



Full wwPDB NMR Structure Validation Report ⓘ

Sep 8, 2025 – 10:11 AM EDT

PDB ID : 9DLU / pdb_00009dlu
BMRB ID : 52595
Title : Solution structure of Staphylococcus aureus response regulator ArlR DNA-binding domain
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Deposited on : 2024-09-11

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

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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 Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
BMRB Restraints Analysis : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

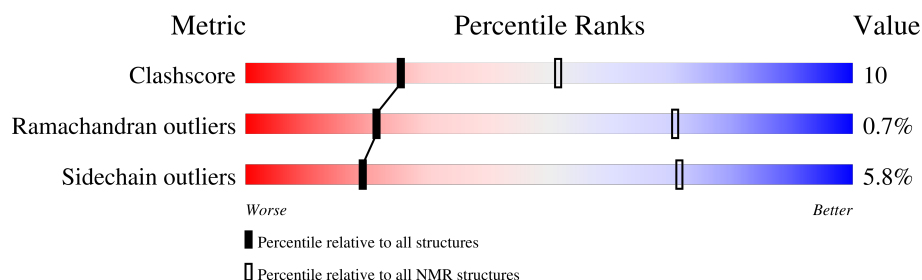
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 89%.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	210492	14027
Ramachandran outliers	207382	12486
Sidechain outliers	206894	12463

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

Mol	Chain	Length	Quality of chain
1	A	105	

2 Ensemble composition and analysis

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

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:124-A:178, A:184-A:219 (91)	0.46	1

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 1 clusters and 7 single-model clusters were found.

Cluster number	Models
1	1, 3, 4
Single-model clusters	2; 5; 6; 7; 8; 9; 10

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1747 atoms, of which 872 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Response regulator ArlR.

Mol	Chain	Residues	Atoms						Trace
1	A	105	Total	C	H	N	O	S	0
			1747	553	872	158	161	3	

There are 8 discrepancies between the modelled and reference sequences:

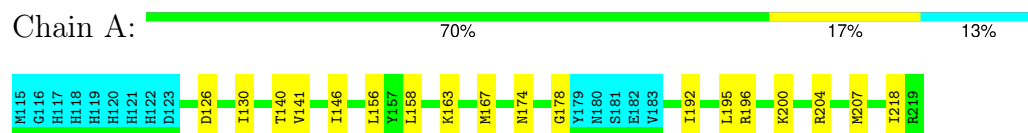
Chain	Residue	Modelled	Actual	Comment	Reference
A	115	MET	-	initiating methionine	UNP Q9KJN4
A	116	GLY	-	expression tag	UNP Q9KJN4
A	117	HIS	-	expression tag	UNP Q9KJN4
A	118	HIS	-	expression tag	UNP Q9KJN4
A	119	HIS	-	expression tag	UNP Q9KJN4
A	120	HIS	-	expression tag	UNP Q9KJN4
A	121	HIS	-	expression tag	UNP Q9KJN4
A	122	HIS	-	expression tag	UNP Q9KJN4

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Response regulator ArlR

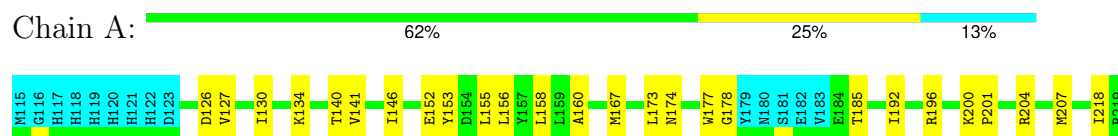


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

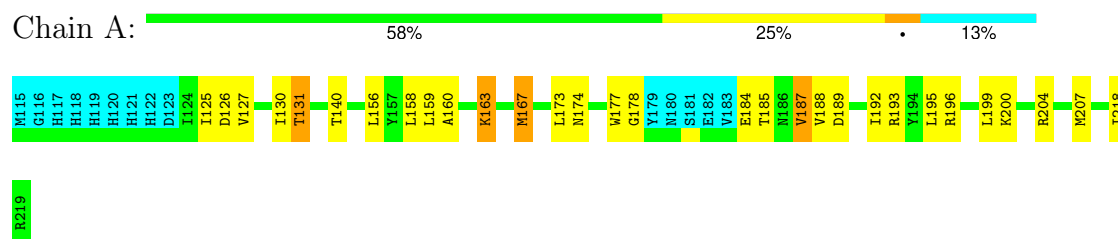
4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Response regulator ArlR



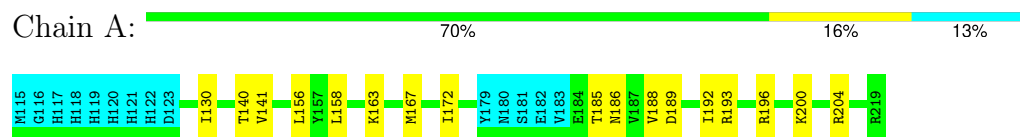
4.2.2 Score per residue for model 2

- Molecule 1: Response regulator ArlR



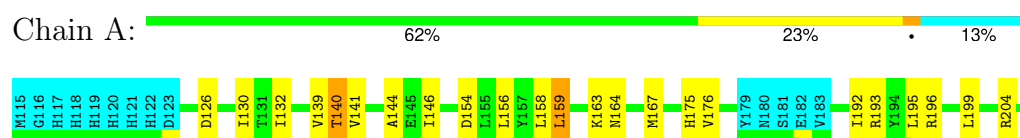
4.2.3 Score per residue for model 3

- Molecule 1: Response regulator ArlR



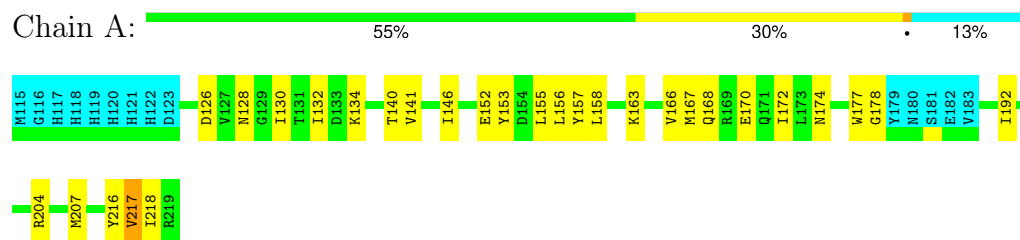
4.2.4 Score per residue for model 4

- Molecule 1: Response regulator ArlR



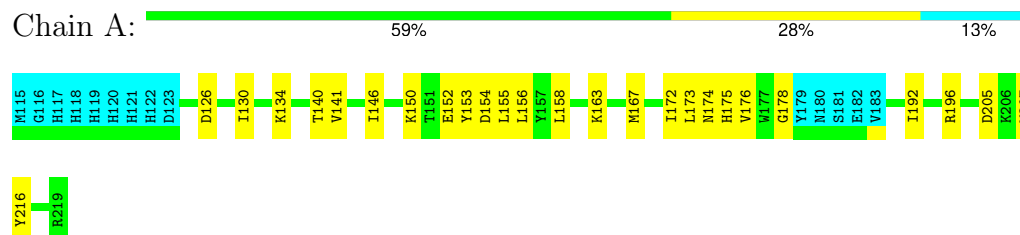
4.2.5 Score per residue for model 5

- Molecule 1: Response regulator ArlR



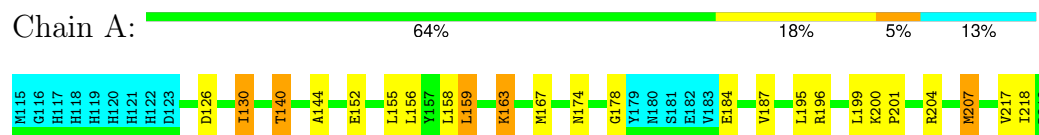
4.2.6 Score per residue for model 6

- Molecule 1: Response regulator ArlR



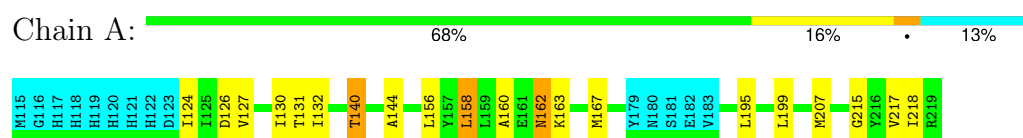
4.2.7 Score per residue for model 7

- Molecule 1: Response regulator ArlR



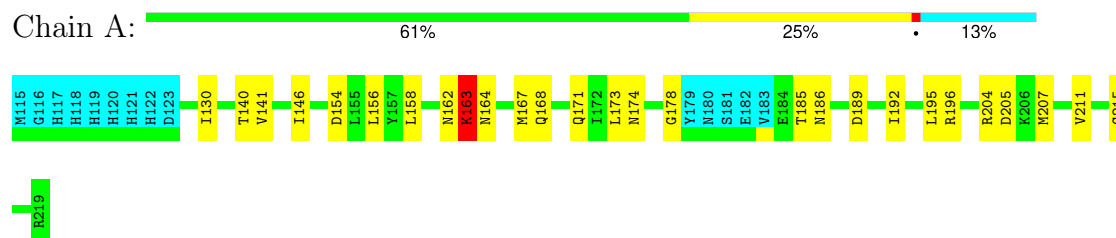
4.2.8 Score per residue for model 8

- Molecule 1: Response regulator ArlR



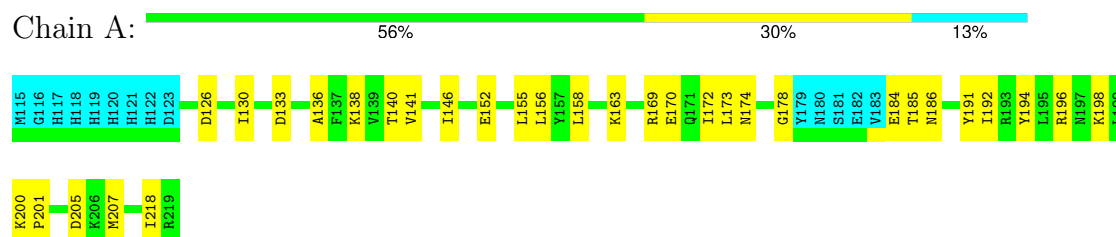
4.2.9 Score per residue for model 9

- Molecule 1: Response regulator ArlR



4.2.10 Score per residue for model 10

- Molecule 1: Response regulator ArlR



5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
ARIA	structure calculation	
ARIA	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	1250
Number of shifts mapped to atoms	1250
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	89%

6 Model quality

6.1 Standard geometry

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	753	771	769	15±3
All	All	7530	7710	7690	154

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 10.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:173:LEU:HG	1:A:185:THR:HG22	0.79	1.55	10	4
1:A:141:VAL:HG12	1:A:146:ILE:HD11	0.74	1.57	10	4
1:A:141:VAL:HG22	1:A:146:ILE:HD11	0.64	1.68	4	1
1:A:166:VAL:HA	1:A:217:VAL:HG21	0.62	1.70	5	1
1:A:126:ASP:HA	1:A:130:ILE:O	0.61	1.96	5	8
1:A:195:LEU:O	1:A:199:LEU:HG	0.60	1.97	7	5
1:A:207:MET:O	1:A:218:ILE:HA	0.60	1.97	8	7
1:A:133:ASP:OD2	1:A:138:LYS:HB3	0.59	1.97	10	1
1:A:189:ASP:O	1:A:193:ARG:HG2	0.59	1.97	2	2
1:A:211:VAL:HG23	1:A:215:GLY:H	0.57	1.59	9	1
1:A:159:LEU:HD22	1:A:167:MET:SD	0.56	2.40	7	1
1:A:169:ARG:NH2	1:A:186:ASN:HA	0.56	2.15	10	1
1:A:158:LEU:CD2	1:A:172:ILE:HA	0.56	2.31	5	4
1:A:204:ARG:O	1:A:207:MET:HB3	0.56	2.00	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:192:ILE:O	1:A:196:ARG:HG2	0.56	2.01	4	6
1:A:196:ARG:O	1:A:200:LYS:HG3	0.56	2.01	5	3
1:A:134:LYS:HA	1:A:153:TYR:OH	0.56	2.01	6	3
1:A:158:LEU:HG	1:A:167:MET:HE2	0.55	1.79	4	7
1:A:158:LEU:HG	1:A:167:MET:HE1	0.55	1.77	7	2
1:A:141:VAL:HB	1:A:204:ARG:NH1	0.54	2.17	9	1
1:A:173:LEU:HG	1:A:185:THR:CG2	0.54	2.32	10	4
1:A:174:ASN:O	1:A:178:GLY:HA3	0.54	2.03	1	7
1:A:133:ASP:OD1	1:A:136:ALA:HB3	0.54	2.02	10	1
1:A:124:ILE:HA	1:A:132:ILE:O	0.53	2.03	8	1
1:A:132:ILE:HD13	1:A:157:TYR:HA	0.53	1.81	5	1
1:A:130:ILE:HD12	1:A:130:ILE:N	0.52	2.20	2	4
1:A:185:THR:O	1:A:188:VAL:HG22	0.52	2.04	3	1
1:A:162:ASN:C	1:A:163:LYS:HD2	0.52	2.29	9	1
1:A:166:VAL:HA	1:A:217:VAL:HG11	0.50	1.82	5	1
1:A:158:LEU:HG	1:A:167:MET:CE	0.50	2.37	7	1
1:A:204:ARG:HD3	1:A:207:MET:SD	0.49	2.46	5	2
1:A:184:GLU:O	1:A:187:VAL:HG22	0.49	2.05	2	1
1:A:141:VAL:HG11	1:A:204:ARG:HD3	0.49	1.84	4	1
1:A:170:GLU:HG2	1:A:185:THR:HG21	0.49	1.82	10	1
1:A:210:THR:HG23	1:A:216:TYR:CE1	0.49	2.42	6	1
1:A:188:VAL:O	1:A:192:ILE:HG12	0.48	2.09	2	2
1:A:140:THR:HA	1:A:144:ALA:O	0.48	2.08	8	3
1:A:163:LYS:HG2	1:A:164:ASN:H	0.48	1.67	9	1
1:A:173:LEU:CG	1:A:185:THR:HG22	0.47	2.36	1	4
1:A:191:TYR:HA	1:A:194:TYR:CD1	0.47	2.44	10	1
1:A:188:VAL:CG2	1:A:189:ASP:N	0.47	2.78	3	1
1:A:158:LEU:O	1:A:162:ASN:HB3	0.47	2.10	8	1
1:A:130:ILE:CD1	1:A:207:MET:SD	0.46	3.04	9	1
1:A:133:ASP:CG	1:A:138:LYS:HB3	0.46	2.35	10	1
1:A:152:GLU:HA	1:A:155:LEU:HD12	0.46	1.87	10	5
1:A:173:LEU:HG	1:A:185:THR:HA	0.46	1.88	10	3
1:A:141:VAL:HB	1:A:204:ARG:CZ	0.45	2.41	9	1
1:A:167:MET:O	1:A:215:GLY:HA3	0.45	2.11	8	2
1:A:159:LEU:HD23	1:A:167:MET:SD	0.45	2.51	2	1
1:A:204:ARG:NE	1:A:204:ARG:HA	0.45	2.27	3	3
1:A:128:ASN:HB2	1:A:207:MET:HE3	0.44	1.88	5	1
1:A:192:ILE:O	1:A:195:LEU:HB2	0.44	2.13	9	1
1:A:173:LEU:C	1:A:173:LEU:HD13	0.44	2.38	10	1
1:A:130:ILE:N	1:A:130:ILE:CD1	0.43	2.81	7	1
1:A:127:VAL:HG11	1:A:160:ALA:O	0.43	2.13	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:159:LEU:HD11	1:A:217:VAL:HA	0.43	1.89	7	2
1:A:162:ASN:ND2	1:A:167:MET:HG2	0.43	2.28	8	1
1:A:186:ASN:HA	1:A:189:ASP:OD2	0.43	2.14	3	1
1:A:188:VAL:HG23	1:A:189:ASP:N	0.43	2.28	3	1
1:A:125:ILE:O	1:A:131:THR:HA	0.43	2.13	2	1
1:A:130:ILE:CG1	1:A:207:MET:HE1	0.43	2.43	6	1
1:A:192:ILE:HG21	1:A:216:TYR:CD1	0.43	2.48	5	1
1:A:154:ASP:OD2	1:A:176:VAL:HA	0.42	2.14	6	2
1:A:184:GLU:O	1:A:187:VAL:HG12	0.42	2.14	7	1
1:A:146:ILE:HD12	1:A:146:ILE:N	0.42	2.29	1	2
1:A:200:LYS:HB2	1:A:201:PRO:HD3	0.41	1.91	7	3
1:A:127:VAL:CG2	1:A:160:ALA:HB1	0.41	2.45	2	1
1:A:158:LEU:HD13	1:A:175:HIS:CD2	0.41	2.51	6	2
1:A:168:GLN:HB3	1:A:170:GLU:OE1	0.41	2.16	5	1
1:A:184:GLU:HB2	1:A:186:ASN:OD1	0.41	2.15	10	1
1:A:198:LYS:O	1:A:201:PRO:HD2	0.41	2.15	10	1
1:A:127:VAL:HG12	1:A:163:LYS:HD2	0.41	1.92	8	1
1:A:162:ASN:HD21	1:A:217:VAL:HA	0.41	1.76	8	1
1:A:154:ASP:O	1:A:158:LEU:HB2	0.40	2.15	9	1
1:A:132:ILE:HG12	1:A:139:VAL:HG22	0.40	1.92	4	1
1:A:168:GLN:HB2	1:A:171:GLN:CG	0.40	2.46	9	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	90/105 (86%)	86±1 (96±1%)	3±1 (3±1%)	1±0 (1±1%)	21	71
All	All	900/1050 (86%)	865 (96%)	29 (3%)	6 (1%)	21	71

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	A	163	LYS	6

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	83/96 (86%)	78±2 (94±2%)	5±2 (6±2%)	19 71
All	All	830/960 (86%)	782 (94%)	48 (6%)	19 71

All 21 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	140	THR	10
1	A	156	LEU	10
1	A	163	LYS	5
1	A	205	ASP	3
1	A	131	THR	2
1	A	141	VAL	2
1	A	159	LEU	2
1	A	167	MET	1
1	A	187	VAL	1
1	A	164	ASN	1
1	A	193	ARG	1
1	A	217	VAL	1
1	A	150	LYS	1
1	A	209	GLU	1
1	A	130	ILE	1
1	A	196	ARG	1
1	A	207	MET	1
1	A	158	LEU	1
1	A	162	ASN	1
1	A	186	ASN	1
1	A	189	ASP	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

