:LYS:HG3	13	0.6
(1,1447)	1:116:A:VAL:HG23	1:118:A:LYS:HG2	13	0.6
(1,1447)	1:116:A:VAL:HG23	1:118:A:LYS:HG3	13	0.6
(1,1425)	1:112:A:LYS:HA	1:145:A:LEU:HD11	3	0.6
(1,1425)	1:112:A:LYS:HA	1:145:A:LEU:HD12	3	0.6
(1,1425)	1:112:A:LYS:HA	1:145:A:LEU:HD13	3	0.6
(1,1425)	1:112:A:LYS:HA	1:145:A:LEU:HD21	3	0.6
(1,1425)	1:112:A:LYS:HA	1:145:A:LEU:HD22	3	0.6
(1,1425)	1:112:A:LYS:HA	1:145:A:LEU:HD23	3	0.6
(1,478)	1:77:A:LEU:HD21	1:78:A:PHE:HA	2	0.6
(1,478)	1:77:A:LEU:HD22	1:78:A:PHE:HA	2	0.6
(1,478)	1:77:A:LEU:HD23	1:78:A:PHE:HA	2	0.6
(1,478)	1:77:A:LEU:HD21	1:78:A:PHE:HA	3	0.6
(1,478)	1:77:A:LEU:HD22	1:78:A:PHE:HA	3	0.6
(1,478)	1:77:A:LEU:HD23	1:78:A:PHE:HA	3	0.6
(1,438)	1:58:A:ILE:HG21	1:59:A:VAL:HG11	20	0.6
(1,438)	1:58:A:ILE:HG21	1:59:A:VAL:HG12	20	0.6
(1,438)	1:58:A:ILE:HG21	1:59:A:VAL:HG13	20	0.6
(1,438)	1:58:A:ILE:HG22	1:59:A:VAL:HG11	20	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,438)	1:58:A:ILE:HG22	1:59:A:VAL:HG12	20	0.6
(1,438)	1:58:A:ILE:HG22	1:59:A:VAL:HG13	20	0.6
(1,438)	1:58:A:ILE:HG23	1:59:A:VAL:HG11	20	0.6
(1,438)	1:58:A:ILE:HG23	1:59:A:VAL:HG12	20	0.6
(1,438)	1:58:A:ILE:HG23	1:59:A:VAL:HG13	20	0.6
(1,204)	1:59:A:VAL:HA	1:103:A:VAL:HG11	17	0.6
(1,204)	1:59:A:VAL:HA	1:103:A:VAL:HG12	17	0.6
(1,204)	1:59:A:VAL:HA	1:103:A:VAL:HG13	17	0.6
(6,1)	2:148:B:SER:H1	2:149:B:PRO:HA	4	0.59
(1,1425)	1:112:A:LYS:HA	1:145:A:LEU:HD11	1	0.59
(1,1425)	1:112:A:LYS:HA	1:145:A:LEU:HD12	1	0.59
(1,1425)	1:112:A:LYS:HA	1:145:A:LEU:HD13	1	0.59
(1,1425)	1:112:A:LYS:HA	1:145:A:LEU:HD21	1	0.59
(1,1425)	1:112:A:LYS:HA	1:145:A:LEU:HD22	1	0.59
(1,1425)	1:112:A:LYS:HA	1:145:A:LEU:HD23	1	0.59
(1,461)	1:101:A:ALA:HB1	1:137:A:MET:HB2	16	0.59
(1,461)	1:101:A:ALA:HB2	1:137:A:MET:HB2	16	0.59
(1,461)	1:101:A:ALA:HB3	1:137:A:MET:HB2	16	0.59
(1,347)	1:104:A:LEU:HD11	1:108:A:ALA:HB1	2	0.59
(1,347)	1:104:A:LEU:HD11	1:108:A:ALA:HB2	2	0.59
(1,347)	1:104:A:LEU:HD11	1:108:A:ALA:HB3	2	0.59
(1,347)	1:104:A:LEU:HD12	1:108:A:ALA:HB1	2	0.59
(1,347)	1:104:A:LEU:HD12	1:108:A:ALA:HB2	2	0.59
(1,347)	1:104:A:LEU:HD12	1:108:A:ALA:HB3	2	0.59
(1,347)	1:104:A:LEU:HD13	1:108:A:ALA:HB1	2	0.59
(1,347)	1:104:A:LEU:HD13	1:108:A:ALA:HB2	2	0.59
(1,347)	1:104:A:LEU:HD13	1:108:A:ALA:HB3	2	0.59
(1,153)	1:63:A:MET:HG2	1:103:A:VAL:HG11	17	0.59
(1,153)	1:63:A:MET:HG2	1:103:A:VAL:HG12	17	0.59
(1,153)	1:63:A:MET:HG2	1:103:A:VAL:HG13	17	0.59
(1,134)	1:59:A:VAL:HB	1:103:A:VAL:HG21	6	0.59
(1,134)	1:59:A:VAL:HB	1:103:A:VAL:HG22	6	0.59
(1,134)	1:59:A:VAL:HB	1:103:A:VAL:HG23	6	0.59
(1,1277)	1:59:A:VAL:HG11	1:103:A:VAL:HA	17	0.58
(1,1277)	1:59:A:VAL:HG12	1:103:A:VAL:HA	17	0.58
(1,1277)	1:59:A:VAL:HG13	1:103:A:VAL:HA	17	0.58
(1,1277)	1:59:A:VAL:HG21	1:103:A:VAL:HA	17	0.58
(1,1277)	1:59:A:VAL:HG22	1:103:A:VAL:HA	17	0.58
(1,1277)	1:59:A:VAL:HG23	1:103:A:VAL:HA	17	0.58
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD11	14	0.58
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD12	14	0.58
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD13	14	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD21	14	0.58
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD22	14	0.58
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD23	14	0.58
(1,838)	1:31:A:PHE:H	1:34:A:VAL:HG21	12	0.58
(1,838)	1:31:A:PHE:H	1:34:A:VAL:HG22	12	0.58
(1,838)	1:31:A:PHE:H	1:34:A:VAL:HG23	12	0.58
(1,838)	1:31:A:PHE:H	1:34:A:VAL:HG21	18	0.58
(1,838)	1:31:A:PHE:H	1:34:A:VAL:HG22	18	0.58
(1,838)	1:31:A:PHE:H	1:34:A:VAL:HG23	18	0.58
(1,478)	1:77:A:LEU:HD21	1:78:A:PHE:HA	18	0.58
(1,478)	1:77:A:LEU:HD22	1:78:A:PHE:HA	18	0.58
(1,478)	1:77:A:LEU:HD23	1:78:A:PHE:HA	18	0.58
(1,438)	1:58:A:ILE:HG21	1:59:A:VAL:HG11	6	0.58
(1,438)	1:58:A:ILE:HG21	1:59:A:VAL:HG12	6	0.58
(1,438)	1:58:A:ILE:HG21	1:59:A:VAL:HG13	6	0.58
(1,438)	1:58:A:ILE:HG22	1:59:A:VAL:HG11	6	0.58
(1,438)	1:58:A:ILE:HG22	1:59:A:VAL:HG12	6	0.58
(1,438)	1:58:A:ILE:HG22	1:59:A:VAL:HG13	6	0.58
(1,438)	1:58:A:ILE:HG23	1:59:A:VAL:HG11	6	0.58
(1,438)	1:58:A:ILE:HG23	1:59:A:VAL:HG12	6	0.58
(1,438)	1:58:A:ILE:HG23	1:59:A:VAL:HG13	6	0.58
(1,438)	1:58:A:ILE:HG21	1:59:A:VAL:HG11	11	0.58
(1,438)	1:58:A:ILE:HG21	1:59:A:VAL:HG12	11	0.58
(1,438)	1:58:A:ILE:HG21	1:59:A:VAL:HG13	11	0.58
(1,438)	1:58:A:ILE:HG22	1:59:A:VAL:HG11	11	0.58
(1,438)	1:58:A:ILE:HG22	1:59:A:VAL:HG12	11	0.58
(1,438)	1:58:A:ILE:HG22	1:59:A:VAL:HG13	11	0.58
(1,438)	1:58:A:ILE:HG23	1:59:A:VAL:HG11	11	0.58
(1,438)	1:58:A:ILE:HG23	1:59:A:VAL:HG12	11	0.58
(1,438)	1:58:A:ILE:HG23	1:59:A:VAL:HG13	11	0.58
(1,336)	1:108:A:ALA:HB1	1:111:A:VAL:HG11	12	0.58
(1,336)	1:108:A:ALA:HB1	1:111:A:VAL:HG12	12	0.58
(1,336)	1:108:A:ALA:HB1	1:111:A:VAL:HG13	12	0.58
(1,336)	1:108:A:ALA:HB2	1:111:A:VAL:HG11	12	0.58
(1,336)	1:108:A:ALA:HB2	1:111:A:VAL:HG12	12	0.58
(1,336)	1:108:A:ALA:HB2	1:111:A:VAL:HG13	12	0.58
(1,336)	1:108:A:ALA:HB3	1:111:A:VAL:HG11	12	0.58
(1,336)	1:108:A:ALA:HB3	1:111:A:VAL:HG12	12	0.58
(1,336)	1:108:A:ALA:HB3	1:111:A:VAL:HG13	12	0.58
(1,204)	1:59:A:VAL:HA	1:103:A:VAL:HG11	15	0.58
(1,204)	1:59:A:VAL:HA	1:103:A:VAL:HG12	15	0.58
(1,204)	1:59:A:VAL:HA	1:103:A:VAL:HG13	15	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,134)	1:59:A:VAL:HB	1:103:A:VAL:HG21	4	0.58
(1,134)	1:59:A:VAL:HB	1:103:A:VAL:HG22	4	0.58
(1,134)	1:59:A:VAL:HB	1:103:A:VAL:HG23	4	0.58
(1,134)	1:59:A:VAL:HB	1:103:A:VAL:HG21	12	0.58
(1,134)	1:59:A:VAL:HB	1:103:A:VAL:HG22	12	0.58
(1,134)	1:59:A:VAL:HB	1:103:A:VAL:HG23	12	0.58
(5,1)	2:155:B:SER:H	1:130:A:ARG:NH2	19	0.57
(1,1202)	1:23:A:LEU:HD11	1:27:A:LEU:HA	11	0.57
(1,1202)	1:23:A:LEU:HD12	1:27:A:LEU:HA	11	0.57
(1,1202)	1:23:A:LEU:HD13	1:27:A:LEU:HA	11	0.57
(1,1202)	1:23:A:LEU:HD21	1:27:A:LEU:HA	11	0.57
(1,1202)	1:23:A:LEU:HD22	1:27:A:LEU:HA	11	0.57
(1,1202)	1:23:A:LEU:HD23	1:27:A:LEU:HA	11	0.57
(1,478)	1:77:A:LEU:HD21	1:78:A:PHE:HA	6	0.57
(1,478)	1:77:A:LEU:HD22	1:78:A:PHE:HA	6	0.57
(1,478)	1:77:A:LEU:HD23	1:78:A:PHE:HA	6	0.57
(1,478)	1:77:A:LEU:HD21	1:78:A:PHE:HA	17	0.57
(1,478)	1:77:A:LEU:HD22	1:78:A:PHE:HA	17	0.57
(1,478)	1:77:A:LEU:HD23	1:78:A:PHE:HA	17	0.57
(1,461)	1:101:A:ALA:HB1	1:137:A:MET:HB2	11	0.57
(1,461)	1:101:A:ALA:HB2	1:137:A:MET:HB2	11	0.57
(1,461)	1:101:A:ALA:HB3	1:137:A:MET:HB2	11	0.57
(1,14)	1:116:A:VAL:HG21	1:118:A:LYS:HG2	7	0.57
(1,14)	1:116:A:VAL:HG21	1:118:A:LYS:HG3	7	0.57
(1,14)	1:116:A:VAL:HG22	1:118:A:LYS:HG2	7	0.57
(1,14)	1:116:A:VAL:HG22	1:118:A:LYS:HG3	7	0.57
(1,14)	1:116:A:VAL:HG23	1:118:A:LYS:HG2	7	0.57
(1,14)	1:116:A:VAL:HG23	1:118:A:LYS:HG3	7	0.57
(1,14)	1:116:A:VAL:HG21	1:118:A:LYS:HG2	11	0.57
(1,14)	1:116:A:VAL:HG21	1:118:A:LYS:HG3	11	0.57
(1,14)	1:116:A:VAL:HG22	1:118:A:LYS:HG2	11	0.57
(1,14)	1:116:A:VAL:HG22	1:118:A:LYS:HG3	11	0.57
(1,14)	1:116:A:VAL:HG23	1:118:A:LYS:HG2	11	0.57
(1,14)	1:116:A:VAL:HG23	1:118:A:LYS:HG3	11	0.57
(1,1447)	1:116:A:VAL:HG11	1:118:A:LYS:HG2	5	0.56
(1,1447)	1:116:A:VAL:HG11	1:118:A:LYS:HG3	5	0.56
(1,1447)	1:116:A:VAL:HG12	1:118:A:LYS:HG2	5	0.56
(1,1447)	1:116:A:VAL:HG12	1:118:A:LYS:HG3	5	0.56
(1,1447)	1:116:A:VAL:HG13	1:118:A:LYS:HG2	5	0.56
(1,1447)	1:116:A:VAL:HG13	1:118:A:LYS:HG3	5	0.56
(1,1447)	1:116:A:VAL:HG21	1:118:A:LYS:HG2	5	0.56
(1,1447)	1:116:A:VAL:HG21	1:118:A:LYS:HG3	5	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1447)	1:116:A:VAL:HG22	1:118:A:LYS:HG2	5	0.56
(1,1447)	1:116:A:VAL:HG22	1:118:A:LYS:HG3	5	0.56
(1,1447)	1:116:A:VAL:HG23	1:118:A:LYS:HG2	5	0.56
(1,1447)	1:116:A:VAL:HG23	1:118:A:LYS:HG3	5	0.56
(1,1403)	1:104:A:LEU:HD11	1:141:A:LEU:HG	10	0.56
(1,1403)	1:104:A:LEU:HD12	1:141:A:LEU:HG	10	0.56
(1,1403)	1:104:A:LEU:HD13	1:141:A:LEU:HG	10	0.56
(1,1403)	1:104:A:LEU:HD21	1:141:A:LEU:HG	10	0.56
(1,1403)	1:104:A:LEU:HD22	1:141:A:LEU:HG	10	0.56
(1,1403)	1:104:A:LEU:HD23	1:141:A:LEU:HG	10	0.56
(1,293)	1:31:A:PHE:HA	1:34:A:VAL:HG11	4	0.56
(1,293)	1:31:A:PHE:HA	1:34:A:VAL:HG12	4	0.56
(1,293)	1:31:A:PHE:HA	1:34:A:VAL:HG13	4	0.56
(1,14)	1:116:A:VAL:HG21	1:118:A:LYS:HG2	20	0.56
(1,14)	1:116:A:VAL:HG21	1:118:A:LYS:HG3	20	0.56
(1,14)	1:116:A:VAL:HG22	1:118:A:LYS:HG2	20	0.56
(1,14)	1:116:A:VAL:HG22	1:118:A:LYS:HG3	20	0.56
(1,14)	1:116:A:VAL:HG23	1:118:A:LYS:HG2	20	0.56
(1,14)	1:116:A:VAL:HG23	1:118:A:LYS:HG3	20	0.56
(1,1425)	1:112:A:LYS:HA	1:145:A:LEU:HD11	14	0.55
(1,1425)	1:112:A:LYS:HA	1:145:A:LEU:HD12	14	0.55
(1,1425)	1:112:A:LYS:HA	1:145:A:LEU:HD13	14	0.55
(1,1425)	1:112:A:LYS:HA	1:145:A:LEU:HD21	14	0.55
(1,1425)	1:112:A:LYS:HA	1:145:A:LEU:HD22	14	0.55
(1,1425)	1:112:A:LYS:HA	1:145:A:LEU:HD23	14	0.55
(1,1281)	1:59:A:VAL:HG11	1:104:A:LEU:H	5	0.55
(1,1281)	1:59:A:VAL:HG12	1:104:A:LEU:H	5	0.55
(1,1281)	1:59:A:VAL:HG13	1:104:A:LEU:H	5	0.55
(1,1281)	1:59:A:VAL:HG21	1:104:A:LEU:H	5	0.55
(1,1281)	1:59:A:VAL:HG22	1:104:A:LEU:H	5	0.55
(1,1281)	1:59:A:VAL:HG23	1:104:A:LEU:H	5	0.55
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD11	1	0.55
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD12	1	0.55
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD13	1	0.55
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD21	1	0.55
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD22	1	0.55
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD23	1	0.55
(1,478)	1:77:A:LEU:HD21	1:78:A:PHE:HA	7	0.55
(1,478)	1:77:A:LEU:HD22	1:78:A:PHE:HA	7	0.55
(1,478)	1:77:A:LEU:HD23	1:78:A:PHE:HA	7	0.55
(1,478)	1:77:A:LEU:HD21	1:78:A:PHE:HA	15	0.55
(1,478)	1:77:A:LEU:HD22	1:78:A:PHE:HA	15	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,478)	1:77:A:LEU:HD23	1:78:A:PHE:HA	15	0.55
(1,153)	1:63:A:MET:HG2	1:103:A:VAL:HG11	1	0.55
(1,153)	1:63:A:MET:HG2	1:103:A:VAL:HG12	1	0.55
(1,153)	1:63:A:MET:HG2	1:103:A:VAL:HG13	1	0.55
(1,1427)	1:112:A:LYS:HB2	1:145:A:LEU:HD11	14	0.54
(1,1427)	1:112:A:LYS:HB2	1:145:A:LEU:HD12	14	0.54
(1,1427)	1:112:A:LYS:HB2	1:145:A:LEU:HD13	14	0.54
(1,1427)	1:112:A:LYS:HB2	1:145:A:LEU:HD21	14	0.54
(1,1427)	1:112:A:LYS:HB2	1:145:A:LEU:HD22	14	0.54
(1,1427)	1:112:A:LYS:HB2	1:145:A:LEU:HD23	14	0.54
(1,1427)	1:112:A:LYS:HB3	1:145:A:LEU:HD11	14	0.54
(1,1427)	1:112:A:LYS:HB3	1:145:A:LEU:HD12	14	0.54
(1,1427)	1:112:A:LYS:HB3	1:145:A:LEU:HD13	14	0.54
(1,1427)	1:112:A:LYS:HB3	1:145:A:LEU:HD21	14	0.54
(1,1427)	1:112:A:LYS:HB3	1:145:A:LEU:HD22	14	0.54
(1,1427)	1:112:A:LYS:HB3	1:145:A:LEU:HD23	14	0.54
(1,1425)	1:112:A:LYS:HA	1:145:A:LEU:HD11	16	0.54
(1,1425)	1:112:A:LYS:HA	1:145:A:LEU:HD12	16	0.54
(1,1425)	1:112:A:LYS:HA	1:145:A:LEU:HD13	16	0.54
(1,1425)	1:112:A:LYS:HA	1:145:A:LEU:HD21	16	0.54
(1,1425)	1:112:A:LYS:HA	1:145:A:LEU:HD22	16	0.54
(1,1425)	1:112:A:LYS:HA	1:145:A:LEU:HD23	16	0.54
(1,1410)	1:108:A:ALA:HB1	1:145:A:LEU:HD11	1	0.54
(1,1410)	1:108:A:ALA:HB1	1:145:A:LEU:HD12	1	0.54
(1,1410)	1:108:A:ALA:HB1	1:145:A:LEU:HD13	1	0.54
(1,1410)	1:108:A:ALA:HB1	1:145:A:LEU:HD21	1	0.54
(1,1410)	1:108:A:ALA:HB1	1:145:A:LEU:HD22	1	0.54
(1,1410)	1:108:A:ALA:HB1	1:145:A:LEU:HD23	1	0.54
(1,1410)	1:108:A:ALA:HB2	1:145:A:LEU:HD11	1	0.54
(1,1410)	1:108:A:ALA:HB2	1:145:A:LEU:HD12	1	0.54
(1,1410)	1:108:A:ALA:HB2	1:145:A:LEU:HD13	1	0.54
(1,1410)	1:108:A:ALA:HB2	1:145:A:LEU:HD21	1	0.54
(1,1410)	1:108:A:ALA:HB2	1:145:A:LEU:HD22	1	0.54
(1,1410)	1:108:A:ALA:HB2	1:145:A:LEU:HD23	1	0.54
(1,1410)	1:108:A:ALA:HB3	1:145:A:LEU:HD11	1	0.54
(1,1410)	1:108:A:ALA:HB3	1:145:A:LEU:HD12	1	0.54
(1,1410)	1:108:A:ALA:HB3	1:145:A:LEU:HD13	1	0.54
(1,1410)	1:108:A:ALA:HB3	1:145:A:LEU:HD21	1	0.54
(1,1410)	1:108:A:ALA:HB3	1:145:A:LEU:HD22	1	0.54
(1,1410)	1:108:A:ALA:HB3	1:145:A:LEU:HD23	1	0.54
(1,1401)	1:104:A:LEU:HD11	1:141:A:LEU:HA	15	0.54
(1,1401)	1:104:A:LEU:HD12	1:141:A:LEU:HA	15	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1401)	1:104:A:LEU:HD13	1:141:A:LEU:HA	15	0.54
(1,1401)	1:104:A:LEU:HD21	1:141:A:LEU:HA	15	0.54
(1,1401)	1:104:A:LEU:HD22	1:141:A:LEU:HA	15	0.54
(1,1401)	1:104:A:LEU:HD23	1:141:A:LEU:HA	15	0.54
(1,1275)	1:59:A:VAL:HG11	1:102:A:ASP:H	17	0.54
(1,1275)	1:59:A:VAL:HG12	1:102:A:ASP:H	17	0.54
(1,1275)	1:59:A:VAL:HG13	1:102:A:ASP:H	17	0.54
(1,1275)	1:59:A:VAL:HG21	1:102:A:ASP:H	17	0.54
(1,1275)	1:59:A:VAL:HG22	1:102:A:ASP:H	17	0.54
(1,1275)	1:59:A:VAL:HG23	1:102:A:ASP:H	17	0.54
(1,1064)	1:139:A:VAL:H	1:139:A:VAL:HB	8	0.54
(1,857)	1:111:A:VAL:HG11	1:112:A:LYS:H	17	0.54
(1,857)	1:111:A:VAL:HG12	1:112:A:LYS:H	17	0.54
(1,857)	1:111:A:VAL:HG13	1:112:A:LYS:H	17	0.54
(1,838)	1:31:A:PHE:H	1:34:A:VAL:HG21	1	0.54
(1,838)	1:31:A:PHE:H	1:34:A:VAL:HG22	1	0.54
(1,838)	1:31:A:PHE:H	1:34:A:VAL:HG23	1	0.54
(1,838)	1:31:A:PHE:H	1:34:A:VAL:HG21	7	0.54
(1,838)	1:31:A:PHE:H	1:34:A:VAL:HG22	7	0.54
(1,838)	1:31:A:PHE:H	1:34:A:VAL:HG23	7	0.54
(1,838)	1:31:A:PHE:H	1:34:A:VAL:HG21	10	0.54
(1,838)	1:31:A:PHE:H	1:34:A:VAL:HG22	10	0.54
(1,838)	1:31:A:PHE:H	1:34:A:VAL:HG23	10	0.54
(1,83)	1:137:A:MET:HB3	1:138:A:ILE:HD11	8	0.54
(1,83)	1:137:A:MET:HB3	1:138:A:ILE:HD12	8	0.54
(1,83)	1:137:A:MET:HB3	1:138:A:ILE:HD13	8	0.54
(1,62)	1:59:A:VAL:HG21	1:100:A:PHE:HD1	3	0.54
(1,62)	1:59:A:VAL:HG21	1:100:A:PHE:HD2	3	0.54
(1,62)	1:59:A:VAL:HG22	1:100:A:PHE:HD1	3	0.54
(1,62)	1:59:A:VAL:HG22	1:100:A:PHE:HD2	3	0.54
(1,62)	1:59:A:VAL:HG23	1:100:A:PHE:HD1	3	0.54
(1,62)	1:59:A:VAL:HG23	1:100:A:PHE:HD2	3	0.54
(1,1422)	1:112:A:LYS:H	1:145:A:LEU:HD11	9	0.53
(1,1422)	1:112:A:LYS:H	1:145:A:LEU:HD12	9	0.53
(1,1422)	1:112:A:LYS:H	1:145:A:LEU:HD13	9	0.53
(1,1422)	1:112:A:LYS:H	1:145:A:LEU:HD21	9	0.53
(1,1422)	1:112:A:LYS:H	1:145:A:LEU:HD22	9	0.53
(1,1422)	1:112:A:LYS:H	1:145:A:LEU:HD23	9	0.53
(1,438)	1:58:A:ILE:HG21	1:59:A:VAL:HG11	2	0.53
(1,438)	1:58:A:ILE:HG21	1:59:A:VAL:HG12	2	0.53
(1,438)	1:58:A:ILE:HG21	1:59:A:VAL:HG13	2	0.53
(1,438)	1:58:A:ILE:HG22	1:59:A:VAL:HG11	2	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,438)	1:58:A:ILE:HG22	1:59:A:VAL:HG12	2	0.53
(1,438)	1:58:A:ILE:HG22	1:59:A:VAL:HG13	2	0.53
(1,438)	1:58:A:ILE:HG23	1:59:A:VAL:HG11	2	0.53
(1,438)	1:58:A:ILE:HG23	1:59:A:VAL:HG12	2	0.53
(1,438)	1:58:A:ILE:HG23	1:59:A:VAL:HG13	2	0.53
(1,134)	1:59:A:VAL:HB	1:103:A:VAL:HG21	2	0.53
(1,134)	1:59:A:VAL:HB	1:103:A:VAL:HG22	2	0.53
(1,134)	1:59:A:VAL:HB	1:103:A:VAL:HG23	2	0.53
(1,14)	1:116:A:VAL:HG21	1:118:A:LYS:HG2	6	0.53
(1,14)	1:116:A:VAL:HG21	1:118:A:LYS:HG3	6	0.53
(1,14)	1:116:A:VAL:HG22	1:118:A:LYS:HG2	6	0.53
(1,14)	1:116:A:VAL:HG22	1:118:A:LYS:HG3	6	0.53
(1,14)	1:116:A:VAL:HG23	1:118:A:LYS:HG2	6	0.53
(1,14)	1:116:A:VAL:HG23	1:118:A:LYS:HG3	6	0.53
(1,14)	1:116:A:VAL:HG21	1:118:A:LYS:HG2	10	0.53
(1,14)	1:116:A:VAL:HG21	1:118:A:LYS:HG3	10	0.53
(1,14)	1:116:A:VAL:HG22	1:118:A:LYS:HG2	10	0.53
(1,14)	1:116:A:VAL:HG22	1:118:A:LYS:HG3	10	0.53
(1,14)	1:116:A:VAL:HG23	1:118:A:LYS:HG2	10	0.53
(1,14)	1:116:A:VAL:HG23	1:118:A:LYS:HG3	10	0.53
(5,1)	2:155:B:SER:H	1:130:A:ARG:NH2	2	0.52
(2,12)	2:158:B:TYR:HD1	1:132:A:VAL:HG11	9	0.52
(2,12)	2:158:B:TYR:HD1	1:132:A:VAL:HG12	9	0.52
(2,12)	2:158:B:TYR:HD1	1:132:A:VAL:HG13	9	0.52
(2,12)	2:158:B:TYR:HD2	1:132:A:VAL:HG11	9	0.52
(2,12)	2:158:B:TYR:HD2	1:132:A:VAL:HG12	9	0.52
(2,12)	2:158:B:TYR:HD2	1:132:A:VAL:HG13	9	0.52
(1,313)	1:34:A:VAL:HG21	1:35:A:THR:HG21	20	0.52
(1,313)	1:34:A:VAL:HG21	1:35:A:THR:HG22	20	0.52
(1,313)	1:34:A:VAL:HG21	1:35:A:THR:HG23	20	0.52
(1,313)	1:34:A:VAL:HG22	1:35:A:THR:HG21	20	0.52
(1,313)	1:34:A:VAL:HG22	1:35:A:THR:HG22	20	0.52
(1,313)	1:34:A:VAL:HG22	1:35:A:THR:HG23	20	0.52
(1,313)	1:34:A:VAL:HG23	1:35:A:THR:HG21	20	0.52
(1,313)	1:34:A:VAL:HG23	1:35:A:THR:HG22	20	0.52
(1,313)	1:34:A:VAL:HG23	1:35:A:THR:HG23	20	0.52
(1,14)	1:116:A:VAL:HG21	1:118:A:LYS:HG2	14	0.52
(1,14)	1:116:A:VAL:HG21	1:118:A:LYS:HG3	14	0.52
(1,14)	1:116:A:VAL:HG22	1:118:A:LYS:HG2	14	0.52
(1,14)	1:116:A:VAL:HG22	1:118:A:LYS:HG3	14	0.52
(1,14)	1:116:A:VAL:HG23	1:118:A:LYS:HG2	14	0.52
(1,14)	1:116:A:VAL:HG23	1:118:A:LYS:HG3	14	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,3)	2:148:B:SER:H1	2:149:B:PRO:HB2	19	0.51
(6,3)	2:148:B:SER:H1	2:149:B:PRO:HB3	19	0.51
(5,1)	2:155:B:SER:H	1:130:A:ARG:NH2	8	0.51
(1,1422)	1:112:A:LYS:H	1:145:A:LEU:HD11	20	0.51
(1,1422)	1:112:A:LYS:H	1:145:A:LEU:HD12	20	0.51
(1,1422)	1:112:A:LYS:H	1:145:A:LEU:HD13	20	0.51
(1,1422)	1:112:A:LYS:H	1:145:A:LEU:HD21	20	0.51
(1,1422)	1:112:A:LYS:H	1:145:A:LEU:HD22	20	0.51
(1,1422)	1:112:A:LYS:H	1:145:A:LEU:HD23	20	0.51
(1,1277)	1:59:A:VAL:HG11	1:103:A:VAL:HA	5	0.51
(1,1277)	1:59:A:VAL:HG12	1:103:A:VAL:HA	5	0.51
(1,1277)	1:59:A:VAL:HG13	1:103:A:VAL:HA	5	0.51
(1,1277)	1:59:A:VAL:HG21	1:103:A:VAL:HA	5	0.51
(1,1277)	1:59:A:VAL:HG22	1:103:A:VAL:HA	5	0.51
(1,1277)	1:59:A:VAL:HG23	1:103:A:VAL:HA	5	0.51
(1,1229)	1:45:A:SER:HB2	1:80:A:LEU:HD11	18	0.51
(1,1229)	1:45:A:SER:HB2	1:80:A:LEU:HD12	18	0.51
(1,1229)	1:45:A:SER:HB2	1:80:A:LEU:HD13	18	0.51
(1,1229)	1:45:A:SER:HB2	1:80:A:LEU:HD21	18	0.51
(1,1229)	1:45:A:SER:HB2	1:80:A:LEU:HD22	18	0.51
(1,1229)	1:45:A:SER:HB2	1:80:A:LEU:HD23	18	0.51
(1,1229)	1:45:A:SER:HB3	1:80:A:LEU:HD11	18	0.51
(1,1229)	1:45:A:SER:HB3	1:80:A:LEU:HD12	18	0.51
(1,1229)	1:45:A:SER:HB3	1:80:A:LEU:HD13	18	0.51
(1,1229)	1:45:A:SER:HB3	1:80:A:LEU:HD21	18	0.51
(1,1229)	1:45:A:SER:HB3	1:80:A:LEU:HD22	18	0.51
(1,1229)	1:45:A:SER:HB3	1:80:A:LEU:HD23	18	0.51
(1,574)	1:108:A:ALA:H	1:111:A:VAL:HG11	20	0.51
(1,574)	1:108:A:ALA:H	1:111:A:VAL:HG12	20	0.51
(1,574)	1:108:A:ALA:H	1:111:A:VAL:HG13	20	0.51
(1,293)	1:31:A:PHE:HA	1:34:A:VAL:HG11	17	0.51
(1,293)	1:31:A:PHE:HA	1:34:A:VAL:HG12	17	0.51
(1,293)	1:31:A:PHE:HA	1:34:A:VAL:HG13	17	0.51
(1,14)	1:116:A:VAL:HG21	1:118:A:LYS:HG2	13	0.51
(1,14)	1:116:A:VAL:HG21	1:118:A:LYS:HG3	13	0.51
(1,14)	1:116:A:VAL:HG22	1:118:A:LYS:HG2	13	0.51
(1,14)	1:116:A:VAL:HG22	1:118:A:LYS:HG3	13	0.51
(1,14)	1:116:A:VAL:HG23	1:118:A:LYS:HG2	13	0.51
(1,14)	1:116:A:VAL:HG23	1:118:A:LYS:HG3	13	0.51
(2,2)	2:149:B:PRO:HG2	1:38:A:MET:HE2	2	0.5
(1,1320)	1:75:A:LEU:HD11	1:111:A:VAL:HG11	7	0.5
(1,1320)	1:75:A:LEU:HD11	1:111:A:VAL:HG12	7	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1320)	1:75:A:LEU:HD11	1:111:A:VAL:HG13	7	0.5
(1,1320)	1:75:A:LEU:HD12	1:111:A:VAL:HG11	7	0.5
(1,1320)	1:75:A:LEU:HD12	1:111:A:VAL:HG12	7	0.5
(1,1320)	1:75:A:LEU:HD12	1:111:A:VAL:HG13	7	0.5
(1,1320)	1:75:A:LEU:HD13	1:111:A:VAL:HG11	7	0.5
(1,1320)	1:75:A:LEU:HD13	1:111:A:VAL:HG12	7	0.5
(1,1320)	1:75:A:LEU:HD13	1:111:A:VAL:HG13	7	0.5
(1,1320)	1:75:A:LEU:HD21	1:111:A:VAL:HG11	7	0.5
(1,1320)	1:75:A:LEU:HD21	1:111:A:VAL:HG12	7	0.5
(1,1320)	1:75:A:LEU:HD21	1:111:A:VAL:HG13	7	0.5
(1,1320)	1:75:A:LEU:HD22	1:111:A:VAL:HG11	7	0.5
(1,1320)	1:75:A:LEU:HD22	1:111:A:VAL:HG12	7	0.5
(1,1320)	1:75:A:LEU:HD22	1:111:A:VAL:HG13	7	0.5
(1,1320)	1:75:A:LEU:HD23	1:111:A:VAL:HG11	7	0.5
(1,1320)	1:75:A:LEU:HD23	1:111:A:VAL:HG12	7	0.5
(1,1320)	1:75:A:LEU:HD23	1:111:A:VAL:HG13	7	0.5
(1,1275)	1:59:A:VAL:HG11	1:102:A:ASP:H	5	0.5
(1,1275)	1:59:A:VAL:HG12	1:102:A:ASP:H	5	0.5
(1,1275)	1:59:A:VAL:HG13	1:102:A:ASP:H	5	0.5
(1,1275)	1:59:A:VAL:HG21	1:102:A:ASP:H	5	0.5
(1,1275)	1:59:A:VAL:HG22	1:102:A:ASP:H	5	0.5
(1,1275)	1:59:A:VAL:HG23	1:102:A:ASP:H	5	0.5
(1,347)	1:104:A:LEU:HD11	1:108:A:ALA:HB1	4	0.5
(1,347)	1:104:A:LEU:HD11	1:108:A:ALA:HB2	4	0.5
(1,347)	1:104:A:LEU:HD11	1:108:A:ALA:HB3	4	0.5
(1,347)	1:104:A:LEU:HD12	1:108:A:ALA:HB1	4	0.5
(1,347)	1:104:A:LEU:HD12	1:108:A:ALA:HB2	4	0.5
(1,347)	1:104:A:LEU:HD12	1:108:A:ALA:HB3	4	0.5
(1,347)	1:104:A:LEU:HD13	1:108:A:ALA:HB1	4	0.5
(1,347)	1:104:A:LEU:HD13	1:108:A:ALA:HB2	4	0.5
(1,347)	1:104:A:LEU:HD13	1:108:A:ALA:HB3	4	0.5
(1,204)	1:59:A:VAL:HA	1:103:A:VAL:HG11	19	0.5
(1,204)	1:59:A:VAL:HA	1:103:A:VAL:HG12	19	0.5
(1,204)	1:59:A:VAL:HA	1:103:A:VAL:HG13	19	0.5
(1,134)	1:59:A:VAL:HB	1:103:A:VAL:HG21	1	0.5
(1,134)	1:59:A:VAL:HB	1:103:A:VAL:HG22	1	0.5
(1,134)	1:59:A:VAL:HB	1:103:A:VAL:HG23	1	0.5
(1,14)	1:116:A:VAL:HG21	1:118:A:LYS:HG2	9	0.5
(1,14)	1:116:A:VAL:HG21	1:118:A:LYS:HG3	9	0.5
(1,14)	1:116:A:VAL:HG22	1:118:A:LYS:HG2	9	0.5
(1,14)	1:116:A:VAL:HG22	1:118:A:LYS:HG3	9	0.5
(1,14)	1:116:A:VAL:HG23	1:118:A:LYS:HG2	9	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,14)	1:116:A:VAL:HG23	1:118:A:LYS:HG3	9	0.5
(1,1077)	1:137:A:MET:HB3	1:141:A:LEU:H	14	0.49
(1,722)	1:34:A:VAL:HG21	1:40:A:SER:H	20	0.49
(1,722)	1:34:A:VAL:HG22	1:40:A:SER:H	20	0.49
(1,722)	1:34:A:VAL:HG23	1:40:A:SER:H	20	0.49
(1,478)	1:77:A:LEU:HD21	1:78:A:PHE:HA	19	0.49
(1,478)	1:77:A:LEU:HD22	1:78:A:PHE:HA	19	0.49
(1,478)	1:77:A:LEU:HD23	1:78:A:PHE:HA	19	0.49
(1,359)	1:75:A:LEU:HD11	1:119:A:SER:HA	5	0.49
(1,359)	1:75:A:LEU:HD12	1:119:A:SER:HA	5	0.49
(1,359)	1:75:A:LEU:HD13	1:119:A:SER:HA	5	0.49
(1,313)	1:34:A:VAL:HG21	1:35:A:THR:HG21	7	0.49
(1,313)	1:34:A:VAL:HG21	1:35:A:THR:HG22	7	0.49
(1,313)	1:34:A:VAL:HG21	1:35:A:THR:HG23	7	0.49
(1,313)	1:34:A:VAL:HG22	1:35:A:THR:HG21	7	0.49
(1,313)	1:34:A:VAL:HG22	1:35:A:THR:HG22	7	0.49
(1,313)	1:34:A:VAL:HG22	1:35:A:THR:HG23	7	0.49
(1,313)	1:34:A:VAL:HG23	1:35:A:THR:HG21	7	0.49
(1,313)	1:34:A:VAL:HG23	1:35:A:THR:HG22	7	0.49
(1,313)	1:34:A:VAL:HG23	1:35:A:THR:HG23	7	0.49
(1,83)	1:137:A:MET:HB3	1:138:A:ILE:HD11	5	0.49
(1,83)	1:137:A:MET:HB3	1:138:A:ILE:HD12	5	0.49
(1,83)	1:137:A:MET:HB3	1:138:A:ILE:HD13	5	0.49
(1,83)	1:137:A:MET:HB3	1:138:A:ILE:HD11	11	0.49
(1,83)	1:137:A:MET:HB3	1:138:A:ILE:HD12	11	0.49
(1,83)	1:137:A:MET:HB3	1:138:A:ILE:HD13	11	0.49
(2,12)	2:158:B:TYR:HD1	1:132:A:VAL:HG11	7	0.48
(2,12)	2:158:B:TYR:HD1	1:132:A:VAL:HG12	7	0.48
(2,12)	2:158:B:TYR:HD1	1:132:A:VAL:HG13	7	0.48
(2,12)	2:158:B:TYR:HD2	1:132:A:VAL:HG11	7	0.48
(2,12)	2:158:B:TYR:HD2	1:132:A:VAL:HG12	7	0.48
(2,12)	2:158:B:TYR:HD2	1:132:A:VAL:HG13	7	0.48
(1,1077)	1:137:A:MET:HB3	1:141:A:LEU:H	4	0.48
(1,14)	1:116:A:VAL:HG21	1:118:A:LYS:HG2	2	0.48
(1,14)	1:116:A:VAL:HG21	1:118:A:LYS:HG3	2	0.48
(1,14)	1:116:A:VAL:HG22	1:118:A:LYS:HG2	2	0.48
(1,14)	1:116:A:VAL:HG22	1:118:A:LYS:HG3	2	0.48
(1,14)	1:116:A:VAL:HG23	1:118:A:LYS:HG2	2	0.48
(1,14)	1:116:A:VAL:HG23	1:118:A:LYS:HG3	2	0.48
(1,1273)	1:59:A:VAL:HG11	1:100:A:PHE:HD1	3	0.47
(1,1273)	1:59:A:VAL:HG11	1:100:A:PHE:HD2	3	0.47
(1,1273)	1:59:A:VAL:HG12	1:100:A:PHE:HD1	3	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1273)	1:59:A:VAL:HG12	1:100:A:PHE:HD2	3	0.47
(1,1273)	1:59:A:VAL:HG13	1:100:A:PHE:HD1	3	0.47
(1,1273)	1:59:A:VAL:HG13	1:100:A:PHE:HD2	3	0.47
(1,1273)	1:59:A:VAL:HG21	1:100:A:PHE:HD1	3	0.47
(1,1273)	1:59:A:VAL:HG21	1:100:A:PHE:HD2	3	0.47
(1,1273)	1:59:A:VAL:HG22	1:100:A:PHE:HD1	3	0.47
(1,1273)	1:59:A:VAL:HG22	1:100:A:PHE:HD2	3	0.47
(1,1273)	1:59:A:VAL:HG23	1:100:A:PHE:HD1	3	0.47
(1,1273)	1:59:A:VAL:HG23	1:100:A:PHE:HD2	3	0.47
(1,952)	1:104:A:LEU:HD21	1:106:A:GLU:H	15	0.47
(1,952)	1:104:A:LEU:HD22	1:106:A:GLU:H	15	0.47
(1,952)	1:104:A:LEU:HD23	1:106:A:GLU:H	15	0.47
(1,134)	1:59:A:VAL:HB	1:103:A:VAL:HG21	20	0.47
(1,134)	1:59:A:VAL:HB	1:103:A:VAL:HG22	20	0.47
(1,134)	1:59:A:VAL:HB	1:103:A:VAL:HG23	20	0.47
(1,83)	1:137:A:MET:HB3	1:138:A:ILE:HD11	1	0.47
(1,83)	1:137:A:MET:HB3	1:138:A:ILE:HD12	1	0.47
(1,83)	1:137:A:MET:HB3	1:138:A:ILE:HD13	1	0.47
(5,1)	2:155:B:SER:H	1:130:A:ARG:NH2	4	0.46
(1,1290)	1:63:A:MET:HB2	1:77:A:LEU:HD11	18	0.46
(1,1290)	1:63:A:MET:HB2	1:77:A:LEU:HD12	18	0.46
(1,1290)	1:63:A:MET:HB2	1:77:A:LEU:HD13	18	0.46
(1,1290)	1:63:A:MET:HB2	1:77:A:LEU:HD21	18	0.46
(1,1290)	1:63:A:MET:HB2	1:77:A:LEU:HD22	18	0.46
(1,1290)	1:63:A:MET:HB2	1:77:A:LEU:HD23	18	0.46
(1,1290)	1:63:A:MET:HB3	1:77:A:LEU:HD11	18	0.46
(1,1290)	1:63:A:MET:HB3	1:77:A:LEU:HD12	18	0.46
(1,1290)	1:63:A:MET:HB3	1:77:A:LEU:HD13	18	0.46
(1,1290)	1:63:A:MET:HB3	1:77:A:LEU:HD21	18	0.46
(1,1290)	1:63:A:MET:HB3	1:77:A:LEU:HD22	18	0.46
(1,1290)	1:63:A:MET:HB3	1:77:A:LEU:HD23	18	0.46
(1,1229)	1:45:A:SER:HB2	1:80:A:LEU:HD11	4	0.46
(1,1229)	1:45:A:SER:HB2	1:80:A:LEU:HD12	4	0.46
(1,1229)	1:45:A:SER:HB2	1:80:A:LEU:HD13	4	0.46
(1,1229)	1:45:A:SER:HB2	1:80:A:LEU:HD21	4	0.46
(1,1229)	1:45:A:SER:HB2	1:80:A:LEU:HD22	4	0.46
(1,1229)	1:45:A:SER:HB2	1:80:A:LEU:HD23	4	0.46
(1,1229)	1:45:A:SER:HB3	1:80:A:LEU:HD11	4	0.46
(1,1229)	1:45:A:SER:HB3	1:80:A:LEU:HD12	4	0.46
(1,1229)	1:45:A:SER:HB3	1:80:A:LEU:HD13	4	0.46
(1,1229)	1:45:A:SER:HB3	1:80:A:LEU:HD21	4	0.46
(1,1229)	1:45:A:SER:HB3	1:80:A:LEU:HD22	4	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1229)	1:45:A:SER:HB3	1:80:A:LEU:HD23	4	0.46
(1,478)	1:77:A:LEU:HD21	1:78:A:PHE:HA	8	0.46
(1,478)	1:77:A:LEU:HD22	1:78:A:PHE:HA	8	0.46
(1,478)	1:77:A:LEU:HD23	1:78:A:PHE:HA	8	0.46
(1,461)	1:101:A:ALA:HB1	1:137:A:MET:HB2	15	0.46
(1,461)	1:101:A:ALA:HB2	1:137:A:MET:HB2	15	0.46
(1,461)	1:101:A:ALA:HB3	1:137:A:MET:HB2	15	0.46
(1,347)	1:104:A:LEU:HD11	1:108:A:ALA:HB1	7	0.46
(1,347)	1:104:A:LEU:HD11	1:108:A:ALA:HB2	7	0.46
(1,347)	1:104:A:LEU:HD11	1:108:A:ALA:HB3	7	0.46
(1,347)	1:104:A:LEU:HD12	1:108:A:ALA:HB1	7	0.46
(1,347)	1:104:A:LEU:HD12	1:108:A:ALA:HB2	7	0.46
(1,347)	1:104:A:LEU:HD12	1:108:A:ALA:HB3	7	0.46
(1,347)	1:104:A:LEU:HD13	1:108:A:ALA:HB1	7	0.46
(1,347)	1:104:A:LEU:HD13	1:108:A:ALA:HB2	7	0.46
(1,347)	1:104:A:LEU:HD13	1:108:A:ALA:HB3	7	0.46
(1,269)	1:104:A:LEU:HD21	1:108:A:ALA:HB1	8	0.46
(1,269)	1:104:A:LEU:HD21	1:108:A:ALA:HB2	8	0.46
(1,269)	1:104:A:LEU:HD21	1:108:A:ALA:HB3	8	0.46
(1,269)	1:104:A:LEU:HD22	1:108:A:ALA:HB1	8	0.46
(1,269)	1:104:A:LEU:HD22	1:108:A:ALA:HB2	8	0.46
(1,269)	1:104:A:LEU:HD22	1:108:A:ALA:HB3	8	0.46
(1,269)	1:104:A:LEU:HD23	1:108:A:ALA:HB1	8	0.46
(1,269)	1:104:A:LEU:HD23	1:108:A:ALA:HB2	8	0.46
(1,269)	1:104:A:LEU:HD23	1:108:A:ALA:HB3	8	0.46
(6,3)	2:148:B:SER:H1	2:149:B:PRO:HB2	15	0.45
(6,3)	2:148:B:SER:H1	2:149:B:PRO:HB3	15	0.45
(6,1)	2:148:B:SER:H1	2:149:B:PRO:HA	17	0.45
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD11	18	0.45
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD12	18	0.45
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD13	18	0.45
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD21	18	0.45
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD22	18	0.45
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD23	18	0.45
(1,1169)	1:34:A:VAL:HG21	1:35:A:THR:H	19	0.45
(1,1169)	1:34:A:VAL:HG22	1:35:A:THR:H	19	0.45
(1,1169)	1:34:A:VAL:HG23	1:35:A:THR:H	19	0.45
(1,446)	1:34:A:VAL:HG21	1:36:A:ASN:H	19	0.45
(1,446)	1:34:A:VAL:HG22	1:36:A:ASN:H	19	0.45
(1,446)	1:34:A:VAL:HG23	1:36:A:ASN:H	19	0.45
(1,438)	1:58:A:ILE:HG21	1:59:A:VAL:HG11	18	0.45
(1,438)	1:58:A:ILE:HG21	1:59:A:VAL:HG12	18	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,438)	1:58:A:ILE:HG21	1:59:A:VAL:HG13	18	0.45
(1,438)	1:58:A:ILE:HG22	1:59:A:VAL:HG11	18	0.45
(1,438)	1:58:A:ILE:HG22	1:59:A:VAL:HG12	18	0.45
(1,438)	1:58:A:ILE:HG22	1:59:A:VAL:HG13	18	0.45
(1,438)	1:58:A:ILE:HG23	1:59:A:VAL:HG11	18	0.45
(1,438)	1:58:A:ILE:HG23	1:59:A:VAL:HG12	18	0.45
(1,438)	1:58:A:ILE:HG23	1:59:A:VAL:HG13	18	0.45
(1,134)	1:59:A:VAL:HB	1:103:A:VAL:HG21	13	0.45
(1,134)	1:59:A:VAL:HB	1:103:A:VAL:HG22	13	0.45
(1,134)	1:59:A:VAL:HB	1:103:A:VAL:HG23	13	0.45
(1,53)	1:58:A:ILE:HG21	1:59:A:VAL:HG21	8	0.45
(1,53)	1:58:A:ILE:HG21	1:59:A:VAL:HG22	8	0.45
(1,53)	1:58:A:ILE:HG21	1:59:A:VAL:HG23	8	0.45
(1,53)	1:58:A:ILE:HG22	1:59:A:VAL:HG21	8	0.45
(1,53)	1:58:A:ILE:HG22	1:59:A:VAL:HG22	8	0.45
(1,53)	1:58:A:ILE:HG22	1:59:A:VAL:HG23	8	0.45
(1,53)	1:58:A:ILE:HG23	1:59:A:VAL:HG21	8	0.45
(1,53)	1:58:A:ILE:HG23	1:59:A:VAL:HG22	8	0.45
(1,53)	1:58:A:ILE:HG23	1:59:A:VAL:HG23	8	0.45
(1,20)	1:132:A:VAL:HG21	1:138:A:ILE:HD11	9	0.45
(1,20)	1:132:A:VAL:HG21	1:138:A:ILE:HD12	9	0.45
(1,20)	1:132:A:VAL:HG21	1:138:A:ILE:HD13	9	0.45
(1,20)	1:132:A:VAL:HG22	1:138:A:ILE:HD11	9	0.45
(1,20)	1:132:A:VAL:HG22	1:138:A:ILE:HD12	9	0.45
(1,20)	1:132:A:VAL:HG22	1:138:A:ILE:HD13	9	0.45
(1,20)	1:132:A:VAL:HG23	1:138:A:ILE:HD11	9	0.45
(1,20)	1:132:A:VAL:HG23	1:138:A:ILE:HD12	9	0.45
(1,20)	1:132:A:VAL:HG23	1:138:A:ILE:HD13	9	0.45
(6,3)	2:148:B:SER:H1	2:149:B:PRO:HB2	17	0.44
(6,3)	2:148:B:SER:H1	2:149:B:PRO:HB3	17	0.44
(6,1)	2:148:B:SER:H1	2:149:B:PRO:HA	15	0.44
(2,2)	2:149:B:PRO:HG2	1:38:A:MET:HE2	18	0.44
(1,1320)	1:75:A:LEU:HD11	1:111:A:VAL:HG11	5	0.44
(1,1320)	1:75:A:LEU:HD11	1:111:A:VAL:HG12	5	0.44
(1,1320)	1:75:A:LEU:HD11	1:111:A:VAL:HG13	5	0.44
(1,1320)	1:75:A:LEU:HD12	1:111:A:VAL:HG11	5	0.44
(1,1320)	1:75:A:LEU:HD12	1:111:A:VAL:HG12	5	0.44
(1,1320)	1:75:A:LEU:HD12	1:111:A:VAL:HG13	5	0.44
(1,1320)	1:75:A:LEU:HD13	1:111:A:VAL:HG11	5	0.44
(1,1320)	1:75:A:LEU:HD13	1:111:A:VAL:HG12	5	0.44
(1,1320)	1:75:A:LEU:HD13	1:111:A:VAL:HG13	5	0.44
(1,1320)	1:75:A:LEU:HD21	1:111:A:VAL:HG11	5	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1320)	1:75:A:LEU:HD21	1:111:A:VAL:HG12	5	0.44
(1,1320)	1:75:A:LEU:HD21	1:111:A:VAL:HG13	5	0.44
(1,1320)	1:75:A:LEU:HD22	1:111:A:VAL:HG11	5	0.44
(1,1320)	1:75:A:LEU:HD22	1:111:A:VAL:HG12	5	0.44
(1,1320)	1:75:A:LEU:HD22	1:111:A:VAL:HG13	5	0.44
(1,1320)	1:75:A:LEU:HD23	1:111:A:VAL:HG11	5	0.44
(1,1320)	1:75:A:LEU:HD23	1:111:A:VAL:HG12	5	0.44
(1,1320)	1:75:A:LEU:HD23	1:111:A:VAL:HG13	5	0.44
(1,963)	1:109:A:ALA:H	1:111:A:VAL:HG11	12	0.44
(1,963)	1:109:A:ALA:H	1:111:A:VAL:HG12	12	0.44
(1,963)	1:109:A:ALA:H	1:111:A:VAL:HG13	12	0.44
(1,952)	1:104:A:LEU:HD21	1:106:A:GLU:H	8	0.44
(1,952)	1:104:A:LEU:HD22	1:106:A:GLU:H	8	0.44
(1,952)	1:104:A:LEU:HD23	1:106:A:GLU:H	8	0.44
(1,478)	1:77:A:LEU:HD21	1:78:A:PHE:HA	1	0.44
(1,478)	1:77:A:LEU:HD22	1:78:A:PHE:HA	1	0.44
(1,478)	1:77:A:LEU:HD23	1:78:A:PHE:HA	1	0.44
(1,478)	1:77:A:LEU:HD21	1:78:A:PHE:HA	5	0.44
(1,478)	1:77:A:LEU:HD22	1:78:A:PHE:HA	5	0.44
(1,478)	1:77:A:LEU:HD23	1:78:A:PHE:HA	5	0.44
(1,478)	1:77:A:LEU:HD21	1:78:A:PHE:HA	20	0.44
(1,478)	1:77:A:LEU:HD22	1:78:A:PHE:HA	20	0.44
(1,478)	1:77:A:LEU:HD23	1:78:A:PHE:HA	20	0.44
(1,442)	1:75:A:LEU:HD11	1:78:A:PHE:HB3	4	0.44
(1,442)	1:75:A:LEU:HD12	1:78:A:PHE:HB3	4	0.44
(1,442)	1:75:A:LEU:HD13	1:78:A:PHE:HB3	4	0.44
(6,1)	2:148:B:SER:H1	2:149:B:PRO:HA	10	0.43
(1,1450)	1:116:A:VAL:HG11	1:120:A:VAL:HG11	17	0.43
(1,1450)	1:116:A:VAL:HG11	1:120:A:VAL:HG12	17	0.43
(1,1450)	1:116:A:VAL:HG11	1:120:A:VAL:HG13	17	0.43
(1,1450)	1:116:A:VAL:HG11	1:120:A:VAL:HG21	17	0.43
(1,1450)	1:116:A:VAL:HG11	1:120:A:VAL:HG22	17	0.43
(1,1450)	1:116:A:VAL:HG11	1:120:A:VAL:HG23	17	0.43
(1,1450)	1:116:A:VAL:HG12	1:120:A:VAL:HG11	17	0.43
(1,1450)	1:116:A:VAL:HG12	1:120:A:VAL:HG12	17	0.43
(1,1450)	1:116:A:VAL:HG12	1:120:A:VAL:HG13	17	0.43
(1,1450)	1:116:A:VAL:HG12	1:120:A:VAL:HG21	17	0.43
(1,1450)	1:116:A:VAL:HG12	1:120:A:VAL:HG22	17	0.43
(1,1450)	1:116:A:VAL:HG12	1:120:A:VAL:HG23	17	0.43
(1,1450)	1:116:A:VAL:HG13	1:120:A:VAL:HG11	17	0.43
(1,1450)	1:116:A:VAL:HG13	1:120:A:VAL:HG12	17	0.43
(1,1450)	1:116:A:VAL:HG13	1:120:A:VAL:HG13	17	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1450)	1:116:A:VAL:HG13	1:120:A:VAL:HG21	17	0.43
(1,1450)	1:116:A:VAL:HG13	1:120:A:VAL:HG22	17	0.43
(1,1450)	1:116:A:VAL:HG13	1:120:A:VAL:HG23	17	0.43
(1,1450)	1:116:A:VAL:HG21	1:120:A:VAL:HG11	17	0.43
(1,1450)	1:116:A:VAL:HG21	1:120:A:VAL:HG12	17	0.43
(1,1450)	1:116:A:VAL:HG21	1:120:A:VAL:HG13	17	0.43
(1,1450)	1:116:A:VAL:HG21	1:120:A:VAL:HG21	17	0.43
(1,1450)	1:116:A:VAL:HG21	1:120:A:VAL:HG22	17	0.43
(1,1450)	1:116:A:VAL:HG21	1:120:A:VAL:HG23	17	0.43
(1,1450)	1:116:A:VAL:HG22	1:120:A:VAL:HG11	17	0.43
(1,1450)	1:116:A:VAL:HG22	1:120:A:VAL:HG12	17	0.43
(1,1450)	1:116:A:VAL:HG22	1:120:A:VAL:HG13	17	0.43
(1,1450)	1:116:A:VAL:HG22	1:120:A:VAL:HG21	17	0.43
(1,1450)	1:116:A:VAL:HG22	1:120:A:VAL:HG22	17	0.43
(1,1450)	1:116:A:VAL:HG22	1:120:A:VAL:HG23	17	0.43
(1,1450)	1:116:A:VAL:HG23	1:120:A:VAL:HG11	17	0.43
(1,1450)	1:116:A:VAL:HG23	1:120:A:VAL:HG12	17	0.43
(1,1450)	1:116:A:VAL:HG23	1:120:A:VAL:HG13	17	0.43
(1,1450)	1:116:A:VAL:HG23	1:120:A:VAL:HG21	17	0.43
(1,1450)	1:116:A:VAL:HG23	1:120:A:VAL:HG22	17	0.43
(1,1450)	1:116:A:VAL:HG23	1:120:A:VAL:HG23	17	0.43
(1,1427)	1:112:A:LYS:HB2	1:145:A:LEU:HD11	15	0.43
(1,1427)	1:112:A:LYS:HB2	1:145:A:LEU:HD12	15	0.43
(1,1427)	1:112:A:LYS:HB2	1:145:A:LEU:HD13	15	0.43
(1,1427)	1:112:A:LYS:HB2	1:145:A:LEU:HD21	15	0.43
(1,1427)	1:112:A:LYS:HB2	1:145:A:LEU:HD22	15	0.43
(1,1427)	1:112:A:LYS:HB2	1:145:A:LEU:HD23	15	0.43
(1,1427)	1:112:A:LYS:HB3	1:145:A:LEU:HD11	15	0.43
(1,1427)	1:112:A:LYS:HB3	1:145:A:LEU:HD12	15	0.43
(1,1427)	1:112:A:LYS:HB3	1:145:A:LEU:HD13	15	0.43
(1,1427)	1:112:A:LYS:HB3	1:145:A:LEU:HD21	15	0.43
(1,1427)	1:112:A:LYS:HB3	1:145:A:LEU:HD22	15	0.43
(1,1427)	1:112:A:LYS:HB3	1:145:A:LEU:HD23	15	0.43
(1,1340)	1:78:A:PHE:HE1	1:104:A:LEU:HD11	7	0.43
(1,1340)	1:78:A:PHE:HE1	1:104:A:LEU:HD12	7	0.43
(1,1340)	1:78:A:PHE:HE1	1:104:A:LEU:HD13	7	0.43
(1,1340)	1:78:A:PHE:HE1	1:104:A:LEU:HD21	7	0.43
(1,1340)	1:78:A:PHE:HE1	1:104:A:LEU:HD22	7	0.43
(1,1340)	1:78:A:PHE:HE1	1:104:A:LEU:HD23	7	0.43
(1,1340)	1:78:A:PHE:HE2	1:104:A:LEU:HD11	7	0.43
(1,1340)	1:78:A:PHE:HE2	1:104:A:LEU:HD12	7	0.43
(1,1340)	1:78:A:PHE:HE2	1:104:A:LEU:HD13	7	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1340)	1:78:A:PHE:HE2	1:104:A:LEU:HD21	7	0.43
(1,1340)	1:78:A:PHE:HE2	1:104:A:LEU:HD22	7	0.43
(1,1340)	1:78:A:PHE:HE2	1:104:A:LEU:HD23	7	0.43
(1,1290)	1:63:A:MET:HB2	1:77:A:LEU:HD11	7	0.43
(1,1290)	1:63:A:MET:HB2	1:77:A:LEU:HD12	7	0.43
(1,1290)	1:63:A:MET:HB2	1:77:A:LEU:HD13	7	0.43
(1,1290)	1:63:A:MET:HB2	1:77:A:LEU:HD21	7	0.43
(1,1290)	1:63:A:MET:HB2	1:77:A:LEU:HD22	7	0.43
(1,1290)	1:63:A:MET:HB2	1:77:A:LEU:HD23	7	0.43
(1,1290)	1:63:A:MET:HB3	1:77:A:LEU:HD11	7	0.43
(1,1290)	1:63:A:MET:HB3	1:77:A:LEU:HD12	7	0.43
(1,1290)	1:63:A:MET:HB3	1:77:A:LEU:HD13	7	0.43
(1,1290)	1:63:A:MET:HB3	1:77:A:LEU:HD21	7	0.43
(1,1290)	1:63:A:MET:HB3	1:77:A:LEU:HD22	7	0.43
(1,1290)	1:63:A:MET:HB3	1:77:A:LEU:HD23	7	0.43
(1,648)	1:75:A:LEU:HD11	1:120:A:VAL:H	1	0.43
(1,648)	1:75:A:LEU:HD12	1:120:A:VAL:H	1	0.43
(1,648)	1:75:A:LEU:HD13	1:120:A:VAL:H	1	0.43
(1,461)	1:101:A:ALA:HB1	1:137:A:MET:HB2	8	0.43
(1,461)	1:101:A:ALA:HB2	1:137:A:MET:HB2	8	0.43
(1,461)	1:101:A:ALA:HB3	1:137:A:MET:HB2	8	0.43
(1,313)	1:34:A:VAL:HG21	1:35:A:THR:HG21	15	0.43
(1,313)	1:34:A:VAL:HG21	1:35:A:THR:HG22	15	0.43
(1,313)	1:34:A:VAL:HG21	1:35:A:THR:HG23	15	0.43
(1,313)	1:34:A:VAL:HG22	1:35:A:THR:HG21	15	0.43
(1,313)	1:34:A:VAL:HG22	1:35:A:THR:HG22	15	0.43
(1,313)	1:34:A:VAL:HG22	1:35:A:THR:HG23	15	0.43
(1,313)	1:34:A:VAL:HG23	1:35:A:THR:HG21	15	0.43
(1,313)	1:34:A:VAL:HG23	1:35:A:THR:HG22	15	0.43
(1,313)	1:34:A:VAL:HG23	1:35:A:THR:HG23	15	0.43
(1,313)	1:34:A:VAL:HG21	1:35:A:THR:HG21	18	0.43
(1,313)	1:34:A:VAL:HG21	1:35:A:THR:HG22	18	0.43
(1,313)	1:34:A:VAL:HG21	1:35:A:THR:HG23	18	0.43
(1,313)	1:34:A:VAL:HG22	1:35:A:THR:HG21	18	0.43
(1,313)	1:34:A:VAL:HG22	1:35:A:THR:HG22	18	0.43
(1,313)	1:34:A:VAL:HG22	1:35:A:THR:HG23	18	0.43
(1,313)	1:34:A:VAL:HG23	1:35:A:THR:HG21	18	0.43
(1,313)	1:34:A:VAL:HG23	1:35:A:THR:HG22	18	0.43
(1,313)	1:34:A:VAL:HG23	1:35:A:THR:HG23	18	0.43
(1,14)	1:116:A:VAL:HG21	1:118:A:LYS:HG2	5	0.43
(1,14)	1:116:A:VAL:HG21	1:118:A:LYS:HG3	5	0.43
(1,14)	1:116:A:VAL:HG22	1:118:A:LYS:HG2	5	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,14)	1:116:A:VAL:HG22	1:118:A:LYS:HG3	5	0.43
(1,14)	1:116:A:VAL:HG23	1:118:A:LYS:HG2	5	0.43
(1,14)	1:116:A:VAL:HG23	1:118:A:LYS:HG3	5	0.43
(6,1)	2:148:B:SER:H1	2:149:B:PRO:HA	1	0.42
(1,1320)	1:75:A:LEU:HD11	1:111:A:VAL:HG11	19	0.42
(1,1320)	1:75:A:LEU:HD11	1:111:A:VAL:HG12	19	0.42
(1,1320)	1:75:A:LEU:HD11	1:111:A:VAL:HG13	19	0.42
(1,1320)	1:75:A:LEU:HD12	1:111:A:VAL:HG11	19	0.42
(1,1320)	1:75:A:LEU:HD12	1:111:A:VAL:HG12	19	0.42
(1,1320)	1:75:A:LEU:HD12	1:111:A:VAL:HG13	19	0.42
(1,1320)	1:75:A:LEU:HD13	1:111:A:VAL:HG11	19	0.42
(1,1320)	1:75:A:LEU:HD13	1:111:A:VAL:HG12	19	0.42
(1,1320)	1:75:A:LEU:HD13	1:111:A:VAL:HG13	19	0.42
(1,1320)	1:75:A:LEU:HD21	1:111:A:VAL:HG11	19	0.42
(1,1320)	1:75:A:LEU:HD21	1:111:A:VAL:HG12	19	0.42
(1,1320)	1:75:A:LEU:HD21	1:111:A:VAL:HG13	19	0.42
(1,1320)	1:75:A:LEU:HD22	1:111:A:VAL:HG11	19	0.42
(1,1320)	1:75:A:LEU:HD22	1:111:A:VAL:HG12	19	0.42
(1,1320)	1:75:A:LEU:HD22	1:111:A:VAL:HG13	19	0.42
(1,1320)	1:75:A:LEU:HD23	1:111:A:VAL:HG11	19	0.42
(1,1320)	1:75:A:LEU:HD23	1:111:A:VAL:HG12	19	0.42
(1,1320)	1:75:A:LEU:HD23	1:111:A:VAL:HG13	19	0.42
(1,1285)	1:62:A:TRP:HE1	1:77:A:LEU:HD11	13	0.42
(1,1285)	1:62:A:TRP:HE1	1:77:A:LEU:HD12	13	0.42
(1,1285)	1:62:A:TRP:HE1	1:77:A:LEU:HD13	13	0.42
(1,1285)	1:62:A:TRP:HE1	1:77:A:LEU:HD21	13	0.42
(1,1285)	1:62:A:TRP:HE1	1:77:A:LEU:HD22	13	0.42
(1,1285)	1:62:A:TRP:HE1	1:77:A:LEU:HD23	13	0.42
(1,1281)	1:59:A:VAL:HG11	1:104:A:LEU:H	14	0.42
(1,1281)	1:59:A:VAL:HG12	1:104:A:LEU:H	14	0.42
(1,1281)	1:59:A:VAL:HG13	1:104:A:LEU:H	14	0.42
(1,1281)	1:59:A:VAL:HG21	1:104:A:LEU:H	14	0.42
(1,1281)	1:59:A:VAL:HG22	1:104:A:LEU:H	14	0.42
(1,1281)	1:59:A:VAL:HG23	1:104:A:LEU:H	14	0.42
(1,1276)	1:59:A:VAL:HG11	1:103:A:VAL:H	16	0.42
(1,1276)	1:59:A:VAL:HG12	1:103:A:VAL:H	16	0.42
(1,1276)	1:59:A:VAL:HG13	1:103:A:VAL:H	16	0.42
(1,1276)	1:59:A:VAL:HG21	1:103:A:VAL:H	16	0.42
(1,1276)	1:59:A:VAL:HG22	1:103:A:VAL:H	16	0.42
(1,1276)	1:59:A:VAL:HG23	1:103:A:VAL:H	16	0.42
(1,818)	1:110:A:LEU:H	1:111:A:VAL:HG11	17	0.42
(1,818)	1:110:A:LEU:H	1:111:A:VAL:HG12	17	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,818)	1:110:A:LEU:H	1:111:A:VAL:HG13	17	0.42
(1,722)	1:34:A:VAL:HG21	1:40:A:SER:H	6	0.42
(1,722)	1:34:A:VAL:HG22	1:40:A:SER:H	6	0.42
(1,722)	1:34:A:VAL:HG23	1:40:A:SER:H	6	0.42
(1,579)	1:48:A:CYS:H	1:84:A:VAL:HG21	17	0.42
(1,579)	1:48:A:CYS:H	1:84:A:VAL:HG22	17	0.42
(1,579)	1:48:A:CYS:H	1:84:A:VAL:HG23	17	0.42
(1,461)	1:101:A:ALA:HB1	1:137:A:MET:HB2	19	0.42
(1,461)	1:101:A:ALA:HB2	1:137:A:MET:HB2	19	0.42
(1,461)	1:101:A:ALA:HB3	1:137:A:MET:HB2	19	0.42
(1,438)	1:58:A:ILE:HG21	1:59:A:VAL:HG11	15	0.42
(1,438)	1:58:A:ILE:HG21	1:59:A:VAL:HG12	15	0.42
(1,438)	1:58:A:ILE:HG21	1:59:A:VAL:HG13	15	0.42
(1,438)	1:58:A:ILE:HG22	1:59:A:VAL:HG11	15	0.42
(1,438)	1:58:A:ILE:HG22	1:59:A:VAL:HG12	15	0.42
(1,438)	1:58:A:ILE:HG22	1:59:A:VAL:HG13	15	0.42
(1,438)	1:58:A:ILE:HG23	1:59:A:VAL:HG11	15	0.42
(1,438)	1:58:A:ILE:HG23	1:59:A:VAL:HG12	15	0.42
(1,438)	1:58:A:ILE:HG23	1:59:A:VAL:HG13	15	0.42
(1,336)	1:108:A:ALA:HB1	1:111:A:VAL:HG11	20	0.42
(1,336)	1:108:A:ALA:HB1	1:111:A:VAL:HG12	20	0.42
(1,336)	1:108:A:ALA:HB1	1:111:A:VAL:HG13	20	0.42
(1,336)	1:108:A:ALA:HB2	1:111:A:VAL:HG11	20	0.42
(1,336)	1:108:A:ALA:HB2	1:111:A:VAL:HG12	20	0.42
(1,336)	1:108:A:ALA:HB2	1:111:A:VAL:HG13	20	0.42
(1,336)	1:108:A:ALA:HB3	1:111:A:VAL:HG11	20	0.42
(1,336)	1:108:A:ALA:HB3	1:111:A:VAL:HG12	20	0.42
(1,336)	1:108:A:ALA:HB3	1:111:A:VAL:HG13	20	0.42
(1,313)	1:34:A:VAL:HG21	1:35:A:THR:HG21	12	0.42
(1,313)	1:34:A:VAL:HG21	1:35:A:THR:HG22	12	0.42
(1,313)	1:34:A:VAL:HG21	1:35:A:THR:HG23	12	0.42
(1,313)	1:34:A:VAL:HG22	1:35:A:THR:HG21	12	0.42
(1,313)	1:34:A:VAL:HG22	1:35:A:THR:HG22	12	0.42
(1,313)	1:34:A:VAL:HG22	1:35:A:THR:HG23	12	0.42
(1,313)	1:34:A:VAL:HG23	1:35:A:THR:HG21	12	0.42
(1,313)	1:34:A:VAL:HG23	1:35:A:THR:HG22	12	0.42
(1,313)	1:34:A:VAL:HG23	1:35:A:THR:HG23	12	0.42
(1,83)	1:137:A:MET:HB3	1:138:A:ILE:HD11	6	0.42
(1,83)	1:137:A:MET:HB3	1:138:A:ILE:HD12	6	0.42
(1,83)	1:137:A:MET:HB3	1:138:A:ILE:HD13	6	0.42
(1,40)	1:85:A:ILE:HG21	1:132:A:VAL:HG11	18	0.42
(1,40)	1:85:A:ILE:HG21	1:132:A:VAL:HG12	18	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,40)	1:85:A:ILE:HG21	1:132:A:VAL:HG13	18	0.42
(1,40)	1:85:A:ILE:HG22	1:132:A:VAL:HG11	18	0.42
(1,40)	1:85:A:ILE:HG22	1:132:A:VAL:HG12	18	0.42
(1,40)	1:85:A:ILE:HG22	1:132:A:VAL:HG13	18	0.42
(1,40)	1:85:A:ILE:HG23	1:132:A:VAL:HG11	18	0.42
(1,40)	1:85:A:ILE:HG23	1:132:A:VAL:HG12	18	0.42
(1,40)	1:85:A:ILE:HG23	1:132:A:VAL:HG13	18	0.42
(6,3)	2:148:B:SER:H1	2:149:B:PRO:HB2	20	0.41
(6,3)	2:148:B:SER:H1	2:149:B:PRO:HB3	20	0.41
(1,1510)	1:139:A:VAL:HG11	1:143:A:GLU:HG2	8	0.41
(1,1510)	1:139:A:VAL:HG11	1:143:A:GLU:HG3	8	0.41
(1,1510)	1:139:A:VAL:HG12	1:143:A:GLU:HG2	8	0.41
(1,1510)	1:139:A:VAL:HG12	1:143:A:GLU:HG3	8	0.41
(1,1510)	1:139:A:VAL:HG13	1:143:A:GLU:HG2	8	0.41
(1,1510)	1:139:A:VAL:HG13	1:143:A:GLU:HG3	8	0.41
(1,1510)	1:139:A:VAL:HG21	1:143:A:GLU:HG2	8	0.41
(1,1510)	1:139:A:VAL:HG21	1:143:A:GLU:HG3	8	0.41
(1,1510)	1:139:A:VAL:HG22	1:143:A:GLU:HG2	8	0.41
(1,1510)	1:139:A:VAL:HG22	1:143:A:GLU:HG3	8	0.41
(1,1510)	1:139:A:VAL:HG23	1:143:A:GLU:HG2	8	0.41
(1,1510)	1:139:A:VAL:HG23	1:143:A:GLU:HG3	8	0.41
(1,1229)	1:45:A:SER:HB2	1:80:A:LEU:HD11	12	0.41
(1,1229)	1:45:A:SER:HB2	1:80:A:LEU:HD12	12	0.41
(1,1229)	1:45:A:SER:HB2	1:80:A:LEU:HD13	12	0.41
(1,1229)	1:45:A:SER:HB2	1:80:A:LEU:HD21	12	0.41
(1,1229)	1:45:A:SER:HB2	1:80:A:LEU:HD22	12	0.41
(1,1229)	1:45:A:SER:HB2	1:80:A:LEU:HD23	12	0.41
(1,1229)	1:45:A:SER:HB3	1:80:A:LEU:HD11	12	0.41
(1,1229)	1:45:A:SER:HB3	1:80:A:LEU:HD12	12	0.41
(1,1229)	1:45:A:SER:HB3	1:80:A:LEU:HD13	12	0.41
(1,1229)	1:45:A:SER:HB3	1:80:A:LEU:HD21	12	0.41
(1,1229)	1:45:A:SER:HB3	1:80:A:LEU:HD22	12	0.41
(1,1229)	1:45:A:SER:HB3	1:80:A:LEU:HD23	12	0.41
(1,1218)	1:44:A:LEU:HB2	1:80:A:LEU:HD11	17	0.41
(1,1218)	1:44:A:LEU:HB2	1:80:A:LEU:HD12	17	0.41
(1,1218)	1:44:A:LEU:HB2	1:80:A:LEU:HD13	17	0.41
(1,1218)	1:44:A:LEU:HB2	1:80:A:LEU:HD21	17	0.41
(1,1218)	1:44:A:LEU:HB2	1:80:A:LEU:HD22	17	0.41
(1,1218)	1:44:A:LEU:HB2	1:80:A:LEU:HD23	17	0.41
(1,857)	1:111:A:VAL:HG11	1:112:A:LYS:H	12	0.41
(1,857)	1:111:A:VAL:HG12	1:112:A:LYS:H	12	0.41
(1,857)	1:111:A:VAL:HG13	1:112:A:LYS:H	12	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,478)	1:77:A:LEU:HD21	1:78:A:PHE:HA	13	0.41
(1,478)	1:77:A:LEU:HD22	1:78:A:PHE:HA	13	0.41
(1,478)	1:77:A:LEU:HD23	1:78:A:PHE:HA	13	0.41
(1,377)	1:62:A:TRP:HZ3	1:103:A:VAL:HG11	7	0.41
(1,377)	1:62:A:TRP:HZ3	1:103:A:VAL:HG12	7	0.41
(1,377)	1:62:A:TRP:HZ3	1:103:A:VAL:HG13	7	0.41
(1,1427)	1:112:A:LYS:HB2	1:145:A:LEU:HD11	9	0.4
(1,1427)	1:112:A:LYS:HB2	1:145:A:LEU:HD12	9	0.4
(1,1427)	1:112:A:LYS:HB2	1:145:A:LEU:HD13	9	0.4
(1,1427)	1:112:A:LYS:HB2	1:145:A:LEU:HD21	9	0.4
(1,1427)	1:112:A:LYS:HB2	1:145:A:LEU:HD22	9	0.4
(1,1427)	1:112:A:LYS:HB2	1:145:A:LEU:HD23	9	0.4
(1,1427)	1:112:A:LYS:HB3	1:145:A:LEU:HD11	9	0.4
(1,1427)	1:112:A:LYS:HB3	1:145:A:LEU:HD12	9	0.4
(1,1427)	1:112:A:LYS:HB3	1:145:A:LEU:HD13	9	0.4
(1,1427)	1:112:A:LYS:HB3	1:145:A:LEU:HD21	9	0.4
(1,1427)	1:112:A:LYS:HB3	1:145:A:LEU:HD22	9	0.4
(1,1427)	1:112:A:LYS:HB3	1:145:A:LEU:HD23	9	0.4
(1,1402)	1:104:A:LEU:HD11	1:141:A:LEU:HB2	14	0.4
(1,1402)	1:104:A:LEU:HD11	1:141:A:LEU:HB3	14	0.4
(1,1402)	1:104:A:LEU:HD12	1:141:A:LEU:HB2	14	0.4
(1,1402)	1:104:A:LEU:HD12	1:141:A:LEU:HB3	14	0.4
(1,1402)	1:104:A:LEU:HD13	1:141:A:LEU:HB2	14	0.4
(1,1402)	1:104:A:LEU:HD13	1:141:A:LEU:HB3	14	0.4
(1,1402)	1:104:A:LEU:HD21	1:141:A:LEU:HB2	14	0.4
(1,1402)	1:104:A:LEU:HD21	1:141:A:LEU:HB3	14	0.4
(1,1402)	1:104:A:LEU:HD22	1:141:A:LEU:HB2	14	0.4
(1,1402)	1:104:A:LEU:HD22	1:141:A:LEU:HB3	14	0.4
(1,1402)	1:104:A:LEU:HD23	1:141:A:LEU:HB2	14	0.4
(1,1402)	1:104:A:LEU:HD23	1:141:A:LEU:HB3	14	0.4
(1,1320)	1:75:A:LEU:HD11	1:111:A:VAL:HG11	11	0.4
(1,1320)	1:75:A:LEU:HD11	1:111:A:VAL:HG12	11	0.4
(1,1320)	1:75:A:LEU:HD11	1:111:A:VAL:HG13	11	0.4
(1,1320)	1:75:A:LEU:HD12	1:111:A:VAL:HG11	11	0.4
(1,1320)	1:75:A:LEU:HD12	1:111:A:VAL:HG12	11	0.4
(1,1320)	1:75:A:LEU:HD12	1:111:A:VAL:HG13	11	0.4
(1,1320)	1:75:A:LEU:HD13	1:111:A:VAL:HG11	11	0.4
(1,1320)	1:75:A:LEU:HD13	1:111:A:VAL:HG12	11	0.4
(1,1320)	1:75:A:LEU:HD13	1:111:A:VAL:HG13	11	0.4
(1,1320)	1:75:A:LEU:HD21	1:111:A:VAL:HG11	11	0.4
(1,1320)	1:75:A:LEU:HD21	1:111:A:VAL:HG12	11	0.4
(1,1320)	1:75:A:LEU:HD21	1:111:A:VAL:HG13	11	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1320)	1:75:A:LEU:HD22	1:111:A:VAL:HG11	11	0.4
(1,1320)	1:75:A:LEU:HD22	1:111:A:VAL:HG12	11	0.4
(1,1320)	1:75:A:LEU:HD22	1:111:A:VAL:HG13	11	0.4
(1,1320)	1:75:A:LEU:HD23	1:111:A:VAL:HG11	11	0.4
(1,1320)	1:75:A:LEU:HD23	1:111:A:VAL:HG12	11	0.4
(1,1320)	1:75:A:LEU:HD23	1:111:A:VAL:HG13	11	0.4
(1,1285)	1:62:A:TRP:HE1	1:77:A:LEU:HD11	15	0.4
(1,1285)	1:62:A:TRP:HE1	1:77:A:LEU:HD12	15	0.4
(1,1285)	1:62:A:TRP:HE1	1:77:A:LEU:HD13	15	0.4
(1,1285)	1:62:A:TRP:HE1	1:77:A:LEU:HD21	15	0.4
(1,1285)	1:62:A:TRP:HE1	1:77:A:LEU:HD22	15	0.4
(1,1285)	1:62:A:TRP:HE1	1:77:A:LEU:HD23	15	0.4
(1,1169)	1:34:A:VAL:HG21	1:35:A:THR:H	20	0.4
(1,1169)	1:34:A:VAL:HG22	1:35:A:THR:H	20	0.4