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 89% for the well-defined parts and 82% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	1250
Number of shifts mapped to atoms	1250
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	97	-0.38 ± 0.28	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	92	0.20 ± 0.19	None needed (< 0.5 ppm)
$^{13}\text{C}'$	95	-0.03 ± 0.22	None needed (< 0.5 ppm)
^{15}N	93	0.53 ± 0.22	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 89%, i.e. 1186 atoms were assigned a chemical shift out of a possible 1336. 0 out of 19 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	452/458 (99%)	184/186 (99%)	180/182 (99%)	88/90 (98%)
Sidechain	662/786 (84%)	450/509 (88%)	212/242 (88%)	0/35 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	72/92 (78%)	36/43 (84%)	35/44 (80%)	1/5 (20%)
Overall	1186/1336 (89%)	670/738 (91%)	427/468 (91%)	89/130 (68%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 82%, i.e. 1250 atoms were assigned a chemical shift out of a possible 1526. 0 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	480/529 (91%)	195/215 (91%)	192/210 (91%)	93/104 (89%)
Sidechain	690/848 (81%)	469/549 (85%)	221/263 (84%)	0/36 (0%)
Aromatic	80/149 (54%)	40/71 (56%)	39/61 (64%)	1/17 (6%)
Overall	1250/1526 (82%)	704/835 (84%)	452/534 (85%)	94/157 (60%)

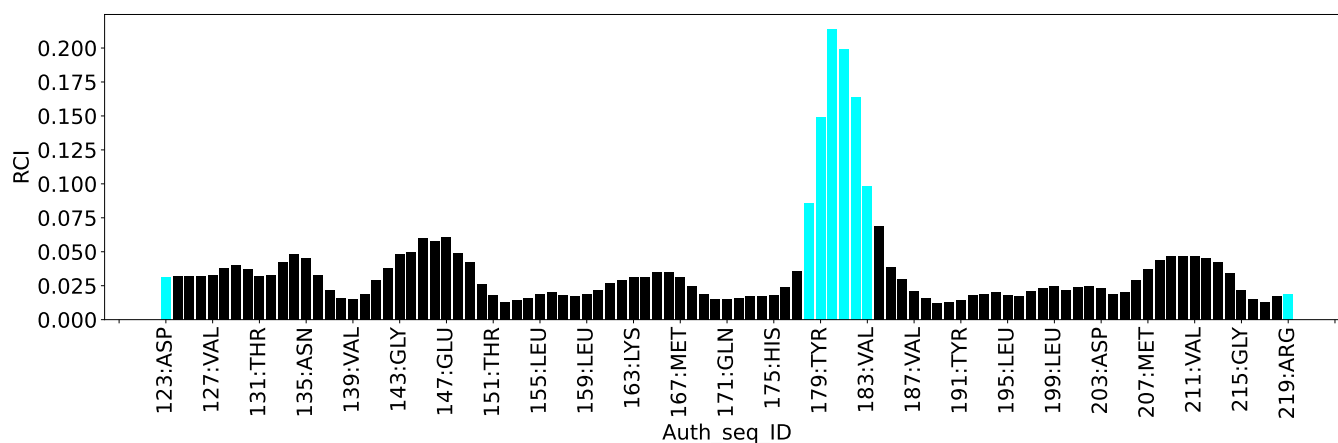
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	1406
Intra-residue ($ i-j =0$)	732
Sequential ($ i-j =1$)	257
Medium range ($ i-j >1$ and $ i-j <5$)	143
Long range ($ i-j \geq 5$)	274
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	174
Number of unmapped restraints	0
Number of restraints per residue	15.0
Number of long range restraints per residue ¹	2.6

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)	61.2	0.2
0.2-0.5 (Medium)	110.0	0.5
>0.5 (Large)	99.3	5.38

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

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

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	7.5	5.41
10.0-20.0 (Medium)	None	None
>20.0 (Large)	1.0	128.62

9 Distance violation analysis ⓘ

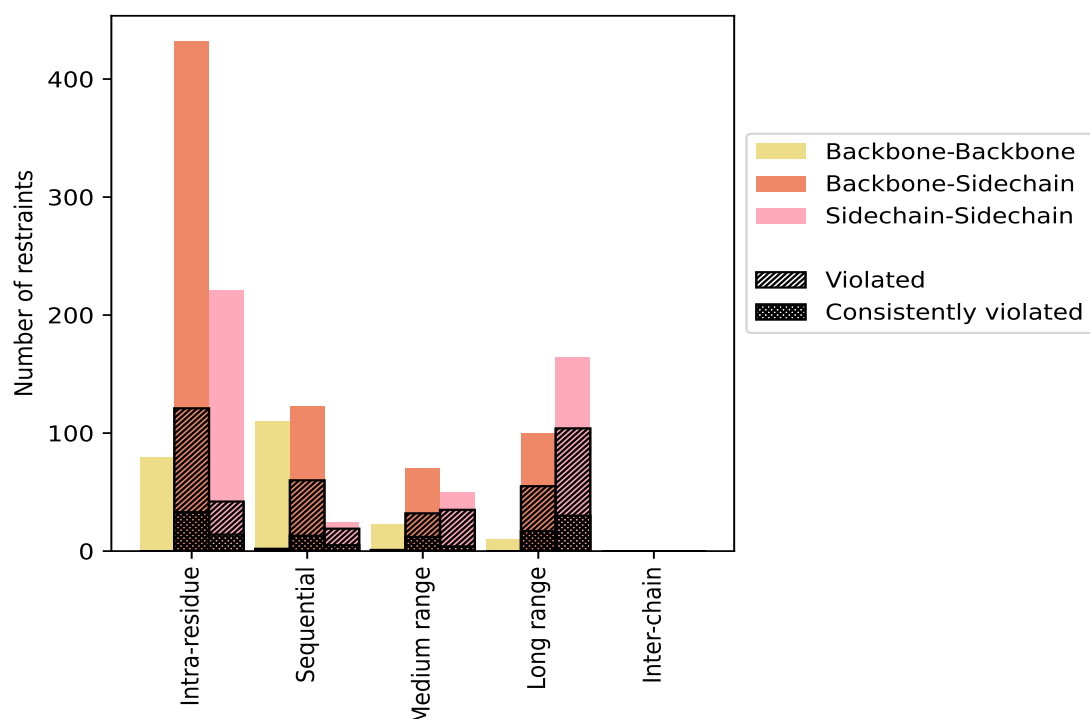
9.1 Summary of distance violations ⓘ

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 ($i-j =0$)	732	52.1	163	22.3	11.6	47	6.4	3.3
Backbone-Backbone	79	5.6	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	432	30.7	121	28.0	8.6	33	7.6	2.3
Sidechain-Sidechain	221	15.7	42	19.0	3.0	14	6.3	1.0
Sequential ($i-j =1$)	257	18.3	81	31.5	5.8	19	7.4	1.4
Backbone-Backbone	110	7.8	2	1.8	0.1	1	0.9	0.1
Backbone-Sidechain	123	8.7	60	48.8	4.3	13	10.6	0.9
Sidechain-Sidechain	24	1.7	19	79.2	1.4	5	20.8	0.4
Medium range ($i-j >1$ & $i-j <5$)	143	10.2	68	47.6	4.8	16	11.2	1.1
Backbone-Backbone	23	1.6	1	4.3	0.1	0	0.0	0.0
Backbone-Sidechain	70	5.0	32	45.7	2.3	12	17.1	0.9
Sidechain-Sidechain	50	3.6	35	70.0	2.5	4	8.0	0.3
Long range ($i-j \geq 5$)	274	19.5	159	58.0	11.3	47	17.2	3.3
Backbone-Backbone	10	0.7	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	100	7.1	55	55.0	3.9	17	17.0	1.2
Sidechain-Sidechain	164	11.7	104	63.4	7.4	30	18.3	2.1
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1406	100.0	471	33.5	33.5	129	9.2	9.2
Backbone-Backbone	222	15.8	3	1.4	0.2	1	0.5	0.1
Backbone-Sidechain	725	51.6	268	37.0	19.1	75	10.3	5.3
Sidechain-Sidechain	459	32.6	200	43.6	14.2	53	11.5	3.8

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

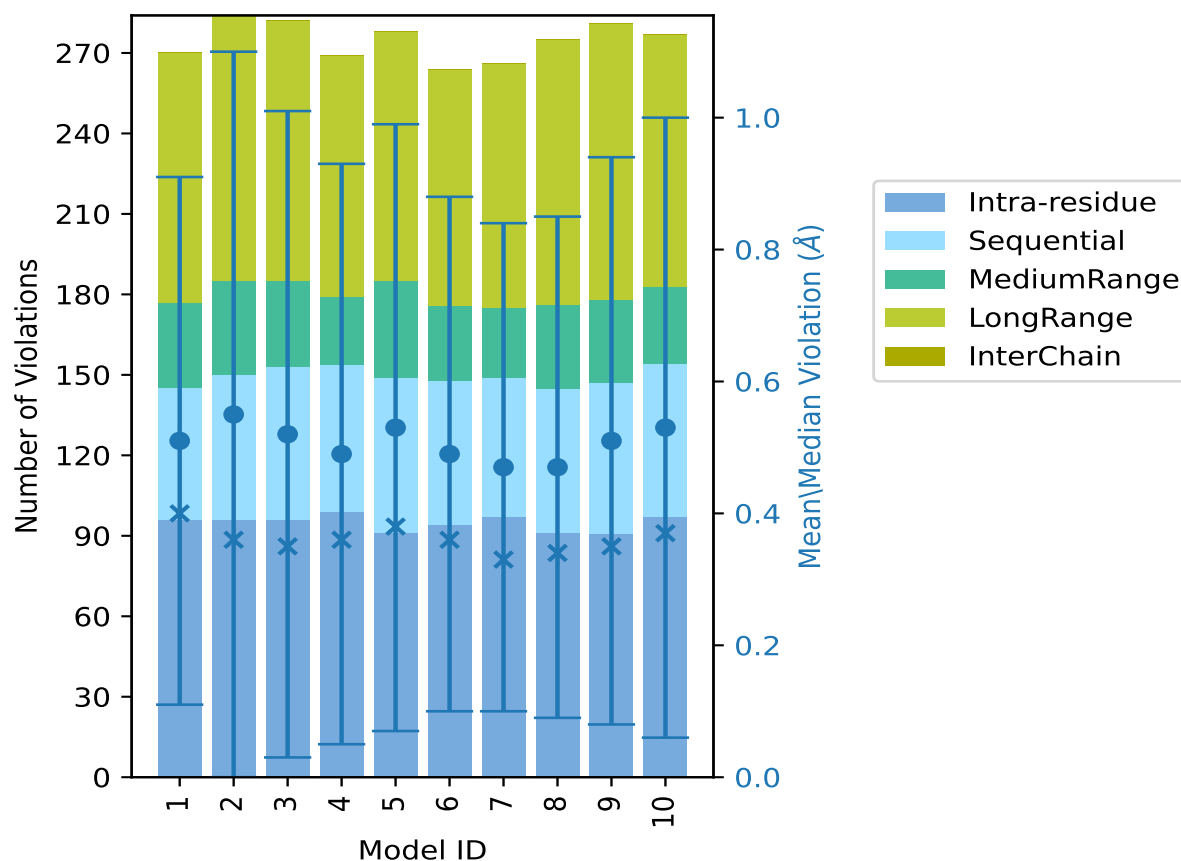
9.2 Distance violation statistics for each model [i](#)

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	96	49	32	93	0	270	0.51	2.77	0.4	0.4
2	96	54	35	99	0	284	0.55	5.38	0.55	0.36
3	96	57	32	97	0	282	0.52	3.22	0.49	0.35
4	99	55	25	90	0	269	0.49	4.16	0.44	0.36
5	91	58	36	93	0	278	0.53	3.19	0.46	0.38
6	94	54	28	88	0	264	0.49	2.55	0.39	0.36
7	97	52	26	91	0	266	0.47	2.08	0.37	0.33
8	91	54	31	99	0	275	0.47	2.58	0.38	0.34
9	91	56	31	103	0	281	0.51	2.7	0.43	0.35
10	97	57	29	94	0	277	0.53	3.57	0.47	0.37

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

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



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

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

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 935(IR:569, SQ:176, MR:75, LR:115, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
41	11	12	25	0	89	1	10.0
10	7	7	12	0	36	2	20.0
9	3	8	12	0	32	3	30.0

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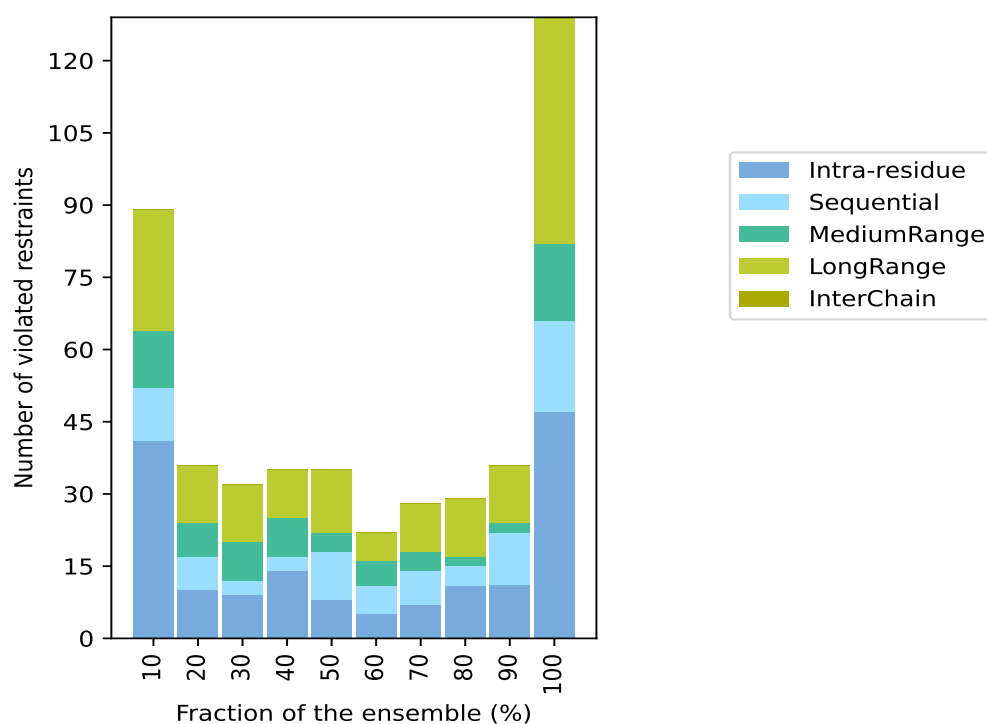
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
14	3	8	10	0	35	4	40.0
8	10	4	13	0	35	5	50.0
5	6	5	6	0	22	6	60.0
7	7	4	10	0	28	7	70.0
11	4	2	12	0	29	8	80.0
11	11	2	12	0	36	9	90.0
47	19	16	47	0	129	10	100.0

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

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

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

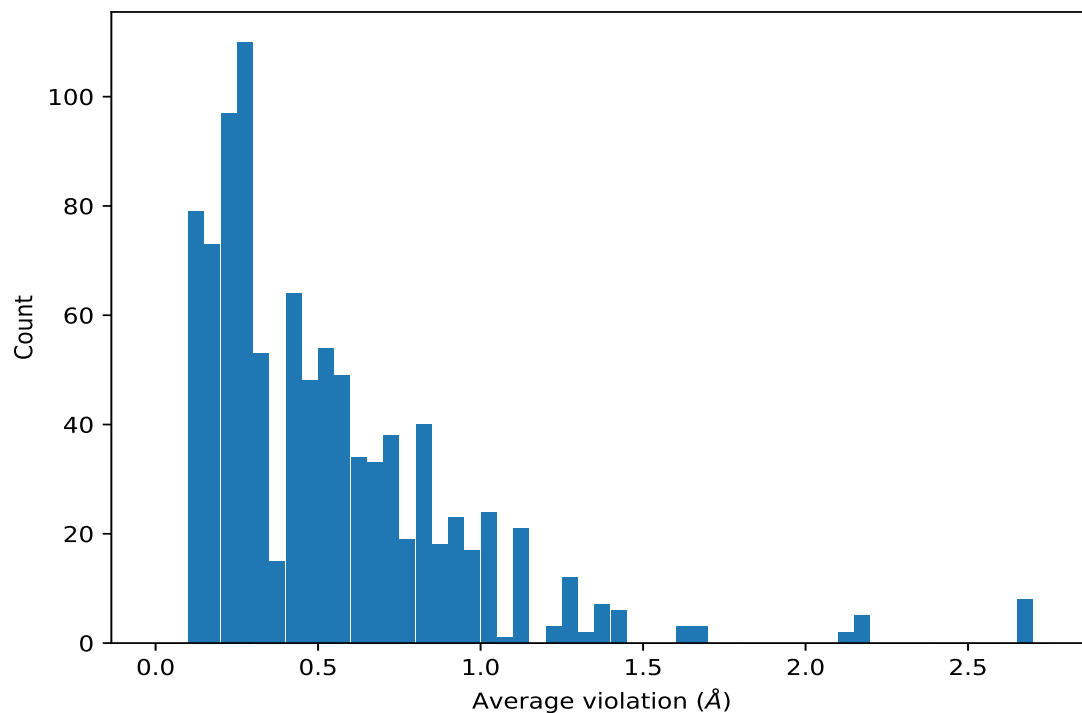


9.4 Most violated distance restraints in the ensemble [i](#)

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

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

in the ensemble



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,166)	1:188:A:VAL:HG23	1:177:A:TRP:HB3	10	2.17	0.37	2.1
(2,166)	1:188:A:VAL:HG23	1:191:A:TYR:HB3	10	2.17	0.37	2.1
(2,166)	1:188:A:VAL:HG21	1:191:A:TYR:HB3	10	2.17	0.37	2.1
(2,166)	1:188:A:VAL:HG22	1:177:A:TRP:HB3	10	2.17	0.37	2.1
(2,166)	1:188:A:VAL:HG21	1:177:A:TRP:HB3	10	2.17	0.37	2.1
(1,697)	1:177:A:TRP:HB2	1:183:A:VAL:HG21	10	1.68	0.12	1.71
(1,697)	1:177:A:TRP:HB2	1:183:A:VAL:HG23	10	1.68	0.12	1.71
(1,697)	1:177:A:TRP:HB2	1:183:A:VAL:HG22	10	1.68	0.12	1.71
(1,742)	1:207:A:MET:HE1	1:218:A:ILE:HG13	10	1.61	0.07	1.6
(1,742)	1:207:A:MET:HE2	1:218:A:ILE:HG13	10	1.61	0.07	1.6
(1,742)	1:207:A:MET:HE3	1:218:A:ILE:HG13	10	1.61	0.07	1.6
(1,340)	1:142:A:ASN:HB3	1:141:A:VAL:HG13	10	1.45	1.19	1.84
(1,340)	1:142:A:ASN:HB3	1:141:A:VAL:HG12	10	1.45	1.19	1.84
(1,340)	1:142:A:ASN:HB3	1:141:A:VAL:HG11	10	1.45	1.19	1.84
(1,751)	1:167:A:MET:HE3	1:158:A:LEU:HB2	10	1.41	0.04	1.41

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,751)	1:167:A:MET:HE1	1:158:A:LEU:HB2	10	1.41	0.04	1.41
(1,751)	1:167:A:MET:HE2	1:158:A:LEU:HB2	10	1.41	0.04	1.41
(2,205)	1:172:A:ILE:HG22	1:158:A:LEU:HD12	10	1.36	0.12	1.35
(2,205)	1:172:A:ILE:HG21	1:158:A:LEU:HD11	10	1.36	0.12	1.35
(2,205)	1:172:A:ILE:HG23	1:158:A:LEU:HD11	10	1.36	0.12	1.35
(2,205)	1:172:A:ILE:HG21	1:158:A:LEU:HD12	10	1.36	0.12	1.35
(2,205)	1:172:A:ILE:HG23	1:158:A:LEU:HD13	10	1.36	0.12	1.35
(2,205)	1:172:A:ILE:HG23	1:158:A:LEU:HD12	10	1.36	0.12	1.35
(2,205)	1:172:A:ILE:HG22	1:158:A:LEU:HD13	10	1.36	0.12	1.35
(2,241)	1:216:A:TYR:HB2	1:159:A:LEU:HB3	10	1.32	0.19	1.38
(2,241)	1:216:A:TYR:HB2	1:217:A:VAL:HB	10	1.32	0.19	1.38
(1,513)	1:156:A:LEU:HB3	1:156:A:LEU:HD21	10	1.02	0.01	1.02
(1,513)	1:156:A:LEU:HB3	1:156:A:LEU:HD23	10	1.02	0.01	1.02
(1,513)	1:156:A:LEU:HB3	1:156:A:LEU:HD22	10	1.02	0.01	1.02
(2,207)	1:208:A:ILE:HG21	1:208:A:ILE:H	10	1.01	0.02	1.02
(2,207)	1:208:A:ILE:HG23	1:208:A:ILE:H	10	1.01	0.02	1.02
(2,207)	1:208:A:ILE:HG22	1:208:A:ILE:H	10	1.01	0.02	1.02
(1,26)	1:190:A:VAL:HA	1:193:A:ARG:HB3	10	1.0	0.51	1.06
(2,288)	1:208:A:ILE:HG21	1:208:A:ILE:H	10	1.0	0.16	1.1
(2,288)	1:208:A:ILE:H	1:199:A:LEU:HD11	10	1.0	0.16	1.1
(2,288)	1:208:A:ILE:HG23	1:208:A:ILE:H	10	1.0	0.16	1.1
(2,288)	1:208:A:ILE:H	1:199:A:LEU:HD13	10	1.0	0.16	1.1
(2,288)	1:208:A:ILE:H	1:199:A:LEU:HD12	10	1.0	0.16	1.1
(2,288)	1:208:A:ILE:HG22	1:208:A:ILE:H	10	1.0	0.16	1.1
(1,300)	1:202:A:TYR:HB2	1:141:A:VAL:HB	10	1.0	0.32	1.08
(2,282)	1:157:A:TYR:H	1:148:A:LEU:HD11	10	1.0	0.1	1.0
(2,282)	1:157:A:TYR:H	1:132:A:ILE:HG12	10	1.0	0.1	1.0
(2,282)	1:157:A:TYR:H	1:148:A:LEU:HD12	10	1.0	0.1	1.0
(2,282)	1:157:A:TYR:H	1:132:A:ILE:HG21	10	1.0	0.1	1.0
(2,282)	1:157:A:TYR:H	1:148:A:LEU:HD13	10	1.0	0.1	1.0
(2,216)	1:192:A:ILE:HG23	1:192:A:ILE:H	10	0.99	0.02	0.98
(2,216)	1:192:A:ILE:HG22	1:192:A:ILE:H	10	0.99	0.02	0.98
(2,216)	1:192:A:ILE:HG21	1:192:A:ILE:H	10	0.99	0.02	0.98
(2,167)	1:151:A:THR:HG22	1:151:A:THR:H	10	0.97	0.01	0.97
(2,167)	1:151:A:THR:HG21	1:177:A:TRP:HE3	10	0.97	0.01	0.97
(2,167)	1:151:A:THR:HG21	1:151:A:THR:H	10	0.97	0.01	0.97
(2,167)	1:151:A:THR:HG23	1:151:A:THR:H	10	0.97	0.01	0.97
(2,151)	1:155:A:LEU:HD11	1:153:A:TYR:H	10	0.95	0.04	0.95
(2,151)	1:155:A:LEU:HD12	1:153:A:TYR:H	10	0.95	0.04	0.95
(2,151)	1:155:A:LEU:HD13	1:153:A:TYR:H	10	0.95	0.04	0.95
(2,151)	1:195:A:LEU:HD11	1:196:A:ARG:H	10	0.95	0.04	0.95
(2,1)	1:131:A:THR:HB	1:124:A:ILE:HG23	10	0.95	0.13	0.94

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1)	1:131:A:THR:HB	1:124:A:ILE:HG21	10	0.95	0.13	0.94
(2,1)	1:131:A:THR:HB	1:124:A:ILE:HG22	10	0.95	0.13	0.94
(2,1)	1:131:A:THR:HB	1:139:A:VAL:HG13	10	0.95	0.13	0.94
(2,1)	1:131:A:THR:HB	1:139:A:VAL:HG11	10	0.95	0.13	0.94
(2,148)	1:199:A:LEU:HD11	1:207:A:MET:HB2	10	0.94	0.93	0.55
(2,148)	1:199:A:LEU:HD13	1:207:A:MET:HB2	10	0.94	0.93	0.55
(2,148)	1:199:A:LEU:HD12	1:207:A:MET:HB2	10	0.94	0.93	0.55
(2,148)	1:199:A:LEU:HD11	1:207:A:MET:HE1	10	0.94	0.93	0.55
(2,209)	1:207:A:MET:HE3	1:207:A:MET:HA	10	0.89	0.08	0.89
(2,209)	1:207:A:MET:HE2	1:207:A:MET:HA	10	0.89	0.08	0.89
(2,209)	1:207:A:MET:HE1	1:207:A:MET:HA	10	0.89	0.08	0.89
(2,209)	1:207:A:MET:HE3	1:208:A:ILE:HA	10	0.89	0.08	0.89
(1,16)	1:188:A:VAL:HA	1:191:A:TYR:HB3	10	0.87	0.14	0.89
(1,111)	1:152:A:GLU:HA	1:155:A:LEU:HB3	10	0.87	0.05	0.86
(1,223)	1:219:A:ARG:HD2	1:219:A:ARG:HB2	10	0.87	0.25	0.95
(1,223)	1:219:A:ARG:HD3	1:219:A:ARG:HB2	10	0.87	0.25	0.95
(2,286)	1:158:A:LEU:H	1:158:A:LEU:HD22	10	0.87	0.11	0.87
(2,286)	1:176:A:VAL:HG21	1:158:A:LEU:H	10	0.87	0.11	0.87
(2,286)	1:158:A:LEU:H	1:158:A:LEU:HD23	10	0.87	0.11	0.87
(2,286)	1:158:A:LEU:H	1:158:A:LEU:HD21	10	0.87	0.11	0.87
(1,633)	1:166:A:VAL:HG11	1:215:A:GLY:H	10	0.86	0.57	0.67
(1,633)	1:166:A:VAL:HG13	1:215:A:GLY:H	10	0.86	0.57	0.67
(1,633)	1:166:A:VAL:HG12	1:215:A:GLY:H	10	0.86	0.57	0.67
(1,255)	1:159:A:LEU:HB2	1:218:A:ILE:HG12	10	0.85	0.33	0.76
(2,219)	1:172:A:ILE:HD11	1:215:A:GLY:HA2	10	0.85	0.11	0.82
(2,219)	1:172:A:ILE:HD13	1:215:A:GLY:HA2	10	0.85	0.11	0.82
(2,219)	1:172:A:ILE:HD13	1:172:A:ILE:HA	10	0.85	0.11	0.82
(2,180)	1:149:A:THR:HG21	1:148:A:LEU:HD22	10	0.82	0.11	0.84
(2,180)	1:149:A:THR:HG21	1:148:A:LEU:HD23	10	0.82	0.11	0.84
(2,180)	1:149:A:THR:HG21	1:148:A:LEU:HD21	10	0.82	0.11	0.84
(2,180)	1:149:A:THR:HG23	1:148:A:LEU:HD21	10	0.82	0.11	0.84
(2,180)	1:149:A:THR:HG22	1:148:A:LEU:HD21	10	0.82	0.11	0.84
(2,180)	1:149:A:THR:HG22	1:148:A:LEU:HD23	10	0.82	0.11	0.84
(2,278)	1:172:A:ILE:H	1:188:A:VAL:HG12	10	0.81	0.05	0.82
(2,278)	1:172:A:ILE:HG22	1:172:A:ILE:H	10	0.81	0.05	0.82
(2,278)	1:172:A:ILE:HG21	1:172:A:ILE:H	10	0.81	0.05	0.82
(2,278)	1:172:A:ILE:HG23	1:172:A:ILE:H	10	0.81	0.05	0.82
(2,278)	1:172:A:ILE:H	1:188:A:VAL:HG11	10	0.81	0.05	0.82
(2,287)	1:159:A:LEU:H	1:156:A:LEU:HD11	10	0.81	0.19	0.73
(2,287)	1:159:A:LEU:H	1:158:A:LEU:HD23	10	0.81	0.19	0.73
(2,287)	1:159:A:LEU:H	1:158:A:LEU:HD21	10	0.81	0.19	0.73
(2,287)	1:159:A:LEU:H	1:158:A:LEU:HD22	10	0.81	0.19	0.73

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,287)	1:159:A:LEU:H	1:156:A:LEU:HD13	10	0.81	0.19	0.73
(2,145)	1:192:A:ILE:HG12	1:195:A:LEU:HD23	10	0.78	0.09	0.78
(2,145)	1:192:A:ILE:HG12	1:172:A:ILE:HD13	10	0.78	0.09	0.78
(2,145)	1:192:A:ILE:HG12	1:195:A:LEU:HD22	10	0.78	0.09	0.78
(2,145)	1:192:A:ILE:HG12	1:172:A:ILE:HD12	10	0.78	0.09	0.78
(1,532)	1:173:A:LEU:HD22	1:174:A:ASN:H	10	0.76	0.51	0.38
(1,532)	1:173:A:LEU:HD23	1:174:A:ASN:H	10	0.76	0.51	0.38
(1,532)	1:173:A:LEU:HD21	1:174:A:ASN:H	10	0.76	0.51	0.38
(1,1086)	1:151:A:THR:H	1:149:A:THR:HG23	10	0.74	0.05	0.75
(1,1086)	1:151:A:THR:H	1:149:A:THR:HG22	10	0.74	0.05	0.75
(1,1086)	1:151:A:THR:H	1:149:A:THR:HG21	10	0.74	0.05	0.75
(2,221)	1:130:A:ILE:HD13	1:127:A:VAL:H	10	0.74	0.37	0.8
(2,221)	1:130:A:ILE:HD11	1:127:A:VAL:H	10	0.74	0.37	0.8
(2,221)	1:130:A:ILE:HD12	1:127:A:VAL:H	10	0.74	0.37	0.8
(2,221)	1:130:A:ILE:HD11	1:131:A:THR:H	10	0.74	0.37	0.8
(2,139)	1:155:A:LEU:HD23	1:155:A:LEU:H	10	0.74	0.08	0.72
(2,139)	1:155:A:LEU:HD21	1:155:A:LEU:H	10	0.74	0.08	0.72
(2,139)	1:155:A:LEU:HD22	1:155:A:LEU:H	10	0.74	0.08	0.72
(2,156)	1:195:A:LEU:HD12	1:152:A:GLU:HG3	10	0.74	0.16	0.68
(2,156)	1:195:A:LEU:HD13	1:152:A:GLU:HG3	10	0.74	0.16	0.68
(2,156)	1:195:A:LEU:HD13	1:152:A:GLU:HB2	10	0.74	0.16	0.68
(2,156)	1:195:A:LEU:HD11	1:152:A:GLU:HG3	10	0.74	0.16	0.68
(1,1042)	1:176:A:VAL:HG11	1:176:A:VAL:H	10	0.73	0.02	0.74
(1,1042)	1:176:A:VAL:HG13	1:176:A:VAL:H	10	0.73	0.02	0.74
(1,1042)	1:176:A:VAL:HG12	1:176:A:VAL:H	10	0.73	0.02	0.74
(2,129)	1:148:A:LEU:HD11	1:149:A:THR:H	10	0.73	0.07	0.74
(2,129)	1:148:A:LEU:HD12	1:149:A:THR:H	10	0.73	0.07	0.74
(2,129)	1:148:A:LEU:HD13	1:149:A:THR:H	10	0.73	0.07	0.74
(2,129)	1:132:A:ILE:HG12	1:140:A:THR:H	10	0.73	0.07	0.74
(2,204)	1:172:A:ILE:HG23	1:155:A:LEU:HG	10	0.73	0.1	0.76
(2,204)	1:172:A:ILE:HG21	1:158:A:LEU:HB2	10	0.73	0.1	0.76
(2,204)	1:172:A:ILE:HG21	1:155:A:LEU:HG	10	0.73	0.1	0.76
(2,204)	1:172:A:ILE:HG23	1:158:A:LEU:HB2	10	0.73	0.1	0.76
(2,204)	1:172:A:ILE:HG22	1:155:A:LEU:HG	10	0.73	0.1	0.76
(2,204)	1:172:A:ILE:HG22	1:158:A:LEU:HB2	10	0.73	0.1	0.76
(2,122)	1:147:A:GLU:HB2	1:146:A:ILE:HG22	10	0.73	0.47	0.5
(2,122)	1:170:A:GLU:HB3	1:173:A:LEU:HD21	10	0.73	0.47	0.5
(2,122)	1:170:A:GLU:HB3	1:173:A:LEU:HD23	10	0.73	0.47	0.5
(2,122)	1:170:A:GLU:HB3	1:173:A:LEU:HD22	10	0.73	0.47	0.5
(2,122)	1:147:A:GLU:HB2	1:146:A:ILE:HG23	10	0.73	0.47	0.5
(2,122)	1:147:A:GLU:HB2	1:146:A:ILE:HG21	10	0.73	0.47	0.5
(2,9)	1:210:A:THR:HA	1:209:A:GLU:HG2	10	0.68	0.32	0.54

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,9)	1:210:A:THR:HA	1:216:A:TYR:HB2	10	0.68	0.32	0.54
(2,9)	1:210:A:THR:HA	1:209:A:GLU:HG3	10	0.68	0.32	0.54
(2,165)	1:188:A:VAL:HG21	1:172:A:ILE:H	10	0.66	0.12	0.65
(2,165)	1:188:A:VAL:HG22	1:186:A:ASN:H	10	0.66	0.12	0.65
(2,165)	1:188:A:VAL:HG21	1:186:A:ASN:H	10	0.66	0.12	0.65
(2,165)	1:188:A:VAL:HG23	1:186:A:ASN:H	10	0.66	0.12	0.65
(2,165)	1:188:A:VAL:HG22	1:172:A:ILE:H	10	0.66	0.12	0.65
(2,206)	1:160:A:ALA:HB2	1:161:A:GLU:HB2	10	0.66	0.1	0.69
(2,206)	1:160:A:ALA:HB3	1:161:A:GLU:HB2	10	0.66	0.1	0.69
(2,206)	1:160:A:ALA:HB1	1:161:A:GLU:HB2	10	0.66	0.1	0.69
(1,784)	1:218:A:ILE:HD12	1:218:A:ILE:HA	10	0.66	0.02	0.66
(1,784)	1:218:A:ILE:HD13	1:218:A:ILE:HA	10	0.66	0.02	0.66
(1,784)	1:218:A:ILE:HD11	1:218:A:ILE:HA	10	0.66	0.02	0.66
(2,229)	1:192:A:ILE:HD13	1:216:A:TYR:HD1	10	0.66	0.26	0.56
(2,229)	1:192:A:ILE:HD13	1:216:A:TYR:HD2	10	0.66	0.26	0.56
(2,229)	1:192:A:ILE:HD12	1:216:A:TYR:HD2	10	0.66	0.26	0.56
(2,229)	1:192:A:ILE:HD11	1:216:A:TYR:HD2	10	0.66	0.26	0.56
(2,229)	1:192:A:ILE:HD12	1:216:A:TYR:HD1	10	0.66	0.26	0.56
(2,227)	1:218:A:ILE:HD13	1:160:A:ALA:HB3	10	0.64	0.14	0.7
(2,227)	1:218:A:ILE:HD11	1:160:A:ALA:HB1	10	0.64	0.14	0.7
(2,227)	1:218:A:ILE:HD13	1:160:A:ALA:HB1	10	0.64	0.14	0.7
(2,227)	1:160:A:ALA:HB3	1:125:A:ILE:HD11	10	0.64	0.14	0.7
(2,227)	1:218:A:ILE:HD11	1:160:A:ALA:HB3	10	0.64	0.14	0.7
(2,227)	1:218:A:ILE:HD11	1:160:A:ALA:HB2	10	0.64	0.14	0.7
(2,227)	1:160:A:ALA:HB1	1:125:A:ILE:HD13	10	0.64	0.14	0.7
(2,227)	1:160:A:ALA:HB2	1:125:A:ILE:HD12	10	0.64	0.14	0.7
(2,196)	1:136:A:ALA:HB3	1:135:A:ASN:H	10	0.63	0.06	0.6
(2,196)	1:136:A:ALA:HB2	1:135:A:ASN:H	10	0.63	0.06	0.6
(2,196)	1:136:A:ALA:HB1	1:135:A:ASN:H	10	0.63	0.06	0.6
(1,849)	1:173:A:LEU:HD11	1:173:A:LEU:H	10	0.62	0.11	0.57
(1,849)	1:173:A:LEU:HD12	1:173:A:LEU:H	10	0.62	0.11	0.57
(1,849)	1:173:A:LEU:HD13	1:173:A:LEU:H	10	0.62	0.11	0.57
(2,301)	1:207:A:MET:H	1:199:A:LEU:HD11	10	0.62	0.32	0.55
(2,301)	1:207:A:MET:H	1:199:A:LEU:HD13	10	0.62	0.32	0.55
(2,301)	1:207:A:MET:H	1:199:A:LEU:HD12	10	0.62	0.32	0.55
(2,301)	1:207:A:MET:H	1:208:A:ILE:HD12	10	0.62	0.32	0.55
(1,1040)	1:190:A:VAL:HG11	1:190:A:VAL:H	10	0.62	0.02	0.62
(1,1040)	1:190:A:VAL:HG12	1:190:A:VAL:H	10	0.62	0.02	0.62
(1,1040)	1:190:A:VAL:HG13	1:190:A:VAL:H	10	0.62	0.02	0.62
(1,1057)	1:131:A:THR:HG21	1:131:A:THR:H	10	0.62	0.05	0.6
(1,1057)	1:131:A:THR:HG23	1:131:A:THR:H	10	0.62	0.05	0.6
(1,1057)	1:131:A:THR:HG22	1:131:A:THR:H	10	0.62	0.05	0.6