(1,1169)	1:34:A:VAL:HG23	1:35:A:THR:H	20	0.4
(1,478)	1:77:A:LEU:HD21	1:78:A:PHE:HA	10	0.4
(1,478)	1:77:A:LEU:HD22	1:78:A:PHE:HA	10	0.4
(1,478)	1:77:A:LEU:HD23	1:78:A:PHE:HA	10	0.4
(1,442)	1:75:A:LEU:HD11	1:78:A:PHE:HB3	2	0.4
(1,442)	1:75:A:LEU:HD12	1:78:A:PHE:HB3	2	0.4
(1,442)	1:75:A:LEU:HD13	1:78:A:PHE:HB3	2	0.4
(1,255)	1:111:A:VAL:HG21	1:120:A:VAL:HA	4	0.4
(1,255)	1:111:A:VAL:HG22	1:120:A:VAL:HA	4	0.4
(1,255)	1:111:A:VAL:HG23	1:120:A:VAL:HA	4	0.4
(1,83)	1:137:A:MET:HB3	1:138:A:ILE:HD11	3	0.4
(1,83)	1:137:A:MET:HB3	1:138:A:ILE:HD12	3	0.4
(1,83)	1:137:A:MET:HB3	1:138:A:ILE:HD13	3	0.4
(1,69)	1:34:A:VAL:HG11	1:41:A:ILE:HD11	3	0.4
(1,69)	1:34:A:VAL:HG11	1:41:A:ILE:HD12	3	0.4
(1,69)	1:34:A:VAL:HG11	1:41:A:ILE:HD13	3	0.4
(1,69)	1:34:A:VAL:HG12	1:41:A:ILE:HD11	3	0.4
(1,69)	1:34:A:VAL:HG12	1:41:A:ILE:HD12	3	0.4
(1,69)	1:34:A:VAL:HG12	1:41:A:ILE:HD13	3	0.4
(1,69)	1:34:A:VAL:HG13	1:41:A:ILE:HD11	3	0.4
(1,69)	1:34:A:VAL:HG13	1:41:A:ILE:HD12	3	0.4
(1,69)	1:34:A:VAL:HG13	1:41:A:ILE:HD13	3	0.4
(6,1)	2:148:B:SER:H1	2:149:B:PRO:HA	16	0.39
(2,12)	2:158:B:TYR:HD1	1:132:A:VAL:HG11	17	0.39
(2,12)	2:158:B:TYR:HD1	1:132:A:VAL:HG12	17	0.39
(2,12)	2:158:B:TYR:HD1	1:132:A:VAL:HG13	17	0.39
(2,12)	2:158:B:TYR:HD2	1:132:A:VAL:HG11	17	0.39
(2,12)	2:158:B:TYR:HD2	1:132:A:VAL:HG12	17	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,12)	2:158:B:TYR:HD2	1:132:A:VAL:HG13	17	0.39
(1,1277)	1:59:A:VAL:HG11	1:103:A:VAL:HA	16	0.39
(1,1277)	1:59:A:VAL:HG12	1:103:A:VAL:HA	16	0.39
(1,1277)	1:59:A:VAL:HG13	1:103:A:VAL:HA	16	0.39
(1,1277)	1:59:A:VAL:HG21	1:103:A:VAL:HA	16	0.39
(1,1277)	1:59:A:VAL:HG22	1:103:A:VAL:HA	16	0.39
(1,1277)	1:59:A:VAL:HG23	1:103:A:VAL:HA	16	0.39
(1,461)	1:101:A:ALA:HB1	1:137:A:MET:HB2	6	0.39
(1,461)	1:101:A:ALA:HB2	1:137:A:MET:HB2	6	0.39
(1,461)	1:101:A:ALA:HB3	1:137:A:MET:HB2	6	0.39
(1,293)	1:31:A:PHE:HA	1:34:A:VAL:HG11	1	0.39
(1,293)	1:31:A:PHE:HA	1:34:A:VAL:HG12	1	0.39
(1,293)	1:31:A:PHE:HA	1:34:A:VAL:HG13	1	0.39
(1,1320)	1:75:A:LEU:HD11	1:111:A:VAL:HG11	8	0.38
(1,1320)	1:75:A:LEU:HD11	1:111:A:VAL:HG12	8	0.38
(1,1320)	1:75:A:LEU:HD11	1:111:A:VAL:HG13	8	0.38
(1,1320)	1:75:A:LEU:HD12	1:111:A:VAL:HG11	8	0.38
(1,1320)	1:75:A:LEU:HD12	1:111:A:VAL:HG12	8	0.38
(1,1320)	1:75:A:LEU:HD12	1:111:A:VAL:HG13	8	0.38
(1,1320)	1:75:A:LEU:HD13	1:111:A:VAL:HG11	8	0.38
(1,1320)	1:75:A:LEU:HD13	1:111:A:VAL:HG12	8	0.38
(1,1320)	1:75:A:LEU:HD13	1:111:A:VAL:HG13	8	0.38
(1,1320)	1:75:A:LEU:HD21	1:111:A:VAL:HG11	8	0.38
(1,1320)	1:75:A:LEU:HD21	1:111:A:VAL:HG12	8	0.38
(1,1320)	1:75:A:LEU:HD21	1:111:A:VAL:HG13	8	0.38
(1,1320)	1:75:A:LEU:HD22	1:111:A:VAL:HG11	8	0.38
(1,1320)	1:75:A:LEU:HD22	1:111:A:VAL:HG12	8	0.38
(1,1320)	1:75:A:LEU:HD22	1:111:A:VAL:HG13	8	0.38
(1,1320)	1:75:A:LEU:HD23	1:111:A:VAL:HG11	8	0.38
(1,1320)	1:75:A:LEU:HD23	1:111:A:VAL:HG12	8	0.38
(1,1320)	1:75:A:LEU:HD23	1:111:A:VAL:HG13	8	0.38
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD11	12	0.38
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD12	12	0.38
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD13	12	0.38
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD21	12	0.38
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD22	12	0.38
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD23	12	0.38
(1,1189)	1:62:A:TRP:HE1	1:77:A:LEU:HD21	11	0.38
(1,1189)	1:62:A:TRP:HE1	1:77:A:LEU:HD22	11	0.38
(1,1189)	1:62:A:TRP:HE1	1:77:A:LEU:HD23	11	0.38
(1,461)	1:101:A:ALA:HB1	1:137:A:MET:HB2	18	0.38
(1,461)	1:101:A:ALA:HB2	1:137:A:MET:HB2	18	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,461)	1:101:A:ALA:HB3	1:137:A:MET:HB2	18	0.38
(1,1500)	1:137:A:MET:HB2	1:141:A:LEU:HD11	3	0.37
(1,1500)	1:137:A:MET:HB2	1:141:A:LEU:HD12	3	0.37
(1,1500)	1:137:A:MET:HB2	1:141:A:LEU:HD13	3	0.37
(1,1500)	1:137:A:MET:HB2	1:141:A:LEU:HD21	3	0.37
(1,1500)	1:137:A:MET:HB2	1:141:A:LEU:HD22	3	0.37
(1,1500)	1:137:A:MET:HB2	1:141:A:LEU:HD23	3	0.37
(1,1432)	1:113:A:ASP:H	1:145:A:LEU:HD11	20	0.37
(1,1432)	1:113:A:ASP:H	1:145:A:LEU:HD12	20	0.37
(1,1432)	1:113:A:ASP:H	1:145:A:LEU:HD13	20	0.37
(1,1432)	1:113:A:ASP:H	1:145:A:LEU:HD21	20	0.37
(1,1432)	1:113:A:ASP:H	1:145:A:LEU:HD22	20	0.37
(1,1432)	1:113:A:ASP:H	1:145:A:LEU:HD23	20	0.37
(1,1320)	1:75:A:LEU:HD11	1:111:A:VAL:HG11	9	0.37
(1,1320)	1:75:A:LEU:HD11	1:111:A:VAL:HG12	9	0.37
(1,1320)	1:75:A:LEU:HD11	1:111:A:VAL:HG13	9	0.37
(1,1320)	1:75:A:LEU:HD12	1:111:A:VAL:HG11	9	0.37
(1,1320)	1:75:A:LEU:HD12	1:111:A:VAL:HG12	9	0.37
(1,1320)	1:75:A:LEU:HD12	1:111:A:VAL:HG13	9	0.37
(1,1320)	1:75:A:LEU:HD13	1:111:A:VAL:HG11	9	0.37
(1,1320)	1:75:A:LEU:HD13	1:111:A:VAL:HG12	9	0.37
(1,1320)	1:75:A:LEU:HD13	1:111:A:VAL:HG13	9	0.37
(1,1320)	1:75:A:LEU:HD21	1:111:A:VAL:HG11	9	0.37
(1,1320)	1:75:A:LEU:HD21	1:111:A:VAL:HG12	9	0.37
(1,1320)	1:75:A:LEU:HD21	1:111:A:VAL:HG13	9	0.37
(1,1320)	1:75:A:LEU:HD22	1:111:A:VAL:HG11	9	0.37
(1,1320)	1:75:A:LEU:HD22	1:111:A:VAL:HG12	9	0.37
(1,1320)	1:75:A:LEU:HD22	1:111:A:VAL:HG13	9	0.37
(1,1320)	1:75:A:LEU:HD23	1:111:A:VAL:HG11	9	0.37
(1,1320)	1:75:A:LEU:HD23	1:111:A:VAL:HG12	9	0.37
(1,1320)	1:75:A:LEU:HD23	1:111:A:VAL:HG13	9	0.37
(1,1318)	1:75:A:LEU:HD11	1:80:A:LEU:H	14	0.37
(1,1318)	1:75:A:LEU:HD12	1:80:A:LEU:H	14	0.37
(1,1318)	1:75:A:LEU:HD13	1:80:A:LEU:H	14	0.37
(1,1318)	1:75:A:LEU:HD21	1:80:A:LEU:H	14	0.37
(1,1318)	1:75:A:LEU:HD22	1:80:A:LEU:H	14	0.37
(1,1318)	1:75:A:LEU:HD23	1:80:A:LEU:H	14	0.37
(1,1219)	1:44:A:LEU:HB3	1:80:A:LEU:HD11	11	0.37
(1,1219)	1:44:A:LEU:HB3	1:80:A:LEU:HD12	11	0.37
(1,1219)	1:44:A:LEU:HB3	1:80:A:LEU:HD13	11	0.37
(1,1219)	1:44:A:LEU:HB3	1:80:A:LEU:HD21	11	0.37
(1,1219)	1:44:A:LEU:HB3	1:80:A:LEU:HD22	11	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1219)	1:44:A:LEU:HB3	1:80:A:LEU:HD23	11	0.37
(1,1202)	1:23:A:LEU:HD11	1:27:A:LEU:HA	19	0.37
(1,1202)	1:23:A:LEU:HD12	1:27:A:LEU:HA	19	0.37
(1,1202)	1:23:A:LEU:HD13	1:27:A:LEU:HA	19	0.37
(1,1202)	1:23:A:LEU:HD21	1:27:A:LEU:HA	19	0.37
(1,1202)	1:23:A:LEU:HD22	1:27:A:LEU:HA	19	0.37
(1,1202)	1:23:A:LEU:HD23	1:27:A:LEU:HA	19	0.37
(1,574)	1:108:A:ALA:H	1:111:A:VAL:HG11	10	0.37
(1,574)	1:108:A:ALA:H	1:111:A:VAL:HG12	10	0.37
(1,574)	1:108:A:ALA:H	1:111:A:VAL:HG13	10	0.37
(1,359)	1:75:A:LEU:HD11	1:119:A:SER:HA	8	0.37
(1,359)	1:75:A:LEU:HD12	1:119:A:SER:HA	8	0.37
(1,359)	1:75:A:LEU:HD13	1:119:A:SER:HA	8	0.37
(1,308)	1:103:A:VAL:HG21	1:107:A:ALA:HA	10	0.37
(1,308)	1:103:A:VAL:HG22	1:107:A:ALA:HA	10	0.37
(1,308)	1:103:A:VAL:HG23	1:107:A:ALA:HA	10	0.37
(1,204)	1:59:A:VAL:HA	1:103:A:VAL:HG11	5	0.37
(1,204)	1:59:A:VAL:HA	1:103:A:VAL:HG12	5	0.37
(1,204)	1:59:A:VAL:HA	1:103:A:VAL:HG13	5	0.37
(1,134)	1:59:A:VAL:HB	1:103:A:VAL:HG21	7	0.37
(1,134)	1:59:A:VAL:HB	1:103:A:VAL:HG22	7	0.37
(1,134)	1:59:A:VAL:HB	1:103:A:VAL:HG23	7	0.37
(6,1)	2:148:B:SER:H1	2:149:B:PRO:HA	2	0.36
(6,1)	2:148:B:SER:H1	2:149:B:PRO:HA	20	0.36
(1,1509)	1:139:A:VAL:HG11	1:143:A:GLU:H	8	0.36
(1,1509)	1:139:A:VAL:HG12	1:143:A:GLU:H	8	0.36
(1,1509)	1:139:A:VAL:HG13	1:143:A:GLU:H	8	0.36
(1,1509)	1:139:A:VAL:HG21	1:143:A:GLU:H	8	0.36
(1,1509)	1:139:A:VAL:HG22	1:143:A:GLU:H	8	0.36
(1,1509)	1:139:A:VAL:HG23	1:143:A:GLU:H	8	0.36
(1,1288)	1:63:A:MET:H	1:77:A:LEU:HD11	6	0.36
(1,1288)	1:63:A:MET:H	1:77:A:LEU:HD12	6	0.36
(1,1288)	1:63:A:MET:H	1:77:A:LEU:HD13	6	0.36
(1,1288)	1:63:A:MET:H	1:77:A:LEU:HD21	6	0.36
(1,1288)	1:63:A:MET:H	1:77:A:LEU:HD22	6	0.36
(1,1288)	1:63:A:MET:H	1:77:A:LEU:HD23	6	0.36
(1,1285)	1:62:A:TRP:HE1	1:77:A:LEU:HD11	2	0.36
(1,1285)	1:62:A:TRP:HE1	1:77:A:LEU:HD12	2	0.36
(1,1285)	1:62:A:TRP:HE1	1:77:A:LEU:HD13	2	0.36
(1,1285)	1:62:A:TRP:HE1	1:77:A:LEU:HD21	2	0.36
(1,1285)	1:62:A:TRP:HE1	1:77:A:LEU:HD22	2	0.36
(1,1285)	1:62:A:TRP:HE1	1:77:A:LEU:HD23	2	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1229)	1:45:A:SER:HB2	1:80:A:LEU:HD11	1	0.36
(1,1229)	1:45:A:SER:HB2	1:80:A:LEU:HD12	1	0.36
(1,1229)	1:45:A:SER:HB2	1:80:A:LEU:HD13	1	0.36
(1,1229)	1:45:A:SER:HB2	1:80:A:LEU:HD21	1	0.36
(1,1229)	1:45:A:SER:HB2	1:80:A:LEU:HD22	1	0.36
(1,1229)	1:45:A:SER:HB2	1:80:A:LEU:HD23	1	0.36
(1,1229)	1:45:A:SER:HB3	1:80:A:LEU:HD11	1	0.36
(1,1229)	1:45:A:SER:HB3	1:80:A:LEU:HD12	1	0.36
(1,1229)	1:45:A:SER:HB3	1:80:A:LEU:HD13	1	0.36
(1,1229)	1:45:A:SER:HB3	1:80:A:LEU:HD21	1	0.36
(1,1229)	1:45:A:SER:HB3	1:80:A:LEU:HD22	1	0.36
(1,1229)	1:45:A:SER:HB3	1:80:A:LEU:HD23	1	0.36
(1,478)	1:77:A:LEU:HD21	1:78:A:PHE:HA	9	0.36
(1,478)	1:77:A:LEU:HD22	1:78:A:PHE:HA	9	0.36
(1,478)	1:77:A:LEU:HD23	1:78:A:PHE:HA	9	0.36
(1,279)	1:77:A:LEU:HD21	1:107:A:ALA:HB1	7	0.36
(1,279)	1:77:A:LEU:HD21	1:107:A:ALA:HB2	7	0.36
(1,279)	1:77:A:LEU:HD21	1:107:A:ALA:HB3	7	0.36
(1,279)	1:77:A:LEU:HD22	1:107:A:ALA:HB1	7	0.36
(1,279)	1:77:A:LEU:HD22	1:107:A:ALA:HB2	7	0.36
(1,279)	1:77:A:LEU:HD22	1:107:A:ALA:HB3	7	0.36
(1,279)	1:77:A:LEU:HD23	1:107:A:ALA:HB1	7	0.36
(1,279)	1:77:A:LEU:HD23	1:107:A:ALA:HB2	7	0.36
(1,279)	1:77:A:LEU:HD23	1:107:A:ALA:HB3	7	0.36
(1,273)	1:75:A:LEU:HA	1:75:A:LEU:HD21	13	0.36
(1,273)	1:75:A:LEU:HA	1:75:A:LEU:HD22	13	0.36
(1,273)	1:75:A:LEU:HA	1:75:A:LEU:HD23	13	0.36
(1,20)	1:132:A:VAL:HG21	1:138:A:ILE:HD11	13	0.36
(1,20)	1:132:A:VAL:HG21	1:138:A:ILE:HD12	13	0.36
(1,20)	1:132:A:VAL:HG21	1:138:A:ILE:HD13	13	0.36
(1,20)	1:132:A:VAL:HG22	1:138:A:ILE:HD11	13	0.36
(1,20)	1:132:A:VAL:HG22	1:138:A:ILE:HD12	13	0.36
(1,20)	1:132:A:VAL:HG22	1:138:A:ILE:HD13	13	0.36
(1,20)	1:132:A:VAL:HG23	1:138:A:ILE:HD11	13	0.36
(1,20)	1:132:A:VAL:HG23	1:138:A:ILE:HD12	13	0.36
(1,20)	1:132:A:VAL:HG23	1:138:A:ILE:HD13	13	0.36
(1,1290)	1:63:A:MET:HB2	1:77:A:LEU:HD11	15	0.35
(1,1290)	1:63:A:MET:HB2	1:77:A:LEU:HD12	15	0.35
(1,1290)	1:63:A:MET:HB2	1:77:A:LEU:HD13	15	0.35
(1,1290)	1:63:A:MET:HB2	1:77:A:LEU:HD21	15	0.35
(1,1290)	1:63:A:MET:HB2	1:77:A:LEU:HD22	15	0.35
(1,1290)	1:63:A:MET:HB2	1:77:A:LEU:HD23	15	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1290)	1:63:A:MET:HB3	1:77:A:LEU:HD11	15	0.35
(1,1290)	1:63:A:MET:HB3	1:77:A:LEU:HD12	15	0.35
(1,1290)	1:63:A:MET:HB3	1:77:A:LEU:HD13	15	0.35
(1,1290)	1:63:A:MET:HB3	1:77:A:LEU:HD21	15	0.35
(1,1290)	1:63:A:MET:HB3	1:77:A:LEU:HD22	15	0.35
(1,1290)	1:63:A:MET:HB3	1:77:A:LEU:HD23	15	0.35
(1,1281)	1:59:A:VAL:HG11	1:104:A:LEU:H	16	0.35
(1,1281)	1:59:A:VAL:HG12	1:104:A:LEU:H	16	0.35
(1,1281)	1:59:A:VAL:HG13	1:104:A:LEU:H	16	0.35
(1,1281)	1:59:A:VAL:HG21	1:104:A:LEU:H	16	0.35
(1,1281)	1:59:A:VAL:HG22	1:104:A:LEU:H	16	0.35
(1,1281)	1:59:A:VAL:HG23	1:104:A:LEU:H	16	0.35
(1,1273)	1:59:A:VAL:HG11	1:100:A:PHE:HD1	5	0.35
(1,1273)	1:59:A:VAL:HG11	1:100:A:PHE:HD2	5	0.35
(1,1273)	1:59:A:VAL:HG12	1:100:A:PHE:HD1	5	0.35
(1,1273)	1:59:A:VAL:HG12	1:100:A:PHE:HD2	5	0.35
(1,1273)	1:59:A:VAL:HG13	1:100:A:PHE:HD1	5	0.35
(1,1273)	1:59:A:VAL:HG13	1:100:A:PHE:HD2	5	0.35
(1,1273)	1:59:A:VAL:HG21	1:100:A:PHE:HD1	5	0.35
(1,1273)	1:59:A:VAL:HG21	1:100:A:PHE:HD2	5	0.35
(1,1273)	1:59:A:VAL:HG22	1:100:A:PHE:HD1	5	0.35
(1,1273)	1:59:A:VAL:HG22	1:100:A:PHE:HD2	5	0.35
(1,1273)	1:59:A:VAL:HG23	1:100:A:PHE:HD1	5	0.35
(1,1273)	1:59:A:VAL:HG23	1:100:A:PHE:HD2	5	0.35
(1,648)	1:75:A:LEU:HD11	1:120:A:VAL:H	4	0.35
(1,648)	1:75:A:LEU:HD12	1:120:A:VAL:H	4	0.35
(1,648)	1:75:A:LEU:HD13	1:120:A:VAL:H	4	0.35
(1,574)	1:108:A:ALA:H	1:111:A:VAL:HG11	14	0.35
(1,574)	1:108:A:ALA:H	1:111:A:VAL:HG12	14	0.35
(1,574)	1:108:A:ALA:H	1:111:A:VAL:HG13	14	0.35
(1,478)	1:77:A:LEU:HD21	1:78:A:PHE:HA	11	0.35
(1,478)	1:77:A:LEU:HD22	1:78:A:PHE:HA	11	0.35
(1,478)	1:77:A:LEU:HD23	1:78:A:PHE:HA	11	0.35
(1,296)	1:34:A:VAL:HG11	1:36:A:ASN:H	5	0.35
(1,296)	1:34:A:VAL:HG12	1:36:A:ASN:H	5	0.35
(1,296)	1:34:A:VAL:HG13	1:36:A:ASN:H	5	0.35
(1,53)	1:58:A:ILE:HG21	1:59:A:VAL:HG21	3	0.35
(1,53)	1:58:A:ILE:HG21	1:59:A:VAL:HG22	3	0.35
(1,53)	1:58:A:ILE:HG21	1:59:A:VAL:HG23	3	0.35
(1,53)	1:58:A:ILE:HG22	1:59:A:VAL:HG21	3	0.35
(1,53)	1:58:A:ILE:HG22	1:59:A:VAL:HG22	3	0.35
(1,53)	1:58:A:ILE:HG22	1:59:A:VAL:HG23	3	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,53)	1:58:A:ILE:HG23	1:59:A:VAL:HG21	3	0.35
(1,53)	1:58:A:ILE:HG23	1:59:A:VAL:HG22	3	0.35
(1,53)	1:58:A:ILE:HG23	1:59:A:VAL:HG23	3	0.35
(6,2)	2:148:B:SER:H1	2:149:B:PRO:HG2	15	0.34
(6,2)	2:148:B:SER:H1	2:149:B:PRO:HG3	15	0.34
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD11	15	0.34
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD12	15	0.34
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD13	15	0.34
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD21	15	0.34
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD22	15	0.34
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD23	15	0.34
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD11	15	0.34
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD12	15	0.34
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD13	15	0.34
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD21	15	0.34
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD22	15	0.34
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD23	15	0.34
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD11	17	0.34
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD12	17	0.34
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD13	17	0.34
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD21	17	0.34
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD22	17	0.34
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD23	17	0.34
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD11	17	0.34
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD12	17	0.34
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD13	17	0.34
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD21	17	0.34
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD22	17	0.34
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD23	17	0.34
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD11	20	0.34
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD12	20	0.34
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD13	20	0.34
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD21	20	0.34
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD22	20	0.34
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD23	20	0.34
(1,847)	1:49:A:ILE:H	1:84:A:VAL:HG11	12	0.34
(1,847)	1:49:A:ILE:H	1:84:A:VAL:HG12	12	0.34
(1,847)	1:49:A:ILE:H	1:84:A:VAL:HG13	12	0.34
(1,648)	1:75:A:LEU:HD11	1:120:A:VAL:H	12	0.34
(1,648)	1:75:A:LEU:HD12	1:120:A:VAL:H	12	0.34
(1,648)	1:75:A:LEU:HD13	1:120:A:VAL:H	12	0.34
(1,442)	1:75:A:LEU:HD11	1:78:A:PHE:HB3	1	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,442)	1:75:A:LEU:HD12	1:78:A:PHE:HB3	1	0.34
(1,442)	1:75:A:LEU:HD13	1:78:A:PHE:HB3	1	0.34
(1,442)	1:75:A:LEU:HD11	1:78:A:PHE:HB3	12	0.34
(1,442)	1:75:A:LEU:HD12	1:78:A:PHE:HB3	12	0.34
(1,442)	1:75:A:LEU:HD13	1:78:A:PHE:HB3	12	0.34
(1,293)	1:31:A:PHE:HA	1:34:A:VAL:HG11	14	0.34
(1,293)	1:31:A:PHE:HA	1:34:A:VAL:HG12	14	0.34
(1,293)	1:31:A:PHE:HA	1:34:A:VAL:HG13	14	0.34
(1,273)	1:75:A:LEU:HA	1:75:A:LEU:HD21	14	0.34
(1,273)	1:75:A:LEU:HA	1:75:A:LEU:HD22	14	0.34
(1,273)	1:75:A:LEU:HA	1:75:A:LEU:HD23	14	0.34
(1,83)	1:137:A:MET:HB3	1:138:A:ILE:HD11	7	0.34
(1,83)	1:137:A:MET:HB3	1:138:A:ILE:HD12	7	0.34
(1,83)	1:137:A:MET:HB3	1:138:A:ILE:HD13	7	0.34
(1,69)	1:34:A:VAL:HG11	1:41:A:ILE:HD11	14	0.34
(1,69)	1:34:A:VAL:HG11	1:41:A:ILE:HD12	14	0.34
(1,69)	1:34:A:VAL:HG11	1:41:A:ILE:HD13	14	0.34
(1,69)	1:34:A:VAL:HG12	1:41:A:ILE:HD11	14	0.34
(1,69)	1:34:A:VAL:HG12	1:41:A:ILE:HD12	14	0.34
(1,69)	1:34:A:VAL:HG12	1:41:A:ILE:HD13	14	0.34
(1,69)	1:34:A:VAL:HG13	1:41:A:ILE:HD11	14	0.34
(1,69)	1:34:A:VAL:HG13	1:41:A:ILE:HD12	14	0.34
(1,69)	1:34:A:VAL:HG13	1:41:A:ILE:HD13	14	0.34
(1,1500)	1:137:A:MET:HB2	1:141:A:LEU:HD11	8	0.33
(1,1500)	1:137:A:MET:HB2	1:141:A:LEU:HD12	8	0.33
(1,1500)	1:137:A:MET:HB2	1:141:A:LEU:HD13	8	0.33
(1,1500)	1:137:A:MET:HB2	1:141:A:LEU:HD21	8	0.33
(1,1500)	1:137:A:MET:HB2	1:141:A:LEU:HD22	8	0.33
(1,1500)	1:137:A:MET:HB2	1:141:A:LEU:HD23	8	0.33
(1,1288)	1:63:A:MET:H	1:77:A:LEU:HD11	19	0.33
(1,1288)	1:63:A:MET:H	1:77:A:LEU:HD12	19	0.33
(1,1288)	1:63:A:MET:H	1:77:A:LEU:HD13	19	0.33
(1,1288)	1:63:A:MET:H	1:77:A:LEU:HD21	19	0.33
(1,1288)	1:63:A:MET:H	1:77:A:LEU:HD22	19	0.33
(1,1288)	1:63:A:MET:H	1:77:A:LEU:HD23	19	0.33
(1,1280)	1:59:A:VAL:HG11	1:103:A:VAL:HG21	3	0.33
(1,1280)	1:59:A:VAL:HG11	1:103:A:VAL:HG22	3	0.33
(1,1280)	1:59:A:VAL:HG11	1:103:A:VAL:HG23	3	0.33
(1,1280)	1:59:A:VAL:HG12	1:103:A:VAL:HG21	3	0.33
(1,1280)	1:59:A:VAL:HG12	1:103:A:VAL:HG22	3	0.33
(1,1280)	1:59:A:VAL:HG12	1:103:A:VAL:HG23	3	0.33
(1,1280)	1:59:A:VAL:HG13	1:103:A:VAL:HG21	3	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1280)	1:59:A:VAL:HG13	1:103:A:VAL:HG22	3	0.33
(1,1280)	1:59:A:VAL:HG13	1:103:A:VAL:HG23	3	0.33
(1,1280)	1:59:A:VAL:HG21	1:103:A:VAL:HG21	3	0.33
(1,1280)	1:59:A:VAL:HG21	1:103:A:VAL:HG22	3	0.33
(1,1280)	1:59:A:VAL:HG21	1:103:A:VAL:HG23	3	0.33
(1,1280)	1:59:A:VAL:HG22	1:103:A:VAL:HG21	3	0.33
(1,1280)	1:59:A:VAL:HG22	1:103:A:VAL:HG22	3	0.33
(1,1280)	1:59:A:VAL:HG22	1:103:A:VAL:HG23	3	0.33
(1,1280)	1:59:A:VAL:HG23	1:103:A:VAL:HG21	3	0.33
(1,1280)	1:59:A:VAL:HG23	1:103:A:VAL:HG22	3	0.33
(1,1280)	1:59:A:VAL:HG23	1:103:A:VAL:HG23	3	0.33
(1,1276)	1:59:A:VAL:HG11	1:103:A:VAL:H	15	0.33
(1,1276)	1:59:A:VAL:HG12	1:103:A:VAL:H	15	0.33
(1,1276)	1:59:A:VAL:HG13	1:103:A:VAL:H	15	0.33
(1,1276)	1:59:A:VAL:HG21	1:103:A:VAL:H	15	0.33
(1,1276)	1:59:A:VAL:HG22	1:103:A:VAL:H	15	0.33
(1,1276)	1:59:A:VAL:HG23	1:103:A:VAL:H	15	0.33
(1,1203)	1:23:A:LEU:HD11	1:27:A:LEU:HB2	15	0.33
(1,1203)	1:23:A:LEU:HD11	1:27:A:LEU:HB3	15	0.33
(1,1203)	1:23:A:LEU:HD12	1:27:A:LEU:HB2	15	0.33
(1,1203)	1:23:A:LEU:HD12	1:27:A:LEU:HB3	15	0.33
(1,1203)	1:23:A:LEU:HD13	1:27:A:LEU:HB2	15	0.33
(1,1203)	1:23:A:LEU:HD13	1:27:A:LEU:HB3	15	0.33
(1,1203)	1:23:A:LEU:HD21	1:27:A:LEU:HB2	15	0.33
(1,1203)	1:23:A:LEU:HD21	1:27:A:LEU:HB3	15	0.33
(1,1203)	1:23:A:LEU:HD22	1:27:A:LEU:HB2	15	0.33
(1,1203)	1:23:A:LEU:HD22	1:27:A:LEU:HB3	15	0.33
(1,1203)	1:23:A:LEU:HD23	1:27:A:LEU:HB2	15	0.33
(1,1203)	1:23:A:LEU:HD23	1:27:A:LEU:HB3	15	0.33
(1,313)	1:34:A:VAL:HG21	1:35:A:THR:HG21	9	0.33
(1,313)	1:34:A:VAL:HG21	1:35:A:THR:HG22	9	0.33
(1,313)	1:34:A:VAL:HG21	1:35:A:THR:HG23	9	0.33
(1,313)	1:34:A:VAL:HG22	1:35:A:THR:HG21	9	0.33
(1,313)	1:34:A:VAL:HG22	1:35:A:THR:HG22	9	0.33
(1,313)	1:34:A:VAL:HG22	1:35:A:THR:HG23	9	0.33
(1,313)	1:34:A:VAL:HG23	1:35:A:THR:HG21	9	0.33
(1,313)	1:34:A:VAL:HG23	1:35:A:THR:HG22	9	0.33
(1,313)	1:34:A:VAL:HG23	1:35:A:THR:HG23	9	0.33
(1,313)	1:34:A:VAL:HG21	1:35:A:THR:HG21	11	0.33
(1,313)	1:34:A:VAL:HG21	1:35:A:THR:HG22	11	0.33
(1,313)	1:34:A:VAL:HG21	1:35:A:THR:HG23	11	0.33
(1,313)	1:34:A:VAL:HG22	1:35:A:THR:HG21	11	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,313)	1:34:A:VAL:HG22	1:35:A:THR:HG22	11	0.33
(1,313)	1:34:A:VAL:HG22	1:35:A:THR:HG23	11	0.33
(1,313)	1:34:A:VAL:HG23	1:35:A:THR:HG21	11	0.33
(1,313)	1:34:A:VAL:HG23	1:35:A:THR:HG22	11	0.33
(1,313)	1:34:A:VAL:HG23	1:35:A:THR:HG23	11	0.33
(1,308)	1:103:A:VAL:HG21	1:107:A:ALA:HA	11	0.33
(1,308)	1:103:A:VAL:HG22	1:107:A:ALA:HA	11	0.33
(1,308)	1:103:A:VAL:HG23	1:107:A:ALA:HA	11	0.33
(1,294)	1:34:A:VAL:H	1:34:A:VAL:HG11	19	0.33
(1,294)	1:34:A:VAL:H	1:34:A:VAL:HG12	19	0.33
(1,294)	1:34:A:VAL:H	1:34:A:VAL:HG13	19	0.33
(1,279)	1:77:A:LEU:HD21	1:107:A:ALA:HB1	16	0.33
(1,279)	1:77:A:LEU:HD21	1:107:A:ALA:HB2	16	0.33
(1,279)	1:77:A:LEU:HD21	1:107:A:ALA:HB3	16	0.33
(1,279)	1:77:A:LEU:HD22	1:107:A:ALA:HB1	16	0.33
(1,279)	1:77:A:LEU:HD22	1:107:A:ALA:HB2	16	0.33
(1,279)	1:77:A:LEU:HD22	1:107:A:ALA:HB3	16	0.33
(1,279)	1:77:A:LEU:HD23	1:107:A:ALA:HB1	16	0.33
(1,279)	1:77:A:LEU:HD23	1:107:A:ALA:HB2	16	0.33
(1,279)	1:77:A:LEU:HD23	1:107:A:ALA:HB3	16	0.33
(1,134)	1:59:A:VAL:HB	1:103:A:VAL:HG21	19	0.33
(1,134)	1:59:A:VAL:HB	1:103:A:VAL:HG22	19	0.33
(1,134)	1:59:A:VAL:HB	1:103:A:VAL:HG23	19	0.33
(1,83)	1:137:A:MET:HB3	1:138:A:ILE:HD11	20	0.33
(1,83)	1:137:A:MET:HB3	1:138:A:ILE:HD12	20	0.33
(1,83)	1:137:A:MET:HB3	1:138:A:ILE:HD13	20	0.33
(6,2)	2:148:B:SER:H1	2:149:B:PRO:HG2	17	0.32
(6,2)	2:148:B:SER:H1	2:149:B:PRO:HG3	17	0.32
(6,2)	2:148:B:SER:H1	2:149:B:PRO:HG2	20	0.32
(6,2)	2:148:B:SER:H1	2:149:B:PRO:HG3	20	0.32
(2,2)	2:149:B:PRO:HB2	1:38:A:MET:HE3	4	0.32
(1,1403)	1:104:A:LEU:HD11	1:141:A:LEU:HG	8	0.32
(1,1403)	1:104:A:LEU:HD12	1:141:A:LEU:HG	8	0.32
(1,1403)	1:104:A:LEU:HD13	1:141:A:LEU:HG	8	0.32
(1,1403)	1:104:A:LEU:HD21	1:141:A:LEU:HG	8	0.32
(1,1403)	1:104:A:LEU:HD22	1:141:A:LEU:HG	8	0.32
(1,1403)	1:104:A:LEU:HD23	1:141:A:LEU:HG	8	0.32
(1,1320)	1:75:A:LEU:HD11	1:111:A:VAL:HG11	18	0.32
(1,1320)	1:75:A:LEU:HD11	1:111:A:VAL:HG12	18	0.32
(1,1320)	1:75:A:LEU:HD11	1:111:A:VAL:HG13	18	0.32
(1,1320)	1:75:A:LEU:HD12	1:111:A:VAL:HG11	18	0.32
(1,1320)	1:75:A:LEU:HD12	1:111:A:VAL:HG12	18	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1320)	1:75:A:LEU:HD12	1:111:A:VAL:HG13	18	0.32
(1,1320)	1:75:A:LEU:HD13	1:111:A:VAL:HG11	18	0.32
(1,1320)	1:75:A:LEU:HD13	1:111:A:VAL:HG12	18	0.32
(1,1320)	1:75:A:LEU:HD13	1:111:A:VAL:HG13	18	0.32
(1,1320)	1:75:A:LEU:HD21	1:111:A:VAL:HG11	18	0.32
(1,1320)	1:75:A:LEU:HD21	1:111:A:VAL:HG12	18	0.32
(1,1320)	1:75:A:LEU:HD21	1:111:A:VAL:HG13	18	0.32
(1,1320)	1:75:A:LEU:HD22	1:111:A:VAL:HG11	18	0.32
(1,1320)	1:75:A:LEU:HD22	1:111:A:VAL:HG12	18	0.32
(1,1320)	1:75:A:LEU:HD22	1:111:A:VAL:HG13	18	0.32
(1,1320)	1:75:A:LEU:HD23	1:111:A:VAL:HG11	18	0.32
(1,1320)	1:75:A:LEU:HD23	1:111:A:VAL:HG12	18	0.32
(1,1320)	1:75:A:LEU:HD23	1:111:A:VAL:HG13	18	0.32
(1,1288)	1:63:A:MET:H	1:77:A:LEU:HD11	8	0.32
(1,1288)	1:63:A:MET:H	1:77:A:LEU:HD12	8	0.32
(1,1288)	1:63:A:MET:H	1:77:A:LEU:HD13	8	0.32
(1,1288)	1:63:A:MET:H	1:77:A:LEU:HD21	8	0.32
(1,1288)	1:63:A:MET:H	1:77:A:LEU:HD22	8	0.32
(1,1288)	1:63:A:MET:H	1:77:A:LEU:HD23	8	0.32
(1,1238)	1:48:A:CYS:HB2	1:84:A:VAL:HG21	8	0.32
(1,1238)	1:48:A:CYS:HB2	1:84:A:VAL:HG22	8	0.32
(1,1238)	1:48:A:CYS:HB2	1:84:A:VAL:HG23	8	0.32
(1,1238)	1:48:A:CYS:HB3	1:84:A:VAL:HG21	8	0.32
(1,1238)	1:48:A:CYS:HB3	1:84:A:VAL:HG22	8	0.32
(1,1238)	1:48:A:CYS:HB3	1:84:A:VAL:HG23	8	0.32
(1,289)	1:101:A:ALA:HB1	1:137:A:MET:HB3	4	0.32
(1,289)	1:101:A:ALA:HB2	1:137:A:MET:HB3	4	0.32
(1,289)	1:101:A:ALA:HB3	1:137:A:MET:HB3	4	0.32
(1,279)	1:77:A:LEU:HD21	1:107:A:ALA:HB1	14	0.32
(1,279)	1:77:A:LEU:HD21	1:107:A:ALA:HB2	14	0.32
(1,279)	1:77:A:LEU:HD21	1:107:A:ALA:HB3	14	0.32
(1,279)	1:77:A:LEU:HD22	1:107:A:ALA:HB1	14	0.32
(1,279)	1:77:A:LEU:HD22	1:107:A:ALA:HB2	14	0.32
(1,279)	1:77:A:LEU:HD22	1:107:A:ALA:HB3	14	0.32
(1,279)	1:77:A:LEU:HD23	1:107:A:ALA:HB1	14	0.32
(1,279)	1:77:A:LEU:HD23	1:107:A:ALA:HB2	14	0.32
(1,279)	1:77:A:LEU:HD23	1:107:A:ALA:HB3	14	0.32
(1,154)	1:139:A:VAL:HG11	1:143:A:GLU:HG2	18	0.32
(1,154)	1:139:A:VAL:HG11	1:143:A:GLU:HG3	18	0.32
(1,154)	1:139:A:VAL:HG12	1:143:A:GLU:HG2	18	0.32
(1,154)	1:139:A:VAL:HG12	1:143:A:GLU:HG3	18	0.32
(1,154)	1:139:A:VAL:HG13	1:143:A:GLU:HG2	18	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,154)	1:139:A:VAL:HG13	1:143:A:GLU:HG3	18	0.32
(1,1238)	1:48:A:CYS:HB2	1:84:A:VAL:HG21	9	0.31
(1,1238)	1:48:A:CYS:HB2	1:84:A:VAL:HG22	9	0.31
(1,1238)	1:48:A:CYS:HB2	1:84:A:VAL:HG23	9	0.31
(1,1238)	1:48:A:CYS:HB3	1:84:A:VAL:HG21	9	0.31
(1,1238)	1:48:A:CYS:HB3	1:84:A:VAL:HG22	9	0.31
(1,1238)	1:48:A:CYS:HB3	1:84:A:VAL:HG23	9	0.31
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD11	17	0.31
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD12	17	0.31
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD13	17	0.31
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD21	17	0.31
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD22	17	0.31
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD23	17	0.31
(1,1189)	1:62:A:TRP:HE1	1:77:A:LEU:HD21	19	0.31
(1,1189)	1:62:A:TRP:HE1	1:77:A:LEU:HD22	19	0.31
(1,1189)	1:62:A:TRP:HE1	1:77:A:LEU:HD23	19	0.31
(1,952)	1:104:A:LEU:HD21	1:106:A:GLU:H	20	0.31
(1,952)	1:104:A:LEU:HD22	1:106:A:GLU:H	20	0.31
(1,952)	1:104:A:LEU:HD23	1:106:A:GLU:H	20	0.31
(1,939)	1:103:A:VAL:HG21	1:104:A:LEU:H	3	0.31
(1,939)	1:103:A:VAL:HG22	1:104:A:LEU:H	3	0.31
(1,939)	1:103:A:VAL:HG23	1:104:A:LEU:H	3	0.31
(1,438)	1:58:A:ILE:HG21	1:59:A:VAL:HG11	4	0.31
(1,438)	1:58:A:ILE:HG21	1:59:A:VAL:HG12	4	0.31
(1,438)	1:58:A:ILE:HG21	1:59:A:VAL:HG13	4	0.31
(1,438)	1:58:A:ILE:HG22	1:59:A:VAL:HG11	4	0.31
(1,438)	1:58:A:ILE:HG22	1:59:A:VAL:HG12	4	0.31
(1,438)	1:58:A:ILE:HG22	1:59:A:VAL:HG13	4	0.31
(1,438)	1:58:A:ILE:HG23	1:59:A:VAL:HG11	4	0.31
(1,438)	1:58:A:ILE:HG23	1:59:A:VAL:HG12	4	0.31
(1,438)	1:58:A:ILE:HG23	1:59:A:VAL:HG13	4	0.31
(1,308)	1:103:A:VAL:HG21	1:107:A:ALA:HA	15	0.31
(1,308)	1:103:A:VAL:HG22	1:107:A:ALA:HA	15	0.31
(1,308)	1:103:A:VAL:HG23	1:107:A:ALA:HA	15	0.31
(1,204)	1:59:A:VAL:HA	1:103:A:VAL:HG11	11	0.31
(1,204)	1:59:A:VAL:HA	1:103:A:VAL:HG12	11	0.31
(1,204)	1:59:A:VAL:HA	1:103:A:VAL:HG13	11	0.31
(1,134)	1:59:A:VAL:HB	1:103:A:VAL:HG21	15	0.31
(1,134)	1:59:A:VAL:HB	1:103:A:VAL:HG22	15	0.31
(1,134)	1:59:A:VAL:HB	1:103:A:VAL:HG23	15	0.31
(6,2)	2:148:B:SER:H1	2:149:B:PRO:HG2	10	0.3
(6,2)	2:148:B:SER:H1	2:149:B:PRO:HG3	10	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1511)	1:140:A:ALA:H	1:141:A:LEU:HD11	20	0.3
(1,1511)	1:140:A:ALA:H	1:141:A:LEU:HD12	20	0.3
(1,1511)	1:140:A:ALA:H	1:141:A:LEU:HD13	20	0.3
(1,1511)	1:140:A:ALA:H	1:141:A:LEU:HD21	20	0.3
(1,1511)	1:140:A:ALA:H	1:141:A:LEU:HD22	20	0.3
(1,1511)	1:140:A:ALA:H	1:141:A:LEU:HD23	20	0.3
(1,1340)	1:78:A:PHE:HE1	1:104:A:LEU:HD11	4	0.3
(1,1340)	1:78:A:PHE:HE1	1:104:A:LEU:HD12	4	0.3
(1,1340)	1:78:A:PHE:HE1	1:104:A:LEU:HD13	4	0.3
(1,1340)	1:78:A:PHE:HE1	1:104:A:LEU:HD21	4	0.3
(1,1340)	1:78:A:PHE:HE1	1:104:A:LEU:HD22	4	0.3
(1,1340)	1:78:A:PHE:HE1	1:104:A:LEU:HD23	4	0.3
(1,1340)	1:78:A:PHE:HE2	1:104:A:LEU:HD11	4	0.3
(1,1340)	1:78:A:PHE:HE2	1:104:A:LEU:HD12	4	0.3
(1,1340)	1:78:A:PHE:HE2	1:104:A:LEU:HD13	4	0.3
(1,1340)	1:78:A:PHE:HE2	1:104:A:LEU:HD21	4	0.3
(1,1340)	1:78:A:PHE:HE2	1:104:A:LEU:HD22	4	0.3
(1,1340)	1:78:A:PHE:HE2	1:104:A:LEU:HD23	4	0.3
(1,1295)	1:66:A:LEU:H	1:66:A:LEU:HD11	18	0.3
(1,1295)	1:66:A:LEU:H	1:66:A:LEU:HD12	18	0.3
(1,1295)	1:66:A:LEU:H	1:66:A:LEU:HD13	18	0.3
(1,1295)	1:66:A:LEU:H	1:66:A:LEU:HD21	18	0.3
(1,1295)	1:66:A:LEU:H	1:66:A:LEU:HD22	18	0.3
(1,1295)	1:66:A:LEU:H	1:66:A:LEU:HD23	18	0.3
(1,1288)	1:63:A:MET:H	1:77:A:LEU:HD11	17	0.3
(1,1288)	1:63:A:MET:H	1:77:A:LEU:HD12	17	0.3
(1,1288)	1:63:A:MET:H	1:77:A:LEU:HD13	17	0.3
(1,1288)	1:63:A:MET:H	1:77:A:LEU:HD21	17	0.3
(1,1288)	1:63:A:MET:H	1:77:A:LEU:HD22	17	0.3
(1,1288)	1:63:A:MET:H	1:77:A:LEU:HD23	17	0.3
(1,1285)	1:62:A:TRP:HE1	1:77:A:LEU:HD11	6	0.3
(1,1285)	1:62:A:TRP:HE1	1:77:A:LEU:HD12	6	0.3
(1,1285)	1:62:A:TRP:HE1	1:77:A:LEU:HD13	6	0.3
(1,1285)	1:62:A:TRP:HE1	1:77:A:LEU:HD21	6	0.3
(1,1285)	1:62:A:TRP:HE1	1:77:A:LEU:HD22	6	0.3
(1,1285)	1:62:A:TRP:HE1	1:77:A:LEU:HD23	6	0.3
(1,1275)	1:59:A:VAL:HG11	1:102:A:ASP:H	2	0.3
(1,1275)	1:59:A:VAL:HG12	1:102:A:ASP:H	2	0.3
(1,1275)	1:59:A:VAL:HG13	1:102:A:ASP:H	2	0.3
(1,1275)	1:59:A:VAL:HG21	1:102:A:ASP:H	2	0.3
(1,1275)	1:59:A:VAL:HG22	1:102:A:ASP:H	2	0.3
(1,1275)	1:59:A:VAL:HG23	1:102:A:ASP:H	2	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1262)	1:59:A:VAL:HG11	1:62:A:TRP:HE3	14	0.3
(1,1262)	1:59:A:VAL:HG12	1:62:A:TRP:HE3	14	0.3
(1,1262)	1:59:A:VAL:HG13	1:62:A:TRP:HE3	14	0.3
(1,1262)	1:59:A:VAL:HG21	1:62:A:TRP:HE3	14	0.3
(1,1262)	1:59:A:VAL:HG22	1:62:A:TRP:HE3	14	0.3
(1,1262)	1:59:A:VAL:HG23	1:62:A:TRP:HE3	14	0.3
(1,1229)	1:45:A:SER:HB2	1:80:A:LEU:HD11	3	0.3
(1,1229)	1:45:A:SER:HB2	1:80:A:LEU:HD12	3	0.3
(1,1229)	1:45:A:SER:HB2	1:80:A:LEU:HD13	3	0.3
(1,1229)	1:45:A:SER:HB2	1:80:A:LEU:HD21	3	0.3
(1,1229)	1:45:A:SER:HB2	1:80:A:LEU:HD22	3	0.3
(1,1229)	1:45:A:SER:HB2	1:80:A:LEU:HD23	3	0.3
(1,1229)	1:45:A:SER:HB3	1:80:A:LEU:HD11	3	0.3
(1,1229)	1:45:A:SER:HB3	1:80:A:LEU:HD12	3	0.3
(1,1229)	1:45:A:SER:HB3	1:80:A:LEU:HD13	3	0.3
(1,1229)	1:45:A:SER:HB3	1:80:A:LEU:HD21	3	0.3
(1,1229)	1:45:A:SER:HB3	1:80:A:LEU:HD22	3	0.3
(1,1229)	1:45:A:SER:HB3	1:80:A:LEU:HD23	3	0.3
(1,1229)	1:45:A:SER:HB2	1:80:A:LEU:HD11	20	0.3
(1,1229)	1:45:A:SER:HB2	1:80:A:LEU:HD12	20	0.3
(1,1229)	1:45:A:SER:HB2	1:80:A:LEU:HD13	20	0.3
(1,1229)	1:45:A:SER:HB2	1:80:A:LEU:HD21	20	0.3
(1,1229)	1:45:A:SER:HB2	1:80:A:LEU:HD22	20	0.3
(1,1229)	1:45:A:SER:HB2	1:80:A:LEU:HD23	20	0.3
(1,1229)	1:45:A:SER:HB3	1:80:A:LEU:HD11	20	0.3
(1,1229)	1:45:A:SER:HB3	1:80:A:LEU:HD12	20	0.3
(1,1229)	1:45:A:SER:HB3	1:80:A:LEU:HD13	20	0.3
(1,1229)	1:45:A:SER:HB3	1:80:A:LEU:HD21	20	0.3
(1,1229)	1:45:A:SER:HB3	1:80:A:LEU:HD22	20	0.3
(1,1229)	1:45:A:SER:HB3	1:80:A:LEU:HD23	20	0.3
(1,1169)	1:34:A:VAL:HG21	1:35:A:THR:H	7	0.3
(1,1169)	1:34:A:VAL:HG22	1:35:A:THR:H	7	0.3
(1,1169)	1:34:A:VAL:HG23	1:35:A:THR:H	7	0.3
(1,1169)	1:34:A:VAL:HG21	1:35:A:THR:H	15	0.3
(1,1169)	1:34:A:VAL:HG22	1:35:A:THR:H	15	0.3
(1,1169)	1:34:A:VAL:HG23	1:35:A:THR:H	15	0.3
(1,376)	1:103:A:VAL:H	1:103:A:VAL:HG11	3	0.3
(1,376)	1:103:A:VAL:H	1:103:A:VAL:HG12	3	0.3
(1,376)	1:103:A:VAL:H	1:103:A:VAL:HG13	3	0.3
(1,369)	1:63:A:MET:HG3	1:103:A:VAL:HG11	9	0.3
(1,369)	1:63:A:MET:HG3	1:103:A:VAL:HG12	9	0.3
(1,369)	1:63:A:MET:HG3	1:103:A:VAL:HG13	9	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,308)	1:103:A:VAL:HG21	1:107:A:ALA:HA	19	0.3
(1,308)	1:103:A:VAL:HG22	1:107:A:ALA:HA	19	0.3
(1,308)	1:103:A:VAL:HG23	1:107:A:ALA:HA	19	0.3
(1,134)	1:59:A:VAL:HB	1:103:A:VAL:HG21	11	0.3
(1,134)	1:59:A:VAL:HB	1:103:A:VAL:HG22	11	0.3
(1,134)	1:59:A:VAL:HB	1:103:A:VAL:HG23	11	0.3
(1,53)	1:58:A:ILE:HG21	1:59:A:VAL:HG21	5	0.3
(1,53)	1:58:A:ILE:HG21	1:59:A:VAL:HG22	5	0.3
(1,53)	1:58:A:ILE:HG21	1:59:A:VAL:HG23	5	0.3
(1,53)	1:58:A:ILE:HG22	1:59:A:VAL:HG21	5	0.3
(1,53)	1:58:A:ILE:HG22	1:59:A:VAL:HG22	5	0.3
(1,53)	1:58:A:ILE:HG22	1:59:A:VAL:HG23	5	0.3
(1,53)	1:58:A:ILE:HG23	1:59:A:VAL:HG21	5	0.3
(1,53)	1:58:A:ILE:HG23	1:59:A:VAL:HG22	5	0.3
(1,53)	1:58:A:ILE:HG23	1:59:A:VAL:HG23	5	0.3
(6,1)	2:148:B:SER:H1	2:149:B:PRO:HA	3	0.29
(1,1494)	1:135:A:GLU:HA	1:139:A:VAL:HG11	14	0.29
(1,1494)	1:135:A:GLU:HA	1:139:A:VAL:HG12	14	0.29
(1,1494)	1:135:A:GLU:HA	1:139:A:VAL:HG13	14	0.29
(1,1494)	1:135:A:GLU:HA	1:139:A:VAL:HG21	14	0.29
(1,1494)	1:135:A:GLU:HA	1:139:A:VAL:HG22	14	0.29
(1,1494)	1:135:A:GLU:HA	1:139:A:VAL:HG23	14	0.29
(1,1490)	1:132:A:VAL:HG11	1:138:A:ILE:HD11	13	0.29
(1,1490)	1:132:A:VAL:HG11	1:138:A:ILE:HD12	13	0.29
(1,1490)	1:132:A:VAL:HG11	1:138:A:ILE:HD13	13	0.29
(1,1490)	1:132:A:VAL:HG12	1:138:A:ILE:HD11	13	0.29
(1,1490)	1:132:A:VAL:HG12	1:138:A:ILE:HD12	13	0.29
(1,1490)	1:132:A:VAL:HG12	1:138:A:ILE:HD13	13	0.29
(1,1490)	1:132:A:VAL:HG13	1:138:A:ILE:HD11	13	0.29
(1,1490)	1:132:A:VAL:HG13	1:138:A:ILE:HD12	13	0.29
(1,1490)	1:132:A:VAL:HG13	1:138:A:ILE:HD13	13	0.29
(1,1490)	1:132:A:VAL:HG21	1:138:A:ILE:HD11	13	0.29
(1,1490)	1:132:A:VAL:HG21	1:138:A:ILE:HD12	13	0.29
(1,1490)	1:132:A:VAL:HG21	1:138:A:ILE:HD13	13	0.29
(1,1490)	1:132:A:VAL:HG22	1:138:A:ILE:HD11	13	0.29
(1,1490)	1:132:A:VAL:HG22	1:138:A:ILE:HD12	13	0.29
(1,1490)	1:132:A:VAL:HG22	1:138:A:ILE:HD13	13	0.29
(1,1490)	1:132:A:VAL:HG23	1:138:A:ILE:HD11	13	0.29
(1,1490)	1:132:A:VAL:HG23	1:138:A:ILE:HD12	13	0.29
(1,1490)	1:132:A:VAL:HG23	1:138:A:ILE:HD13	13	0.29
(1,1432)	1:113:A:ASP:H	1:145:A:LEU:HD11	19	0.29
(1,1432)	1:113:A:ASP:H	1:145:A:LEU:HD12	19	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1432)	1:113:A:ASP:H	1:145:A:LEU:HD13	19	0.29
(1,1432)	1:113:A:ASP:H	1:145:A:LEU:HD21	19	0.29
(1,1432)	1:113:A:ASP:H	1:145:A:LEU:HD22	19	0.29
(1,1432)	1:113:A:ASP:H	1:145:A:LEU:HD23	19	0.29
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD11	2	0.29
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD12	2	0.29
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD13	2	0.29
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD21	2	0.29
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD22	2	0.29
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD23	2	0.29
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD11	2	0.29
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD12	2	0.29
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD13	2	0.29
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD21	2	0.29
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD22	2	0.29
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD23	2	0.29
(1,1285)	1:62:A:TRP:HE1	1:77:A:LEU:HD11	1	0.29
(1,1285)	1:62:A:TRP:HE1	1:77:A:LEU:HD12	1	0.29
(1,1285)	1:62:A:TRP:HE1	1:77:A:LEU:HD13	1	0.29
(1,1285)	1:62:A:TRP:HE1	1:77:A:LEU:HD21	1	0.29
(1,1285)	1:62:A:TRP:HE1	1:77:A:LEU:HD22	1	0.29
(1,1285)	1:62:A:TRP:HE1	1:77:A:LEU:HD23	1	0.29
(1,1275)	1:59:A:VAL:HG11	1:102:A:ASP:H	7	0.29
(1,1275)	1:59:A:VAL:HG12	1:102:A:ASP:H	7	0.29
(1,1275)	1:59:A:VAL:HG13	1:102:A:ASP:H	7	0.29
(1,1275)	1:59:A:VAL:HG21	1:102:A:ASP:H	7	0.29
(1,1275)	1:59:A:VAL:HG22	1:102:A:ASP:H	7	0.29
(1,1275)	1:59:A:VAL:HG23	1:102:A:ASP:H	7	0.29
(1,1275)	1:59:A:VAL:HG11	1:102:A:ASP:H	15	0.29
(1,1275)	1:59:A:VAL:HG12	1:102:A:ASP:H	15	0.29
(1,1275)	1:59:A:VAL:HG13	1:102:A:ASP:H	15	0.29
(1,1275)	1:59:A:VAL:HG21	1:102:A:ASP:H	15	0.29
(1,1275)	1:59:A:VAL:HG22	1:102:A:ASP:H	15	0.29
(1,1275)	1:59:A:VAL:HG23	1:102:A:ASP:H	15	0.29
(1,1203)	1:23:A:LEU:HD11	1:27:A:LEU:HB2	14	0.29
(1,1203)	1:23:A:LEU:HD11	1:27:A:LEU:HB3	14	0.29
(1,1203)	1:23:A:LEU:HD12	1:27:A:LEU:HB2	14	0.29
(1,1203)	1:23:A:LEU:HD12	1:27:A:LEU:HB3	14	0.29
(1,1203)	1:23:A:LEU:HD13	1:27:A:LEU:HB2	14	0.29
(1,1203)	1:23:A:LEU:HD13	1:27:A:LEU:HB3	14	0.29
(1,1203)	1:23:A:LEU:HD21	1:27:A:LEU:HB2	14	0.29
(1,1203)	1:23:A:LEU:HD21	1:27:A:LEU:HB3	14	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1203)	1:23:A:LEU:HD22	1:27:A:LEU:HB2	14	0.29
(1,1203)	1:23:A:LEU:HD22	1:27:A:LEU:HB3	14	0.29
(1,1203)	1:23:A:LEU:HD23	1:27:A:LEU:HB2	14	0.29
(1,1203)	1:23:A:LEU:HD23	1:27:A:LEU:HB3	14	0.29
(1,952)	1:104:A:LEU:HD21	1:106:A:GLU:H	5	0.29
(1,952)	1:104:A:LEU:HD22	1:106:A:GLU:H	5	0.29
(1,952)	1:104:A:LEU:HD23	1:106:A:GLU:H	5	0.29
(1,308)	1:103:A:VAL:HG21	1:107:A:ALA:HA	5	0.29
(1,308)	1:103:A:VAL:HG22	1:107:A:ALA:HA	5	0.29
(1,308)	1:103:A:VAL:HG23	1:107:A:ALA:HA	5	0.29
(1,259)	1:111:A:VAL:HG21	1:124:A:PHE:HB2	5	0.29
(1,259)	1:111:A:VAL:HG21	1:124:A:PHE:HB3	5	0.29
(1,259)	1:111:A:VAL:HG22	1:124:A:PHE:HB2	5	0.29
(1,259)	1:111:A:VAL:HG22	1:124:A:PHE:HB3	5	0.29
(1,259)	1:111:A:VAL:HG23	1:124:A:PHE:HB2	5	0.29
(1,259)	1:111:A:VAL:HG23	1:124:A:PHE:HB3	5	0.29
(1,64)	1:78:A:PHE:HD1	1:120:A:VAL:HG11	20	0.29
(1,64)	1:78:A:PHE:HD1	1:120:A:VAL:HG12	20	0.29
(1,64)	1:78:A:PHE:HD1	1:120:A:VAL:HG13	20	0.29
(1,64)	1:78:A:PHE:HD2	1:120:A:VAL:HG11	20	0.29
(1,64)	1:78:A:PHE:HD2	1:120:A:VAL:HG12	20	0.29
(1,64)	1:78:A:PHE:HD2	1:120:A:VAL:HG13	20	0.29
(4,1)	2:151:B:TYR:HH	1:82:A:ASN:ND2	12	0.28
(1,1450)	1:116:A:VAL:HG11	1:120:A:VAL:HG11	4	0.28
(1,1450)	1:116:A:VAL:HG11	1:120:A:VAL:HG12	4	0.28
(1,1450)	1:116:A:VAL:HG11	1:120:A:VAL:HG13	4	0.28
(1,1450)	1:116:A:VAL:HG11	1:120:A:VAL:HG21	4	0.28
(1,1450)	1:116:A:VAL:HG11	1:120:A:VAL:HG22	4	0.28
(1,1450)	1:116:A:VAL:HG11	1:120:A:VAL:HG23	4	0.28
(1,1450)	1:116:A:VAL:HG12	1:120:A:VAL:HG11	4	0.28
(1,1450)	1:116:A:VAL:HG12	1:120:A:VAL:HG12	4	0.28
(1,1450)	1:116:A:VAL:HG12	1:120:A:VAL:HG13	4	0.28
(1,1450)	1:116:A:VAL:HG12	1:120:A:VAL:HG21	4	0.28
(1,1450)	1:116:A:VAL:HG12	1:120:A:VAL:HG22	4	0.28
(1,1450)	1:116:A:VAL:HG12	1:120:A:VAL:HG23	4	0.28
(1,1450)	1:116:A:VAL:HG13	1:120:A:VAL:HG11	4	0.28
(1,1450)	1:116:A:VAL:HG13	1:120:A:VAL:HG12	4	0.28
(1,1450)	1:116:A:VAL:HG13	1:120:A:VAL:HG13	4	0.28
(1,1450)	1:116:A:VAL:HG13	1:120:A:VAL:HG21	4	0.28
(1,1450)	1:116:A:VAL:HG13	1:120:A:VAL:HG22	4	0.28
(1,1450)	1:116:A:VAL:HG13	1:120:A:VAL:HG23	4	0.28
(1,1450)	1:116:A:VAL:HG21	1:120:A:VAL:HG11	4	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1450)	1:116:A:VAL:HG21	1:120:A:VAL:HG12	4	0.28
(1,1450)	1:116:A:VAL:HG21	1:120:A:VAL:HG13	4	0.28
(1,1450)	1:116:A:VAL:HG21	1:120:A:VAL:HG21	4	0.28
(1,1450)	1:116:A:VAL:HG21	1:120:A:VAL:HG22	4	0.28
(1,1450)	1:116:A:VAL:HG21	1:120:A:VAL:HG23	4	0.28
(1,1450)	1:116:A:VAL:HG22	1:120:A:VAL:HG11	4	0.28
(1,1450)	1:116:A:VAL:HG22	1:120:A:VAL:HG12	4	0.28
(1,1450)	1:116:A:VAL:HG22	1:120:A:VAL:HG13	4	0.28
(1,1450)	1:116:A:VAL:HG22	1:120:A:VAL:HG21	4	0.28
(1,1450)	1:116:A:VAL:HG22	1:120:A:VAL:HG22	4	0.28
(1,1450)	1:116:A:VAL:HG22	1:120:A:VAL:HG23	4	0.28
(1,1450)	1:116:A:VAL:HG23	1:120:A:VAL:HG11	4	0.28
(1,1450)	1:116:A:VAL:HG23	1:120:A:VAL:HG12	4	0.28
(1,1450)	1:116:A:VAL:HG23	1:120:A:VAL:HG13	4	0.28
(1,1450)	1:116:A:VAL:HG23	1:120:A:VAL:HG21	4	0.28
(1,1450)	1:116:A:VAL:HG23	1:120:A:VAL:HG22	4	0.28
(1,1450)	1:116:A:VAL:HG23	1:120:A:VAL:HG23	4	0.28
(1,1444)	1:116:A:VAL:HB	1:120:A:VAL:HG11	20	0.28
(1,1444)	1:116:A:VAL:HB	1:120:A:VAL:HG12	20	0.28
(1,1444)	1:116:A:VAL:HB	1:120:A:VAL:HG13	20	0.28
(1,1444)	1:116:A:VAL:HB	1:120:A:VAL:HG21	20	0.28
(1,1444)	1:116:A:VAL:HB	1:120:A:VAL:HG22	20	0.28
(1,1444)	1:116:A:VAL:HB	1:120:A:VAL:HG23	20	0.28
(1,1347)	1:84:A:VAL:HG11	1:85:A:ILE:HG12	18	0.28
(1,1347)	1:84:A:VAL:HG11	1:85:A:ILE:HG13	18	0.28
(1,1347)	1:84:A:VAL:HG12	1:85:A:ILE:HG12	18	0.28
(1,1347)	1:84:A:VAL:HG12	1:85:A:ILE:HG13	18	0.28
(1,1347)	1:84:A:VAL:HG13	1:85:A:ILE:HG12	18	0.28
(1,1347)	1:84:A:VAL:HG13	1:85:A:ILE:HG13	18	0.28
(1,1340)	1:78:A:PHE:HE1	1:104:A:LEU:HD11	2	0.28
(1,1340)	1:78:A:PHE:HE1	1:104:A:LEU:HD12	2	0.28
(1,1340)	1:78:A:PHE:HE1	1:104:A:LEU:HD13	2	0.28
(1,1340)	1:78:A:PHE:HE1	1:104:A:LEU:HD21	2	0.28
(1,1340)	1:78:A:PHE:HE1	1:104:A:LEU:HD22	2	0.28
(1,1340)	1:78:A:PHE:HE1	1:104:A:LEU:HD23	2	0.28
(1,1340)	1:78:A:PHE:HE2	1:104:A:LEU:HD11	2	0.28
(1,1340)	1:78:A:PHE:HE2	1:104:A:LEU:HD12	2	0.28
(1,1340)	1:78:A:PHE:HE2	1:104:A:LEU:HD13	2	0.28
(1,1340)	1:78:A:PHE:HE2	1:104:A:LEU:HD21	2	0.28
(1,1340)	1:78:A:PHE:HE2	1:104:A:LEU:HD22	2	0.28
(1,1340)	1:78:A:PHE:HE2	1:104:A:LEU:HD23	2	0.28
(1,1276)	1:59:A:VAL:HG11	1:103:A:VAL:H	18	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1276)	1:59:A:VAL:HG12	1:103:A:VAL:H	18	0.28
(1,1276)	1:59:A:VAL:HG13	1:103:A:VAL:H	18	0.28
(1,1276)	1:59:A:VAL:HG21	1:103:A:VAL:H	18	0.28
(1,1276)	1:59:A:VAL:HG22	1:103:A:VAL:H	18	0.28
(1,1276)	1:59:A:VAL:HG23	1:103:A:VAL:H	18	0.28
(1,1085)	1:141:A:LEU:HG	1:142:A:ARG:H	10	0.28
(1,857)	1:111:A:VAL:HG11	1:112:A:LYS:H	10	0.28
(1,857)	1:111:A:VAL:HG12	1:112:A:LYS:H	10	0.28
(1,857)	1:111:A:VAL:HG13	1:112:A:LYS:H	10	0.28
(1,857)	1:111:A:VAL:HG11	1:112:A:LYS:H	15	0.28
(1,857)	1:111:A:VAL:HG12	1:112:A:LYS:H	15	0.28
(1,857)	1:111:A:VAL:HG13	1:112:A:LYS:H	15	0.28
(1,563)	1:66:A:LEU:HB2	1:69:A:SER:H	7	0.28
(1,563)	1:66:A:LEU:HB3	1:69:A:SER:H	7	0.28
(1,442)	1:75:A:LEU:HD11	1:78:A:PHE:HB3	7	0.28
(1,442)	1:75:A:LEU:HD12	1:78:A:PHE:HB3	7	0.28
(1,442)	1:75:A:LEU:HD13	1:78:A:PHE:HB3	7	0.28
(1,308)	1:103:A:VAL:HG21	1:107:A:ALA:HA	1	0.28
(1,308)	1:103:A:VAL:HG22	1:107:A:ALA:HA	1	0.28
(1,308)	1:103:A:VAL:HG23	1:107:A:ALA:HA	1	0.28
(1,279)	1:77:A:LEU:HD21	1:107:A:ALA:HB1	8	0.28
(1,279)	1:77:A:LEU:HD21	1:107:A:ALA:HB2	8	0.28
(1,279)	1:77:A:LEU:HD21	1:107:A:ALA:HB3	8	0.28
(1,279)	1:77:A:LEU:HD22	1:107:A:ALA:HB1	8	0.28
(1,279)	1:77:A:LEU:HD22	1:107:A:ALA:HB2	8	0.28
(1,279)	1:77:A:LEU:HD22	1:107:A:ALA:HB3	8	0.28
(1,279)	1:77:A:LEU:HD23	1:107:A:ALA:HB1	8	0.28
(1,279)	1:77:A:LEU:HD23	1:107:A:ALA:HB2	8	0.28
(1,279)	1:77:A:LEU:HD23	1:107:A:ALA:HB3	8	0.28
(1,262)	1:59:A:VAL:HG11	1:62:A:TRP:HE3	14	0.28
(1,262)	1:59:A:VAL:HG12	1:62:A:TRP:HE3	14	0.28
(1,262)	1:59:A:VAL:HG13	1:62:A:TRP:HE3	14	0.28
(1,259)	1:111:A:VAL:HG21	1:124:A:PHE:HB2	1	0.28
(1,259)	1:111:A:VAL:HG21	1:124:A:PHE:HB3	1	0.28
(1,259)	1:111:A:VAL:HG22	1:124:A:PHE:HB2	1	0.28
(1,259)	1:111:A:VAL:HG22	1:124:A:PHE:HB3	1	0.28
(1,259)	1:111:A:VAL:HG23	1:124:A:PHE:HB2	1	0.28
(1,259)	1:111:A:VAL:HG23	1:124:A:PHE:HB3	1	0.28
(1,259)	1:111:A:VAL:HG21	1:124:A:PHE:HB2	14	0.28
(1,259)	1:111:A:VAL:HG21	1:124:A:PHE:HB3	14	0.28
(1,259)	1:111:A:VAL:HG22	1:124:A:PHE:HB2	14	0.28
(1,259)	1:111:A:VAL:HG22	1:124:A:PHE:HB3	14	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,259)	1:111:A:VAL:HG23	1:124:A:PHE:HB2	14	0.28
(1,259)	1:111:A:VAL:HG23	1:124:A:PHE:HB3	14	0.28
(1,83)	1:137:A:MET:HB3	1:138:A:ILE:HD11	10	0.28
(1,83)	1:137:A:MET:HB3	1:138:A:ILE:HD12	10	0.28
(1,83)	1:137:A:MET:HB3	1:138:A:ILE:HD13	10	0.28
(1,61)	1:59:A:VAL:HG21	1:62:A:TRP:HE3	14	0.28
(1,61)	1:59:A:VAL:HG22	1:62:A:TRP:HE3	14	0.28
(1,61)	1:59:A:VAL:HG23	1:62:A:TRP:HE3	14	0.28
(1,1494)	1:135:A:GLU:HA	1:139:A:VAL:HG11	15	0.27
(1,1494)	1:135:A:GLU:HA	1:139:A:VAL:HG12	15	0.27
(1,1494)	1:135:A:GLU:HA	1:139:A:VAL:HG13	15	0.27
(1,1494)	1:135:A:GLU:HA	1:139:A:VAL:HG21	15	0.27
(1,1494)	1:135:A:GLU:HA	1:139:A:VAL:HG22	15	0.27
(1,1494)	1:135:A:GLU:HA	1:139:A:VAL:HG23	15	0.27
(1,1402)	1:104:A:LEU:HD11	1:141:A:LEU:HB2	10	0.27
(1,1402)	1:104:A:LEU:HD11	1:141:A:LEU:HB3	10	0.27
(1,1402)	1:104:A:LEU:HD12	1:141:A:LEU:HB2	10	0.27
(1,1402)	1:104:A:LEU:HD12	1:141:A:LEU:HB3	10	0.27
(1,1402)	1:104:A:LEU:HD13	1:141:A:LEU:HB2	10	0.27
(1,1402)	1:104:A:LEU:HD13	1:141:A:LEU:HB3	10	0.27
(1,1402)	1:104:A:LEU:HD21	1:141:A:LEU:HB2	10	0.27
(1,1402)	1:104:A:LEU:HD21	1:141:A:LEU:HB3	10	0.27
(1,1402)	1:104:A:LEU:HD22	1:141:A:LEU:HB2	10	0.27
(1,1402)	1:104:A:LEU:HD22	1:141:A:LEU:HB3	10	0.27
(1,1402)	1:104:A:LEU:HD23	1:141:A:LEU:HB2	10	0.27
(1,1402)	1:104:A:LEU:HD23	1:141:A:LEU:HB3	10	0.27
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD11	1	0.27
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD12	1	0.27
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD13	1	0.27
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD21	1	0.27
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD22	1	0.27
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD23	1	0.27
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD11	1	0.27
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD12	1	0.27
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD13	1	0.27
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD21	1	0.27
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD22	1	0.27
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD23	1	0.27
(1,1285)	1:62:A:TRP:HE1	1:77:A:LEU:HD11	19	0.27
(1,1285)	1:62:A:TRP:HE1	1:77:A:LEU:HD12	19	0.27
(1,1285)	1:62:A:TRP:HE1	1:77:A:LEU:HD13	19	0.27
(1,1285)	1:62:A:TRP:HE1	1:77:A:LEU:HD21	19	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1285)	1:62:A:TRP:HE1	1:77:A:LEU:HD22	19	0.27
(1,1285)	1:62:A:TRP:HE1	1:77:A:LEU:HD23	19	0.27
(1,1238)	1:48:A:CYS:HB2	1:84:A:VAL:HG21	17	0.27
(1,1238)	1:48:A:CYS:HB2	1:84:A:VAL:HG22	17	0.27
(1,1238)	1:48:A:CYS:HB2	1:84:A:VAL:HG23	17	0.27
(1,1238)	1:48:A:CYS:HB3	1:84:A:VAL:HG21	17	0.27
(1,1238)	1:48:A:CYS:HB3	1:84:A:VAL:HG22	17	0.27
(1,1238)	1:48:A:CYS:HB3	1:84:A:VAL:HG23	17	0.27
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD11	13	0.27
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD12	13	0.27
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD13	13	0.27
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD21	13	0.27
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD22	13	0.27
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD23	13	0.27
(1,1189)	1:62:A:TRP:HE1	1:77:A:LEU:HD21	18	0.27
(1,1189)	1:62:A:TRP:HE1	1:77:A:LEU:HD22	18	0.27
(1,1189)	1:62:A:TRP:HE1	1:77:A:LEU:HD23	18	0.27
(1,1085)	1:141:A:LEU:HG	1:142:A:ARG:H	16	0.27
(1,857)	1:111:A:VAL:HG11	1:112:A:LYS:H	4	0.27
(1,857)	1:111:A:VAL:HG12	1:112:A:LYS:H	4	0.27
(1,857)	1:111:A:VAL:HG13	1:112:A:LYS:H	4	0.27
(1,857)	1:111:A:VAL:HG11	1:112:A:LYS:H	13	0.27
(1,857)	1:111:A:VAL:HG12	1:112:A:LYS:H	13	0.27
(1,857)	1:111:A:VAL:HG13	1:112:A:LYS:H	13	0.27
(1,857)	1:111:A:VAL:HG11	1:112:A:LYS:H	20	0.27
(1,857)	1:111:A:VAL:HG12	1:112:A:LYS:H	20	0.27
(1,857)	1:111:A:VAL:HG13	1:112:A:LYS:H	20	0.27
(1,478)	1:77:A:LEU:HD21	1:78:A:PHE:HA	14	0.27
(1,478)	1:77:A:LEU:HD22	1:78:A:PHE:HA	14	0.27
(1,478)	1:77:A:LEU:HD23	1:78:A:PHE:HA	14	0.27