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,754)	1:158:A:LEU:HD11	1:167:A:MET:HE1	10	0.59	0.17	0.52
(1,754)	1:158:A:LEU:HD13	1:167:A:MET:HE2	10	0.59	0.17	0.52
(1,754)	1:158:A:LEU:HD13	1:167:A:MET:HE1	10	0.59	0.17	0.52
(1,754)	1:158:A:LEU:HD12	1:167:A:MET:HE3	10	0.59	0.17	0.52
(1,754)	1:158:A:LEU:HD11	1:167:A:MET:HE2	10	0.59	0.17	0.52
(1,754)	1:158:A:LEU:HD12	1:167:A:MET:HE2	10	0.59	0.17	0.52
(1,754)	1:158:A:LEU:HD11	1:167:A:MET:HE3	10	0.59	0.17	0.52
(1,1003)	1:159:A:LEU:HB3	1:159:A:LEU:H	10	0.59	0.21	0.7
(1,834)	1:173:A:LEU:HD22	1:173:A:LEU:H	10	0.58	0.08	0.63
(1,834)	1:173:A:LEU:HD21	1:173:A:LEU:H	10	0.58	0.08	0.63
(1,834)	1:173:A:LEU:HD23	1:173:A:LEU:H	10	0.58	0.08	0.63
(1,820)	1:151:A:THR:HB	1:176:A:VAL:HG12	10	0.58	0.09	0.6
(1,820)	1:151:A:THR:HB	1:176:A:VAL:HG11	10	0.58	0.09	0.6
(1,820)	1:151:A:THR:HB	1:176:A:VAL:HG13	10	0.58	0.09	0.6
(1,768)	1:216:A:TYR:HB3	1:172:A:ILE:HD12	10	0.57	0.08	0.54
(1,768)	1:216:A:TYR:HB3	1:172:A:ILE:HD11	10	0.57	0.08	0.54
(1,578)	1:151:A:THR:HG22	1:191:A:TYR:HB2	10	0.57	0.12	0.6
(1,578)	1:151:A:THR:HG23	1:191:A:TYR:HB2	10	0.57	0.12	0.6
(1,578)	1:151:A:THR:HG21	1:191:A:TYR:HB2	10	0.57	0.12	0.6
(1,1085)	1:151:A:THR:HG22	1:151:A:THR:H	10	0.55	0.01	0.55
(1,1085)	1:151:A:THR:HG21	1:151:A:THR:H	10	0.55	0.01	0.55
(1,1085)	1:151:A:THR:HG23	1:151:A:THR:H	10	0.55	0.01	0.55
(1,972)	1:169:A:ARG:H	1:168:A:GLN:HB2	10	0.54	0.1	0.55
(2,184)	1:183:A:VAL:HG13	1:177:A:TRP:HD1	10	0.53	0.16	0.57
(2,184)	1:183:A:VAL:HG12	1:177:A:TRP:HD1	10	0.53	0.16	0.57
(2,184)	1:187:A:VAL:HG21	1:177:A:TRP:HD1	10	0.53	0.16	0.57
(2,184)	1:183:A:VAL:HG11	1:177:A:TRP:HD1	10	0.53	0.16	0.57
(2,284)	1:132:A:ILE:H	1:125:A:ILE:HG22	10	0.52	0.08	0.5
(2,284)	1:132:A:ILE:H	1:125:A:ILE:HG21	10	0.52	0.08	0.5
(2,284)	1:132:A:ILE:H	1:125:A:ILE:HG23	10	0.52	0.08	0.5
(2,163)	1:154:A:ASP:HA	1:176:A:VAL:HG23	10	0.51	0.04	0.52
(2,163)	1:154:A:ASP:HA	1:176:A:VAL:HG21	10	0.51	0.04	0.52
(2,163)	1:154:A:ASP:HA	1:176:A:VAL:HG22	10	0.51	0.04	0.52
(1,624)	1:149:A:THR:HG21	1:152:A:GLU:HB3	10	0.51	0.29	0.33
(1,624)	1:149:A:THR:HG23	1:152:A:GLU:HB3	10	0.51	0.29	0.33
(1,624)	1:149:A:THR:HG22	1:152:A:GLU:HB3	10	0.51	0.29	0.33
(2,27)	1:207:A:MET:HA	1:218:A:ILE:HG21	10	0.5	0.12	0.5
(2,27)	1:154:A:ASP:HA	1:176:A:VAL:HG23	10	0.5	0.12	0.5
(2,27)	1:207:A:MET:HA	1:218:A:ILE:HG23	10	0.5	0.12	0.5
(2,27)	1:207:A:MET:HA	1:218:A:ILE:HG22	10	0.5	0.12	0.5
(2,27)	1:154:A:ASP:HA	1:176:A:VAL:HG21	10	0.5	0.12	0.5
(1,579)	1:151:A:THR:HG21	1:154:A:ASP:HB3	10	0.49	0.06	0.48

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,579)	1:151:A:THR:HG23	1:154:A:ASP:HB3	10	0.49	0.06	0.48
(1,579)	1:151:A:THR:HG22	1:154:A:ASP:HB3	10	0.49	0.06	0.48
(1,643)	1:166:A:VAL:HG13	1:167:A:MET:H	10	0.49	0.38	0.38
(1,643)	1:166:A:VAL:HG11	1:167:A:MET:H	10	0.49	0.38	0.38
(2,213)	1:167:A:MET:HE2	1:168:A:GLN:H	10	0.48	0.17	0.46
(2,213)	1:167:A:MET:HE2	1:167:A:MET:H	10	0.48	0.17	0.46
(2,213)	1:167:A:MET:HE3	1:168:A:GLN:H	10	0.48	0.17	0.46
(2,213)	1:167:A:MET:HE3	1:167:A:MET:H	10	0.48	0.17	0.46
(2,213)	1:167:A:MET:HE1	1:168:A:GLN:H	10	0.48	0.17	0.46
(2,223)	1:208:A:ILE:HD11	1:196:A:ARG:HA	10	0.48	0.15	0.48
(2,223)	1:208:A:ILE:HD13	1:196:A:ARG:HA	10	0.48	0.15	0.48
(2,223)	1:208:A:ILE:HD12	1:192:A:ILE:HA	10	0.48	0.15	0.48
(2,223)	1:208:A:ILE:HD12	1:196:A:ARG:HA	10	0.48	0.15	0.48
(2,228)	1:218:A:ILE:HD12	1:128:A:ASN:HB2	10	0.46	0.14	0.46
(2,228)	1:218:A:ILE:HD13	1:128:A:ASN:HB2	10	0.46	0.14	0.46
(2,228)	1:218:A:ILE:HD11	1:128:A:ASN:HB2	10	0.46	0.14	0.46
(2,127)	1:132:A:ILE:HG12	1:157:A:TYR:HB2	10	0.46	0.05	0.45
(2,178)	1:149:A:THR:HG21	1:148:A:LEU:HB3	10	0.46	0.09	0.44
(2,178)	1:149:A:THR:HG23	1:148:A:LEU:HB3	10	0.46	0.09	0.44
(2,178)	1:149:A:THR:HG22	1:148:A:LEU:HB3	10	0.46	0.09	0.44
(1,233)	1:155:A:LEU:HB3	1:155:A:LEU:H	10	0.45	0.01	0.45
(1,342)	1:170:A:GLU:HG3	1:170:A:GLU:HB3	10	0.44	0.09	0.47
(1,444)	1:177:A:TRP:HB3	1:177:A:TRP:HE3	10	0.43	0.02	0.43
(1,793)	1:146:A:ILE:HD11	1:202:A:TYR:HD2	10	0.43	0.11	0.42
(1,793)	1:146:A:ILE:HD12	1:202:A:TYR:HD2	10	0.43	0.11	0.42
(1,793)	1:146:A:ILE:HD13	1:202:A:TYR:HD1	10	0.43	0.11	0.42
(1,793)	1:146:A:ILE:HD13	1:202:A:TYR:HD2	10	0.43	0.11	0.42
(1,793)	1:146:A:ILE:HD12	1:202:A:TYR:HD1	10	0.43	0.11	0.42
(1,793)	1:146:A:ILE:HD11	1:202:A:TYR:HD1	10	0.43	0.11	0.42
(1,446)	1:168:A:GLN:HB3	1:168:A:GLN:H	10	0.43	0.02	0.43
(1,1030)	1:195:A:LEU:HD23	1:195:A:LEU:H	10	0.42	0.02	0.42
(1,1030)	1:195:A:LEU:HD22	1:195:A:LEU:H	10	0.42	0.02	0.42
(1,1030)	1:195:A:LEU:HD21	1:195:A:LEU:H	10	0.42	0.02	0.42
(1,652)	1:141:A:VAL:HG11	1:146:A:ILE:HG12	10	0.42	0.28	0.34
(1,652)	1:141:A:VAL:HG13	1:146:A:ILE:HG12	10	0.42	0.28	0.34
(1,652)	1:141:A:VAL:HG12	1:146:A:ILE:HG12	10	0.42	0.28	0.34
(1,689)	1:214:A:VAL:HG22	1:215:A:GLY:H	10	0.42	0.02	0.42
(1,689)	1:214:A:VAL:HG23	1:215:A:GLY:H	10	0.42	0.02	0.42
(1,689)	1:214:A:VAL:HG21	1:215:A:GLY:H	10	0.42	0.02	0.42
(1,774)	1:208:A:ILE:HD11	1:208:A:ILE:H	10	0.4	0.03	0.41
(1,774)	1:208:A:ILE:HD13	1:208:A:ILE:H	10	0.4	0.03	0.41
(1,774)	1:208:A:ILE:HD12	1:208:A:ILE:H	10	0.4	0.03	0.41

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,765)	1:172:A:ILE:HD11	1:172:A:ILE:H	10	0.4	0.02	0.4
(1,765)	1:172:A:ILE:HD13	1:172:A:ILE:H	10	0.4	0.02	0.4
(1,832)	1:153:A:TYR:HB3	1:148:A:LEU:HD12	10	0.4	0.08	0.4
(1,832)	1:153:A:TYR:HB3	1:148:A:LEU:HD13	10	0.4	0.08	0.4
(1,832)	1:153:A:TYR:HB3	1:148:A:LEU:HD11	10	0.4	0.08	0.4
(1,1072)	1:195:A:LEU:HD11	1:196:A:ARG:H	10	0.4	0.04	0.4
(1,1072)	1:195:A:LEU:HD12	1:196:A:ARG:H	10	0.4	0.04	0.4
(1,508)	1:156:A:LEU:HD21	1:156:A:LEU:H	10	0.37	0.07	0.38
(1,508)	1:156:A:LEU:HD23	1:156:A:LEU:H	10	0.37	0.07	0.38
(1,508)	1:156:A:LEU:HD22	1:156:A:LEU:H	10	0.37	0.07	0.38
(1,522)	1:191:A:TYR:HB2	1:155:A:LEU:HD22	10	0.37	0.09	0.36
(1,522)	1:191:A:TYR:HB2	1:155:A:LEU:HD23	10	0.37	0.09	0.36
(1,522)	1:191:A:TYR:HB2	1:155:A:LEU:HD21	10	0.37	0.09	0.36
(2,316)	1:176:A:VAL:HG23	1:154:A:ASP:H	10	0.36	0.07	0.37
(2,316)	1:176:A:VAL:HG21	1:154:A:ASP:H	10	0.36	0.07	0.37
(2,316)	1:176:A:VAL:HG22	1:154:A:ASP:H	10	0.36	0.07	0.37
(1,757)	1:192:A:ILE:HG23	1:196:A:ARG:H	10	0.34	0.04	0.35
(1,757)	1:192:A:ILE:HG22	1:196:A:ARG:H	10	0.34	0.04	0.35
(1,757)	1:192:A:ILE:HG21	1:196:A:ARG:H	10	0.34	0.04	0.35
(2,62)	1:125:A:ILE:HB	1:126:A:ASP:H	10	0.34	0.03	0.34
(2,30)	1:205:A:ASP:HA	1:196:A:ARG:HB3	10	0.34	0.14	0.24
(2,30)	1:205:A:ASP:HA	1:199:A:LEU:HG	10	0.34	0.14	0.24
(1,651)	1:127:A:VAL:HG12	1:163:A:LYS:HG2	10	0.33	0.06	0.32
(1,651)	1:127:A:VAL:HG13	1:163:A:LYS:HG2	10	0.33	0.06	0.32
(1,651)	1:127:A:VAL:HG11	1:163:A:LYS:HG2	10	0.33	0.06	0.32
(1,651)	1:127:A:VAL:HG13	1:163:A:LYS:HG3	10	0.33	0.06	0.32
(1,651)	1:127:A:VAL:HG11	1:163:A:LYS:HG3	10	0.33	0.06	0.32
(1,1076)	1:154:A:ASP:H	1:155:A:LEU:HD11	10	0.33	0.03	0.32
(1,1076)	1:154:A:ASP:H	1:155:A:LEU:HD12	10	0.33	0.03	0.32
(1,1076)	1:154:A:ASP:H	1:155:A:LEU:HD13	10	0.33	0.03	0.32
(1,531)	1:192:A:ILE:HG13	1:192:A:ILE:H	10	0.32	0.02	0.32
(1,1045)	1:192:A:ILE:HG23	1:192:A:ILE:H	10	0.31	0.02	0.31
(1,1045)	1:192:A:ILE:HG22	1:192:A:ILE:H	10	0.31	0.02	0.31
(1,1045)	1:192:A:ILE:HG21	1:192:A:ILE:H	10	0.31	0.02	0.31
(1,70)	1:192:A:ILE:HA	1:192:A:ILE:HG13	10	0.3	0.02	0.3
(2,232)	1:192:A:ILE:HD12	1:208:A:ILE:HG23	10	0.3	0.04	0.3
(2,232)	1:208:A:ILE:HD12	1:192:A:ILE:HD11	10	0.3	0.04	0.3
(2,232)	1:192:A:ILE:HD12	1:208:A:ILE:HG21	10	0.3	0.04	0.3
(2,232)	1:192:A:ILE:HD13	1:208:A:ILE:HG22	10	0.3	0.04	0.3
(2,232)	1:192:A:ILE:HD12	1:208:A:ILE:HG22	10	0.3	0.04	0.3
(2,232)	1:192:A:ILE:HD13	1:208:A:ILE:HG23	10	0.3	0.04	0.3
(2,232)	1:192:A:ILE:HD11	1:208:A:ILE:HG23	10	0.3	0.04	0.3

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,306)	1:190:A:VAL:HG23	1:191:A:TYR:H	10	0.3	0.06	0.29
(2,306)	1:190:A:VAL:HG22	1:191:A:TYR:H	10	0.3	0.06	0.29
(2,306)	1:190:A:VAL:HG21	1:191:A:TYR:H	10	0.3	0.06	0.29
(1,443)	1:177:A:TRP:HB3	1:177:A:TRP:H	10	0.3	0.01	0.29
(1,583)	1:139:A:VAL:HG23	1:133:A:ASP:H	10	0.3	0.03	0.29
(1,583)	1:139:A:VAL:HG21	1:133:A:ASP:H	10	0.3	0.03	0.29
(1,583)	1:139:A:VAL:HG22	1:133:A:ASP:H	10	0.3	0.03	0.29
(1,449)	1:161:A:GLU:HB2	1:125:A:ILE:HG23	10	0.28	0.07	0.3
(1,449)	1:161:A:GLU:HB2	1:125:A:ILE:HG22	10	0.28	0.07	0.3
(1,449)	1:161:A:GLU:HB2	1:125:A:ILE:HG21	10	0.28	0.07	0.3
(1,427)	1:219:A:ARG:HB3	1:219:A:ARG:H	10	0.28	0.06	0.29
(1,467)	1:171:A:GLN:HB3	1:171:A:GLN:H	10	0.28	0.02	0.27
(1,147)	1:219:A:ARG:HA	1:219:A:ARG:HB2	10	0.27	0.01	0.28
(2,162)	1:148:A:LEU:HD22	1:149:A:THR:H	10	0.27	0.07	0.26
(2,162)	1:148:A:LEU:HD23	1:149:A:THR:H	10	0.27	0.07	0.26
(2,162)	1:148:A:LEU:HD21	1:149:A:THR:H	10	0.27	0.07	0.26
(1,662)	1:176:A:VAL:HG11	1:177:A:TRP:HE3	10	0.27	0.06	0.28
(1,662)	1:176:A:VAL:HG13	1:177:A:TRP:HE3	10	0.27	0.06	0.28
(1,662)	1:176:A:VAL:HG12	1:177:A:TRP:HE3	10	0.27	0.06	0.28
(1,730)	1:216:A:TYR:HB2	1:208:A:ILE:HG21	10	0.27	0.1	0.28
(1,730)	1:216:A:TYR:HB2	1:208:A:ILE:HG23	10	0.27	0.1	0.28
(1,730)	1:216:A:TYR:HB2	1:208:A:ILE:HG22	10	0.27	0.1	0.28
(1,724)	1:132:A:ILE:HG21	1:139:A:VAL:HA	10	0.26	0.03	0.27
(1,724)	1:132:A:ILE:HG22	1:139:A:VAL:HA	10	0.26	0.03	0.27
(1,724)	1:132:A:ILE:HG23	1:139:A:VAL:HA	10	0.26	0.03	0.27
(1,781)	1:130:A:ILE:HG12	1:130:A:ILE:HD12	10	0.26	0.02	0.27
(1,781)	1:130:A:ILE:HG12	1:130:A:ILE:HD13	10	0.26	0.02	0.27
(1,781)	1:130:A:ILE:HG12	1:130:A:ILE:HD11	10	0.26	0.02	0.27
(1,618)	1:190:A:VAL:HG22	1:190:A:VAL:HG12	10	0.26	0.01	0.26
(1,618)	1:190:A:VAL:HG21	1:190:A:VAL:HG13	10	0.26	0.01	0.26
(1,618)	1:190:A:VAL:HG23	1:190:A:VAL:HG12	10	0.26	0.01	0.26
(1,618)	1:190:A:VAL:HG23	1:190:A:VAL:HG11	10	0.26	0.01	0.26
(1,618)	1:190:A:VAL:HG22	1:190:A:VAL:HG11	10	0.26	0.01	0.26
(1,618)	1:190:A:VAL:HG22	1:190:A:VAL:HG13	10	0.26	0.01	0.26
(1,618)	1:190:A:VAL:HG23	1:190:A:VAL:HG13	10	0.26	0.01	0.26
(2,102)	1:167:A:MET:HG3	1:167:A:MET:HA	10	0.26	0.13	0.22
(2,102)	1:167:A:MET:HG3	1:217:A:VAL:HA	10	0.26	0.13	0.22
(1,291)	1:191:A:TYR:HB3	1:191:A:TYR:H	10	0.26	0.03	0.26
(2,48)	1:173:A:LEU:HB2	1:174:A:ASN:H	10	0.25	0.05	0.25
(1,818)	1:149:A:THR:HG22	1:149:A:THR:HB	10	0.25	0.01	0.25
(1,818)	1:149:A:THR:HG23	1:149:A:THR:HB	10	0.25	0.01	0.25
(1,818)	1:149:A:THR:HG21	1:149:A:THR:HB	10	0.25	0.01	0.25

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,665)	1:211:A:VAL:HA	1:211:A:VAL:HG22	10	0.25	0.28	0.16
(1,665)	1:211:A:VAL:HA	1:211:A:VAL:HG21	10	0.25	0.28	0.16
(1,665)	1:211:A:VAL:HA	1:211:A:VAL:HG23	10	0.25	0.28	0.16
(1,661)	1:190:A:VAL:HG11	1:191:A:TYR:H	10	0.25	0.02	0.24
(1,661)	1:190:A:VAL:HG12	1:191:A:TYR:H	10	0.25	0.02	0.24
(1,661)	1:190:A:VAL:HG13	1:191:A:TYR:H	10	0.25	0.02	0.24
(1,641)	1:166:A:VAL:HB	1:166:A:VAL:HG21	10	0.24	0.01	0.24
(1,641)	1:166:A:VAL:HB	1:166:A:VAL:HG22	10	0.24	0.01	0.24
(1,641)	1:166:A:VAL:HB	1:166:A:VAL:HG23	10	0.24	0.01	0.24
(1,158)	1:184:A:GLU:HA	1:184:A:GLU:HG3	10	0.23	0.04	0.24
(1,514)	1:156:A:LEU:HD21	1:156:A:LEU:HG	10	0.23	0.01	0.24
(1,514)	1:156:A:LEU:HD22	1:156:A:LEU:HG	10	0.23	0.01	0.24
(1,514)	1:156:A:LEU:HD23	1:156:A:LEU:HG	10	0.23	0.01	0.24
(2,211)	1:125:A:ILE:HB	1:125:A:ILE:HG22	10	0.21	0.02	0.22
(2,211)	1:125:A:ILE:HB	1:125:A:ILE:HG21	10	0.21	0.02	0.22
(2,211)	1:125:A:ILE:HB	1:125:A:ILE:HG23	10	0.21	0.02	0.22
(1,1024)	1:146:A:ILE:HG12	1:146:A:ILE:H	10	0.2	0.04	0.2
(1,632)	1:140:A:THR:HG22	1:141:A:VAL:H	10	0.18	0.01	0.18
(1,632)	1:140:A:THR:HG21	1:141:A:VAL:H	10	0.18	0.01	0.18
(1,632)	1:140:A:THR:HG23	1:141:A:VAL:H	10	0.18	0.01	0.18
(1,519)	1:192:A:ILE:HA	1:155:A:LEU:HD21	10	0.17	0.03	0.18
(1,519)	1:192:A:ILE:HA	1:155:A:LEU:HD22	10	0.17	0.03	0.18
(1,519)	1:192:A:ILE:HA	1:155:A:LEU:HD23	10	0.17	0.03	0.18
(1,975)	1:158:A:LEU:H	1:157:A:TYR:HB2	10	0.16	0.04	0.16
(1,177)	1:126:A:ASP:HA	1:125:A:ILE:HG22	10	0.16	0.04	0.16
(1,177)	1:126:A:ASP:HA	1:125:A:ILE:HG21	10	0.16	0.04	0.16
(1,177)	1:126:A:ASP:HA	1:125:A:ILE:HG23	10	0.16	0.04	0.16
(2,10)	1:157:A:TYR:HA	1:156:A:LEU:HB3	10	0.15	0.02	0.16
(1,356)	1:194:A:TYR:HB3	1:194:A:TYR:H	10	0.15	0.01	0.15
(1,445)	1:177:A:TRP:HB2	1:177:A:TRP:HD1	10	0.14	0.01	0.15
(1,616)	1:199:A:LEU:HG	1:199:A:LEU:HD21	10	0.13	0.01	0.13
(1,616)	1:199:A:LEU:HG	1:199:A:LEU:HD22	10	0.13	0.01	0.13
(1,616)	1:199:A:LEU:HG	1:199:A:LEU:HD23	10	0.13	0.01	0.13
(2,158)	1:195:A:LEU:HG	1:195:A:LEU:HD12	10	0.13	0.0	0.13
(2,158)	1:195:A:LEU:HG	1:195:A:LEU:HD21	10	0.13	0.0	0.13
(2,158)	1:195:A:LEU:HG	1:195:A:LEU:HD13	10	0.13	0.0	0.13
(2,6)	1:191:A:TYR:HA	1:192:A:ILE:H	10	0.13	0.01	0.13
(1,185)	1:201:A:PRO:HD3	1:201:A:PRO:HB2	10	0.11	0.01	0.11
(2,88)	1:184:A:GLU:HG2	1:183:A:VAL:HG12	9	1.27	0.45	1.25
(2,88)	1:182:A:GLU:HG3	1:183:A:VAL:HG22	9	1.27	0.45	1.25
(2,88)	1:184:A:GLU:HG2	1:183:A:VAL:HG13	9	1.27	0.45	1.25
(2,88)	1:182:A:GLU:HG2	1:183:A:VAL:HG22	9	1.27	0.45	1.25

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,88)	1:182:A:GLU:HG3	1:183:A:VAL:HG21	9	1.27	0.45	1.25
(1,746)	1:207:A:MET:HG3	1:218:A:ILE:HG21	9	1.26	0.34	1.34
(1,746)	1:207:A:MET:HG3	1:218:A:ILE:HG23	9	1.26	0.34	1.34
(1,746)	1:207:A:MET:HG3	1:218:A:ILE:HG22	9	1.26	0.34	1.34
(1,49)	1:181:A:SER:HB3	1:177:A:TRP:HB2	9	1.22	0.18	1.18
(2,105)	1:207:A:MET:HG3	1:130:A:ILE:HD11	9	1.13	0.33	1.26
(2,105)	1:207:A:MET:HG3	1:130:A:ILE:HD13	9	1.13	0.33	1.26
(2,105)	1:207:A:MET:HG3	1:218:A:ILE:HG23	9	1.13	0.33	1.26
(2,105)	1:207:A:MET:HG3	1:218:A:ILE:HG22	9	1.13	0.33	1.26
(2,105)	1:207:A:MET:HG3	1:218:A:ILE:HG21	9	1.13	0.33	1.26
(2,78)	1:197:A:ASN:HB3	1:200:A:LYS:HD2	9	0.98	0.38	1.05
(2,78)	1:197:A:ASN:HB3	1:198:A:LYS:HB3	9	0.98	0.38	1.05
(1,750)	1:167:A:MET:HG2	1:167:A:MET:HE3	9	0.96	0.07	0.99
(1,750)	1:167:A:MET:HG2	1:167:A:MET:HE2	9	0.96	0.07	0.99
(1,750)	1:167:A:MET:HG2	1:167:A:MET:HE1	9	0.96	0.07	0.99
(2,198)	1:187:A:VAL:HG11	1:188:A:VAL:HB	9	0.84	0.06	0.83
(2,198)	1:187:A:VAL:HG12	1:188:A:VAL:HB	9	0.84	0.06	0.83
(2,198)	1:187:A:VAL:HG13	1:188:A:VAL:HB	9	0.84	0.06	0.83
(2,198)	1:187:A:VAL:HG13	1:190:A:VAL:HB	9	0.84	0.06	0.83
(2,182)	1:214:A:VAL:HG11	1:168:A:GLN:H	9	0.82	0.14	0.74
(2,182)	1:214:A:VAL:HG13	1:168:A:GLN:H	9	0.82	0.14	0.74
(2,182)	1:166:A:VAL:HG23	1:167:A:MET:H	9	0.82	0.14	0.74
(2,182)	1:214:A:VAL:HG12	1:168:A:GLN:H	9	0.82	0.14	0.74
(1,987)	1:147:A:GLU:HB3	1:147:A:GLU:H	9	0.79	0.03	0.79
(1,596)	1:167:A:MET:HG2	1:159:A:LEU:HD23	9	0.76	0.6	0.49
(1,596)	1:167:A:MET:HG2	1:159:A:LEU:HD22	9	0.76	0.6	0.49
(1,596)	1:167:A:MET:HG2	1:159:A:LEU:HD21	9	0.76	0.6	0.49
(2,171)	1:188:A:VAL:HG13	1:188:A:VAL:H	9	0.73	0.16	0.82
(2,171)	1:188:A:VAL:HG11	1:188:A:VAL:H	9	0.73	0.16	0.82
(2,171)	1:173:A:LEU:HG	1:178:A:GLY:H	9	0.73	0.16	0.82
(2,179)	1:146:A:ILE:HB	1:139:A:VAL:HG13	9	0.62	0.2	0.62
(2,179)	1:146:A:ILE:HB	1:139:A:VAL:HG11	9	0.62	0.2	0.62
(2,179)	1:146:A:ILE:HB	1:139:A:VAL:HG12	9	0.62	0.2	0.62
(1,29)	1:190:A:VAL:HA	1:189:A:ASP:HB3	9	0.59	0.42	0.56
(2,230)	1:216:A:TYR:HB3	1:192:A:ILE:HD12	9	0.59	0.13	0.63
(2,230)	1:216:A:TYR:HB3	1:192:A:ILE:HD11	9	0.59	0.13	0.63
(2,230)	1:216:A:TYR:HB3	1:192:A:ILE:HD13	9	0.59	0.13	0.63
(1,986)	1:147:A:GLU:HB2	1:148:A:LEU:H	9	0.56	0.08	0.56
(2,294)	1:183:A:VAL:HG12	1:187:A:VAL:H	9	0.53	0.19	0.5
(2,294)	1:183:A:VAL:HG13	1:187:A:VAL:H	9	0.53	0.19	0.5
(2,294)	1:183:A:VAL:HG11	1:187:A:VAL:H	9	0.53	0.19	0.5
(2,75)	1:128:A:ASN:HB3	1:218:A:ILE:HG21	9	0.51	0.21	0.6

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,75)	1:128:A:ASN:HB3	1:218:A:ILE:HG23	9	0.51	0.21	0.6
(2,75)	1:128:A:ASN:HB3	1:218:A:ILE:HG22	9	0.51	0.21	0.6
(2,297)	1:205:A:ASP:H	1:199:A:LEU:HD11	9	0.46	0.14	0.44
(2,297)	1:205:A:ASP:H	1:199:A:LEU:HD13	9	0.46	0.14	0.44
(2,297)	1:205:A:ASP:H	1:199:A:LEU:HD12	9	0.46	0.14	0.44
(2,297)	1:205:A:ASP:H	1:199:A:LEU:HD22	9	0.46	0.14	0.44
(2,233)	1:207:A:MET:HE2	1:160:A:ALA:HA	9	0.45	0.16	0.44
(2,233)	1:207:A:MET:HE3	1:160:A:ALA:HA	9	0.45	0.16	0.44
(2,233)	1:207:A:MET:HE1	1:160:A:ALA:HA	9	0.45	0.16	0.44
(2,281)	1:148:A:LEU:HD11	1:153:A:TYR:H	9	0.45	0.14	0.49
(2,281)	1:148:A:LEU:HD12	1:153:A:TYR:H	9	0.45	0.14	0.49
(2,281)	1:148:A:LEU:HD13	1:153:A:TYR:H	9	0.45	0.14	0.49
(2,89)	1:137:A:PHE:HB3	1:137:A:PHE:H	9	0.4	0.02	0.4
(1,1039)	1:159:A:LEU:H	1:159:A:LEU:HD12	9	0.4	0.28	0.21
(1,1039)	1:159:A:LEU:H	1:159:A:LEU:HD13	9	0.4	0.28	0.21
(1,1039)	1:159:A:LEU:H	1:159:A:LEU:HD11	9	0.4	0.28	0.21
(1,563)	1:188:A:VAL:HG22	1:189:A:ASP:H	9	0.38	0.06	0.38
(1,563)	1:188:A:VAL:HG21	1:189:A:ASP:H	9	0.38	0.06	0.38
(1,563)	1:188:A:VAL:HG23	1:189:A:ASP:H	9	0.38	0.06	0.38
(1,463)	1:172:A:ILE:HG12	1:172:A:ILE:H	9	0.29	0.06	0.25
(1,705)	1:217:A:VAL:HG12	1:217:A:VAL:HA	9	0.28	0.01	0.28
(1,705)	1:217:A:VAL:HG11	1:217:A:VAL:HA	9	0.28	0.01	0.28
(1,705)	1:217:A:VAL:HG13	1:217:A:VAL:HA	9	0.28	0.01	0.28
(1,682)	1:136:A:ALA:HB1	1:135:A:ASN:HB3	9	0.27	0.06	0.28
(1,682)	1:136:A:ALA:HB3	1:135:A:ASN:HB2	9	0.27	0.06	0.28
(1,682)	1:136:A:ALA:HB3	1:135:A:ASN:HB3	9	0.27	0.06	0.28
(1,682)	1:136:A:ALA:HB1	1:135:A:ASN:HB2	9	0.27	0.06	0.28
(1,829)	1:147:A:GLU:HB2	1:147:A:GLU:HA	9	0.27	0.01	0.27
(1,810)	1:124:A:ILE:HG13	1:124:A:ILE:HA	9	0.26	0.02	0.26
(2,279)	1:140:A:THR:H	1:140:A:THR:HG21	9	0.22	0.04	0.21
(2,279)	1:140:A:THR:H	1:140:A:THR:HG23	9	0.22	0.04	0.21
(2,279)	1:140:A:THR:H	1:140:A:THR:HG22	9	0.22	0.04	0.21
(1,805)	1:192:A:ILE:HD11	1:192:A:ILE:H	9	0.22	0.07	0.17
(1,805)	1:192:A:ILE:HD12	1:192:A:ILE:H	9	0.22	0.07	0.17
(1,805)	1:192:A:ILE:HD13	1:192:A:ILE:H	9	0.22	0.07	0.17
(1,686)	1:144:A:ALA:HB2	1:145:A:GLU:H	9	0.2	0.03	0.21
(1,686)	1:144:A:ALA:HB3	1:145:A:GLU:H	9	0.2	0.03	0.21
(1,686)	1:144:A:ALA:HB1	1:145:A:GLU:H	9	0.2	0.03	0.21
(2,164)	1:176:A:VAL:HG21	1:155:A:LEU:H	9	0.2	0.08	0.18
(2,164)	1:176:A:VAL:HG22	1:155:A:LEU:H	9	0.2	0.08	0.18
(2,164)	1:176:A:VAL:HG23	1:155:A:LEU:H	9	0.2	0.08	0.18
(1,419)	1:187:A:VAL:HB	1:188:A:VAL:H	9	0.19	0.02	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,280)	1:148:A:LEU:H	1:148:A:LEU:HD21	9	0.18	0.08	0.14
(2,280)	1:148:A:LEU:H	1:148:A:LEU:HD22	9	0.18	0.08	0.14
(2,280)	1:148:A:LEU:H	1:148:A:LEU:HD23	9	0.18	0.08	0.14
(1,800)	1:146:A:ILE:HD12	1:139:A:VAL:HG13	9	0.13	0.02	0.13
(1,800)	1:146:A:ILE:HD13	1:139:A:VAL:HG11	9	0.13	0.02	0.13
(1,800)	1:146:A:ILE:HD11	1:139:A:VAL:HG13	9	0.13	0.02	0.13
(1,800)	1:146:A:ILE:HD13	1:139:A:VAL:HG13	9	0.13	0.02	0.13
(1,800)	1:146:A:ILE:HD12	1:139:A:VAL:HG12	9	0.13	0.02	0.13
(1,800)	1:146:A:ILE:HD12	1:139:A:VAL:HG11	9	0.13	0.02	0.13
(2,168)	1:151:A:THR:HB	1:151:A:THR:HG22	9	0.12	0.01	0.13
(2,168)	1:151:A:THR:HA	1:151:A:THR:HG21	9	0.12	0.01	0.13
(2,168)	1:151:A:THR:HB	1:151:A:THR:HG23	9	0.12	0.01	0.13
(2,168)	1:151:A:THR:HB	1:151:A:THR:HG21	9	0.12	0.01	0.13
(2,189)	1:217:A:VAL:HG23	1:165:A:HIS:HB2	8	1.11	0.79	0.92
(2,189)	1:217:A:VAL:HG23	1:165:A:HIS:HB3	8	1.11	0.79	0.92
(2,189)	1:217:A:VAL:HG21	1:165:A:HIS:HB2	8	1.11	0.79	0.92
(2,189)	1:217:A:VAL:HG22	1:165:A:HIS:HB3	8	1.11	0.79	0.92
(2,189)	1:141:A:VAL:HG13	1:204:A:ARG:HD3	8	1.11	0.79	0.92
(2,189)	1:141:A:VAL:HG12	1:204:A:ARG:HD3	8	1.11	0.79	0.92
(2,189)	1:141:A:VAL:HG11	1:204:A:ARG:HD3	8	1.11	0.79	0.92
(1,739)	1:207:A:MET:HG3	1:207:A:MET:HE3	8	1.02	0.02	1.02
(1,739)	1:207:A:MET:HG3	1:207:A:MET:HE2	8	1.02	0.02	1.02
(1,739)	1:207:A:MET:HG3	1:207:A:MET:HE1	8	1.02	0.02	1.02
(1,194)	1:215:A:GLY:HA2	1:169:A:ARG:HB2	8	0.98	0.32	0.92
(1,607)	1:159:A:LEU:HD21	1:217:A:VAL:HA	8	0.81	1.03	0.24
(1,607)	1:159:A:LEU:HD23	1:217:A:VAL:HA	8	0.81	1.03	0.24
(1,607)	1:159:A:LEU:HD22	1:217:A:VAL:HA	8	0.81	1.03	0.24
(1,541)	1:134:A:LYS:HG3	1:134:A:LYS:H	8	0.59	0.03	0.6
(1,541)	1:134:A:LYS:HG2	1:134:A:LYS:H	8	0.59	0.03	0.6
(2,100)	1:167:A:MET:HG2	1:159:A:LEU:HD23	8	0.54	0.29	0.5
(2,100)	1:167:A:MET:HG2	1:159:A:LEU:HD22	8	0.54	0.29	0.5
(2,100)	1:167:A:MET:HG2	1:159:A:LEU:HD21	8	0.54	0.29	0.5
(2,100)	1:204:A:ARG:HB2	1:130:A:ILE:HD13	8	0.54	0.29	0.5
(2,100)	1:204:A:ARG:HB2	1:130:A:ILE:HD12	8	0.54	0.29	0.5
(1,1000)	1:169:A:ARG:HB2	1:169:A:ARG:H	8	0.54	0.03	0.53
(2,191)	1:211:A:VAL:HG21	1:217:A:VAL:H	8	0.53	0.08	0.52
(2,191)	1:211:A:VAL:HG23	1:217:A:VAL:H	8	0.53	0.08	0.52
(2,191)	1:211:A:VAL:HG22	1:217:A:VAL:H	8	0.53	0.08	0.52
(1,81)	1:169:A:ARG:HA	1:169:A:ARG:HG3	8	0.51	0.04	0.51
(1,81)	1:169:A:ARG:HA	1:169:A:ARG:HG2	8	0.51	0.04	0.51
(1,286)	1:205:A:ASP:HB2	1:196:A:ARG:HB2	8	0.49	0.39	0.42
(2,92)	1:171:A:GLN:HG3	1:167:A:MET:HA	8	0.45	0.25	0.39