(1,369)	1:63:A:MET:HG3	1:103:A:VAL:HG11	14	0.27
(1,369)	1:63:A:MET:HG3	1:103:A:VAL:HG12	14	0.27
(1,369)	1:63:A:MET:HG3	1:103:A:VAL:HG13	14	0.27
(1,1494)	1:135:A:GLU:HA	1:139:A:VAL:HG11	16	0.26
(1,1494)	1:135:A:GLU:HA	1:139:A:VAL:HG12	16	0.26
(1,1494)	1:135:A:GLU:HA	1:139:A:VAL:HG13	16	0.26
(1,1494)	1:135:A:GLU:HA	1:139:A:VAL:HG21	16	0.26
(1,1494)	1:135:A:GLU:HA	1:139:A:VAL:HG22	16	0.26
(1,1494)	1:135:A:GLU:HA	1:139:A:VAL:HG23	16	0.26
(1,1276)	1:59:A:VAL:HG11	1:103:A:VAL:H	9	0.26
(1,1276)	1:59:A:VAL:HG12	1:103:A:VAL:H	9	0.26
(1,1276)	1:59:A:VAL:HG13	1:103:A:VAL:H	9	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1276)	1:59:A:VAL:HG21	1:103:A:VAL:H	9	0.26
(1,1276)	1:59:A:VAL:HG22	1:103:A:VAL:H	9	0.26
(1,1276)	1:59:A:VAL:HG23	1:103:A:VAL:H	9	0.26
(1,1085)	1:141:A:LEU:HG	1:142:A:ARG:H	14	0.26
(1,963)	1:109:A:ALA:H	1:111:A:VAL:HG11	20	0.26
(1,963)	1:109:A:ALA:H	1:111:A:VAL:HG12	20	0.26
(1,963)	1:109:A:ALA:H	1:111:A:VAL:HG13	20	0.26
(1,952)	1:104:A:LEU:HD21	1:106:A:GLU:H	11	0.26
(1,952)	1:104:A:LEU:HD22	1:106:A:GLU:H	11	0.26
(1,952)	1:104:A:LEU:HD23	1:106:A:GLU:H	11	0.26
(1,722)	1:34:A:VAL:HG21	1:40:A:SER:H	18	0.26
(1,722)	1:34:A:VAL:HG22	1:40:A:SER:H	18	0.26
(1,722)	1:34:A:VAL:HG23	1:40:A:SER:H	18	0.26
(1,574)	1:108:A:ALA:H	1:111:A:VAL:HG11	4	0.26
(1,574)	1:108:A:ALA:H	1:111:A:VAL:HG12	4	0.26
(1,574)	1:108:A:ALA:H	1:111:A:VAL:HG13	4	0.26
(1,574)	1:108:A:ALA:H	1:111:A:VAL:HG11	6	0.26
(1,574)	1:108:A:ALA:H	1:111:A:VAL:HG12	6	0.26
(1,574)	1:108:A:ALA:H	1:111:A:VAL:HG13	6	0.26
(1,461)	1:101:A:ALA:HB1	1:137:A:MET:HB2	1	0.26
(1,461)	1:101:A:ALA:HB2	1:137:A:MET:HB2	1	0.26
(1,461)	1:101:A:ALA:HB3	1:137:A:MET:HB2	1	0.26
(1,371)	1:100:A:PHE:HA	1:103:A:VAL:HG11	18	0.26
(1,371)	1:100:A:PHE:HA	1:103:A:VAL:HG12	18	0.26
(1,371)	1:100:A:PHE:HA	1:103:A:VAL:HG13	18	0.26
(1,359)	1:75:A:LEU:HD11	1:119:A:SER:HA	19	0.26
(1,359)	1:75:A:LEU:HD12	1:119:A:SER:HA	19	0.26
(1,359)	1:75:A:LEU:HD13	1:119:A:SER:HA	19	0.26
(1,308)	1:103:A:VAL:HG21	1:107:A:ALA:HA	2	0.26
(1,308)	1:103:A:VAL:HG22	1:107:A:ALA:HA	2	0.26
(1,308)	1:103:A:VAL:HG23	1:107:A:ALA:HA	2	0.26
(1,308)	1:103:A:VAL:HG21	1:107:A:ALA:HA	6	0.26
(1,308)	1:103:A:VAL:HG22	1:107:A:ALA:HA	6	0.26
(1,308)	1:103:A:VAL:HG23	1:107:A:ALA:HA	6	0.26
(1,308)	1:103:A:VAL:HG21	1:107:A:ALA:HA	9	0.26
(1,308)	1:103:A:VAL:HG22	1:107:A:ALA:HA	9	0.26
(1,308)	1:103:A:VAL:HG23	1:107:A:ALA:HA	9	0.26
(1,308)	1:103:A:VAL:HG21	1:107:A:ALA:HA	16	0.26
(1,308)	1:103:A:VAL:HG22	1:107:A:ALA:HA	16	0.26
(1,308)	1:103:A:VAL:HG23	1:107:A:ALA:HA	16	0.26
(1,259)	1:111:A:VAL:HG21	1:124:A:PHE:HB2	15	0.26
(1,259)	1:111:A:VAL:HG21	1:124:A:PHE:HB3	15	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,259)	1:111:A:VAL:HG22	1:124:A:PHE:HB2	15	0.26
(1,259)	1:111:A:VAL:HG22	1:124:A:PHE:HB3	15	0.26
(1,259)	1:111:A:VAL:HG23	1:124:A:PHE:HB2	15	0.26
(1,259)	1:111:A:VAL:HG23	1:124:A:PHE:HB3	15	0.26
(1,19)	1:78:A:PHE:HD1	1:120:A:VAL:HG21	14	0.26
(1,19)	1:78:A:PHE:HD1	1:120:A:VAL:HG22	14	0.26
(1,19)	1:78:A:PHE:HD1	1:120:A:VAL:HG23	14	0.26
(1,19)	1:78:A:PHE:HD2	1:120:A:VAL:HG21	14	0.26
(1,19)	1:78:A:PHE:HD2	1:120:A:VAL:HG22	14	0.26
(1,19)	1:78:A:PHE:HD2	1:120:A:VAL:HG23	14	0.26
(1,1511)	1:140:A:ALA:H	1:141:A:LEU:HD11	19	0.25
(1,1511)	1:140:A:ALA:H	1:141:A:LEU:HD12	19	0.25
(1,1511)	1:140:A:ALA:H	1:141:A:LEU:HD13	19	0.25
(1,1511)	1:140:A:ALA:H	1:141:A:LEU:HD21	19	0.25
(1,1511)	1:140:A:ALA:H	1:141:A:LEU:HD22	19	0.25
(1,1511)	1:140:A:ALA:H	1:141:A:LEU:HD23	19	0.25
(1,1494)	1:135:A:GLU:HA	1:139:A:VAL:HG11	18	0.25
(1,1494)	1:135:A:GLU:HA	1:139:A:VAL:HG12	18	0.25
(1,1494)	1:135:A:GLU:HA	1:139:A:VAL:HG13	18	0.25
(1,1494)	1:135:A:GLU:HA	1:139:A:VAL:HG21	18	0.25
(1,1494)	1:135:A:GLU:HA	1:139:A:VAL:HG22	18	0.25
(1,1494)	1:135:A:GLU:HA	1:139:A:VAL:HG23	18	0.25
(1,1450)	1:116:A:VAL:HG11	1:120:A:VAL:HG11	7	0.25
(1,1450)	1:116:A:VAL:HG11	1:120:A:VAL:HG12	7	0.25
(1,1450)	1:116:A:VAL:HG11	1:120:A:VAL:HG13	7	0.25
(1,1450)	1:116:A:VAL:HG11	1:120:A:VAL:HG21	7	0.25
(1,1450)	1:116:A:VAL:HG11	1:120:A:VAL:HG22	7	0.25
(1,1450)	1:116:A:VAL:HG11	1:120:A:VAL:HG23	7	0.25
(1,1450)	1:116:A:VAL:HG12	1:120:A:VAL:HG11	7	0.25
(1,1450)	1:116:A:VAL:HG12	1:120:A:VAL:HG12	7	0.25
(1,1450)	1:116:A:VAL:HG12	1:120:A:VAL:HG13	7	0.25
(1,1450)	1:116:A:VAL:HG12	1:120:A:VAL:HG21	7	0.25
(1,1450)	1:116:A:VAL:HG12	1:120:A:VAL:HG22	7	0.25
(1,1450)	1:116:A:VAL:HG12	1:120:A:VAL:HG23	7	0.25
(1,1450)	1:116:A:VAL:HG13	1:120:A:VAL:HG11	7	0.25
(1,1450)	1:116:A:VAL:HG13	1:120:A:VAL:HG12	7	0.25
(1,1450)	1:116:A:VAL:HG13	1:120:A:VAL:HG13	7	0.25
(1,1450)	1:116:A:VAL:HG13	1:120:A:VAL:HG21	7	0.25
(1,1450)	1:116:A:VAL:HG13	1:120:A:VAL:HG22	7	0.25
(1,1450)	1:116:A:VAL:HG13	1:120:A:VAL:HG23	7	0.25
(1,1450)	1:116:A:VAL:HG21	1:120:A:VAL:HG11	7	0.25
(1,1450)	1:116:A:VAL:HG21	1:120:A:VAL:HG12	7	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1450)	1:116:A:VAL:HG21	1:120:A:VAL:HG13	7	0.25
(1,1450)	1:116:A:VAL:HG21	1:120:A:VAL:HG21	7	0.25
(1,1450)	1:116:A:VAL:HG21	1:120:A:VAL:HG22	7	0.25
(1,1450)	1:116:A:VAL:HG21	1:120:A:VAL:HG23	7	0.25
(1,1450)	1:116:A:VAL:HG22	1:120:A:VAL:HG11	7	0.25
(1,1450)	1:116:A:VAL:HG22	1:120:A:VAL:HG12	7	0.25
(1,1450)	1:116:A:VAL:HG22	1:120:A:VAL:HG13	7	0.25
(1,1450)	1:116:A:VAL:HG22	1:120:A:VAL:HG21	7	0.25
(1,1450)	1:116:A:VAL:HG22	1:120:A:VAL:HG22	7	0.25
(1,1450)	1:116:A:VAL:HG22	1:120:A:VAL:HG23	7	0.25
(1,1450)	1:116:A:VAL:HG23	1:120:A:VAL:HG11	7	0.25
(1,1450)	1:116:A:VAL:HG23	1:120:A:VAL:HG12	7	0.25
(1,1450)	1:116:A:VAL:HG23	1:120:A:VAL:HG13	7	0.25
(1,1450)	1:116:A:VAL:HG23	1:120:A:VAL:HG21	7	0.25
(1,1450)	1:116:A:VAL:HG23	1:120:A:VAL:HG22	7	0.25
(1,1450)	1:116:A:VAL:HG23	1:120:A:VAL:HG23	7	0.25
(1,1295)	1:66:A:LEU:H	1:66:A:LEU:HD11	7	0.25
(1,1295)	1:66:A:LEU:H	1:66:A:LEU:HD12	7	0.25
(1,1295)	1:66:A:LEU:H	1:66:A:LEU:HD13	7	0.25
(1,1295)	1:66:A:LEU:H	1:66:A:LEU:HD21	7	0.25
(1,1295)	1:66:A:LEU:H	1:66:A:LEU:HD22	7	0.25
(1,1295)	1:66:A:LEU:H	1:66:A:LEU:HD23	7	0.25
(1,1285)	1:62:A:TRP:HE1	1:77:A:LEU:HD11	3	0.25
(1,1285)	1:62:A:TRP:HE1	1:77:A:LEU:HD12	3	0.25
(1,1285)	1:62:A:TRP:HE1	1:77:A:LEU:HD13	3	0.25
(1,1285)	1:62:A:TRP:HE1	1:77:A:LEU:HD21	3	0.25
(1,1285)	1:62:A:TRP:HE1	1:77:A:LEU:HD22	3	0.25
(1,1285)	1:62:A:TRP:HE1	1:77:A:LEU:HD23	3	0.25
(1,1279)	1:59:A:VAL:HG11	1:103:A:VAL:HG11	18	0.25
(1,1279)	1:59:A:VAL:HG11	1:103:A:VAL:HG12	18	0.25
(1,1279)	1:59:A:VAL:HG11	1:103:A:VAL:HG13	18	0.25
(1,1279)	1:59:A:VAL:HG12	1:103:A:VAL:HG11	18	0.25
(1,1279)	1:59:A:VAL:HG12	1:103:A:VAL:HG12	18	0.25
(1,1279)	1:59:A:VAL:HG12	1:103:A:VAL:HG13	18	0.25
(1,1279)	1:59:A:VAL:HG13	1:103:A:VAL:HG11	18	0.25
(1,1279)	1:59:A:VAL:HG13	1:103:A:VAL:HG12	18	0.25
(1,1279)	1:59:A:VAL:HG13	1:103:A:VAL:HG13	18	0.25
(1,1279)	1:59:A:VAL:HG21	1:103:A:VAL:HG11	18	0.25
(1,1279)	1:59:A:VAL:HG21	1:103:A:VAL:HG12	18	0.25
(1,1279)	1:59:A:VAL:HG21	1:103:A:VAL:HG13	18	0.25
(1,1279)	1:59:A:VAL:HG22	1:103:A:VAL:HG11	18	0.25
(1,1279)	1:59:A:VAL:HG22	1:103:A:VAL:HG12	18	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1279)	1:59:A:VAL:HG22	1:103:A:VAL:HG13	18	0.25
(1,1279)	1:59:A:VAL:HG23	1:103:A:VAL:HG11	18	0.25
(1,1279)	1:59:A:VAL:HG23	1:103:A:VAL:HG12	18	0.25
(1,1279)	1:59:A:VAL:HG23	1:103:A:VAL:HG13	18	0.25
(1,1189)	1:62:A:TRP:HE1	1:77:A:LEU:HD21	1	0.25
(1,1189)	1:62:A:TRP:HE1	1:77:A:LEU:HD22	1	0.25
(1,1189)	1:62:A:TRP:HE1	1:77:A:LEU:HD23	1	0.25
(1,1085)	1:141:A:LEU:HG	1:142:A:ARG:H	3	0.25
(1,857)	1:111:A:VAL:HG11	1:112:A:LYS:H	11	0.25
(1,857)	1:111:A:VAL:HG12	1:112:A:LYS:H	11	0.25
(1,857)	1:111:A:VAL:HG13	1:112:A:LYS:H	11	0.25
(1,857)	1:111:A:VAL:HG11	1:112:A:LYS:H	14	0.25
(1,857)	1:111:A:VAL:HG12	1:112:A:LYS:H	14	0.25
(1,857)	1:111:A:VAL:HG13	1:112:A:LYS:H	14	0.25
(1,442)	1:75:A:LEU:HD11	1:78:A:PHE:HB3	9	0.25
(1,442)	1:75:A:LEU:HD12	1:78:A:PHE:HB3	9	0.25
(1,442)	1:75:A:LEU:HD13	1:78:A:PHE:HB3	9	0.25
(1,379)	1:139:A:VAL:HG21	1:143:A:GLU:HG2	6	0.25
(1,379)	1:139:A:VAL:HG21	1:143:A:GLU:HG3	6	0.25
(1,379)	1:139:A:VAL:HG22	1:143:A:GLU:HG2	6	0.25
(1,379)	1:139:A:VAL:HG22	1:143:A:GLU:HG3	6	0.25
(1,379)	1:139:A:VAL:HG23	1:143:A:GLU:HG2	6	0.25
(1,379)	1:139:A:VAL:HG23	1:143:A:GLU:HG3	6	0.25
(1,308)	1:103:A:VAL:HG21	1:107:A:ALA:HA	13	0.25
(1,308)	1:103:A:VAL:HG22	1:107:A:ALA:HA	13	0.25
(1,308)	1:103:A:VAL:HG23	1:107:A:ALA:HA	13	0.25
(1,259)	1:111:A:VAL:HG21	1:124:A:PHE:HB2	7	0.25
(1,259)	1:111:A:VAL:HG21	1:124:A:PHE:HB3	7	0.25
(1,259)	1:111:A:VAL:HG22	1:124:A:PHE:HB2	7	0.25
(1,259)	1:111:A:VAL:HG22	1:124:A:PHE:HB3	7	0.25
(1,259)	1:111:A:VAL:HG23	1:124:A:PHE:HB2	7	0.25
(1,259)	1:111:A:VAL:HG23	1:124:A:PHE:HB3	7	0.25
(1,134)	1:59:A:VAL:HB	1:103:A:VAL:HG21	18	0.25
(1,134)	1:59:A:VAL:HB	1:103:A:VAL:HG22	18	0.25
(1,134)	1:59:A:VAL:HB	1:103:A:VAL:HG23	18	0.25
(1,69)	1:34:A:VAL:HG11	1:41:A:ILE:HD11	6	0.25
(1,69)	1:34:A:VAL:HG11	1:41:A:ILE:HD12	6	0.25
(1,69)	1:34:A:VAL:HG11	1:41:A:ILE:HD13	6	0.25
(1,69)	1:34:A:VAL:HG12	1:41:A:ILE:HD11	6	0.25
(1,69)	1:34:A:VAL:HG12	1:41:A:ILE:HD12	6	0.25
(1,69)	1:34:A:VAL:HG12	1:41:A:ILE:HD13	6	0.25
(1,69)	1:34:A:VAL:HG13	1:41:A:ILE:HD11	6	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,69)	1:34:A:VAL:HG13	1:41:A:ILE:HD12	6	0.25
(1,69)	1:34:A:VAL:HG13	1:41:A:ILE:HD13	6	0.25
(1,53)	1:58:A:ILE:HG21	1:59:A:VAL:HG21	9	0.25
(1,53)	1:58:A:ILE:HG21	1:59:A:VAL:HG22	9	0.25
(1,53)	1:58:A:ILE:HG21	1:59:A:VAL:HG23	9	0.25
(1,53)	1:58:A:ILE:HG22	1:59:A:VAL:HG21	9	0.25
(1,53)	1:58:A:ILE:HG22	1:59:A:VAL:HG22	9	0.25
(1,53)	1:58:A:ILE:HG22	1:59:A:VAL:HG23	9	0.25
(1,53)	1:58:A:ILE:HG23	1:59:A:VAL:HG21	9	0.25
(1,53)	1:58:A:ILE:HG23	1:59:A:VAL:HG22	9	0.25
(1,53)	1:58:A:ILE:HG23	1:59:A:VAL:HG23	9	0.25
(1,53)	1:58:A:ILE:HG21	1:59:A:VAL:HG21	14	0.25
(1,53)	1:58:A:ILE:HG21	1:59:A:VAL:HG22	14	0.25
(1,53)	1:58:A:ILE:HG21	1:59:A:VAL:HG23	14	0.25
(1,53)	1:58:A:ILE:HG22	1:59:A:VAL:HG21	14	0.25
(1,53)	1:58:A:ILE:HG22	1:59:A:VAL:HG22	14	0.25
(1,53)	1:58:A:ILE:HG22	1:59:A:VAL:HG23	14	0.25
(1,53)	1:58:A:ILE:HG23	1:59:A:VAL:HG21	14	0.25
(1,53)	1:58:A:ILE:HG23	1:59:A:VAL:HG22	14	0.25
(1,53)	1:58:A:ILE:HG23	1:59:A:VAL:HG23	14	0.25
(6,3)	2:148:B:SER:H1	2:149:B:PRO:HB2	8	0.24
(6,3)	2:148:B:SER:H1	2:149:B:PRO:HB3	8	0.24
(1,1494)	1:135:A:GLU:HA	1:139:A:VAL:HG11	4	0.24
(1,1494)	1:135:A:GLU:HA	1:139:A:VAL:HG12	4	0.24
(1,1494)	1:135:A:GLU:HA	1:139:A:VAL:HG13	4	0.24
(1,1494)	1:135:A:GLU:HA	1:139:A:VAL:HG21	4	0.24
(1,1494)	1:135:A:GLU:HA	1:139:A:VAL:HG22	4	0.24
(1,1494)	1:135:A:GLU:HA	1:139:A:VAL:HG23	4	0.24
(1,1487)	1:132:A:VAL:HG11	1:133:A:TYR:H	12	0.24
(1,1487)	1:132:A:VAL:HG12	1:133:A:TYR:H	12	0.24
(1,1487)	1:132:A:VAL:HG13	1:133:A:TYR:H	12	0.24
(1,1487)	1:132:A:VAL:HG21	1:133:A:TYR:H	12	0.24
(1,1487)	1:132:A:VAL:HG22	1:133:A:TYR:H	12	0.24
(1,1487)	1:132:A:VAL:HG23	1:133:A:TYR:H	12	0.24
(1,1450)	1:116:A:VAL:HG11	1:120:A:VAL:HG11	11	0.24
(1,1450)	1:116:A:VAL:HG11	1:120:A:VAL:HG12	11	0.24
(1,1450)	1:116:A:VAL:HG11	1:120:A:VAL:HG13	11	0.24
(1,1450)	1:116:A:VAL:HG11	1:120:A:VAL:HG21	11	0.24
(1,1450)	1:116:A:VAL:HG11	1:120:A:VAL:HG22	11	0.24
(1,1450)	1:116:A:VAL:HG11	1:120:A:VAL:HG23	11	0.24
(1,1450)	1:116:A:VAL:HG12	1:120:A:VAL:HG11	11	0.24
(1,1450)	1:116:A:VAL:HG12	1:120:A:VAL:HG12	11	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1450)	1:116:A:VAL:HG12	1:120:A:VAL:HG13	11	0.24
(1,1450)	1:116:A:VAL:HG12	1:120:A:VAL:HG21	11	0.24
(1,1450)	1:116:A:VAL:HG12	1:120:A:VAL:HG22	11	0.24
(1,1450)	1:116:A:VAL:HG12	1:120:A:VAL:HG23	11	0.24
(1,1450)	1:116:A:VAL:HG13	1:120:A:VAL:HG11	11	0.24
(1,1450)	1:116:A:VAL:HG13	1:120:A:VAL:HG12	11	0.24
(1,1450)	1:116:A:VAL:HG13	1:120:A:VAL:HG13	11	0.24
(1,1450)	1:116:A:VAL:HG13	1:120:A:VAL:HG21	11	0.24
(1,1450)	1:116:A:VAL:HG13	1:120:A:VAL:HG22	11	0.24
(1,1450)	1:116:A:VAL:HG13	1:120:A:VAL:HG23	11	0.24
(1,1450)	1:116:A:VAL:HG21	1:120:A:VAL:HG11	11	0.24
(1,1450)	1:116:A:VAL:HG21	1:120:A:VAL:HG12	11	0.24
(1,1450)	1:116:A:VAL:HG21	1:120:A:VAL:HG13	11	0.24
(1,1450)	1:116:A:VAL:HG21	1:120:A:VAL:HG21	11	0.24
(1,1450)	1:116:A:VAL:HG21	1:120:A:VAL:HG22	11	0.24
(1,1450)	1:116:A:VAL:HG21	1:120:A:VAL:HG23	11	0.24
(1,1450)	1:116:A:VAL:HG22	1:120:A:VAL:HG11	11	0.24
(1,1450)	1:116:A:VAL:HG22	1:120:A:VAL:HG12	11	0.24
(1,1450)	1:116:A:VAL:HG22	1:120:A:VAL:HG13	11	0.24
(1,1450)	1:116:A:VAL:HG22	1:120:A:VAL:HG21	11	0.24
(1,1450)	1:116:A:VAL:HG22	1:120:A:VAL:HG22	11	0.24
(1,1450)	1:116:A:VAL:HG22	1:120:A:VAL:HG23	11	0.24
(1,1450)	1:116:A:VAL:HG23	1:120:A:VAL:HG11	11	0.24
(1,1450)	1:116:A:VAL:HG23	1:120:A:VAL:HG12	11	0.24
(1,1450)	1:116:A:VAL:HG23	1:120:A:VAL:HG13	11	0.24
(1,1450)	1:116:A:VAL:HG23	1:120:A:VAL:HG21	11	0.24
(1,1450)	1:116:A:VAL:HG23	1:120:A:VAL:HG22	11	0.24
(1,1450)	1:116:A:VAL:HG23	1:120:A:VAL:HG23	11	0.24
(1,1432)	1:113:A:ASP:H	1:145:A:LEU:HD11	5	0.24
(1,1432)	1:113:A:ASP:H	1:145:A:LEU:HD12	5	0.24
(1,1432)	1:113:A:ASP:H	1:145:A:LEU:HD13	5	0.24
(1,1432)	1:113:A:ASP:H	1:145:A:LEU:HD21	5	0.24
(1,1432)	1:113:A:ASP:H	1:145:A:LEU:HD22	5	0.24
(1,1432)	1:113:A:ASP:H	1:145:A:LEU:HD23	5	0.24
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD11	14	0.24
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD12	14	0.24
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD13	14	0.24
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD21	14	0.24
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD22	14	0.24
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD23	14	0.24
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD11	14	0.24
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD12	14	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD13	14	0.24
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD21	14	0.24
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD22	14	0.24
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD23	14	0.24
(1,1320)	1:75:A:LEU:HD11	1:111:A:VAL:HG11	6	0.24
(1,1320)	1:75:A:LEU:HD11	1:111:A:VAL:HG12	6	0.24
(1,1320)	1:75:A:LEU:HD11	1:111:A:VAL:HG13	6	0.24
(1,1320)	1:75:A:LEU:HD12	1:111:A:VAL:HG11	6	0.24
(1,1320)	1:75:A:LEU:HD12	1:111:A:VAL:HG12	6	0.24
(1,1320)	1:75:A:LEU:HD12	1:111:A:VAL:HG13	6	0.24
(1,1320)	1:75:A:LEU:HD13	1:111:A:VAL:HG11	6	0.24
(1,1320)	1:75:A:LEU:HD13	1:111:A:VAL:HG12	6	0.24
(1,1320)	1:75:A:LEU:HD13	1:111:A:VAL:HG13	6	0.24
(1,1320)	1:75:A:LEU:HD21	1:111:A:VAL:HG11	6	0.24
(1,1320)	1:75:A:LEU:HD21	1:111:A:VAL:HG12	6	0.24
(1,1320)	1:75:A:LEU:HD21	1:111:A:VAL:HG13	6	0.24
(1,1320)	1:75:A:LEU:HD22	1:111:A:VAL:HG11	6	0.24
(1,1320)	1:75:A:LEU:HD22	1:111:A:VAL:HG12	6	0.24
(1,1320)	1:75:A:LEU:HD22	1:111:A:VAL:HG13	6	0.24
(1,1320)	1:75:A:LEU:HD23	1:111:A:VAL:HG11	6	0.24
(1,1320)	1:75:A:LEU:HD23	1:111:A:VAL:HG12	6	0.24
(1,1320)	1:75:A:LEU:HD23	1:111:A:VAL:HG13	6	0.24
(1,1278)	1:59:A:VAL:HG11	1:103:A:VAL:HB	14	0.24
(1,1278)	1:59:A:VAL:HG12	1:103:A:VAL:HB	14	0.24
(1,1278)	1:59:A:VAL:HG13	1:103:A:VAL:HB	14	0.24
(1,1278)	1:59:A:VAL:HG21	1:103:A:VAL:HB	14	0.24
(1,1278)	1:59:A:VAL:HG22	1:103:A:VAL:HB	14	0.24
(1,1278)	1:59:A:VAL:HG23	1:103:A:VAL:HB	14	0.24
(1,857)	1:111:A:VAL:HG11	1:112:A:LYS:H	3	0.24
(1,857)	1:111:A:VAL:HG12	1:112:A:LYS:H	3	0.24
(1,857)	1:111:A:VAL:HG13	1:112:A:LYS:H	3	0.24
(1,857)	1:111:A:VAL:HG11	1:112:A:LYS:H	6	0.24
(1,857)	1:111:A:VAL:HG12	1:112:A:LYS:H	6	0.24
(1,857)	1:111:A:VAL:HG13	1:112:A:LYS:H	6	0.24
(1,722)	1:34:A:VAL:HG21	1:40:A:SER:H	12	0.24
(1,722)	1:34:A:VAL:HG22	1:40:A:SER:H	12	0.24
(1,722)	1:34:A:VAL:HG23	1:40:A:SER:H	12	0.24
(1,371)	1:100:A:PHE:HA	1:103:A:VAL:HG11	11	0.24
(1,371)	1:100:A:PHE:HA	1:103:A:VAL:HG12	11	0.24
(1,371)	1:100:A:PHE:HA	1:103:A:VAL:HG13	11	0.24
(1,308)	1:103:A:VAL:HG21	1:107:A:ALA:HA	4	0.24
(1,308)	1:103:A:VAL:HG22	1:107:A:ALA:HA	4	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,308)	1:103:A:VAL:HG23	1:107:A:ALA:HA	4	0.24
(1,308)	1:103:A:VAL:HG21	1:107:A:ALA:HA	12	0.24
(1,308)	1:103:A:VAL:HG22	1:107:A:ALA:HA	12	0.24
(1,308)	1:103:A:VAL:HG23	1:107:A:ALA:HA	12	0.24
(1,296)	1:34:A:VAL:HG11	1:36:A:ASN:H	13	0.24
(1,296)	1:34:A:VAL:HG12	1:36:A:ASN:H	13	0.24
(1,296)	1:34:A:VAL:HG13	1:36:A:ASN:H	13	0.24
(1,259)	1:111:A:VAL:HG21	1:124:A:PHE:HB2	2	0.24
(1,259)	1:111:A:VAL:HG21	1:124:A:PHE:HB3	2	0.24
(1,259)	1:111:A:VAL:HG22	1:124:A:PHE:HB2	2	0.24
(1,259)	1:111:A:VAL:HG22	1:124:A:PHE:HB3	2	0.24
(1,259)	1:111:A:VAL:HG23	1:124:A:PHE:HB2	2	0.24
(1,259)	1:111:A:VAL:HG23	1:124:A:PHE:HB3	2	0.24
(1,259)	1:111:A:VAL:HG21	1:124:A:PHE:HB2	3	0.24
(1,259)	1:111:A:VAL:HG21	1:124:A:PHE:HB3	3	0.24
(1,259)	1:111:A:VAL:HG22	1:124:A:PHE:HB2	3	0.24
(1,259)	1:111:A:VAL:HG22	1:124:A:PHE:HB3	3	0.24
(1,259)	1:111:A:VAL:HG23	1:124:A:PHE:HB2	3	0.24
(1,259)	1:111:A:VAL:HG23	1:124:A:PHE:HB3	3	0.24
(1,259)	1:111:A:VAL:HG21	1:124:A:PHE:HB2	6	0.24
(1,259)	1:111:A:VAL:HG21	1:124:A:PHE:HB3	6	0.24
(1,259)	1:111:A:VAL:HG22	1:124:A:PHE:HB2	6	0.24
(1,259)	1:111:A:VAL:HG22	1:124:A:PHE:HB3	6	0.24
(1,259)	1:111:A:VAL:HG23	1:124:A:PHE:HB2	6	0.24
(1,259)	1:111:A:VAL:HG23	1:124:A:PHE:HB3	6	0.24
(1,259)	1:111:A:VAL:HG21	1:124:A:PHE:HB2	18	0.24
(1,259)	1:111:A:VAL:HG21	1:124:A:PHE:HB3	18	0.24
(1,259)	1:111:A:VAL:HG22	1:124:A:PHE:HB2	18	0.24
(1,259)	1:111:A:VAL:HG22	1:124:A:PHE:HB3	18	0.24
(1,259)	1:111:A:VAL:HG23	1:124:A:PHE:HB2	18	0.24
(1,259)	1:111:A:VAL:HG23	1:124:A:PHE:HB3	18	0.24
(1,252)	1:111:A:VAL:HG21	1:121:A:GLU:H	10	0.24
(1,252)	1:111:A:VAL:HG22	1:121:A:GLU:H	10	0.24
(1,252)	1:111:A:VAL:HG23	1:121:A:GLU:H	10	0.24
(1,61)	1:59:A:VAL:HG21	1:62:A:TRP:HE3	18	0.24
(1,61)	1:59:A:VAL:HG22	1:62:A:TRP:HE3	18	0.24
(1,61)	1:59:A:VAL:HG23	1:62:A:TRP:HE3	18	0.24
(2,2)	2:149:B:PRO:HG2	1:38:A:MET:HE2	10	0.23
(1,1487)	1:132:A:VAL:HG11	1:133:A:TYR:H	13	0.23
(1,1487)	1:132:A:VAL:HG12	1:133:A:TYR:H	13	0.23
(1,1487)	1:132:A:VAL:HG13	1:133:A:TYR:H	13	0.23
(1,1487)	1:132:A:VAL:HG21	1:133:A:TYR:H	13	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1487)	1:132:A:VAL:HG22	1:133:A:TYR:H	13	0.23
(1,1487)	1:132:A:VAL:HG23	1:133:A:TYR:H	13	0.23
(1,1295)	1:66:A:LEU:H	1:66:A:LEU:HD11	20	0.23
(1,1295)	1:66:A:LEU:H	1:66:A:LEU:HD12	20	0.23
(1,1295)	1:66:A:LEU:H	1:66:A:LEU:HD13	20	0.23
(1,1295)	1:66:A:LEU:H	1:66:A:LEU:HD21	20	0.23
(1,1295)	1:66:A:LEU:H	1:66:A:LEU:HD22	20	0.23
(1,1295)	1:66:A:LEU:H	1:66:A:LEU:HD23	20	0.23
(1,1279)	1:59:A:VAL:HG11	1:103:A:VAL:HG11	15	0.23
(1,1279)	1:59:A:VAL:HG11	1:103:A:VAL:HG12	15	0.23
(1,1279)	1:59:A:VAL:HG11	1:103:A:VAL:HG13	15	0.23
(1,1279)	1:59:A:VAL:HG12	1:103:A:VAL:HG11	15	0.23
(1,1279)	1:59:A:VAL:HG12	1:103:A:VAL:HG12	15	0.23
(1,1279)	1:59:A:VAL:HG12	1:103:A:VAL:HG13	15	0.23
(1,1279)	1:59:A:VAL:HG13	1:103:A:VAL:HG11	15	0.23
(1,1279)	1:59:A:VAL:HG13	1:103:A:VAL:HG12	15	0.23
(1,1279)	1:59:A:VAL:HG13	1:103:A:VAL:HG13	15	0.23
(1,1279)	1:59:A:VAL:HG21	1:103:A:VAL:HG11	15	0.23
(1,1279)	1:59:A:VAL:HG21	1:103:A:VAL:HG12	15	0.23
(1,1279)	1:59:A:VAL:HG21	1:103:A:VAL:HG13	15	0.23
(1,1279)	1:59:A:VAL:HG22	1:103:A:VAL:HG11	15	0.23
(1,1279)	1:59:A:VAL:HG22	1:103:A:VAL:HG12	15	0.23
(1,1279)	1:59:A:VAL:HG22	1:103:A:VAL:HG13	15	0.23
(1,1279)	1:59:A:VAL:HG23	1:103:A:VAL:HG11	15	0.23
(1,1279)	1:59:A:VAL:HG23	1:103:A:VAL:HG12	15	0.23
(1,1279)	1:59:A:VAL:HG23	1:103:A:VAL:HG13	15	0.23
(1,1275)	1:59:A:VAL:HG11	1:102:A:ASP:H	18	0.23
(1,1275)	1:59:A:VAL:HG12	1:102:A:ASP:H	18	0.23
(1,1275)	1:59:A:VAL:HG13	1:102:A:ASP:H	18	0.23
(1,1275)	1:59:A:VAL:HG21	1:102:A:ASP:H	18	0.23
(1,1275)	1:59:A:VAL:HG22	1:102:A:ASP:H	18	0.23
(1,1275)	1:59:A:VAL:HG23	1:102:A:ASP:H	18	0.23
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD11	9	0.23
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD12	9	0.23
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD13	9	0.23
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD21	9	0.23
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD22	9	0.23
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD23	9	0.23
(1,1085)	1:141:A:LEU:HG	1:142:A:ARG:H	15	0.23
(1,857)	1:111:A:VAL:HG11	1:112:A:LYS:H	8	0.23
(1,857)	1:111:A:VAL:HG12	1:112:A:LYS:H	8	0.23
(1,857)	1:111:A:VAL:HG13	1:112:A:LYS:H	8	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,857)	1:111:A:VAL:HG11	1:112:A:LYS:H	18	0.23
(1,857)	1:111:A:VAL:HG12	1:112:A:LYS:H	18	0.23
(1,857)	1:111:A:VAL:HG13	1:112:A:LYS:H	18	0.23
(1,838)	1:31:A:PHE:H	1:34:A:VAL:HG21	8	0.23
(1,838)	1:31:A:PHE:H	1:34:A:VAL:HG22	8	0.23
(1,838)	1:31:A:PHE:H	1:34:A:VAL:HG23	8	0.23
(1,583)	1:48:A:CYS:H	1:51:A:ASN:HB2	4	0.23
(1,583)	1:48:A:CYS:H	1:51:A:ASN:HB2	9	0.23
(1,279)	1:77:A:LEU:HD21	1:107:A:ALA:HB1	18	0.23
(1,279)	1:77:A:LEU:HD21	1:107:A:ALA:HB2	18	0.23
(1,279)	1:77:A:LEU:HD21	1:107:A:ALA:HB3	18	0.23
(1,279)	1:77:A:LEU:HD22	1:107:A:ALA:HB1	18	0.23
(1,279)	1:77:A:LEU:HD22	1:107:A:ALA:HB2	18	0.23
(1,279)	1:77:A:LEU:HD22	1:107:A:ALA:HB3	18	0.23
(1,279)	1:77:A:LEU:HD23	1:107:A:ALA:HB1	18	0.23
(1,279)	1:77:A:LEU:HD23	1:107:A:ALA:HB2	18	0.23
(1,279)	1:77:A:LEU:HD23	1:107:A:ALA:HB3	18	0.23
(1,259)	1:111:A:VAL:HG21	1:124:A:PHE:HB2	8	0.23
(1,259)	1:111:A:VAL:HG21	1:124:A:PHE:HB3	8	0.23
(1,259)	1:111:A:VAL:HG22	1:124:A:PHE:HB2	8	0.23
(1,259)	1:111:A:VAL:HG22	1:124:A:PHE:HB3	8	0.23
(1,259)	1:111:A:VAL:HG23	1:124:A:PHE:HB2	8	0.23
(1,259)	1:111:A:VAL:HG23	1:124:A:PHE:HB3	8	0.23
(1,259)	1:111:A:VAL:HG21	1:124:A:PHE:HB2	9	0.23
(1,259)	1:111:A:VAL:HG21	1:124:A:PHE:HB3	9	0.23
(1,259)	1:111:A:VAL:HG22	1:124:A:PHE:HB2	9	0.23
(1,259)	1:111:A:VAL:HG22	1:124:A:PHE:HB3	9	0.23
(1,259)	1:111:A:VAL:HG23	1:124:A:PHE:HB2	9	0.23
(1,259)	1:111:A:VAL:HG23	1:124:A:PHE:HB3	9	0.23
(1,252)	1:111:A:VAL:HG21	1:121:A:GLU:H	16	0.23
(1,252)	1:111:A:VAL:HG22	1:121:A:GLU:H	16	0.23
(1,252)	1:111:A:VAL:HG23	1:121:A:GLU:H	16	0.23
(1,252)	1:111:A:VAL:HG21	1:121:A:GLU:H	17	0.23
(1,252)	1:111:A:VAL:HG22	1:121:A:GLU:H	17	0.23
(1,252)	1:111:A:VAL:HG23	1:121:A:GLU:H	17	0.23
(1,204)	1:59:A:VAL:HA	1:103:A:VAL:HG11	7	0.23
(1,204)	1:59:A:VAL:HA	1:103:A:VAL:HG12	7	0.23
(1,204)	1:59:A:VAL:HA	1:103:A:VAL:HG13	7	0.23
(1,53)	1:58:A:ILE:HG21	1:59:A:VAL:HG21	10	0.23
(1,53)	1:58:A:ILE:HG21	1:59:A:VAL:HG22	10	0.23
(1,53)	1:58:A:ILE:HG21	1:59:A:VAL:HG23	10	0.23
(1,53)	1:58:A:ILE:HG22	1:59:A:VAL:HG21	10	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,53)	1:58:A:ILE:HG22	1:59:A:VAL:HG22	10	0.23
(1,53)	1:58:A:ILE:HG22	1:59:A:VAL:HG23	10	0.23
(1,53)	1:58:A:ILE:HG23	1:59:A:VAL:HG21	10	0.23
(1,53)	1:58:A:ILE:HG23	1:59:A:VAL:HG22	10	0.23
(1,53)	1:58:A:ILE:HG23	1:59:A:VAL:HG23	10	0.23
(1,1494)	1:135:A:GLU:HA	1:139:A:VAL:HG11	1	0.22
(1,1494)	1:135:A:GLU:HA	1:139:A:VAL:HG12	1	0.22
(1,1494)	1:135:A:GLU:HA	1:139:A:VAL:HG13	1	0.22
(1,1494)	1:135:A:GLU:HA	1:139:A:VAL:HG21	1	0.22
(1,1494)	1:135:A:GLU:HA	1:139:A:VAL:HG22	1	0.22
(1,1494)	1:135:A:GLU:HA	1:139:A:VAL:HG23	1	0.22
(1,1494)	1:135:A:GLU:HA	1:139:A:VAL:HG11	12	0.22
(1,1494)	1:135:A:GLU:HA	1:139:A:VAL:HG12	12	0.22
(1,1494)	1:135:A:GLU:HA	1:139:A:VAL:HG13	12	0.22
(1,1494)	1:135:A:GLU:HA	1:139:A:VAL:HG21	12	0.22
(1,1494)	1:135:A:GLU:HA	1:139:A:VAL:HG22	12	0.22
(1,1494)	1:135:A:GLU:HA	1:139:A:VAL:HG23	12	0.22
(1,1487)	1:132:A:VAL:HG11	1:133:A:TYR:H	2	0.22
(1,1487)	1:132:A:VAL:HG12	1:133:A:TYR:H	2	0.22
(1,1487)	1:132:A:VAL:HG13	1:133:A:TYR:H	2	0.22
(1,1487)	1:132:A:VAL:HG21	1:133:A:TYR:H	2	0.22
(1,1487)	1:132:A:VAL:HG22	1:133:A:TYR:H	2	0.22
(1,1487)	1:132:A:VAL:HG23	1:133:A:TYR:H	2	0.22
(1,1381)	1:97:A:ARG:HB2	1:101:A:ALA:H	14	0.22
(1,1381)	1:97:A:ARG:HB3	1:101:A:ALA:H	14	0.22
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD11	6	0.22
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD12	6	0.22
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD13	6	0.22
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD21	6	0.22
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD22	6	0.22
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD23	6	0.22
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD11	6	0.22
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD12	6	0.22
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD13	6	0.22
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD21	6	0.22
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD22	6	0.22
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD23	6	0.22
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD11	9	0.22
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD12	9	0.22
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD13	9	0.22
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD21	9	0.22
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD22	9	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD23	9	0.22
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD11	9	0.22
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD12	9	0.22
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD13	9	0.22
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD21	9	0.22
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD22	9	0.22
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD23	9	0.22
(1,1294)	1:63:A:MET:HG2	1:103:A:VAL:HG11	14	0.22
(1,1294)	1:63:A:MET:HG2	1:103:A:VAL:HG12	14	0.22
(1,1294)	1:63:A:MET:HG2	1:103:A:VAL:HG13	14	0.22
(1,1294)	1:63:A:MET:HG3	1:103:A:VAL:HG11	14	0.22
(1,1294)	1:63:A:MET:HG3	1:103:A:VAL:HG12	14	0.22
(1,1294)	1:63:A:MET:HG3	1:103:A:VAL:HG13	14	0.22
(1,1293)	1:63:A:MET:HG2	1:77:A:LEU:HD11	8	0.22
(1,1293)	1:63:A:MET:HG2	1:77:A:LEU:HD12	8	0.22
(1,1293)	1:63:A:MET:HG2	1:77:A:LEU:HD13	8	0.22
(1,1293)	1:63:A:MET:HG2	1:77:A:LEU:HD21	8	0.22
(1,1293)	1:63:A:MET:HG2	1:77:A:LEU:HD22	8	0.22
(1,1293)	1:63:A:MET:HG2	1:77:A:LEU:HD23	8	0.22
(1,1293)	1:63:A:MET:HG3	1:77:A:LEU:HD11	8	0.22
(1,1293)	1:63:A:MET:HG3	1:77:A:LEU:HD12	8	0.22
(1,1293)	1:63:A:MET:HG3	1:77:A:LEU:HD13	8	0.22
(1,1293)	1:63:A:MET:HG3	1:77:A:LEU:HD21	8	0.22
(1,1293)	1:63:A:MET:HG3	1:77:A:LEU:HD22	8	0.22
(1,1293)	1:63:A:MET:HG3	1:77:A:LEU:HD23	8	0.22
(1,1277)	1:59:A:VAL:HG11	1:103:A:VAL:HA	15	0.22
(1,1277)	1:59:A:VAL:HG12	1:103:A:VAL:HA	15	0.22
(1,1277)	1:59:A:VAL:HG13	1:103:A:VAL:HA	15	0.22
(1,1277)	1:59:A:VAL:HG21	1:103:A:VAL:HA	15	0.22
(1,1277)	1:59:A:VAL:HG22	1:103:A:VAL:HA	15	0.22
(1,1277)	1:59:A:VAL:HG23	1:103:A:VAL:HA	15	0.22
(1,1259)	1:59:A:VAL:HG11	1:61:A:HIS:H	20	0.22
(1,1259)	1:59:A:VAL:HG12	1:61:A:HIS:H	20	0.22
(1,1259)	1:59:A:VAL:HG13	1:61:A:HIS:H	20	0.22
(1,1259)	1:59:A:VAL:HG21	1:61:A:HIS:H	20	0.22
(1,1259)	1:59:A:VAL:HG22	1:61:A:HIS:H	20	0.22
(1,1259)	1:59:A:VAL:HG23	1:61:A:HIS:H	20	0.22
(1,1238)	1:48:A:CYS:HB2	1:84:A:VAL:HG21	3	0.22
(1,1238)	1:48:A:CYS:HB2	1:84:A:VAL:HG22	3	0.22
(1,1238)	1:48:A:CYS:HB2	1:84:A:VAL:HG23	3	0.22
(1,1238)	1:48:A:CYS:HB3	1:84:A:VAL:HG21	3	0.22
(1,1238)	1:48:A:CYS:HB3	1:84:A:VAL:HG22	3	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1238)	1:48:A:CYS:HB3	1:84:A:VAL:HG23	3	0.22
(1,1189)	1:62:A:TRP:HE1	1:77:A:LEU:HD21	15	0.22
(1,1189)	1:62:A:TRP:HE1	1:77:A:LEU:HD22	15	0.22
(1,1189)	1:62:A:TRP:HE1	1:77:A:LEU:HD23	15	0.22
(1,1112)	1:61:A:HIS:H	1:61:A:HIS:HD2	4	0.22
(1,1112)	1:61:A:HIS:H	1:61:A:HIS:HD2	19	0.22
(1,857)	1:111:A:VAL:HG11	1:112:A:LYS:H	16	0.22
(1,857)	1:111:A:VAL:HG12	1:112:A:LYS:H	16	0.22
(1,857)	1:111:A:VAL:HG13	1:112:A:LYS:H	16	0.22
(1,847)	1:49:A:ILE:H	1:84:A:VAL:HG11	15	0.22
(1,847)	1:49:A:ILE:H	1:84:A:VAL:HG12	15	0.22
(1,847)	1:49:A:ILE:H	1:84:A:VAL:HG13	15	0.22
(1,841)	1:68:A:ARG:HB2	1:69:A:SER:H	8	0.22
(1,841)	1:68:A:ARG:HB3	1:69:A:SER:H	8	0.22
(1,583)	1:48:A:CYS:H	1:51:A:ASN:HB2	12	0.22
(1,583)	1:48:A:CYS:H	1:51:A:ASN:HB2	18	0.22
(1,574)	1:108:A:ALA:H	1:111:A:VAL:HG11	13	0.22
(1,574)	1:108:A:ALA:H	1:111:A:VAL:HG12	13	0.22
(1,574)	1:108:A:ALA:H	1:111:A:VAL:HG13	13	0.22
(1,574)	1:108:A:ALA:H	1:111:A:VAL:HG11	18	0.22
(1,574)	1:108:A:ALA:H	1:111:A:VAL:HG12	18	0.22
(1,574)	1:108:A:ALA:H	1:111:A:VAL:HG13	18	0.22
(1,344)	1:49:A:ILE:H	1:84:A:VAL:HG21	17	0.22
(1,344)	1:49:A:ILE:H	1:84:A:VAL:HG22	17	0.22
(1,344)	1:49:A:ILE:H	1:84:A:VAL:HG23	17	0.22
(1,308)	1:103:A:VAL:HG21	1:107:A:ALA:HA	17	0.22
(1,308)	1:103:A:VAL:HG22	1:107:A:ALA:HA	17	0.22
(1,308)	1:103:A:VAL:HG23	1:107:A:ALA:HA	17	0.22
(1,259)	1:111:A:VAL:HG21	1:124:A:PHE:HB2	10	0.22
(1,259)	1:111:A:VAL:HG21	1:124:A:PHE:HB3	10	0.22
(1,259)	1:111:A:VAL:HG22	1:124:A:PHE:HB2	10	0.22
(1,259)	1:111:A:VAL:HG22	1:124:A:PHE:HB3	10	0.22
(1,259)	1:111:A:VAL:HG23	1:124:A:PHE:HB2	10	0.22
(1,259)	1:111:A:VAL:HG23	1:124:A:PHE:HB3	10	0.22
(1,259)	1:111:A:VAL:HG21	1:124:A:PHE:HB2	19	0.22
(1,259)	1:111:A:VAL:HG21	1:124:A:PHE:HB3	19	0.22
(1,259)	1:111:A:VAL:HG22	1:124:A:PHE:HB2	19	0.22
(1,259)	1:111:A:VAL:HG22	1:124:A:PHE:HB3	19	0.22
(1,259)	1:111:A:VAL:HG23	1:124:A:PHE:HB2	19	0.22
(1,259)	1:111:A:VAL:HG23	1:124:A:PHE:HB3	19	0.22
(1,83)	1:137:A:MET:HB3	1:138:A:ILE:HD11	12	0.22
(1,83)	1:137:A:MET:HB3	1:138:A:ILE:HD12	12	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,83)	1:137:A:MET:HB3	1:138:A:ILE:HD13	12	0.22
(1,53)	1:58:A:ILE:HG21	1:59:A:VAL:HG21	16	0.22
(1,53)	1:58:A:ILE:HG21	1:59:A:VAL:HG22	16	0.22
(1,53)	1:58:A:ILE:HG21	1:59:A:VAL:HG23	16	0.22
(1,53)	1:58:A:ILE:HG22	1:59:A:VAL:HG21	16	0.22
(1,53)	1:58:A:ILE:HG22	1:59:A:VAL:HG22	16	0.22
(1,53)	1:58:A:ILE:HG22	1:59:A:VAL:HG23	16	0.22
(1,53)	1:58:A:ILE:HG23	1:59:A:VAL:HG21	16	0.22
(1,53)	1:58:A:ILE:HG23	1:59:A:VAL:HG22	16	0.22
(1,53)	1:58:A:ILE:HG23	1:59:A:VAL:HG23	16	0.22
(1,20)	1:132:A:VAL:HG21	1:138:A:ILE:HD11	1	0.22
(1,20)	1:132:A:VAL:HG21	1:138:A:ILE:HD12	1	0.22
(1,20)	1:132:A:VAL:HG21	1:138:A:ILE:HD13	1	0.22
(1,20)	1:132:A:VAL:HG22	1:138:A:ILE:HD11	1	0.22
(1,20)	1:132:A:VAL:HG22	1:138:A:ILE:HD12	1	0.22
(1,20)	1:132:A:VAL:HG22	1:138:A:ILE:HD13	1	0.22
(1,20)	1:132:A:VAL:HG23	1:138:A:ILE:HD11	1	0.22
(1,20)	1:132:A:VAL:HG23	1:138:A:ILE:HD12	1	0.22
(1,20)	1:132:A:VAL:HG23	1:138:A:ILE:HD13	1	0.22
(6,2)	2:148:B:SER:H1	2:149:B:PRO:HG2	2	0.21
(6,2)	2:148:B:SER:H1	2:149:B:PRO:HG3	2	0.21
(1,1511)	1:140:A:ALA:H	1:141:A:LEU:HD11	2	0.21
(1,1511)	1:140:A:ALA:H	1:141:A:LEU:HD12	2	0.21
(1,1511)	1:140:A:ALA:H	1:141:A:LEU:HD13	2	0.21
(1,1511)	1:140:A:ALA:H	1:141:A:LEU:HD21	2	0.21
(1,1511)	1:140:A:ALA:H	1:141:A:LEU:HD22	2	0.21
(1,1511)	1:140:A:ALA:H	1:141:A:LEU:HD23	2	0.21
(1,1508)	1:139:A:VAL:HG11	1:140:A:ALA:HB1	10	0.21
(1,1508)	1:139:A:VAL:HG11	1:140:A:ALA:HB2	10	0.21
(1,1508)	1:139:A:VAL:HG11	1:140:A:ALA:HB3	10	0.21
(1,1508)	1:139:A:VAL:HG12	1:140:A:ALA:HB1	10	0.21
(1,1508)	1:139:A:VAL:HG12	1:140:A:ALA:HB2	10	0.21
(1,1508)	1:139:A:VAL:HG12	1:140:A:ALA:HB3	10	0.21
(1,1508)	1:139:A:VAL:HG13	1:140:A:ALA:HB1	10	0.21
(1,1508)	1:139:A:VAL:HG13	1:140:A:ALA:HB2	10	0.21
(1,1508)	1:139:A:VAL:HG13	1:140:A:ALA:HB3	10	0.21
(1,1508)	1:139:A:VAL:HG21	1:140:A:ALA:HB1	10	0.21
(1,1508)	1:139:A:VAL:HG21	1:140:A:ALA:HB2	10	0.21
(1,1508)	1:139:A:VAL:HG21	1:140:A:ALA:HB3	10	0.21
(1,1508)	1:139:A:VAL:HG22	1:140:A:ALA:HB1	10	0.21
(1,1508)	1:139:A:VAL:HG22	1:140:A:ALA:HB2	10	0.21
(1,1508)	1:139:A:VAL:HG22	1:140:A:ALA:HB3	10	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1508)	1:139:A:VAL:HG23	1:140:A:ALA:HB1	10	0.21
(1,1508)	1:139:A:VAL:HG23	1:140:A:ALA:HB2	10	0.21
(1,1508)	1:139:A:VAL:HG23	1:140:A:ALA:HB3	10	0.21
(1,1508)	1:139:A:VAL:HG11	1:140:A:ALA:HB1	13	0.21
(1,1508)	1:139:A:VAL:HG11	1:140:A:ALA:HB2	13	0.21
(1,1508)	1:139:A:VAL:HG11	1:140:A:ALA:HB3	13	0.21
(1,1508)	1:139:A:VAL:HG12	1:140:A:ALA:HB1	13	0.21
(1,1508)	1:139:A:VAL:HG12	1:140:A:ALA:HB2	13	0.21
(1,1508)	1:139:A:VAL:HG12	1:140:A:ALA:HB3	13	0.21
(1,1508)	1:139:A:VAL:HG13	1:140:A:ALA:HB1	13	0.21
(1,1508)	1:139:A:VAL:HG13	1:140:A:ALA:HB2	13	0.21
(1,1508)	1:139:A:VAL:HG13	1:140:A:ALA:HB3	13	0.21
(1,1508)	1:139:A:VAL:HG21	1:140:A:ALA:HB1	13	0.21
(1,1508)	1:139:A:VAL:HG21	1:140:A:ALA:HB2	13	0.21
(1,1508)	1:139:A:VAL:HG21	1:140:A:ALA:HB3	13	0.21
(1,1508)	1:139:A:VAL:HG22	1:140:A:ALA:HB1	13	0.21
(1,1508)	1:139:A:VAL:HG22	1:140:A:ALA:HB2	13	0.21
(1,1508)	1:139:A:VAL:HG22	1:140:A:ALA:HB3	13	0.21
(1,1508)	1:139:A:VAL:HG23	1:140:A:ALA:HB1	13	0.21
(1,1508)	1:139:A:VAL:HG23	1:140:A:ALA:HB2	13	0.21
(1,1508)	1:139:A:VAL:HG23	1:140:A:ALA:HB3	13	0.21
(1,1487)	1:132:A:VAL:HG11	1:133:A:TYR:H	4	0.21
(1,1487)	1:132:A:VAL:HG12	1:133:A:TYR:H	4	0.21
(1,1487)	1:132:A:VAL:HG13	1:133:A:TYR:H	4	0.21
(1,1487)	1:132:A:VAL:HG21	1:133:A:TYR:H	4	0.21
(1,1487)	1:132:A:VAL:HG22	1:133:A:TYR:H	4	0.21
(1,1487)	1:132:A:VAL:HG23	1:133:A:TYR:H	4	0.21
(1,1410)	1:108:A:ALA:HB1	1:145:A:LEU:HD11	13	0.21
(1,1410)	1:108:A:ALA:HB1	1:145:A:LEU:HD12	13	0.21
(1,1410)	1:108:A:ALA:HB1	1:145:A:LEU:HD13	13	0.21
(1,1410)	1:108:A:ALA:HB1	1:145:A:LEU:HD21	13	0.21
(1,1410)	1:108:A:ALA:HB1	1:145:A:LEU:HD22	13	0.21
(1,1410)	1:108:A:ALA:HB1	1:145:A:LEU:HD23	13	0.21
(1,1410)	1:108:A:ALA:HB2	1:145:A:LEU:HD11	13	0.21
(1,1410)	1:108:A:ALA:HB2	1:145:A:LEU:HD12	13	0.21
(1,1410)	1:108:A:ALA:HB2	1:145:A:LEU:HD13	13	0.21
(1,1410)	1:108:A:ALA:HB2	1:145:A:LEU:HD21	13	0.21
(1,1410)	1:108:A:ALA:HB2	1:145:A:LEU:HD22	13	0.21
(1,1410)	1:108:A:ALA:HB2	1:145:A:LEU:HD23	13	0.21
(1,1410)	1:108:A:ALA:HB3	1:145:A:LEU:HD11	13	0.21
(1,1410)	1:108:A:ALA:HB3	1:145:A:LEU:HD12	13	0.21
(1,1410)	1:108:A:ALA:HB3	1:145:A:LEU:HD13	13	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1410)	1:108:A:ALA:HB3	1:145:A:LEU:HD21	13	0.21
(1,1410)	1:108:A:ALA:HB3	1:145:A:LEU:HD22	13	0.21
(1,1410)	1:108:A:ALA:HB3	1:145:A:LEU:HD23	13	0.21
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD11	12	0.21
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD12	12	0.21
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD13	12	0.21
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD21	12	0.21
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD22	12	0.21
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD23	12	0.21
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD11	12	0.21
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD12	12	0.21
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD13	12	0.21
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD21	12	0.21
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD22	12	0.21
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD23	12	0.21
(1,1294)	1:63:A:MET:HG2	1:103:A:VAL:HG11	2	0.21
(1,1294)	1:63:A:MET:HG2	1:103:A:VAL:HG12	2	0.21
(1,1294)	1:63:A:MET:HG2	1:103:A:VAL:HG13	2	0.21
(1,1294)	1:63:A:MET:HG3	1:103:A:VAL:HG11	2	0.21
(1,1294)	1:63:A:MET:HG3	1:103:A:VAL:HG12	2	0.21
(1,1294)	1:63:A:MET:HG3	1:103:A:VAL:HG13	2	0.21
(1,1278)	1:59:A:VAL:HG11	1:103:A:VAL:HB	3	0.21
(1,1278)	1:59:A:VAL:HG12	1:103:A:VAL:HB	3	0.21
(1,1278)	1:59:A:VAL:HG13	1:103:A:VAL:HB	3	0.21
(1,1278)	1:59:A:VAL:HG21	1:103:A:VAL:HB	3	0.21
(1,1278)	1:59:A:VAL:HG22	1:103:A:VAL:HB	3	0.21
(1,1278)	1:59:A:VAL:HG23	1:103:A:VAL:HB	3	0.21
(1,1259)	1:59:A:VAL:HG11	1:61:A:HIS:H	12	0.21
(1,1259)	1:59:A:VAL:HG12	1:61:A:HIS:H	12	0.21
(1,1259)	1:59:A:VAL:HG13	1:61:A:HIS:H	12	0.21
(1,1259)	1:59:A:VAL:HG21	1:61:A:HIS:H	12	0.21
(1,1259)	1:59:A:VAL:HG22	1:61:A:HIS:H	12	0.21
(1,1259)	1:59:A:VAL:HG23	1:61:A:HIS:H	12	0.21
(1,1189)	1:62:A:TRP:HE1	1:77:A:LEU:HD21	14	0.21
(1,1189)	1:62:A:TRP:HE1	1:77:A:LEU:HD22	14	0.21
(1,1189)	1:62:A:TRP:HE1	1:77:A:LEU:HD23	14	0.21
(1,950)	1:103:A:VAL:HG21	1:107:A:ALA:H	15	0.21
(1,950)	1:103:A:VAL:HG22	1:107:A:ALA:H	15	0.21
(1,950)	1:103:A:VAL:HG23	1:107:A:ALA:H	15	0.21
(1,847)	1:49:A:ILE:H	1:84:A:VAL:HG11	16	0.21
(1,847)	1:49:A:ILE:H	1:84:A:VAL:HG12	16	0.21
(1,847)	1:49:A:ILE:H	1:84:A:VAL:HG13	16	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,583)	1:48:A:CYS:H	1:51:A:ASN:HB2	1	0.21
(1,579)	1:48:A:CYS:H	1:84:A:VAL:HG21	3	0.21
(1,579)	1:48:A:CYS:H	1:84:A:VAL:HG22	3	0.21
(1,579)	1:48:A:CYS:H	1:84:A:VAL:HG23	3	0.21
(1,296)	1:34:A:VAL:HG11	1:36:A:ASN:H	14	0.21
(1,296)	1:34:A:VAL:HG12	1:36:A:ASN:H	14	0.21
(1,296)	1:34:A:VAL:HG13	1:36:A:ASN:H	14	0.21
(1,259)	1:111:A:VAL:HG21	1:124:A:PHE:HB2	4	0.21
(1,259)	1:111:A:VAL:HG21	1:124:A:PHE:HB3	4	0.21
(1,259)	1:111:A:VAL:HG22	1:124:A:PHE:HB2	4	0.21
(1,259)	1:111:A:VAL:HG22	1:124:A:PHE:HB3	4	0.21
(1,259)	1:111:A:VAL:HG23	1:124:A:PHE:HB2	4	0.21
(1,259)	1:111:A:VAL:HG23	1:124:A:PHE:HB3	4	0.21
(1,259)	1:111:A:VAL:HG21	1:124:A:PHE:HB2	11	0.21
(1,259)	1:111:A:VAL:HG21	1:124:A:PHE:HB3	11	0.21
(1,259)	1:111:A:VAL:HG22	1:124:A:PHE:HB2	11	0.21
(1,259)	1:111:A:VAL:HG22	1:124:A:PHE:HB3	11	0.21
(1,259)	1:111:A:VAL:HG23	1:124:A:PHE:HB2	11	0.21
(1,259)	1:111:A:VAL:HG23	1:124:A:PHE:HB3	11	0.21
(1,259)	1:111:A:VAL:HG21	1:124:A:PHE:HB2	12	0.21
(1,259)	1:111:A:VAL:HG21	1:124:A:PHE:HB3	12	0.21
(1,259)	1:111:A:VAL:HG22	1:124:A:PHE:HB2	12	0.21
(1,259)	1:111:A:VAL:HG22	1:124:A:PHE:HB3	12	0.21
(1,259)	1:111:A:VAL:HG23	1:124:A:PHE:HB2	12	0.21
(1,259)	1:111:A:VAL:HG23	1:124:A:PHE:HB3	12	0.21
(1,252)	1:111:A:VAL:HG21	1:121:A:GLU:H	12	0.21
(1,252)	1:111:A:VAL:HG22	1:121:A:GLU:H	12	0.21
(1,252)	1:111:A:VAL:HG23	1:121:A:GLU:H	12	0.21
(1,245)	1:72:A:PRO:HA	1:116:A:VAL:HG21	18	0.21
(1,245)	1:72:A:PRO:HA	1:116:A:VAL:HG22	18	0.21
(1,245)	1:72:A:PRO:HA	1:116:A:VAL:HG23	18	0.21
(1,134)	1:59:A:VAL:HB	1:103:A:VAL:HG21	17	0.21
(1,134)	1:59:A:VAL:HB	1:103:A:VAL:HG22	17	0.21
(1,134)	1:59:A:VAL:HB	1:103:A:VAL:HG23	17	0.21
(1,1511)	1:140:A:ALA:H	1:141:A:LEU:HD11	17	0.2
(1,1511)	1:140:A:ALA:H	1:141:A:LEU:HD12	17	0.2
(1,1511)	1:140:A:ALA:H	1:141:A:LEU:HD13	17	0.2
(1,1511)	1:140:A:ALA:H	1:141:A:LEU:HD21	17	0.2
(1,1511)	1:140:A:ALA:H	1:141:A:LEU:HD22	17	0.2
(1,1511)	1:140:A:ALA:H	1:141:A:LEU:HD23	17	0.2
(1,1505)	1:139:A:VAL:H	1:141:A:LEU:HD11	10	0.2
(1,1505)	1:139:A:VAL:H	1:141:A:LEU:HD12	10	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1505)	1:139:A:VAL:H	1:141:A:LEU:HD13	10	0.2
(1,1505)	1:139:A:VAL:H	1:141:A:LEU:HD21	10	0.2
(1,1505)	1:139:A:VAL:H	1:141:A:LEU:HD22	10	0.2
(1,1505)	1:139:A:VAL:H	1:141:A:LEU:HD23	10	0.2
(1,1494)	1:135:A:GLU:HA	1:139:A:VAL:HG11	5	0.2
(1,1494)	1:135:A:GLU:HA	1:139:A:VAL:HG12	5	0.2
(1,1494)	1:135:A:GLU:HA	1:139:A:VAL:HG13	5	0.2
(1,1494)	1:135:A:GLU:HA	1:139:A:VAL:HG21	5	0.2
(1,1494)	1:135:A:GLU:HA	1:139:A:VAL:HG22	5	0.2
(1,1494)	1:135:A:GLU:HA	1:139:A:VAL:HG23	5	0.2
(1,1381)	1:97:A:ARG:HB2	1:101:A:ALA:H	11	0.2
(1,1381)	1:97:A:ARG:HB3	1:101:A:ALA:H	11	0.2
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD11	10	0.2
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD12	10	0.2
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD13	10	0.2
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD21	10	0.2
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD22	10	0.2
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD23	10	0.2
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD11	10	0.2
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD12	10	0.2
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD13	10	0.2
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD21	10	0.2
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD22	10	0.2
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD23	10	0.2
(1,1294)	1:63:A:MET:HG2	1:103:A:VAL:HG11	9	0.2
(1,1294)	1:63:A:MET:HG2	1:103:A:VAL:HG12	9	0.2
(1,1294)	1:63:A:MET:HG2	1:103:A:VAL:HG13	9	0.2
(1,1294)	1:63:A:MET:HG3	1:103:A:VAL:HG11	9	0.2
(1,1294)	1:63:A:MET:HG3	1:103:A:VAL:HG12	9	0.2
(1,1294)	1:63:A:MET:HG3	1:103:A:VAL:HG13	9	0.2
(1,1169)	1:34:A:VAL:HG21	1:35:A:THR:H	18	0.2
(1,1169)	1:34:A:VAL:HG22	1:35:A:THR:H	18	0.2
(1,1169)	1:34:A:VAL:HG23	1:35:A:THR:H	18	0.2
(1,1085)	1:141:A:LEU:HG	1:142:A:ARG:H	1	0.2
(1,953)	1:103:A:VAL:HG21	1:106:A:GLU:H	3	0.2
(1,953)	1:103:A:VAL:HG22	1:106:A:GLU:H	3	0.2
(1,953)	1:103:A:VAL:HG23	1:106:A:GLU:H	3	0.2
(1,950)	1:103:A:VAL:HG21	1:107:A:ALA:H	10	0.2
(1,950)	1:103:A:VAL:HG22	1:107:A:ALA:H	10	0.2
(1,950)	1:103:A:VAL:HG23	1:107:A:ALA:H	10	0.2
(1,950)	1:103:A:VAL:HG21	1:107:A:ALA:H	19	0.2
(1,950)	1:103:A:VAL:HG22	1:107:A:ALA:H	19	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,950)	1:103:A:VAL:HG23	1:107:A:ALA:H	19	0.2
(1,719)	1:109:A:ALA:H	1:112:A:LYS:H	1	0.2
(1,719)	1:109:A:ALA:H	1:112:A:LYS:H	4	0.2
(1,719)	1:109:A:ALA:H	1:112:A:LYS:H	6	0.2
(1,583)	1:48:A:CYS:H	1:51:A:ASN:HB2	20	0.2
(1,574)	1:108:A:ALA:H	1:111:A:VAL:HG11	11	0.2
(1,574)	1:108:A:ALA:H	1:111:A:VAL:HG12	11	0.2
(1,574)	1:108:A:ALA:H	1:111:A:VAL:HG13	11	0.2
(1,442)	1:75:A:LEU:HD11	1:78:A:PHE:HB3	17	0.2
(1,442)	1:75:A:LEU:HD12	1:78:A:PHE:HB3	17	0.2
(1,442)	1:75:A:LEU:HD13	1:78:A:PHE:HB3	17	0.2
(1,424)	1:84:A:VAL:HG11	1:88:A:CYS:HB2	7	0.2
(1,424)	1:84:A:VAL:HG11	1:88:A:CYS:HB3	7	0.2
(1,424)	1:84:A:VAL:HG12	1:88:A:CYS:HB2	7	0.2
(1,424)	1:84:A:VAL:HG12	1:88:A:CYS:HB3	7	0.2
(1,424)	1:84:A:VAL:HG13	1:88:A:CYS:HB2	7	0.2
(1,424)	1:84:A:VAL:HG13	1:88:A:CYS:HB3	7	0.2
(1,424)	1:84:A:VAL:HG11	1:88:A:CYS:HB2	11	0.2
(1,424)	1:84:A:VAL:HG11	1:88:A:CYS:HB3	11	0.2
(1,424)	1:84:A:VAL:HG12	1:88:A:CYS:HB2	11	0.2
(1,424)	1:84:A:VAL:HG12	1:88:A:CYS:HB3	11	0.2
(1,424)	1:84:A:VAL:HG13	1:88:A:CYS:HB2	11	0.2
(1,424)	1:84:A:VAL:HG13	1:88:A:CYS:HB3	11	0.2
(1,371)	1:100:A:PHE:HA	1:103:A:VAL:HG11	14	0.2
(1,371)	1:100:A:PHE:HA	1:103:A:VAL:HG12	14	0.2
(1,371)	1:100:A:PHE:HA	1:103:A:VAL:HG13	14	0.2
(1,369)	1:63:A:MET:HG3	1:103:A:VAL:HG11	19	0.2
(1,369)	1:63:A:MET:HG3	1:103:A:VAL:HG12	19	0.2
(1,369)	1:63:A:MET:HG3	1:103:A:VAL:HG13	19	0.2
(1,308)	1:103:A:VAL:HG21	1:107:A:ALA:HA	7	0.2
(1,308)	1:103:A:VAL:HG22	1:107:A:ALA:HA	7	0.2
(1,308)	1:103:A:VAL:HG23	1:107:A:ALA:HA	7	0.2
(1,279)	1:77:A:LEU:HD21	1:107:A:ALA:HB1	5	0.2
(1,279)	1:77:A:LEU:HD21	1:107:A:ALA:HB2	5	0.2
(1,279)	1:77:A:LEU:HD21	1:107:A:ALA:HB3	5	0.2
(1,279)	1:77:A:LEU:HD22	1:107:A:ALA:HB1	5	0.2
(1,279)	1:77:A:LEU:HD22	1:107:A:ALA:HB2	5	0.2
(1,279)	1:77:A:LEU:HD22	1:107:A:ALA:HB3	5	0.2
(1,279)	1:77:A:LEU:HD23	1:107:A:ALA:HB1	5	0.2
(1,279)	1:77:A:LEU:HD23	1:107:A:ALA:HB2	5	0.2
(1,279)	1:77:A:LEU:HD23	1:107:A:ALA:HB3	5	0.2
(1,259)	1:111:A:VAL:HG21	1:124:A:PHE:HB2	13	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,259)	1:111:A:VAL:HG21	1:124:A:PHE:HB3	13	0.2
(1,259)	1:111:A:VAL:HG22	1:124:A:PHE:HB2	13	0.2
(1,259)	1:111:A:VAL:HG22	1:124:A:PHE:HB3	13	0.2
(1,259)	1:111:A:VAL:HG23	1:124:A:PHE:HB2	13	0.2
(1,259)	1:111:A:VAL:HG23	1:124:A:PHE:HB3	13	0.2
(1,259)	1:111:A:VAL:HG21	1:124:A:PHE:HB2	16	0.2
(1,259)	1:111:A:VAL:HG21	1:124:A:PHE:HB3	16	0.2
(1,259)	1:111:A:VAL:HG22	1:124:A:PHE:HB2	16	0.2
(1,259)	1:111:A:VAL:HG22	1:124:A:PHE:HB3	16	0.2
(1,259)	1:111:A:VAL:HG23	1:124:A:PHE:HB2	16	0.2
(1,259)	1:111:A:VAL:HG23	1:124:A:PHE:HB3	16	0.2
(1,259)	1:111:A:VAL:HG21	1:124:A:PHE:HB2	17	0.2
(1,259)	1:111:A:VAL:HG21	1:124:A:PHE:HB3	17	0.2
(1,259)	1:111:A:VAL:HG22	1:124:A:PHE:HB2	17	0.2
(1,259)	1:111:A:VAL:HG22	1:124:A:PHE:HB3	17	0.2
(1,259)	1:111:A:VAL:HG23	1:124:A:PHE:HB2	17	0.2
(1,259)	1:111:A:VAL:HG23	1:124:A:PHE:HB3	17	0.2
(1,259)	1:111:A:VAL:HG21	1:124:A:PHE:HB2	20	0.2
(1,259)	1:111:A:VAL:HG21	1:124:A:PHE:HB3	20	0.2
(1,259)	1:111:A:VAL:HG22	1:124:A:PHE:HB2	20	0.2
(1,259)	1:111:A:VAL:HG22	1:124:A:PHE:HB3	20	0.2
(1,259)	1:111:A:VAL:HG23	1:124:A:PHE:HB2	20	0.2
(1,259)	1:111:A:VAL:HG23	1:124:A:PHE:HB3	20	0.2
(1,82)	1:132:A:VAL:HG11	1:138:A:ILE:HD11	6	0.2
(1,82)	1:132:A:VAL:HG11	1:138:A:ILE:HD12	6	0.2
(1,82)	1:132:A:VAL:HG11	1:138:A:ILE:HD13	6	0.2
(1,82)	1:132:A:VAL:HG12	1:138:A:ILE:HD11	6	0.2
(1,82)	1:132:A:VAL:HG12	1:138:A:ILE:HD12	6	0.2
(1,82)	1:132:A:VAL:HG12	1:138:A:ILE:HD13	6	0.2
(1,82)	1:132:A:VAL:HG13	1:138:A:ILE:HD11	6	0.2
(1,82)	1:132:A:VAL:HG13	1:138:A:ILE:HD12	6	0.2
(1,82)	1:132:A:VAL:HG13	1:138:A:ILE:HD13	6	0.2
(1,62)	1:59:A:VAL:HG21	1:100:A:PHE:HD1	9	0.2
(1,62)	1:59:A:VAL:HG21	1:100:A:PHE:HD2	9	0.2
(1,62)	1:59:A:VAL:HG22	1:100:A:PHE:HD1	9	0.2
(1,62)	1:59:A:VAL:HG22	1:100:A:PHE:HD2	9	0.2
(1,62)	1:59:A:VAL:HG23	1:100:A:PHE:HD1	9	0.2
(1,62)	1:59:A:VAL:HG23	1:100:A:PHE:HD2	9	0.2
(1,1425)	1:112:A:LYS:HA	1:145:A:LEU:HD11	9	0.19
(1,1425)	1:112:A:LYS:HA	1:145:A:LEU:HD12	9	0.19
(1,1425)	1:112:A:LYS:HA	1:145:A:LEU:HD13	9	0.19
(1,1425)	1:112:A:LYS:HA	1:145:A:LEU:HD21	9	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1425)	1:112:A:LYS:HA	1:145:A:LEU:HD22	9	0.19
(1,1425)	1:112:A:LYS:HA	1:145:A:LEU:HD23	9	0.19
(1,1402)	1:104:A:LEU:HD11	1:141:A:LEU:HB2	16	0.19