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,113)	1:200:A:LYS:HB3	1:200:A:LYS:HE2	8	0.4	0.08	0.4
(2,113)	1:205:A:ASP:HB3	1:200:A:LYS:HB2	8	0.4	0.08	0.4
(2,113)	1:200:A:LYS:HB2	1:200:A:LYS:HE2	8	0.4	0.08	0.4
(2,113)	1:200:A:LYS:HB3	1:200:A:LYS:HE3	8	0.4	0.08	0.4
(2,113)	1:200:A:LYS:HB2	1:200:A:LYS:HE3	8	0.4	0.08	0.4
(2,317)	1:172:A:ILE:H	1:171:A:GLN:HG2	8	0.26	0.07	0.25
(2,317)	1:172:A:ILE:H	1:168:A:GLN:HB2	8	0.26	0.07	0.25
(2,318)	1:175:A:HIS:H	1:158:A:LEU:HD23	8	0.24	0.06	0.24
(2,318)	1:175:A:HIS:H	1:158:A:LEU:HD21	8	0.24	0.06	0.24
(2,318)	1:175:A:HIS:H	1:176:A:VAL:HG22	8	0.24	0.06	0.24
(2,318)	1:175:A:HIS:H	1:176:A:VAL:HG23	8	0.24	0.06	0.24
(1,48)	1:181:A:SER:HB2	1:181:A:SER:HA	8	0.24	0.0	0.24
(1,396)	1:167:A:MET:HG2	1:167:A:MET:HB3	8	0.24	0.01	0.24
(2,97)	1:127:A:VAL:HB	1:163:A:LYS:HB3	8	0.23	0.08	0.23
(2,71)	1:202:A:TYR:HB3	1:141:A:VAL:HB	8	0.22	0.04	0.24
(2,43)	1:195:A:LEU:HB3	1:192:A:ILE:HA	8	0.2	0.06	0.2
(2,43)	1:196:A:ARG:HA	1:195:A:LEU:HB3	8	0.2	0.06	0.2
(1,1084)	1:124:A:ILE:H	1:124:A:ILE:HG13	8	0.19	0.06	0.19
(1,812)	1:192:A:ILE:HD12	1:208:A:ILE:HG23	8	0.19	0.02	0.18
(1,812)	1:192:A:ILE:HD11	1:208:A:ILE:HG22	8	0.19	0.02	0.18
(1,812)	1:192:A:ILE:HD12	1:208:A:ILE:HG22	8	0.19	0.02	0.18
(1,812)	1:192:A:ILE:HD13	1:208:A:ILE:HG23	8	0.19	0.02	0.18
(1,812)	1:192:A:ILE:HD11	1:208:A:ILE:HG23	8	0.19	0.02	0.18
(2,26)	1:219:A:ARG:HA	1:219:A:ARG:HG2	8	0.19	0.06	0.17
(2,200)	1:187:A:VAL:HG12	1:187:A:VAL:HG21	8	0.18	0.04	0.16
(2,200)	1:187:A:VAL:HG13	1:187:A:VAL:HG22	8	0.18	0.04	0.16
(2,200)	1:187:A:VAL:HG11	1:187:A:VAL:HG21	8	0.18	0.04	0.16
(2,200)	1:183:A:VAL:HG12	1:187:A:VAL:HG11	8	0.18	0.04	0.16
(2,200)	1:187:A:VAL:HG13	1:187:A:VAL:HG21	8	0.18	0.04	0.16
(2,200)	1:187:A:VAL:HG12	1:187:A:VAL:HG22	8	0.18	0.04	0.16
(1,521)	1:191:A:TYR:HB3	1:155:A:LEU:HD21	8	0.18	0.03	0.18
(1,521)	1:191:A:TYR:HB3	1:155:A:LEU:HD23	8	0.18	0.03	0.18
(1,521)	1:191:A:TYR:HB3	1:155:A:LEU:HD22	8	0.18	0.03	0.18
(1,587)	1:139:A:VAL:HG22	1:138:A:LYS:HA	8	0.17	0.05	0.18
(1,587)	1:139:A:VAL:HG23	1:138:A:LYS:HA	8	0.17	0.05	0.18
(1,587)	1:139:A:VAL:HG21	1:138:A:LYS:HA	8	0.17	0.05	0.18
(1,333)	1:197:A:ASN:HB2	1:198:A:LYS:H	8	0.14	0.02	0.14
(1,182)	1:201:A:PRO:HD2	1:200:A:LYS:HB2	8	0.14	0.03	0.12
(1,182)	1:201:A:PRO:HD2	1:200:A:LYS:HB3	8	0.14	0.03	0.12
(1,323)	1:128:A:ASN:HB2	1:128:A:ASN:HA	8	0.12	0.01	0.12
(2,137)	1:156:A:LEU:HG	1:156:A:LEU:HD13	8	0.11	0.01	0.11
(2,137)	1:156:A:LEU:HG	1:156:A:LEU:HD12	8	0.11	0.01	0.11

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,137)	1:124:A:ILE:HG13	1:124:A:ILE:HD13	8	0.11	0.01	0.11
(2,137)	1:124:A:ILE:HG13	1:124:A:ILE:HD12	8	0.11	0.01	0.11
(2,137)	1:156:A:LEU:HG	1:156:A:LEU:HD11	8	0.11	0.01	0.11
(1,613)	1:190:A:VAL:HG23	1:189:A:ASP:HB3	7	1.25	0.16	1.19
(1,613)	1:190:A:VAL:HG21	1:189:A:ASP:HB3	7	1.25	0.16	1.19
(2,86)	1:145:A:GLU:HG3	1:138:A:LYS:HE3	7	1.11	0.55	0.91
(2,86)	1:147:A:GLU:HG2	1:138:A:LYS:HE2	7	1.11	0.55	0.91
(2,86)	1:145:A:GLU:HG3	1:138:A:LYS:HE2	7	1.11	0.55	0.91
(1,408)	1:167:A:MET:HG2	1:172:A:ILE:HD12	7	1.03	0.08	1.05
(1,408)	1:167:A:MET:HG2	1:172:A:ILE:HD11	7	1.03	0.08	1.05
(2,215)	1:167:A:MET:HE1	1:175:A:HIS:HB2	7	0.92	0.26	0.97
(2,215)	1:167:A:MET:HE1	1:162:A:ASN:HB3	7	0.92	0.26	0.97
(2,215)	1:167:A:MET:HE2	1:162:A:ASN:HB3	7	0.92	0.26	0.97
(2,215)	1:167:A:MET:HE2	1:175:A:HIS:HB2	7	0.92	0.26	0.97
(2,215)	1:167:A:MET:HE3	1:175:A:HIS:HB2	7	0.92	0.26	0.97
(1,1037)	1:165:A:HIS:H	1:217:A:VAL:HG21	7	0.67	1.03	0.27
(1,1037)	1:165:A:HIS:H	1:217:A:VAL:HG23	7	0.67	1.03	0.27
(1,1037)	1:165:A:HIS:H	1:217:A:VAL:HG22	7	0.67	1.03	0.27
(1,527)	1:159:A:LEU:HD13	1:216:A:TYR:HB2	7	0.54	0.2	0.54
(1,527)	1:159:A:LEU:HD12	1:216:A:TYR:HB2	7	0.54	0.2	0.54
(1,527)	1:159:A:LEU:HD11	1:216:A:TYR:HB2	7	0.54	0.2	0.54
(2,183)	1:140:A:THR:HG21	1:138:A:LYS:HD2	7	0.54	0.35	0.36
(2,183)	1:140:A:THR:HG23	1:138:A:LYS:HD2	7	0.54	0.35	0.36
(2,183)	1:140:A:THR:HG22	1:138:A:LYS:HD2	7	0.54	0.35	0.36
(2,183)	1:140:A:THR:HG23	1:138:A:LYS:HB3	7	0.54	0.35	0.36
(1,1004)	1:207:A:MET:H	1:206:A:LYS:HB3	7	0.53	0.05	0.53
(1,658)	1:163:A:LYS:HE2	1:127:A:VAL:HG12	7	0.53	0.15	0.58
(1,658)	1:163:A:LYS:HE2	1:127:A:VAL:HG11	7	0.53	0.15	0.58
(1,658)	1:163:A:LYS:HE2	1:127:A:VAL:HG13	7	0.53	0.15	0.58
(1,658)	1:163:A:LYS:HE3	1:127:A:VAL:HG13	7	0.53	0.15	0.58
(1,658)	1:163:A:LYS:HE3	1:127:A:VAL:HG12	7	0.53	0.15	0.58
(2,197)	1:187:A:VAL:HG13	1:177:A:TRP:HH2	7	0.48	0.53	0.29
(2,197)	1:187:A:VAL:HG12	1:177:A:TRP:HH2	7	0.48	0.53	0.29
(2,197)	1:187:A:VAL:HG11	1:177:A:TRP:HH2	7	0.48	0.53	0.29
(2,87)	1:209:A:GLU:HG3	1:217:A:VAL:HG12	7	0.41	0.34	0.27
(2,87)	1:209:A:GLU:HG3	1:217:A:VAL:HG13	7	0.41	0.34	0.27
(2,87)	1:209:A:GLU:HG2	1:217:A:VAL:HG11	7	0.41	0.34	0.27
(2,87)	1:182:A:GLU:HG3	1:183:A:VAL:HG21	7	0.41	0.34	0.27
(2,87)	1:209:A:GLU:HG2	1:217:A:VAL:HG12	7	0.41	0.34	0.27
(2,44)	1:196:A:ARG:HD2	1:195:A:LEU:HB3	7	0.39	0.07	0.41
(2,44)	1:196:A:ARG:HD3	1:195:A:LEU:HB3	7	0.39	0.07	0.41
(1,492)	1:130:A:ILE:HG13	1:130:A:ILE:H	7	0.35	0.14	0.42

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,42)	1:204:A:ARG:HD3	1:130:A:ILE:HD11	7	0.34	0.12	0.34
(2,42)	1:204:A:ARG:HD3	1:130:A:ILE:HD13	7	0.34	0.12	0.34
(2,42)	1:204:A:ARG:HD3	1:130:A:ILE:HD12	7	0.34	0.12	0.34
(1,225)	1:204:A:ARG:HD3	1:204:A:ARG:HB2	7	0.33	0.1	0.29
(2,199)	1:136:A:ALA:HB3	1:138:A:LYS:HB3	7	0.31	0.1	0.29
(2,199)	1:136:A:ALA:HB2	1:138:A:LYS:HB3	7	0.31	0.1	0.29
(2,199)	1:136:A:ALA:HB1	1:138:A:LYS:HB3	7	0.31	0.1	0.29
(2,199)	1:136:A:ALA:HB3	1:138:A:LYS:HB2	7	0.31	0.1	0.29
(1,1080)	1:169:A:ARG:H	1:169:A:ARG:HD2	7	0.3	0.09	0.27
(1,1080)	1:169:A:ARG:H	1:169:A:ARG:HD3	7	0.3	0.09	0.27
(1,796)	1:146:A:ILE:HA	1:146:A:ILE:HD12	7	0.29	0.1	0.36
(1,796)	1:146:A:ILE:HA	1:146:A:ILE:HD11	7	0.29	0.1	0.36
(1,796)	1:146:A:ILE:HA	1:146:A:ILE:HD13	7	0.29	0.1	0.36
(2,74)	1:153:A:TYR:HB2	1:148:A:LEU:HD12	7	0.28	0.09	0.25
(2,74)	1:128:A:ASN:HB2	1:218:A:ILE:HG23	7	0.28	0.09	0.25
(2,74)	1:128:A:ASN:HB2	1:218:A:ILE:HG22	7	0.28	0.09	0.25
(1,355)	1:184:A:GLU:HG2	1:184:A:GLU:H	7	0.27	0.04	0.26
(1,735)	1:125:A:ILE:HG21	1:126:A:ASP:H	7	0.26	0.07	0.25
(1,735)	1:125:A:ILE:HG23	1:126:A:ASP:H	7	0.26	0.07	0.25
(1,735)	1:125:A:ILE:HG22	1:126:A:ASP:H	7	0.26	0.07	0.25
(1,1048)	1:207:A:MET:H	1:206:A:LYS:HG3	7	0.26	0.05	0.29
(1,1048)	1:207:A:MET:H	1:206:A:LYS:HG2	7	0.26	0.05	0.29
(2,309)	1:140:A:THR:H	1:132:A:ILE:HG13	7	0.22	0.08	0.23
(1,220)	1:216:A:TYR:HB3	1:192:A:ILE:HD12	7	0.22	0.06	0.2
(1,220)	1:216:A:TYR:HB3	1:192:A:ILE:HD11	7	0.22	0.06	0.2
(1,220)	1:216:A:TYR:HB3	1:192:A:ILE:HD13	7	0.22	0.06	0.2
(1,121)	1:140:A:THR:HA	1:141:A:VAL:HG11	7	0.19	0.11	0.15
(1,121)	1:140:A:THR:HA	1:141:A:VAL:HG13	7	0.19	0.11	0.15
(1,121)	1:140:A:THR:HA	1:141:A:VAL:HG12	7	0.19	0.11	0.15
(1,745)	1:160:A:ALA:HA	1:218:A:ILE:HG23	7	0.18	0.04	0.17
(1,745)	1:160:A:ALA:HA	1:218:A:ILE:HG22	7	0.18	0.04	0.17
(1,745)	1:160:A:ALA:HA	1:218:A:ILE:HG21	7	0.18	0.04	0.17
(1,367)	1:171:A:GLN:HG3	1:171:A:GLN:H	7	0.14	0.02	0.14
(1,554)	1:148:A:LEU:HB3	1:148:A:LEU:HD22	7	0.12	0.01	0.13
(1,554)	1:148:A:LEU:HB3	1:148:A:LEU:HD23	7	0.12	0.01	0.13
(1,554)	1:148:A:LEU:HB3	1:148:A:LEU:HD21	7	0.12	0.01	0.13
(1,617)	1:159:A:LEU:HD21	1:159:A:LEU:HB2	6	0.88	0.02	0.88
(1,617)	1:159:A:LEU:HD23	1:159:A:LEU:HB2	6	0.88	0.02	0.88
(1,617)	1:159:A:LEU:HD22	1:159:A:LEU:HB2	6	0.88	0.02	0.88
(2,190)	1:141:A:VAL:HG23	1:142:A:ASN:HB3	6	0.82	0.4	0.68
(2,190)	1:141:A:VAL:HG21	1:142:A:ASN:HB3	6	0.82	0.4	0.68
(2,172)	1:199:A:LEU:HD22	1:202:A:TYR:HD2	6	0.7	0.54	0.51