(1,1402)	1:104:A:LEU:HD11	1:141:A:LEU:HB3	16	0.19
(1,1402)	1:104:A:LEU:HD12	1:141:A:LEU:HB2	16	0.19
(1,1402)	1:104:A:LEU:HD12	1:141:A:LEU:HB3	16	0.19
(1,1402)	1:104:A:LEU:HD13	1:141:A:LEU:HB2	16	0.19
(1,1402)	1:104:A:LEU:HD13	1:141:A:LEU:HB3	16	0.19
(1,1402)	1:104:A:LEU:HD21	1:141:A:LEU:HB2	16	0.19
(1,1402)	1:104:A:LEU:HD21	1:141:A:LEU:HB3	16	0.19
(1,1402)	1:104:A:LEU:HD22	1:141:A:LEU:HB2	16	0.19
(1,1402)	1:104:A:LEU:HD22	1:141:A:LEU:HB3	16	0.19
(1,1402)	1:104:A:LEU:HD23	1:141:A:LEU:HB2	16	0.19
(1,1402)	1:104:A:LEU:HD23	1:141:A:LEU:HB3	16	0.19
(1,1381)	1:97:A:ARG:HB2	1:101:A:ALA:H	18	0.19
(1,1381)	1:97:A:ARG:HB3	1:101:A:ALA:H	18	0.19
(1,1288)	1:63:A:MET:H	1:77:A:LEU:HD11	13	0.19
(1,1288)	1:63:A:MET:H	1:77:A:LEU:HD12	13	0.19
(1,1288)	1:63:A:MET:H	1:77:A:LEU:HD13	13	0.19
(1,1288)	1:63:A:MET:H	1:77:A:LEU:HD21	13	0.19
(1,1288)	1:63:A:MET:H	1:77:A:LEU:HD22	13	0.19
(1,1288)	1:63:A:MET:H	1:77:A:LEU:HD23	13	0.19
(1,1285)	1:62:A:TRP:HE1	1:77:A:LEU:HD11	18	0.19
(1,1285)	1:62:A:TRP:HE1	1:77:A:LEU:HD12	18	0.19
(1,1285)	1:62:A:TRP:HE1	1:77:A:LEU:HD13	18	0.19
(1,1285)	1:62:A:TRP:HE1	1:77:A:LEU:HD21	18	0.19
(1,1285)	1:62:A:TRP:HE1	1:77:A:LEU:HD22	18	0.19
(1,1285)	1:62:A:TRP:HE1	1:77:A:LEU:HD23	18	0.19
(1,1275)	1:59:A:VAL:HG11	1:102:A:ASP:H	12	0.19
(1,1275)	1:59:A:VAL:HG12	1:102:A:ASP:H	12	0.19
(1,1275)	1:59:A:VAL:HG13	1:102:A:ASP:H	12	0.19
(1,1275)	1:59:A:VAL:HG21	1:102:A:ASP:H	12	0.19
(1,1275)	1:59:A:VAL:HG22	1:102:A:ASP:H	12	0.19
(1,1275)	1:59:A:VAL:HG23	1:102:A:ASP:H	12	0.19
(1,1273)	1:59:A:VAL:HG11	1:100:A:PHE:HD1	9	0.19
(1,1273)	1:59:A:VAL:HG11	1:100:A:PHE:HD2	9	0.19
(1,1273)	1:59:A:VAL:HG12	1:100:A:PHE:HD1	9	0.19
(1,1273)	1:59:A:VAL:HG12	1:100:A:PHE:HD2	9	0.19
(1,1273)	1:59:A:VAL:HG13	1:100:A:PHE:HD1	9	0.19
(1,1273)	1:59:A:VAL:HG13	1:100:A:PHE:HD2	9	0.19
(1,1273)	1:59:A:VAL:HG21	1:100:A:PHE:HD1	9	0.19
(1,1273)	1:59:A:VAL:HG21	1:100:A:PHE:HD2	9	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1273)	1:59:A:VAL:HG22	1:100:A:PHE:HD1	9	0.19
(1,1273)	1:59:A:VAL:HG22	1:100:A:PHE:HD2	9	0.19
(1,1273)	1:59:A:VAL:HG23	1:100:A:PHE:HD1	9	0.19
(1,1273)	1:59:A:VAL:HG23	1:100:A:PHE:HD2	9	0.19
(1,1259)	1:59:A:VAL:HG11	1:61:A:HIS:H	2	0.19
(1,1259)	1:59:A:VAL:HG12	1:61:A:HIS:H	2	0.19
(1,1259)	1:59:A:VAL:HG13	1:61:A:HIS:H	2	0.19
(1,1259)	1:59:A:VAL:HG21	1:61:A:HIS:H	2	0.19
(1,1259)	1:59:A:VAL:HG22	1:61:A:HIS:H	2	0.19
(1,1259)	1:59:A:VAL:HG23	1:61:A:HIS:H	2	0.19
(1,1259)	1:59:A:VAL:HG11	1:61:A:HIS:H	17	0.19
(1,1259)	1:59:A:VAL:HG12	1:61:A:HIS:H	17	0.19
(1,1259)	1:59:A:VAL:HG13	1:61:A:HIS:H	17	0.19
(1,1259)	1:59:A:VAL:HG21	1:61:A:HIS:H	17	0.19
(1,1259)	1:59:A:VAL:HG22	1:61:A:HIS:H	17	0.19
(1,1259)	1:59:A:VAL:HG23	1:61:A:HIS:H	17	0.19
(1,1169)	1:34:A:VAL:HG21	1:35:A:THR:H	9	0.19
(1,1169)	1:34:A:VAL:HG22	1:35:A:THR:H	9	0.19
(1,1169)	1:34:A:VAL:HG23	1:35:A:THR:H	9	0.19
(1,952)	1:104:A:LEU:HD21	1:106:A:GLU:H	13	0.19
(1,952)	1:104:A:LEU:HD22	1:106:A:GLU:H	13	0.19
(1,952)	1:104:A:LEU:HD23	1:106:A:GLU:H	13	0.19
(1,771)	1:76:A:ASN:H	1:78:A:PHE:HB2	13	0.19
(1,656)	1:50:A:GLU:H	1:51:A:ASN:HD21	3	0.19
(1,625)	1:100:A:PHE:HD1	1:102:A:ASP:H	19	0.19
(1,625)	1:100:A:PHE:HD2	1:102:A:ASP:H	19	0.19
(1,583)	1:48:A:CYS:H	1:51:A:ASN:HB2	13	0.19
(1,579)	1:48:A:CYS:H	1:84:A:VAL:HG21	15	0.19
(1,579)	1:48:A:CYS:H	1:84:A:VAL:HG22	15	0.19
(1,579)	1:48:A:CYS:H	1:84:A:VAL:HG23	15	0.19
(1,574)	1:108:A:ALA:H	1:111:A:VAL:HG11	7	0.19
(1,574)	1:108:A:ALA:H	1:111:A:VAL:HG12	7	0.19
(1,574)	1:108:A:ALA:H	1:111:A:VAL:HG13	7	0.19
(1,536)	1:122:A:ARG:H	1:122:A:ARG:HD2	7	0.19
(1,536)	1:122:A:ARG:H	1:122:A:ARG:HD3	7	0.19
(1,536)	1:122:A:ARG:H	1:122:A:ARG:HD2	19	0.19
(1,536)	1:122:A:ARG:H	1:122:A:ARG:HD3	19	0.19
(1,471)	1:47:A:TRP:HA	1:47:A:TRP:HD1	18	0.19
(1,424)	1:84:A:VAL:HG11	1:88:A:CYS:HB2	13	0.19
(1,424)	1:84:A:VAL:HG11	1:88:A:CYS:HB3	13	0.19
(1,424)	1:84:A:VAL:HG12	1:88:A:CYS:HB2	13	0.19
(1,424)	1:84:A:VAL:HG12	1:88:A:CYS:HB3	13	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,424)	1:84:A:VAL:HG13	1:88:A:CYS:HB2	13	0.19
(1,424)	1:84:A:VAL:HG13	1:88:A:CYS:HB3	13	0.19
(1,424)	1:84:A:VAL:HG11	1:88:A:CYS:HB2	14	0.19
(1,424)	1:84:A:VAL:HG11	1:88:A:CYS:HB3	14	0.19
(1,424)	1:84:A:VAL:HG12	1:88:A:CYS:HB2	14	0.19
(1,424)	1:84:A:VAL:HG12	1:88:A:CYS:HB3	14	0.19
(1,424)	1:84:A:VAL:HG13	1:88:A:CYS:HB2	14	0.19
(1,424)	1:84:A:VAL:HG13	1:88:A:CYS:HB3	14	0.19
(1,379)	1:139:A:VAL:HG21	1:143:A:GLU:HG2	11	0.19
(1,379)	1:139:A:VAL:HG21	1:143:A:GLU:HG3	11	0.19
(1,379)	1:139:A:VAL:HG22	1:143:A:GLU:HG2	11	0.19
(1,379)	1:139:A:VAL:HG22	1:143:A:GLU:HG3	11	0.19
(1,379)	1:139:A:VAL:HG23	1:143:A:GLU:HG2	11	0.19
(1,379)	1:139:A:VAL:HG23	1:143:A:GLU:HG3	11	0.19
(1,371)	1:100:A:PHE:HA	1:103:A:VAL:HG11	15	0.19
(1,371)	1:100:A:PHE:HA	1:103:A:VAL:HG12	15	0.19
(1,371)	1:100:A:PHE:HA	1:103:A:VAL:HG13	15	0.19
(1,308)	1:103:A:VAL:HG21	1:107:A:ALA:HA	8	0.19
(1,308)	1:103:A:VAL:HG22	1:107:A:ALA:HA	8	0.19
(1,308)	1:103:A:VAL:HG23	1:107:A:ALA:HA	8	0.19
(1,296)	1:34:A:VAL:HG11	1:36:A:ASN:H	8	0.19
(1,296)	1:34:A:VAL:HG12	1:36:A:ASN:H	8	0.19
(1,296)	1:34:A:VAL:HG13	1:36:A:ASN:H	8	0.19
(1,296)	1:34:A:VAL:HG11	1:36:A:ASN:H	16	0.19
(1,296)	1:34:A:VAL:HG12	1:36:A:ASN:H	16	0.19
(1,296)	1:34:A:VAL:HG13	1:36:A:ASN:H	16	0.19
(1,61)	1:59:A:VAL:HG21	1:62:A:TRP:HE3	17	0.19
(1,61)	1:59:A:VAL:HG22	1:62:A:TRP:HE3	17	0.19
(1,61)	1:59:A:VAL:HG23	1:62:A:TRP:HE3	17	0.19
(1,1487)	1:132:A:VAL:HG11	1:133:A:TYR:H	16	0.18
(1,1487)	1:132:A:VAL:HG12	1:133:A:TYR:H	16	0.18
(1,1487)	1:132:A:VAL:HG13	1:133:A:TYR:H	16	0.18
(1,1487)	1:132:A:VAL:HG21	1:133:A:TYR:H	16	0.18
(1,1487)	1:132:A:VAL:HG22	1:133:A:TYR:H	16	0.18
(1,1487)	1:132:A:VAL:HG23	1:133:A:TYR:H	16	0.18
(1,1443)	1:116:A:VAL:HA	1:120:A:VAL:HG11	17	0.18
(1,1443)	1:116:A:VAL:HA	1:120:A:VAL:HG12	17	0.18
(1,1443)	1:116:A:VAL:HA	1:120:A:VAL:HG13	17	0.18
(1,1443)	1:116:A:VAL:HA	1:120:A:VAL:HG21	17	0.18
(1,1443)	1:116:A:VAL:HA	1:120:A:VAL:HG22	17	0.18
(1,1443)	1:116:A:VAL:HA	1:120:A:VAL:HG23	17	0.18
(1,1427)	1:112:A:LYS:HB2	1:145:A:LEU:HD11	6	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1427)	1:112:A:LYS:HB2	1:145:A:LEU:HD12	6	0.18
(1,1427)	1:112:A:LYS:HB2	1:145:A:LEU:HD13	6	0.18
(1,1427)	1:112:A:LYS:HB2	1:145:A:LEU:HD21	6	0.18
(1,1427)	1:112:A:LYS:HB2	1:145:A:LEU:HD22	6	0.18
(1,1427)	1:112:A:LYS:HB2	1:145:A:LEU:HD23	6	0.18
(1,1427)	1:112:A:LYS:HB3	1:145:A:LEU:HD11	6	0.18
(1,1427)	1:112:A:LYS:HB3	1:145:A:LEU:HD12	6	0.18
(1,1427)	1:112:A:LYS:HB3	1:145:A:LEU:HD13	6	0.18
(1,1427)	1:112:A:LYS:HB3	1:145:A:LEU:HD21	6	0.18
(1,1427)	1:112:A:LYS:HB3	1:145:A:LEU:HD22	6	0.18
(1,1427)	1:112:A:LYS:HB3	1:145:A:LEU:HD23	6	0.18
(1,1410)	1:108:A:ALA:HB1	1:145:A:LEU:HD11	9	0.18
(1,1410)	1:108:A:ALA:HB1	1:145:A:LEU:HD12	9	0.18
(1,1410)	1:108:A:ALA:HB1	1:145:A:LEU:HD13	9	0.18
(1,1410)	1:108:A:ALA:HB1	1:145:A:LEU:HD21	9	0.18
(1,1410)	1:108:A:ALA:HB1	1:145:A:LEU:HD22	9	0.18
(1,1410)	1:108:A:ALA:HB1	1:145:A:LEU:HD23	9	0.18
(1,1410)	1:108:A:ALA:HB2	1:145:A:LEU:HD11	9	0.18
(1,1410)	1:108:A:ALA:HB2	1:145:A:LEU:HD12	9	0.18
(1,1410)	1:108:A:ALA:HB2	1:145:A:LEU:HD13	9	0.18
(1,1410)	1:108:A:ALA:HB2	1:145:A:LEU:HD21	9	0.18
(1,1410)	1:108:A:ALA:HB2	1:145:A:LEU:HD22	9	0.18
(1,1410)	1:108:A:ALA:HB2	1:145:A:LEU:HD23	9	0.18
(1,1410)	1:108:A:ALA:HB3	1:145:A:LEU:HD11	9	0.18
(1,1410)	1:108:A:ALA:HB3	1:145:A:LEU:HD12	9	0.18
(1,1410)	1:108:A:ALA:HB3	1:145:A:LEU:HD13	9	0.18
(1,1410)	1:108:A:ALA:HB3	1:145:A:LEU:HD21	9	0.18
(1,1410)	1:108:A:ALA:HB3	1:145:A:LEU:HD22	9	0.18
(1,1410)	1:108:A:ALA:HB3	1:145:A:LEU:HD23	9	0.18
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD11	4	0.18
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD12	4	0.18
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD13	4	0.18
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD21	4	0.18
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD22	4	0.18
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD23	4	0.18
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD11	4	0.18
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD12	4	0.18
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD13	4	0.18
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD21	4	0.18
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD22	4	0.18
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD23	4	0.18
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD11	18	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD12	18	0.18
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD13	18	0.18
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD21	18	0.18
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD22	18	0.18
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD23	18	0.18
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD11	18	0.18
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD12	18	0.18
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD13	18	0.18
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD21	18	0.18
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD22	18	0.18
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD23	18	0.18
(1,1277)	1:59:A:VAL:HG11	1:103:A:VAL:HA	9	0.18
(1,1277)	1:59:A:VAL:HG12	1:103:A:VAL:HA	9	0.18
(1,1277)	1:59:A:VAL:HG13	1:103:A:VAL:HA	9	0.18
(1,1277)	1:59:A:VAL:HG21	1:103:A:VAL:HA	9	0.18
(1,1277)	1:59:A:VAL:HG22	1:103:A:VAL:HA	9	0.18
(1,1277)	1:59:A:VAL:HG23	1:103:A:VAL:HA	9	0.18
(1,1277)	1:59:A:VAL:HG11	1:103:A:VAL:HA	18	0.18
(1,1277)	1:59:A:VAL:HG12	1:103:A:VAL:HA	18	0.18
(1,1277)	1:59:A:VAL:HG13	1:103:A:VAL:HA	18	0.18
(1,1277)	1:59:A:VAL:HG21	1:103:A:VAL:HA	18	0.18
(1,1277)	1:59:A:VAL:HG22	1:103:A:VAL:HA	18	0.18
(1,1277)	1:59:A:VAL:HG23	1:103:A:VAL:HA	18	0.18
(1,1276)	1:59:A:VAL:HG11	1:103:A:VAL:H	19	0.18
(1,1276)	1:59:A:VAL:HG12	1:103:A:VAL:H	19	0.18
(1,1276)	1:59:A:VAL:HG13	1:103:A:VAL:H	19	0.18
(1,1276)	1:59:A:VAL:HG21	1:103:A:VAL:H	19	0.18
(1,1276)	1:59:A:VAL:HG22	1:103:A:VAL:H	19	0.18
(1,1276)	1:59:A:VAL:HG23	1:103:A:VAL:H	19	0.18
(1,1259)	1:59:A:VAL:HG11	1:61:A:HIS:H	1	0.18
(1,1259)	1:59:A:VAL:HG12	1:61:A:HIS:H	1	0.18
(1,1259)	1:59:A:VAL:HG13	1:61:A:HIS:H	1	0.18
(1,1259)	1:59:A:VAL:HG21	1:61:A:HIS:H	1	0.18
(1,1259)	1:59:A:VAL:HG22	1:61:A:HIS:H	1	0.18
(1,1259)	1:59:A:VAL:HG23	1:61:A:HIS:H	1	0.18
(1,1189)	1:62:A:TRP:HE1	1:77:A:LEU:HD21	13	0.18
(1,1189)	1:62:A:TRP:HE1	1:77:A:LEU:HD22	13	0.18
(1,1189)	1:62:A:TRP:HE1	1:77:A:LEU:HD23	13	0.18
(1,1078)	1:141:A:LEU:H	1:142:A:ARG:HG2	11	0.18
(1,1078)	1:141:A:LEU:H	1:142:A:ARG:HG3	11	0.18
(1,857)	1:111:A:VAL:HG11	1:112:A:LYS:H	1	0.18
(1,857)	1:111:A:VAL:HG12	1:112:A:LYS:H	1	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,857)	1:111:A:VAL:HG13	1:112:A:LYS:H	1	0.18
(1,857)	1:111:A:VAL:HG11	1:112:A:LYS:H	2	0.18
(1,857)	1:111:A:VAL:HG12	1:112:A:LYS:H	2	0.18
(1,857)	1:111:A:VAL:HG13	1:112:A:LYS:H	2	0.18
(1,847)	1:49:A:ILE:H	1:84:A:VAL:HG11	1	0.18
(1,847)	1:49:A:ILE:H	1:84:A:VAL:HG12	1	0.18
(1,847)	1:49:A:ILE:H	1:84:A:VAL:HG13	1	0.18
(1,824)	1:98:A:GLU:H	1:133:A:TYR:HD1	1	0.18
(1,824)	1:98:A:GLU:H	1:133:A:TYR:HD2	1	0.18
(1,719)	1:109:A:ALA:H	1:112:A:LYS:H	15	0.18
(1,625)	1:100:A:PHE:HD1	1:102:A:ASP:H	10	0.18
(1,625)	1:100:A:PHE:HD2	1:102:A:ASP:H	10	0.18
(1,583)	1:48:A:CYS:H	1:51:A:ASN:HB2	6	0.18
(1,583)	1:48:A:CYS:H	1:51:A:ASN:HB2	11	0.18
(1,583)	1:48:A:CYS:H	1:51:A:ASN:HB2	16	0.18
(1,574)	1:108:A:ALA:H	1:111:A:VAL:HG11	8	0.18
(1,574)	1:108:A:ALA:H	1:111:A:VAL:HG12	8	0.18
(1,574)	1:108:A:ALA:H	1:111:A:VAL:HG13	8	0.18
(1,471)	1:47:A:TRP:HA	1:47:A:TRP:HD1	12	0.18
(1,442)	1:75:A:LEU:HD11	1:78:A:PHE:HB3	19	0.18
(1,442)	1:75:A:LEU:HD12	1:78:A:PHE:HB3	19	0.18
(1,442)	1:75:A:LEU:HD13	1:78:A:PHE:HB3	19	0.18
(1,359)	1:75:A:LEU:HD11	1:119:A:SER:HA	11	0.18
(1,359)	1:75:A:LEU:HD12	1:119:A:SER:HA	11	0.18
(1,359)	1:75:A:LEU:HD13	1:119:A:SER:HA	11	0.18
(1,1505)	1:139:A:VAL:H	1:141:A:LEU:HD11	12	0.17
(1,1505)	1:139:A:VAL:H	1:141:A:LEU:HD12	12	0.17
(1,1505)	1:139:A:VAL:H	1:141:A:LEU:HD13	12	0.17
(1,1505)	1:139:A:VAL:H	1:141:A:LEU:HD21	12	0.17
(1,1505)	1:139:A:VAL:H	1:141:A:LEU:HD22	12	0.17
(1,1505)	1:139:A:VAL:H	1:141:A:LEU:HD23	12	0.17
(1,1500)	1:137:A:MET:HB2	1:141:A:LEU:HD11	15	0.17
(1,1500)	1:137:A:MET:HB2	1:141:A:LEU:HD12	15	0.17
(1,1500)	1:137:A:MET:HB2	1:141:A:LEU:HD13	15	0.17
(1,1500)	1:137:A:MET:HB2	1:141:A:LEU:HD21	15	0.17
(1,1500)	1:137:A:MET:HB2	1:141:A:LEU:HD22	15	0.17
(1,1500)	1:137:A:MET:HB2	1:141:A:LEU:HD23	15	0.17
(1,1487)	1:132:A:VAL:HG11	1:133:A:TYR:H	1	0.17
(1,1487)	1:132:A:VAL:HG12	1:133:A:TYR:H	1	0.17
(1,1487)	1:132:A:VAL:HG13	1:133:A:TYR:H	1	0.17
(1,1487)	1:132:A:VAL:HG21	1:133:A:TYR:H	1	0.17
(1,1487)	1:132:A:VAL:HG22	1:133:A:TYR:H	1	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1487)	1:132:A:VAL:HG23	1:133:A:TYR:H	1	0.17
(1,1347)	1:84:A:VAL:HG11	1:85:A:ILE:HG12	15	0.17
(1,1347)	1:84:A:VAL:HG11	1:85:A:ILE:HG13	15	0.17
(1,1347)	1:84:A:VAL:HG12	1:85:A:ILE:HG12	15	0.17
(1,1347)	1:84:A:VAL:HG12	1:85:A:ILE:HG13	15	0.17
(1,1347)	1:84:A:VAL:HG13	1:85:A:ILE:HG12	15	0.17
(1,1347)	1:84:A:VAL:HG13	1:85:A:ILE:HG13	15	0.17
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD11	5	0.17
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD12	5	0.17
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD13	5	0.17
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD21	5	0.17
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD22	5	0.17
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD23	5	0.17
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD11	5	0.17
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD12	5	0.17
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD13	5	0.17
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD21	5	0.17
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD22	5	0.17
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD23	5	0.17
(1,1294)	1:63:A:MET:HG2	1:103:A:VAL:HG11	19	0.17
(1,1294)	1:63:A:MET:HG2	1:103:A:VAL:HG12	19	0.17
(1,1294)	1:63:A:MET:HG2	1:103:A:VAL:HG13	19	0.17
(1,1294)	1:63:A:MET:HG3	1:103:A:VAL:HG11	19	0.17
(1,1294)	1:63:A:MET:HG3	1:103:A:VAL:HG12	19	0.17
(1,1294)	1:63:A:MET:HG3	1:103:A:VAL:HG13	19	0.17
(1,1275)	1:59:A:VAL:HG11	1:102:A:ASP:H	3	0.17
(1,1275)	1:59:A:VAL:HG12	1:102:A:ASP:H	3	0.17
(1,1275)	1:59:A:VAL:HG13	1:102:A:ASP:H	3	0.17
(1,1275)	1:59:A:VAL:HG21	1:102:A:ASP:H	3	0.17
(1,1275)	1:59:A:VAL:HG22	1:102:A:ASP:H	3	0.17
(1,1275)	1:59:A:VAL:HG23	1:102:A:ASP:H	3	0.17
(1,1218)	1:44:A:LEU:HB2	1:80:A:LEU:HD11	11	0.17
(1,1218)	1:44:A:LEU:HB2	1:80:A:LEU:HD12	11	0.17
(1,1218)	1:44:A:LEU:HB2	1:80:A:LEU:HD13	11	0.17
(1,1218)	1:44:A:LEU:HB2	1:80:A:LEU:HD21	11	0.17
(1,1218)	1:44:A:LEU:HB2	1:80:A:LEU:HD22	11	0.17
(1,1218)	1:44:A:LEU:HB2	1:80:A:LEU:HD23	11	0.17
(1,1112)	1:61:A:HIS:H	1:61:A:HIS:HD2	12	0.17
(1,1078)	1:141:A:LEU:H	1:142:A:ARG:HG2	7	0.17
(1,1078)	1:141:A:LEU:H	1:142:A:ARG:HG3	7	0.17
(1,963)	1:109:A:ALA:H	1:111:A:VAL:HG11	14	0.17
(1,963)	1:109:A:ALA:H	1:111:A:VAL:HG12	14	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,963)	1:109:A:ALA:H	1:111:A:VAL:HG13	14	0.17
(1,857)	1:111:A:VAL:HG11	1:112:A:LYS:H	5	0.17
(1,857)	1:111:A:VAL:HG12	1:112:A:LYS:H	5	0.17
(1,857)	1:111:A:VAL:HG13	1:112:A:LYS:H	5	0.17
(1,857)	1:111:A:VAL:HG11	1:112:A:LYS:H	7	0.17
(1,857)	1:111:A:VAL:HG12	1:112:A:LYS:H	7	0.17
(1,857)	1:111:A:VAL:HG13	1:112:A:LYS:H	7	0.17
(1,847)	1:49:A:ILE:H	1:84:A:VAL:HG11	2	0.17
(1,847)	1:49:A:ILE:H	1:84:A:VAL:HG12	2	0.17
(1,847)	1:49:A:ILE:H	1:84:A:VAL:HG13	2	0.17
(1,847)	1:49:A:ILE:H	1:84:A:VAL:HG11	5	0.17
(1,847)	1:49:A:ILE:H	1:84:A:VAL:HG12	5	0.17
(1,847)	1:49:A:ILE:H	1:84:A:VAL:HG13	5	0.17
(1,847)	1:49:A:ILE:H	1:84:A:VAL:HG11	17	0.17
(1,847)	1:49:A:ILE:H	1:84:A:VAL:HG12	17	0.17
(1,847)	1:49:A:ILE:H	1:84:A:VAL:HG13	17	0.17
(1,831)	1:92:A:ASN:H	1:93:A:ALA:H	18	0.17
(1,818)	1:110:A:LEU:H	1:111:A:VAL:HG11	12	0.17
(1,818)	1:110:A:LEU:H	1:111:A:VAL:HG12	12	0.17
(1,818)	1:110:A:LEU:H	1:111:A:VAL:HG13	12	0.17
(1,771)	1:76:A:ASN:H	1:78:A:PHE:HB2	9	0.17
(1,771)	1:76:A:ASN:H	1:78:A:PHE:HB2	15	0.17
(1,656)	1:50:A:GLU:H	1:51:A:ASN:HD21	4	0.17
(1,656)	1:50:A:GLU:H	1:51:A:ASN:HD21	11	0.17
(1,583)	1:48:A:CYS:H	1:51:A:ASN:HB2	7	0.17
(1,583)	1:48:A:CYS:H	1:51:A:ASN:HB2	8	0.17
(1,574)	1:108:A:ALA:H	1:111:A:VAL:HG11	16	0.17
(1,574)	1:108:A:ALA:H	1:111:A:VAL:HG12	16	0.17
(1,574)	1:108:A:ALA:H	1:111:A:VAL:HG13	16	0.17
(1,424)	1:84:A:VAL:HG11	1:88:A:CYS:HB2	2	0.17
(1,424)	1:84:A:VAL:HG11	1:88:A:CYS:HB3	2	0.17
(1,424)	1:84:A:VAL:HG12	1:88:A:CYS:HB2	2	0.17
(1,424)	1:84:A:VAL:HG12	1:88:A:CYS:HB3	2	0.17
(1,424)	1:84:A:VAL:HG13	1:88:A:CYS:HB2	2	0.17
(1,424)	1:84:A:VAL:HG13	1:88:A:CYS:HB3	2	0.17
(1,424)	1:84:A:VAL:HG11	1:88:A:CYS:HB2	16	0.17
(1,424)	1:84:A:VAL:HG11	1:88:A:CYS:HB3	16	0.17
(1,424)	1:84:A:VAL:HG12	1:88:A:CYS:HB2	16	0.17
(1,424)	1:84:A:VAL:HG12	1:88:A:CYS:HB3	16	0.17
(1,424)	1:84:A:VAL:HG13	1:88:A:CYS:HB2	16	0.17
(1,424)	1:84:A:VAL:HG13	1:88:A:CYS:HB3	16	0.17
(1,424)	1:84:A:VAL:HG11	1:88:A:CYS:HB2	17	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,424)	1:84:A:VAL:HG11	1:88:A:CYS:HB3	17	0.17
(1,424)	1:84:A:VAL:HG12	1:88:A:CYS:HB2	17	0.17
(1,424)	1:84:A:VAL:HG12	1:88:A:CYS:HB3	17	0.17
(1,424)	1:84:A:VAL:HG13	1:88:A:CYS:HB2	17	0.17
(1,424)	1:84:A:VAL:HG13	1:88:A:CYS:HB3	17	0.17
(1,388)	1:78:A:PHE:HB3	1:111:A:VAL:HG11	6	0.17
(1,388)	1:78:A:PHE:HB3	1:111:A:VAL:HG12	6	0.17
(1,388)	1:78:A:PHE:HB3	1:111:A:VAL:HG13	6	0.17
(1,371)	1:100:A:PHE:HA	1:103:A:VAL:HG11	17	0.17
(1,371)	1:100:A:PHE:HA	1:103:A:VAL:HG12	17	0.17
(1,371)	1:100:A:PHE:HA	1:103:A:VAL:HG13	17	0.17
(1,297)	1:37:A:THR:HG21	1:38:A:MET:HB2	10	0.17
(1,297)	1:37:A:THR:HG21	1:38:A:MET:HB3	10	0.17
(1,297)	1:37:A:THR:HG22	1:38:A:MET:HB2	10	0.17
(1,297)	1:37:A:THR:HG22	1:38:A:MET:HB3	10	0.17
(1,297)	1:37:A:THR:HG23	1:38:A:MET:HB2	10	0.17
(1,297)	1:37:A:THR:HG23	1:38:A:MET:HB3	10	0.17
(1,296)	1:34:A:VAL:HG11	1:36:A:ASN:H	17	0.17
(1,296)	1:34:A:VAL:HG12	1:36:A:ASN:H	17	0.17
(1,296)	1:34:A:VAL:HG13	1:36:A:ASN:H	17	0.17
(1,252)	1:111:A:VAL:HG21	1:121:A:GLU:H	1	0.17
(1,252)	1:111:A:VAL:HG22	1:121:A:GLU:H	1	0.17
(1,252)	1:111:A:VAL:HG23	1:121:A:GLU:H	1	0.17
(1,252)	1:111:A:VAL:HG21	1:121:A:GLU:H	14	0.17
(1,252)	1:111:A:VAL:HG22	1:121:A:GLU:H	14	0.17
(1,252)	1:111:A:VAL:HG23	1:121:A:GLU:H	14	0.17
(2,12)	2:158:B:TYR:HD1	1:132:A:VAL:HG11	3	0.16
(2,12)	2:158:B:TYR:HD1	1:132:A:VAL:HG12	3	0.16
(2,12)	2:158:B:TYR:HD1	1:132:A:VAL:HG13	3	0.16
(2,12)	2:158:B:TYR:HD2	1:132:A:VAL:HG11	3	0.16
(2,12)	2:158:B:TYR:HD2	1:132:A:VAL:HG12	3	0.16
(2,12)	2:158:B:TYR:HD2	1:132:A:VAL:HG13	3	0.16
(1,1511)	1:140:A:ALA:H	1:141:A:LEU:HD11	13	0.16
(1,1511)	1:140:A:ALA:H	1:141:A:LEU:HD12	13	0.16
(1,1511)	1:140:A:ALA:H	1:141:A:LEU:HD13	13	0.16
(1,1511)	1:140:A:ALA:H	1:141:A:LEU:HD21	13	0.16
(1,1511)	1:140:A:ALA:H	1:141:A:LEU:HD22	13	0.16
(1,1511)	1:140:A:ALA:H	1:141:A:LEU:HD23	13	0.16
(1,1505)	1:139:A:VAL:H	1:141:A:LEU:HD11	3	0.16
(1,1505)	1:139:A:VAL:H	1:141:A:LEU:HD12	3	0.16
(1,1505)	1:139:A:VAL:H	1:141:A:LEU:HD13	3	0.16
(1,1505)	1:139:A:VAL:H	1:141:A:LEU:HD21	3	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1505)	1:139:A:VAL:H	1:141:A:LEU:HD22	3	0.16
(1,1505)	1:139:A:VAL:H	1:141:A:LEU:HD23	3	0.16
(1,1487)	1:132:A:VAL:HG11	1:133:A:TYR:H	7	0.16
(1,1487)	1:132:A:VAL:HG12	1:133:A:TYR:H	7	0.16
(1,1487)	1:132:A:VAL:HG13	1:133:A:TYR:H	7	0.16
(1,1487)	1:132:A:VAL:HG21	1:133:A:TYR:H	7	0.16
(1,1487)	1:132:A:VAL:HG22	1:133:A:TYR:H	7	0.16
(1,1487)	1:132:A:VAL:HG23	1:133:A:TYR:H	7	0.16
(1,1450)	1:116:A:VAL:HG11	1:120:A:VAL:HG11	8	0.16
(1,1450)	1:116:A:VAL:HG11	1:120:A:VAL:HG12	8	0.16
(1,1450)	1:116:A:VAL:HG11	1:120:A:VAL:HG13	8	0.16
(1,1450)	1:116:A:VAL:HG11	1:120:A:VAL:HG21	8	0.16
(1,1450)	1:116:A:VAL:HG11	1:120:A:VAL:HG22	8	0.16
(1,1450)	1:116:A:VAL:HG11	1:120:A:VAL:HG23	8	0.16
(1,1450)	1:116:A:VAL:HG12	1:120:A:VAL:HG11	8	0.16
(1,1450)	1:116:A:VAL:HG12	1:120:A:VAL:HG12	8	0.16
(1,1450)	1:116:A:VAL:HG12	1:120:A:VAL:HG13	8	0.16
(1,1450)	1:116:A:VAL:HG12	1:120:A:VAL:HG21	8	0.16
(1,1450)	1:116:A:VAL:HG12	1:120:A:VAL:HG22	8	0.16
(1,1450)	1:116:A:VAL:HG12	1:120:A:VAL:HG23	8	0.16
(1,1450)	1:116:A:VAL:HG13	1:120:A:VAL:HG11	8	0.16
(1,1450)	1:116:A:VAL:HG13	1:120:A:VAL:HG12	8	0.16
(1,1450)	1:116:A:VAL:HG13	1:120:A:VAL:HG13	8	0.16
(1,1450)	1:116:A:VAL:HG13	1:120:A:VAL:HG21	8	0.16
(1,1450)	1:116:A:VAL:HG13	1:120:A:VAL:HG22	8	0.16
(1,1450)	1:116:A:VAL:HG13	1:120:A:VAL:HG23	8	0.16
(1,1450)	1:116:A:VAL:HG21	1:120:A:VAL:HG11	8	0.16
(1,1450)	1:116:A:VAL:HG21	1:120:A:VAL:HG12	8	0.16
(1,1450)	1:116:A:VAL:HG21	1:120:A:VAL:HG13	8	0.16
(1,1450)	1:116:A:VAL:HG21	1:120:A:VAL:HG21	8	0.16
(1,1450)	1:116:A:VAL:HG21	1:120:A:VAL:HG22	8	0.16
(1,1450)	1:116:A:VAL:HG21	1:120:A:VAL:HG23	8	0.16
(1,1450)	1:116:A:VAL:HG22	1:120:A:VAL:HG11	8	0.16
(1,1450)	1:116:A:VAL:HG22	1:120:A:VAL:HG12	8	0.16
(1,1450)	1:116:A:VAL:HG22	1:120:A:VAL:HG13	8	0.16
(1,1450)	1:116:A:VAL:HG22	1:120:A:VAL:HG21	8	0.16
(1,1450)	1:116:A:VAL:HG22	1:120:A:VAL:HG22	8	0.16
(1,1450)	1:116:A:VAL:HG22	1:120:A:VAL:HG23	8	0.16
(1,1450)	1:116:A:VAL:HG23	1:120:A:VAL:HG11	8	0.16
(1,1450)	1:116:A:VAL:HG23	1:120:A:VAL:HG12	8	0.16
(1,1450)	1:116:A:VAL:HG23	1:120:A:VAL:HG13	8	0.16
(1,1450)	1:116:A:VAL:HG23	1:120:A:VAL:HG21	8	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1450)	1:116:A:VAL:HG23	1:120:A:VAL:HG22	8	0.16
(1,1450)	1:116:A:VAL:HG23	1:120:A:VAL:HG23	8	0.16
(1,1450)	1:116:A:VAL:HG11	1:120:A:VAL:HG11	9	0.16
(1,1450)	1:116:A:VAL:HG11	1:120:A:VAL:HG12	9	0.16
(1,1450)	1:116:A:VAL:HG11	1:120:A:VAL:HG13	9	0.16
(1,1450)	1:116:A:VAL:HG11	1:120:A:VAL:HG21	9	0.16
(1,1450)	1:116:A:VAL:HG11	1:120:A:VAL:HG22	9	0.16
(1,1450)	1:116:A:VAL:HG11	1:120:A:VAL:HG23	9	0.16
(1,1450)	1:116:A:VAL:HG12	1:120:A:VAL:HG11	9	0.16
(1,1450)	1:116:A:VAL:HG12	1:120:A:VAL:HG12	9	0.16
(1,1450)	1:116:A:VAL:HG12	1:120:A:VAL:HG13	9	0.16
(1,1450)	1:116:A:VAL:HG12	1:120:A:VAL:HG21	9	0.16
(1,1450)	1:116:A:VAL:HG12	1:120:A:VAL:HG22	9	0.16
(1,1450)	1:116:A:VAL:HG12	1:120:A:VAL:HG23	9	0.16
(1,1450)	1:116:A:VAL:HG13	1:120:A:VAL:HG11	9	0.16
(1,1450)	1:116:A:VAL:HG13	1:120:A:VAL:HG12	9	0.16
(1,1450)	1:116:A:VAL:HG13	1:120:A:VAL:HG13	9	0.16
(1,1450)	1:116:A:VAL:HG13	1:120:A:VAL:HG21	9	0.16
(1,1450)	1:116:A:VAL:HG13	1:120:A:VAL:HG22	9	0.16
(1,1450)	1:116:A:VAL:HG13	1:120:A:VAL:HG23	9	0.16
(1,1450)	1:116:A:VAL:HG21	1:120:A:VAL:HG11	9	0.16
(1,1450)	1:116:A:VAL:HG21	1:120:A:VAL:HG12	9	0.16
(1,1450)	1:116:A:VAL:HG21	1:120:A:VAL:HG13	9	0.16
(1,1450)	1:116:A:VAL:HG21	1:120:A:VAL:HG21	9	0.16
(1,1450)	1:116:A:VAL:HG21	1:120:A:VAL:HG22	9	0.16
(1,1450)	1:116:A:VAL:HG21	1:120:A:VAL:HG23	9	0.16
(1,1450)	1:116:A:VAL:HG22	1:120:A:VAL:HG11	9	0.16
(1,1450)	1:116:A:VAL:HG22	1:120:A:VAL:HG12	9	0.16
(1,1450)	1:116:A:VAL:HG22	1:120:A:VAL:HG13	9	0.16
(1,1450)	1:116:A:VAL:HG22	1:120:A:VAL:HG21	9	0.16
(1,1450)	1:116:A:VAL:HG22	1:120:A:VAL:HG22	9	0.16
(1,1450)	1:116:A:VAL:HG22	1:120:A:VAL:HG23	9	0.16
(1,1450)	1:116:A:VAL:HG23	1:120:A:VAL:HG11	9	0.16
(1,1450)	1:116:A:VAL:HG23	1:120:A:VAL:HG12	9	0.16
(1,1450)	1:116:A:VAL:HG23	1:120:A:VAL:HG13	9	0.16
(1,1450)	1:116:A:VAL:HG23	1:120:A:VAL:HG21	9	0.16
(1,1450)	1:116:A:VAL:HG23	1:120:A:VAL:HG22	9	0.16
(1,1450)	1:116:A:VAL:HG23	1:120:A:VAL:HG23	9	0.16
(1,1285)	1:62:A:TRP:HE1	1:77:A:LEU:HD11	4	0.16
(1,1285)	1:62:A:TRP:HE1	1:77:A:LEU:HD12	4	0.16
(1,1285)	1:62:A:TRP:HE1	1:77:A:LEU:HD13	4	0.16
(1,1285)	1:62:A:TRP:HE1	1:77:A:LEU:HD21	4	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1285)	1:62:A:TRP:HE1	1:77:A:LEU:HD22	4	0.16
(1,1285)	1:62:A:TRP:HE1	1:77:A:LEU:HD23	4	0.16
(1,1285)	1:62:A:TRP:HE1	1:77:A:LEU:HD11	9	0.16
(1,1285)	1:62:A:TRP:HE1	1:77:A:LEU:HD12	9	0.16
(1,1285)	1:62:A:TRP:HE1	1:77:A:LEU:HD13	9	0.16
(1,1285)	1:62:A:TRP:HE1	1:77:A:LEU:HD21	9	0.16
(1,1285)	1:62:A:TRP:HE1	1:77:A:LEU:HD22	9	0.16
(1,1285)	1:62:A:TRP:HE1	1:77:A:LEU:HD23	9	0.16
(1,1280)	1:59:A:VAL:HG11	1:103:A:VAL:HG21	5	0.16
(1,1280)	1:59:A:VAL:HG11	1:103:A:VAL:HG22	5	0.16
(1,1280)	1:59:A:VAL:HG11	1:103:A:VAL:HG23	5	0.16
(1,1280)	1:59:A:VAL:HG12	1:103:A:VAL:HG21	5	0.16
(1,1280)	1:59:A:VAL:HG12	1:103:A:VAL:HG22	5	0.16
(1,1280)	1:59:A:VAL:HG12	1:103:A:VAL:HG23	5	0.16
(1,1280)	1:59:A:VAL:HG13	1:103:A:VAL:HG21	5	0.16
(1,1280)	1:59:A:VAL:HG13	1:103:A:VAL:HG22	5	0.16
(1,1280)	1:59:A:VAL:HG13	1:103:A:VAL:HG23	5	0.16
(1,1280)	1:59:A:VAL:HG21	1:103:A:VAL:HG21	5	0.16
(1,1280)	1:59:A:VAL:HG21	1:103:A:VAL:HG22	5	0.16
(1,1280)	1:59:A:VAL:HG21	1:103:A:VAL:HG23	5	0.16
(1,1280)	1:59:A:VAL:HG22	1:103:A:VAL:HG21	5	0.16
(1,1280)	1:59:A:VAL:HG22	1:103:A:VAL:HG22	5	0.16
(1,1280)	1:59:A:VAL:HG22	1:103:A:VAL:HG23	5	0.16
(1,1280)	1:59:A:VAL:HG23	1:103:A:VAL:HG21	5	0.16
(1,1280)	1:59:A:VAL:HG23	1:103:A:VAL:HG22	5	0.16
(1,1280)	1:59:A:VAL:HG23	1:103:A:VAL:HG23	5	0.16
(1,1259)	1:59:A:VAL:HG11	1:61:A:HIS:H	6	0.16
(1,1259)	1:59:A:VAL:HG12	1:61:A:HIS:H	6	0.16
(1,1259)	1:59:A:VAL:HG13	1:61:A:HIS:H	6	0.16
(1,1259)	1:59:A:VAL:HG21	1:61:A:HIS:H	6	0.16
(1,1259)	1:59:A:VAL:HG22	1:61:A:HIS:H	6	0.16
(1,1259)	1:59:A:VAL:HG23	1:61:A:HIS:H	6	0.16
(1,1196)	1:82:A:ASN:H	1:127:A:TRP:HE1	1	0.16
(1,1072)	1:139:A:VAL:HG21	1:140:A:ALA:H	10	0.16
(1,1072)	1:139:A:VAL:HG22	1:140:A:ALA:H	10	0.16
(1,1072)	1:139:A:VAL:HG23	1:140:A:ALA:H	10	0.16
(1,981)	1:112:A:LYS:HB2	1:113:A:ASP:H	17	0.16
(1,981)	1:112:A:LYS:HB3	1:113:A:ASP:H	17	0.16
(1,950)	1:103:A:VAL:HG21	1:107:A:ALA:H	11	0.16
(1,950)	1:103:A:VAL:HG22	1:107:A:ALA:H	11	0.16
(1,950)	1:103:A:VAL:HG23	1:107:A:ALA:H	11	0.16
(1,656)	1:50:A:GLU:H	1:51:A:ASN:HD21	6	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,656)	1:50:A:GLU:H	1:51:A:ASN:HD21	8	0.16
(1,583)	1:48:A:CYS:H	1:51:A:ASN:HB2	5	0.16
(1,574)	1:108:A:ALA:H	1:111:A:VAL:HG11	15	0.16
(1,574)	1:108:A:ALA:H	1:111:A:VAL:HG12	15	0.16
(1,574)	1:108:A:ALA:H	1:111:A:VAL:HG13	15	0.16
(1,536)	1:122:A:ARG:H	1:122:A:ARG:HD2	15	0.16
(1,536)	1:122:A:ARG:H	1:122:A:ARG:HD3	15	0.16
(1,442)	1:75:A:LEU:HD11	1:78:A:PHE:HB3	5	0.16
(1,442)	1:75:A:LEU:HD12	1:78:A:PHE:HB3	5	0.16
(1,442)	1:75:A:LEU:HD13	1:78:A:PHE:HB3	5	0.16
(1,433)	1:84:A:VAL:HG11	1:96:A:PHE:HE1	3	0.16
(1,433)	1:84:A:VAL:HG11	1:96:A:PHE:HE2	3	0.16
(1,433)	1:84:A:VAL:HG12	1:96:A:PHE:HE1	3	0.16
(1,433)	1:84:A:VAL:HG12	1:96:A:PHE:HE2	3	0.16
(1,433)	1:84:A:VAL:HG13	1:96:A:PHE:HE1	3	0.16
(1,433)	1:84:A:VAL:HG13	1:96:A:PHE:HE2	3	0.16
(1,371)	1:100:A:PHE:HA	1:103:A:VAL:HG11	19	0.16
(1,371)	1:100:A:PHE:HA	1:103:A:VAL:HG12	19	0.16
(1,371)	1:100:A:PHE:HA	1:103:A:VAL:HG13	19	0.16
(1,297)	1:37:A:THR:HG21	1:38:A:MET:HB2	2	0.16
(1,297)	1:37:A:THR:HG21	1:38:A:MET:HB3	2	0.16
(1,297)	1:37:A:THR:HG22	1:38:A:MET:HB2	2	0.16
(1,297)	1:37:A:THR:HG22	1:38:A:MET:HB3	2	0.16
(1,297)	1:37:A:THR:HG23	1:38:A:MET:HB2	2	0.16
(1,297)	1:37:A:THR:HG23	1:38:A:MET:HB3	2	0.16
(1,252)	1:111:A:VAL:HG21	1:121:A:GLU:H	8	0.16
(1,252)	1:111:A:VAL:HG22	1:121:A:GLU:H	8	0.16
(1,252)	1:111:A:VAL:HG23	1:121:A:GLU:H	8	0.16
(1,252)	1:111:A:VAL:HG21	1:121:A:GLU:H	9	0.16
(1,252)	1:111:A:VAL:HG22	1:121:A:GLU:H	9	0.16
(1,252)	1:111:A:VAL:HG23	1:121:A:GLU:H	9	0.16
(1,252)	1:111:A:VAL:HG21	1:121:A:GLU:H	19	0.16
(1,252)	1:111:A:VAL:HG22	1:121:A:GLU:H	19	0.16
(1,252)	1:111:A:VAL:HG23	1:121:A:GLU:H	19	0.16
(1,62)	1:59:A:VAL:HG21	1:100:A:PHE:HD1	5	0.16
(1,62)	1:59:A:VAL:HG21	1:100:A:PHE:HD2	5	0.16
(1,62)	1:59:A:VAL:HG22	1:100:A:PHE:HD1	5	0.16
(1,62)	1:59:A:VAL:HG22	1:100:A:PHE:HD2	5	0.16
(1,62)	1:59:A:VAL:HG23	1:100:A:PHE:HD1	5	0.16
(1,62)	1:59:A:VAL:HG23	1:100:A:PHE:HD2	5	0.16
(5,1)	2:155:B:SER:H	1:130:A:ARG:NH2	20	0.15
(4,1)	2:151:B:TYR:HH	1:82:A:ASN:ND2	4	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1511)	1:140:A:ALA:H	1:141:A:LEU:HD11	18	0.15
(1,1511)	1:140:A:ALA:H	1:141:A:LEU:HD12	18	0.15
(1,1511)	1:140:A:ALA:H	1:141:A:LEU:HD13	18	0.15
(1,1511)	1:140:A:ALA:H	1:141:A:LEU:HD21	18	0.15
(1,1511)	1:140:A:ALA:H	1:141:A:LEU:HD22	18	0.15
(1,1511)	1:140:A:ALA:H	1:141:A:LEU:HD23	18	0.15
(1,1443)	1:116:A:VAL:HA	1:120:A:VAL:HG11	9	0.15
(1,1443)	1:116:A:VAL:HA	1:120:A:VAL:HG12	9	0.15
(1,1443)	1:116:A:VAL:HA	1:120:A:VAL:HG13	9	0.15
(1,1443)	1:116:A:VAL:HA	1:120:A:VAL:HG21	9	0.15
(1,1443)	1:116:A:VAL:HA	1:120:A:VAL:HG22	9	0.15
(1,1443)	1:116:A:VAL:HA	1:120:A:VAL:HG23	9	0.15
(1,1422)	1:112:A:LYS:H	1:145:A:LEU:HD11	19	0.15
(1,1422)	1:112:A:LYS:H	1:145:A:LEU:HD12	19	0.15
(1,1422)	1:112:A:LYS:H	1:145:A:LEU:HD13	19	0.15
(1,1422)	1:112:A:LYS:H	1:145:A:LEU:HD21	19	0.15
(1,1422)	1:112:A:LYS:H	1:145:A:LEU:HD22	19	0.15
(1,1422)	1:112:A:LYS:H	1:145:A:LEU:HD23	19	0.15
(1,1347)	1:84:A:VAL:HG11	1:85:A:ILE:HG12	4	0.15
(1,1347)	1:84:A:VAL:HG11	1:85:A:ILE:HG13	4	0.15
(1,1347)	1:84:A:VAL:HG12	1:85:A:ILE:HG12	4	0.15
(1,1347)	1:84:A:VAL:HG12	1:85:A:ILE:HG13	4	0.15
(1,1347)	1:84:A:VAL:HG13	1:85:A:ILE:HG12	4	0.15
(1,1347)	1:84:A:VAL:HG13	1:85:A:ILE:HG13	4	0.15
(1,1340)	1:78:A:PHE:HE1	1:104:A:LEU:HD11	9	0.15
(1,1340)	1:78:A:PHE:HE1	1:104:A:LEU:HD12	9	0.15
(1,1340)	1:78:A:PHE:HE1	1:104:A:LEU:HD13	9	0.15
(1,1340)	1:78:A:PHE:HE1	1:104:A:LEU:HD21	9	0.15
(1,1340)	1:78:A:PHE:HE1	1:104:A:LEU:HD22	9	0.15
(1,1340)	1:78:A:PHE:HE1	1:104:A:LEU:HD23	9	0.15
(1,1340)	1:78:A:PHE:HE2	1:104:A:LEU:HD11	9	0.15
(1,1340)	1:78:A:PHE:HE2	1:104:A:LEU:HD12	9	0.15
(1,1340)	1:78:A:PHE:HE2	1:104:A:LEU:HD13	9	0.15
(1,1340)	1:78:A:PHE:HE2	1:104:A:LEU:HD21	9	0.15
(1,1340)	1:78:A:PHE:HE2	1:104:A:LEU:HD22	9	0.15
(1,1340)	1:78:A:PHE:HE2	1:104:A:LEU:HD23	9	0.15
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD11	13	0.15
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD12	13	0.15
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD13	13	0.15
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD21	13	0.15
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD22	13	0.15
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD23	13	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD11	13	0.15
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD12	13	0.15
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD13	13	0.15
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD21	13	0.15
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD22	13	0.15
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD23	13	0.15
(1,1288)	1:63:A:MET:H	1:77:A:LEU:HD11	4	0.15
(1,1288)	1:63:A:MET:H	1:77:A:LEU:HD12	4	0.15
(1,1288)	1:63:A:MET:H	1:77:A:LEU:HD13	4	0.15
(1,1288)	1:63:A:MET:H	1:77:A:LEU:HD21	4	0.15
(1,1288)	1:63:A:MET:H	1:77:A:LEU:HD22	4	0.15
(1,1288)	1:63:A:MET:H	1:77:A:LEU:HD23	4	0.15
(1,1280)	1:59:A:VAL:HG11	1:103:A:VAL:HG21	14	0.15
(1,1280)	1:59:A:VAL:HG11	1:103:A:VAL:HG22	14	0.15
(1,1280)	1:59:A:VAL:HG11	1:103:A:VAL:HG23	14	0.15
(1,1280)	1:59:A:VAL:HG12	1:103:A:VAL:HG21	14	0.15
(1,1280)	1:59:A:VAL:HG12	1:103:A:VAL:HG22	14	0.15
(1,1280)	1:59:A:VAL:HG12	1:103:A:VAL:HG23	14	0.15
(1,1280)	1:59:A:VAL:HG13	1:103:A:VAL:HG21	14	0.15
(1,1280)	1:59:A:VAL:HG13	1:103:A:VAL:HG22	14	0.15
(1,1280)	1:59:A:VAL:HG13	1:103:A:VAL:HG23	14	0.15
(1,1280)	1:59:A:VAL:HG21	1:103:A:VAL:HG21	14	0.15
(1,1280)	1:59:A:VAL:HG21	1:103:A:VAL:HG22	14	0.15
(1,1280)	1:59:A:VAL:HG21	1:103:A:VAL:HG23	14	0.15
(1,1280)	1:59:A:VAL:HG22	1:103:A:VAL:HG21	14	0.15
(1,1280)	1:59:A:VAL:HG22	1:103:A:VAL:HG22	14	0.15
(1,1280)	1:59:A:VAL:HG22	1:103:A:VAL:HG23	14	0.15
(1,1280)	1:59:A:VAL:HG23	1:103:A:VAL:HG21	14	0.15
(1,1280)	1:59:A:VAL:HG23	1:103:A:VAL:HG22	14	0.15
(1,1280)	1:59:A:VAL:HG23	1:103:A:VAL:HG23	14	0.15
(1,1259)	1:59:A:VAL:HG11	1:61:A:HIS:H	19	0.15
(1,1259)	1:59:A:VAL:HG12	1:61:A:HIS:H	19	0.15
(1,1259)	1:59:A:VAL:HG13	1:61:A:HIS:H	19	0.15
(1,1259)	1:59:A:VAL:HG21	1:61:A:HIS:H	19	0.15
(1,1259)	1:59:A:VAL:HG22	1:61:A:HIS:H	19	0.15
(1,1259)	1:59:A:VAL:HG23	1:61:A:HIS:H	19	0.15
(1,1189)	1:62:A:TRP:HE1	1:77:A:LEU:HD21	3	0.15
(1,1189)	1:62:A:TRP:HE1	1:77:A:LEU:HD22	3	0.15
(1,1189)	1:62:A:TRP:HE1	1:77:A:LEU:HD23	3	0.15
(1,1169)	1:34:A:VAL:HG21	1:35:A:THR:H	12	0.15
(1,1169)	1:34:A:VAL:HG22	1:35:A:THR:H	12	0.15
(1,1169)	1:34:A:VAL:HG23	1:35:A:THR:H	12	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1077)	1:137:A:MET:HB3	1:141:A:LEU:H	3	0.15
(1,1073)	1:139:A:VAL:HB	1:140:A:ALA:H	15	0.15
(1,981)	1:112:A:LYS:HB2	1:113:A:ASP:H	20	0.15
(1,981)	1:112:A:LYS:HB3	1:113:A:ASP:H	20	0.15
(1,719)	1:109:A:ALA:H	1:112:A:LYS:H	3	0.15
(1,719)	1:109:A:ALA:H	1:112:A:LYS:H	16	0.15
(1,656)	1:50:A:GLU:H	1:51:A:ASN:HD21	18	0.15
(1,583)	1:48:A:CYS:H	1:51:A:ASN:HB2	2	0.15
(1,583)	1:48:A:CYS:H	1:51:A:ASN:HB2	15	0.15
(1,583)	1:48:A:CYS:H	1:51:A:ASN:HB2	19	0.15
(1,516)	1:77:A:LEU:HD21	1:78:A:PHE:H	12	0.15
(1,516)	1:77:A:LEU:HD22	1:78:A:PHE:H	12	0.15
(1,516)	1:77:A:LEU:HD23	1:78:A:PHE:H	12	0.15
(1,496)	1:85:A:ILE:HD11	1:86:A:GLN:H	9	0.15
(1,496)	1:85:A:ILE:HD12	1:86:A:GLN:H	9	0.15
(1,496)	1:85:A:ILE:HD13	1:86:A:GLN:H	9	0.15
(1,457)	1:95:A:ILE:HA	1:97:A:ARG:HG2	11	0.15
(1,457)	1:95:A:ILE:HA	1:97:A:ARG:HG3	11	0.15
(1,457)	1:95:A:ILE:HA	1:97:A:ARG:HG2	14	0.15
(1,457)	1:95:A:ILE:HA	1:97:A:ARG:HG3	14	0.15
(1,457)	1:95:A:ILE:HA	1:97:A:ARG:HG2	18	0.15
(1,457)	1:95:A:ILE:HA	1:97:A:ARG:HG3	18	0.15
(1,388)	1:78:A:PHE:HB3	1:111:A:VAL:HG11	3	0.15
(1,388)	1:78:A:PHE:HB3	1:111:A:VAL:HG12	3	0.15
(1,388)	1:78:A:PHE:HB3	1:111:A:VAL:HG13	3	0.15
(1,297)	1:37:A:THR:HG21	1:38:A:MET:HB2	19	0.15
(1,297)	1:37:A:THR:HG21	1:38:A:MET:HB3	19	0.15
(1,297)	1:37:A:THR:HG22	1:38:A:MET:HB2	19	0.15
(1,297)	1:37:A:THR:HG22	1:38:A:MET:HB3	19	0.15
(1,297)	1:37:A:THR:HG23	1:38:A:MET:HB2	19	0.15
(1,297)	1:37:A:THR:HG23	1:38:A:MET:HB3	19	0.15
(1,296)	1:34:A:VAL:HG11	1:36:A:ASN:H	11	0.15
(1,296)	1:34:A:VAL:HG12	1:36:A:ASN:H	11	0.15
(1,296)	1:34:A:VAL:HG13	1:36:A:ASN:H	11	0.15
(1,252)	1:111:A:VAL:HG21	1:121:A:GLU:H	6	0.15
(1,252)	1:111:A:VAL:HG22	1:121:A:GLU:H	6	0.15
(1,252)	1:111:A:VAL:HG23	1:121:A:GLU:H	6	0.15
(1,171)	1:34:A:VAL:H	1:36:A:ASN:HA	7	0.15
(1,171)	1:34:A:VAL:H	1:36:A:ASN:HA	15	0.15
(1,135)	1:101:A:ALA:HA	1:103:A:VAL:HG21	3	0.15
(1,135)	1:101:A:ALA:HA	1:103:A:VAL:HG22	3	0.15
(1,135)	1:101:A:ALA:HA	1:103:A:VAL:HG23	3	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,82)	1:132:A:VAL:HG11	1:138:A:ILE:HD11	5	0.15
(1,82)	1:132:A:VAL:HG11	1:138:A:ILE:HD12	5	0.15
(1,82)	1:132:A:VAL:HG11	1:138:A:ILE:HD13	5	0.15
(1,82)	1:132:A:VAL:HG12	1:138:A:ILE:HD11	5	0.15
(1,82)	1:132:A:VAL:HG12	1:138:A:ILE:HD12	5	0.15
(1,82)	1:132:A:VAL:HG12	1:138:A:ILE:HD13	5	0.15
(1,82)	1:132:A:VAL:HG13	1:138:A:ILE:HD11	5	0.15
(1,82)	1:132:A:VAL:HG13	1:138:A:ILE:HD12	5	0.15
(1,82)	1:132:A:VAL:HG13	1:138:A:ILE:HD13	5	0.15
(1,1511)	1:140:A:ALA:H	1:141:A:LEU:HD11	11	0.14
(1,1511)	1:140:A:ALA:H	1:141:A:LEU:HD12	11	0.14
(1,1511)	1:140:A:ALA:H	1:141:A:LEU:HD13	11	0.14
(1,1511)	1:140:A:ALA:H	1:141:A:LEU:HD21	11	0.14
(1,1511)	1:140:A:ALA:H	1:141:A:LEU:HD22	11	0.14
(1,1511)	1:140:A:ALA:H	1:141:A:LEU:HD23	11	0.14
(1,1502)	1:138:A:ILE:H	1:141:A:LEU:HD11	8	0.14
(1,1502)	1:138:A:ILE:H	1:141:A:LEU:HD12	8	0.14
(1,1502)	1:138:A:ILE:H	1:141:A:LEU:HD13	8	0.14
(1,1502)	1:138:A:ILE:H	1:141:A:LEU:HD21	8	0.14
(1,1502)	1:138:A:ILE:H	1:141:A:LEU:HD22	8	0.14
(1,1502)	1:138:A:ILE:H	1:141:A:LEU:HD23	8	0.14
(1,1502)	1:138:A:ILE:H	1:141:A:LEU:HD11	10	0.14
(1,1502)	1:138:A:ILE:H	1:141:A:LEU:HD12	10	0.14
(1,1502)	1:138:A:ILE:H	1:141:A:LEU:HD13	10	0.14
(1,1502)	1:138:A:ILE:H	1:141:A:LEU:HD21	10	0.14
(1,1502)	1:138:A:ILE:H	1:141:A:LEU:HD22	10	0.14
(1,1502)	1:138:A:ILE:H	1:141:A:LEU:HD23	10	0.14
(1,1487)	1:132:A:VAL:HG11	1:133:A:TYR:H	19	0.14
(1,1487)	1:132:A:VAL:HG12	1:133:A:TYR:H	19	0.14
(1,1487)	1:132:A:VAL:HG13	1:133:A:TYR:H	19	0.14
(1,1487)	1:132:A:VAL:HG21	1:133:A:TYR:H	19	0.14
(1,1487)	1:132:A:VAL:HG22	1:133:A:TYR:H	19	0.14
(1,1487)	1:132:A:VAL:HG23	1:133:A:TYR:H	19	0.14
(1,1427)	1:112:A:LYS:HB2	1:145:A:LEU:HD11	5	0.14
(1,1427)	1:112:A:LYS:HB2	1:145:A:LEU:HD12	5	0.14
(1,1427)	1:112:A:LYS:HB2	1:145:A:LEU:HD13	5	0.14
(1,1427)	1:112:A:LYS:HB2	1:145:A:LEU:HD21	5	0.14
(1,1427)	1:112:A:LYS:HB2	1:145:A:LEU:HD22	5	0.14
(1,1427)	1:112:A:LYS:HB2	1:145:A:LEU:HD23	5	0.14
(1,1427)	1:112:A:LYS:HB3	1:145:A:LEU:HD11	5	0.14
(1,1427)	1:112:A:LYS:HB3	1:145:A:LEU:HD12	5	0.14
(1,1427)	1:112:A:LYS:HB3	1:145:A:LEU:HD13	5	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1427)	1:112:A:LYS:HB3	1:145:A:LEU:HD21	5	0.14
(1,1427)	1:112:A:LYS:HB3	1:145:A:LEU:HD22	5	0.14
(1,1427)	1:112:A:LYS:HB3	1:145:A:LEU:HD23	5	0.14
(1,1422)	1:112:A:LYS:H	1:145:A:LEU:HD11	5	0.14
(1,1422)	1:112:A:LYS:H	1:145:A:LEU:HD12	5	0.14
(1,1422)	1:112:A:LYS:H	1:145:A:LEU:HD13	5	0.14
(1,1422)	1:112:A:LYS:H	1:145:A:LEU:HD21	5	0.14
(1,1422)	1:112:A:LYS:H	1:145:A:LEU:HD22	5	0.14
(1,1422)	1:112:A:LYS:H	1:145:A:LEU:HD23	5	0.14
(1,1366)	1:91:A:LYS:H	1:92:A:ASN:HB2	2	0.14
(1,1366)	1:91:A:LYS:H	1:92:A:ASN:HB3	2	0.14
(1,1362)	1:88:A:CYS:H	1:89:A:LYS:HB2	8	0.14
(1,1362)	1:88:A:CYS:H	1:89:A:LYS:HB3	8	0.14
(1,1340)	1:78:A:PHE:HE1	1:104:A:LEU:HD11	8	0.14
(1,1340)	1:78:A:PHE:HE1	1:104:A:LEU:HD12	8	0.14
(1,1340)	1:78:A:PHE:HE1	1:104:A:LEU:HD13	8	0.14
(1,1340)	1:78:A:PHE:HE1	1:104:A:LEU:HD21	8	0.14
(1,1340)	1:78:A:PHE:HE1	1:104:A:LEU:HD22	8	0.14
(1,1340)	1:78:A:PHE:HE1	1:104:A:LEU:HD23	8	0.14
(1,1340)	1:78:A:PHE:HE2	1:104:A:LEU:HD11	8	0.14
(1,1340)	1:78:A:PHE:HE2	1:104:A:LEU:HD12	8	0.14
(1,1340)	1:78:A:PHE:HE2	1:104:A:LEU:HD13	8	0.14
(1,1340)	1:78:A:PHE:HE2	1:104:A:LEU:HD21	8	0.14
(1,1340)	1:78:A:PHE:HE2	1:104:A:LEU:HD22	8	0.14
(1,1340)	1:78:A:PHE:HE2	1:104:A:LEU:HD23	8	0.14
(1,1320)	1:75:A:LEU:HD11	1:111:A:VAL:HG11	15	0.14
(1,1320)	1:75:A:LEU:HD11	1:111:A:VAL:HG12	15	0.14
(1,1320)	1:75:A:LEU:HD11	1:111:A:VAL:HG13	15	0.14
(1,1320)	1:75:A:LEU:HD12	1:111:A:VAL:HG11	15	0.14
(1,1320)	1:75:A:LEU:HD12	1:111:A:VAL:HG12	15	0.14
(1,1320)	1:75:A:LEU:HD12	1:111:A:VAL:HG13	15	0.14
(1,1320)	1:75:A:LEU:HD13	1:111:A:VAL:HG11	15	0.14
(1,1320)	1:75:A:LEU:HD13	1:111:A:VAL:HG12	15	0.14
(1,1320)	1:75:A:LEU:HD13	1:111:A:VAL:HG13	15	0.14
(1,1320)	1:75:A:LEU:HD21	1:111:A:VAL:HG11	15	0.14
(1,1320)	1:75:A:LEU:HD21	1:111:A:VAL:HG12	15	0.14
(1,1320)	1:75:A:LEU:HD21	1:111:A:VAL:HG13	15	0.14
(1,1320)	1:75:A:LEU:HD22	1:111:A:VAL:HG11	15	0.14
(1,1320)	1:75:A:LEU:HD22	1:111:A:VAL:HG12	15	0.14
(1,1320)	1:75:A:LEU:HD22	1:111:A:VAL:HG13	15	0.14
(1,1320)	1:75:A:LEU:HD23	1:111:A:VAL:HG11	15	0.14
(1,1320)	1:75:A:LEU:HD23	1:111:A:VAL:HG12	15	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1320)	1:75:A:LEU:HD23	1:111:A:VAL:HG13	15	0.14
(1,1286)	1:62:A:TRP:HE1	1:80:A:LEU:HD11	16	0.14
(1,1286)	1:62:A:TRP:HE1	1:80:A:LEU:HD12	16	0.14
(1,1286)	1:62:A:TRP:HE1	1:80:A:LEU:HD13	16	0.14
(1,1286)	1:62:A:TRP:HE1	1:80:A:LEU:HD21	16	0.14
(1,1286)	1:62:A:TRP:HE1	1:80:A:LEU:HD22	16	0.14
(1,1286)	1:62:A:TRP:HE1	1:80:A:LEU:HD23	16	0.14
(1,1196)	1:82:A:ASN:H	1:127:A:TRP:HE1	3	0.14
(1,981)	1:112:A:LYS:HB2	1:113:A:ASP:H	5	0.14
(1,981)	1:112:A:LYS:HB3	1:113:A:ASP:H	5	0.14
(1,981)	1:112:A:LYS:HB2	1:113:A:ASP:H	7	0.14
(1,981)	1:112:A:LYS:HB3	1:113:A:ASP:H	7	0.14
(1,981)	1:112:A:LYS:HB2	1:113:A:ASP:H	8	0.14
(1,981)	1:112:A:LYS:HB3	1:113:A:ASP:H	8	0.14
(1,981)	1:112:A:LYS:HB2	1:113:A:ASP:H	12	0.14
(1,981)	1:112:A:LYS:HB3	1:113:A:ASP:H	12	0.14
(1,963)	1:109:A:ALA:H	1:111:A:VAL:HG11	10	0.14
(1,963)	1:109:A:ALA:H	1:111:A:VAL:HG12	10	0.14
(1,963)	1:109:A:ALA:H	1:111:A:VAL:HG13	10	0.14
(1,952)	1:104:A:LEU:HD21	1:106:A:GLU:H	1	0.14
(1,952)	1:104:A:LEU:HD22	1:106:A:GLU:H	1	0.14
(1,952)	1:104:A:LEU:HD23	1:106:A:GLU:H	1	0.14
(1,771)	1:76:A:ASN:H	1:78:A:PHE:HB2	17	0.14
(1,604)	1:132:A:VAL:HG21	1:133:A:TYR:H	13	0.14
(1,604)	1:132:A:VAL:HG22	1:133:A:TYR:H	13	0.14
(1,604)	1:132:A:VAL:HG23	1:133:A:TYR:H	13	0.14
(1,496)	1:85:A:ILE:HD11	1:86:A:GLN:H	8	0.14
(1,496)	1:85:A:ILE:HD12	1:86:A:GLN:H	8	0.14
(1,496)	1:85:A:ILE:HD13	1:86:A:GLN:H	8	0.14
(1,496)	1:85:A:ILE:HD11	1:86:A:GLN:H	14	0.14
(1,496)	1:85:A:ILE:HD12	1:86:A:GLN:H	14	0.14
(1,496)	1:85:A:ILE:HD13	1:86:A:GLN:H	14	0.14
(1,461)	1:101:A:ALA:HB1	1:137:A:MET:HB2	5	0.14
(1,461)	1:101:A:ALA:HB2	1:137:A:MET:HB2	5	0.14
(1,461)	1:101:A:ALA:HB3	1:137:A:MET:HB2	5	0.14
(1,344)	1:49:A:ILE:H	1:84:A:VAL:HG21	19	0.14
(1,344)	1:49:A:ILE:H	1:84:A:VAL:HG22	19	0.14
(1,344)	1:49:A:ILE:H	1:84:A:VAL:HG23	19	0.14
(1,13)	1:142:A:ARG:HA	1:145:A:LEU:HB3	11	0.14
(1,1511)	1:140:A:ALA:H	1:141:A:LEU:HD11	6	0.13
(1,1511)	1:140:A:ALA:H	1:141:A:LEU:HD12	6	0.13
(1,1511)	1:140:A:ALA:H	1:141:A:LEU:HD13	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1511)	1:140:A:ALA:H	1:141:A:LEU:HD21	6	0.13
(1,1511)	1:140:A:ALA:H	1:141:A:LEU:HD22	6	0.13
(1,1511)	1:140:A:ALA:H	1:141:A:LEU:HD23	6	0.13
(1,1511)	1:140:A:ALA:H	1:141:A:LEU:HD11	8	0.13
(1,1511)	1:140:A:ALA:H	1:141:A:LEU:HD12	8	0.13
(1,1511)	1:140:A:ALA:H	1:141:A:LEU:HD13	8	0.13
(1,1511)	1:140:A:ALA:H	1:141:A:LEU:HD21	8	0.13
(1,1511)	1:140:A:ALA:H	1:141:A:LEU:HD22	8	0.13
(1,1511)	1:140:A:ALA:H	1:141:A:LEU:HD23	8	0.13
(1,1508)	1:139:A:VAL:HG11	1:140:A:ALA:HB1	3	0.13
(1,1508)	1:139:A:VAL:HG11	1:140:A:ALA:HB2	3	0.13
(1,1508)	1:139:A:VAL:HG11	1:140:A:ALA:HB3	3	0.13
(1,1508)	1:139:A:VAL:HG12	1:140:A:ALA:HB1	3	0.13
(1,1508)	1:139:A:VAL:HG12	1:140:A:ALA:HB2	3	0.13
(1,1508)	1:139:A:VAL:HG12	1:140:A:ALA:HB3	3	0.13
(1,1508)	1:139:A:VAL:HG13	1:140:A:ALA:HB1	3	0.13
(1,1508)	1:139:A:VAL:HG13	1:140:A:ALA:HB2	3	0.13
(1,1508)	1:139:A:VAL:HG13	1:140:A:ALA:HB3	3	0.13
(1,1508)	1:139:A:VAL:HG21	1:140:A:ALA:HB1	3	0.13
(1,1508)	1:139:A:VAL:HG21	1:140:A:ALA:HB2	3	0.13
(1,1508)	1:139:A:VAL:HG21	1:140:A:ALA:HB3	3	0.13
(1,1508)	1:139:A:VAL:HG22	1:140:A:ALA:HB1	3	0.13
(1,1508)	1:139:A:VAL:HG22	1:140:A:ALA:HB2	3	0.13
(1,1508)	1:139:A:VAL:HG22	1:140:A:ALA:HB3	3	0.13
(1,1508)	1:139:A:VAL:HG23	1:140:A:ALA:HB1	3	0.13
(1,1508)	1:139:A:VAL:HG23	1:140:A:ALA:HB2	3	0.13
(1,1508)	1:139:A:VAL:HG23	1:140:A:ALA:HB3	3	0.13
(1,1508)	1:139:A:VAL:HG11	1:140:A:ALA:HB1	6	0.13
(1,1508)	1:139:A:VAL:HG11	1:140:A:ALA:HB2	6	0.13
(1,1508)	1:139:A:VAL:HG11	1:140:A:ALA:HB3	6	0.13
(1,1508)	1:139:A:VAL:HG12	1:140:A:ALA:HB1	6	0.13
(1,1508)	1:139:A:VAL:HG12	1:140:A:ALA:HB2	6	0.13
(1,1508)	1:139:A:VAL:HG12	1:140:A:ALA:HB3	6	0.13
(1,1508)	1:139:A:VAL:HG13	1:140:A:ALA:HB1	6	0.13
(1,1508)	1:139:A:VAL:HG13	1:140:A:ALA:HB2	6	0.13
(1,1508)	1:139:A:VAL:HG13	1:140:A:ALA:HB3	6	0.13
(1,1508)	1:139:A:VAL:HG21	1:140:A:ALA:HB1	6	0.13
(1,1508)	1:139:A:VAL:HG21	1:140:A:ALA:HB2	6	0.13
(1,1508)	1:139:A:VAL:HG21	1:140:A:ALA:HB3	6	0.13
(1,1508)	1:139:A:VAL:HG22	1:140:A:ALA:HB1	6	0.13
(1,1508)	1:139:A:VAL:HG22	1:140:A:ALA:HB2	6	0.13
(1,1508)	1:139:A:VAL:HG22	1:140:A:ALA:HB3	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1508)	1:139:A:VAL:HG23	1:140:A:ALA:HB1	6	0.13
(1,1508)	1:139:A:VAL:HG23	1:140:A:ALA:HB2	6	0.13
(1,1508)	1:139:A:VAL:HG23	1:140:A:ALA:HB3	6	0.13
(1,1508)	1:139:A:VAL:HG11	1:140:A:ALA:HB1	11	0.13
(1,1508)	1:139:A:VAL:HG11	1:140:A:ALA:HB2	11	0.13
(1,1508)	1:139:A:VAL:HG11	1:140:A:ALA:HB3	11	0.13
(1,1508)	1:139:A:VAL:HG12	1:140:A:ALA:HB1	11	0.13
(1,1508)	1:139:A:VAL:HG12	1:140:A:ALA:HB2	11	0.13
(1,1508)	1:139:A:VAL:HG12	1:140:A:ALA:HB3	11	0.13
(1,1508)	1:139:A:VAL:HG13	1:140:A:ALA:HB1	11	0.13
(1,1508)	1:139:A:VAL:HG13	1:140:A:ALA:HB2	11	0.13
(1,1508)	1:139:A:VAL:HG13	1:140:A:ALA:HB3	11	0.13
(1,1508)	1:139:A:VAL:HG21	1:140:A:ALA:HB1	11	0.13
(1,1508)	1:139:A:VAL:HG21	1:140:A:ALA:HB2	11	0.13
(1,1508)	1:139:A:VAL:HG21	1:140:A:ALA:HB3	11	0.13
(1,1508)	1:139:A:VAL:HG22	1:140:A:ALA:HB1	11	0.13
(1,1508)	1:139:A:VAL:HG22	1:140:A:ALA:HB2	11	0.13
(1,1508)	1:139:A:VAL:HG22	1:140:A:ALA:HB3	11	0.13
(1,1508)	1:139:A:VAL:HG23	1:140:A:ALA:HB1	11	0.13
(1,1508)	1:139:A:VAL:HG23	1:140:A:ALA:HB2	11	0.13
(1,1508)	1:139:A:VAL:HG23	1:140:A:ALA:HB3	11	0.13
(1,1500)	1:137:A:MET:HB2	1:141:A:LEU:HD11	16	0.13
(1,1500)	1:137:A:MET:HB2	1:141:A:LEU:HD12	16	0.13
(1,1500)	1:137:A:MET:HB2	1:141:A:LEU:HD13	16	0.13
(1,1500)	1:137:A:MET:HB2	1:141:A:LEU:HD21	16	0.13
(1,1500)	1:137:A:MET:HB2	1:141:A:LEU:HD22	16	0.13
(1,1500)	1:137:A:MET:HB2	1:141:A:LEU:HD23	16	0.13
(1,1492)	1:133:A:TYR:H	1:141:A:LEU:HD11	4	0.13
(1,1492)	1:133:A:TYR:H	1:141:A:LEU:HD12	4	0.13
(1,1492)	1:133:A:TYR:H	1:141:A:LEU:HD13	4	0.13
(1,1492)	1:133:A:TYR:H	1:141:A:LEU:HD21	4	0.13
(1,1492)	1:133:A:TYR:H	1:141:A:LEU:HD22	4	0.13
(1,1492)	1:133:A:TYR:H	1:141:A:LEU:HD23	4	0.13
(1,1490)	1:132:A:VAL:HG11	1:138:A:ILE:HD11	11	0.13
(1,1490)	1:132:A:VAL:HG11	1:138:A:ILE:HD12	11	0.13
(1,1490)	1:132:A:VAL:HG11	1:138:A:ILE:HD13	11	0.13
(1,1490)	1:132:A:VAL:HG12	1:138:A:ILE:HD11	11	0.13
(1,1490)	1:132:A:VAL:HG12	1:138:A:ILE:HD12	11	0.13
(1,1490)	1:132:A:VAL:HG12	1:138:A:ILE:HD13	11	0.13
(1,1490)	1:132:A:VAL:HG13	1:138:A:ILE:HD11	11	0.13
(1,1490)	1:132:A:VAL:HG13	1:138:A:ILE:HD12	11	0.13
(1,1490)	1:132:A:VAL:HG13	1:138:A:ILE:HD13	11	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1490)	1:132:A:VAL:HG21	1:138:A:ILE:HD11	11	0.13
(1,1490)	1:132:A:VAL:HG21	1:138:A:ILE:HD12	11	0.13
(1,1490)	1:132:A:VAL:HG21	1:138:A:ILE:HD13	11	0.13
(1,1490)	1:132:A:VAL:HG22	1:138:A:ILE:HD11	11	0.13
(1,1490)	1:132:A:VAL:HG22	1:138:A:ILE:HD12	11	0.13
(1,1490)	1:132:A:VAL:HG22	1:138:A:ILE:HD13	11	0.13
(1,1490)	1:132:A:VAL:HG23	1:138:A:ILE:HD11	11	0.13
(1,1490)	1:132:A:VAL:HG23	1:138:A:ILE:HD12	11	0.13
(1,1490)	1:132:A:VAL:HG23	1:138:A:ILE:HD13	11	0.13
(1,1487)	1:132:A:VAL:HG11	1:133:A:TYR:H	8	0.13
(1,1487)	1:132:A:VAL:HG12	1:133:A:TYR:H	8	0.13
(1,1487)	1:132:A:VAL:HG13	1:133:A:TYR:H	8	0.13
(1,1487)	1:132:A:VAL:HG21	1:133:A:TYR:H	8	0.13
(1,1487)	1:132:A:VAL:HG22	1:133:A:TYR:H	8	0.13
(1,1487)	1:132:A:VAL:HG23	1:133:A:TYR:H	8	0.13
(1,1347)	1:84:A:VAL:HG11	1:85:A:ILE:HG12	6	0.13
(1,1347)	1:84:A:VAL:HG11	1:85:A:ILE:HG13	6	0.13
(1,1347)	1:84:A:VAL:HG12	1:85:A:ILE:HG12	6	0.13
(1,1347)	1:84:A:VAL:HG12	1:85:A:ILE:HG13	6	0.13
(1,1347)	1:84:A:VAL:HG13	1:85:A:ILE:HG12	6	0.13
(1,1347)	1:84:A:VAL:HG13	1:85:A:ILE:HG13	6	0.13
(1,1347)	1:84:A:VAL:HG11	1:85:A:ILE:HG12	16	0.13
(1,1347)	1:84:A:VAL:HG11	1:85:A:ILE:HG13	16	0.13
(1,1347)	1:84:A:VAL:HG12	1:85:A:ILE:HG12	16	0.13
(1,1347)	1:84:A:VAL:HG12	1:85:A:ILE:HG13	16	0.13
(1,1347)	1:84:A:VAL:HG13	1:85:A:ILE:HG12	16	0.13
(1,1347)	1:84:A:VAL:HG13	1:85:A:ILE:HG13	16	0.13
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD11	11	0.13
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD12	11	0.13
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD13	11	0.13
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD21	11	0.13
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD22	11	0.13
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD23	11	0.13
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD11	11	0.13
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD12	11	0.13
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD13	11	0.13
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD21	11	0.13
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD22	11	0.13
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD23	11	0.13
(1,1320)	1:75:A:LEU:HD11	1:111:A:VAL:HG11	10	0.13
(1,1320)	1:75:A:LEU:HD11	1:111:A:VAL:HG12	10	0.13
(1,1320)	1:75:A:LEU:HD11	1:111:A:VAL:HG13	10	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1320)	1:75:A:LEU:HD12	1:111:A:VAL:HG11	10	0.13
(1,1320)	1:75:A:LEU:HD12	1:111:A:VAL:HG12	10	0.13
(1,1320)	1:75:A:LEU:HD12	1:111:A:VAL:HG13	10	0.13
(1,1320)	1:75:A:LEU:HD13	1:111:A:VAL:HG11	10	0.13
(1,1320)	1:75:A:LEU:HD13	1:111:A:VAL:HG12	10	0.13
(1,1320)	1:75:A:LEU:HD13	1:111:A:VAL:HG13	10	0.13
(1,1320)	1:75:A:LEU:HD21	1:111:A:VAL:HG11	10	0.13
(1,1320)	1:75:A:LEU:HD21	1:111:A:VAL:HG12	10	0.13
(1,1320)	1:75:A:LEU:HD21	1:111:A:VAL:HG13	10	0.13
(1,1320)	1:75:A:LEU:HD22	1:111:A:VAL:HG11	10	0.13
(1,1320)	1:75:A:LEU:HD22	1:111:A:VAL:HG12	10	0.13
(1,1320)	1:75:A:LEU:HD22	1:111:A:VAL:HG13	10	0.13
(1,1320)	1:75:A:LEU:HD23	1:111:A:VAL:HG11	10	0.13
(1,1320)	1:75:A:LEU:HD23	1:111:A:VAL:HG12	10	0.13
(1,1320)	1:75:A:LEU:HD23	1:111:A:VAL:HG13	10	0.13
(1,1288)	1:63:A:MET:H	1:77:A:LEU:HD11	11	0.13
(1,1288)	1:63:A:MET:H	1:77:A:LEU:HD12	11	0.13
(1,1288)	1:63:A:MET:H	1:77:A:LEU:HD13	11	0.13
(1,1288)	1:63:A:MET:H	1:77:A:LEU:HD21	11	0.13
(1,1288)	1:63:A:MET:H	1:77:A:LEU:HD22	11	0.13
(1,1288)	1:63:A:MET:H	1:77:A:LEU:HD23	11	0.13
(1,1073)	1:139:A:VAL:HB	1:140:A:ALA:H	1	0.13
(1,1073)	1:139:A:VAL:HB	1:140:A:ALA:H	12	0.13
(1,1073)	1:139:A:VAL:HB	1:140:A:ALA:H	14	0.13
(1,1073)	1:139:A:VAL:HB	1:140:A:ALA:H	16	0.13
(1,1073)	1:139:A:VAL:HB	1:140:A:ALA:H	18	0.13
(1,1033)	1:128:A:GLU:H	1:138:A:ILE:HG12	12	0.13
(1,1033)	1:128:A:GLU:H	1:138:A:ILE:HG13	12	0.13
(1,1032)	1:127:A:TRP:HB3	1:128:A:GLU:H	1	0.13
(1,981)	1:112:A:LYS:HB2	1:113:A:ASP:H	19	0.13
(1,981)	1:112:A:LYS:HB3	1:113:A:ASP:H	19	0.13
(1,950)	1:103:A:VAL:HG21	1:107:A:ALA:H	9	0.13
(1,950)	1:103:A:VAL:HG22	1:107:A:ALA:H	9	0.13
(1,950)	1:103:A:VAL:HG23	1:107:A:ALA:H	9	0.13
(1,950)	1:103:A:VAL:HG21	1:107:A:ALA:H	17	0.13
(1,950)	1:103:A:VAL:HG22	1:107:A:ALA:H	17	0.13
(1,950)	1:103:A:VAL:HG23	1:107:A:ALA:H	17	0.13
(1,847)	1:49:A:ILE:H	1:84:A:VAL:HG11	19	0.13
(1,847)	1:49:A:ILE:H	1:84:A:VAL:HG12	19	0.13
(1,847)	1:49:A:ILE:H	1:84:A:VAL:HG13	19	0.13
(1,846)	1:45:A:SER:HA	1:85:A:ILE:H	12	0.13
(1,846)	1:45:A:SER:HA	1:85:A:ILE:H	15	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,824)	1:98:A:GLU:H	1:133:A:TYR:HD1	4	0.13
(1,824)	1:98:A:GLU:H	1:133:A:TYR:HD2	4	0.13
(1,804)	1:84:A:VAL:HB	1:87:A:ASN:H	10	0.13
(1,804)	1:84:A:VAL:HB	1:87:A:ASN:H	18	0.13
(1,771)	1:76:A:ASN:H	1:78:A:PHE:HB2	2	0.13
(1,771)	1:76:A:ASN:H	1:78:A:PHE:HB2	3	0.13
(1,771)	1:76:A:ASN:H	1:78:A:PHE:HB2	19	0.13
(1,719)	1:109:A:ALA:H	1:112:A:LYS:H	13	0.13
(1,656)	1:50:A:GLU:H	1:51:A:ASN:HD21	5	0.13
(1,656)	1:50:A:GLU:H	1:51:A:ASN:HD21	20	0.13
(1,604)	1:132:A:VAL:HG21	1:133:A:TYR:H	1	0.13
(1,604)	1:132:A:VAL:HG22	1:133:A:TYR:H	1	0.13
(1,604)	1:132:A:VAL:HG23	1:133:A:TYR:H	1	0.13
(1,596)	1:101:A:ALA:H	1:133:A:TYR:HD1	5	0.13
(1,596)	1:101:A:ALA:H	1:133:A:TYR:HD2	5	0.13
(1,596)	1:101:A:ALA:H	1:133:A:TYR:HD1	16	0.13
(1,596)	1:101:A:ALA:H	1:133:A:TYR:HD2	16	0.13
(1,579)	1:48:A:CYS:H	1:84:A:VAL:HG21	10	0.13
(1,579)	1:48:A:CYS:H	1:84:A:VAL:HG22	10	0.13
(1,579)	1:48:A:CYS:H	1:84:A:VAL:HG23	10	0.13
(1,536)	1:122:A:ARG:H	1:122:A:ARG:HD2	2	0.13
(1,536)	1:122:A:ARG:H	1:122:A:ARG:HD3	2	0.13
(1,496)	1:85:A:ILE:HD11	1:86:A:GLN:H	10	0.13
(1,496)	1:85:A:ILE:HD12	1:86:A:GLN:H	10	0.13
(1,496)	1:85:A:ILE:HD13	1:86:A:GLN:H	10	0.13
(1,461)	1:101:A:ALA:HB1	1:137:A:MET:HB2	13	0.13
(1,461)	1:101:A:ALA:HB2	1:137:A:MET:HB2	13	0.13
(1,461)	1:101:A:ALA:HB3	1:137:A:MET:HB2	13	0.13
(1,377)	1:62:A:TRP:HZ3	1:103:A:VAL:HG11	17	0.13
(1,377)	1:62:A:TRP:HZ3	1:103:A:VAL:HG12	17	0.13
(1,377)	1:62:A:TRP:HZ3	1:103:A:VAL:HG13	17	0.13
(1,336)	1:108:A:ALA:HB1	1:111:A:VAL:HG11	14	0.13
(1,336)	1:108:A:ALA:HB1	1:111:A:VAL:HG12	14	0.13
(1,336)	1:108:A:ALA:HB1	1:111:A:VAL:HG13	14	0.13
(1,336)	1:108:A:ALA:HB2	1:111:A:VAL:HG11	14	0.13
(1,336)	1:108:A:ALA:HB2	1:111:A:VAL:HG12	14	0.13
(1,336)	1:108:A:ALA:HB2	1:111:A:VAL:HG13	14	0.13
(1,336)	1:108:A:ALA:HB3	1:111:A:VAL:HG11	14	0.13
(1,336)	1:108:A:ALA:HB3	1:111:A:VAL:HG12	14	0.13
(1,336)	1:108:A:ALA:HB3	1:111:A:VAL:HG13	14	0.13
(1,297)	1:37:A:THR:HG21	1:38:A:MET:HB2	11	0.13
(1,297)	1:37:A:THR:HG21	1:38:A:MET:HB3	11	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,297)	1:37:A:THR:HG22	1:38:A:MET:HB2	11	0.13
(1,297)	1:37:A:THR:HG22	1:38:A:MET:HB3	11	0.13
(1,297)	1:37:A:THR:HG23	1:38:A:MET:HB2	11	0.13
(1,297)	1:37:A:THR:HG23	1:38:A:MET:HB3	11	0.13
(1,279)	1:77:A:LEU:HD21	1:107:A:ALA:HB1	10	0.13
(1,279)	1:77:A:LEU:HD21	1:107:A:ALA:HB2	10	0.13
(1,279)	1:77:A:LEU:HD21	1:107:A:ALA:HB3	10	0.13
(1,279)	1:77:A:LEU:HD22	1:107:A:ALA:HB1	10	0.13
(1,279)	1:77:A:LEU:HD22	1:107:A:ALA:HB2	10	0.13
(1,279)	1:77:A:LEU:HD22	1:107:A:ALA:HB3	10	0.13
(1,279)	1:77:A:LEU:HD23	1:107:A:ALA:HB1	10	0.13
(1,279)	1:77:A:LEU:HD23	1:107:A:ALA:HB2	10	0.13
(1,279)	1:77:A:LEU:HD23	1:107:A:ALA:HB3	10	0.13
(1,252)	1:111:A:VAL:HG21	1:121:A:GLU:H	15	0.13
(1,252)	1:111:A:VAL:HG22	1:121:A:GLU:H	15	0.13
(1,252)	1:111:A:VAL:HG23	1:121:A:GLU:H	15	0.13
(1,252)	1:111:A:VAL:HG21	1:121:A:GLU:H	18	0.13
(1,252)	1:111:A:VAL:HG22	1:121:A:GLU:H	18	0.13
(1,252)	1:111:A:VAL:HG23	1:121:A:GLU:H	18	0.13
(1,171)	1:34:A:VAL:H	1:36:A:ASN:HA	20	0.13
(1,162)	1:93:A:ALA:HA	1:94:A:ILE:HG21	8	0.13
(1,162)	1:93:A:ALA:HA	1:94:A:ILE:HG22	8	0.13
(1,162)	1:93:A:ALA:HA	1:94:A:ILE:HG23	8	0.13
(1,74)	1:49:A:ILE:HD11	1:84:A:VAL:HG11	12	0.13
(1,74)	1:49:A:ILE:HD11	1:84:A:VAL:HG12	12	0.13
(1,74)	1:49:A:ILE:HD11	1:84:A:VAL:HG13	12	0.13
(1,74)	1:49:A:ILE:HD12	1:84:A:VAL:HG11	12	0.13
(1,74)	1:49:A:ILE:HD12	1:84:A:VAL:HG12	12	0.13
(1,74)	1:49:A:ILE:HD12	1:84:A:VAL:HG13	12	0.13
(1,74)	1:49:A:ILE:HD13	1:84:A:VAL:HG11	12	0.13
(1,74)	1:49:A:ILE:HD13	1:84:A:VAL:HG12	12	0.13
(1,74)	1:49:A:ILE:HD13	1:84:A:VAL:HG13	12	0.13
(1,1519)	1:145:A:LEU:HB2	1:146:A:SER:H	7	0.12
(1,1519)	1:145:A:LEU:HB3	1:146:A:SER:H	7	0.12
(1,1511)	1:140:A:ALA:H	1:141:A:LEU:HD11	9	0.12
(1,1511)	1:140:A:ALA:H	1:141:A:LEU:HD12	9	0.12
(1,1511)	1:140:A:ALA:H	1:141:A:LEU:HD13	9	0.12
(1,1511)	1:140:A:ALA:H	1:141:A:LEU:HD21	9	0.12
(1,1511)	1:140:A:ALA:H	1:141:A:LEU:HD22	9	0.12
(1,1511)	1:140:A:ALA:H	1:141:A:LEU:HD23	9	0.12
(1,1491)	1:132:A:VAL:HG11	1:141:A:LEU:HD11	11	0.12
(1,1491)	1:132:A:VAL:HG11	1:141:A:LEU:HD12	11	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1491)	1:132:A:VAL:HG11	1:141:A:LEU:HD13	11	0.12
(1,1491)	1:132:A:VAL:HG11	1:141:A:LEU:HD21	11	0.12
(1,1491)	1:132:A:VAL:HG11	1:141:A:LEU:HD22	11	0.12
(1,1491)	1:132:A:VAL:HG11	1:141:A:LEU:HD23	11	0.12
(1,1491)	1:132:A:VAL:HG12	1:141:A:LEU:HD11	11	0.12
(1,1491)	1:132:A:VAL:HG12	1:141:A:LEU:HD12	11	0.12
(1,1491)	1:132:A:VAL:HG12	1:141:A:LEU:HD13	11	0.12
(1,1491)	1:132:A:VAL:HG12	1:141:A:LEU:HD21	11	0.12
(1,1491)	1:132:A:VAL:HG12	1:141:A:LEU:HD22	11	0.12
(1,1491)	1:132:A:VAL:HG12	1:141:A:LEU:HD23	11	0.12
(1,1491)	1:132:A:VAL:HG13	1:141:A:LEU:HD11	11	0.12
(1,1491)	1:132:A:VAL:HG13	1:141:A:LEU:HD12	11	0.12
(1,1491)	1:132:A:VAL:HG13	1:141:A:LEU:HD13	11	0.12
(1,1491)	1:132:A:VAL:HG13	1:141:A:LEU:HD21	11	0.12
(1,1491)	1:132:A:VAL:HG13	1:141:A:LEU:HD22	11	0.12
(1,1491)	1:132:A:VAL:HG13	1:141:A:LEU:HD23	11	0.12
(1,1491)	1:132:A:VAL:HG21	1:141:A:LEU:HD11	11	0.12
(1,1491)	1:132:A:VAL:HG21	1:141:A:LEU:HD12	11	0.12
(1,1491)	1:132:A:VAL:HG21	1:141:A:LEU:HD13	11	0.12
(1,1491)	1:132:A:VAL:HG21	1:141:A:LEU:HD21	11	0.12
(1,1491)	1:132:A:VAL:HG21	1:141:A:LEU:HD22	11	0.12
(1,1491)	1:132:A:VAL:HG21	1:141:A:LEU:HD23	11	0.12
(1,1491)	1:132:A:VAL:HG22	1:141:A:LEU:HD11	11	0.12
(1,1491)	1:132:A:VAL:HG22	1:141:A:LEU:HD12	11	0.12
(1,1491)	1:132:A:VAL:HG22	1:141:A:LEU:HD13	11	0.12
(1,1491)	1:132:A:VAL:HG22	1:141:A:LEU:HD21	11	0.12
(1,1491)	1:132:A:VAL:HG22	1:141:A:LEU:HD22	11	0.12
(1,1491)	1:132:A:VAL:HG22	1:141:A:LEU:HD23	11	0.12
(1,1491)	1:132:A:VAL:HG23	1:141:A:LEU:HD11	11	0.12
(1,1491)	1:132:A:VAL:HG23	1:141:A:LEU:HD12	11	0.12
(1,1491)	1:132:A:VAL:HG23	1:141:A:LEU:HD13	11	0.12
(1,1491)	1:132:A:VAL:HG23	1:141:A:LEU:HD21	11	0.12
(1,1491)	1:132:A:VAL:HG23	1:141:A:LEU:HD22	11	0.12
(1,1491)	1:132:A:VAL:HG23	1:141:A:LEU:HD23	11	0.12
(1,1487)	1:132:A:VAL:HG11	1:133:A:TYR:H	10	0.12
(1,1487)	1:132:A:VAL:HG12	1:133:A:TYR:H	10	0.12
(1,1487)	1:132:A:VAL:HG13	1:133:A:TYR:H	10	0.12
(1,1487)	1:132:A:VAL:HG21	1:133:A:TYR:H	10	0.12
(1,1487)	1:132:A:VAL:HG22	1:133:A:TYR:H	10	0.12
(1,1487)	1:132:A:VAL:HG23	1:133:A:TYR:H	10	0.12
(1,1469)	1:121:A:GLU:HA	1:145:A:LEU:HD11	17	0.12
(1,1469)	1:121:A:GLU:HA	1:145:A:LEU:HD12	17	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1469)	1:121:A:GLU:HA	1:145:A:LEU:HD13	17	0.12
(1,1469)	1:121:A:GLU:HA	1:145:A:LEU:HD21	17	0.12
(1,1469)	1:121:A:GLU:HA	1:145:A:LEU:HD22	17	0.12
(1,1469)	1:121:A:GLU:HA	1:145:A:LEU:HD23	17	0.12
(1,1450)	1:116:A:VAL:HG11	1:120:A:VAL:HG11	6	0.12
(1,1450)	1:116:A:VAL:HG11	1:120:A:VAL:HG12	6	0.12
(1,1450)	1:116:A:VAL:HG11	1:120:A:VAL:HG13	6	0.12
(1,1450)	1:116:A:VAL:HG11	1:120:A:VAL:HG21	6	0.12
(1,1450)	1:116:A:VAL:HG11	1:120:A:VAL:HG22	6	0.12
(1,1450)	1:116:A:VAL:HG11	1:120:A:VAL:HG23	6	0.12
(1,1450)	1:116:A:VAL:HG12	1:120:A:VAL:HG11	6	0.12
(1,1450)	1:116:A:VAL:HG12	1:120:A:VAL:HG12	6	0.12
(1,1450)	1:116:A:VAL:HG12	1:120:A:VAL:HG13	6	0.12
(1,1450)	1:116:A:VAL:HG12	1:120:A:VAL:HG21	6	0.12
(1,1450)	1:116:A:VAL:HG12	1:120:A:VAL:HG22	6	0.12
(1,1450)	1:116:A:VAL:HG12	1:120:A:VAL:HG23	6	0.12
(1,1450)	1:116:A:VAL:HG13	1:120:A:VAL:HG11	6	0.12
(1,1450)	1:116:A:VAL:HG13	1:120:A:VAL:HG12	6	0.12
(1,1450)	1:116:A:VAL:HG13	1:120:A:VAL:HG13	6	0.12
(1,1450)	1:116:A:VAL:HG13	1:120:A:VAL:HG21	6	0.12
(1,1450)	1:116:A:VAL:HG13	1:120:A:VAL:HG22	6	0.12
(1,1450)	1:116:A:VAL:HG13	1:120:A:VAL:HG23	6	0.12
(1,1450)	1:116:A:VAL:HG21	1:120:A:VAL:HG11	6	0.12
(1,1450)	1:116:A:VAL:HG21	1:120:A:VAL:HG12	6	0.12
(1,1450)	1:116:A:VAL:HG21	1:120:A:VAL:HG13	6	0.12
(1,1450)	1:116:A:VAL:HG21	1:120:A:VAL:HG21	6	0.12
(1,1450)	1:116:A:VAL:HG21	1:120:A:VAL:HG22	6	0.12
(1,1450)	1:116:A:VAL:HG21	1:120:A:VAL:HG23	6	0.12
(1,1450)	1:116:A:VAL:HG22	1:120:A:VAL:HG11	6	0.12
(1,1450)	1:116:A:VAL:HG22	1:120:A:VAL:HG12	6	0.12
(1,1450)	1:116:A:VAL:HG22	1:120:A:VAL:HG13	6	0.12
(1,1450)	1:116:A:VAL:HG22	1:120:A:VAL:HG21	6	0.12
(1,1450)	1:116:A:VAL:HG22	1:120:A:VAL:HG22	6	0.12
(1,1450)	1:116:A:VAL:HG22	1:120:A:VAL:HG23	6	0.12
(1,1450)	1:116:A:VAL:HG23	1:120:A:VAL:HG11	6	0.12
(1,1450)	1:116:A:VAL:HG23	1:120:A:VAL:HG12	6	0.12
(1,1450)	1:116:A:VAL:HG23	1:120:A:VAL:HG13	6	0.12
(1,1450)	1:116:A:VAL:HG23	1:120:A:VAL:HG21	6	0.12
(1,1450)	1:116:A:VAL:HG23	1:120:A:VAL:HG22	6	0.12
(1,1450)	1:116:A:VAL:HG23	1:120:A:VAL:HG23	6	0.12
(1,1366)	1:91:A:LYS:H	1:92:A:ASN:HB2	10	0.12
(1,1366)	1:91:A:LYS:H	1:92:A:ASN:HB3	10	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1362)	1:88:A:CYS:H	1:89:A:LYS:HB2	7	0.12
(1,1362)	1:88:A:CYS:H	1:89:A:LYS:HB3	7	0.12
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD11	3	0.12
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD12	3	0.12
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD13	3	0.12
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD21	3	0.12
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD22	3	0.12
(1,1331)	1:76:A:ASN:HB2	1:77:A:LEU:HD23	3	0.12
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD11	3	0.12
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD12	3	0.12
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD13	3	0.12
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD21	3	0.12
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD22	3	0.12
(1,1331)	1:76:A:ASN:HB3	1:77:A:LEU:HD23	3	0.12
(1,1275)	1:59:A:VAL:HG11	1:102:A:ASP:H	1	0.12
(1,1275)	1:59:A:VAL:HG12	1:102:A:ASP:H	1	0.12
(1,1275)	1:59:A:VAL:HG13	1:102:A:ASP:H	1	0.12
(1,1275)	1:59:A:VAL:HG21	1:102:A:ASP:H	1	0.12
(1,1275)	1:59:A:VAL:HG22	1:102:A:ASP:H	1	0.12
(1,1275)	1:59:A:VAL:HG23	1:102:A:ASP:H	1	0.12
(1,1243)	1:53:A:LYS:HB2	1:54:A:HIS:HB2	2	0.12
(1,1243)	1:53:A:LYS:HB2	1:54:A:HIS:HB3	2	0.12
(1,1243)	1:53:A:LYS:HB3	1:54:A:HIS:HB2	2	0.12
(1,1243)	1:53:A:LYS:HB3	1:54:A:HIS:HB3	2	0.12
(1,1243)	1:53:A:LYS:HB2	1:54:A:HIS:HB2	5	0.12
(1,1243)	1:53:A:LYS:HB2	1:54:A:HIS:HB3	5	0.12
(1,1243)	1:53:A:LYS:HB3	1:54:A:HIS:HB2	5	0.12
(1,1243)	1:53:A:LYS:HB3	1:54:A:HIS:HB3	5	0.12
(1,1243)	1:53:A:LYS:HB2	1:54:A:HIS:HB2	15	0.12
(1,1243)	1:53:A:LYS:HB2	1:54:A:HIS:HB3	15	0.12
(1,1243)	1:53:A:LYS:HB3	1:54:A:HIS:HB2	15	0.12
(1,1243)	1:53:A:LYS:HB3	1:54:A:HIS:HB3	15	0.12
(1,1072)	1:139:A:VAL:HG21	1:140:A:ALA:H	3	0.12
(1,1072)	1:139:A:VAL:HG22	1:140:A:ALA:H	3	0.12
(1,1072)	1:139:A:VAL:HG23	1:140:A:ALA:H	3	0.12
(1,993)	1:78:A:PHE:HD1	1:120:A:VAL:H	19	0.12
(1,993)	1:78:A:PHE:HD2	1:120:A:VAL:H	19	0.12
(1,981)	1:112:A:LYS:HB2	1:113:A:ASP:H	2	0.12
(1,981)	1:112:A:LYS:HB3	1:113:A:ASP:H	2	0.12
(1,981)	1:112:A:LYS:HB2	1:113:A:ASP:H	11	0.12
(1,981)	1:112:A:LYS:HB3	1:113:A:ASP:H	11	0.12
(1,981)	1:112:A:LYS:HB2	1:113:A:ASP:H	14	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,981)	1:112:A:LYS:HB3	1:113:A:ASP:H	14	0.12
(1,950)	1:103:A:VAL:HG21	1:107:A:ALA:H	1	0.12
(1,950)	1:103:A:VAL:HG22	1:107:A:ALA:H	1	0.12
(1,950)	1:103:A:VAL:HG23	1:107:A:ALA:H	1	0.12
(1,936)	1:102:A:ASP:HB2	1:104:A:LEU:H	17	0.12
(1,936)	1:102:A:ASP:HB3	1:104:A:LEU:H	17	0.12
(1,857)	1:111:A:VAL:HG11	1:112:A:LYS:H	9	0.12
(1,857)	1:111:A:VAL:HG12	1:112:A:LYS:H	9	0.12
(1,857)	1:111:A:VAL:HG13	1:112:A:LYS:H	9	0.12
(1,857)	1:111:A:VAL:HG11	1:112:A:LYS:H	19	0.12
(1,857)	1:111:A:VAL:HG12	1:112:A:LYS:H	19	0.12
(1,857)	1:111:A:VAL:HG13	1:112:A:LYS:H	19	0.12
(1,847)	1:49:A:ILE:H	1:84:A:VAL:HG11	7	0.12
(1,847)	1:49:A:ILE:H	1:84:A:VAL:HG12	7	0.12
(1,847)	1:49:A:ILE:H	1:84:A:VAL:HG13	7	0.12
(1,847)	1:49:A:ILE:H	1:84:A:VAL:HG11	20	0.12
(1,847)	1:49:A:ILE:H	1:84:A:VAL:HG12	20	0.12
(1,847)	1:49:A:ILE:H	1:84:A:VAL:HG13	20	0.12
(1,826)	1:82:A:ASN:H	1:84:A:VAL:HB	7	0.12
(1,818)	1:110:A:LEU:H	1:111:A:VAL:HG11	10	0.12
(1,818)	1:110:A:LEU:H	1:111:A:VAL:HG12	10	0.12
(1,818)	1:110:A:LEU:H	1:111:A:VAL:HG13	10	0.12
(1,804)	1:84:A:VAL:HB	1:87:A:ASN:H	19	0.12
(1,771)	1:76:A:ASN:H	1:78:A:PHE:HB2	1	0.12
(1,771)	1:76:A:ASN:H	1:78:A:PHE:HB2	6	0.12
(1,771)	1:76:A:ASN:H	1:78:A:PHE:HB2	11	0.12
(1,771)	1:76:A:ASN:H	1:78:A:PHE:HB2	18	0.12
(1,734)	1:65:A:TRP:H	1:67:A:ARG:HB2	7	0.12
(1,734)	1:65:A:TRP:H	1:67:A:ARG:HB3	7	0.12
(1,719)	1:109:A:ALA:H	1:112:A:LYS:H	18	0.12
(1,672)	1:26:A:SER:H	1:28:A:ASP:HB2	4	0.12
(1,672)	1:26:A:SER:H	1:28:A:ASP:HB3	4	0.12
(1,656)	1:50:A:GLU:H	1:51:A:ASN:HD21	9	0.12
(1,656)	1:50:A:GLU:H	1:51:A:ASN:HD21	16	0.12
(1,656)	1:50:A:GLU:H	1:51:A:ASN:HD21	19	0.12
(1,648)	1:75:A:LEU:HD11	1:120:A:VAL:H	16	0.12
(1,648)	1:75:A:LEU:HD12	1:120:A:VAL:H	16	0.12
(1,648)	1:75:A:LEU:HD13	1:120:A:VAL:H	16	0.12
(1,630)	1:65:A:TRP:HA	1:68:A:ARG:H	3	0.12
(1,604)	1:132:A:VAL:HG21	1:133:A:TYR:H	12	0.12
(1,604)	1:132:A:VAL:HG22	1:133:A:TYR:H	12	0.12
(1,604)	1:132:A:VAL:HG23	1:133:A:TYR:H	12	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,583)	1:48:A:CYS:H	1:51:A:ASN:HB2	3	0.12
(1,583)	1:48:A:CYS:H	1:51:A:ASN:HB2	14	0.12
(1,583)	1:48:A:CYS:H	1:51:A:ASN:HB2	17	0.12
(1,579)	1:48:A:CYS:H	1:84:A:VAL:HG21	9	0.12
(1,579)	1:48:A:CYS:H	1:84:A:VAL:HG22	9	0.12
(1,579)	1:48:A:CYS:H	1:84:A:VAL:HG23	9	0.12
(1,537)	1:32:A:GLN:H	1:32:A:GLN:HB3	9	0.12
(1,496)	1:85:A:ILE:HD11	1:86:A:GLN:H	3	0.12
(1,496)	1:85:A:ILE:HD12	1:86:A:GLN:H	3	0.12
(1,496)	1:85:A:ILE:HD13	1:86:A:GLN:H	3	0.12
(1,442)	1:75:A:LEU:HD11	1:78:A:PHE:HB3	11	0.12
(1,442)	1:75:A:LEU:HD12	1:78:A:PHE:HB3	11	0.12
(1,442)	1:75:A:LEU:HD13	1:78:A:PHE:HB3	11	0.12
(1,433)	1:84:A:VAL:HG11	1:96:A:PHE:HE1	9	0.12
(1,433)	1:84:A:VAL:HG11	1:96:A:PHE:HE2	9	0.12
(1,433)	1:84:A:VAL:HG12	1:96:A:PHE:HE1	9	0.12
(1,433)	1:84:A:VAL:HG12	1:96:A:PHE:HE2	9	0.12
(1,433)	1:84:A:VAL:HG13	1:96:A:PHE:HE1	9	0.12
(1,433)	1:84:A:VAL:HG13	1:96:A:PHE:HE2	9	0.12
(1,369)	1:63:A:MET:HG3	1:103:A:VAL:HG11	18	0.12
(1,369)	1:63:A:MET:HG3	1:103:A:VAL:HG12	18	0.12
(1,369)	1:63:A:MET:HG3	1:103:A:VAL:HG13	18	0.12
(1,359)	1:75:A:LEU:HD11	1:119:A:SER:HA	20	0.12
(1,359)	1:75:A:LEU:HD12	1:119:A:SER:HA	20	0.12
(1,359)	1:75:A:LEU:HD13	1:119:A:SER:HA	20	0.12
(1,322)	1:142:A:ARG:HA	1:142:A:ARG:HD2	18	0.12
(1,322)	1:142:A:ARG:HA	1:142:A:ARG:HD3	18	0.12
(1,319)	1:27:A:LEU:HB2	1:58:A:ILE:HA	5	0.12
(1,319)	1:27:A:LEU:HB3	1:58:A:ILE:HA	5	0.12
(1,297)	1:37:A:THR:HG21	1:38:A:MET:HB2	13	0.12
(1,297)	1:37:A:THR:HG21	1:38:A:MET:HB3	13	0.12
(1,297)	1:37:A:THR:HG22	1:38:A:MET:HB2	13	0.12
(1,297)	1:37:A:THR:HG22	1:38:A:MET:HB3	13	0.12
(1,297)	1:37:A:THR:HG23	1:38:A:MET:HB2	13	0.12
(1,297)	1:37:A:THR:HG23	1:38:A:MET:HB3	13	0.12
(1,296)	1:34:A:VAL:HG11	1:36:A:ASN:H	1	0.12
(1,296)	1:34:A:VAL:HG12	1:36:A:ASN:H	1	0.12
(1,296)	1:34:A:VAL:HG13	1:36:A:ASN:H	1	0.12
(1,296)	1:34:A:VAL:HG11	1:36:A:ASN:H	4	0.12
(1,296)	1:34:A:VAL:HG12	1:36:A:ASN:H	4	0.12
(1,296)	1:34:A:VAL:HG13	1:36:A:ASN:H	4	0.12
(1,252)	1:111:A:VAL:HG21	1:121:A:GLU:H	2	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,252)	1:111:A:VAL:HG22	1:121:A:GLU:H	2	0.12
(1,252)	1:111:A:VAL:HG23	1:121:A:GLU:H	2	0.12
(1,252)	1:111:A:VAL:HG21	1:121:A:GLU:H	13	0.12
(1,252)	1:111:A:VAL:HG22	1:121:A:GLU:H	13	0.12
(1,252)	1:111:A:VAL:HG23	1:121:A:GLU:H	13	0.12
(1,252)	1:111:A:VAL:HG21	1:121:A:GLU:H	20	0.12
(1,252)	1:111:A:VAL:HG22	1:121:A:GLU:H	20	0.12
(1,252)	1:111:A:VAL:HG23	1:121:A:GLU:H	20	0.12
(1,227)	1:85:A:ILE:HD11	1:101:A:ALA:H	20	0.12
(1,227)	1:85:A:ILE:HD12	1:101:A:ALA:H	20	0.12
(1,227)	1:85:A:ILE:HD13	1:101:A:ALA:H	20	0.12
(1,206)	1:48:A:CYS:HA	1:51:A:ASN:HA	1	0.12
(1,155)	1:90:A:ARG:HD2	1:91:A:LYS:HA	9	0.12
(1,155)	1:90:A:ARG:HD3	1:91:A:LYS:HA	9	0.12
(1,83)	1:137:A:MET:HB3	1:138:A:ILE:HD11	4	0.12
(1,83)	1:137:A:MET:HB3	1:138:A:ILE:HD12	4	0.12
(1,83)	1:137:A:MET:HB3	1:138:A:ILE:HD13	4	0.12
(1,74)	1:49:A:ILE:HD11	1:84:A:VAL:HG11	1	0.12
(1,74)	1:49:A:ILE:HD11	1:84:A:VAL:HG12	1	0.12
(1,74)	1:49:A:ILE:HD11	1:84:A:VAL:HG13	1	0.12
(1,74)	1:49:A:ILE:HD12	1:84:A:VAL:HG11	1	0.12
(1,74)	1:49:A:ILE:HD12	1:84:A:VAL:HG12	1	0.12
(1,74)	1:49:A:ILE:HD12	1:84:A:VAL:HG13	1	0.12
(1,74)	1:49:A:ILE:HD13	1:84:A:VAL:HG11	1	0.12
(1,74)	1:49:A:ILE:HD13	1:84:A:VAL:HG12	1	0.12
(1,74)	1:49:A:ILE:HD13	1:84:A:VAL:HG13	1	0.12
(1,74)	1:49:A:ILE:HD11	1:84:A:VAL:HG11	20	0.12
(1,74)	1:49:A:ILE:HD11	1:84:A:VAL:HG12	20	0.12
(1,74)	1:49:A:ILE:HD11	1:84:A:VAL:HG13	20	0.12
(1,74)	1:49:A:ILE:HD12	1:84:A:VAL:HG11	20	0.12
(1,74)	1:49:A:ILE:HD12	1:84:A:VAL:HG12	20	0.12
(1,74)	1:49:A:ILE:HD12	1:84:A:VAL:HG13	20	0.12
(1,74)	1:49:A:ILE:HD13	1:84:A:VAL:HG11	20	0.12
(1,74)	1:49:A:ILE:HD13	1:84:A:VAL:HG12	20	0.12
(1,74)	1:49:A:ILE:HD13	1:84:A:VAL:HG13	20	0.12
(1,20)	1:132:A:VAL:HG21	1:138:A:ILE:HD11	20	0.12
(1,20)	1:132:A:VAL:HG21	1:138:A:ILE:HD12	20	0.12
(1,20)	1:132:A:VAL:HG21	1:138:A:ILE:HD13	20	0.12
(1,20)	1:132:A:VAL:HG22	1:138:A:ILE:HD11	20	0.12
(1,20)	1:132:A:VAL:HG22	1:138:A:ILE:HD12	20	0.12
(1,20)	1:132:A:VAL:HG22	1:138:A:ILE:HD13	20	0.12
(1,20)	1:132:A:VAL:HG23	1:138:A:ILE:HD11	20	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,20)	1:132:A:VAL:HG23	1:138:A:ILE:HD12	20	0.12
(1,20)	1:132:A:VAL:HG23	1:138:A:ILE:HD13	20	0.12
(8,1)	2:152:B:SER:O	2:155:B:SER:H	20	0.11
(6,6)	2:154:B:TPO:HG21	2:153:B:PRO:HB2	1	0.11
(6,6)	2:154:B:TPO:HG21	2:153:B:PRO:HB3	1	0.11
(6,6)	2:154:B:TPO:HG21	2:153:B:PRO:HB2	5	0.11
(6,6)	2:154:B:TPO:HG21	2:153:B:PRO:HB3	5	0.11
(6,6)	2:154:B:TPO:HG21	2:153:B:PRO:HB2	14	0.11
(6,6)	2:154:B:TPO:HG21	2:153:B:PRO:HB3	14	0.11
(1,1511)	1:140:A:ALA:H	1:141:A:LEU:HD11	12	0.11
(1,1511)	1:140:A:ALA:H	1:141:A:LEU:HD12	12	0.11
(1,1511)	1:140:A:ALA:H	1:141:A:LEU:HD13	12	0.11
(1,1511)	1:140:A:ALA:H	1:141:A:LEU:HD21	12	0.11
(1,1511)	1:140:A:ALA:H	1:141:A:LEU:HD22	12	0.11
(1,1511)	1:140:A:ALA:H	1:141:A:LEU:HD23	12	0.11
(1,1501)	1:137:A:MET:HB3	1:141:A:LEU:HD11	14	0.11
(1,1501)	1:137:A:MET:HB3	1:141:A:LEU:HD12	14	0.11
(1,1501)	1:137:A:MET:HB3	1:141:A:LEU:HD13	14	0.11
(1,1501)	1:137:A:MET:HB3	1:141:A:LEU:HD21	14	0.11
(1,1501)	1:137:A:MET:HB3	1:141:A:LEU:HD22	14	0.11
(1,1501)	1:137:A:MET:HB3	1:141:A:LEU:HD23	14	0.11
(1,1459)	1:120:A:VAL:HG11	1:123:A:ILE:HD11	14	0.11
(1,1459)	1:120:A:VAL:HG11	1:123:A:ILE:HD12	14	0.11
(1,1459)	1:120:A:VAL:HG11	1:123:A:ILE:HD13	14	0.11
(1,1459)	1:120:A:VAL:HG12	1:123:A:ILE:HD11	14	0.11
(1,1459)	1:120:A:VAL:HG12	1:123:A:ILE:HD12	14	0.11
(1,1459)	1:120:A:VAL:HG12	1:123:A:ILE:HD13	14	0.11
(1,1459)	1:120:A:VAL:HG13	1:123:A:ILE:HD11	14	0.11
(1,1459)	1:120:A:VAL:HG13	1:123:A:ILE:HD12	14	0.11
(1,1459)	1:120:A:VAL:HG13	1:123:A:ILE:HD13	14	0.11
(1,1459)	1:120:A:VAL:HG21	1:123:A:ILE:HD11	14	0.11
(1,1459)	1:120:A:VAL:HG21	1:123:A:ILE:HD12	14	0.11
(1,1459)	1:120:A:VAL:HG21	1:123:A:ILE:HD13	14	0.11
(1,1459)	1:120:A:VAL:HG22	1:123:A:ILE:HD11	14	0.11
(1,1459)	1:120:A:VAL:HG22	1:123:A:ILE:HD12	14	0.11
(1,1459)	1:120:A:VAL:HG22	1:123:A:ILE:HD13	14	0.11
(1,1459)	1:120:A:VAL:HG23	1:123:A:ILE:HD11	14	0.11
(1,1459)	1:120:A:VAL:HG23	1:123:A:ILE:HD12	14	0.11
(1,1459)	1:120:A:VAL:HG23	1:123:A:ILE:HD13	14	0.11
(1,1432)	1:113:A:ASP:H	1:145:A:LEU:HD11	11	0.11
(1,1432)	1:113:A:ASP:H	1:145:A:LEU:HD12	11	0.11
(1,1432)	1:113:A:ASP:H	1:145:A:LEU:HD13	11	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1432)	1:113:A:ASP:H	1:145:A:LEU:HD21	11	0.11
(1,1432)	1:113:A:ASP:H	1:145:A:LEU:HD22	11	0.11
(1,1432)	1:113:A:ASP:H	1:145:A:LEU:HD23	11	0.11
(1,1366)	1:91:A:LYS:H	1:92:A:ASN:HB2	1	0.11
(1,1366)	1:91:A:LYS:H	1:92:A:ASN:HB3	1	0.11
(1,1366)	1:91:A:LYS:H	1:92:A:ASN:HB2	18	0.11
(1,1366)	1:91:A:LYS:H	1:92:A:ASN:HB3	18	0.11
(1,1364)	1:89:A:LYS:H	1:94:A:ILE:HG12	18	0.11
(1,1364)	1:89:A:LYS:H	1:94:A:ILE:HG13	18	0.11
(1,1362)	1:88:A:CYS:H	1:89:A:LYS:HB2	1	0.11
(1,1362)	1:88:A:CYS:H	1:89:A:LYS:HB3	1	0.11
(1,1320)	1:75:A:LEU:HD11	1:111:A:VAL:HG11	2	0.11
(1,1320)	1:75:A:LEU:HD11	1:111:A:VAL:HG12	2	0.11
(1,1320)	1:75:A:LEU:HD11	1:111:A:VAL:HG13	2	0.11
(1,1320)	1:75:A:LEU:HD12	1:111:A:VAL:HG11	2	0.11
(1,1320)	1:75:A:LEU:HD12	1:111:A:VAL:HG12	2	0.11
(1,1320)	1:75:A:LEU:HD12	1:111:A:VAL:HG13	2	0.11
(1,1320)	1:75:A:LEU:HD13	1:111:A:VAL:HG11	2	0.11
(1,1320)	1:75:A:LEU:HD13	1:111:A:VAL:HG12	2	0.11
(1,1320)	1:75:A:LEU:HD13	1:111:A:VAL:HG13	2	0.11
(1,1320)	1:75:A:LEU:HD21	1:111:A:VAL:HG11	2	0.11
(1,1320)	1:75:A:LEU:HD21	1:111:A:VAL:HG12	2	0.11
(1,1320)	1:75:A:LEU:HD21	1:111:A:VAL:HG13	2	0.11
(1,1320)	1:75:A:LEU:HD22	1:111:A:VAL:HG11	2	0.11
(1,1320)	1:75:A:LEU:HD22	1:111:A:VAL:HG12	2	0.11
(1,1320)	1:75:A:LEU:HD22	1:111:A:VAL:HG13	2	0.11
(1,1320)	1:75:A:LEU:HD23	1:111:A:VAL:HG11	2	0.11
(1,1320)	1:75:A:LEU:HD23	1:111:A:VAL:HG12	2	0.11
(1,1320)	1:75:A:LEU:HD23	1:111:A:VAL:HG13	2	0.11
(1,1280)	1:59:A:VAL:HG11	1:103:A:VAL:HG21	16	0.11
(1,1280)	1:59:A:VAL:HG11	1:103:A:VAL:HG22	16	0.11
(1,1280)	1:59:A:VAL:HG11	1:103:A:VAL:HG23	16	0.11
(1,1280)	1:59:A:VAL:HG12	1:103:A:VAL:HG21	16	0.11
(1,1280)	1:59:A:VAL:HG12	1:103:A:VAL:HG22	16	0.11
(1,1280)	1:59:A:VAL:HG12	1:103:A:VAL:HG23	16	0.11
(1,1280)	1:59:A:VAL:HG13	1:103:A:VAL:HG21	16	0.11
(1,1280)	1:59:A:VAL:HG13	1:103:A:VAL:HG22	16	0.11
(1,1280)	1:59:A:VAL:HG13	1:103:A:VAL:HG23	16	0.11
(1,1280)	1:59:A:VAL:HG21	1:103:A:VAL:HG21	16	0.11
(1,1280)	1:59:A:VAL:HG21	1:103:A:VAL:HG22	16	0.11
(1,1280)	1:59:A:VAL:HG21	1:103:A:VAL:HG23	16	0.11
(1,1280)	1:59:A:VAL:HG22	1:103:A:VAL:HG21	16	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1280)	1:59:A:VAL:HG22	1:103:A:VAL:HG22	16	0.11
(1,1280)	1:59:A:VAL:HG22	1:103:A:VAL:HG23	16	0.11
(1,1280)	1:59:A:VAL:HG23	1:103:A:VAL:HG21	16	0.11
(1,1280)	1:59:A:VAL:HG23	1:103:A:VAL:HG22	16	0.11
(1,1280)	1:59:A:VAL:HG23	1:103:A:VAL:HG23	16	0.11
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD11	6	0.11
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD12	6	0.11
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD13	6	0.11
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD21	6	0.11
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD22	6	0.11
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD23	6	0.11
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD11	7	0.11
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD12	7	0.11
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD13	7	0.11
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD21	7	0.11
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD22	7	0.11
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD23	7	0.11
(1,1169)	1:34:A:VAL:HG21	1:35:A:THR:H	11	0.11
(1,1169)	1:34:A:VAL:HG22	1:35:A:THR:H	11	0.11
(1,1169)	1:34:A:VAL:HG23	1:35:A:THR:H	11	0.11
(1,1147)	1:75:A:LEU:H	1:111:A:VAL:HG11	7	0.11
(1,1147)	1:75:A:LEU:H	1:111:A:VAL:HG12	7	0.11
(1,1147)	1:75:A:LEU:H	1:111:A:VAL:HG13	7	0.11
(1,1147)	1:75:A:LEU:H	1:111:A:VAL:HG11	19	0.11
(1,1147)	1:75:A:LEU:H	1:111:A:VAL:HG12	19	0.11
(1,1147)	1:75:A:LEU:H	1:111:A:VAL:HG13	19	0.11
(1,1132)	1:66:A:LEU:HD11	1:67:A:ARG:H	5	0.11
(1,1132)	1:66:A:LEU:HD12	1:67:A:ARG:H	5	0.11
(1,1132)	1:66:A:LEU:HD13	1:67:A:ARG:H	5	0.11
(1,1112)	1:61:A:HIS:H	1:61:A:HIS:HD2	9	0.11
(1,1108)	1:58:A:ILE:HG21	1:60:A:TYR:H	1	0.11
(1,1108)	1:58:A:ILE:HG22	1:60:A:TYR:H	1	0.11
(1,1108)	1:58:A:ILE:HG23	1:60:A:TYR:H	1	0.11
(1,1108)	1:58:A:ILE:HG21	1:60:A:TYR:H	7	0.11
(1,1108)	1:58:A:ILE:HG22	1:60:A:TYR:H	7	0.11
(1,1108)	1:58:A:ILE:HG23	1:60:A:TYR:H	7	0.11
(1,1108)	1:58:A:ILE:HG21	1:60:A:TYR:H	11	0.11
(1,1108)	1:58:A:ILE:HG22	1:60:A:TYR:H	11	0.11
(1,1108)	1:58:A:ILE:HG23	1:60:A:TYR:H	11	0.11
(1,1108)	1:58:A:ILE:HG21	1:60:A:TYR:H	12	0.11
(1,1108)	1:58:A:ILE:HG22	1:60:A:TYR:H	12	0.11
(1,1108)	1:58:A:ILE:HG23	1:60:A:TYR:H	12	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1057)	1:136:A:GLU:HB2	1:137:A:MET:H	11	0.11
(1,1057)	1:136:A:GLU:HB3	1:137:A:MET:H	11	0.11
(1,1033)	1:128:A:GLU:H	1:138:A:ILE:HG12	7	0.11
(1,1033)	1:128:A:GLU:H	1:138:A:ILE:HG13	7	0.11
(1,981)	1:112:A:LYS:HB2	1:113:A:ASP:H	1	0.11
(1,981)	1:112:A:LYS:HB3	1:113:A:ASP:H	1	0.11
(1,981)	1:112:A:LYS:HB2	1:113:A:ASP:H	13	0.11
(1,981)	1:112:A:LYS:HB3	1:113:A:ASP:H	13	0.11
(1,981)	1:112:A:LYS:HB2	1:113:A:ASP:H	15	0.11
(1,981)	1:112:A:LYS:HB3	1:113:A:ASP:H	15	0.11
(1,981)	1:112:A:LYS:HB2	1:113:A:ASP:H	16	0.11
(1,981)	1:112:A:LYS:HB3	1:113:A:ASP:H	16	0.11
(1,952)	1:104:A:LEU:HD21	1:106:A:GLU:H	19	0.11
(1,952)	1:104:A:LEU:HD22	1:106:A:GLU:H	19	0.11
(1,952)	1:104:A:LEU:HD23	1:106:A:GLU:H	19	0.11
(1,950)	1:103:A:VAL:HG21	1:107:A:ALA:H	6	0.11
(1,950)	1:103:A:VAL:HG22	1:107:A:ALA:H	6	0.11
(1,950)	1:103:A:VAL:HG23	1:107:A:ALA:H	6	0.11
(1,947)	1:103:A:VAL:HB	1:107:A:ALA:H	3	0.11
(1,938)	1:101:A:ALA:HB1	1:104:A:LEU:H	10	0.11
(1,938)	1:101:A:ALA:HB2	1:104:A:LEU:H	10	0.11
(1,938)	1:101:A:ALA:HB3	1:104:A:LEU:H	10	0.11
(1,881)	1:51:A:ASN:H	1:51:A:ASN:HD21	9	0.11
(1,847)	1:49:A:ILE:H	1:84:A:VAL:HG11	11	0.11
(1,847)	1:49:A:ILE:H	1:84:A:VAL:HG12	11	0.11
(1,847)	1:49:A:ILE:H	1:84:A:VAL:HG13	11	0.11
(1,846)	1:45:A:SER:HA	1:85:A:ILE:H	6	0.11
(1,826)	1:82:A:ASN:H	1:84:A:VAL:HB	12	0.11
(1,819)	1:100:A:PHE:HD1	1:104:A:LEU:H	10	0.11
(1,819)	1:100:A:PHE:HD2	1:104:A:LEU:H	10	0.11
(1,819)	1:100:A:PHE:HD1	1:104:A:LEU:H	19	0.11
(1,819)	1:100:A:PHE:HD2	1:104:A:LEU:H	19	0.11
(1,804)	1:84:A:VAL:HB	1:87:A:ASN:H	3	0.11
(1,804)	1:84:A:VAL:HB	1:87:A:ASN:H	4	0.11
(1,804)	1:84:A:VAL:HB	1:87:A:ASN:H	12	0.11
(1,771)	1:76:A:ASN:H	1:78:A:PHE:HB2	7	0.11
(1,771)	1:76:A:ASN:H	1:78:A:PHE:HB2	8	0.11
(1,771)	1:76:A:ASN:H	1:78:A:PHE:HB2	14	0.11
(1,727)	1:139:A:VAL:H	1:142:A:ARG:HD2	7	0.11
(1,727)	1:139:A:VAL:H	1:142:A:ARG:HD3	7	0.11
(1,656)	1:50:A:GLU:H	1:51:A:ASN:HD21	2	0.11
(1,656)	1:50:A:GLU:H	1:51:A:ASN:HD21	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,656)	1:50:A:GLU:H	1:51:A:ASN:HD21	10	0.11
(1,656)	1:50:A:GLU:H	1:51:A:ASN:HD21	14	0.11
(1,646)	1:41:A:ILE:HA	1:44:A:LEU:H	10	0.11
(1,645)	1:42:A:GLN:H	1:44:A:LEU:H	10	0.11
(1,600)	1:101:A:ALA:H	1:103:A:VAL:HG21	3	0.11
(1,600)	1:101:A:ALA:H	1:103:A:VAL:HG22	3	0.11
(1,600)	1:101:A:ALA:H	1:103:A:VAL:HG23	3	0.11
(1,574)	1:108:A:ALA:H	1:111:A:VAL:HG11	1	0.11
(1,574)	1:108:A:ALA:H	1:111:A:VAL:HG12	1	0.11
(1,574)	1:108:A:ALA:H	1:111:A:VAL:HG13	1	0.11
(1,537)	1:32:A:GLN:H	1:32:A:GLN:HB3	2	0.11
(1,537)	1:32:A:GLN:H	1:32:A:GLN:HB3	5	0.11
(1,537)	1:32:A:GLN:H	1:32:A:GLN:HB3	11	0.11
(1,537)	1:32:A:GLN:H	1:32:A:GLN:HB3	12	0.11
(1,537)	1:32:A:GLN:H	1:32:A:GLN:HB3	14	0.11
(1,537)	1:32:A:GLN:H	1:32:A:GLN:HB3	15	0.11
(1,537)	1:32:A:GLN:H	1:32:A:GLN:HB3	16	0.11
(1,537)	1:32:A:GLN:H	1:32:A:GLN:HB3	19	0.11
(1,496)	1:85:A:ILE:HD11	1:86:A:GLN:H	2	0.11
(1,496)	1:85:A:ILE:HD12	1:86:A:GLN:H	2	0.11
(1,496)	1:85:A:ILE:HD13	1:86:A:GLN:H	2	0.11
(1,496)	1:85:A:ILE:HD11	1:86:A:GLN:H	11	0.11
(1,496)	1:85:A:ILE:HD12	1:86:A:GLN:H	11	0.11
(1,496)	1:85:A:ILE:HD13	1:86:A:GLN:H	11	0.11
(1,379)	1:139:A:VAL:HG21	1:143:A:GLU:HG2	17	0.11
(1,379)	1:139:A:VAL:HG21	1:143:A:GLU:HG3	17	0.11
(1,379)	1:139:A:VAL:HG22	1:143:A:GLU:HG2	17	0.11
(1,379)	1:139:A:VAL:HG22	1:143:A:GLU:HG3	17	0.11
(1,379)	1:139:A:VAL:HG23	1:143:A:GLU:HG2	17	0.11
(1,379)	1:139:A:VAL:HG23	1:143:A:GLU:HG3	17	0.11
(1,371)	1:100:A:PHE:HA	1:103:A:VAL:HG11	10	0.11
(1,371)	1:100:A:PHE:HA	1:103:A:VAL:HG12	10	0.11
(1,371)	1:100:A:PHE:HA	1:103:A:VAL:HG13	10	0.11
(1,322)	1:142:A:ARG:HA	1:142:A:ARG:HD2	20	0.11
(1,322)	1:142:A:ARG:HA	1:142:A:ARG:HD3	20	0.11
(1,297)	1:37:A:THR:HG21	1:38:A:MET:HB2	8	0.11
(1,297)	1:37:A:THR:HG21	1:38:A:MET:HB3	8	0.11
(1,297)	1:37:A:THR:HG22	1:38:A:MET:HB2	8	0.11
(1,297)	1:37:A:THR:HG22	1:38:A:MET:HB3	8	0.11
(1,297)	1:37:A:THR:HG23	1:38:A:MET:HB2	8	0.11
(1,297)	1:37:A:THR:HG23	1:38:A:MET:HB3	8	0.11
(1,227)	1:85:A:ILE:HD11	1:101:A:ALA:H	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,227)	1:85:A:ILE:HD12	1:101:A:ALA:H	3	0.11
(1,227)	1:85:A:ILE:HD13	1:101:A:ALA:H	3	0.11
(1,227)	1:85:A:ILE:HD11	1:101:A:ALA:H	7	0.11
(1,227)	1:85:A:ILE:HD12	1:101:A:ALA:H	7	0.11
(1,227)	1:85:A:ILE:HD13	1:101:A:ALA:H	7	0.11
(1,204)	1:59:A:VAL:HA	1:103:A:VAL:HG11	9	0.11
(1,204)	1:59:A:VAL:HA	1:103:A:VAL:HG12	9	0.11
(1,204)	1:59:A:VAL:HA	1:103:A:VAL:HG13	9	0.11
(1,162)	1:93:A:ALA:HA	1:94:A:ILE:HG21	7	0.11
(1,162)	1:93:A:ALA:HA	1:94:A:ILE:HG22	7	0.11
(1,162)	1:93:A:ALA:HA	1:94:A:ILE:HG23	7	0.11
(1,74)	1:49:A:ILE:HD11	1:84:A:VAL:HG11	9	0.11
(1,74)	1:49:A:ILE:HD11	1:84:A:VAL:HG12	9	0.11
(1,74)	1:49:A:ILE:HD11	1:84:A:VAL:HG13	9	0.11
(1,74)	1:49:A:ILE:HD12	1:84:A:VAL:HG11	9	0.11
(1,74)	1:49:A:ILE:HD12	1:84:A:VAL:HG12	9	0.11
(1,74)	1:49:A:ILE:HD12	1:84:A:VAL:HG13	9	0.11
(1,74)	1:49:A:ILE:HD13	1:84:A:VAL:HG11	9	0.11
(1,74)	1:49:A:ILE:HD13	1:84:A:VAL:HG12	9	0.11
(1,74)	1:49:A:ILE:HD13	1:84:A:VAL:HG13	9	0.11
(1,66)	1:49:A:ILE:HA	1:84:A:VAL:HG11	4	0.11
(1,66)	1:49:A:ILE:HA	1:84:A:VAL:HG12	4	0.11
(1,66)	1:49:A:ILE:HA	1:84:A:VAL:HG13	4	0.11
(1,66)	1:49:A:ILE:HA	1:84:A:VAL:HG11	9	0.11
(1,66)	1:49:A:ILE:HA	1:84:A:VAL:HG12	9	0.11
(1,66)	1:49:A:ILE:HA	1:84:A:VAL:HG13	9	0.11
(1,61)	1:59:A:VAL:HG21	1:62:A:TRP:HE3	10	0.11
(1,61)	1:59:A:VAL:HG22	1:62:A:TRP:HE3	10	0.11
(1,61)	1:59:A:VAL:HG23	1:62:A:TRP:HE3	10	0.11
(1,1450)	1:116:A:VAL:HG11	1:120:A:VAL:HG11	2	0.1
(1,1450)	1:116:A:VAL:HG11	1:120:A:VAL:HG12	2	0.1
(1,1450)	1:116:A:VAL:HG11	1:120:A:VAL:HG13	2	0.1
(1,1450)	1:116:A:VAL:HG11	1:120:A:VAL:HG21	2	0.1
(1,1450)	1:116:A:VAL:HG11	1:120:A:VAL:HG22	2	0.1
(1,1450)	1:116:A:VAL:HG11	1:120:A:VAL:HG23	2	0.1
(1,1450)	1:116:A:VAL:HG12	1:120:A:VAL:HG11	2	0.1
(1,1450)	1:116:A:VAL:HG12	1:120:A:VAL:HG12	2	0.1
(1,1450)	1:116:A:VAL:HG12	1:120:A:VAL:HG13	2	0.1
(1,1450)	1:116:A:VAL:HG12	1:120:A:VAL:HG21	2	0.1
(1,1450)	1:116:A:VAL:HG12	1:120:A:VAL:HG22	2	0.1
(1,1450)	1:116:A:VAL:HG12	1:120:A:VAL:HG23	2	0.1
(1,1450)	1:116:A:VAL:HG13	1:120:A:VAL:HG11	2	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1450)	1:116:A:VAL:HG13	1:120:A:VAL:HG12	2	0.1
(1,1450)	1:116:A:VAL:HG13	1:120:A:VAL:HG13	2	0.1
(1,1450)	1:116:A:VAL:HG13	1:120:A:VAL:HG21	2	0.1
(1,1450)	1:116:A:VAL:HG13	1:120:A:VAL:HG22	2	0.1
(1,1450)	1:116:A:VAL:HG13	1:120:A:VAL:HG23	2	0.1
(1,1450)	1:116:A:VAL:HG21	1:120:A:VAL:HG11	2	0.1
(1,1450)	1:116:A:VAL:HG21	1:120:A:VAL:HG12	2	0.1
(1,1450)	1:116:A:VAL:HG21	1:120:A:VAL:HG13	2	0.1
(1,1450)	1:116:A:VAL:HG21	1:120:A:VAL:HG21	2	0.1
(1,1450)	1:116:A:VAL:HG21	1:120:A:VAL:HG22	2	0.1
(1,1450)	1:116:A:VAL:HG21	1:120:A:VAL:HG23	2	0.1
(1,1450)	1:116:A:VAL:HG22	1:120:A:VAL:HG11	2	0.1
(1,1450)	1:116:A:VAL:HG22	1:120:A:VAL:HG12	2	0.1
(1,1450)	1:116:A:VAL:HG22	1:120:A:VAL:HG13	2	0.1
(1,1450)	1:116:A:VAL:HG22	1:120:A:VAL:HG21	2	0.1
(1,1450)	1:116:A:VAL:HG22	1:120:A:VAL:HG22	2	0.1
(1,1450)	1:116:A:VAL:HG22	1:120:A:VAL:HG23	2	0.1
(1,1450)	1:116:A:VAL:HG23	1:120:A:VAL:HG11	2	0.1
(1,1450)	1:116:A:VAL:HG23	1:120:A:VAL:HG12	2	0.1
(1,1450)	1:116:A:VAL:HG23	1:120:A:VAL:HG13	2	0.1
(1,1450)	1:116:A:VAL:HG23	1:120:A:VAL:HG21	2	0.1
(1,1450)	1:116:A:VAL:HG23	1:120:A:VAL:HG22	2	0.1
(1,1450)	1:116:A:VAL:HG23	1:120:A:VAL:HG23	2	0.1
(1,1447)	1:116:A:VAL:HG11	1:118:A:LYS:HG2	16	0.1
(1,1447)	1:116:A:VAL:HG11	1:118:A:LYS:HG3	16	0.1
(1,1447)	1:116:A:VAL:HG12	1:118:A:LYS:HG2	16	0.1
(1,1447)	1:116:A:VAL:HG12	1:118:A:LYS:HG3	16	0.1
(1,1447)	1:116:A:VAL:HG13	1:118:A:LYS:HG2	16	0.1
(1,1447)	1:116:A:VAL:HG13	1:118:A:LYS:HG3	16	0.1
(1,1447)	1:116:A:VAL:HG21	1:118:A:LYS:HG2	16	0.1
(1,1447)	1:116:A:VAL:HG21	1:118:A:LYS:HG3	16	0.1
(1,1447)	1:116:A:VAL:HG22	1:118:A:LYS:HG2	16	0.1
(1,1447)	1:116:A:VAL:HG22	1:118:A:LYS:HG3	16	0.1
(1,1447)	1:116:A:VAL:HG23	1:118:A:LYS:HG2	16	0.1
(1,1447)	1:116:A:VAL:HG23	1:118:A:LYS:HG3	16	0.1
(1,1347)	1:84:A:VAL:HG11	1:85:A:ILE:HG12	12	0.1
(1,1347)	1:84:A:VAL:HG11	1:85:A:ILE:HG13	12	0.1
(1,1347)	1:84:A:VAL:HG12	1:85:A:ILE:HG12	12	0.1
(1,1347)	1:84:A:VAL:HG12	1:85:A:ILE:HG13	12	0.1
(1,1347)	1:84:A:VAL:HG13	1:85:A:ILE:HG12	12	0.1
(1,1347)	1:84:A:VAL:HG13	1:85:A:ILE:HG13	12	0.1
(1,1347)	1:84:A:VAL:HG11	1:85:A:ILE:HG12	17	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1347)	1:84:A:VAL:HG11	1:85:A:ILE:HG13	17	0.1
(1,1347)	1:84:A:VAL:HG12	1:85:A:ILE:HG12	17	0.1
(1,1347)	1:84:A:VAL:HG12	1:85:A:ILE:HG13	17	0.1
(1,1347)	1:84:A:VAL:HG13	1:85:A:ILE:HG12	17	0.1
(1,1347)	1:84:A:VAL:HG13	1:85:A:ILE:HG13	17	0.1
(1,1297)	1:66:A:LEU:HD11	1:67:A:ARG:H	6	0.1
(1,1297)	1:66:A:LEU:HD12	1:67:A:ARG:H	6	0.1
(1,1297)	1:66:A:LEU:HD13	1:67:A:ARG:H	6	0.1
(1,1297)	1:66:A:LEU:HD21	1:67:A:ARG:H	6	0.1
(1,1297)	1:66:A:LEU:HD22	1:67:A:ARG:H	6	0.1
(1,1297)	1:66:A:LEU:HD23	1:67:A:ARG:H	6	0.1
(1,1262)	1:59:A:VAL:HG11	1:62:A:TRP:HE3	10	0.1
(1,1262)	1:59:A:VAL:HG12	1:62:A:TRP:HE3	10	0.1
(1,1262)	1:59:A:VAL:HG13	1:62:A:TRP:HE3	10	0.1
(1,1262)	1:59:A:VAL:HG21	1:62:A:TRP:HE3	10	0.1
(1,1262)	1:59:A:VAL:HG22	1:62:A:TRP:HE3	10	0.1
(1,1262)	1:59:A:VAL:HG23	1:62:A:TRP:HE3	10	0.1
(1,1259)	1:59:A:VAL:HG11	1:61:A:HIS:H	7	0.1
(1,1259)	1:59:A:VAL:HG12	1:61:A:HIS:H	7	0.1
(1,1259)	1:59:A:VAL:HG13	1:61:A:HIS:H	7	0.1
(1,1259)	1:59:A:VAL:HG21	1:61:A:HIS:H	7	0.1
(1,1259)	1:59:A:VAL:HG22	1:61:A:HIS:H	7	0.1
(1,1259)	1:59:A:VAL:HG23	1:61:A:HIS:H	7	0.1
(1,1238)	1:48:A:CYS:HB2	1:84:A:VAL:HG21	18	0.1
(1,1238)	1:48:A:CYS:HB2	1:84:A:VAL:HG22	18	0.1
(1,1238)	1:48:A:CYS:HB2	1:84:A:VAL:HG23	18	0.1
(1,1238)	1:48:A:CYS:HB3	1:84:A:VAL:HG21	18	0.1
(1,1238)	1:48:A:CYS:HB3	1:84:A:VAL:HG22	18	0.1
(1,1238)	1:48:A:CYS:HB3	1:84:A:VAL:HG23	18	0.1
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD11	19	0.1
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD12	19	0.1
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD13	19	0.1
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD21	19	0.1
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD22	19	0.1
(1,1228)	1:45:A:SER:H	1:80:A:LEU:HD23	19	0.1
(1,1223)	1:44:A:LEU:HD11	1:81:A:ALA:H	3	0.1
(1,1223)	1:44:A:LEU:HD12	1:81:A:ALA:H	3	0.1
(1,1223)	1:44:A:LEU:HD13	1:81:A:ALA:H	3	0.1
(1,1223)	1:44:A:LEU:HD21	1:81:A:ALA:H	3	0.1
(1,1223)	1:44:A:LEU:HD22	1:81:A:ALA:H	3	0.1
(1,1223)	1:44:A:LEU:HD23	1:81:A:ALA:H	3	0.1
(1,1189)	1:62:A:TRP:HE1	1:77:A:LEU:HD21	5	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1189)	1:62:A:TRP:HE1	1:77:A:LEU:HD22	5	0.1
(1,1189)	1:62:A:TRP:HE1	1:77:A:LEU:HD23	5	0.1
(1,1177)	1:47:A:TRP:H	1:47:A:TRP:HD1	5	0.1
(1,1147)	1:75:A:LEU:H	1:111:A:VAL:HG11	5	0.1
(1,1147)	1:75:A:LEU:H	1:111:A:VAL:HG12	5	0.1
(1,1147)	1:75:A:LEU:H	1:111:A:VAL:HG13	5	0.1
(1,1108)	1:58:A:ILE:HG21	1:60:A:TYR:H	13	0.1
(1,1108)	1:58:A:ILE:HG22	1:60:A:TYR:H	13	0.1
(1,1108)	1:58:A:ILE:HG23	1:60:A:TYR:H	13	0.1
(1,1108)	1:58:A:ILE:HG21	1:60:A:TYR:H	19	0.1
(1,1108)	1:58:A:ILE:HG22	1:60:A:TYR:H	19	0.1
(1,1108)	1:58:A:ILE:HG23	1:60:A:TYR:H	19	0.1
(1,1099)	1:146:A:SER:H	1:146:A:SER:HB2	13	0.1
(1,1099)	1:146:A:SER:H	1:146:A:SER:HB3	13	0.1
(1,1073)	1:139:A:VAL:HB	1:140:A:ALA:H	4	0.1
(1,1033)	1:128:A:GLU:H	1:138:A:ILE:HG12	3	0.1
(1,1033)	1:128:A:GLU:H	1:138:A:ILE:HG13	3	0.1
(1,981)	1:112:A:LYS:HB2	1:113:A:ASP:H	3	0.1
(1,981)	1:112:A:LYS:HB3	1:113:A:ASP:H	3	0.1
(1,981)	1:112:A:LYS:HB2	1:113:A:ASP:H	6	0.1
(1,981)	1:112:A:LYS:HB3	1:113:A:ASP:H	6	0.1
(1,981)	1:112:A:LYS:HB2	1:113:A:ASP:H	9	0.1
(1,981)	1:112:A:LYS:HB3	1:113:A:ASP:H	9	0.1
(1,962)	1:107:A:ALA:HB1	1:109:A:ALA:H	17	0.1
(1,962)	1:107:A:ALA:HB2	1:109:A:ALA:H	17	0.1
(1,962)	1:107:A:ALA:HB3	1:109:A:ALA:H	17	0.1
(1,847)	1:49:A:ILE:H	1:84:A:VAL:HG11	6	0.1
(1,847)	1:49:A:ILE:H	1:84:A:VAL:HG12	6	0.1
(1,847)	1:49:A:ILE:H	1:84:A:VAL:HG13	6	0.1
(1,826)	1:82:A:ASN:H	1:84:A:VAL:HB	4	0.1
(1,826)	1:82:A:ASN:H	1:84:A:VAL:HB	16	0.1
(1,816)	1:87:A:ASN:H	1:88:A:CYS:HA	15	0.1
(1,804)	1:84:A:VAL:HB	1:87:A:ASN:H	15	0.1
(1,766)	1:73:A:HIS:H	1:76:A:ASN:H	12	0.1
(1,719)	1:109:A:ALA:H	1:112:A:LYS:H	8	0.1
(1,719)	1:109:A:ALA:H	1:112:A:LYS:H	12	0.1
(1,591)	1:108:A:ALA:H	1:111:A:VAL:H	17	0.1
(1,583)	1:48:A:CYS:H	1:51:A:ASN:HB2	10	0.1
(1,579)	1:48:A:CYS:H	1:84:A:VAL:HG21	18	0.1
(1,579)	1:48:A:CYS:H	1:84:A:VAL:HG22	18	0.1
(1,579)	1:48:A:CYS:H	1:84:A:VAL:HG23	18	0.1
(1,537)	1:32:A:GLN:H	1:32:A:GLN:HB3	6	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,493)	1:51:A:ASN:HD21	1:58:A:ILE:HG21	4	0.1
(1,493)	1:51:A:ASN:HD21	1:58:A:ILE:HG22	4	0.1
(1,493)	1:51:A:ASN:HD21	1:58:A:ILE:HG23	4	0.1
(1,359)	1:75:A:LEU:HD11	1:119:A:SER:HA	16	0.1
(1,359)	1:75:A:LEU:HD12	1:119:A:SER:HA	16	0.1
(1,359)	1:75:A:LEU:HD13	1:119:A:SER:HA	16	0.1
(1,299)	1:90:A:ARG:HA	1:91:A:LYS:HG2	15	0.1
(1,299)	1:90:A:ARG:HA	1:91:A:LYS:HG3	15	0.1
(1,227)	1:85:A:ILE:HD11	1:101:A:ALA:H	10	0.1
(1,227)	1:85:A:ILE:HD12	1:101:A:ALA:H	10	0.1
(1,227)	1:85:A:ILE:HD13	1:101:A:ALA:H	10	0.1
(1,227)	1:85:A:ILE:HD11	1:101:A:ALA:H	11	0.1
(1,227)	1:85:A:ILE:HD12	1:101:A:ALA:H	11	0.1
(1,227)	1:85:A:ILE:HD13	1:101:A:ALA:H	11	0.1
(1,227)	1:85:A:ILE:HD11	1:101:A:ALA:H	16	0.1
(1,227)	1:85:A:ILE:HD12	1:101:A:ALA:H	16	0.1
(1,227)	1:85:A:ILE:HD13	1:101:A:ALA:H	16	0.1
(1,227)	1:85:A:ILE:HD11	1:101:A:ALA:H	19	0.1
(1,227)	1:85:A:ILE:HD12	1:101:A:ALA:H	19	0.1
(1,227)	1:85:A:ILE:HD13	1:101:A:ALA:H	19	0.1
(1,185)	1:75:A:LEU:H	1:111:A:VAL:HA	5	0.1
(1,185)	1:75:A:LEU:H	1:111:A:VAL:HA	9	0.1
(1,155)	1:90:A:ARG:HD2	1:91:A:LYS:HA	7	0.1
(1,155)	1:90:A:ARG:HD3	1:91:A:LYS:HA	7	0.1
(1,97)	1:95:A:ILE:HD11	1:98:A:GLU:HA	10	0.1
(1,97)	1:95:A:ILE:HD12	1:98:A:GLU:HA	10	0.1
(1,97)	1:95:A:ILE:HD13	1:98:A:GLU:HA	10	0.1
(1,74)	1:49:A:ILE:HD11	1:84:A:VAL:HG11	6	0.1
(1,74)	1:49:A:ILE:HD11	1:84:A:VAL:HG12	6	0.1
(1,74)	1:49:A:ILE:HD11	1:84:A:VAL:HG13	6	0.1
(1,74)	1:49:A:ILE:HD12	1:84:A:VAL:HG11	6	0.1
(1,74)	1:49:A:ILE:HD12	1:84:A:VAL:HG12	6	0.1
(1,74)	1:49:A:ILE:HD12	1:84:A:VAL:HG13	6	0.1
(1,74)	1:49:A:ILE:HD13	1:84:A:VAL:HG11	6	0.1
(1,74)	1:49:A:ILE:HD13	1:84:A:VAL:HG12	6	0.1
(1,74)	1:49:A:ILE:HD13	1:84:A:VAL:HG13	6	0.1
(1,74)	1:49:A:ILE:HD11	1:84:A:VAL:HG11	7	0.1
(1,74)	1:49:A:ILE:HD11	1:84:A:VAL:HG12	7	0.1
(1,74)	1:49:A:ILE:HD11	1:84:A:VAL:HG13	7	0.1
(1,74)	1:49:A:ILE:HD12	1:84:A:VAL:HG11	7	0.1
(1,74)	1:49:A:ILE:HD12	1:84:A:VAL:HG12	7	0.1
(1,74)	1:49:A:ILE:HD12	1:84:A:VAL:HG13	7	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,74)	1:49:A:ILE:HD13	1:84:A:VAL:HG11	7	0.1
(1,74)	1:49:A:ILE:HD13	1:84:A:VAL:HG12	7	0.1
(1,74)	1:49:A:ILE:HD13	1:84:A:VAL:HG13	7	0.1
(1,74)	1:49:A:ILE:HD11	1:84:A:VAL:HG11	19	0.1
(1,74)	1:49:A:ILE:HD11	1:84:A:VAL:HG12	19	0.1
(1,74)	1:49:A:ILE:HD11	1:84:A:VAL:HG13	19	0.1
(1,74)	1:49:A:ILE:HD12	1:84:A:VAL:HG11	19	0.1
(1,74)	1:49:A:ILE:HD12	1:84:A:VAL:HG12	19	0.1
(1,74)	1:49:A:ILE:HD12	1:84:A:VAL:HG13	19	0.1
(1,74)	1:49:A:ILE:HD13	1:84:A:VAL:HG11	19	0.1
(1,74)	1:49:A:ILE:HD13	1:84:A:VAL:HG12	19	0.1
(1,74)	1:49:A:ILE:HD13	1:84:A:VAL:HG13	19	0.1
(1,66)	1:49:A:ILE:HA	1:84:A:VAL:HG11	1	0.1
(1,66)	1:49:A:ILE:HA	1:84:A:VAL:HG12	1	0.1
(1,66)	1:49:A:ILE:HA	1:84:A:VAL:HG13	1	0.1
(1,20)	1:132:A:VAL:HG21	1:138:A:ILE:HD11	14	0.1
(1,20)	1:132:A:VAL:HG21	1:138:A:ILE:HD12	14	0.1
(1,20)	1:132:A:VAL:HG21	1:138:A:ILE:HD13	14	0.1
(1,20)	1:132:A:VAL:HG22	1:138:A:ILE:HD11	14	0.1
(1,20)	1:132:A:VAL:HG22	1:138:A:ILE:HD12	14	0.1
(1,20)	1:132:A:VAL:HG22	1:138:A:ILE:HD13	14	0.1
(1,20)	1:132:A:VAL:HG23	1:138:A:ILE:HD11	14	0.1
(1,20)	1:132:A:VAL:HG23	1:138:A:ILE:HD12	14	0.1
(1,20)	1:132:A:VAL:HG23	1:138:A:ILE:HD13	14	0.1