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,172)	1:199:A:LEU:HD21	1:202:A:TYR:HD2	6	0.7	0.54	0.51
(2,172)	1:199:A:LEU:HD21	1:202:A:TYR:HD1	6	0.7	0.54	0.51
(2,55)	1:200:A:LYS:HE3	1:196:A:ARG:HB2	6	0.56	0.38	0.52
(2,55)	1:200:A:LYS:HE2	1:196:A:ARG:HB2	6	0.56	0.38	0.52
(2,55)	1:198:A:LYS:HE2	1:152:A:GLU:HB3	6	0.56	0.38	0.52
(2,55)	1:198:A:LYS:HE3	1:152:A:GLU:HB3	6	0.56	0.38	0.52
(2,55)	1:163:A:LYS:HE3	1:161:A:GLU:HG2	6	0.56	0.38	0.52
(1,823)	1:124:A:ILE:HD12	1:133:A:ASP:HB3	6	0.4	0.07	0.41
(1,823)	1:124:A:ILE:HD11	1:133:A:ASP:HB3	6	0.4	0.07	0.41
(1,823)	1:124:A:ILE:HD13	1:133:A:ASP:HB3	6	0.4	0.07	0.41
(1,581)	1:185:A:THR:HG22	1:173:A:LEU:HD11	6	0.4	0.02	0.39
(1,581)	1:185:A:THR:HG22	1:173:A:LEU:HD13	6	0.4	0.02	0.39
(1,581)	1:185:A:THR:HG23	1:173:A:LEU:HD13	6	0.4	0.02	0.39
(1,581)	1:185:A:THR:HG21	1:173:A:LEU:HD13	6	0.4	0.02	0.39
(1,581)	1:185:A:THR:HG23	1:173:A:LEU:HD12	6	0.4	0.02	0.39
(1,581)	1:185:A:THR:HG23	1:173:A:LEU:HD11	6	0.4	0.02	0.39
(1,144)	1:189:A:ASP:HA	1:189:A:ASP:HB2	6	0.36	0.01	0.36
(1,461)	1:212:A:ARG:HB2	1:210:A:THR:HG23	6	0.32	0.23	0.24
(1,461)	1:212:A:ARG:HB2	1:210:A:THR:HG21	6	0.32	0.23	0.24
(1,461)	1:212:A:ARG:HB3	1:210:A:THR:HG23	6	0.32	0.23	0.24
(1,461)	1:212:A:ARG:HB3	1:210:A:THR:HG22	6	0.32	0.23	0.24
(1,461)	1:212:A:ARG:HB2	1:210:A:THR:HG22	6	0.32	0.23	0.24
(1,1068)	1:181:A:SER:H	1:180:A:ASN:HB2	6	0.28	0.14	0.26
(2,222)	1:205:A:ASP:HA	1:208:A:ILE:HD13	6	0.26	0.16	0.18
(2,222)	1:205:A:ASP:HA	1:208:A:ILE:HD12	6	0.26	0.16	0.18
(1,844)	1:200:A:LYS:HD2	1:200:A:LYS:H	6	0.25	0.11	0.25
(1,844)	1:200:A:LYS:HD3	1:200:A:LYS:H	6	0.25	0.11	0.25
(2,212)	1:207:A:MET:HE3	1:218:A:ILE:HG21	6	0.23	0.07	0.22
(2,212)	1:207:A:MET:HE2	1:130:A:ILE:HD11	6	0.23	0.07	0.22
(2,212)	1:207:A:MET:HE1	1:218:A:ILE:HG23	6	0.23	0.07	0.22
(2,212)	1:207:A:MET:HE2	1:130:A:ILE:HD13	6	0.23	0.07	0.22
(2,212)	1:207:A:MET:HE2	1:218:A:ILE:HG23	6	0.23	0.07	0.22
(2,212)	1:207:A:MET:HE1	1:218:A:ILE:HG22	6	0.23	0.07	0.22
(1,762)	1:192:A:ILE:HG22	1:208:A:ILE:HD12	6	0.22	0.06	0.24
(1,762)	1:192:A:ILE:HG21	1:208:A:ILE:HD11	6	0.22	0.06	0.24
(1,762)	1:192:A:ILE:HG23	1:208:A:ILE:HD11	6	0.22	0.06	0.24
(1,266)	1:189:A:ASP:HB3	1:189:A:ASP:H	6	0.21	0.01	0.22
(1,605)	1:210:A:THR:HG23	1:211:A:VAL:H	6	0.2	0.06	0.21
(1,605)	1:210:A:THR:HG22	1:211:A:VAL:H	6	0.2	0.06	0.21
(2,185)	1:187:A:VAL:HB	1:183:A:VAL:HG12	6	0.2	0.08	0.2
(2,185)	1:166:A:VAL:HG12	1:217:A:VAL:HB	6	0.2	0.08	0.2
(2,185)	1:187:A:VAL:HB	1:183:A:VAL:HG11	6	0.2	0.08	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,185)	1:166:A:VAL:HG13	1:217:A:VAL:HB	6	0.2	0.08	0.2
(2,185)	1:187:A:VAL:HB	1:183:A:VAL:HG13	6	0.2	0.08	0.2
(1,683)	1:136:A:ALA:HB3	1:133:A:ASP:HB2	6	0.18	0.02	0.18
(1,683)	1:136:A:ALA:HB2	1:133:A:ASP:HB2	6	0.18	0.02	0.18
(1,990)	1:145:A:GLU:HB3	1:146:A:ILE:H	6	0.17	0.03	0.17
(1,589)	1:185:A:THR:HG21	1:184:A:GLU:HA	6	0.16	0.03	0.16
(1,589)	1:185:A:THR:HG22	1:184:A:GLU:HA	6	0.16	0.03	0.16
(1,589)	1:185:A:THR:HG23	1:184:A:GLU:HA	6	0.16	0.03	0.16
(1,282)	1:203:A:ASP:HB3	1:203:A:ASP:HA	6	0.14	0.01	0.14
(1,98)	1:170:A:GLU:HA	1:173:A:LEU:HB2	6	0.14	0.02	0.12
(1,377)	1:183:A:VAL:HB	1:184:A:GLU:H	6	0.12	0.01	0.12
(1,548)	1:173:A:LEU:HD13	1:187:A:VAL:HG11	5	2.69	1.66	2.7
(1,548)	1:173:A:LEU:HD11	1:187:A:VAL:HG13	5	2.69	1.66	2.7
(1,548)	1:173:A:LEU:HD12	1:187:A:VAL:HG12	5	2.69	1.66	2.7
(1,548)	1:173:A:LEU:HD11	1:187:A:VAL:HG11	5	2.69	1.66	2.7
(1,569)	1:173:A:LEU:HD11	1:188:A:VAL:HG21	5	2.69	0.11	2.76
(1,569)	1:173:A:LEU:HD12	1:188:A:VAL:HG21	5	2.69	0.11	2.76
(1,569)	1:173:A:LEU:HD11	1:188:A:VAL:HG22	5	2.69	0.11	2.76
(1,569)	1:173:A:LEU:HD12	1:188:A:VAL:HG22	5	2.69	0.11	2.76
(1,440)	1:184:A:GLU:HB2	1:186:A:ASN:HB3	5	1.07	0.19	1.11
(1,165)	1:164:A:ASN:HA	1:217:A:VAL:HG21	5	0.99	0.8	0.61
(1,165)	1:164:A:ASN:HA	1:217:A:VAL:HG23	5	0.99	0.8	0.61
(1,456)	1:134:A:LYS:HD3	1:157:A:TYR:HE1	5	0.7	0.42	0.65
(1,456)	1:134:A:LYS:HD3	1:157:A:TYR:HE2	5	0.7	0.42	0.65
(1,148)	1:189:A:ASP:HA	1:188:A:VAL:HG12	5	0.67	1.04	0.17
(1,148)	1:189:A:ASP:HA	1:188:A:VAL:HG11	5	0.67	1.04	0.17
(1,148)	1:189:A:ASP:HA	1:188:A:VAL:HG13	5	0.67	1.04	0.17
(1,649)	1:190:A:VAL:HB	1:187:A:VAL:HG23	5	0.64	0.74	0.28
(1,649)	1:190:A:VAL:HB	1:187:A:VAL:HG22	5	0.64	0.74	0.28
(1,649)	1:190:A:VAL:HB	1:187:A:VAL:HG21	5	0.64	0.74	0.28
(1,448)	1:212:A:ARG:HD3	1:212:A:ARG:HB2	5	0.56	0.29	0.77
(1,448)	1:212:A:ARG:HD3	1:212:A:ARG:HB3	5	0.56	0.29	0.77
(1,776)	1:204:A:ARG:HB2	1:130:A:ILE:HD11	5	0.55	0.37	0.51
(1,776)	1:204:A:ARG:HB2	1:130:A:ILE:HD13	5	0.55	0.37	0.51
(1,776)	1:204:A:ARG:HB2	1:130:A:ILE:HD12	5	0.55	0.37	0.51
(2,40)	1:204:A:ARG:HD2	1:204:A:ARG:HB2	5	0.55	0.14	0.61
(1,1011)	1:151:A:THR:H	1:150:A:LYS:HB2	5	0.45	0.08	0.42
(1,252)	1:138:A:LYS:HE2	1:138:A:LYS:HG2	5	0.35	0.04	0.35
(1,252)	1:138:A:LYS:HE3	1:138:A:LYS:HG2	5	0.35	0.04	0.35
(1,171)	1:186:A:ASN:HA	1:186:A:ASN:HB2	5	0.35	0.01	0.35
(2,307)	1:211:A:VAL:H	1:216:A:TYR:HD2	5	0.33	0.18	0.3
(2,307)	1:211:A:VAL:H	1:216:A:TYR:HD1	5	0.33	0.18	0.3

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,314)	1:204:A:ARG:H	1:199:A:LEU:HD23	5	0.33	0.11	0.29
(2,314)	1:204:A:ARG:H	1:199:A:LEU:HD21	5	0.33	0.11	0.29
(2,314)	1:204:A:ARG:H	1:199:A:LEU:HD22	5	0.33	0.11	0.29
(2,226)	1:159:A:LEU:HB3	1:218:A:ILE:HD13	5	0.31	0.12	0.31
(2,226)	1:125:A:ILE:HD13	1:132:A:ILE:HB	5	0.31	0.12	0.31
(2,226)	1:159:A:LEU:HB3	1:218:A:ILE:HD11	5	0.31	0.12	0.31
(2,47)	1:204:A:ARG:HD2	1:199:A:LEU:HD22	5	0.31	0.15	0.3
(2,47)	1:204:A:ARG:HD2	1:141:A:VAL:HG22	5	0.31	0.15	0.3
(2,47)	1:204:A:ARG:HD2	1:199:A:LEU:HD23	5	0.31	0.15	0.3
(2,47)	1:204:A:ARG:HD2	1:141:A:VAL:HG21	5	0.31	0.15	0.3
(1,733)	1:130:A:ILE:HG21	1:131:A:THR:H	5	0.3	0.05	0.29
(1,733)	1:130:A:ILE:HG22	1:131:A:THR:H	5	0.3	0.05	0.29
(1,733)	1:130:A:ILE:HG23	1:131:A:THR:H	5	0.3	0.05	0.29
(2,214)	1:167:A:MET:HE3	1:159:A:LEU:HA	5	0.28	0.11	0.34
(2,214)	1:167:A:MET:HE1	1:159:A:LEU:HA	5	0.28	0.11	0.34
(2,214)	1:167:A:MET:HE1	1:158:A:LEU:HA	5	0.28	0.11	0.34
(2,214)	1:167:A:MET:HE2	1:159:A:LEU:HA	5	0.28	0.11	0.34
(1,479)	1:193:A:ARG:HG3	1:193:A:ARG:HA	5	0.27	0.07	0.3
(2,187)	1:127:A:VAL:HG22	1:126:A:ASP:HA	5	0.26	0.06	0.26
(2,187)	1:127:A:VAL:HG21	1:126:A:ASP:HA	5	0.26	0.06	0.26
(2,187)	1:127:A:VAL:HG23	1:126:A:ASP:HA	5	0.26	0.06	0.26
(1,466)	1:193:A:ARG:HB3	1:193:A:ARG:H	5	0.23	0.02	0.24
(1,634)	1:183:A:VAL:HG12	1:187:A:VAL:H	5	0.21	0.06	0.22
(1,634)	1:183:A:VAL:HG11	1:187:A:VAL:H	5	0.21	0.06	0.22
(1,634)	1:183:A:VAL:HG13	1:187:A:VAL:H	5	0.21	0.06	0.22
(2,193)	1:176:A:VAL:HG11	1:177:A:TRP:HZ3	5	0.21	0.05	0.22
(2,193)	1:176:A:VAL:HG12	1:177:A:TRP:HZ3	5	0.21	0.05	0.22
(1,211)	1:216:A:TYR:HB2	1:217:A:VAL:H	5	0.2	0.09	0.18
(1,360)	1:147:A:GLU:HG3	1:147:A:GLU:HA	5	0.19	0.06	0.2
(1,573)	1:151:A:THR:HG22	1:152:A:GLU:H	5	0.16	0.03	0.14
(1,573)	1:151:A:THR:HG21	1:152:A:GLU:H	5	0.16	0.03	0.14
(1,573)	1:151:A:THR:HG23	1:152:A:GLU:H	5	0.16	0.03	0.14
(1,41)	1:185:A:THR:HA	1:173:A:LEU:HB3	5	0.15	0.02	0.14
(2,289)	1:214:A:VAL:HG13	1:215:A:GLY:H	5	0.14	0.05	0.12
(2,289)	1:214:A:VAL:HG11	1:215:A:GLY:H	5	0.14	0.05	0.12
(2,289)	1:214:A:VAL:HG12	1:215:A:GLY:H	5	0.14	0.05	0.12
(1,168)	1:160:A:ALA:HA	1:127:A:VAL:HB	5	0.14	0.02	0.15
(1,482)	1:148:A:LEU:HD11	1:153:A:TYR:H	5	0.14	0.02	0.13
(1,482)	1:148:A:LEU:HD13	1:153:A:TYR:H	5	0.14	0.02	0.13
(1,482)	1:148:A:LEU:HD12	1:153:A:TYR:H	5	0.14	0.02	0.13
(1,979)	1:175:A:HIS:H	1:174:A:ASN:HB2	5	0.14	0.02	0.14
(1,594)	1:156:A:LEU:HA	1:156:A:LEU:HD12	5	0.13	0.02	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,594)	1:156:A:LEU:HA	1:156:A:LEU:HD11	5	0.13	0.02	0.13
(1,594)	1:156:A:LEU:HA	1:156:A:LEU:HD13	5	0.13	0.02	0.13
(1,390)	1:204:A:ARG:HB3	1:204:A:ARG:H	5	0.12	0.02	0.12
(1,1075)	1:147:A:GLU:H	1:146:A:ILE:HB	5	0.12	0.02	0.12
(1,542)	1:173:A:LEU:HD11	1:177:A:TRP:HE3	4	1.25	0.1	1.25
(1,542)	1:173:A:LEU:HD12	1:177:A:TRP:HE3	4	1.25	0.1	1.25
(1,101)	1:170:A:GLU:HA	1:173:A:LEU:HD21	4	1.14	0.16	1.08
(1,101)	1:170:A:GLU:HA	1:173:A:LEU:HD22	4	1.14	0.16	1.08
(1,101)	1:170:A:GLU:HA	1:173:A:LEU:HD23	4	1.14	0.16	1.08
(1,604)	1:185:A:THR:HG21	1:173:A:LEU:HD21	4	0.92	0.13	0.98
(1,604)	1:185:A:THR:HG21	1:173:A:LEU:HD22	4	0.92	0.13	0.98
(1,604)	1:185:A:THR:HG23	1:173:A:LEU:HD23	4	0.92	0.13	0.98
(1,46)	1:185:A:THR:HA	1:173:A:LEU:HD13	4	0.82	0.05	0.84
(1,46)	1:185:A:THR:HA	1:173:A:LEU:HD11	4	0.82	0.05	0.84
(1,709)	1:209:A:GLU:HG3	1:217:A:VAL:HG13	4	0.79	0.98	0.28
(1,709)	1:209:A:GLU:HG3	1:217:A:VAL:HG11	4	0.79	0.98	0.28
(1,709)	1:209:A:GLU:HG2	1:217:A:VAL:HG13	4	0.79	0.98	0.28
(1,709)	1:209:A:GLU:HG3	1:217:A:VAL:HG12	4	0.79	0.98	0.28
(2,174)	1:173:A:LEU:HG	1:177:A:TRP:HB2	4	0.78	0.07	0.8
(2,300)	1:172:A:ILE:HG23	1:174:A:ASN:H	4	0.76	0.03	0.77
(2,300)	1:172:A:ILE:HG22	1:174:A:ASN:H	4	0.76	0.03	0.77
(2,300)	1:174:A:ASN:H	1:173:A:LEU:HG	4	0.76	0.03	0.77
(1,219)	1:216:A:TYR:HB3	1:159:A:LEU:HD22	4	0.65	0.42	0.66
(2,106)	1:190:A:VAL:HB	1:187:A:VAL:HG21	4	0.63	0.79	0.18
(2,106)	1:190:A:VAL:HB	1:187:A:VAL:HG23	4	0.63	0.79	0.18
(2,106)	1:190:A:VAL:HB	1:187:A:VAL:HG22	4	0.63	0.79	0.18
(1,547)	1:173:A:LEU:HD12	1:173:A:LEU:HB2	4	0.6	0.01	0.6
(1,547)	1:173:A:LEU:HD13	1:173:A:LEU:HB2	4	0.6	0.01	0.6
(1,530)	1:159:A:LEU:HB2	1:159:A:LEU:HD11	4	0.55	0.06	0.55
(2,262)	1:193:A:ARG:H	1:193:A:ARG:HD3	4	0.55	0.17	0.58
(2,262)	1:193:A:ARG:H	1:193:A:ARG:HD2	4	0.55	0.17	0.58
(2,263)	1:166:A:VAL:H	1:165:A:HIS:HB3	4	0.48	0.09	0.46
(2,263)	1:166:A:VAL:H	1:165:A:HIS:HB2	4	0.48	0.09	0.46
(2,290)	1:124:A:ILE:H	1:124:A:ILE:HG22	4	0.43	0.19	0.39
(2,290)	1:124:A:ILE:HD12	1:124:A:ILE:H	4	0.43	0.19	0.39
(2,290)	1:124:A:ILE:HD11	1:124:A:ILE:H	4	0.43	0.19	0.39
(2,142)	1:173:A:LEU:HD21	1:184:A:GLU:HA	4	0.43	0.21	0.34
(2,142)	1:173:A:LEU:HD22	1:184:A:GLU:HA	4	0.43	0.21	0.34
(2,153)	1:173:A:LEU:HD11	1:177:A:TRP:H	4	0.4	0.1	0.36
(2,153)	1:173:A:LEU:HD12	1:177:A:TRP:H	4	0.4	0.1	0.36
(1,544)	1:173:A:LEU:HD11	1:173:A:LEU:HA	4	0.35	0.02	0.35
(1,544)	1:173:A:LEU:HD12	1:173:A:LEU:HA	4	0.35	0.02	0.35