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

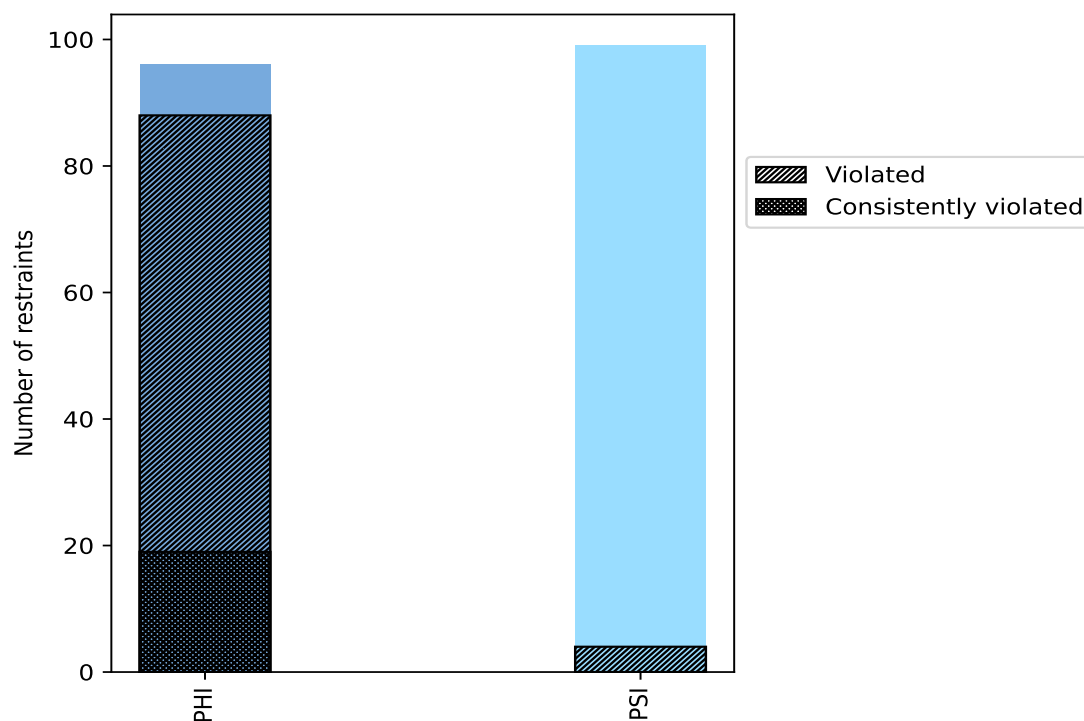
10.1 Summary of dihedral-angle violations [i](#)

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	96	49.2	88	91.7	45.1	19	19.8	9.7
PSI	99	50.8	4	4.0	2.1	0	0.0	0.0
Total	195	100.0	92	47.2	47.2	19	9.7	9.7

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

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



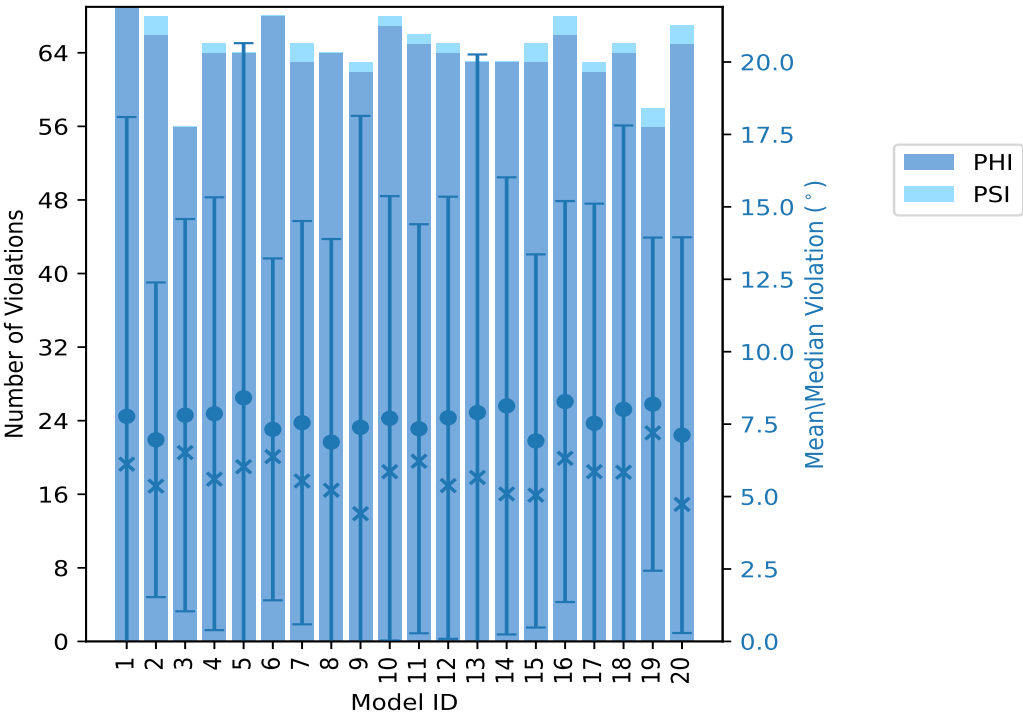
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	69	0	69	7.77	80.83	10.33	6.12
2	66	2	68	6.96	31.43	5.43	5.36
3	56	0	56	7.81	41.43	6.77	6.52
4	64	1	65	7.86	42.25	7.47	5.6
5	64	0	64	8.41	93.07	12.24	6.03
6	68	0	68	7.32	41.1	5.9	6.38
7	63	2	65	7.55	36.98	6.96	5.54
8	64	0	64	6.88	47.14	7.01	5.22
9	62	1	63	7.39	82.57	10.75	4.41
10	67	1	68	7.7	51.33	7.67	5.86
11	65	1	66	7.34	44.92	7.06	6.22
12	64	1	65	7.72	46.72	7.63	5.38
13	63	0	63	7.9	97.45	12.36	5.66
14	63	0	63	8.13	32.79	7.89	5.09
15	63	2	65	6.92	36.44	6.44	5.05
16	66	2	68	8.28	30.08	6.92	6.32
17	62	1	63	7.53	39.09	7.58	5.86
18	64	1	65	8.01	61.43	9.8	5.84
19	56	2	58	8.19	28.96	5.75	7.2
20	65	2	67	7.12	36.36	6.83	4.73

10.2.1 Bar graph : Dihedral violation statistics for each model [i](#)



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

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

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

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

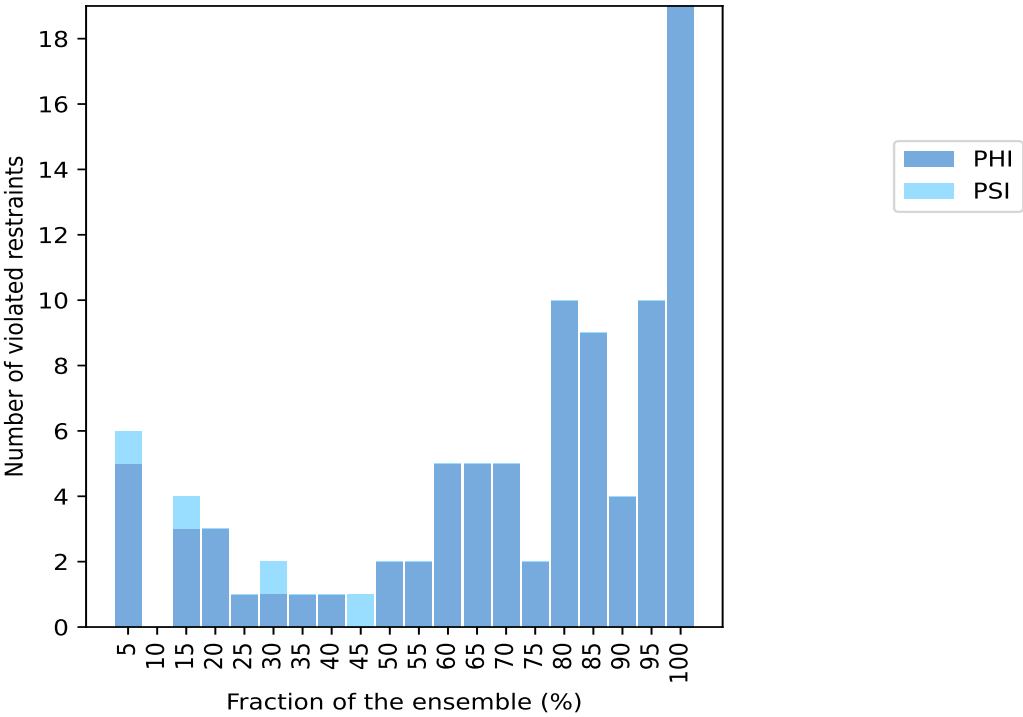
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Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
5	0	5	12	60.0
5	0	5	13	65.0
5	0	5	14	70.0
2	0	2	15	75.0
10	0	10	16	80.0
9	0	9	17	85.0
4	0	4	18	90.0
10	0	10	19	95.0
19	0	19	20	100.0

¹ Number of models with violations

10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble ⓘ

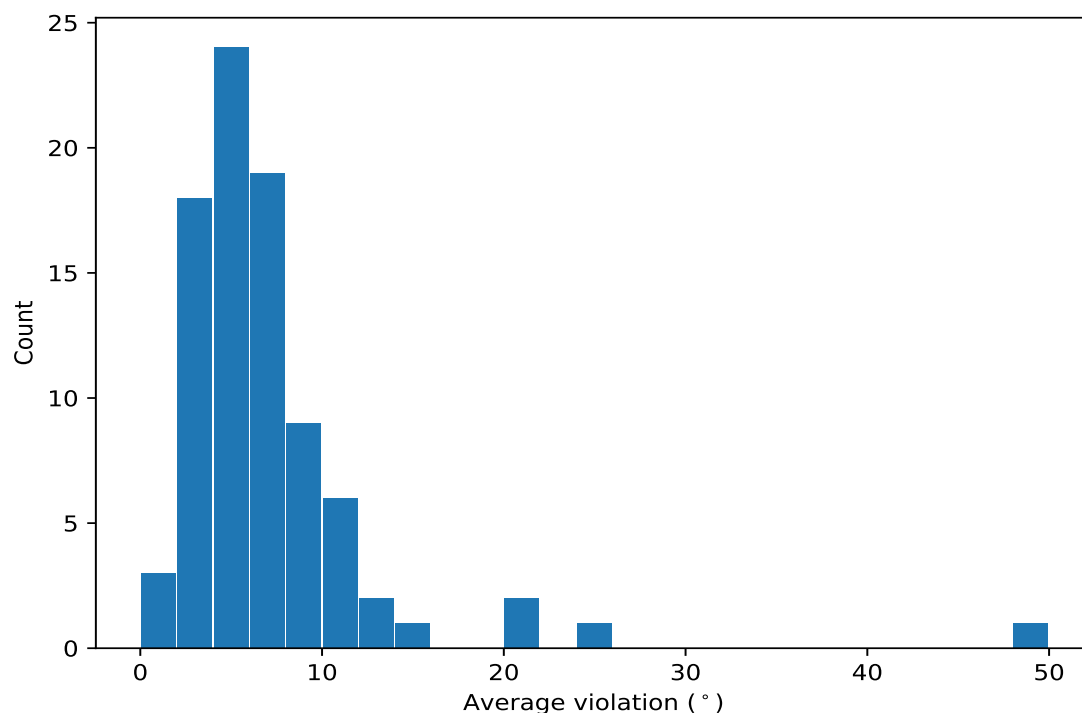


10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

10.4.1 Histogram : Distribution of mean dihedral-angle violations ⓘ

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

in the ensemble



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
(1,34)	1:39:A:GLU:C	1:40:A:SER:N	1:40:A:SER:CA	1:40:A:SER:C	20	48.02	22.29	41.84
(1,178)	1:136:A:GLU:C	1:137:A:MET:N	1:137:A:MET:CA	1:137:A:MET:C	20	21.7	9.34	19.13
(1,150)	1:118:A:LYS:C	1:119:A:SER:N	1:119:A:SER:CA	1:119:A:SER:C	20	21.2	4.26	21.16
(1,54)	1:49:A:ILE:C	1:50:A:GLU:N	1:50:A:GLU:CA	1:50:A:GLU:C	20	14.33	7.6	13.0
(1,115)	1:85:A:ILE:C	1:86:A:GLN:N	1:86:A:GLN:CA	1:86:A:GLN:C	20	13.52	4.12	12.66
(1,186)	1:140:A:ALA:C	1:141:A:LEU:N	1:141:A:LEU:CA	1:141:A:LEU:C	20	12.11	8.11	10.3
(1,93)	1:74:A:ARG:C	1:75:A:LEU:N	1:75:A:LEU:CA	1:75:A:LEU:C	20	10.68	4.9	9.98
(1,172)	1:129:A:ASP:C	1:130:A:ARG:N	1:130:A:ARG:CA	1:130:A:ARG:C	20	9.89	5.08	8.28
(1,140)	1:106:A:GLU:C	1:107:A:ALA:N	1:107:A:ALA:CA	1:107:A:ALA:C	20	8.85	2.27	8.83
(1,64)	1:58:A:ILE:C	1:59:A:VAL:N	1:59:A:VAL:CA	1:59:A:VAL:C	20	7.57	2.34	7.74
(1,129)	1:99:A:SER:C	1:100:A:PHE:N	1:100:A:PHE:CA	1:100:A:PHE:C	20	7.43	3.39	7.1
(1,66)	1:59:A:VAL:C	1:60:A:TYR:N	1:60:A:TYR:CA	1:60:A:TYR:C	20	7.35	3.01	7.78
(1,97)	1:76:A:ASN:C	1:77:A:LEU:N	1:77:A:LEU:CA	1:77:A:LEU:C	20	6.77	2.95	7.3
(1,144)	1:108:A:ALA:C	1:109:A:ALA:N	1:109:A:ALA:CA	1:109:A:ALA:C	20	6.42	2.19	6.42
(1,113)	1:84:A:VAL:C	1:85:A:ILE:N	1:85:A:ILE:CA	1:85:A:ILE:C	20	6.1	2.02	5.54
(1,95)	1:75:A:LEU:C	1:76:A:ASN:N	1:76:A:ASN:CA	1:76:A:ASN:C	20	5.16	3.09	4.8
(1,111)	1:83:A:ASP:C	1:84:A:VAL:N	1:84:A:VAL:CA	1:84:A:VAL:C	20	4.54	2.47	4.23
(1,89)	1:72:A:PRO:C	1:73:A:HIS:N	1:73:A:HIS:CA	1:73:A:HIS:C	20	4.48	1.86	4.74
(1,160)	1:123:A:ILE:C	1:124:A:PHE:N	1:124:A:PHE:CA	1:124:A:PHE:C	20	4.34	2.69	4.04
(1,103)	1:79:A:TYR:C	1:80:A:LEU:N	1:80:A:LEU:CA	1:80:A:LEU:C	19	10.04	6.05	9.69

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,68)	1:60:A:TYR:C	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	19	8.59	3.63	8.22
(1,16)	1:26:A:SER:C	1:27:A:LEU:N	1:27:A:LEU:CA	1:27:A:LEU:C	19	7.84	4.72	7.42
(1,52)	1:48:A:CYS:C	1:49:A:ILE:N	1:49:A:ILE:CA	1:49:A:ILE:C	19	7.74	3.01	7.64
(1,127)	1:98:A:GLU:C	1:99:A:SER:N	1:99:A:SER:CA	1:99:A:SER:C	19	7.12	4.21	6.77
(1,190)	1:142:A:ARG:C	1:143:A:GLU:N	1:143:A:GLU:CA	1:143:A:GLU:C	19	6.86	3.12	7.1
(1,28)	1:32:A:GLN:C	1:33:A:SER:N	1:33:A:SER:CA	1:33:A:SER:C	19	4.95	3.24	3.93
(1,156)	1:121:A:GLU:C	1:122:A:ARG:N	1:122:A:ARG:CA	1:122:A:ARG:C	19	4.65	2.18	4.15
(1,164)	1:125:A:LYS:C	1:126:A:ILE:N	1:126:A:ILE:CA	1:126:A:ILE:C	19	4.49	2.39	4.43
(1,138)	1:105:A:PRO:C	1:106:A:GLU:N	1:106:A:GLU:CA	1:106:A:GLU:C	19	4.35	2.06	4.41
(1,82)	1:67:A:ARG:C	1:68:A:ARG:N	1:68:A:ARG:CA	1:68:A:ARG:C	18	8.97	5.54	7.9
(1,24)	1:30:A:LYS:C	1:31:A:PHE:N	1:31:A:PHE:CA	1:31:A:PHE:C	18	6.92	3.64	6.77
(1,99)	1:77:A:LEU:C	1:78:A:PHE:N	1:78:A:PHE:CA	1:78:A:PHE:C	18	4.85	2.32	4.64
(1,142)	1:107:A:ALA:C	1:108:A:ALA:N	1:108:A:ALA:CA	1:108:A:ALA:C	18	3.18	1.49	2.66
(1,72)	1:62:A:TRP:C	1:63:A:MET:N	1:63:A:MET:CA	1:63:A:MET:C	17	9.85	4.73	10.54
(1,26)	1:31:A:PHE:C	1:32:A:GLN:N	1:32:A:GLN:CA	1:32:A:GLN:C	17	8.79	3.9	8.88
(1,74)	1:63:A:MET:C	1:64:A:LYS:N	1:64:A:LYS:CA	1:64:A:LYS:C	17	8.3	6.17	7.44
(1,78)	1:65:A:TRP:C	1:66:A:LEU:N	1:66:A:LEU:CA	1:66:A:LEU:C	17	7.78	5.08	6.46
(1,14)	1:25:A:SER:C	1:26:A:SER:N	1:26:A:SER:CA	1:26:A:SER:C	17	7.06	3.25	6.91
(1,166)	1:126:A:ILE:C	1:127:A:TRP:N	1:127:A:TRP:CA	1:127:A:TRP:C	17	6.71	4.42	6.58
(1,168)	1:127:A:TRP:C	1:128:A:GLU:N	1:128:A:GLU:CA	1:128:A:GLU:C	17	6.34	4.54	4.89
(1,22)	1:29:A:ARG:C	1:30:A:LYS:N	1:30:A:LYS:CA	1:30:A:LYS:C	17	4.16	2.33	3.67
(1,12)	1:24:A:GLU:C	1:25:A:SER:N	1:25:A:SER:CA	1:25:A:SER:C	17	3.32	1.54	2.89
(1,76)	1:64:A:LYS:C	1:65:A:TRP:N	1:65:A:TRP:CA	1:65:A:TRP:C	16	11.79	7.64	9.86
(1,194)	1:144:A:ALA:C	1:145:A:LEU:N	1:145:A:LEU:CA	1:145:A:LEU:C	16	11.36	10.19	7.02
(1,60)	1:56:A:SER:C	1:57:A:THR:N	1:57:A:THR:CA	1:57:A:THR:C	16	8.41	5.61	5.7
(1,158)	1:122:A:ARG:C	1:123:A:ILE:N	1:123:A:ILE:CA	1:123:A:ILE:C	16	8.0	6.33	7.2
(1,32)	1:38:A:MET:C	1:39:A:GLU:N	1:39:A:GLU:CA	1:39:A:GLU:C	16	6.0	4.66	3.54
(1,162)	1:124:A:PHE:C	1:125:A:LYS:N	1:125:A:LYS:CA	1:125:A:LYS:C	16	5.93	3.25	5.78
(1,62)	1:57:A:THR:C	1:58:A:ILE:N	1:58:A:ILE:CA	1:58:A:ILE:C	16	3.83	2.2	3.11
(1,192)	1:143:A:GLU:C	1:144:A:ALA:N	1:144:A:ALA:CA	1:144:A:ALA:C	16	3.56	1.99	3.0
(1,101)	1:78:A:PHE:C	1:79:A:TYR:N	1:79:A:TYR:CA	1:79:A:TYR:C	16	2.99	1.58	2.76
(1,44)	1:44:A:LEU:C	1:45:A:SER:N	1:45:A:SER:CA	1:45:A:SER:C	16	2.47	1.86	1.6
(1,170)	1:128:A:GLU:C	1:129:A:ASP:N	1:129:A:ASP:CA	1:129:A:ASP:C	15	6.38	3.38	6.94
(1,105)	1:80:A:LEU:C	1:81:A:ALA:N	1:81:A:ALA:CA	1:81:A:ALA:C	15	4.68	3.72	3.52
(1,188)	1:141:A:LEU:C	1:142:A:ARG:N	1:142:A:ARG:CA	1:142:A:ARG:C	14	11.03	5.32	11.18
(1,46)	1:45:A:SER:C	1:46:A:SER:N	1:46:A:SER:CA	1:46:A:SER:C	14	6.99	3.45	5.82
(1,117)	1:86:A:GLN:C	1:87:A:ASN:N	1:87:A:ASN:CA	1:87:A:ASN:C	14	5.99	3.58	5.06
(1,133)	1:101:A:ALA:C	1:102:A:ASP:N	1:102:A:ASP:CA	1:102:A:ASP:C	14	5.39	4.4	5.41
(1,36)	1:40:A:SER:C	1:41:A:ILE:N	1:41:A:ILE:CA	1:41:A:ILE:C	14	4.33	2.35	3.81
(1,8)	1:22:A:ALA:C	1:23:A:LEU:N	1:23:A:LEU:CA	1:23:A:LEU:C	13	6.05	3.64	7.26
(1,58)	1:55:A:HIS:C	1:56:A:SER:N	1:56:A:SER:CA	1:56:A:SER:C	13	4.28	3.35	2.78
(1,18)	1:27:A:LEU:C	1:28:A:ASP:N	1:28:A:ASP:CA	1:28:A:ASP:C	13	3.63	3.16	3.25
(1,6)	1:21:A:GLY:C	1:22:A:ALA:N	1:22:A:ALA:CA	1:22:A:ALA:C	13	3.4	2.29	3.62
(1,80)	1:66:A:LEU:C	1:67:A:ARG:N	1:67:A:ARG:CA	1:67:A:ARG:C	13	2.57	2.12	1.85
(1,125)	1:97:A:ARG:C	1:98:A:GLU:N	1:98:A:GLU:CA	1:98:A:GLU:C	12	4.34	2.54	4.27
(1,20)	1:28:A:ASP:C	1:29:A:ARG:N	1:29:A:ARG:CA	1:29:A:ARG:C	12	4.24	2.55	3.75
(1,109)	1:82:A:ASN:C	1:83:A:ASP:N	1:83:A:ASP:CA	1:83:A:ASP:C	12	3.21	2.56	2.13
(1,38)	1:41:A:ILE:C	1:42:A:GLN:N	1:42:A:GLN:CA	1:42:A:GLN:C	12	2.65	1.3	2.4
(1,180)	1:137:A:MET:C	1:138:A:ILE:N	1:138:A:ILE:CA	1:138:A:ILE:C	12	2.22	0.74	1.98
(1,152)	1:119:A:SER:C	1:120:A:VAL:N	1:120:A:VAL:CA	1:120:A:VAL:C	11	5.92	4.44	3.74
(1,10)	1:23:A:LEU:C	1:24:A:GLU:N	1:24:A:GLU:CA	1:24:A:GLU:C	11	3.57	3.04	2.68

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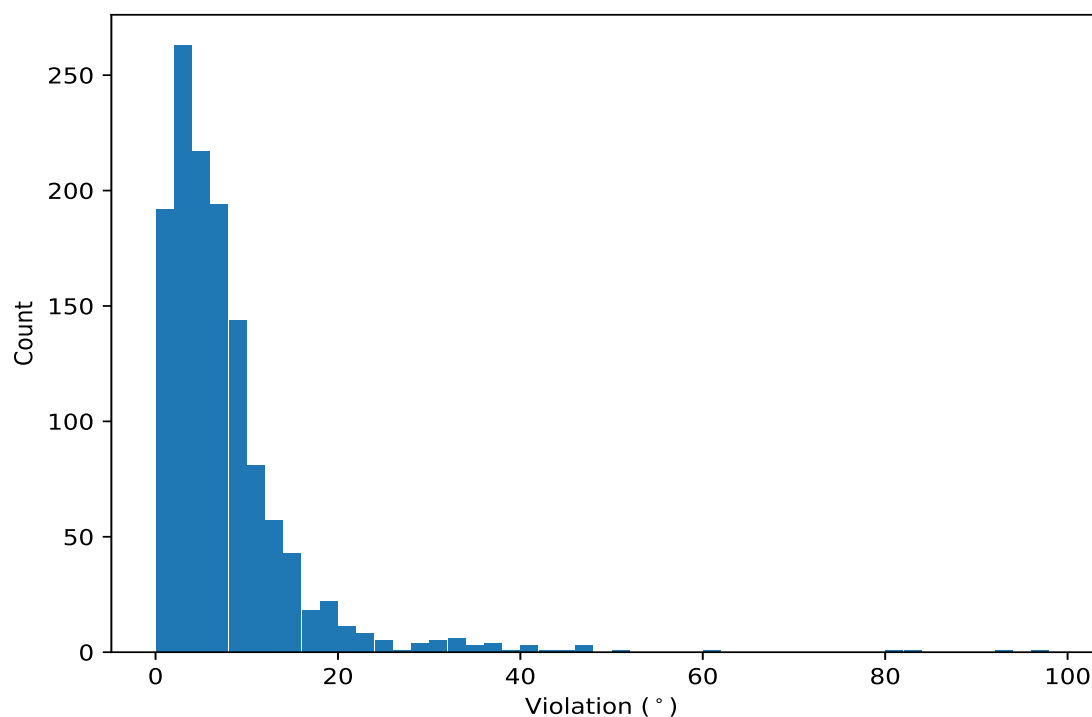
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,84)	1:68:A:ARG:C	1:69:A:SER:N	1:69:A:SER:CA	1:69:A:SER:C	10	11.07	9.44	7.86
(1,182)	1:138:A:ILE:C	1:139:A:VAL:N	1:139:A:VAL:CA	1:139:A:VAL:C	10	5.67	3.9	3.34
(1,173)	1:130:A:ARG:N	1:130:A:ARG:CA	1:130:A:ARG:C	1:131:A:ASN:N	9	4.54	3.11	3.58
(1,123)	1:96:A:PHE:C	1:97:A:ARG:N	1:97:A:ARG:CA	1:97:A:ARG:C	8	3.48	1.78	3.72
(1,184)	1:139:A:VAL:C	1:140:A:ALA:N	1:140:A:ALA:CA	1:140:A:ALA:C	7	3.75	4.42	2.01
(1,90)	1:73:A:HIS:N	1:73:A:HIS:CA	1:73:A:HIS:C	1:74:A:ARG:N	6	3.39	2.24	2.3
(1,121)	1:95:A:ILE:C	1:96:A:PHE:N	1:96:A:PHE:CA	1:96:A:PHE:C	6	1.77	0.84	1.51
(1,48)	1:46:A:SER:C	1:47:A:TRP:N	1:47:A:TRP:CA	1:47:A:TRP:C	5	1.71	0.59	1.56
(1,91)	1:73:A:HIS:C	1:74:A:ARG:N	1:74:A:ARG:CA	1:74:A:ARG:C	4	5.14	1.64	5.38
(1,176)	1:135:A:GLU:C	1:136:A:GLU:N	1:136:A:GLU:CA	1:136:A:GLU:C	4	4.65	4.19	3.11
(1,70)	1:61:A:HIS:C	1:62:A:TRP:N	1:62:A:TRP:CA	1:62:A:TRP:C	4	3.88	2.59	3.14
(1,85)	1:69:A:SER:N	1:69:A:SER:CA	1:69:A:SER:C	1:70:A:ALA:N	3	25.93	25.72	15.04
(1,148)	1:117:A:SER:C	1:118:A:LYS:N	1:118:A:LYS:CA	1:118:A:LYS:C	3	4.03	2.1	4.73
(1,42)	1:43:A:GLY:C	1:44:A:LEU:N	1:44:A:LEU:CA	1:44:A:LEU:C	3	3.9	1.97	4.95
(1,40)	1:42:A:GLN:C	1:43:A:GLY:N	1:43:A:GLY:CA	1:43:A:GLY:C	3	1.1	0.14	1.01

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 (°)
(1,34)	1:39:A:GLU:C	1:40:A:SER:N	1:40:A:SER:CA	1:40:A:SER:C	13	97.45
(1,34)	1:39:A:GLU:C	1:40:A:SER:N	1:40:A:SER:CA	1:40:A:SER:C	5	93.07
(1,34)	1:39:A:GLU:C	1:40:A:SER:N	1:40:A:SER:CA	1:40:A:SER:C	9	82.57
(1,34)	1:39:A:GLU:C	1:40:A:SER:N	1:40:A:SER:CA	1:40:A:SER:C	1	80.83
(1,85)	1:69:A:SER:N	1:69:A:SER:CA	1:69:A:SER:C	1:70:A:ALA:N	18	61.43
(1,34)	1:39:A:GLU:C	1:40:A:SER:N	1:40:A:SER:CA	1:40:A:SER:C	10	51.33
(1,34)	1:39:A:GLU:C	1:40:A:SER:N	1:40:A:SER:CA	1:40:A:SER:C	18	47.22
(1,34)	1:39:A:GLU:C	1:40:A:SER:N	1:40:A:SER:CA	1:40:A:SER:C	8	47.14
(1,34)	1:39:A:GLU:C	1:40:A:SER:N	1:40:A:SER:CA	1:40:A:SER:C	12	46.72
(1,34)	1:39:A:GLU:C	1:40:A:SER:N	1:40:A:SER:CA	1:40:A:SER:C	11	44.92
(1,34)	1:39:A:GLU:C	1:40:A:SER:N	1:40:A:SER:CA	1:40:A:SER:C	4	42.25
(1,34)	1:39:A:GLU:C	1:40:A:SER:N	1:40:A:SER:CA	1:40:A:SER:C	3	41.43
(1,178)	1:136:A:GLU:C	1:137:A:MET:N	1:137:A:MET:CA	1:137:A:MET:C	5	41.29
(1,34)	1:39:A:GLU:C	1:40:A:SER:N	1:40:A:SER:CA	1:40:A:SER:C	6	41.1
(1,34)	1:39:A:GLU:C	1:40:A:SER:N	1:40:A:SER:CA	1:40:A:SER:C	17	39.09
(1,34)	1:39:A:GLU:C	1:40:A:SER:N	1:40:A:SER:CA	1:40:A:SER:C	7	36.98
(1,186)	1:140:A:ALA:C	1:141:A:LEU:N	1:141:A:LEU:CA	1:141:A:LEU:C	7	36.57
(1,34)	1:39:A:GLU:C	1:40:A:SER:N	1:40:A:SER:CA	1:40:A:SER:C	15	36.44
(1,34)	1:39:A:GLU:C	1:40:A:SER:N	1:40:A:SER:CA	1:40:A:SER:C	20	36.36
(1,178)	1:136:A:GLU:C	1:137:A:MET:N	1:137:A:MET:CA	1:137:A:MET:C	1	35.14
(1,84)	1:68:A:ARG:C	1:69:A:SER:N	1:69:A:SER:CA	1:69:A:SER:C	20	35.08
(1,178)	1:136:A:GLU:C	1:137:A:MET:N	1:137:A:MET:CA	1:137:A:MET:C	4	34.05
(1,194)	1:144:A:ALA:C	1:145:A:LEU:N	1:145:A:LEU:CA	1:145:A:LEU:C	17	33.69
(1,194)	1:144:A:ALA:C	1:145:A:LEU:N	1:145:A:LEU:CA	1:145:A:LEU:C	12	33.47
(1,76)	1:64:A:LYS:C	1:65:A:TRP:N	1:65:A:TRP:CA	1:65:A:TRP:C	14	32.79
(1,54)	1:49:A:ILE:C	1:50:A:GLU:N	1:50:A:GLU:CA	1:50:A:GLU:C	17	32.69
(1,178)	1:136:A:GLU:C	1:137:A:MET:N	1:137:A:MET:CA	1:137:A:MET:C	15	32.41
(1,186)	1:140:A:ALA:C	1:141:A:LEU:N	1:141:A:LEU:CA	1:141:A:LEU:C	11	32.07
(1,34)	1:39:A:GLU:C	1:40:A:SER:N	1:40:A:SER:CA	1:40:A:SER:C	2	31.43
(1,178)	1:136:A:GLU:C	1:137:A:MET:N	1:137:A:MET:CA	1:137:A:MET:C	14	30.68
(1,54)	1:49:A:ILE:C	1:50:A:GLU:N	1:50:A:GLU:CA	1:50:A:GLU:C	14	30.34
(1,178)	1:136:A:GLU:C	1:137:A:MET:N	1:137:A:MET:CA	1:137:A:MET:C	16	30.08
(1,178)	1:136:A:GLU:C	1:137:A:MET:N	1:137:A:MET:CA	1:137:A:MET:C	18	30.07
(1,34)	1:39:A:GLU:C	1:40:A:SER:N	1:40:A:SER:CA	1:40:A:SER:C	14	29.68
(1,103)	1:79:A:TYR:C	1:80:A:LEU:N	1:80:A:LEU:CA	1:80:A:LEU:C	16	29.48
(1,150)	1:118:A:LYS:C	1:119:A:SER:N	1:119:A:SER:CA	1:119:A:SER:C	19	28.96
(1,54)	1:49:A:ILE:C	1:50:A:GLU:N	1:50:A:GLU:CA	1:50:A:GLU:C	10	28.55
(1,150)	1:118:A:LYS:C	1:119:A:SER:N	1:119:A:SER:CA	1:119:A:SER:C	14	27.42
(1,16)	1:26:A:SER:C	1:27:A:LEU:N	1:27:A:LEU:CA	1:27:A:LEU:C	16	25.98
(1,115)	1:85:A:ILE:C	1:86:A:GLN:N	1:86:A:GLN:CA	1:86:A:GLN:C	13	25.17
(1,150)	1:118:A:LYS:C	1:119:A:SER:N	1:119:A:SER:CA	1:119:A:SER:C	4	24.64
(1,150)	1:118:A:LYS:C	1:119:A:SER:N	1:119:A:SER:CA	1:119:A:SER:C	9	24.35
(1,150)	1:118:A:LYS:C	1:119:A:SER:N	1:119:A:SER:CA	1:119:A:SER:C	18	24.0
(1,60)	1:56:A:SER:C	1:57:A:THR:N	1:57:A:THR:CA	1:57:A:THR:C	8	23.95
(1,158)	1:122:A:ARG:C	1:123:A:ILE:N	1:123:A:ILE:CA	1:123:A:ILE:C	19	23.23
(1,178)	1:136:A:GLU:C	1:137:A:MET:N	1:137:A:MET:CA	1:137:A:MET:C	3	23.1
(1,150)	1:118:A:LYS:C	1:119:A:SER:N	1:119:A:SER:CA	1:119:A:SER:C	16	22.96

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,150)	1:118:A:LYS:C	1:119:A:SER:N	1:119:A:SER:CA	1:119:A:SER:C	20	22.94
(1,34)	1:39:A:GLU:C	1:40:A:SER:N	1:40:A:SER:CA	1:40:A:SER:C	16	22.82
(1,150)	1:118:A:LYS:C	1:119:A:SER:N	1:119:A:SER:CA	1:119:A:SER:C	17	22.74
(1,150)	1:118:A:LYS:C	1:119:A:SER:N	1:119:A:SER:CA	1:119:A:SER:C	3	22.44
(1,188)	1:141:A:LEU:C	1:142:A:ARG:N	1:142:A:ARG:CA	1:142:A:ARG:C	2	21.43
(1,150)	1:118:A:LYS:C	1:119:A:SER:N	1:119:A:SER:CA	1:119:A:SER:C	12	21.37
(1,172)	1:129:A:ASP:C	1:130:A:ARG:N	1:130:A:ARG:CA	1:130:A:ARG:C	14	20.98
(1,150)	1:118:A:LYS:C	1:119:A:SER:N	1:119:A:SER:CA	1:119:A:SER:C	10	20.95
(1,150)	1:118:A:LYS:C	1:119:A:SER:N	1:119:A:SER:CA	1:119:A:SER:C	1	20.92
(1,150)	1:118:A:LYS:C	1:119:A:SER:N	1:119:A:SER:CA	1:119:A:SER:C	15	20.85
(1,150)	1:118:A:LYS:C	1:119:A:SER:N	1:119:A:SER:CA	1:119:A:SER:C	13	20.83
(1,194)	1:144:A:ALA:C	1:145:A:LEU:N	1:145:A:LEU:CA	1:145:A:LEU:C	20	20.77
(1,93)	1:74:A:ARG:C	1:75:A:LEU:N	1:75:A:LEU:CA	1:75:A:LEU:C	13	20.35
(1,172)	1:129:A:ASP:C	1:130:A:ARG:N	1:130:A:ARG:CA	1:130:A:ARG:C	16	20.16
(1,82)	1:67:A:ARG:C	1:68:A:ARG:N	1:68:A:ARG:CA	1:68:A:ARG:C	7	20.06
(1,150)	1:118:A:LYS:C	1:119:A:SER:N	1:119:A:SER:CA	1:119:A:SER:C	5	19.99
(1,74)	1:63:A:MET:C	1:64:A:LYS:N	1:64:A:LYS:CA	1:64:A:LYS:C	10	19.88
(1,178)	1:136:A:GLU:C	1:137:A:MET:N	1:137:A:MET:CA	1:137:A:MET:C	12	19.76
(1,150)	1:118:A:LYS:C	1:119:A:SER:N	1:119:A:SER:CA	1:119:A:SER:C	6	19.63
(1,82)	1:67:A:ARG:C	1:68:A:ARG:N	1:68:A:ARG:CA	1:68:A:ARG:C	15	19.55
(1,150)	1:118:A:LYS:C	1:119:A:SER:N	1:119:A:SER:CA	1:119:A:SER:C	8	19.49
(1,178)	1:136:A:GLU:C	1:137:A:MET:N	1:137:A:MET:CA	1:137:A:MET:C	9	19.4
(1,178)	1:136:A:GLU:C	1:137:A:MET:N	1:137:A:MET:CA	1:137:A:MET:C	8	18.87
(1,72)	1:62:A:TRP:C	1:63:A:MET:N	1:63:A:MET:CA	1:63:A:MET:C	4	18.69
(1,78)	1:65:A:TRP:C	1:66:A:LEU:N	1:66:A:LEU:CA	1:66:A:LEU:C	2	18.64
(1,74)	1:63:A:MET:C	1:64:A:LYS:N	1:64:A:LYS:CA	1:64:A:LYS:C	4	18.57
(1,115)	1:85:A:ILE:C	1:86:A:GLN:N	1:86:A:GLN:CA	1:86:A:GLN:C	7	18.51
(1,194)	1:144:A:ALA:C	1:145:A:LEU:N	1:145:A:LEU:CA	1:145:A:LEU:C	7	18.42
(1,103)	1:79:A:TYR:C	1:80:A:LEU:N	1:80:A:LEU:CA	1:80:A:LEU:C	6	18.4
(1,74)	1:63:A:MET:C	1:64:A:LYS:N	1:64:A:LYS:CA	1:64:A:LYS:C	16	18.37
(1,168)	1:127:A:TRP:C	1:128:A:GLU:N	1:128:A:GLU:CA	1:128:A:GLU:C	19	18.33
(1,194)	1:144:A:ALA:C	1:145:A:LEU:N	1:145:A:LEU:CA	1:145:A:LEU:C	2	18.29
(1,93)	1:74:A:ARG:C	1:75:A:LEU:N	1:75:A:LEU:CA	1:75:A:LEU:C	15	18.29
(1,76)	1:64:A:LYS:C	1:65:A:TRP:N	1:65:A:TRP:CA	1:65:A:TRP:C	11	18.21
(1,166)	1:126:A:ILE:C	1:127:A:TRP:N	1:127:A:TRP:CA	1:127:A:TRP:C	5	18.19
(1,72)	1:62:A:TRP:C	1:63:A:MET:N	1:63:A:MET:CA	1:63:A:MET:C	12	18.17
(1,68)	1:60:A:TYR:C	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	4	18.0
(1,84)	1:68:A:ARG:C	1:69:A:SER:N	1:69:A:SER:CA	1:69:A:SER:C	18	17.72
(1,115)	1:85:A:ILE:C	1:86:A:GLN:N	1:86:A:GLN:CA	1:86:A:GLN:C	19	17.6
(1,115)	1:85:A:ILE:C	1:86:A:GLN:N	1:86:A:GLN:CA	1:86:A:GLN:C	16	17.52
(1,172)	1:129:A:ASP:C	1:130:A:ARG:N	1:130:A:ARG:CA	1:130:A:ARG:C	10	17.5
(1,158)	1:122:A:ARG:C	1:123:A:ILE:N	1:123:A:ILE:CA	1:123:A:ILE:C	5	17.48
(1,76)	1:64:A:LYS:C	1:65:A:TRP:N	1:65:A:TRP:CA	1:65:A:TRP:C	12	17.48
(1,158)	1:122:A:ARG:C	1:123:A:ILE:N	1:123:A:ILE:CA	1:123:A:ILE:C	12	17.41
(1,54)	1:49:A:ILE:C	1:50:A:GLU:N	1:50:A:GLU:CA	1:50:A:GLU:C	19	17.41
(1,76)	1:64:A:LYS:C	1:65:A:TRP:N	1:65:A:TRP:CA	1:65:A:TRP:C	16	17.07
(1,78)	1:65:A:TRP:C	1:66:A:LEU:N	1:66:A:LEU:CA	1:66:A:LEU:C	1	17.06
(1,76)	1:64:A:LYS:C	1:65:A:TRP:N	1:65:A:TRP:CA	1:65:A:TRP:C	8	16.96
(1,26)	1:31:A:PHE:C	1:32:A:GLN:N	1:32:A:GLN:CA	1:32:A:GLN:C	11	16.74
(1,188)	1:141:A:LEU:C	1:142:A:ARG:N	1:142:A:ARG:CA	1:142:A:ARG:C	4	16.7
(1,115)	1:85:A:ILE:C	1:86:A:GLN:N	1:86:A:GLN:CA	1:86:A:GLN:C	10	16.52

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,32)	1:38:A:MET:C	1:39:A:GLU:N	1:39:A:GLU:CA	1:39:A:GLU:C	19	16.45
(1,186)	1:140:A:ALA:C	1:141:A:LEU:N	1:141:A:LEU:CA	1:141:A:LEU:C	9	16.43
(1,178)	1:136:A:GLU:C	1:137:A:MET:N	1:137:A:MET:CA	1:137:A:MET:C	19	16.16
(1,78)	1:65:A:TRP:C	1:66:A:LEU:N	1:66:A:LEU:CA	1:66:A:LEU:C	3	16.11
(1,76)	1:64:A:LYS:C	1:65:A:TRP:N	1:65:A:TRP:CA	1:65:A:TRP:C	4	15.88
(1,188)	1:141:A:LEU:C	1:142:A:ARG:N	1:142:A:ARG:CA	1:142:A:ARG:C	19	15.83
(1,93)	1:74:A:ARG:C	1:75:A:LEU:N	1:75:A:LEU:CA	1:75:A:LEU:C	17	15.81
(1,133)	1:101:A:ALA:C	1:102:A:ASP:N	1:102:A:ASP:CA	1:102:A:ASP:C	10	15.69
(1,93)	1:74:A:ARG:C	1:75:A:LEU:N	1:75:A:LEU:CA	1:75:A:LEU:C	9	15.57
(1,150)	1:118:A:LYS:C	1:119:A:SER:N	1:119:A:SER:CA	1:119:A:SER:C	7	15.56
(1,93)	1:74:A:ARG:C	1:75:A:LEU:N	1:75:A:LEU:CA	1:75:A:LEU:C	7	15.51
(1,54)	1:49:A:ILE:C	1:50:A:GLU:N	1:50:A:GLU:CA	1:50:A:GLU:C	16	15.45
(1,152)	1:119:A:SER:C	1:120:A:VAL:N	1:120:A:VAL:CA	1:120:A:VAL:C	14	15.44
(1,54)	1:49:A:ILE:C	1:50:A:GLU:N	1:50:A:GLU:CA	1:50:A:GLU:C	3	15.4
(1,162)	1:124:A:PHE:C	1:125:A:LYS:N	1:125:A:LYS:CA	1:125:A:LYS:C	17	15.32
(1,82)	1:67:A:ARG:C	1:68:A:ARG:N	1:68:A:ARG:CA	1:68:A:ARG:C	14	15.31
(1,188)	1:141:A:LEU:C	1:142:A:ARG:N	1:142:A:ARG:CA	1:142:A:ARG:C	9	15.28
(1,103)	1:79:A:TYR:C	1:80:A:LEU:N	1:80:A:LEU:CA	1:80:A:LEU:C	4	15.18
(1,85)	1:69:A:SER:N	1:69:A:SER:CA	1:69:A:SER:C	1:70:A:ALA:N	20	15.04
(1,26)	1:31:A:PHE:C	1:32:A:GLN:N	1:32:A:GLN:CA	1:32:A:GLN:C	3	14.91
(1,46)	1:45:A:SER:C	1:46:A:SER:N	1:46:A:SER:CA	1:46:A:SER:C	16	14.88
(1,93)	1:74:A:ARG:C	1:75:A:LEU:N	1:75:A:LEU:CA	1:75:A:LEU:C	19	14.8
(1,54)	1:49:A:ILE:C	1:50:A:GLU:N	1:50:A:GLU:CA	1:50:A:GLU:C	6	14.79
(1,115)	1:85:A:ILE:C	1:86:A:GLN:N	1:86:A:GLN:CA	1:86:A:GLN:C	17	14.77
(1,129)	1:99:A:SER:C	1:100:A:PHE:N	1:100:A:PHE:CA	1:100:A:PHE:C	14	14.71
(1,150)	1:118:A:LYS:C	1:119:A:SER:N	1:119:A:SER:CA	1:119:A:SER:C	2	14.66
(1,105)	1:80:A:LEU:C	1:81:A:ALA:N	1:81:A:ALA:CA	1:81:A:ALA:C	14	14.62
(1,115)	1:85:A:ILE:C	1:86:A:GLN:N	1:86:A:GLN:CA	1:86:A:GLN:C	8	14.6
(1,84)	1:68:A:ARG:C	1:69:A:SER:N	1:69:A:SER:CA	1:69:A:SER:C	2	14.57
(1,178)	1:136:A:GLU:C	1:137:A:MET:N	1:137:A:MET:CA	1:137:A:MET:C	7	14.49
(1,115)	1:85:A:ILE:C	1:86:A:GLN:N	1:86:A:GLN:CA	1:86:A:GLN:C	11	14.44
(1,184)	1:139:A:VAL:C	1:140:A:ALA:N	1:140:A:ALA:CA	1:140:A:ALA:C	12	14.33
(1,178)	1:136:A:GLU:C	1:137:A:MET:N	1:137:A:MET:CA	1:137:A:MET:C	10	14.3
(1,168)	1:127:A:TRP:C	1:128:A:GLU:N	1:128:A:GLU:CA	1:128:A:GLU:C	1	14.3
(1,188)	1:141:A:LEU:C	1:142:A:ARG:N	1:142:A:ARG:CA	1:142:A:ARG:C	6	14.28
(1,117)	1:86:A:GLN:C	1:87:A:ASN:N	1:87:A:ASN:CA	1:87:A:ASN:C	12	14.26
(1,178)	1:136:A:GLU:C	1:137:A:MET:N	1:137:A:MET:CA	1:137:A:MET:C	20	14.24
(1,60)	1:56:A:SER:C	1:57:A:THR:N	1:57:A:THR:CA	1:57:A:THR:C	10	14.2
(1,74)	1:63:A:MET:C	1:64:A:LYS:N	1:64:A:LYS:CA	1:64:A:LYS:C	11	14.19
(1,178)	1:136:A:GLU:C	1:137:A:MET:N	1:137:A:MET:CA	1:137:A:MET:C	2	14.16
(1,186)	1:140:A:ALA:C	1:141:A:LEU:N	1:141:A:LEU:CA	1:141:A:LEU:C	4	14.12
(1,127)	1:98:A:GLU:C	1:99:A:SER:N	1:99:A:SER:CA	1:99:A:SER:C	9	14.1
(1,82)	1:67:A:ARG:C	1:68:A:ARG:N	1:68:A:ARG:CA	1:68:A:ARG:C	13	14.07
(1,172)	1:129:A:ASP:C	1:130:A:ARG:N	1:130:A:ARG:CA	1:130:A:ARG:C	19	14.02
(1,72)	1:62:A:TRP:C	1:63:A:MET:N	1:63:A:MET:CA	1:63:A:MET:C	14	14.02
(1,97)	1:76:A:ASN:C	1:77:A:LEU:N	1:77:A:LEU:CA	1:77:A:LEU:C	20	14.01
(1,76)	1:64:A:LYS:C	1:65:A:TRP:N	1:65:A:TRP:CA	1:65:A:TRP:C	7	14.01
(1,182)	1:138:A:ILE:C	1:139:A:VAL:N	1:139:A:VAL:CA	1:139:A:VAL:C	18	13.94
(1,172)	1:129:A:ASP:C	1:130:A:ARG:N	1:130:A:ARG:CA	1:130:A:ARG:C	3	13.93
(1,127)	1:98:A:GLU:C	1:99:A:SER:N	1:99:A:SER:CA	1:99:A:SER:C	3	13.87
(1,60)	1:56:A:SER:C	1:57:A:THR:N	1:57:A:THR:CA	1:57:A:THR:C	9	13.84

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,115)	1:85:A:ILE:C	1:86:A:GLN:N	1:86:A:GLN:CA	1:86:A:GLN:C	15	13.68
(1,54)	1:49:A:ILE:C	1:50:A:GLU:N	1:50:A:GLU:CA	1:50:A:GLU:C	15	13.65
(1,93)	1:74:A:ARG:C	1:75:A:LEU:N	1:75:A:LEU:CA	1:75:A:LEU:C	14	13.6
(1,72)	1:62:A:TRP:C	1:63:A:MET:N	1:63:A:MET:CA	1:63:A:MET:C	11	13.55
(1,52)	1:48:A:CYS:C	1:49:A:ILE:N	1:49:A:ILE:CA	1:49:A:ILE:C	1	13.55
(1,54)	1:49:A:ILE:C	1:50:A:GLU:N	1:50:A:GLU:CA	1:50:A:GLU:C	2	13.47
(1,133)	1:101:A:ALA:C	1:102:A:ASP:N	1:102:A:ASP:CA	1:102:A:ASP:C	19	13.46
(1,60)	1:56:A:SER:C	1:57:A:THR:N	1:57:A:THR:CA	1:57:A:THR:C	5	13.44
(1,68)	1:60:A:TYR:C	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	7	13.43
(1,28)	1:32:A:GLN:C	1:33:A:SER:N	1:33:A:SER:CA	1:33:A:SER:C	6	13.41
(1,66)	1:59:A:VAL:C	1:60:A:TYR:N	1:60:A:TYR:CA	1:60:A:TYR:C	14	13.35
(1,54)	1:49:A:ILE:C	1:50:A:GLU:N	1:50:A:GLU:CA	1:50:A:GLU:C	7	13.32
(1,68)	1:60:A:TYR:C	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	16	13.17
(1,58)	1:55:A:HIS:C	1:56:A:SER:N	1:56:A:SER:CA	1:56:A:SER:C	10	13.16
(1,178)	1:136:A:GLU:C	1:137:A:MET:N	1:137:A:MET:CA	1:137:A:MET:C	17	13.15
(1,93)	1:74:A:ARG:C	1:75:A:LEU:N	1:75:A:LEU:CA	1:75:A:LEU:C	10	13.12
(1,24)	1:30:A:LYS:C	1:31:A:PHE:N	1:31:A:PHE:CA	1:31:A:PHE:C	7	13.06
(1,32)	1:38:A:MET:C	1:39:A:GLU:N	1:39:A:GLU:CA	1:39:A:GLU:C	8	13.05
(1,160)	1:123:A:ILE:C	1:124:A:PHE:N	1:124:A:PHE:CA	1:124:A:PHE:C	12	13.03
(1,127)	1:98:A:GLU:C	1:99:A:SER:N	1:99:A:SER:CA	1:99:A:SER:C	6	13.01
(1,84)	1:68:A:ARG:C	1:69:A:SER:N	1:69:A:SER:CA	1:69:A:SER:C	1	12.89
(1,97)	1:76:A:ASN:C	1:77:A:LEU:N	1:77:A:LEU:CA	1:77:A:LEU:C	16	12.85
(1,140)	1:106:A:GLU:C	1:107:A:ALA:N	1:107:A:ALA:CA	1:107:A:ALA:C	16	12.84
(1,115)	1:85:A:ILE:C	1:86:A:GLN:N	1:86:A:GLN:CA	1:86:A:GLN:C	5	12.82
(1,72)	1:62:A:TRP:C	1:63:A:MET:N	1:63:A:MET:CA	1:63:A:MET:C	20	12.8
(1,82)	1:67:A:ARG:C	1:68:A:ARG:N	1:68:A:ARG:CA	1:68:A:ARG:C	19	12.74
(1,54)	1:49:A:ILE:C	1:50:A:GLU:N	1:50:A:GLU:CA	1:50:A:GLU:C	18	12.69
(1,140)	1:106:A:GLU:C	1:107:A:ALA:N	1:107:A:ALA:CA	1:107:A:ALA:C	4	12.65
(1,18)	1:27:A:LEU:C	1:28:A:ASP:N	1:28:A:ASP:CA	1:28:A:ASP:C	7	12.65
(1,26)	1:31:A:PHE:C	1:32:A:GLN:N	1:32:A:GLN:CA	1:32:A:GLN:C	16	12.63
(1,10)	1:23:A:LEU:C	1:24:A:GLU:N	1:24:A:GLU:CA	1:24:A:GLU:C	16	12.62
(1,186)	1:140:A:ALA:C	1:141:A:LEU:N	1:141:A:LEU:CA	1:141:A:LEU:C	6	12.59
(1,14)	1:25:A:SER:C	1:26:A:SER:N	1:26:A:SER:CA	1:26:A:SER:C	4	12.59
(1,172)	1:129:A:ASP:C	1:130:A:ARG:N	1:130:A:ARG:CA	1:130:A:ARG:C	2	12.58
(1,186)	1:140:A:ALA:C	1:141:A:LEU:N	1:141:A:LEU:CA	1:141:A:LEU:C	19	12.54
(1,64)	1:58:A:ILE:C	1:59:A:VAL:N	1:59:A:VAL:CA	1:59:A:VAL:C	17	12.52
(1,115)	1:85:A:ILE:C	1:86:A:GLN:N	1:86:A:GLN:CA	1:86:A:GLN:C	14	12.51
(1,103)	1:79:A:TYR:C	1:80:A:LEU:N	1:80:A:LEU:CA	1:80:A:LEU:C	11	12.49
(1,170)	1:128:A:GLU:C	1:129:A:ASP:N	1:129:A:ASP:CA	1:129:A:ASP:C	5	12.46
(1,26)	1:31:A:PHE:C	1:32:A:GLN:N	1:32:A:GLN:CA	1:32:A:GLN:C	1	12.36
(1,115)	1:85:A:ILE:C	1:86:A:GLN:N	1:86:A:GLN:CA	1:86:A:GLN:C	6	12.28
(1,72)	1:62:A:TRP:C	1:63:A:MET:N	1:63:A:MET:CA	1:63:A:MET:C	3	12.27
(1,103)	1:79:A:TYR:C	1:80:A:LEU:N	1:80:A:LEU:CA	1:80:A:LEU:C	13	12.25
(1,74)	1:63:A:MET:C	1:64:A:LYS:N	1:64:A:LYS:CA	1:64:A:LYS:C	12	12.24
(1,60)	1:56:A:SER:C	1:57:A:THR:N	1:57:A:THR:CA	1:57:A:THR:C	3	12.22
(1,115)	1:85:A:ILE:C	1:86:A:GLN:N	1:86:A:GLN:CA	1:86:A:GLN:C	3	12.2
(1,93)	1:74:A:ARG:C	1:75:A:LEU:N	1:75:A:LEU:CA	1:75:A:LEU:C	11	12.19
(1,24)	1:30:A:LYS:C	1:31:A:PHE:N	1:31:A:PHE:CA	1:31:A:PHE:C	13	12.18
(1,24)	1:30:A:LYS:C	1:31:A:PHE:N	1:31:A:PHE:CA	1:31:A:PHE:C	2	12.15
(1,166)	1:126:A:ILE:C	1:127:A:TRP:N	1:127:A:TRP:CA	1:127:A:TRP:C	1	12.08
(1,54)	1:49:A:ILE:C	1:50:A:GLU:N	1:50:A:GLU:CA	1:50:A:GLU:C	11	12.06

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,178)	1:136:A:GLU:C	1:137:A:MET:N	1:137:A:MET:CA	1:137:A:MET:C	6	12.05
(1,66)	1:59:A:VAL:C	1:60:A:TYR:N	1:60:A:TYR:CA	1:60:A:TYR:C	20	12.03
(1,105)	1:80:A:LEU:C	1:81:A:ALA:N	1:81:A:ALA:CA	1:81:A:ALA:C	10	11.91
(1,82)	1:67:A:ARG:C	1:68:A:ARG:N	1:68:A:ARG:CA	1:68:A:ARG:C	8	11.91
(1,72)	1:62:A:TRP:C	1:63:A:MET:N	1:63:A:MET:CA	1:63:A:MET:C	10	11.9
(1,140)	1:106:A:GLU:C	1:107:A:ALA:N	1:107:A:ALA:CA	1:107:A:ALA:C	8	11.87
(1,115)	1:85:A:ILE:C	1:86:A:GLN:N	1:86:A:GLN:CA	1:86:A:GLN:C	1	11.78
(1,95)	1:75:A:LEU:C	1:76:A:ASN:N	1:76:A:ASN:CA	1:76:A:ASN:C	17	11.74
(1,46)	1:45:A:SER:C	1:46:A:SER:N	1:46:A:SER:CA	1:46:A:SER:C	1	11.74
(1,28)	1:32:A:GLN:C	1:33:A:SER:N	1:33:A:SER:CA	1:33:A:SER:C	9	11.7
(1,129)	1:99:A:SER:C	1:100:A:PHE:N	1:100:A:PHE:CA	1:100:A:PHE:C	15	11.69
(1,127)	1:98:A:GLU:C	1:99:A:SER:N	1:99:A:SER:CA	1:99:A:SER:C	14	11.68
(1,190)	1:142:A:ARG:C	1:143:A:GLU:N	1:143:A:GLU:CA	1:143:A:GLU:C	11	11.67
(1,115)	1:85:A:ILE:C	1:86:A:GLN:N	1:86:A:GLN:CA	1:86:A:GLN:C	20	11.67
(1,54)	1:49:A:ILE:C	1:50:A:GLU:N	1:50:A:GLU:CA	1:50:A:GLU:C	4	11.67
(1,34)	1:39:A:GLU:C	1:40:A:SER:N	1:40:A:SER:CA	1:40:A:SER:C	19	11.64
(1,188)	1:141:A:LEU:C	1:142:A:ARG:N	1:142:A:ARG:CA	1:142:A:ARG:C	20	11.59
(1,186)	1:140:A:ALA:C	1:141:A:LEU:N	1:141:A:LEU:CA	1:141:A:LEU:C	20	11.52
(1,68)	1:60:A:TYR:C	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	11	11.52
(1,115)	1:85:A:ILE:C	1:86:A:GLN:N	1:86:A:GLN:CA	1:86:A:GLN:C	9	11.49
(1,54)	1:49:A:ILE:C	1:50:A:GLU:N	1:50:A:GLU:CA	1:50:A:GLU:C	5	11.49
(1,170)	1:128:A:GLU:C	1:129:A:ASP:N	1:129:A:ASP:CA	1:129:A:ASP:C	3	11.47
(1,152)	1:119:A:SER:C	1:120:A:VAL:N	1:120:A:VAL:CA	1:120:A:VAL:C	8	11.47
(1,188)	1:141:A:LEU:C	1:142:A:ARG:N	1:142:A:ARG:CA	1:142:A:ARG:C	8	11.43
(1,68)	1:60:A:TYR:C	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	9	11.43
(1,140)	1:106:A:GLU:C	1:107:A:ALA:N	1:107:A:ALA:CA	1:107:A:ALA:C	14	11.41
(1,186)	1:140:A:ALA:C	1:141:A:LEU:N	1:141:A:LEU:CA	1:141:A:LEU:C	13	11.36
(1,52)	1:48:A:CYS:C	1:49:A:ILE:N	1:49:A:ILE:CA	1:49:A:ILE:C	8	11.36
(1,176)	1:135:A:GLU:C	1:136:A:GLU:N	1:136:A:GLU:CA	1:136:A:GLU:C	18	11.33
(1,172)	1:129:A:ASP:C	1:130:A:ARG:N	1:130:A:ARG:CA	1:130:A:ARG:C	12	11.32
(1,66)	1:59:A:VAL:C	1:60:A:TYR:N	1:60:A:TYR:CA	1:60:A:TYR:C	9	11.32
(1,14)	1:25:A:SER:C	1:26:A:SER:N	1:26:A:SER:CA	1:26:A:SER:C	2	11.3
(1,103)	1:79:A:TYR:C	1:80:A:LEU:N	1:80:A:LEU:CA	1:80:A:LEU:C	19	11.26
(1,140)	1:106:A:GLU:C	1:107:A:ALA:N	1:107:A:ALA:CA	1:107:A:ALA:C	20	11.24
(1,186)	1:140:A:ALA:C	1:141:A:LEU:N	1:141:A:LEU:CA	1:141:A:LEU:C	15	11.19
(1,168)	1:127:A:TRP:C	1:128:A:GLU:N	1:128:A:GLU:CA	1:128:A:GLU:C	16	11.19
(1,26)	1:31:A:PHE:C	1:32:A:GLN:N	1:32:A:GLN:CA	1:32:A:GLN:C	9	11.15
(1,117)	1:86:A:GLN:C	1:87:A:ASN:N	1:87:A:ASN:CA	1:87:A:ASN:C	6	11.13
(1,164)	1:125:A:LYS:C	1:126:A:ILE:N	1:126:A:ILE:CA	1:126:A:ILE:C	11	11.12
(1,8)	1:22:A:ALA:C	1:23:A:LEU:N	1:23:A:LEU:CA	1:23:A:LEU:C	6	11.11
(1,82)	1:67:A:ARG:C	1:68:A:ARG:N	1:68:A:ARG:CA	1:68:A:ARG:C	5	11.08
(1,173)	1:130:A:ARG:N	1:130:A:ARG:CA	1:130:A:ARG:C	1:131:A:ASN:N	10	11.02
(1,46)	1:45:A:SER:C	1:46:A:SER:N	1:46:A:SER:CA	1:46:A:SER:C	13	11.02
(1,78)	1:65:A:TRP:C	1:66:A:LEU:N	1:66:A:LEU:CA	1:66:A:LEU:C	12	11.01
(1,62)	1:57:A:THR:C	1:58:A:ILE:N	1:58:A:ILE:CA	1:58:A:ILE:C	12	11.0
(1,172)	1:129:A:ASP:C	1:130:A:ARG:N	1:130:A:ARG:CA	1:130:A:ARG:C	13	10.98
(1,190)	1:142:A:ARG:C	1:143:A:GLU:N	1:143:A:GLU:CA	1:143:A:GLU:C	18	10.97
(1,188)	1:141:A:LEU:C	1:142:A:ARG:N	1:142:A:ARG:CA	1:142:A:ARG:C	12	10.94
(1,178)	1:136:A:GLU:C	1:137:A:MET:N	1:137:A:MET:CA	1:137:A:MET:C	13	10.94
(1,64)	1:58:A:ILE:C	1:59:A:VAL:N	1:59:A:VAL:CA	1:59:A:VAL:C	15	10.93
(1,127)	1:98:A:GLU:C	1:99:A:SER:N	1:99:A:SER:CA	1:99:A:SER:C	10	10.88

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,93)	1:74:A:ARG:C	1:75:A:LEU:N	1:75:A:LEU:CA	1:75:A:LEU:C	1	10.88
(1,152)	1:119:A:SER:C	1:120:A:VAL:N	1:120:A:VAL:CA	1:120:A:VAL:C	11	10.82
(1,156)	1:121:A:GLU:C	1:122:A:ARG:N	1:122:A:ARG:CA	1:122:A:ARG:C	19	10.8
(1,74)	1:63:A:MET:C	1:64:A:LYS:N	1:64:A:LYS:CA	1:64:A:LYS:C	17	10.8
(1,144)	1:108:A:ALA:C	1:109:A:ALA:N	1:109:A:ALA:CA	1:109:A:ALA:C	10	10.78
(1,166)	1:126:A:ILE:C	1:127:A:TRP:N	1:127:A:TRP:CA	1:127:A:TRP:C	18	10.73
(1,127)	1:98:A:GLU:C	1:99:A:SER:N	1:99:A:SER:CA	1:99:A:SER:C	20	10.71
(1,190)	1:142:A:ARG:C	1:143:A:GLU:N	1:143:A:GLU:CA	1:143:A:GLU:C	4	10.7
(1,52)	1:48:A:CYS:C	1:49:A:ILE:N	1:49:A:ILE:CA	1:49:A:ILE:C	5	10.7
(1,129)	1:99:A:SER:C	1:100:A:PHE:N	1:100:A:PHE:CA	1:100:A:PHE:C	18	10.69
(1,72)	1:62:A:TRP:C	1:63:A:MET:N	1:63:A:MET:CA	1:63:A:MET:C	18	10.67
(1,129)	1:99:A:SER:C	1:100:A:PHE:N	1:100:A:PHE:CA	1:100:A:PHE:C	2	10.66
(1,103)	1:79:A:TYR:C	1:80:A:LEU:N	1:80:A:LEU:CA	1:80:A:LEU:C	1	10.59
(1,186)	1:140:A:ALA:C	1:141:A:LEU:N	1:141:A:LEU:CA	1:141:A:LEU:C	2	10.56
(1,32)	1:38:A:MET:C	1:39:A:GLU:N	1:39:A:GLU:CA	1:39:A:GLU:C	6	10.56
(1,52)	1:48:A:CYS:C	1:49:A:ILE:N	1:49:A:ILE:CA	1:49:A:ILE:C	13	10.55
(1,8)	1:22:A:ALA:C	1:23:A:LEU:N	1:23:A:LEU:CA	1:23:A:LEU:C	2	10.55
(1,72)	1:62:A:TRP:C	1:63:A:MET:N	1:63:A:MET:CA	1:63:A:MET:C	16	10.54
(1,24)	1:30:A:LYS:C	1:31:A:PHE:N	1:31:A:PHE:CA	1:31:A:PHE:C	20	10.54
(1,129)	1:99:A:SER:C	1:100:A:PHE:N	1:100:A:PHE:CA	1:100:A:PHE:C	17	10.46
(1,54)	1:49:A:ILE:C	1:50:A:GLU:N	1:50:A:GLU:CA	1:50:A:GLU:C	13	10.42
(1,158)	1:122:A:ARG:C	1:123:A:ILE:N	1:123:A:ILE:CA	1:123:A:ILE:C	11	10.34
(1,129)	1:99:A:SER:C	1:100:A:PHE:N	1:100:A:PHE:CA	1:100:A:PHE:C	4	10.23
(1,103)	1:79:A:TYR:C	1:80:A:LEU:N	1:80:A:LEU:CA	1:80:A:LEU:C	12	10.21
(1,26)	1:31:A:PHE:C	1:32:A:GLN:N	1:32:A:GLN:CA	1:32:A:GLN:C	17	10.2
(1,95)	1:75:A:LEU:C	1:76:A:ASN:N	1:76:A:ASN:CA	1:76:A:ASN:C	2	10.17
(1,194)	1:144:A:ALA:C	1:145:A:LEU:N	1:145:A:LEU:CA	1:145:A:LEU:C	16	10.14
(1,32)	1:38:A:MET:C	1:39:A:GLU:N	1:39:A:GLU:CA	1:39:A:GLU:C	10	10.09
(1,14)	1:25:A:SER:C	1:26:A:SER:N	1:26:A:SER:CA	1:26:A:SER:C	18	10.07
(1,186)	1:140:A:ALA:C	1:141:A:LEU:N	1:141:A:LEU:CA	1:141:A:LEU:C	18	10.03
(1,144)	1:108:A:ALA:C	1:109:A:ALA:N	1:109:A:ALA:CA	1:109:A:ALA:C	15	10.03
(1,46)	1:45:A:SER:C	1:46:A:SER:N	1:46:A:SER:CA	1:46:A:SER:C	14	10.0
(1,16)	1:26:A:SER:C	1:27:A:LEU:N	1:27:A:LEU:CA	1:27:A:LEU:C	6	9.99
(1,76)	1:64:A:LYS:C	1:65:A:TRP:N	1:65:A:TRP:CA	1:65:A:TRP:C	6	9.98
(1,109)	1:82:A:ASN:C	1:83:A:ASP:N	1:83:A:ASP:CA	1:83:A:ASP:C	16	9.97
(1,190)	1:142:A:ARG:C	1:143:A:GLU:N	1:143:A:GLU:CA	1:143:A:GLU:C	3	9.95
(1,103)	1:79:A:TYR:C	1:80:A:LEU:N	1:80:A:LEU:CA	1:80:A:LEU:C	3	9.92
(1,24)	1:30:A:LYS:C	1:31:A:PHE:N	1:31:A:PHE:CA	1:31:A:PHE:C	10	9.88
(1,190)	1:142:A:ARG:C	1:143:A:GLU:N	1:143:A:GLU:CA	1:143:A:GLU:C	9	9.8
(1,26)	1:31:A:PHE:C	1:32:A:GLN:N	1:32:A:GLN:CA	1:32:A:GLN:C	7	9.79
(1,26)	1:31:A:PHE:C	1:32:A:GLN:N	1:32:A:GLN:CA	1:32:A:GLN:C	6	9.78
(1,186)	1:140:A:ALA:C	1:141:A:LEU:N	1:141:A:LEU:CA	1:141:A:LEU:C	17	9.77
(1,178)	1:136:A:GLU:C	1:137:A:MET:N	1:137:A:MET:CA	1:137:A:MET:C	11	9.76
(1,16)	1:26:A:SER:C	1:27:A:LEU:N	1:27:A:LEU:CA	1:27:A:LEU:C	2	9.75
(1,76)	1:64:A:LYS:C	1:65:A:TRP:N	1:65:A:TRP:CA	1:65:A:TRP:C	10	9.74
(1,32)	1:38:A:MET:C	1:39:A:GLU:N	1:39:A:GLU:CA	1:39:A:GLU:C	4	9.74
(1,168)	1:127:A:TRP:C	1:128:A:GLU:N	1:128:A:GLU:CA	1:128:A:GLU:C	11	9.73
(1,182)	1:138:A:ILE:C	1:139:A:VAL:N	1:139:A:VAL:CA	1:139:A:VAL:C	20	9.71
(1,188)	1:141:A:LEU:C	1:142:A:ARG:N	1:142:A:ARG:CA	1:142:A:ARG:C	5	9.7
(1,103)	1:79:A:TYR:C	1:80:A:LEU:N	1:80:A:LEU:CA	1:80:A:LEU:C	2	9.69
(1,115)	1:85:A:ILE:C	1:86:A:GLN:N	1:86:A:GLN:CA	1:86:A:GLN:C	12	9.68

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,60)	1:56:A:SER:C	1:57:A:THR:N	1:57:A:THR:CA	1:57:A:THR:C	2	9.68
(1,52)	1:48:A:CYS:C	1:49:A:ILE:N	1:49:A:ILE:CA	1:49:A:ILE:C	6	9.68
(1,66)	1:59:A:VAL:C	1:60:A:TYR:N	1:60:A:TYR:CA	1:60:A:TYR:C	8	9.67
(1,64)	1:58:A:ILE:C	1:59:A:VAL:N	1:59:A:VAL:CA	1:59:A:VAL:C	9	9.65
(1,52)	1:48:A:CYS:C	1:49:A:ILE:N	1:49:A:ILE:CA	1:49:A:ILE:C	11	9.65
(1,166)	1:126:A:ILE:C	1:127:A:TRP:N	1:127:A:TRP:CA	1:127:A:TRP:C	6	9.62
(1,103)	1:79:A:TYR:C	1:80:A:LEU:N	1:80:A:LEU:CA	1:80:A:LEU:C	17	9.59
(1,188)	1:141:A:LEU:C	1:142:A:ARG:N	1:142:A:ARG:CA	1:142:A:ARG:C	13	9.58
(1,78)	1:65:A:TRP:C	1:66:A:LEU:N	1:66:A:LEU:CA	1:66:A:LEU:C	5	9.57
(1,64)	1:58:A:ILE:C	1:59:A:VAL:N	1:59:A:VAL:CA	1:59:A:VAL:C	5	9.57
(1,190)	1:142:A:ARG:C	1:143:A:GLU:N	1:143:A:GLU:CA	1:143:A:GLU:C	5	9.56
(1,186)	1:140:A:ALA:C	1:141:A:LEU:N	1:141:A:LEU:CA	1:141:A:LEU:C	5	9.55
(1,144)	1:108:A:ALA:C	1:109:A:ALA:N	1:109:A:ALA:CA	1:109:A:ALA:C	13	9.51
(1,140)	1:106:A:GLU:C	1:107:A:ALA:N	1:107:A:ALA:CA	1:107:A:ALA:C	3	9.51
(1,113)	1:84:A:VAL:C	1:85:A:ILE:N	1:85:A:ILE:CA	1:85:A:ILE:C	4	9.49
(1,170)	1:128:A:GLU:C	1:129:A:ASP:N	1:129:A:ASP:CA	1:129:A:ASP:C	6	9.47
(1,8)	1:22:A:ALA:C	1:23:A:LEU:N	1:23:A:LEU:CA	1:23:A:LEU:C	4	9.47
(1,52)	1:48:A:CYS:C	1:49:A:ILE:N	1:49:A:ILE:CA	1:49:A:ILE:C	16	9.45
(1,68)	1:60:A:TYR:C	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	18	9.43
(1,14)	1:25:A:SER:C	1:26:A:SER:N	1:26:A:SER:CA	1:26:A:SER:C	17	9.43
(1,129)	1:99:A:SER:C	1:100:A:PHE:N	1:100:A:PHE:CA	1:100:A:PHE:C	5	9.42
(1,158)	1:122:A:ARG:C	1:123:A:ILE:N	1:123:A:ILE:CA	1:123:A:ILE:C	2	9.41
(1,140)	1:106:A:GLU:C	1:107:A:ALA:N	1:107:A:ALA:CA	1:107:A:ALA:C	12	9.39
(1,64)	1:58:A:ILE:C	1:59:A:VAL:N	1:59:A:VAL:CA	1:59:A:VAL:C	14	9.39
(1,158)	1:122:A:ARG:C	1:123:A:ILE:N	1:123:A:ILE:CA	1:123:A:ILE:C	6	9.32
(1,99)	1:77:A:LEU:C	1:78:A:PHE:N	1:78:A:PHE:CA	1:78:A:PHE:C	7	9.31
(1,24)	1:30:A:LYS:C	1:31:A:PHE:N	1:31:A:PHE:CA	1:31:A:PHE:C	4	9.3
(1,113)	1:84:A:VAL:C	1:85:A:ILE:N	1:85:A:ILE:CA	1:85:A:ILE:C	17	9.28
(1,64)	1:58:A:ILE:C	1:59:A:VAL:N	1:59:A:VAL:CA	1:59:A:VAL:C	3	9.27
(1,150)	1:118:A:LYS:C	1:119:A:SER:N	1:119:A:SER:CA	1:119:A:SER:C	11	9.24
(1,140)	1:106:A:GLU:C	1:107:A:ALA:N	1:107:A:ALA:CA	1:107:A:ALA:C	17	9.23
(1,117)	1:86:A:GLN:C	1:87:A:ASN:N	1:87:A:ASN:CA	1:87:A:ASN:C	1	9.21
(1,186)	1:140:A:ALA:C	1:141:A:LEU:N	1:141:A:LEU:CA	1:141:A:LEU:C	12	9.2
(1,113)	1:84:A:VAL:C	1:85:A:ILE:N	1:85:A:ILE:CA	1:85:A:ILE:C	6	9.2
(1,170)	1:128:A:GLU:C	1:129:A:ASP:N	1:129:A:ASP:CA	1:129:A:ASP:C	20	9.18
(1,84)	1:68:A:ARG:C	1:69:A:SER:N	1:69:A:SER:CA	1:69:A:SER:C	3	9.17
(1,16)	1:26:A:SER:C	1:27:A:LEU:N	1:27:A:LEU:CA	1:27:A:LEU:C	1	9.14
(1,162)	1:124:A:PHE:C	1:125:A:LYS:N	1:125:A:LYS:CA	1:125:A:LYS:C	8	9.13
(1,82)	1:67:A:ARG:C	1:68:A:ARG:N	1:68:A:ARG:CA	1:68:A:ARG:C	20	9.12
(1,140)	1:106:A:GLU:C	1:107:A:ALA:N	1:107:A:ALA:CA	1:107:A:ALA:C	7	9.1
(1,80)	1:66:A:LEU:C	1:67:A:ARG:N	1:67:A:ARG:CA	1:67:A:ARG:C	7	9.1
(1,66)	1:59:A:VAL:C	1:60:A:TYR:N	1:60:A:TYR:CA	1:60:A:TYR:C	16	9.1
(1,93)	1:74:A:ARG:C	1:75:A:LEU:N	1:75:A:LEU:CA	1:75:A:LEU:C	16	9.08
(1,186)	1:140:A:ALA:C	1:141:A:LEU:N	1:141:A:LEU:CA	1:141:A:LEU:C	8	9.07
(1,172)	1:129:A:ASP:C	1:130:A:ARG:N	1:130:A:ARG:CA	1:130:A:ARG:C	5	9.07
(1,14)	1:25:A:SER:C	1:26:A:SER:N	1:26:A:SER:CA	1:26:A:SER:C	9	9.07
(1,14)	1:25:A:SER:C	1:26:A:SER:N	1:26:A:SER:CA	1:26:A:SER:C	3	9.03
(1,111)	1:83:A:ASP:C	1:84:A:VAL:N	1:84:A:VAL:CA	1:84:A:VAL:C	13	9.02
(1,20)	1:28:A:ASP:C	1:29:A:ARG:N	1:29:A:ARG:CA	1:29:A:ARG:C	19	9.0
(1,166)	1:126:A:ILE:C	1:127:A:TRP:N	1:127:A:TRP:CA	1:127:A:TRP:C	20	8.99
(1,66)	1:59:A:VAL:C	1:60:A:TYR:N	1:60:A:TYR:CA	1:60:A:TYR:C	19	8.99

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,14)	1:25:A:SER:C	1:26:A:SER:N	1:26:A:SER:CA	1:26:A:SER:C	10	8.94
(1,64)	1:58:A:ILE:C	1:59:A:VAL:N	1:59:A:VAL:CA	1:59:A:VAL:C	16	8.93
(1,113)	1:84:A:VAL:C	1:85:A:ILE:N	1:85:A:ILE:CA	1:85:A:ILE:C	10	8.92
(1,14)	1:25:A:SER:C	1:26:A:SER:N	1:26:A:SER:CA	1:26:A:SER:C	5	8.92
(1,68)	1:60:A:TYR:C	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	20	8.91
(1,26)	1:31:A:PHE:C	1:32:A:GLN:N	1:32:A:GLN:CA	1:32:A:GLN:C	5	8.88
(1,127)	1:98:A:GLU:C	1:99:A:SER:N	1:99:A:SER:CA	1:99:A:SER:C	19	8.86
(1,68)	1:60:A:TYR:C	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	3	8.84
(1,140)	1:106:A:GLU:C	1:107:A:ALA:N	1:107:A:ALA:CA	1:107:A:ALA:C	1	8.83
(1,140)	1:106:A:GLU:C	1:107:A:ALA:N	1:107:A:ALA:CA	1:107:A:ALA:C	11	8.83
(1,129)	1:99:A:SER:C	1:100:A:PHE:N	1:100:A:PHE:CA	1:100:A:PHE:C	16	8.82
(1,166)	1:126:A:ILE:C	1:127:A:TRP:N	1:127:A:TRP:CA	1:127:A:TRP:C	4	8.8
(1,140)	1:106:A:GLU:C	1:107:A:ALA:N	1:107:A:ALA:CA	1:107:A:ALA:C	6	8.8
(1,66)	1:59:A:VAL:C	1:60:A:TYR:N	1:60:A:TYR:CA	1:60:A:TYR:C	10	8.79
(1,144)	1:108:A:ALA:C	1:109:A:ALA:N	1:109:A:ALA:CA	1:109:A:ALA:C	11	8.72
(1,16)	1:26:A:SER:C	1:27:A:LEU:N	1:27:A:LEU:CA	1:27:A:LEU:C	12	8.71
(1,58)	1:55:A:HIS:C	1:56:A:SER:N	1:56:A:SER:CA	1:56:A:SER:C	9	8.66
(1,24)	1:30:A:LYS:C	1:31:A:PHE:N	1:31:A:PHE:CA	1:31:A:PHE:C	14	8.66
(1,166)	1:126:A:ILE:C	1:127:A:TRP:N	1:127:A:TRP:CA	1:127:A:TRP:C	19	8.63
(1,64)	1:58:A:ILE:C	1:59:A:VAL:N	1:59:A:VAL:CA	1:59:A:VAL:C	10	8.61
(1,144)	1:108:A:ALA:C	1:109:A:ALA:N	1:109:A:ALA:CA	1:109:A:ALA:C	17	8.6
(1,93)	1:74:A:ARG:C	1:75:A:LEU:N	1:75:A:LEU:CA	1:75:A:LEU:C	3	8.59
(1,8)	1:22:A:ALA:C	1:23:A:LEU:N	1:23:A:LEU:CA	1:23:A:LEU:C	5	8.58
(1,117)	1:86:A:GLN:C	1:87:A:ASN:N	1:87:A:ASN:CA	1:87:A:ASN:C	3	8.56
(1,68)	1:60:A:TYR:C	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	13	8.56
(1,32)	1:38:A:MET:C	1:39:A:GLU:N	1:39:A:GLU:CA	1:39:A:GLU:C	20	8.56
(1,26)	1:31:A:PHE:C	1:32:A:GLN:N	1:32:A:GLN:CA	1:32:A:GLN:C	15	8.56
(1,111)	1:83:A:ASP:C	1:84:A:VAL:N	1:84:A:VAL:CA	1:84:A:VAL:C	11	8.55
(1,192)	1:143:A:GLU:C	1:144:A:ALA:N	1:144:A:ALA:CA	1:144:A:ALA:C	13	8.54
(1,101)	1:78:A:PHE:C	1:79:A:TYR:N	1:79:A:TYR:CA	1:79:A:TYR:C	14	8.53
(1,125)	1:97:A:ARG:C	1:98:A:GLU:N	1:98:A:GLU:CA	1:98:A:GLU:C	16	8.52
(1,115)	1:85:A:ILE:C	1:86:A:GLN:N	1:86:A:GLN:CA	1:86:A:GLN:C	18	8.51
(1,22)	1:29:A:ARG:C	1:30:A:LYS:N	1:30:A:LYS:CA	1:30:A:LYS:C	18	8.5
(1,95)	1:75:A:LEU:C	1:76:A:ASN:N	1:76:A:ASN:CA	1:76:A:ASN:C	15	8.48
(1,172)	1:129:A:ASP:C	1:130:A:ARG:N	1:130:A:ARG:CA	1:130:A:ARG:C	18	8.45
(1,8)	1:22:A:ALA:C	1:23:A:LEU:N	1:23:A:LEU:CA	1:23:A:LEU:C	15	8.45
(1,138)	1:105:A:PRO:C	1:106:A:GLU:N	1:106:A:GLU:CA	1:106:A:GLU:C	10	8.44
(1,95)	1:75:A:LEU:C	1:76:A:ASN:N	1:76:A:ASN:CA	1:76:A:ASN:C	6	8.42
(1,156)	1:121:A:GLU:C	1:122:A:ARG:N	1:122:A:ARG:CA	1:122:A:ARG:C	6	8.41
(1,16)	1:26:A:SER:C	1:27:A:LEU:N	1:27:A:LEU:CA	1:27:A:LEU:C	13	8.41
(1,158)	1:122:A:ARG:C	1:123:A:ILE:N	1:123:A:ILE:CA	1:123:A:ILE:C	20	8.4
(1,97)	1:76:A:ASN:C	1:77:A:LEU:N	1:77:A:LEU:CA	1:77:A:LEU:C	3	8.37
(1,115)	1:85:A:ILE:C	1:86:A:GLN:N	1:86:A:GLN:CA	1:86:A:GLN:C	2	8.36
(1,95)	1:75:A:LEU:C	1:76:A:ASN:N	1:76:A:ASN:CA	1:76:A:ASN:C	1	8.36
(1,52)	1:48:A:CYS:C	1:49:A:ILE:N	1:49:A:ILE:CA	1:49:A:ILE:C	4	8.35
(1,140)	1:106:A:GLU:C	1:107:A:ALA:N	1:107:A:ALA:CA	1:107:A:ALA:C	5	8.34
(1,182)	1:138:A:ILE:C	1:139:A:VAL:N	1:139:A:VAL:CA	1:139:A:VAL:C	13	8.32
(1,99)	1:77:A:LEU:C	1:78:A:PHE:N	1:78:A:PHE:CA	1:78:A:PHE:C	8	8.32
(1,182)	1:138:A:ILE:C	1:139:A:VAL:N	1:139:A:VAL:CA	1:139:A:VAL:C	1	8.29
(1,64)	1:58:A:ILE:C	1:59:A:VAL:N	1:59:A:VAL:CA	1:59:A:VAL:C	18	8.28
(1,89)	1:72:A:PRO:C	1:73:A:HIS:N	1:73:A:HIS:CA	1:73:A:HIS:C	18	8.26

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,140)	1:106:A:GLU:C	1:107:A:ALA:N	1:107:A:ALA:CA	1:107:A:ALA:C	18	8.24
(1,22)	1:29:A:ARG:C	1:30:A:LYS:N	1:30:A:LYS:CA	1:30:A:LYS:C	16	8.23
(1,97)	1:76:A:ASN:C	1:77:A:LEU:N	1:77:A:LEU:CA	1:77:A:LEU:C	2	8.22
(1,68)	1:60:A:TYR:C	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	17	8.22
(1,170)	1:128:A:GLU:C	1:129:A:ASP:N	1:129:A:ASP:CA	1:129:A:ASP:C	4	8.19
(1,129)	1:99:A:SER:C	1:100:A:PHE:N	1:100:A:PHE:CA	1:100:A:PHE:C	1	8.19
(1,190)	1:142:A:ARG:C	1:143:A:GLU:N	1:143:A:GLU:CA	1:143:A:GLU:C	7	8.18
(1,66)	1:59:A:VAL:C	1:60:A:TYR:N	1:60:A:TYR:CA	1:60:A:TYR:C	13	8.18
(1,44)	1:44:A:LEU:C	1:45:A:SER:N	1:45:A:SER:CA	1:45:A:SER:C	19	8.16
(1,194)	1:144:A:ALA:C	1:145:A:LEU:N	1:145:A:LEU:CA	1:145:A:LEU:C	14	8.15
(1,113)	1:84:A:VAL:C	1:85:A:ILE:N	1:85:A:ILE:CA	1:85:A:ILE:C	18	8.15
(1,68)	1:60:A:TYR:C	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	15	8.15
(1,66)	1:59:A:VAL:C	1:60:A:TYR:N	1:60:A:TYR:CA	1:60:A:TYR:C	6	8.15
(1,16)	1:26:A:SER:C	1:27:A:LEU:N	1:27:A:LEU:CA	1:27:A:LEU:C	19	8.14
(1,170)	1:128:A:GLU:C	1:129:A:ASP:N	1:129:A:ASP:CA	1:129:A:ASP:C	16	8.13
(1,160)	1:123:A:ILE:C	1:124:A:PHE:N	1:124:A:PHE:CA	1:124:A:PHE:C	11	8.13
(1,66)	1:59:A:VAL:C	1:60:A:TYR:N	1:60:A:TYR:CA	1:60:A:TYR:C	11	8.13
(1,172)	1:129:A:ASP:C	1:130:A:ARG:N	1:130:A:ARG:CA	1:130:A:ARG:C	17	8.12
(1,158)	1:122:A:ARG:C	1:123:A:ILE:N	1:123:A:ILE:CA	1:123:A:ILE:C	10	8.1
(1,72)	1:62:A:TRP:C	1:63:A:MET:N	1:63:A:MET:CA	1:63:A:MET:C	6	8.1
(1,6)	1:21:A:GLY:C	1:22:A:ALA:N	1:22:A:ALA:CA	1:22:A:ALA:C	2	8.09
(1,173)	1:130:A:ARG:N	1:130:A:ARG:CA	1:130:A:ARG:C	1:131:A:ASN:N	16	8.05
(1,82)	1:67:A:ARG:C	1:68:A:ARG:N	1:68:A:ARG:CA	1:68:A:ARG:C	11	8.0
(1,97)	1:76:A:ASN:C	1:77:A:LEU:N	1:77:A:LEU:CA	1:77:A:LEU:C	18	7.96
(1,74)	1:63:A:MET:C	1:64:A:LYS:N	1:64:A:LYS:CA	1:64:A:LYS:C	3	7.96
(1,54)	1:49:A:ILE:C	1:50:A:GLU:N	1:50:A:GLU:CA	1:50:A:GLU:C	8	7.92
(1,36)	1:40:A:SER:C	1:41:A:ILE:N	1:41:A:ILE:CA	1:41:A:ILE:C	16	7.92
(1,52)	1:48:A:CYS:C	1:49:A:ILE:N	1:49:A:ILE:CA	1:49:A:ILE:C	12	7.87
(1,162)	1:124:A:PHE:C	1:125:A:LYS:N	1:125:A:LYS:CA	1:125:A:LYS:C	6	7.86
(1,60)	1:56:A:SER:C	1:57:A:THR:N	1:57:A:THR:CA	1:57:A:THR:C	1	7.86
(1,78)	1:65:A:TRP:C	1:66:A:LEU:N	1:66:A:LEU:CA	1:66:A:LEU:C	6	7.84
(1,64)	1:58:A:ILE:C	1:59:A:VAL:N	1:59:A:VAL:CA	1:59:A:VAL:C	19	7.84
(1,78)	1:65:A:TRP:C	1:66:A:LEU:N	1:66:A:LEU:CA	1:66:A:LEU:C	9	7.83
(1,97)	1:76:A:ASN:C	1:77:A:LEU:N	1:77:A:LEU:CA	1:77:A:LEU:C	4	7.82
(1,97)	1:76:A:ASN:C	1:77:A:LEU:N	1:77:A:LEU:CA	1:77:A:LEU:C	7	7.82
(1,82)	1:67:A:ARG:C	1:68:A:ARG:N	1:68:A:ARG:CA	1:68:A:ARG:C	6	7.81
(1,70)	1:61:A:HIS:C	1:62:A:TRP:N	1:62:A:TRP:CA	1:62:A:TRP:C	7	7.8
(1,36)	1:40:A:SER:C	1:41:A:ILE:N	1:41:A:ILE:CA	1:41:A:ILE:C	17	7.78
(1,111)	1:83:A:ASP:C	1:84:A:VAL:N	1:84:A:VAL:CA	1:84:A:VAL:C	1	7.76
(1,8)	1:22:A:ALA:C	1:23:A:LEU:N	1:23:A:LEU:CA	1:23:A:LEU:C	1	7.75
(1,194)	1:144:A:ALA:C	1:145:A:LEU:N	1:145:A:LEU:CA	1:145:A:LEU:C	18	7.7
(1,89)	1:72:A:PRO:C	1:73:A:HIS:N	1:73:A:HIS:CA	1:73:A:HIS:C	10	7.7
(1,74)	1:63:A:MET:C	1:64:A:LYS:N	1:64:A:LYS:CA	1:64:A:LYS:C	2	7.68
(1,54)	1:49:A:ILE:C	1:50:A:GLU:N	1:50:A:GLU:CA	1:50:A:GLU:C	12	7.67
(1,190)	1:142:A:ARG:C	1:143:A:GLU:N	1:143:A:GLU:CA	1:143:A:GLU:C	19	7.66
(1,99)	1:77:A:LEU:C	1:78:A:PHE:N	1:78:A:PHE:CA	1:78:A:PHE:C	17	7.65
(1,64)	1:58:A:ILE:C	1:59:A:VAL:N	1:59:A:VAL:CA	1:59:A:VAL:C	4	7.64
(1,52)	1:48:A:CYS:C	1:49:A:ILE:N	1:49:A:ILE:CA	1:49:A:ILE:C	9	7.64
(1,190)	1:142:A:ARG:C	1:143:A:GLU:N	1:143:A:GLU:CA	1:143:A:GLU:C	14	7.62
(1,186)	1:140:A:ALA:C	1:141:A:LEU:N	1:141:A:LEU:CA	1:141:A:LEU:C	3	7.62
(1,16)	1:26:A:SER:C	1:27:A:LEU:N	1:27:A:LEU:CA	1:27:A:LEU:C	8	7.61

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,72)	1:62:A:TRP:C	1:63:A:MET:N	1:63:A:MET:CA	1:63:A:MET:C	7	7.6
(1,28)	1:32:A:GLN:C	1:33:A:SER:N	1:33:A:SER:CA	1:33:A:SER:C	11	7.59
(1,129)	1:99:A:SER:C	1:100:A:PHE:N	1:100:A:PHE:CA	1:100:A:PHE:C	6	7.57
(1,16)	1:26:A:SER:C	1:27:A:LEU:N	1:27:A:LEU:CA	1:27:A:LEU:C	9	7.57
(1,103)	1:79:A:TYR:C	1:80:A:LEU:N	1:80:A:LEU:CA	1:80:A:LEU:C	18	7.56
(1,20)	1:28:A:ASP:C	1:29:A:ARG:N	1:29:A:ARG:CA	1:29:A:ARG:C	1	7.56
(1,140)	1:106:A:GLU:C	1:107:A:ALA:N	1:107:A:ALA:CA	1:107:A:ALA:C	2	7.54
(1,78)	1:65:A:TRP:C	1:66:A:LEU:N	1:66:A:LEU:CA	1:66:A:LEU:C	13	7.54
(1,164)	1:125:A:LYS:C	1:126:A:ILE:N	1:126:A:ILE:CA	1:126:A:ILE:C	1	7.53
(1,28)	1:32:A:GLN:C	1:33:A:SER:N	1:33:A:SER:CA	1:33:A:SER:C	14	7.53
(1,24)	1:30:A:LYS:C	1:31:A:PHE:N	1:31:A:PHE:CA	1:31:A:PHE:C	8	7.52
(1,52)	1:48:A:CYS:C	1:49:A:ILE:N	1:49:A:ILE:CA	1:49:A:ILE:C	20	7.51
(1,68)	1:60:A:TYR:C	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	10	7.49
(1,58)	1:55:A:HIS:C	1:56:A:SER:N	1:56:A:SER:CA	1:56:A:SER:C	1	7.49
(1,90)	1:73:A:HIS:N	1:73:A:HIS:CA	1:73:A:HIS:C	1:74:A:ARG:N	16	7.48
(1,162)	1:124:A:PHE:C	1:125:A:LYS:N	1:125:A:LYS:CA	1:125:A:LYS:C	4	7.46
(1,127)	1:98:A:GLU:C	1:99:A:SER:N	1:99:A:SER:CA	1:99:A:SER:C	8	7.46
(1,97)	1:76:A:ASN:C	1:77:A:LEU:N	1:77:A:LEU:CA	1:77:A:LEU:C	15	7.46
(1,93)	1:74:A:ARG:C	1:75:A:LEU:N	1:75:A:LEU:CA	1:75:A:LEU:C	20	7.45
(1,76)	1:64:A:LYS:C	1:65:A:TRP:N	1:65:A:TRP:CA	1:65:A:TRP:C	15	7.44
(1,74)	1:63:A:MET:C	1:64:A:LYS:N	1:64:A:LYS:CA	1:64:A:LYS:C	1	7.44
(1,164)	1:125:A:LYS:C	1:126:A:ILE:N	1:126:A:ILE:CA	1:126:A:ILE:C	17	7.43
(1,68)	1:60:A:TYR:C	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	5	7.43
(1,127)	1:98:A:GLU:C	1:99:A:SER:N	1:99:A:SER:CA	1:99:A:SER:C	16	7.42
(1,125)	1:97:A:ARG:C	1:98:A:GLU:N	1:98:A:GLU:CA	1:98:A:GLU:C	10	7.42
(1,66)	1:59:A:VAL:C	1:60:A:TYR:N	1:60:A:TYR:CA	1:60:A:TYR:C	5	7.42
(1,16)	1:26:A:SER:C	1:27:A:LEU:N	1:27:A:LEU:CA	1:27:A:LEU:C	20	7.42
(1,170)	1:128:A:GLU:C	1:129:A:ASP:N	1:129:A:ASP:CA	1:129:A:ASP:C	19	7.41
(1,111)	1:83:A:ASP:C	1:84:A:VAL:N	1:84:A:VAL:CA	1:84:A:VAL:C	5	7.41
(1,144)	1:108:A:ALA:C	1:109:A:ALA:N	1:109:A:ALA:CA	1:109:A:ALA:C	4	7.39
(1,97)	1:76:A:ASN:C	1:77:A:LEU:N	1:77:A:LEU:CA	1:77:A:LEU:C	5	7.36
(1,36)	1:40:A:SER:C	1:41:A:ILE:N	1:41:A:ILE:CA	1:41:A:ILE:C	5	7.33
(1,97)	1:76:A:ASN:C	1:77:A:LEU:N	1:77:A:LEU:CA	1:77:A:LEU:C	9	7.32
(1,24)	1:30:A:LYS:C	1:31:A:PHE:N	1:31:A:PHE:CA	1:31:A:PHE:C	19	7.32
(1,160)	1:123:A:ILE:C	1:124:A:PHE:N	1:124:A:PHE:CA	1:124:A:PHE:C	8	7.31
(1,52)	1:48:A:CYS:C	1:49:A:ILE:N	1:49:A:ILE:CA	1:49:A:ILE:C	19	7.31
(1,26)	1:31:A:PHE:C	1:32:A:GLN:N	1:32:A:GLN:CA	1:32:A:GLN:C	19	7.29
(1,16)	1:26:A:SER:C	1:27:A:LEU:N	1:27:A:LEU:CA	1:27:A:LEU:C	7	7.28
(1,97)	1:76:A:ASN:C	1:77:A:LEU:N	1:77:A:LEU:CA	1:77:A:LEU:C	10	7.27
(1,113)	1:84:A:VAL:C	1:85:A:ILE:N	1:85:A:ILE:CA	1:85:A:ILE:C	13	7.26
(1,8)	1:22:A:ALA:C	1:23:A:LEU:N	1:23:A:LEU:CA	1:23:A:LEU:C	10	7.26
(1,138)	1:105:A:PRO:C	1:106:A:GLU:N	1:106:A:GLU:CA	1:106:A:GLU:C	19	7.22
(1,93)	1:74:A:ARG:C	1:75:A:LEU:N	1:75:A:LEU:CA	1:75:A:LEU:C	5	7.22
(1,76)	1:64:A:LYS:C	1:65:A:TRP:N	1:65:A:TRP:CA	1:65:A:TRP:C	17	7.22
(1,133)	1:101:A:ALA:C	1:102:A:ASP:N	1:102:A:ASP:CA	1:102:A:ASP:C	5	7.21
(1,103)	1:79:A:TYR:C	1:80:A:LEU:N	1:80:A:LEU:CA	1:80:A:LEU:C	15	7.2
(1,99)	1:77:A:LEU:C	1:78:A:PHE:N	1:78:A:PHE:CA	1:78:A:PHE:C	12	7.2
(1,95)	1:75:A:LEU:C	1:76:A:ASN:N	1:76:A:ASN:CA	1:76:A:ASN:C	4	7.2
(1,188)	1:141:A:LEU:C	1:142:A:ARG:N	1:142:A:ARG:CA	1:142:A:ARG:C	18	7.19
(1,72)	1:62:A:TRP:C	1:63:A:MET:N	1:63:A:MET:CA	1:63:A:MET:C	19	7.19
(1,168)	1:127:A:TRP:C	1:128:A:GLU:N	1:128:A:GLU:CA	1:128:A:GLU:C	14	7.16

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,138)	1:105:A:PRO:C	1:106:A:GLU:N	1:106:A:GLU:CA	1:106:A:GLU:C	18	7.16
(1,54)	1:49:A:ILE:C	1:50:A:GLU:N	1:50:A:GLU:CA	1:50:A:GLU:C	20	7.16
(1,162)	1:124:A:PHE:C	1:125:A:LYS:N	1:125:A:LYS:CA	1:125:A:LYS:C	7	7.14
(1,113)	1:84:A:VAL:C	1:85:A:ILE:N	1:85:A:ILE:CA	1:85:A:ILE:C	14	7.14
(1,22)	1:29:A:ARG:C	1:30:A:LYS:N	1:30:A:LYS:CA	1:30:A:LYS:C	12	7.12
(1,8)	1:22:A:ALA:C	1:23:A:LEU:N	1:23:A:LEU:CA	1:23:A:LEU:C	7	7.12
(1,190)	1:142:A:ARG:C	1:143:A:GLU:N	1:143:A:GLU:CA	1:143:A:GLU:C	10	7.1
(1,138)	1:105:A:PRO:C	1:106:A:GLU:N	1:106:A:GLU:CA	1:106:A:GLU:C	15	7.09
(1,133)	1:101:A:ALA:C	1:102:A:ASP:N	1:102:A:ASP:CA	1:102:A:ASP:C	12	7.07
(1,66)	1:59:A:VAL:C	1:60:A:TYR:N	1:60:A:TYR:CA	1:60:A:TYR:C	18	7.07
(1,52)	1:48:A:CYS:C	1:49:A:ILE:N	1:49:A:ILE:CA	1:49:A:ILE:C	3	7.06
(1,46)	1:45:A:SER:C	1:46:A:SER:N	1:46:A:SER:CA	1:46:A:SER:C	11	7.06
(1,144)	1:108:A:ALA:C	1:109:A:ALA:N	1:109:A:ALA:CA	1:109:A:ALA:C	12	7.02
(1,117)	1:86:A:GLN:C	1:87:A:ASN:N	1:87:A:ASN:CA	1:87:A:ASN:C	20	7.02
(1,142)	1:107:A:ALA:C	1:108:A:ALA:N	1:108:A:ALA:CA	1:108:A:ALA:C	6	7.0
(1,168)	1:127:A:TRP:C	1:128:A:GLU:N	1:128:A:GLU:CA	1:128:A:GLU:C	10	6.99
(1,162)	1:124:A:PHE:C	1:125:A:LYS:N	1:125:A:LYS:CA	1:125:A:LYS:C	2	6.99
(1,144)	1:108:A:ALA:C	1:109:A:ALA:N	1:109:A:ALA:CA	1:109:A:ALA:C	3	6.99
(1,166)	1:126:A:ILE:C	1:127:A:TRP:N	1:127:A:TRP:CA	1:127:A:TRP:C	11	6.98
(1,95)	1:75:A:LEU:C	1:76:A:ASN:N	1:76:A:ASN:CA	1:76:A:ASN:C	3	6.98
(1,46)	1:45:A:SER:C	1:46:A:SER:N	1:46:A:SER:CA	1:46:A:SER:C	15	6.97
(1,172)	1:129:A:ASP:C	1:130:A:ARG:N	1:130:A:ARG:CA	1:130:A:ARG:C	1	6.96
(1,170)	1:128:A:GLU:C	1:129:A:ASP:N	1:129:A:ASP:CA	1:129:A:ASP:C	1	6.94
(1,125)	1:97:A:ARG:C	1:98:A:GLU:N	1:98:A:GLU:CA	1:98:A:GLU:C	2	6.94
(1,76)	1:64:A:LYS:C	1:65:A:TRP:N	1:65:A:TRP:CA	1:65:A:TRP:C	5	6.94
(1,140)	1:106:A:GLU:C	1:107:A:ALA:N	1:107:A:ALA:CA	1:107:A:ALA:C	13	6.91
(1,14)	1:25:A:SER:C	1:26:A:SER:N	1:26:A:SER:CA	1:26:A:SER:C	11	6.91
(1,28)	1:32:A:GLN:C	1:33:A:SER:N	1:33:A:SER:CA	1:33:A:SER:C	17	6.88
(1,18)	1:27:A:LEU:C	1:28:A:ASP:N	1:28:A:ASP:CA	1:28:A:ASP:C	15	6.87
(1,190)	1:142:A:ARG:C	1:143:A:GLU:N	1:143:A:GLU:CA	1:143:A:GLU:C	16	6.85
(1,91)	1:73:A:HIS:C	1:74:A:ARG:N	1:74:A:ARG:CA	1:74:A:ARG:C	6	6.85
(1,64)	1:58:A:ILE:C	1:59:A:VAL:N	1:59:A:VAL:CA	1:59:A:VAL:C	7	6.83
(1,172)	1:129:A:ASP:C	1:130:A:ARG:N	1:130:A:ARG:CA	1:130:A:ARG:C	4	6.82
(1,99)	1:77:A:LEU:C	1:78:A:PHE:N	1:78:A:PHE:CA	1:78:A:PHE:C	14	6.82
(1,52)	1:48:A:CYS:C	1:49:A:ILE:N	1:49:A:ILE:CA	1:49:A:ILE:C	18	6.79
(1,14)	1:25:A:SER:C	1:26:A:SER:N	1:26:A:SER:CA	1:26:A:SER:C	6	6.79
(1,127)	1:98:A:GLU:C	1:99:A:SER:N	1:99:A:SER:CA	1:99:A:SER:C	15	6.77
(1,93)	1:74:A:ARG:C	1:75:A:LEU:N	1:75:A:LEU:CA	1:75:A:LEU:C	2	6.76
(1,14)	1:25:A:SER:C	1:26:A:SER:N	1:26:A:SER:CA	1:26:A:SER:C	15	6.76
(1,95)	1:75:A:LEU:C	1:76:A:ASN:N	1:76:A:ASN:CA	1:76:A:ASN:C	18	6.74
(1,105)	1:80:A:LEU:C	1:81:A:ALA:N	1:81:A:ALA:CA	1:81:A:ALA:C	15	6.72
(1,64)	1:58:A:ILE:C	1:59:A:VAL:N	1:59:A:VAL:CA	1:59:A:VAL:C	11	6.71
(1,188)	1:141:A:LEU:C	1:142:A:ARG:N	1:142:A:ARG:CA	1:142:A:ARG:C	17	6.69
(1,113)	1:84:A:VAL:C	1:85:A:ILE:N	1:85:A:ILE:CA	1:85:A:ILE:C	2	6.69
(1,113)	1:84:A:VAL:C	1:85:A:ILE:N	1:85:A:ILE:CA	1:85:A:ILE:C	15	6.69
(1,172)	1:129:A:ASP:C	1:130:A:ARG:N	1:130:A:ARG:CA	1:130:A:ARG:C	7	6.66
(1,129)	1:99:A:SER:C	1:100:A:PHE:N	1:100:A:PHE:CA	1:100:A:PHE:C	9	6.64
(1,111)	1:83:A:ASP:C	1:84:A:VAL:N	1:84:A:VAL:CA	1:84:A:VAL:C	8	6.63
(1,28)	1:32:A:GLN:C	1:33:A:SER:N	1:33:A:SER:CA	1:33:A:SER:C	19	6.63
(1,172)	1:129:A:ASP:C	1:130:A:ARG:N	1:130:A:ARG:CA	1:130:A:ARG:C	15	6.62
(1,144)	1:108:A:ALA:C	1:109:A:ALA:N	1:109:A:ALA:CA	1:109:A:ALA:C	16	6.61

Continued on next page...

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,20)	1:28:A:ASP:C	1:29:A:ARG:N	1:29:A:ARG:CA	1:29:A:ARG:C	4	6.61
(1,6)	1:21:A:GLY:C	1:22:A:ALA:N	1:22:A:ALA:CA	1:22:A:ALA:C	4	6.61
(1,91)	1:73:A:HIS:C	1:74:A:ARG:N	1:74:A:ARG:CA	1:74:A:ARG:C	1	6.6
(1,190)	1:142:A:ARG:C	1:143:A:GLU:N	1:143:A:GLU:CA	1:143:A:GLU:C	2	6.59
(1,144)	1:108:A:ALA:C	1:109:A:ALA:N	1:109:A:ALA:CA	1:109:A:ALA:C	19	6.59
(1,16)	1:26:A:SER:C	1:27:A:LEU:N	1:27:A:LEU:CA	1:27:A:LEU:C	3	6.59
(1,166)	1:126:A:ILE:C	1:127:A:TRP:N	1:127:A:TRP:CA	1:127:A:TRP:C	12	6.58
(1,129)	1:99:A:SER:C	1:100:A:PHE:N	1:100:A:PHE:CA	1:100:A:PHE:C	11	6.58
(1,129)	1:99:A:SER:C	1:100:A:PHE:N	1:100:A:PHE:CA	1:100:A:PHE:C	20	6.57
(1,62)	1:57:A:THR:C	1:58:A:ILE:N	1:58:A:ILE:CA	1:58:A:ILE:C	19	6.57
(1,84)	1:68:A:ARG:C	1:69:A:SER:N	1:69:A:SER:CA	1:69:A:SER:C	9	6.56
(1,66)	1:59:A:VAL:C	1:60:A:TYR:N	1:60:A:TYR:CA	1:60:A:TYR:C	15	6.56
(1,46)	1:45:A:SER:C	1:46:A:SER:N	1:46:A:SER:CA	1:46:A:SER:C	19	6.56
(1,192)	1:143:A:GLU:C	1:144:A:ALA:N	1:144:A:ALA:CA	1:144:A:ALA:C	5	6.55
(1,111)	1:83:A:ASP:C	1:84:A:VAL:N	1:84:A:VAL:CA	1:84:A:VAL:C	14	6.55
(1,32)	1:38:A:MET:C	1:39:A:GLU:N	1:39:A:GLU:CA	1:39:A:GLU:C	2	6.55
(1,16)	1:26:A:SER:C	1:27:A:LEU:N	1:27:A:LEU:CA	1:27:A:LEU:C	15	6.55
(1,164)	1:125:A:LYS:C	1:126:A:ILE:N	1:126:A:ILE:CA	1:126:A:ILE:C	14	6.51
(1,89)	1:72:A:PRO:C	1:73:A:HIS:N	1:73:A:HIS:CA	1:73:A:HIS:C	1	6.5
(1,127)	1:98:A:GLU:C	1:99:A:SER:N	1:99:A:SER:CA	1:99:A:SER:C	13	6.47
(1,125)	1:97:A:ARG:C	1:98:A:GLU:N	1:98:A:GLU:CA	1:98:A:GLU:C	13	6.46
(1,78)	1:65:A:TRP:C	1:66:A:LEU:N	1:66:A:LEU:CA	1:66:A:LEU:C	19	6.46
(1,12)	1:24:A:GLU:C	1:25:A:SER:N	1:25:A:SER:CA	1:25:A:SER:C	3	6.45
(1,123)	1:96:A:PHE:C	1:97:A:ARG:N	1:97:A:ARG:CA	1:97:A:ARG:C	17	6.43
(1,138)	1:105:A:PRO:C	1:106:A:GLU:N	1:106:A:GLU:CA	1:106:A:GLU:C	3	6.42
(1,103)	1:79:A:TYR:C	1:80:A:LEU:N	1:80:A:LEU:CA	1:80:A:LEU:C	7	6.42
(1,156)	1:121:A:GLU:C	1:122:A:ARG:N	1:122:A:ARG:CA	1:122:A:ARG:C	8	6.39
(1,64)	1:58:A:ILE:C	1:59:A:VAL:N	1:59:A:VAL:CA	1:59:A:VAL:C	6	6.39
(1,168)	1:127:A:TRP:C	1:128:A:GLU:N	1:128:A:GLU:CA	1:128:A:GLU:C	17	6.36
(1,160)	1:123:A:ILE:C	1:124:A:PHE:N	1:124:A:PHE:CA	1:124:A:PHE:C	6	6.36
(1,89)	1:72:A:PRO:C	1:73:A:HIS:N	1:73:A:HIS:CA	1:73:A:HIS:C	19	6.36
(1,194)	1:144:A:ALA:C	1:145:A:LEU:N	1:145:A:LEU:CA	1:145:A:LEU:C	11	6.35
(1,68)	1:60:A:TYR:C	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	12	6.35
(1,115)	1:85:A:ILE:C	1:86:A:GLN:N	1:86:A:GLN:CA	1:86:A:GLN:C	4	6.34
(1,52)	1:48:A:CYS:C	1:49:A:ILE:N	1:49:A:ILE:CA	1:49:A:ILE:C	7	6.32
(1,152)	1:119:A:SER:C	1:120:A:VAL:N	1:120:A:VAL:CA	1:120:A:VAL:C	13	6.3
(1,68)	1:60:A:TYR:C	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	1	6.3
(1,158)	1:122:A:ARG:C	1:123:A:ILE:N	1:123:A:ILE:CA	1:123:A:ILE:C	1	6.29
(1,72)	1:62:A:TRP:C	1:63:A:MET:N	1:63:A:MET:CA	1:63:A:MET:C	1	6.29
(1,97)	1:76:A:ASN:C	1:77:A:LEU:N	1:77:A:LEU:CA	1:77:A:LEU:C	6	6.28
(1,97)	1:76:A:ASN:C	1:77:A:LEU:N	1:77:A:LEU:CA	1:77:A:LEU:C	11	6.26
(1,82)	1:67:A:ARG:C	1:68:A:ARG:N	1:68:A:ARG:CA	1:68:A:ARG:C	17	6.26
(1,162)	1:124:A:PHE:C	1:125:A:LYS:N	1:125:A:LYS:CA	1:125:A:LYS:C	14	6.25
(1,144)	1:108:A:ALA:C	1:109:A:ALA:N	1:109:A:ALA:CA	1:109:A:ALA:C	14	6.25
(1,133)	1:101:A:ALA:C	1:102:A:ASP:N	1:102:A:ASP:CA	1:102:A:ASP:C	1	6.25
(1,36)	1:40:A:SER:C	1:41:A:ILE:N	1:41:A:ILE:CA	1:41:A:ILE:C	2	6.25
(1,93)	1:74:A:ARG:C	1:75:A:LEU:N	1:75:A:LEU:CA	1:75:A:LEU:C	18	6.23
(1,24)	1:30:A:LYS:C	1:31:A:PHE:N	1:31:A:PHE:CA	1:31:A:PHE:C	9	6.22
(1,22)	1:29:A:ARG:C	1:30:A:LYS:N	1:30:A:LYS:CA	1:30:A:LYS:C	17	6.22
(1,78)	1:65:A:TRP:C	1:66:A:LEU:N	1:66:A:LEU:CA	1:66:A:LEU:C	10	6.2
(1,148)	1:117:A:SER:C	1:118:A:LYS:N	1:118:A:LYS:CA	1:118:A:LYS:C	11	6.18

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,16)	1:26:A:SER:C	1:27:A:LEU:N	1:27:A:LEU:CA	1:27:A:LEU:C	5	6.18
(1,113)	1:84:A:VAL:C	1:85:A:ILE:N	1:85:A:ILE:CA	1:85:A:ILE:C	3	6.14
(1,66)	1:59:A:VAL:C	1:60:A:TYR:N	1:60:A:TYR:CA	1:60:A:TYR:C	7	6.14
(1,172)	1:129:A:ASP:C	1:130:A:ARG:N	1:130:A:ARG:CA	1:130:A:ARG:C	8	6.13
(1,99)	1:77:A:LEU:C	1:78:A:PHE:N	1:78:A:PHE:CA	1:78:A:PHE:C	11	6.12
(1,54)	1:49:A:ILE:C	1:50:A:GLU:N	1:50:A:GLU:CA	1:50:A:GLU:C	1	6.12
(1,156)	1:121:A:GLU:C	1:122:A:ARG:N	1:122:A:ARG:CA	1:122:A:ARG:C	18	6.09
(1,140)	1:106:A:GLU:C	1:107:A:ALA:N	1:107:A:ALA:CA	1:107:A:ALA:C	15	6.07
(1,20)	1:28:A:ASP:C	1:29:A:ARG:N	1:29:A:ARG:CA	1:29:A:ARG:C	3	6.06
(1,186)	1:140:A:ALA:C	1:141:A:LEU:N	1:141:A:LEU:CA	1:141:A:LEU:C	16	6.03
(1,133)	1:101:A:ALA:C	1:102:A:ASP:N	1:102:A:ASP:CA	1:102:A:ASP:C	2	6.03
(1,64)	1:58:A:ILE:C	1:59:A:VAL:N	1:59:A:VAL:CA	1:59:A:VAL:C	13	6.01
(1,60)	1:56:A:SER:C	1:57:A:THR:N	1:57:A:THR:CA	1:57:A:THR:C	7	6.0
(1,144)	1:108:A:ALA:C	1:109:A:ALA:N	1:109:A:ALA:CA	1:109:A:ALA:C	8	5.97
(1,26)	1:31:A:PHE:C	1:32:A:GLN:N	1:32:A:GLN:CA	1:32:A:GLN:C	20	5.97
(1,82)	1:67:A:ARG:C	1:68:A:ARG:N	1:68:A:ARG:CA	1:68:A:ARG:C	10	5.96
(1,129)	1:99:A:SER:C	1:100:A:PHE:N	1:100:A:PHE:CA	1:100:A:PHE:C	13	5.92
(1,36)	1:40:A:SER:C	1:41:A:ILE:N	1:41:A:ILE:CA	1:41:A:ILE:C	8	5.91
(1,162)	1:124:A:PHE:C	1:125:A:LYS:N	1:125:A:LYS:CA	1:125:A:LYS:C	5	5.88
(1,142)	1:107:A:ALA:C	1:108:A:ALA:N	1:108:A:ALA:CA	1:108:A:ALA:C	1	5.87
(1,36)	1:40:A:SER:C	1:41:A:ILE:N	1:41:A:ILE:CA	1:41:A:ILE:C	1	5.87
(1,111)	1:83:A:ASP:C	1:84:A:VAL:N	1:84:A:VAL:CA	1:84:A:VAL:C	17	5.86
(1,74)	1:63:A:MET:C	1:64:A:LYS:N	1:64:A:LYS:CA	1:64:A:LYS:C	8	5.85
(1,99)	1:77:A:LEU:C	1:78:A:PHE:N	1:78:A:PHE:CA	1:78:A:PHE:C	18	5.84
(1,72)	1:62:A:TRP:C	1:63:A:MET:N	1:63:A:MET:CA	1:63:A:MET:C	13	5.83
(1,52)	1:48:A:CYS:C	1:49:A:ILE:N	1:49:A:ILE:CA	1:49:A:ILE:C	2	5.81
(1,140)	1:106:A:GLU:C	1:107:A:ALA:N	1:107:A:ALA:CA	1:107:A:ALA:C	9	5.79
(1,93)	1:74:A:ARG:C	1:75:A:LEU:N	1:75:A:LEU:CA	1:75:A:LEU:C	6	5.78
(1,93)	1:74:A:ARG:C	1:75:A:LEU:N	1:75:A:LEU:CA	1:75:A:LEU:C	12	5.78
(1,24)	1:30:A:LYS:C	1:31:A:PHE:N	1:31:A:PHE:CA	1:31:A:PHE:C	1	5.78
(1,14)	1:25:A:SER:C	1:26:A:SER:N	1:26:A:SER:CA	1:26:A:SER:C	12	5.77
(1,140)	1:106:A:GLU:C	1:107:A:ALA:N	1:107:A:ALA:CA	1:107:A:ALA:C	10	5.76
(1,109)	1:82:A:ASN:C	1:83:A:ASP:N	1:83:A:ASP:CA	1:83:A:ASP:C	13	5.72
(1,162)	1:124:A:PHE:C	1:125:A:LYS:N	1:125:A:LYS:CA	1:125:A:LYS:C	18	5.67
(1,66)	1:59:A:VAL:C	1:60:A:TYR:N	1:60:A:TYR:CA	1:60:A:TYR:C	4	5.67
(1,89)	1:72:A:PRO:C	1:73:A:HIS:N	1:73:A:HIS:CA	1:73:A:HIS:C	13	5.66
(1,22)	1:29:A:ARG:C	1:30:A:LYS:N	1:30:A:LYS:CA	1:30:A:LYS:C	6	5.66
(1,133)	1:101:A:ALA:C	1:102:A:ASP:N	1:102:A:ASP:CA	1:102:A:ASP:C	7	5.65
(1,38)	1:41:A:ILE:C	1:42:A:GLN:N	1:42:A:GLN:CA	1:42:A:GLN:C	5	5.62
(1,42)	1:43:A:GLY:C	1:44:A:LEU:N	1:44:A:LEU:CA	1:44:A:LEU:C	7	5.61
(1,127)	1:98:A:GLU:C	1:99:A:SER:N	1:99:A:SER:CA	1:99:A:SER:C	4	5.6
(1,97)	1:76:A:ASN:C	1:77:A:LEU:N	1:77:A:LEU:CA	1:77:A:LEU:C	12	5.59
(1,125)	1:97:A:ARG:C	1:98:A:GLU:N	1:98:A:GLU:CA	1:98:A:GLU:C	15	5.57
(1,192)	1:143:A:GLU:C	1:144:A:ALA:N	1:144:A:ALA:CA	1:144:A:ALA:C	8	5.56
(1,64)	1:58:A:ILE:C	1:59:A:VAL:N	1:59:A:VAL:CA	1:59:A:VAL:C	2	5.56
(1,129)	1:99:A:SER:C	1:100:A:PHE:N	1:100:A:PHE:CA	1:100:A:PHE:C	7	5.54
(1,117)	1:86:A:GLN:C	1:87:A:ASN:N	1:87:A:ASN:CA	1:87:A:ASN:C	18	5.54
(1,111)	1:83:A:ASP:C	1:84:A:VAL:N	1:84:A:VAL:CA	1:84:A:VAL:C	7	5.54
(1,164)	1:125:A:LYS:C	1:126:A:ILE:N	1:126:A:ILE:CA	1:126:A:ILE:C	8	5.5
(1,105)	1:80:A:LEU:C	1:81:A:ALA:N	1:81:A:ALA:CA	1:81:A:ALA:C	18	5.5
(1,12)	1:24:A:GLU:C	1:25:A:SER:N	1:25:A:SER:CA	1:25:A:SER:C	8	5.5

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,22)	1:29:A:ARG:C	1:30:A:LYS:N	1:30:A:LYS:CA	1:30:A:LYS:C	9	5.48
(1,172)	1:129:A:ASP:C	1:130:A:ARG:N	1:130:A:ARG:CA	1:130:A:ARG:C	6	5.45
(1,168)	1:127:A:TRP:C	1:128:A:GLU:N	1:128:A:GLU:CA	1:128:A:GLU:C	5	5.45
(1,12)	1:24:A:GLU:C	1:25:A:SER:N	1:25:A:SER:CA	1:25:A:SER:C	14	5.45
(1,64)	1:58:A:ILE:C	1:59:A:VAL:N	1:59:A:VAL:CA	1:59:A:VAL:C	1	5.43
(1,84)	1:68:A:ARG:C	1:69:A:SER:N	1:69:A:SER:CA	1:69:A:SER:C	17	5.42
(1,76)	1:64:A:LYS:C	1:65:A:TRP:N	1:65:A:TRP:CA	1:65:A:TRP:C	19	5.42
(1,173)	1:130:A:ARG:N	1:130:A:ARG:CA	1:130:A:ARG:C	1:131:A:ASN:N	4	5.41
(1,60)	1:56:A:SER:C	1:57:A:THR:N	1:57:A:THR:CA	1:57:A:THR:C	4	5.39
(1,89)	1:72:A:PRO:C	1:73:A:HIS:N	1:73:A:HIS:CA	1:73:A:HIS:C	12	5.38
(1,84)	1:68:A:ARG:C	1:69:A:SER:N	1:69:A:SER:CA	1:69:A:SER:C	12	5.38
(1,20)	1:28:A:ASP:C	1:29:A:ARG:N	1:29:A:ARG:CA	1:29:A:ARG:C	11	5.37
(1,89)	1:72:A:PRO:C	1:73:A:HIS:N	1:73:A:HIS:CA	1:73:A:HIS:C	5	5.36
(1,18)	1:27:A:LEU:C	1:28:A:ASP:N	1:28:A:ASP:CA	1:28:A:ASP:C	1	5.34
(1,44)	1:44:A:LEU:C	1:45:A:SER:N	1:45:A:SER:CA	1:45:A:SER:C	20	5.31
(1,64)	1:58:A:ILE:C	1:59:A:VAL:N	1:59:A:VAL:CA	1:59:A:VAL:C	12	5.29
(1,6)	1:21:A:GLY:C	1:22:A:ALA:N	1:22:A:ALA:CA	1:22:A:ALA:C	7	5.28
(1,190)	1:142:A:ARG:C	1:143:A:GLU:N	1:143:A:GLU:CA	1:143:A:GLU:C	15	5.26
(1,158)	1:122:A:ARG:C	1:123:A:ILE:N	1:123:A:ILE:CA	1:123:A:ILE:C	8	5.26
(1,90)	1:73:A:HIS:N	1:73:A:HIS:CA	1:73:A:HIS:C	1:74:A:ARG:N	15	5.26
(1,72)	1:62:A:TRP:C	1:63:A:MET:N	1:63:A:MET:CA	1:63:A:MET:C	8	5.26
(1,123)	1:96:A:PHE:C	1:97:A:ARG:N	1:97:A:ARG:CA	1:97:A:ARG:C	7	5.23
(1,117)	1:86:A:GLN:C	1:87:A:ASN:N	1:87:A:ASN:CA	1:87:A:ASN:C	7	5.22
(1,99)	1:77:A:LEU:C	1:78:A:PHE:N	1:78:A:PHE:CA	1:78:A:PHE:C	10	5.22
(1,133)	1:101:A:ALA:C	1:102:A:ASP:N	1:102:A:ASP:CA	1:102:A:ASP:C	8	5.17
(1,111)	1:83:A:ASP:C	1:84:A:VAL:N	1:84:A:VAL:CA	1:84:A:VAL:C	16	5.17
(1,26)	1:31:A:PHE:C	1:32:A:GLN:N	1:32:A:GLN:CA	1:32:A:GLN:C	2	5.17
(1,164)	1:125:A:LYS:C	1:126:A:ILE:N	1:126:A:ILE:CA	1:126:A:ILE:C	7	5.15
(1,176)	1:135:A:GLU:C	1:136:A:GLU:N	1:136:A:GLU:CA	1:136:A:GLU:C	1	5.12
(1,156)	1:121:A:GLU:C	1:122:A:ARG:N	1:122:A:ARG:CA	1:122:A:ARG:C	7	5.12
(1,144)	1:108:A:ALA:C	1:109:A:ALA:N	1:109:A:ALA:CA	1:109:A:ALA:C	20	5.12
(1,142)	1:107:A:ALA:C	1:108:A:ALA:N	1:108:A:ALA:CA	1:108:A:ALA:C	13	5.12
(1,89)	1:72:A:PRO:C	1:73:A:HIS:N	1:73:A:HIS:CA	1:73:A:HIS:C	17	5.11
(1,26)	1:31:A:PHE:C	1:32:A:GLN:N	1:32:A:GLN:CA	1:32:A:GLN:C	10	5.11
(1,173)	1:130:A:ARG:N	1:130:A:ARG:CA	1:130:A:ARG:C	1:131:A:ASN:N	2	5.1
(1,97)	1:76:A:ASN:C	1:77:A:LEU:N	1:77:A:LEU:CA	1:77:A:LEU:C	19	5.1
(1,89)	1:72:A:PRO:C	1:73:A:HIS:N	1:73:A:HIS:CA	1:73:A:HIS:C	16	5.09
(1,46)	1:45:A:SER:C	1:46:A:SER:N	1:46:A:SER:CA	1:46:A:SER:C	6	5.09
(1,10)	1:23:A:LEU:C	1:24:A:GLU:N	1:24:A:GLU:CA	1:24:A:GLU:C	14	5.09
(1,172)	1:129:A:ASP:C	1:130:A:ARG:N	1:130:A:ARG:CA	1:130:A:ARG:C	11	5.08
(1,105)	1:80:A:LEU:C	1:81:A:ALA:N	1:81:A:ALA:CA	1:81:A:ALA:C	11	5.08
(1,170)	1:128:A:GLU:C	1:129:A:ASP:N	1:129:A:ASP:CA	1:129:A:ASP:C	18	5.07
(1,162)	1:124:A:PHE:C	1:125:A:LYS:N	1:125:A:LYS:CA	1:125:A:LYS:C	1	5.05
(1,156)	1:121:A:GLU:C	1:122:A:ARG:N	1:122:A:ARG:CA	1:122:A:ARG:C	15	5.05
(1,156)	1:121:A:GLU:C	1:122:A:ARG:N	1:122:A:ARG:CA	1:122:A:ARG:C	4	5.03
(1,28)	1:32:A:GLN:C	1:33:A:SER:N	1:33:A:SER:CA	1:33:A:SER:C	15	5.03
(1,152)	1:119:A:SER:C	1:120:A:VAL:N	1:120:A:VAL:CA	1:120:A:VAL:C	3	5.02
(1,95)	1:75:A:LEU:C	1:76:A:ASN:N	1:76:A:ASN:CA	1:76:A:ASN:C	14	5.02
(1,192)	1:143:A:GLU:C	1:144:A:ALA:N	1:144:A:ALA:CA	1:144:A:ALA:C	10	5.0
(1,103)	1:79:A:TYR:C	1:80:A:LEU:N	1:80:A:LEU:CA	1:80:A:LEU:C	20	5.0
(1,82)	1:67:A:ARG:C	1:68:A:ARG:N	1:68:A:ARG:CA	1:68:A:ARG:C	18	4.99

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,166)	1:126:A:ILE:C	1:127:A:TRP:N	1:127:A:TRP:CA	1:127:A:TRP:C	13	4.98
(1,60)	1:56:A:SER:C	1:57:A:THR:N	1:57:A:THR:CA	1:57:A:THR:C	14	4.96
(1,113)	1:84:A:VAL:C	1:85:A:ILE:N	1:85:A:ILE:CA	1:85:A:ILE:C	12	4.95
(1,95)	1:75:A:LEU:C	1:76:A:ASN:N	1:76:A:ASN:CA	1:76:A:ASN:C	12	4.95
(1,42)	1:43:A:GLY:C	1:44:A:LEU:N	1:44:A:LEU:CA	1:44:A:LEU:C	20	4.95
(1,162)	1:124:A:PHE:C	1:125:A:LYS:N	1:125:A:LYS:CA	1:125:A:LYS:C	16	4.94
(1,138)	1:105:A:PRO:C	1:106:A:GLU:N	1:106:A:GLU:CA	1:106:A:GLU:C	6	4.94
(1,109)	1:82:A:ASN:C	1:83:A:ASP:N	1:83:A:ASP:CA	1:83:A:ASP:C	17	4.93
(1,76)	1:64:A:LYS:C	1:65:A:TRP:N	1:65:A:TRP:CA	1:65:A:TRP:C	9	4.93
(1,190)	1:142:A:ARG:C	1:143:A:GLU:N	1:143:A:GLU:CA	1:143:A:GLU:C	1	4.92
(1,46)	1:45:A:SER:C	1:46:A:SER:N	1:46:A:SER:CA	1:46:A:SER:C	8	4.92
(1,113)	1:84:A:VAL:C	1:85:A:ILE:N	1:85:A:ILE:CA	1:85:A:ILE:C	8	4.91
(1,117)	1:86:A:GLN:C	1:87:A:ASN:N	1:87:A:ASN:CA	1:87:A:ASN:C	8	4.9
(1,168)	1:127:A:TRP:C	1:128:A:GLU:N	1:128:A:GLU:CA	1:128:A:GLU:C	15	4.89
(1,26)	1:31:A:PHE:C	1:32:A:GLN:N	1:32:A:GLN:CA	1:32:A:GLN:C	14	4.88
(1,144)	1:108:A:ALA:C	1:109:A:ALA:N	1:109:A:ALA:CA	1:109:A:ALA:C	7	4.87
(1,117)	1:86:A:GLN:C	1:87:A:ASN:N	1:87:A:ASN:CA	1:87:A:ASN:C	5	4.87
(1,113)	1:84:A:VAL:C	1:85:A:ILE:N	1:85:A:ILE:CA	1:85:A:ILE:C	11	4.87
(1,164)	1:125:A:LYS:C	1:126:A:ILE:N	1:126:A:ILE:CA	1:126:A:ILE:C	3	4.86
(1,113)	1:84:A:VAL:C	1:85:A:ILE:N	1:85:A:ILE:CA	1:85:A:ILE:C	19	4.86
(1,89)	1:72:A:PRO:C	1:73:A:HIS:N	1:73:A:HIS:CA	1:73:A:HIS:C	2	4.82
(1,164)	1:125:A:LYS:C	1:126:A:ILE:N	1:126:A:ILE:CA	1:126:A:ILE:C	9	4.81
(1,125)	1:97:A:ARG:C	1:98:A:GLU:N	1:98:A:GLU:CA	1:98:A:GLU:C	3	4.81
(1,103)	1:79:A:TYR:C	1:80:A:LEU:N	1:80:A:LEU:CA	1:80:A:LEU:C	9	4.81
(1,74)	1:63:A:MET:C	1:64:A:LYS:N	1:64:A:LYS:CA	1:64:A:LYS:C	7	4.8
(1,58)	1:55:A:HIS:C	1:56:A:SER:N	1:56:A:SER:CA	1:56:A:SER:C	15	4.8
(1,170)	1:128:A:GLU:C	1:129:A:ASP:N	1:129:A:ASP:CA	1:129:A:ASP:C	11	4.78
(1,66)	1:59:A:VAL:C	1:60:A:TYR:N	1:60:A:TYR:CA	1:60:A:TYR:C	3	4.78
(1,6)	1:21:A:GLY:C	1:22:A:ALA:N	1:22:A:ALA:CA	1:22:A:ALA:C	6	4.78
(1,68)	1:60:A:TYR:C	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	14	4.77
(1,194)	1:144:A:ALA:C	1:145:A:LEU:N	1:145:A:LEU:CA	1:145:A:LEU:C	15	4.76
(1,160)	1:123:A:ILE:C	1:124:A:PHE:N	1:124:A:PHE:CA	1:124:A:PHE:C	3	4.76
(1,60)	1:56:A:SER:C	1:57:A:THR:N	1:57:A:THR:CA	1:57:A:THR:C	16	4.76
(1,52)	1:48:A:CYS:C	1:49:A:ILE:N	1:49:A:ILE:CA	1:49:A:ILE:C	15	4.76
(1,12)	1:24:A:GLU:C	1:25:A:SER:N	1:25:A:SER:CA	1:25:A:SER:C	19	4.75
(1,62)	1:57:A:THR:C	1:58:A:ILE:N	1:58:A:ILE:CA	1:58:A:ILE:C	3	4.74
(1,148)	1:117:A:SER:C	1:118:A:LYS:N	1:118:A:LYS:CA	1:118:A:LYS:C	20	4.73
(1,46)	1:45:A:SER:C	1:46:A:SER:N	1:46:A:SER:CA	1:46:A:SER:C	12	4.72
(1,144)	1:108:A:ALA:C	1:109:A:ALA:N	1:109:A:ALA:CA	1:109:A:ALA:C	2	4.71
(1,138)	1:105:A:PRO:C	1:106:A:GLU:N	1:106:A:GLU:CA	1:106:A:GLU:C	12	4.71
(1,12)	1:24:A:GLU:C	1:25:A:SER:N	1:25:A:SER:CA	1:25:A:SER:C	15	4.7
(1,166)	1:126:A:ILE:C	1:127:A:TRP:N	1:127:A:TRP:CA	1:127:A:TRP:C	9	4.69
(1,156)	1:121:A:GLU:C	1:122:A:ARG:N	1:122:A:ARG:CA	1:122:A:ARG:C	14	4.69
(1,14)	1:25:A:SER:C	1:26:A:SER:N	1:26:A:SER:CA	1:26:A:SER:C	14	4.69
(1,24)	1:30:A:LYS:C	1:31:A:PHE:N	1:31:A:PHE:CA	1:31:A:PHE:C	18	4.68
(1,99)	1:77:A:LEU:C	1:78:A:PHE:N	1:78:A:PHE:CA	1:78:A:PHE:C	4	4.67
(1,186)	1:140:A:ALA:C	1:141:A:LEU:N	1:141:A:LEU:CA	1:141:A:LEU:C	10	4.66
(1,142)	1:107:A:ALA:C	1:108:A:ALA:N	1:108:A:ALA:CA	1:108:A:ALA:C	4	4.66
(1,138)	1:105:A:PRO:C	1:106:A:GLU:N	1:106:A:GLU:CA	1:106:A:GLU:C	1	4.66
(1,62)	1:57:A:THR:C	1:58:A:ILE:N	1:58:A:ILE:CA	1:58:A:ILE:C	7	4.66
(1,95)	1:75:A:LEU:C	1:76:A:ASN:N	1:76:A:ASN:CA	1:76:A:ASN:C	13	4.65

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,89)	1:72:A:PRO:C	1:73:A:HIS:N	1:73:A:HIS:CA	1:73:A:HIS:C	11	4.65
(1,70)	1:61:A:HIS:C	1:62:A:TRP:N	1:62:A:TRP:CA	1:62:A:TRP:C	16	4.64
(1,140)	1:106:A:GLU:C	1:107:A:ALA:N	1:107:A:ALA:CA	1:107:A:ALA:C	19	4.63
(1,68)	1:60:A:TYR:C	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	2	4.63
(1,99)	1:77:A:LEU:C	1:78:A:PHE:N	1:78:A:PHE:CA	1:78:A:PHE:C	13	4.62
(1,78)	1:65:A:TRP:C	1:66:A:LEU:N	1:66:A:LEU:CA	1:66:A:LEU:C	4	4.61
(1,14)	1:25:A:SER:C	1:26:A:SER:N	1:26:A:SER:CA	1:26:A:SER:C	20	4.61
(1,129)	1:99:A:SER:C	1:100:A:PHE:N	1:100:A:PHE:CA	1:100:A:PHE:C	19	4.57
(1,78)	1:65:A:TRP:C	1:66:A:LEU:N	1:66:A:LEU:CA	1:66:A:LEU:C	16	4.57
(1,127)	1:98:A:GLU:C	1:99:A:SER:N	1:99:A:SER:CA	1:99:A:SER:C	18	4.56
(1,28)	1:32:A:GLN:C	1:33:A:SER:N	1:33:A:SER:CA	1:33:A:SER:C	3	4.56
(1,162)	1:124:A:PHE:C	1:125:A:LYS:N	1:125:A:LYS:CA	1:125:A:LYS:C	15	4.54
(1,144)	1:108:A:ALA:C	1:109:A:ALA:N	1:109:A:ALA:CA	1:109:A:ALA:C	5	4.54
(1,194)	1:144:A:ALA:C	1:145:A:LEU:N	1:145:A:LEU:CA	1:145:A:LEU:C	6	4.53
(1,78)	1:65:A:TRP:C	1:66:A:LEU:N	1:66:A:LEU:CA	1:66:A:LEU:C	11	4.53
(1,60)	1:56:A:SER:C	1:57:A:THR:N	1:57:A:THR:CA	1:57:A:THR:C	12	4.53
(1,138)	1:105:A:PRO:C	1:106:A:GLU:N	1:106:A:GLU:CA	1:106:A:GLU:C	5	4.51
(1,127)	1:98:A:GLU:C	1:99:A:SER:N	1:99:A:SER:CA	1:99:A:SER:C	1	4.51
(1,117)	1:86:A:GLN:C	1:87:A:ASN:N	1:87:A:ASN:CA	1:87:A:ASN:C	9	4.49
(1,160)	1:123:A:ILE:C	1:124:A:PHE:N	1:124:A:PHE:CA	1:124:A:PHE:C	16	4.47
(1,160)	1:123:A:ILE:C	1:124:A:PHE:N	1:124:A:PHE:CA	1:124:A:PHE:C	17	4.46
(1,22)	1:29:A:ARG:C	1:30:A:LYS:N	1:30:A:LYS:CA	1:30:A:LYS:C	10	4.46
(1,164)	1:125:A:LYS:C	1:126:A:ILE:N	1:126:A:ILE:CA	1:126:A:ILE:C	15	4.45
(1,24)	1:30:A:LYS:C	1:31:A:PHE:N	1:31:A:PHE:CA	1:31:A:PHE:C	16	4.45
(1,164)	1:125:A:LYS:C	1:126:A:ILE:N	1:126:A:ILE:CA	1:126:A:ILE:C	5	4.43
(1,6)	1:21:A:GLY:C	1:22:A:ALA:N	1:22:A:ALA:CA	1:22:A:ALA:C	5	4.43
(1,138)	1:105:A:PRO:C	1:106:A:GLU:N	1:106:A:GLU:CA	1:106:A:GLU:C	9	4.41
(1,192)	1:143:A:GLU:C	1:144:A:ALA:N	1:144:A:ALA:CA	1:144:A:ALA:C	12	4.4
(1,78)	1:65:A:TRP:C	1:66:A:LEU:N	1:66:A:LEU:CA	1:66:A:LEU:C	15	4.4
(1,29)	1:33:A:SER:N	1:33:A:SER:CA	1:33:A:SER:C	1:34:A:VAL:N	11	4.4
(1,16)	1:26:A:SER:C	1:27:A:LEU:N	1:27:A:LEU:CA	1:27:A:LEU:C	14	4.4
(1,160)	1:123:A:ILE:C	1:124:A:PHE:N	1:124:A:PHE:CA	1:124:A:PHE:C	9	4.38
(1,82)	1:67:A:ARG:C	1:68:A:ARG:N	1:68:A:ARG:CA	1:68:A:ARG:C	9	4.38
(1,12)	1:24:A:GLU:C	1:25:A:SER:N	1:25:A:SER:CA	1:25:A:SER:C	2	4.38
(1,190)	1:142:A:ARG:C	1:143:A:GLU:N	1:143:A:GLU:CA	1:143:A:GLU:C	6	4.35
(1,103)	1:79:A:TYR:C	1:80:A:LEU:N	1:80:A:LEU:CA	1:80:A:LEU:C	8	4.35
(1,160)	1:123:A:ILE:C	1:124:A:PHE:N	1:124:A:PHE:CA	1:124:A:PHE:C	2	4.34
(1,156)	1:121:A:GLU:C	1:122:A:ARG:N	1:122:A:ARG:CA	1:122:A:ARG:C	20	4.34
(1,111)	1:83:A:ASP:C	1:84:A:VAL:N	1:84:A:VAL:CA	1:84:A:VAL:C	6	4.34
(1,109)	1:82:A:ASN:C	1:83:A:ASP:N	1:83:A:ASP:CA	1:83:A:ASP:C	6	4.34
(1,144)	1:108:A:ALA:C	1:109:A:ALA:N	1:109:A:ALA:CA	1:109:A:ALA:C	6	4.32
(1,36)	1:40:A:SER:C	1:41:A:ILE:N	1:41:A:ILE:CA	1:41:A:ILE:C	13	4.32
(1,18)	1:27:A:LEU:C	1:28:A:ASP:N	1:28:A:ASP:CA	1:28:A:ASP:C	14	4.32
(1,97)	1:76:A:ASN:C	1:77:A:LEU:N	1:77:A:LEU:CA	1:77:A:LEU:C	17	4.28
(1,46)	1:45:A:SER:C	1:46:A:SER:N	1:46:A:SER:CA	1:46:A:SER:C	7	4.28
(1,123)	1:96:A:PHE:C	1:97:A:ARG:N	1:97:A:ARG:CA	1:97:A:ARG:C	4	4.26
(1,38)	1:41:A:ILE:C	1:42:A:GLN:N	1:42:A:GLN:CA	1:42:A:GLN:C	2	4.25
(1,28)	1:32:A:GLN:C	1:33:A:SER:N	1:33:A:SER:CA	1:33:A:SER:C	5	4.25
(1,54)	1:49:A:ILE:C	1:50:A:GLU:N	1:50:A:GLU:CA	1:50:A:GLU:C	9	4.23
(1,20)	1:28:A:ASP:C	1:29:A:ARG:N	1:29:A:ARG:CA	1:29:A:ARG:C	13	4.23
(1,166)	1:126:A:ILE:C	1:127:A:TRP:N	1:127:A:TRP:CA	1:127:A:TRP:C	15	4.2

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,194)	1:144:A:ALA:C	1:145:A:LEU:N	1:145:A:LEU:CA	1:145:A:LEU:C	10	4.19
(1,160)	1:123:A:ILE:C	1:124:A:PHE:N	1:124:A:PHE:CA	1:124:A:PHE:C	7	4.19
(1,60)	1:56:A:SER:C	1:57:A:THR:N	1:57:A:THR:CA	1:57:A:THR:C	13	4.18
(1,192)	1:143:A:GLU:C	1:144:A:ALA:N	1:144:A:ALA:CA	1:144:A:ALA:C	2	4.17
(1,91)	1:73:A:HIS:C	1:74:A:ARG:N	1:74:A:ARG:CA	1:74:A:ARG:C	2	4.16
(1,74)	1:63:A:MET:C	1:64:A:LYS:N	1:64:A:LYS:CA	1:64:A:LYS:C	18	4.16
(1,156)	1:121:A:GLU:C	1:122:A:ARG:N	1:122:A:ARG:CA	1:122:A:ARG:C	1	4.15
(1,170)	1:128:A:GLU:C	1:129:A:ASP:N	1:129:A:ASP:CA	1:129:A:ASP:C	13	4.14
(1,60)	1:56:A:SER:C	1:57:A:THR:N	1:57:A:THR:CA	1:57:A:THR:C	6	4.14
(1,6)	1:21:A:GLY:C	1:22:A:ALA:N	1:22:A:ALA:CA	1:22:A:ALA:C	15	4.13
(1,113)	1:84:A:VAL:C	1:85:A:ILE:N	1:85:A:ILE:CA	1:85:A:ILE:C	9	4.12
(1,111)	1:83:A:ASP:C	1:84:A:VAL:N	1:84:A:VAL:CA	1:84:A:VAL:C	20	4.12
(1,97)	1:76:A:ASN:C	1:77:A:LEU:N	1:77:A:LEU:CA	1:77:A:LEU:C	8	4.12
(1,164)	1:125:A:LYS:C	1:126:A:ILE:N	1:126:A:ILE:CA	1:126:A:ILE:C	16	4.1
(1,113)	1:84:A:VAL:C	1:85:A:ILE:N	1:85:A:ILE:CA	1:85:A:ILE:C	16	4.09
(1,172)	1:129:A:ASP:C	1:130:A:ARG:N	1:130:A:ARG:CA	1:130:A:ARG:C	9	4.07
(1,156)	1:121:A:GLU:C	1:122:A:ARG:N	1:122:A:ARG:CA	1:122:A:ARG:C	2	4.07
(1,22)	1:29:A:ARG:C	1:30:A:LYS:N	1:30:A:LYS:CA	1:30:A:LYS:C	7	4.06
(1,168)	1:127:A:TRP:C	1:128:A:GLU:N	1:128:A:GLU:CA	1:128:A:GLU:C	20	4.05
(1,89)	1:72:A:PRO:C	1:73:A:HIS:N	1:73:A:HIS:CA	1:73:A:HIS:C	20	4.05
(1,190)	1:142:A:ARG:C	1:143:A:GLU:N	1:143:A:GLU:CA	1:143:A:GLU:C	8	4.04
(1,144)	1:108:A:ALA:C	1:109:A:ALA:N	1:109:A:ALA:CA	1:109:A:ALA:C	18	4.04
(1,16)	1:26:A:SER:C	1:27:A:LEU:N	1:27:A:LEU:CA	1:27:A:LEU:C	18	4.03
(1,103)	1:79:A:TYR:C	1:80:A:LEU:N	1:80:A:LEU:CA	1:80:A:LEU:C	5	4.02
(1,26)	1:31:A:PHE:C	1:32:A:GLN:N	1:32:A:GLN:CA	1:32:A:GLN:C	8	4.02
(1,156)	1:121:A:GLU:C	1:122:A:ARG:N	1:122:A:ARG:CA	1:122:A:ARG:C	10	4.0
(1,62)	1:57:A:THR:C	1:58:A:ILE:N	1:58:A:ILE:CA	1:58:A:ILE:C	20	3.97
(1,16)	1:26:A:SER:C	1:27:A:LEU:N	1:27:A:LEU:CA	1:27:A:LEU:C	17	3.97
(1,46)	1:45:A:SER:C	1:46:A:SER:N	1:46:A:SER:CA	1:46:A:SER:C	17	3.95
(1,113)	1:84:A:VAL:C	1:85:A:ILE:N	1:85:A:ILE:CA	1:85:A:ILE:C	7	3.93
(1,28)	1:32:A:GLN:C	1:33:A:SER:N	1:33:A:SER:CA	1:33:A:SER:C	7	3.93
(1,168)	1:127:A:TRP:C	1:128:A:GLU:N	1:128:A:GLU:CA	1:128:A:GLU:C	2	3.92
(1,113)	1:84:A:VAL:C	1:85:A:ILE:N	1:85:A:ILE:CA	1:85:A:ILE:C	20	3.92
(1,105)	1:80:A:LEU:C	1:81:A:ALA:N	1:81:A:ALA:CA	1:81:A:ALA:C	16	3.92
(1,160)	1:123:A:ILE:C	1:124:A:PHE:N	1:124:A:PHE:CA	1:124:A:PHE:C	18	3.9
(1,156)	1:121:A:GLU:C	1:122:A:ARG:N	1:122:A:ARG:CA	1:122:A:ARG:C	17	3.9
(1,113)	1:84:A:VAL:C	1:85:A:ILE:N	1:85:A:ILE:CA	1:85:A:ILE:C	1	3.9
(1,168)	1:127:A:TRP:C	1:128:A:GLU:N	1:128:A:GLU:CA	1:128:A:GLU:C	18	3.88
(1,123)	1:96:A:PHE:C	1:97:A:ARG:N	1:97:A:ARG:CA	1:97:A:ARG:C	12	3.88
(1,111)	1:83:A:ASP:C	1:84:A:VAL:N	1:84:A:VAL:CA	1:84:A:VAL:C	4	3.88
(1,160)	1:123:A:ILE:C	1:124:A:PHE:N	1:124:A:PHE:CA	1:124:A:PHE:C	10	3.87
(1,186)	1:140:A:ALA:C	1:141:A:LEU:N	1:141:A:LEU:CA	1:141:A:LEU:C	14	3.85
(1,105)	1:80:A:LEU:C	1:81:A:ALA:N	1:81:A:ALA:CA	1:81:A:ALA:C	12	3.85
(1,24)	1:30:A:LYS:C	1:31:A:PHE:N	1:31:A:PHE:CA	1:31:A:PHE:C	12	3.85
(1,24)	1:30:A:LYS:C	1:31:A:PHE:N	1:31:A:PHE:CA	1:31:A:PHE:C	15	3.85
(1,18)	1:27:A:LEU:C	1:28:A:ASP:N	1:28:A:ASP:CA	1:28:A:ASP:C	12	3.85
(1,44)	1:44:A:LEU:C	1:45:A:SER:N	1:45:A:SER:CA	1:45:A:SER:C	12	3.84
(1,28)	1:32:A:GLN:C	1:33:A:SER:N	1:33:A:SER:CA	1:33:A:SER:C	16	3.83
(1,16)	1:26:A:SER:C	1:27:A:LEU:N	1:27:A:LEU:CA	1:27:A:LEU:C	11	3.83
(1,66)	1:59:A:VAL:C	1:60:A:TYR:N	1:60:A:TYR:CA	1:60:A:TYR:C	2	3.82
(1,58)	1:55:A:HIS:C	1:56:A:SER:N	1:56:A:SER:CA	1:56:A:SER:C	19	3.82

Continued on next page...

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,164)	1:125:A:LYS:C	1:126:A:ILE:N	1:126:A:ILE:CA	1:126:A:ILE:C	19	3.78
(1,62)	1:57:A:THR:C	1:58:A:ILE:N	1:58:A:ILE:CA	1:58:A:ILE:C	6	3.78
(1,194)	1:144:A:ALA:C	1:145:A:LEU:N	1:145:A:LEU:CA	1:145:A:LEU:C	4	3.77
(1,194)	1:144:A:ALA:C	1:145:A:LEU:N	1:145:A:LEU:CA	1:145:A:LEU:C	9	3.77
(1,156)	1:121:A:GLU:C	1:122:A:ARG:N	1:122:A:ARG:CA	1:122:A:ARG:C	9	3.77
(1,180)	1:137:A:MET:C	1:138:A:ILE:N	1:138:A:ILE:CA	1:138:A:ILE:C	10	3.76
(1,80)	1:66:A:LEU:C	1:67:A:ARG:N	1:67:A:ARG:CA	1:67:A:ARG:C	13	3.75
(1,152)	1:119:A:SER:C	1:120:A:VAL:N	1:120:A:VAL:CA	1:120:A:VAL:C	9	3.74
(1,125)	1:97:A:ARG:C	1:98:A:GLU:N	1:98:A:GLU:CA	1:98:A:GLU:C	19	3.73
(1,62)	1:57:A:THR:C	1:58:A:ILE:N	1:58:A:ILE:CA	1:58:A:ILE:C	1	3.73
(1,93)	1:74:A:ARG:C	1:75:A:LEU:N	1:75:A:LEU:CA	1:75:A:LEU:C	4	3.68
(1,152)	1:119:A:SER:C	1:120:A:VAL:N	1:120:A:VAL:CA	1:120:A:VAL:C	6	3.67
(1,80)	1:66:A:LEU:C	1:67:A:ARG:N	1:67:A:ARG:CA	1:67:A:ARG:C	9	3.67
(1,22)	1:29:A:ARG:C	1:30:A:LYS:N	1:30:A:LYS:CA	1:30:A:LYS:C	20	3.67
(1,99)	1:77:A:LEU:C	1:78:A:PHE:N	1:78:A:PHE:CA	1:78:A:PHE:C	6	3.65
(1,184)	1:139:A:VAL:C	1:140:A:ALA:N	1:140:A:ALA:CA	1:140:A:ALA:C	13	3.63
(1,156)	1:121:A:GLU:C	1:122:A:ARG:N	1:122:A:ARG:CA	1:122:A:ARG:C	5	3.63
(1,152)	1:119:A:SER:C	1:120:A:VAL:N	1:120:A:VAL:CA	1:120:A:VAL:C	7	3.63
(1,129)	1:99:A:SER:C	1:100:A:PHE:N	1:100:A:PHE:CA	1:100:A:PHE:C	12	3.63
(1,101)	1:78:A:PHE:C	1:79:A:TYR:N	1:79:A:TYR:CA	1:79:A:TYR:C	8	3.63
(1,32)	1:38:A:MET:C	1:39:A:GLU:N	1:39:A:GLU:CA	1:39:A:GLU:C	14	3.63
(1,138)	1:105:A:PRO:C	1:106:A:GLU:N	1:106:A:GLU:CA	1:106:A:GLU:C	16	3.62
(1,6)	1:21:A:GLY:C	1:22:A:ALA:N	1:22:A:ALA:CA	1:22:A:ALA:C	10	3.62
(1,99)	1:77:A:LEU:C	1:78:A:PHE:N	1:78:A:PHE:CA	1:78:A:PHE:C	19	3.6
(1,173)	1:130:A:ARG:N	1:130:A:ARG:CA	1:130:A:ARG:C	1:131:A:ASN:N	15	3.58
(1,168)	1:127:A:TRP:C	1:128:A:GLU:N	1:128:A:GLU:CA	1:128:A:GLU:C	13	3.58
(1,101)	1:78:A:PHE:C	1:79:A:TYR:N	1:79:A:TYR:CA	1:79:A:TYR:C	15	3.57
(1,78)	1:65:A:TRP:C	1:66:A:LEU:N	1:66:A:LEU:CA	1:66:A:LEU:C	17	3.56
(1,123)	1:96:A:PHE:C	1:97:A:ARG:N	1:97:A:ARG:CA	1:97:A:ARG:C	6	3.55
(1,82)	1:67:A:ARG:C	1:68:A:ARG:N	1:68:A:ARG:CA	1:68:A:ARG:C	3	3.55
(1,80)	1:66:A:LEU:C	1:67:A:ARG:N	1:67:A:ARG:CA	1:67:A:ARG:C	5	3.53
(1,105)	1:80:A:LEU:C	1:81:A:ALA:N	1:81:A:ALA:CA	1:81:A:ALA:C	20	3.52
(1,46)	1:45:A:SER:C	1:46:A:SER:N	1:46:A:SER:CA	1:46:A:SER:C	5	3.52
(1,28)	1:32:A:GLN:C	1:33:A:SER:N	1:33:A:SER:CA	1:33:A:SER:C	2	3.52
(1,60)	1:56:A:SER:C	1:57:A:THR:N	1:57:A:THR:CA	1:57:A:THR:C	20	3.5
(1,10)	1:23:A:LEU:C	1:24:A:GLU:N	1:24:A:GLU:CA	1:24:A:GLU:C	1	3.5
(1,68)	1:60:A:TYR:C	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	6	3.49
(1,121)	1:95:A:ILE:C	1:96:A:PHE:N	1:96:A:PHE:CA	1:96:A:PHE:C	6	3.48
(1,113)	1:84:A:VAL:C	1:85:A:ILE:N	1:85:A:ILE:CA	1:85:A:ILE:C	5	3.46
(1,32)	1:38:A:MET:C	1:39:A:GLU:N	1:39:A:GLU:CA	1:39:A:GLU:C	16	3.44
(1,192)	1:143:A:GLU:C	1:144:A:ALA:N	1:144:A:ALA:CA	1:144:A:ALA:C	17	3.43
(1,28)	1:32:A:GLN:C	1:33:A:SER:N	1:33:A:SER:CA	1:33:A:SER:C	4	3.43
(1,22)	1:29:A:ARG:C	1:30:A:LYS:N	1:30:A:LYS:CA	1:30:A:LYS:C	4	3.43
(1,186)	1:140:A:ALA:C	1:141:A:LEU:N	1:141:A:LEU:CA	1:141:A:LEU:C	1	3.42
(1,64)	1:58:A:ILE:C	1:59:A:VAL:N	1:59:A:VAL:CA	1:59:A:VAL:C	8	3.42
(1,156)	1:121:A:GLU:C	1:122:A:ARG:N	1:122:A:ARG:CA	1:122:A:ARG:C	12	3.41
(1,144)	1:108:A:ALA:C	1:109:A:ALA:N	1:109:A:ALA:CA	1:109:A:ALA:C	9	3.41
(1,101)	1:78:A:PHE:C	1:79:A:TYR:N	1:79:A:TYR:CA	1:79:A:TYR:C	9	3.41
(1,76)	1:64:A:LYS:C	1:65:A:TRP:N	1:65:A:TRP:CA	1:65:A:TRP:C	13	3.41
(1,18)	1:27:A:LEU:C	1:28:A:ASP:N	1:28:A:ASP:CA	1:28:A:ASP:C	2	3.41
(1,99)	1:77:A:LEU:C	1:78:A:PHE:N	1:78:A:PHE:CA	1:78:A:PHE:C	5	3.4

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,86)	1:70:A:ALA:C	1:71:A:TYR:N	1:71:A:TYR:CA	1:71:A:TYR:C	2	3.4
(1,182)	1:138:A:ILE:C	1:139:A:VAL:N	1:139:A:VAL:CA	1:139:A:VAL:C	4	3.38
(1,16)	1:26:A:SER:C	1:27:A:LEU:N	1:27:A:LEU:CA	1:27:A:LEU:C	10	3.38
(1,156)	1:121:A:GLU:C	1:122:A:ARG:N	1:122:A:ARG:CA	1:122:A:ARG:C	16	3.37
(1,138)	1:105:A:PRO:C	1:106:A:GLU:N	1:106:A:GLU:CA	1:106:A:GLU:C	14	3.37
(1,72)	1:62:A:TRP:C	1:63:A:MET:N	1:63:A:MET:CA	1:63:A:MET:C	2	3.37
(1,89)	1:72:A:PRO:C	1:73:A:HIS:N	1:73:A:HIS:CA	1:73:A:HIS:C	8	3.36
(1,164)	1:125:A:LYS:C	1:126:A:ILE:N	1:126:A:ILE:CA	1:126:A:ILE:C	2	3.35
(1,142)	1:107:A:ALA:C	1:108:A:ALA:N	1:108:A:ALA:CA	1:108:A:ALA:C	7	3.35
(1,62)	1:57:A:THR:C	1:58:A:ILE:N	1:58:A:ILE:CA	1:58:A:ILE:C	5	3.35
(1,38)	1:41:A:ILE:C	1:42:A:GLN:N	1:42:A:GLN:CA	1:42:A:GLN:C	20	3.33
(1,12)	1:24:A:GLU:C	1:25:A:SER:N	1:25:A:SER:CA	1:25:A:SER:C	6	3.33
(1,142)	1:107:A:ALA:C	1:108:A:ALA:N	1:108:A:ALA:CA	1:108:A:ALA:C	3	3.3
(1,36)	1:40:A:SER:C	1:41:A:ILE:N	1:41:A:ILE:CA	1:41:A:ILE:C	10	3.3
(1,182)	1:138:A:ILE:C	1:139:A:VAL:N	1:139:A:VAL:CA	1:139:A:VAL:C	14	3.29
(1,142)	1:107:A:ALA:C	1:108:A:ALA:N	1:108:A:ALA:CA	1:108:A:ALA:C	18	3.29
(1,95)	1:75:A:LEU:C	1:76:A:ASN:N	1:76:A:ASN:CA	1:76:A:ASN:C	8	3.29
(1,129)	1:99:A:SER:C	1:100:A:PHE:N	1:100:A:PHE:CA	1:100:A:PHE:C	10	3.28
(1,117)	1:86:A:GLN:C	1:87:A:ASN:N	1:87:A:ASN:CA	1:87:A:ASN:C	17	3.28
(1,38)	1:41:A:ILE:C	1:42:A:GLN:N	1:42:A:GLN:CA	1:42:A:GLN:C	7	3.28
(1,164)	1:125:A:LYS:C	1:126:A:ILE:N	1:126:A:ILE:CA	1:126:A:ILE:C	13	3.27
(1,101)	1:78:A:PHE:C	1:79:A:TYR:N	1:79:A:TYR:CA	1:79:A:TYR:C	5	3.27
(1,20)	1:28:A:ASP:C	1:29:A:ARG:N	1:29:A:ARG:CA	1:29:A:ARG:C	16	3.27
(1,99)	1:77:A:LEU:C	1:78:A:PHE:N	1:78:A:PHE:CA	1:78:A:PHE:C	15	3.26
(1,22)	1:29:A:ARG:C	1:30:A:LYS:N	1:30:A:LYS:CA	1:30:A:LYS:C	19	3.26
(1,18)	1:27:A:LEU:C	1:28:A:ASP:N	1:28:A:ASP:CA	1:28:A:ASP:C	8	3.25
(1,158)	1:122:A:ARG:C	1:123:A:ILE:N	1:123:A:ILE:CA	1:123:A:ILE:C	7	3.24
(1,95)	1:75:A:LEU:C	1:76:A:ASN:N	1:76:A:ASN:CA	1:76:A:ASN:C	19	3.24
(1,180)	1:137:A:MET:C	1:138:A:ILE:N	1:138:A:ILE:CA	1:138:A:ILE:C	3	3.21
(1,166)	1:126:A:ILE:C	1:127:A:TRP:N	1:127:A:TRP:CA	1:127:A:TRP:C	8	3.21
(1,105)	1:80:A:LEU:C	1:81:A:ALA:N	1:81:A:ALA:CA	1:81:A:ALA:C	1	3.21
(1,82)	1:67:A:ARG:C	1:68:A:ARG:N	1:68:A:ARG:CA	1:68:A:ARG:C	4	3.21
(1,46)	1:45:A:SER:C	1:46:A:SER:N	1:46:A:SER:CA	1:46:A:SER:C	20	3.21
(1,38)	1:41:A:ILE:C	1:42:A:GLN:N	1:42:A:GLN:CA	1:42:A:GLN:C	18	3.21
(1,173)	1:130:A:ARG:N	1:130:A:ARG:CA	1:130:A:ARG:C	1:131:A:ASN:N	19	3.18
(1,22)	1:29:A:ARG:C	1:30:A:LYS:N	1:30:A:LYS:CA	1:30:A:LYS:C	2	3.18
(1,32)	1:38:A:MET:C	1:39:A:GLU:N	1:39:A:GLU:CA	1:39:A:GLU:C	18	3.17
(1,64)	1:58:A:ILE:C	1:59:A:VAL:N	1:59:A:VAL:CA	1:59:A:VAL:C	20	3.15
(1,180)	1:137:A:MET:C	1:138:A:ILE:N	1:138:A:ILE:CA	1:138:A:ILE:C	13	3.13
(1,125)	1:97:A:ARG:C	1:98:A:GLU:N	1:98:A:GLU:CA	1:98:A:GLU:C	20	3.13
(1,138)	1:105:A:PRO:C	1:106:A:GLU:N	1:106:A:GLU:CA	1:106:A:GLU:C	11	3.12
(1,111)	1:83:A:ASP:C	1:84:A:VAL:N	1:84:A:VAL:CA	1:84:A:VAL:C	15	3.12
(1,10)	1:23:A:LEU:C	1:24:A:GLU:N	1:24:A:GLU:CA	1:24:A:GLU:C	5	3.12
(1,138)	1:105:A:PRO:C	1:106:A:GLU:N	1:106:A:GLU:CA	1:106:A:GLU:C	8	3.11
(1,109)	1:82:A:ASN:C	1:83:A:ASP:N	1:83:A:ASP:CA	1:83:A:ASP:C	2	3.11
(1,32)	1:38:A:MET:C	1:39:A:GLU:N	1:39:A:GLU:CA	1:39:A:GLU:C	9	3.11
(1,168)	1:127:A:TRP:C	1:128:A:GLU:N	1:128:A:GLU:CA	1:128:A:GLU:C	4	3.1
(1,192)	1:143:A:GLU:C	1:144:A:ALA:N	1:144:A:ALA:CA	1:144:A:ALA:C	4	3.09
(1,58)	1:55:A:HIS:C	1:56:A:SER:N	1:56:A:SER:CA	1:56:A:SER:C	13	3.07
(1,89)	1:72:A:PRO:C	1:73:A:HIS:N	1:73:A:HIS:CA	1:73:A:HIS:C	14	3.06
(1,89)	1:72:A:PRO:C	1:73:A:HIS:N	1:73:A:HIS:CA	1:73:A:HIS:C	15	3.06

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,160)	1:123:A:ILE:C	1:124:A:PHE:N	1:124:A:PHE:CA	1:124:A:PHE:C	14	3.05
(1,101)	1:78:A:PHE:C	1:79:A:TYR:N	1:79:A:TYR:CA	1:79:A:TYR:C	3	3.04
(1,101)	1:78:A:PHE:C	1:79:A:TYR:N	1:79:A:TYR:CA	1:79:A:TYR:C	10	3.03
(1,170)	1:128:A:GLU:C	1:129:A:ASP:N	1:129:A:ASP:CA	1:129:A:ASP:C	12	3.02
(1,68)	1:60:A:TYR:C	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	8	3.02
(1,127)	1:98:A:GLU:C	1:99:A:SER:N	1:99:A:SER:CA	1:99:A:SER:C	5	3.01
(1,184)	1:139:A:VAL:C	1:140:A:ALA:N	1:140:A:ALA:CA	1:140:A:ALA:C	16	2.99
(1,166)	1:126:A:ILE:C	1:127:A:TRP:N	1:127:A:TRP:CA	1:127:A:TRP:C	16	2.99
(1,95)	1:75:A:LEU:C	1:76:A:ASN:N	1:76:A:ASN:CA	1:76:A:ASN:C	5	2.99
(1,142)	1:107:A:ALA:C	1:108:A:ALA:N	1:108:A:ALA:CA	1:108:A:ALA:C	14	2.98
(1,93)	1:74:A:ARG:C	1:75:A:LEU:N	1:75:A:LEU:CA	1:75:A:LEU:C	8	2.97
(1,91)	1:73:A:HIS:C	1:74:A:ARG:N	1:74:A:ARG:CA	1:74:A:ARG:C	12	2.95
(1,66)	1:59:A:VAL:C	1:60:A:TYR:N	1:60:A:TYR:CA	1:60:A:TYR:C	1	2.95
(1,12)	1:24:A:GLU:C	1:25:A:SER:N	1:25:A:SER:CA	1:25:A:SER:C	12	2.95
(1,101)	1:78:A:PHE:C	1:79:A:TYR:N	1:79:A:TYR:CA	1:79:A:TYR:C	4	2.94
(1,182)	1:138:A:ILE:C	1:139:A:VAL:N	1:139:A:VAL:CA	1:139:A:VAL:C	15	2.92
(1,105)	1:80:A:LEU:C	1:81:A:ALA:N	1:81:A:ALA:CA	1:81:A:ALA:C	8	2.92
(1,97)	1:76:A:ASN:C	1:77:A:LEU:N	1:77:A:LEU:CA	1:77:A:LEU:C	13	2.91
(1,44)	1:44:A:LEU:C	1:45:A:SER:N	1:45:A:SER:CA	1:45:A:SER:C	15	2.91
(1,192)	1:143:A:GLU:C	1:144:A:ALA:N	1:144:A:ALA:CA	1:144:A:ALA:C	9	2.9
(1,144)	1:108:A:ALA:C	1:109:A:ALA:N	1:109:A:ALA:CA	1:109:A:ALA:C	1	2.9
(1,99)	1:77:A:LEU:C	1:78:A:PHE:N	1:78:A:PHE:CA	1:78:A:PHE:C	16	2.89
(1,12)	1:24:A:GLU:C	1:25:A:SER:N	1:25:A:SER:CA	1:25:A:SER:C	16	2.89
(1,12)	1:24:A:GLU:C	1:25:A:SER:N	1:25:A:SER:CA	1:25:A:SER:C	18	2.89
(1,62)	1:57:A:THR:C	1:58:A:ILE:N	1:58:A:ILE:CA	1:58:A:ILE:C	14	2.87
(1,105)	1:80:A:LEU:C	1:81:A:ALA:N	1:81:A:ALA:CA	1:81:A:ALA:C	4	2.86
(1,164)	1:125:A:LYS:C	1:126:A:ILE:N	1:126:A:ILE:CA	1:126:A:ILE:C	6	2.85
(1,62)	1:57:A:THR:C	1:58:A:ILE:N	1:58:A:ILE:CA	1:58:A:ILE:C	2	2.85
(1,10)	1:23:A:LEU:C	1:24:A:GLU:N	1:24:A:GLU:CA	1:24:A:GLU:C	2	2.85
(1,138)	1:105:A:PRO:C	1:106:A:GLU:N	1:106:A:GLU:CA	1:106:A:GLU:C	17	2.83
(1,12)	1:24:A:GLU:C	1:25:A:SER:N	1:25:A:SER:CA	1:25:A:SER:C	4	2.83
(1,172)	1:129:A:ASP:C	1:130:A:ARG:N	1:130:A:ARG:CA	1:130:A:ARG:C	20	2.82
(1,44)	1:44:A:LEU:C	1:45:A:SER:N	1:45:A:SER:CA	1:45:A:SER:C	17	2.81
(1,95)	1:75:A:LEU:C	1:76:A:ASN:N	1:76:A:ASN:CA	1:76:A:ASN:C	10	2.8
(1,89)	1:72:A:PRO:C	1:73:A:HIS:N	1:73:A:HIS:CA	1:73:A:HIS:C	4	2.79
(1,58)	1:55:A:HIS:C	1:56:A:SER:N	1:56:A:SER:CA	1:56:A:SER:C	11	2.78
(1,160)	1:123:A:ILE:C	1:124:A:PHE:N	1:124:A:PHE:CA	1:124:A:PHE:C	13	2.77
(1,182)	1:138:A:ILE:C	1:139:A:VAL:N	1:139:A:VAL:CA	1:139:A:VAL:C	17	2.75
(1,194)	1:144:A:ALA:C	1:145:A:LEU:N	1:145:A:LEU:CA	1:145:A:LEU:C	8	2.73
(1,162)	1:124:A:PHE:C	1:125:A:LYS:N	1:125:A:LYS:CA	1:125:A:LYS:C	20	2.73
(1,44)	1:44:A:LEU:C	1:45:A:SER:N	1:45:A:SER:CA	1:45:A:SER:C	16	2.73
(1,36)	1:40:A:SER:C	1:41:A:ILE:N	1:41:A:ILE:CA	1:41:A:ILE:C	19	2.73
(1,89)	1:72:A:PRO:C	1:73:A:HIS:N	1:73:A:HIS:CA	1:73:A:HIS:C	3	2.72
(1,158)	1:122:A:ARG:C	1:123:A:ILE:N	1:123:A:ILE:CA	1:123:A:ILE:C	15	2.71
(1,142)	1:107:A:ALA:C	1:108:A:ALA:N	1:108:A:ALA:CA	1:108:A:ALA:C	5	2.7
(1,62)	1:57:A:THR:C	1:58:A:ILE:N	1:58:A:ILE:CA	1:58:A:ILE:C	9	2.7
(1,62)	1:57:A:THR:C	1:58:A:ILE:N	1:58:A:ILE:CA	1:58:A:ILE:C	4	2.69
(1,48)	1:46:A:SER:C	1:47:A:TRP:N	1:47:A:TRP:CA	1:47:A:TRP:C	1	2.69
(1,74)	1:63:A:MET:C	1:64:A:LYS:N	1:64:A:LYS:CA	1:64:A:LYS:C	20	2.68
(1,58)	1:55:A:HIS:C	1:56:A:SER:N	1:56:A:SER:CA	1:56:A:SER:C	17	2.68
(1,10)	1:23:A:LEU:C	1:24:A:GLU:N	1:24:A:GLU:CA	1:24:A:GLU:C	11	2.68

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,168)	1:127:A:TRP:C	1:128:A:GLU:N	1:128:A:GLU:CA	1:128:A:GLU:C	3	2.67
(1,138)	1:105:A:PRO:C	1:106:A:GLU:N	1:106:A:GLU:CA	1:106:A:GLU:C	20	2.65
(1,142)	1:107:A:ALA:C	1:108:A:ALA:N	1:108:A:ALA:CA	1:108:A:ALA:C	10	2.63
(1,97)	1:76:A:ASN:C	1:77:A:LEU:N	1:77:A:LEU:CA	1:77:A:LEU:C	1	2.63
(1,89)	1:72:A:PRO:C	1:73:A:HIS:N	1:73:A:HIS:CA	1:73:A:HIS:C	7	2.63
(1,38)	1:41:A:ILE:C	1:42:A:GLN:N	1:42:A:GLN:CA	1:42:A:GLN:C	17	2.63
(1,192)	1:143:A:GLU:C	1:144:A:ALA:N	1:144:A:ALA:CA	1:144:A:ALA:C	11	2.62
(1,111)	1:83:A:ASP:C	1:84:A:VAL:N	1:84:A:VAL:CA	1:84:A:VAL:C	10	2.6
(1,99)	1:77:A:LEU:C	1:78:A:PHE:N	1:78:A:PHE:CA	1:78:A:PHE:C	2	2.6
(1,160)	1:123:A:ILE:C	1:124:A:PHE:N	1:124:A:PHE:CA	1:124:A:PHE:C	15	2.59
(1,84)	1:68:A:ARG:C	1:69:A:SER:N	1:69:A:SER:CA	1:69:A:SER:C	16	2.59
(1,109)	1:82:A:ASN:C	1:83:A:ASP:N	1:83:A:ASP:CA	1:83:A:ASP:C	15	2.58
(1,142)	1:107:A:ALA:C	1:108:A:ALA:N	1:108:A:ALA:CA	1:108:A:ALA:C	16	2.57
(1,101)	1:78:A:PHE:C	1:79:A:TYR:N	1:79:A:TYR:CA	1:79:A:TYR:C	7	2.57
(1,101)	1:78:A:PHE:C	1:79:A:TYR:N	1:79:A:TYR:CA	1:79:A:TYR:C	19	2.57
(1,160)	1:123:A:ILE:C	1:124:A:PHE:N	1:124:A:PHE:CA	1:124:A:PHE:C	20	2.56
(1,192)	1:143:A:GLU:C	1:144:A:ALA:N	1:144:A:ALA:CA	1:144:A:ALA:C	16	2.55
(1,182)	1:138:A:ILE:C	1:139:A:VAL:N	1:139:A:VAL:CA	1:139:A:VAL:C	12	2.55
(1,162)	1:124:A:PHE:C	1:125:A:LYS:N	1:125:A:LYS:CA	1:125:A:LYS:C	13	2.55
(1,152)	1:119:A:SER:C	1:120:A:VAL:N	1:120:A:VAL:CA	1:120:A:VAL:C	5	2.55
(1,74)	1:63:A:MET:C	1:64:A:LYS:N	1:64:A:LYS:CA	1:64:A:LYS:C	9	2.55
(1,188)	1:141:A:LEU:C	1:142:A:ARG:N	1:142:A:ARG:CA	1:142:A:ARG:C	11	2.54
(1,160)	1:123:A:ILE:C	1:124:A:PHE:N	1:124:A:PHE:CA	1:124:A:PHE:C	1	2.54
(1,20)	1:28:A:ASP:C	1:29:A:ARG:N	1:29:A:ARG:CA	1:29:A:ARG:C	2	2.54
(1,20)	1:28:A:ASP:C	1:29:A:ARG:N	1:29:A:ARG:CA	1:29:A:ARG:C	8	2.54
(1,28)	1:32:A:GLN:C	1:33:A:SER:N	1:33:A:SER:CA	1:33:A:SER:C	20	2.53
(1,66)	1:59:A:VAL:C	1:60:A:TYR:N	1:60:A:TYR:CA	1:60:A:TYR:C	17	2.52
(1,14)	1:25:A:SER:C	1:26:A:SER:N	1:26:A:SER:CA	1:26:A:SER:C	13	2.52
(1,192)	1:143:A:GLU:C	1:144:A:ALA:N	1:144:A:ALA:CA	1:144:A:ALA:C	1	2.51
(1,10)	1:23:A:LEU:C	1:24:A:GLU:N	1:24:A:GLU:CA	1:24:A:GLU:C	6	2.5
(1,170)	1:128:A:GLU:C	1:129:A:ASP:N	1:129:A:ASP:CA	1:129:A:ASP:C	15	2.49
(1,58)	1:55:A:HIS:C	1:56:A:SER:N	1:56:A:SER:CA	1:56:A:SER:C	14	2.49
(1,62)	1:57:A:THR:C	1:58:A:ILE:N	1:58:A:ILE:CA	1:58:A:ILE:C	18	2.47
(1,24)	1:30:A:LYS:C	1:31:A:PHE:N	1:31:A:PHE:CA	1:31:A:PHE:C	5	2.46
(1,28)	1:32:A:GLN:C	1:33:A:SER:N	1:33:A:SER:CA	1:33:A:SER:C	18	2.44
(1,180)	1:137:A:MET:C	1:138:A:ILE:N	1:138:A:ILE:CA	1:138:A:ILE:C	7	2.43
(1,142)	1:107:A:ALA:C	1:108:A:ALA:N	1:108:A:ALA:CA	1:108:A:ALA:C	11	2.42
(1,111)	1:83:A:ASP:C	1:84:A:VAL:N	1:84:A:VAL:CA	1:84:A:VAL:C	9	2.4
(1,123)	1:96:A:PHE:C	1:97:A:ARG:N	1:97:A:ARG:CA	1:97:A:ARG:C	9	2.39
(1,82)	1:67:A:ARG:C	1:68:A:ARG:N	1:68:A:ARG:CA	1:68:A:ARG:C	1	2.39
(1,190)	1:142:A:ARG:C	1:143:A:GLU:N	1:143:A:GLU:CA	1:143:A:GLU:C	20	2.37
(1,90)	1:73:A:HIS:N	1:73:A:HIS:CA	1:73:A:HIS:C	1:74:A:ARG:N	20	2.37
(1,10)	1:23:A:LEU:C	1:24:A:GLU:N	1:24:A:GLU:CA	1:24:A:GLU:C	12	2.37
(1,22)	1:29:A:ARG:C	1:30:A:LYS:N	1:30:A:LYS:CA	1:30:A:LYS:C	15	2.35
(1,158)	1:122:A:ARG:C	1:123:A:ILE:N	1:123:A:ILE:CA	1:123:A:ILE:C	13	2.34
(1,111)	1:83:A:ASP:C	1:84:A:VAL:N	1:84:A:VAL:CA	1:84:A:VAL:C	12	2.34
(1,117)	1:86:A:GLN:C	1:87:A:ASN:N	1:87:A:ASN:CA	1:87:A:ASN:C	10	2.33
(1,173)	1:130:A:ARG:N	1:130:A:ARG:CA	1:130:A:ARG:C	1:131:A:ASN:N	12	2.32
(1,107)	1:81:A:ALA:C	1:82:A:ASN:N	1:82:A:ASN:CA	1:82:A:ASN:C	8	2.32
(1,62)	1:57:A:THR:C	1:58:A:ILE:N	1:58:A:ILE:CA	1:58:A:ILE:C	15	2.3
(1,142)	1:107:A:ALA:C	1:108:A:ALA:N	1:108:A:ALA:CA	1:108:A:ALA:C	12	2.29

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,66)	1:59:A:VAL:C	1:60:A:TYR:N	1:60:A:TYR:CA	1:60:A:TYR:C	12	2.29
(1,103)	1:79:A:TYR:C	1:80:A:LEU:N	1:80:A:LEU:CA	1:80:A:LEU:C	10	2.28
(1,58)	1:55:A:HIS:C	1:56:A:SER:N	1:56:A:SER:CA	1:56:A:SER:C	18	2.24
(1,10)	1:23:A:LEU:C	1:24:A:GLU:N	1:24:A:GLU:CA	1:24:A:GLU:C	10	2.24
(1,105)	1:80:A:LEU:C	1:81:A:ALA:N	1:81:A:ALA:CA	1:81:A:ALA:C	17	2.23
(1,90)	1:73:A:HIS:N	1:73:A:HIS:CA	1:73:A:HIS:C	1:74:A:ARG:N	9	2.23
(1,32)	1:38:A:MET:C	1:39:A:GLU:N	1:39:A:GLU:CA	1:39:A:GLU:C	1	2.23
(1,32)	1:38:A:MET:C	1:39:A:GLU:N	1:39:A:GLU:CA	1:39:A:GLU:C	12	2.23
(1,28)	1:32:A:GLN:C	1:33:A:SER:N	1:33:A:SER:CA	1:33:A:SER:C	13	2.23
(1,180)	1:137:A:MET:C	1:138:A:ILE:N	1:138:A:ILE:CA	1:138:A:ILE:C	9	2.22
(1,129)	1:99:A:SER:C	1:100:A:PHE:N	1:100:A:PHE:CA	1:100:A:PHE:C	3	2.2
(1,36)	1:40:A:SER:C	1:41:A:ILE:N	1:41:A:ILE:CA	1:41:A:ILE:C	9	2.2
(1,101)	1:78:A:PHE:C	1:79:A:TYR:N	1:79:A:TYR:CA	1:79:A:TYR:C	6	2.18
(1,38)	1:41:A:ILE:C	1:42:A:GLN:N	1:42:A:GLN:CA	1:42:A:GLN:C	10	2.17
(1,142)	1:107:A:ALA:C	1:108:A:ALA:N	1:108:A:ALA:CA	1:108:A:ALA:C	2	2.15
(1,12)	1:24:A:GLU:C	1:25:A:SER:N	1:25:A:SER:CA	1:25:A:SER:C	10	2.13
(1,36)	1:40:A:SER:C	1:41:A:ILE:N	1:41:A:ILE:CA	1:41:A:ILE:C	6	2.12
(1,80)	1:66:A:LEU:C	1:67:A:ARG:N	1:67:A:ARG:CA	1:67:A:ARG:C	18	2.11
(1,180)	1:137:A:MET:C	1:138:A:ILE:N	1:138:A:ILE:CA	1:138:A:ILE:C	11	2.1
(1,101)	1:78:A:PHE:C	1:79:A:TYR:N	1:79:A:TYR:CA	1:79:A:TYR:C	18	2.1
(1,8)	1:22:A:ALA:C	1:23:A:LEU:N	1:23:A:LEU:CA	1:23:A:LEU:C	17	2.1
(1,101)	1:78:A:PHE:C	1:79:A:TYR:N	1:79:A:TYR:CA	1:79:A:TYR:C	13	2.06
(1,127)	1:98:A:GLU:C	1:99:A:SER:N	1:99:A:SER:CA	1:99:A:SER:C	11	2.05
(1,117)	1:86:A:GLN:C	1:87:A:ASN:N	1:87:A:ASN:CA	1:87:A:ASN:C	4	2.04
(1,22)	1:29:A:ARG:C	1:30:A:LYS:N	1:30:A:LYS:CA	1:30:A:LYS:C	11	2.03
(1,121)	1:95:A:ILE:C	1:96:A:PHE:N	1:96:A:PHE:CA	1:96:A:PHE:C	18	2.02
(1,62)	1:57:A:THR:C	1:58:A:ILE:N	1:58:A:ILE:CA	1:58:A:ILE:C	13	2.02
(1,48)	1:46:A:SER:C	1:47:A:TRP:N	1:47:A:TRP:CA	1:47:A:TRP:C	4	2.02
(1,184)	1:139:A:VAL:C	1:140:A:ALA:N	1:140:A:ALA:CA	1:140:A:ALA:C	14	2.01
(1,164)	1:125:A:LYS:C	1:126:A:ILE:N	1:126:A:ILE:CA	1:126:A:ILE:C	20	2.01
(1,138)	1:105:A:PRO:C	1:106:A:GLU:N	1:106:A:GLU:CA	1:106:A:GLU:C	4	2.01
(1,101)	1:78:A:PHE:C	1:79:A:TYR:N	1:79:A:TYR:CA	1:79:A:TYR:C	20	2.0
(1,95)	1:75:A:LEU:C	1:76:A:ASN:N	1:76:A:ASN:CA	1:76:A:ASN:C	9	2.0
(1,80)	1:66:A:LEU:C	1:67:A:ARG:N	1:67:A:ARG:CA	1:67:A:ARG:C	3	2.0
(1,36)	1:40:A:SER:C	1:41:A:ILE:N	1:41:A:ILE:CA	1:41:A:ILE:C	11	1.99
(1,26)	1:31:A:PHE:C	1:32:A:GLN:N	1:32:A:GLN:CA	1:32:A:GLN:C	13	1.98
(1,58)	1:55:A:HIS:C	1:56:A:SER:N	1:56:A:SER:CA	1:56:A:SER:C	7	1.96
(1,158)	1:122:A:ARG:C	1:123:A:ILE:N	1:123:A:ILE:CA	1:123:A:ILE:C	14	1.91
(1,60)	1:56:A:SER:C	1:57:A:THR:N	1:57:A:THR:CA	1:57:A:THR:C	18	1.91
(1,133)	1:101:A:ALA:C	1:102:A:ASP:N	1:102:A:ASP:CA	1:102:A:ASP:C	3	1.89
(1,44)	1:44:A:LEU:C	1:45:A:SER:N	1:45:A:SER:CA	1:45:A:SER:C	7	1.89
(1,142)	1:107:A:ALA:C	1:108:A:ALA:N	1:108:A:ALA:CA	1:108:A:ALA:C	15	1.88
(1,162)	1:124:A:PHE:C	1:125:A:LYS:N	1:125:A:LYS:CA	1:125:A:LYS:C	11	1.87
(1,142)	1:107:A:ALA:C	1:108:A:ALA:N	1:108:A:ALA:CA	1:108:A:ALA:C	17	1.87
(1,180)	1:137:A:MET:C	1:138:A:ILE:N	1:138:A:ILE:CA	1:138:A:ILE:C	17	1.86
(1,95)	1:75:A:LEU:C	1:76:A:ASN:N	1:76:A:ASN:CA	1:76:A:ASN:C	16	1.86
(1,80)	1:66:A:LEU:C	1:67:A:ARG:N	1:67:A:ARG:CA	1:67:A:ARG:C	1	1.85
(1,180)	1:137:A:MET:C	1:138:A:ILE:N	1:138:A:ILE:CA	1:138:A:ILE:C	4	1.82
(1,111)	1:83:A:ASP:C	1:84:A:VAL:N	1:84:A:VAL:CA	1:84:A:VAL:C	3	1.82
(1,90)	1:73:A:HIS:N	1:73:A:HIS:CA	1:73:A:HIS:C	1:74:A:ARG:N	2	1.81
(1,12)	1:24:A:GLU:C	1:25:A:SER:N	1:25:A:SER:CA	1:25:A:SER:C	20	1.81

Continued on next page...

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,97)	1:76:A:ASN:C	1:77:A:LEU:N	1:77:A:LEU:CA	1:77:A:LEU:C	14	1.8
(1,95)	1:75:A:LEU:C	1:76:A:ASN:N	1:76:A:ASN:CA	1:76:A:ASN:C	11	1.78
(1,180)	1:137:A:MET:C	1:138:A:ILE:N	1:138:A:ILE:CA	1:138:A:ILE:C	19	1.76
(1,12)	1:24:A:GLU:C	1:25:A:SER:N	1:25:A:SER:CA	1:25:A:SER:C	1	1.76
(1,8)	1:22:A:ALA:C	1:23:A:LEU:N	1:23:A:LEU:CA	1:23:A:LEU:C	12	1.75
(1,101)	1:78:A:PHE:C	1:79:A:TYR:N	1:79:A:TYR:CA	1:79:A:TYR:C	12	1.74
(1,28)	1:32:A:GLN:C	1:33:A:SER:N	1:33:A:SER:CA	1:33:A:SER:C	12	1.74
(1,170)	1:128:A:GLU:C	1:129:A:ASP:N	1:129:A:ASP:CA	1:129:A:ASP:C	7	1.73
(1,133)	1:101:A:ALA:C	1:102:A:ASP:N	1:102:A:ASP:CA	1:102:A:ASP:C	13	1.73
(1,12)	1:24:A:GLU:C	1:25:A:SER:N	1:25:A:SER:CA	1:25:A:SER:C	5	1.73
(1,127)	1:98:A:GLU:C	1:99:A:SER:N	1:99:A:SER:CA	1:99:A:SER:C	2	1.71
(1,38)	1:41:A:ILE:C	1:42:A:GLN:N	1:42:A:GLN:CA	1:42:A:GLN:C	19	1.71
(1,190)	1:142:A:ARG:C	1:143:A:GLU:N	1:143:A:GLU:CA	1:143:A:GLU:C	12	1.69
(1,121)	1:95:A:ILE:C	1:96:A:PHE:N	1:96:A:PHE:CA	1:96:A:PHE:C	17	1.69
(1,38)	1:41:A:ILE:C	1:42:A:GLN:N	1:42:A:GLN:CA	1:42:A:GLN:C	12	1.69
(1,109)	1:82:A:ASN:C	1:83:A:ASP:N	1:83:A:ASP:CA	1:83:A:ASP:C	4	1.68
(1,89)	1:72:A:PRO:C	1:73:A:HIS:N	1:73:A:HIS:CA	1:73:A:HIS:C	6	1.67
(1,70)	1:61:A:HIS:C	1:62:A:TRP:N	1:62:A:TRP:CA	1:62:A:TRP:C	8	1.64
(1,52)	1:48:A:CYS:C	1:49:A:ILE:N	1:49:A:ILE:CA	1:49:A:ILE:C	14	1.64
(1,164)	1:125:A:LYS:C	1:126:A:ILE:N	1:126:A:ILE:CA	1:126:A:ILE:C	10	1.63
(1,36)	1:40:A:SER:C	1:41:A:ILE:N	1:41:A:ILE:CA	1:41:A:ILE:C	4	1.63
(1,133)	1:101:A:ALA:C	1:102:A:ASP:N	1:102:A:ASP:CA	1:102:A:ASP:C	16	1.62
(1,44)	1:44:A:LEU:C	1:45:A:SER:N	1:45:A:SER:CA	1:45:A:SER:C	13	1.62
(1,192)	1:143:A:GLU:C	1:144:A:ALA:N	1:144:A:ALA:CA	1:144:A:ALA:C	7	1.61
(1,74)	1:63:A:MET:C	1:64:A:LYS:N	1:64:A:LYS:CA	1:64:A:LYS:C	14	1.61
(1,109)	1:82:A:ASN:C	1:83:A:ASP:N	1:83:A:ASP:CA	1:83:A:ASP:C	14	1.6
(1,182)	1:138:A:ILE:C	1:139:A:VAL:N	1:139:A:VAL:CA	1:139:A:VAL:C	16	1.59
(1,142)	1:107:A:ALA:C	1:108:A:ALA:N	1:108:A:ALA:CA	1:108:A:ALA:C	8	1.59
(1,44)	1:44:A:LEU:C	1:45:A:SER:N	1:45:A:SER:CA	1:45:A:SER:C	2	1.59
(1,28)	1:32:A:GLN:C	1:33:A:SER:N	1:33:A:SER:CA	1:33:A:SER:C	10	1.59
(1,160)	1:123:A:ILE:C	1:124:A:PHE:N	1:124:A:PHE:CA	1:124:A:PHE:C	19	1.57
(1,142)	1:107:A:ALA:C	1:108:A:ALA:N	1:108:A:ALA:CA	1:108:A:ALA:C	9	1.57
(1,24)	1:30:A:LYS:C	1:31:A:PHE:N	1:31:A:PHE:CA	1:31:A:PHE:C	17	1.57
(1,105)	1:80:A:LEU:C	1:81:A:ALA:N	1:81:A:ALA:CA	1:81:A:ALA:C	9	1.56
(1,62)	1:57:A:THR:C	1:58:A:ILE:N	1:58:A:ILE:CA	1:58:A:ILE:C	10	1.56
(1,48)	1:46:A:SER:C	1:47:A:TRP:N	1:47:A:TRP:CA	1:47:A:TRP:C	17	1.56
(1,44)	1:44:A:LEU:C	1:45:A:SER:N	1:45:A:SER:CA	1:45:A:SER:C	3	1.56
(1,12)	1:24:A:GLU:C	1:25:A:SER:N	1:25:A:SER:CA	1:25:A:SER:C	17	1.56
(1,8)	1:22:A:ALA:C	1:23:A:LEU:N	1:23:A:LEU:CA	1:23:A:LEU:C	8	1.56
(1,18)	1:27:A:LEU:C	1:28:A:ASP:N	1:28:A:ASP:CA	1:28:A:ASP:C	17	1.54
(1,18)	1:27:A:LEU:C	1:28:A:ASP:N	1:28:A:ASP:CA	1:28:A:ASP:C	10	1.5
(1,162)	1:124:A:PHE:C	1:125:A:LYS:N	1:125:A:LYS:CA	1:125:A:LYS:C	9	1.49
(1,8)	1:22:A:ALA:C	1:23:A:LEU:N	1:23:A:LEU:CA	1:23:A:LEU:C	11	1.49
(1,127)	1:98:A:GLU:C	1:99:A:SER:N	1:99:A:SER:CA	1:99:A:SER:C	12	1.47
(1,80)	1:66:A:LEU:C	1:67:A:ARG:N	1:67:A:ARG:CA	1:67:A:ARG:C	17	1.46
(1,70)	1:61:A:HIS:C	1:62:A:TRP:N	1:62:A:TRP:CA	1:62:A:TRP:C	11	1.46
(1,180)	1:137:A:MET:C	1:138:A:ILE:N	1:138:A:ILE:CA	1:138:A:ILE:C	2	1.45
(1,6)	1:21:A:GLY:C	1:22:A:ALA:N	1:22:A:ALA:CA	1:22:A:ALA:C	20	1.45
(1,180)	1:137:A:MET:C	1:138:A:ILE:N	1:138:A:ILE:CA	1:138:A:ILE:C	8	1.44
(1,111)	1:83:A:ASP:C	1:84:A:VAL:N	1:84:A:VAL:CA	1:84:A:VAL:C	2	1.44
(1,192)	1:143:A:GLU:C	1:144:A:ALA:N	1:144:A:ALA:CA	1:144:A:ALA:C	19	1.42

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,160)	1:123:A:ILE:C	1:124:A:PHE:N	1:124:A:PHE:CA	1:124:A:PHE:C	4	1.42
(1,125)	1:97:A:ARG:C	1:98:A:GLU:N	1:98:A:GLU:CA	1:98:A:GLU:C	17	1.41
(1,8)	1:22:A:ALA:C	1:23:A:LEU:N	1:23:A:LEU:CA	1:23:A:LEU:C	3	1.41
(1,180)	1:137:A:MET:C	1:138:A:ILE:N	1:138:A:ILE:CA	1:138:A:ILE:C	1	1.4
(1,164)	1:125:A:LYS:C	1:126:A:ILE:N	1:126:A:ILE:CA	1:126:A:ILE:C	4	1.4
(1,133)	1:101:A:ALA:C	1:102:A:ASP:N	1:102:A:ASP:CA	1:102:A:ASP:C	4	1.4
(1,38)	1:41:A:ILE:C	1:42:A:GLN:N	1:42:A:GLN:CA	1:42:A:GLN:C	14	1.4
(1,38)	1:41:A:ILE:C	1:42:A:GLN:N	1:42:A:GLN:CA	1:42:A:GLN:C	15	1.4
(1,78)	1:65:A:TRP:C	1:66:A:LEU:N	1:66:A:LEU:CA	1:66:A:LEU:C	14	1.39
(1,12)	1:24:A:GLU:C	1:25:A:SER:N	1:25:A:SER:CA	1:25:A:SER:C	11	1.38
(1,4)	1:20:A:ALA:C	1:21:A:GLY:N	1:21:A:GLY:CA	1:21:A:GLY:C	5	1.38
(1,158)	1:122:A:ARG:C	1:123:A:ILE:N	1:123:A:ILE:CA	1:123:A:ILE:C	18	1.37
(1,192)	1:143:A:GLU:C	1:144:A:ALA:N	1:144:A:ALA:CA	1:144:A:ALA:C	20	1.36
(1,152)	1:119:A:SER:C	1:120:A:VAL:N	1:120:A:VAL:CA	1:120:A:VAL:C	20	1.36
(1,125)	1:97:A:ARG:C	1:98:A:GLU:N	1:98:A:GLU:CA	1:98:A:GLU:C	18	1.36
(1,125)	1:97:A:ARG:C	1:98:A:GLU:N	1:98:A:GLU:CA	1:98:A:GLU:C	6	1.35
(1,84)	1:68:A:ARG:C	1:69:A:SER:N	1:69:A:SER:CA	1:69:A:SER:C	7	1.35
(1,44)	1:44:A:LEU:C	1:45:A:SER:N	1:45:A:SER:CA	1:45:A:SER:C	6	1.35
(1,138)	1:105:A:PRO:C	1:106:A:GLU:N	1:106:A:GLU:CA	1:106:A:GLU:C	2	1.34
(1,109)	1:82:A:ASN:C	1:83:A:ASP:N	1:83:A:ASP:CA	1:83:A:ASP:C	10	1.34
(1,125)	1:97:A:ARG:C	1:98:A:GLU:N	1:98:A:GLU:CA	1:98:A:GLU:C	9	1.33
(1,121)	1:95:A:ILE:C	1:96:A:PHE:N	1:96:A:PHE:CA	1:96:A:PHE:C	11	1.33
(1,89)	1:72:A:PRO:C	1:73:A:HIS:N	1:73:A:HIS:CA	1:73:A:HIS:C	9	1.33
(1,85)	1:69:A:SER:N	1:69:A:SER:CA	1:69:A:SER:C	1:70:A:ALA:N	7	1.31
(1,80)	1:66:A:LEU:C	1:67:A:ARG:N	1:67:A:ARG:CA	1:67:A:ARG:C	10	1.31
(1,20)	1:28:A:ASP:C	1:29:A:ARG:N	1:29:A:ARG:CA	1:29:A:ARG:C	10	1.31
(1,10)	1:23:A:LEU:C	1:24:A:GLU:N	1:24:A:GLU:CA	1:24:A:GLU:C	18	1.31
(1,58)	1:55:A:HIS:C	1:56:A:SER:N	1:56:A:SER:CA	1:56:A:SER:C	20	1.3
(1,40)	1:42:A:GLN:C	1:43:A:GLY:N	1:43:A:GLY:CA	1:43:A:GLY:C	20	1.3
(1,188)	1:141:A:LEU:C	1:142:A:ARG:N	1:142:A:ARG:CA	1:142:A:ARG:C	1	1.29
(1,44)	1:44:A:LEU:C	1:45:A:SER:N	1:45:A:SER:CA	1:45:A:SER:C	1	1.29
(1,36)	1:40:A:SER:C	1:41:A:ILE:N	1:41:A:ILE:CA	1:41:A:ILE:C	3	1.29
(1,14)	1:25:A:SER:C	1:26:A:SER:N	1:26:A:SER:CA	1:26:A:SER:C	7	1.29
(1,95)	1:75:A:LEU:C	1:76:A:ASN:N	1:76:A:ASN:CA	1:76:A:ASN:C	20	1.28
(1,28)	1:32:A:GLN:C	1:33:A:SER:N	1:33:A:SER:CA	1:33:A:SER:C	8	1.28
(1,133)	1:101:A:ALA:C	1:102:A:ASP:N	1:102:A:ASP:CA	1:102:A:ASP:C	6	1.26
(1,101)	1:78:A:PHE:C	1:79:A:TYR:N	1:79:A:TYR:CA	1:79:A:TYR:C	1	1.26
(1,18)	1:27:A:LEU:C	1:28:A:ASP:N	1:28:A:ASP:CA	1:28:A:ASP:C	5	1.26
(1,14)	1:25:A:SER:C	1:26:A:SER:N	1:26:A:SER:CA	1:26:A:SER:C	19	1.26
(1,111)	1:83:A:ASP:C	1:84:A:VAL:N	1:84:A:VAL:CA	1:84:A:VAL:C	19	1.25
(1,48)	1:46:A:SER:C	1:47:A:TRP:N	1:47:A:TRP:CA	1:47:A:TRP:C	10	1.25
(1,166)	1:126:A:ILE:C	1:127:A:TRP:N	1:127:A:TRP:CA	1:127:A:TRP:C	3	1.24
(1,95)	1:75:A:LEU:C	1:76:A:ASN:N	1:76:A:ASN:CA	1:76:A:ASN:C	7	1.24
(1,170)	1:128:A:GLU:C	1:129:A:ASP:N	1:129:A:ASP:CA	1:129:A:ASP:C	9	1.23
(1,80)	1:66:A:LEU:C	1:67:A:ARG:N	1:67:A:ARG:CA	1:67:A:ARG:C	8	1.23
(1,44)	1:44:A:LEU:C	1:45:A:SER:N	1:45:A:SER:CA	1:45:A:SER:C	18	1.23
(1,72)	1:62:A:TRP:C	1:63:A:MET:N	1:63:A:MET:CA	1:63:A:MET:C	5	1.22
(1,58)	1:55:A:HIS:C	1:56:A:SER:N	1:56:A:SER:CA	1:56:A:SER:C	16	1.22
(1,20)	1:28:A:ASP:C	1:29:A:ARG:N	1:29:A:ARG:CA	1:29:A:ARG:C	14	1.22
(1,6)	1:21:A:GLY:C	1:22:A:ALA:N	1:22:A:ALA:CA	1:22:A:ALA:C	9	1.22
(1,80)	1:66:A:LEU:C	1:67:A:ARG:N	1:67:A:ARG:CA	1:67:A:ARG:C	15	1.21

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,192)	1:143:A:GLU:C	1:144:A:ALA:N	1:144:A:ALA:CA	1:144:A:ALA:C	14	1.2
(1,174)	1:134:A:PRO:C	1:135:A:GLU:N	1:135:A:GLU:CA	1:135:A:GLU:C	18	1.19
(1,109)	1:82:A:ASN:C	1:83:A:ASP:N	1:83:A:ASP:CA	1:83:A:ASP:C	8	1.19
(1,6)	1:21:A:GLY:C	1:22:A:ALA:N	1:22:A:ALA:CA	1:22:A:ALA:C	1	1.19
(1,184)	1:139:A:VAL:C	1:140:A:ALA:N	1:140:A:ALA:CA	1:140:A:ALA:C	10	1.18
(1,129)	1:99:A:SER:C	1:100:A:PHE:N	1:100:A:PHE:CA	1:100:A:PHE:C	8	1.18
(1,6)	1:21:A:GLY:C	1:22:A:ALA:N	1:22:A:ALA:CA	1:22:A:ALA:C	14	1.18
(1,6)	1:21:A:GLY:C	1:22:A:ALA:N	1:22:A:ALA:CA	1:22:A:ALA:C	16	1.18
(1,148)	1:117:A:SER:C	1:118:A:LYS:N	1:118:A:LYS:CA	1:118:A:LYS:C	6	1.17
(1,90)	1:73:A:HIS:N	1:73:A:HIS:CA	1:73:A:HIS:C	1:74:A:ARG:N	19	1.17
(1,32)	1:38:A:MET:C	1:39:A:GLU:N	1:39:A:GLU:CA	1:39:A:GLU:C	3	1.17
(1,158)	1:122:A:ARG:C	1:123:A:ILE:N	1:123:A:ILE:CA	1:123:A:ILE:C	9	1.16
(1,164)	1:125:A:LYS:C	1:126:A:ILE:N	1:126:A:ILE:CA	1:126:A:ILE:C	18	1.15
(1,74)	1:63:A:MET:C	1:64:A:LYS:N	1:64:A:LYS:CA	1:64:A:LYS:C	15	1.15
(1,42)	1:43:A:GLY:C	1:44:A:LEU:N	1:44:A:LEU:CA	1:44:A:LEU:C	4	1.15
(1,18)	1:27:A:LEU:C	1:28:A:ASP:N	1:28:A:ASP:CA	1:28:A:ASP:C	16	1.15
(1,105)	1:80:A:LEU:C	1:81:A:ALA:N	1:81:A:ALA:CA	1:81:A:ALA:C	7	1.14
(1,99)	1:77:A:LEU:C	1:78:A:PHE:N	1:78:A:PHE:CA	1:78:A:PHE:C	20	1.14
(1,80)	1:66:A:LEU:C	1:67:A:ARG:N	1:67:A:ARG:CA	1:67:A:ARG:C	14	1.14
(1,166)	1:126:A:ILE:C	1:127:A:TRP:N	1:127:A:TRP:CA	1:127:A:TRP:C	14	1.13
(1,105)	1:80:A:LEU:C	1:81:A:ALA:N	1:81:A:ALA:CA	1:81:A:ALA:C	6	1.13
(1,74)	1:63:A:MET:C	1:64:A:LYS:N	1:64:A:LYS:CA	1:64:A:LYS:C	5	1.12
(1,20)	1:28:A:ASP:C	1:29:A:ARG:N	1:29:A:ARG:CA	1:29:A:ARG:C	5	1.12
(1,44)	1:44:A:LEU:C	1:45:A:SER:N	1:45:A:SER:CA	1:45:A:SER:C	9	1.11
(1,194)	1:144:A:ALA:C	1:145:A:LEU:N	1:145:A:LEU:CA	1:145:A:LEU:C	3	1.1
(1,176)	1:135:A:GLU:C	1:136:A:GLU:N	1:136:A:GLU:CA	1:136:A:GLU:C	11	1.1
(1,173)	1:130:A:ARG:N	1:130:A:ARG:CA	1:130:A:ARG:C	1:131:A:ASN:N	17	1.1
(1,168)	1:127:A:TRP:C	1:128:A:GLU:N	1:128:A:GLU:CA	1:128:A:GLU:C	6	1.1
(1,52)	1:48:A:CYS:C	1:49:A:ILE:N	1:49:A:ILE:CA	1:49:A:ILE:C	17	1.1
(1,173)	1:130:A:ARG:N	1:130:A:ARG:CA	1:130:A:ARG:C	1:131:A:ASN:N	7	1.09
(1,152)	1:119:A:SER:C	1:120:A:VAL:N	1:120:A:VAL:CA	1:120:A:VAL:C	10	1.09
(1,123)	1:96:A:PHE:C	1:97:A:ARG:N	1:97:A:ARG:CA	1:97:A:ARG:C	10	1.09
(1,121)	1:95:A:ILE:C	1:96:A:PHE:N	1:96:A:PHE:CA	1:96:A:PHE:C	12	1.09
(1,111)	1:83:A:ASP:C	1:84:A:VAL:N	1:84:A:VAL:CA	1:84:A:VAL:C	18	1.09
(1,82)	1:67:A:ARG:C	1:68:A:ARG:N	1:68:A:ARG:CA	1:68:A:ARG:C	2	1.09
(1,76)	1:64:A:LYS:C	1:65:A:TRP:N	1:65:A:TRP:CA	1:65:A:TRP:C	3	1.09
(1,22)	1:29:A:ARG:C	1:30:A:LYS:N	1:30:A:LYS:CA	1:30:A:LYS:C	5	1.09
(1,6)	1:21:A:GLY:C	1:22:A:ALA:N	1:22:A:ALA:CA	1:22:A:ALA:C	18	1.09
(1,184)	1:139:A:VAL:C	1:140:A:ALA:N	1:140:A:ALA:CA	1:140:A:ALA:C	8	1.08
(1,24)	1:30:A:LYS:C	1:31:A:PHE:N	1:31:A:PHE:CA	1:31:A:PHE:C	11	1.08
(1,18)	1:27:A:LEU:C	1:28:A:ASP:N	1:28:A:ASP:CA	1:28:A:ASP:C	6	1.08
(1,38)	1:41:A:ILE:C	1:42:A:GLN:N	1:42:A:GLN:CA	1:42:A:GLN:C	6	1.07
(1,176)	1:135:A:GLU:C	1:136:A:GLU:N	1:136:A:GLU:CA	1:136:A:GLU:C	13	1.06
(1,154)	1:120:A:VAL:C	1:121:A:GLU:N	1:121:A:GLU:CA	1:121:A:GLU:C	11	1.06
(1,109)	1:82:A:ASN:C	1:83:A:ASP:N	1:83:A:ASP:CA	1:83:A:ASP:C	12	1.06
(1,168)	1:127:A:TRP:C	1:128:A:GLU:N	1:128:A:GLU:CA	1:128:A:GLU:C	8	1.05
(1,127)	1:98:A:GLU:C	1:99:A:SER:N	1:99:A:SER:CA	1:99:A:SER:C	17	1.05
(1,44)	1:44:A:LEU:C	1:45:A:SER:N	1:45:A:SER:CA	1:45:A:SER:C	4	1.05
(1,32)	1:38:A:MET:C	1:39:A:GLU:N	1:39:A:GLU:CA	1:39:A:GLU:C	11	1.05
(1,99)	1:77:A:LEU:C	1:78:A:PHE:N	1:78:A:PHE:CA	1:78:A:PHE:C	1	1.04
(1,48)	1:46:A:SER:C	1:47:A:TRP:N	1:47:A:TRP:CA	1:47:A:TRP:C	2	1.04

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,10)	1:23:A:LEU:C	1:24:A:GLU:N	1:24:A:GLU:CA	1:24:A:GLU:C	15	1.04
(1,166)	1:126:A:ILE:C	1:127:A:TRP:N	1:127:A:TRP:CA	1:127:A:TRP:C	2	1.03
(1,156)	1:121:A:GLU:C	1:122:A:ARG:N	1:122:A:ARG:CA	1:122:A:ARG:C	11	1.03
(1,123)	1:96:A:PHE:C	1:97:A:ARG:N	1:97:A:ARG:CA	1:97:A:ARG:C	16	1.03
(1,44)	1:44:A:LEU:C	1:45:A:SER:N	1:45:A:SER:CA	1:45:A:SER:C	11	1.03
(1,32)	1:38:A:MET:C	1:39:A:GLU:N	1:39:A:GLU:CA	1:39:A:GLU:C	15	1.03
(1,22)	1:29:A:ARG:C	1:30:A:LYS:N	1:30:A:LYS:CA	1:30:A:LYS:C	13	1.03
(1,160)	1:123:A:ILE:C	1:124:A:PHE:N	1:124:A:PHE:CA	1:124:A:PHE:C	5	1.02
(1,133)	1:101:A:ALA:C	1:102:A:ASP:N	1:102:A:ASP:CA	1:102:A:ASP:C	14	1.02
(1,117)	1:86:A:GLN:C	1:87:A:ASN:N	1:87:A:ASN:CA	1:87:A:ASN:C	16	1.02
(1,78)	1:65:A:TRP:C	1:66:A:LEU:N	1:66:A:LEU:CA	1:66:A:LEU:C	18	1.02
(1,18)	1:27:A:LEU:C	1:28:A:ASP:N	1:28:A:ASP:CA	1:28:A:ASP:C	20	1.02
(1,190)	1:142:A:ARG:C	1:143:A:GLU:N	1:143:A:GLU:CA	1:143:A:GLU:C	13	1.01
(1,184)	1:139:A:VAL:C	1:140:A:ALA:N	1:140:A:ALA:CA	1:140:A:ALA:C	1	1.01
(1,156)	1:121:A:GLU:C	1:122:A:ARG:N	1:122:A:ARG:CA	1:122:A:ARG:C	13	1.01
(1,138)	1:105:A:PRO:C	1:106:A:GLU:N	1:106:A:GLU:CA	1:106:A:GLU:C	13	1.01
(1,109)	1:82:A:ASN:C	1:83:A:ASP:N	1:83:A:ASP:CA	1:83:A:ASP:C	9	1.01
(1,80)	1:66:A:LEU:C	1:67:A:ARG:N	1:67:A:ARG:CA	1:67:A:ARG:C	16	1.01
(1,40)	1:42:A:GLN:C	1:43:A:GLY:N	1:43:A:GLY:CA	1:43:A:GLY:C	7	1.01
(1,22)	1:29:A:ARG:C	1:30:A:LYS:N	1:30:A:LYS:CA	1:30:A:LYS:C	8	1.01
(1,121)	1:95:A:ILE:C	1:96:A:PHE:N	1:96:A:PHE:CA	1:96:A:PHE:C	15	1.0
(1,40)	1:42:A:GLN:C	1:43:A:GLY:N	1:43:A:GLY:CA	1:43:A:GLY:C	1	1.0