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,978)	1:126:A:ASP:HB2	1:126:A:ASP:H	4	0.33	0.01	0.34
(2,291)	1:199:A:LEU:HD21	1:199:A:LEU:H	4	0.29	0.1	0.26
(2,291)	1:199:A:LEU:HD23	1:199:A:LEU:H	4	0.29	0.1	0.26
(2,291)	1:199:A:LEU:HD22	1:199:A:LEU:H	4	0.29	0.1	0.26
(1,736)	1:207:A:MET:HE2	1:130:A:ILE:H	4	0.28	0.03	0.28
(1,736)	1:207:A:MET:HE3	1:130:A:ILE:H	4	0.28	0.03	0.28
(1,1078)	1:165:A:HIS:H	1:163:A:LYS:HG3	4	0.26	0.06	0.24
(1,1078)	1:165:A:HIS:H	1:163:A:LYS:HG2	4	0.26	0.06	0.24
(1,642)	1:183:A:VAL:HG13	1:187:A:VAL:HG13	4	0.24	0.09	0.22
(1,642)	1:183:A:VAL:HG13	1:187:A:VAL:HG12	4	0.24	0.09	0.22
(1,642)	1:183:A:VAL:HG12	1:187:A:VAL:HG13	4	0.24	0.09	0.22
(1,642)	1:183:A:VAL:HG11	1:187:A:VAL:HG11	4	0.24	0.09	0.22
(1,585)	1:139:A:VAL:HG23	1:153:A:TYR:HE1	4	0.24	0.06	0.24
(1,585)	1:139:A:VAL:HG22	1:153:A:TYR:HE1	4	0.24	0.06	0.24
(1,585)	1:139:A:VAL:HG21	1:153:A:TYR:HE1	4	0.24	0.06	0.24
(2,31)	1:205:A:ASP:HA	1:196:A:ARG:HD2	4	0.24	0.18	0.15
(2,170)	1:199:A:LEU:HD21	1:199:A:LEU:H	4	0.23	0.08	0.23
(2,170)	1:159:A:LEU:HD22	1:159:A:LEU:H	4	0.23	0.08	0.23
(2,170)	1:159:A:LEU:HD21	1:159:A:LEU:H	4	0.23	0.08	0.23
(2,126)	1:132:A:ILE:HG13	1:139:A:VAL:HA	4	0.22	0.06	0.22
(1,621)	1:131:A:THR:HG22	1:126:A:ASP:HA	4	0.2	0.03	0.18
(1,621)	1:131:A:THR:HG21	1:126:A:ASP:HA	4	0.2	0.03	0.18
(2,238)	1:128:A:ASN:HB2	1:128:A:ASN:HA	4	0.18	0.01	0.18
(1,1029)	1:130:A:ILE:HG12	1:130:A:ILE:H	4	0.17	0.01	0.18
(2,277)	1:172:A:ILE:HG23	1:173:A:LEU:H	4	0.15	0.02	0.15
(2,277)	1:172:A:ILE:HG22	1:173:A:LEU:H	4	0.15	0.02	0.15
(2,91)	1:171:A:GLN:HG3	1:168:A:GLN:H	4	0.14	0.02	0.14
(1,195)	1:215:A:GLY:HA2	1:169:A:ARG:HG2	4	0.12	0.02	0.12
(2,234)	1:214:A:VAL:HG11	1:214:A:VAL:HA	4	0.12	0.01	0.12
(2,234)	1:214:A:VAL:HG13	1:214:A:VAL:HA	4	0.12	0.01	0.12
(2,234)	1:214:A:VAL:HG12	1:214:A:VAL:HA	4	0.12	0.01	0.12
(1,433)	1:184:A:GLU:HB3	1:184:A:GLU:H	4	0.11	0.01	0.12
(2,90)	1:214:A:VAL:HB	1:214:A:VAL:HG11	4	0.1	0.0	0.1
(2,90)	1:214:A:VAL:HB	1:214:A:VAL:HG21	4	0.1	0.0	0.1
(2,124)	1:171:A:GLN:HB3	1:172:A:ILE:HG12	3	1.13	0.56	1.3
(2,124)	1:171:A:GLN:HB3	1:167:A:MET:HE2	3	1.13	0.56	1.3
(2,124)	1:171:A:GLN:HB3	1:167:A:MET:HE1	3	1.13	0.56	1.3
(1,398)	1:167:A:MET:HB3	1:172:A:ILE:HD12	3	0.96	0.23	0.97
(1,398)	1:167:A:MET:HB3	1:172:A:ILE:HD11	3	0.96	0.23	0.97
(1,802)	1:124:A:ILE:HD12	1:133:A:ASP:HB2	3	0.92	0.12	0.87
(1,802)	1:124:A:ILE:HD11	1:133:A:ASP:HB2	3	0.92	0.12	0.87
(2,224)	1:207:A:MET:HE1	1:130:A:ILE:HD12	3	0.85	0.18	0.78

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,224)	1:130:A:ILE:HD11	1:130:A:ILE:HB	3	0.85	0.18	0.78
(2,224)	1:207:A:MET:HE1	1:130:A:ILE:HD13	3	0.85	0.18	0.78
(1,399)	1:167:A:MET:HB3	1:172:A:ILE:HG13	3	0.83	0.44	0.8
(2,143)	1:199:A:LEU:HD13	1:196:A:ARG:HD2	3	0.74	0.3	0.75
(2,143)	1:199:A:LEU:HD12	1:196:A:ARG:HD2	3	0.74	0.3	0.75
(1,50)	1:181:A:SER:HB2	1:177:A:TRP:HB2	3	0.63	0.34	0.42
(1,748)	1:167:A:MET:HE2	1:167:A:MET:HA	3	0.59	0.17	0.5
(1,748)	1:167:A:MET:HE1	1:167:A:MET:HA	3	0.59	0.17	0.5
(2,60)	1:159:A:LEU:HB2	1:218:A:ILE:HD11	3	0.55	0.05	0.58
(2,60)	1:159:A:LEU:HB2	1:159:A:LEU:HD11	3	0.55	0.05	0.58
(1,753)	1:158:A:LEU:HD23	1:167:A:MET:HE3	3	0.54	0.12	0.52
(1,753)	1:158:A:LEU:HD23	1:167:A:MET:HE2	3	0.54	0.12	0.52
(1,753)	1:158:A:LEU:HD23	1:167:A:MET:HE1	3	0.54	0.12	0.52
(2,203)	1:217:A:VAL:HG11	1:219:A:ARG:HG3	3	0.49	0.34	0.35
(2,203)	1:217:A:VAL:HG12	1:219:A:ARG:HG2	3	0.49	0.34	0.35
(2,203)	1:217:A:VAL:HG11	1:219:A:ARG:HG2	3	0.49	0.34	0.35
(1,280)	1:203:A:ASP:HB2	1:203:A:ASP:H	3	0.45	0.01	0.45
(2,39)	1:219:A:ARG:HD3	1:217:A:VAL:HG12	3	0.4	0.15	0.4
(2,39)	1:219:A:ARG:HD3	1:217:A:VAL:HG21	3	0.4	0.15	0.4
(2,39)	1:219:A:ARG:HD3	1:217:A:VAL:HG11	3	0.4	0.15	0.4
(1,794)	1:146:A:ILE:HD12	1:202:A:TYR:HE2	3	0.24	0.15	0.18
(1,794)	1:146:A:ILE:HD13	1:202:A:TYR:HE2	3	0.24	0.15	0.18
(1,794)	1:146:A:ILE:HD12	1:202:A:TYR:HE1	3	0.24	0.15	0.18
(2,36)	1:193:A:ARG:HA	1:196:A:ARG:HD3	3	0.23	0.14	0.16
(2,36)	1:205:A:ASP:HA	1:196:A:ARG:HD2	3	0.23	0.14	0.16
(1,574)	1:151:A:THR:HG23	1:191:A:TYR:HE2	3	0.22	0.04	0.25
(1,716)	1:160:A:ALA:HB2	1:156:A:LEU:HD13	3	0.22	0.08	0.27
(1,716)	1:160:A:ALA:HB3	1:156:A:LEU:HD11	3	0.22	0.08	0.27
(1,716)	1:160:A:ALA:HB3	1:156:A:LEU:HD12	3	0.22	0.08	0.27
(1,36)	1:187:A:VAL:HA	1:190:A:VAL:HG22	3	0.21	0.02	0.19
(1,36)	1:187:A:VAL:HA	1:190:A:VAL:HG23	3	0.21	0.02	0.19
(1,772)	1:132:A:ILE:HD12	1:157:A:TYR:H	3	0.2	0.08	0.22
(1,772)	1:132:A:ILE:HD13	1:157:A:TYR:H	3	0.2	0.08	0.22
(2,217)	1:192:A:ILE:HG21	1:216:A:TYR:HE2	3	0.18	0.02	0.18
(2,217)	1:192:A:ILE:HG23	1:216:A:TYR:HE1	3	0.18	0.02	0.18
(2,2)	1:185:A:THR:HB	1:173:A:LEU:HB3	3	0.18	0.01	0.17
(2,2)	1:185:A:THR:HB	1:169:A:ARG:HB2	3	0.18	0.01	0.17
(1,516)	1:155:A:LEU:HD21	1:192:A:ILE:H	3	0.17	0.04	0.17
(1,516)	1:155:A:LEU:HD22	1:192:A:ILE:H	3	0.17	0.04	0.17
(1,516)	1:155:A:LEU:HD23	1:192:A:ILE:H	3	0.17	0.04	0.17
(1,550)	1:150:A:LYS:HG3	1:149:A:THR:HB	3	0.16	0.03	0.15
(1,550)	1:150:A:LYS:HG2	1:149:A:THR:HB	3	0.16	0.03	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,246)	1:133:A:ASP:HB3	1:133:A:ASP:H	3	0.16	0.02	0.15
(1,528)	1:159:A:LEU:HB3	1:159:A:LEU:HD13	3	0.16	0.04	0.16
(1,528)	1:159:A:LEU:HB3	1:159:A:LEU:HD12	3	0.16	0.04	0.16
(2,239)	1:153:A:TYR:HB3	1:148:A:LEU:HB3	3	0.16	0.02	0.15
(1,707)	1:166:A:VAL:HA	1:217:A:VAL:HG11	3	0.14	0.04	0.12
(1,707)	1:166:A:VAL:HA	1:217:A:VAL:HG12	3	0.14	0.04	0.12
(1,734)	1:146:A:ILE:HG21	1:147:A:GLU:H	3	0.14	0.01	0.14
(1,734)	1:146:A:ILE:HG23	1:147:A:GLU:H	3	0.14	0.01	0.14
(1,623)	1:149:A:THR:HG22	1:149:A:THR:HA	3	0.13	0.01	0.13
(1,623)	1:149:A:THR:HG21	1:149:A:THR:HA	3	0.13	0.01	0.13
(1,388)	1:167:A:MET:HG3	1:167:A:MET:H	3	0.13	0.01	0.13
(1,898)	1:154:A:ASP:H	1:153:A:TYR:HD2	3	0.12	0.01	0.12
(2,160)	1:134:A:LYS:HG2	1:134:A:LYS:HD3	3	0.11	0.01	0.11
(2,160)	1:138:A:LYS:HB2	1:138:A:LYS:HG3	3	0.11	0.01	0.11
(1,570)	1:188:A:VAL:HG22	1:187:A:VAL:HG11	2	2.13	0.8	2.13
(1,570)	1:188:A:VAL:HG22	1:187:A:VAL:HG13	2	2.13	0.8	2.13
(2,147)	1:204:A:ARG:HB2	1:199:A:LEU:HD13	2	1.23	1.04	1.23
(2,147)	1:204:A:ARG:HB2	1:199:A:LEU:HD11	2	1.23	1.04	1.23
(1,339)	1:128:A:ASN:HB3	1:207:A:MET:HG2	2	0.85	0.72	0.85
(1,775)	1:130:A:ILE:HD12	1:130:A:ILE:HA	2	0.69	0.03	0.69
(1,775)	1:130:A:ILE:HD11	1:130:A:ILE:HA	2	0.69	0.03	0.69
(1,51)	1:181:A:SER:HB3	1:183:A:VAL:HG21	2	0.5	0.38	0.5
(1,51)	1:181:A:SER:HB3	1:183:A:VAL:HG22	2	0.5	0.38	0.5
(2,117)	1:165:A:HIS:HB2	1:162:A:ASN:HB2	2	0.47	0.32	0.47
(2,117)	1:165:A:HIS:HB3	1:162:A:ASN:HB2	2	0.47	0.32	0.47
(1,773)	1:130:A:ILE:HD13	1:130:A:ILE:H	2	0.45	0.04	0.45
(1,773)	1:130:A:ILE:HD12	1:130:A:ILE:H	2	0.45	0.04	0.45
(1,1010)	1:135:A:ASN:H	1:134:A:LYS:HB3	2	0.44	0.03	0.44
(1,1010)	1:135:A:ASN:H	1:134:A:LYS:HB2	2	0.44	0.03	0.44
(1,133)	1:159:A:LEU:HA	1:162:A:ASN:HB2	2	0.42	0.32	0.42
(1,575)	1:151:A:THR:HG22	1:177:A:TRP:HH2	2	0.32	0.02	0.32
(2,173)	1:210:A:THR:HG22	1:216:A:TYR:HE1	2	0.32	0.02	0.32
(1,801)	1:124:A:ILE:HD11	1:124:A:ILE:H	2	0.32	0.2	0.32
(1,352)	1:147:A:GLU:HG3	1:147:A:GLU:H	2	0.29	0.1	0.29
(1,555)	1:175:A:HIS:HB2	1:176:A:VAL:HG22	2	0.29	0.01	0.29
(1,555)	1:175:A:HIS:HB2	1:176:A:VAL:HG23	2	0.29	0.01	0.29
(2,104)	1:167:A:MET:HB2	1:167:A:MET:HG2	2	0.29	0.0	0.29
(1,766)	1:172:A:ILE:HD13	1:216:A:TYR:HD2	2	0.28	0.01	0.28
(2,82)	1:138:A:LYS:HB3	1:133:A:ASP:HB3	2	0.24	0.04	0.24
(1,738)	1:128:A:ASN:HB3	1:207:A:MET:HE2	2	0.24	0.1	0.24
(1,738)	1:128:A:ASN:HB3	1:207:A:MET:HE1	2	0.24	0.1	0.24
(2,79)	1:152:A:GLU:HG3	1:155:A:LEU:HD11	2	0.24	0.08	0.24

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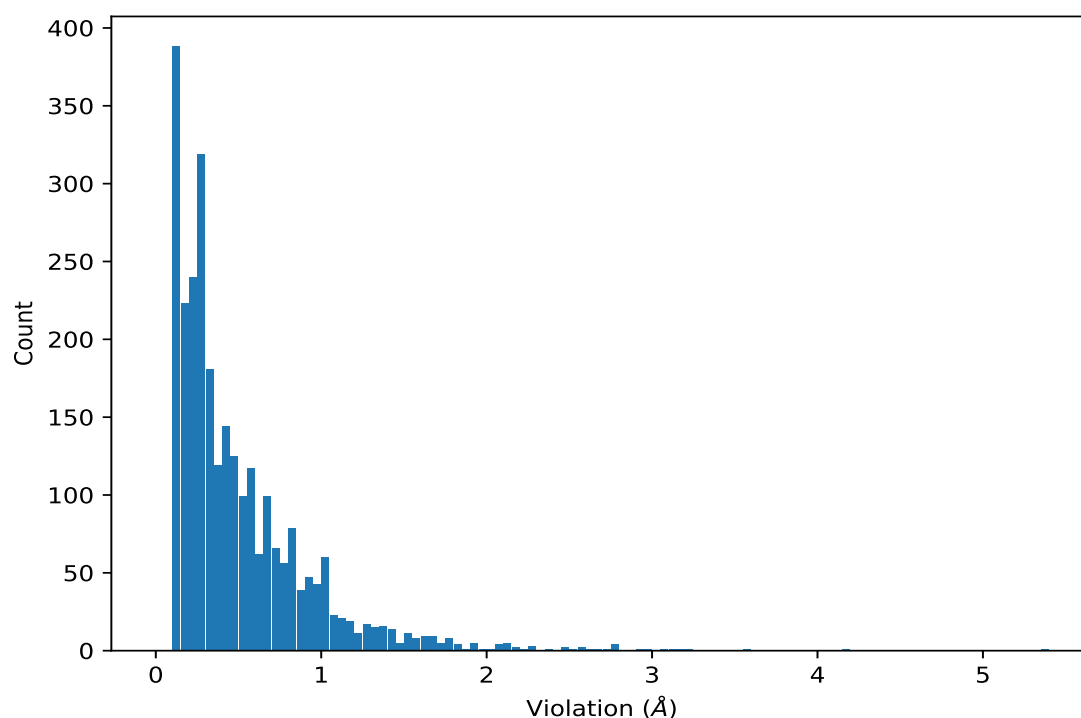
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,79)	1:152:A:GLU:HG3	1:155:A:LEU:HD12	2	0.24	0.08	0.24
(1,619)	1:159:A:LEU:HD21	1:192:A:ILE:HD13	2	0.23	0.07	0.23
(1,619)	1:159:A:LEU:HD23	1:192:A:ILE:HD13	2	0.23	0.07	0.23
(1,375)	1:141:A:VAL:HB	1:141:A:VAL:H	2	0.22	0.12	0.22
(1,659)	1:202:A:TYR:HB2	1:141:A:VAL:HG12	2	0.22	0.03	0.22
(2,56)	1:133:A:ASP:HB2	1:138:A:LYS:HB2	2	0.19	0.09	0.19
(2,56)	1:133:A:ASP:HB2	1:138:A:LYS:HB3	2	0.19	0.09	0.19
(1,69)	1:153:A:TYR:HA	1:156:A:LEU:HB2	2	0.18	0.03	0.18
(2,208)	1:130:A:ILE:HG23	1:131:A:THR:HA	2	0.17	0.03	0.17
(2,208)	1:130:A:ILE:HG21	1:131:A:THR:HA	2	0.17	0.03	0.17
(1,717)	1:160:A:ALA:HB2	1:132:A:ILE:HD13	2	0.16	0.02	0.16
(1,726)	1:132:A:ILE:HG23	1:134:A:LYS:HA	2	0.16	0.04	0.16
(2,15)	1:152:A:GLU:HA	1:152:A:GLU:HG3	2	0.16	0.01	0.16
(2,15)	1:152:A:GLU:HA	1:152:A:GLU:HB2	2	0.16	0.01	0.16
(1,153)	1:206:A:LYS:HA	1:206:A:LYS:HG2	2	0.15	0.01	0.15
(1,993)	1:194:A:TYR:H	1:193:A:ARG:HB2	2	0.15	0.03	0.15
(1,496)	1:130:A:ILE:HG12	1:130:A:ILE:HA	2	0.15	0.04	0.15
(1,1001)	1:159:A:LEU:HB3	1:160:A:ALA:H	2	0.15	0.02	0.15
(1,576)	1:151:A:THR:HG23	1:177:A:TRP:HZ2	2	0.14	0.03	0.14
(1,169)	1:160:A:ALA:HA	1:218:A:ILE:HB	2	0.12	0.02	0.12
(1,928)	1:180:A:ASN:H	1:179:A:TYR:HA	2	0.11	0.0	0.11
(1,778)	1:130:A:ILE:HG13	1:130:A:ILE:HD12	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)
(1,548)	1:173:A:LEU:HD11	1:187:A:VAL:HG13	2	5.38
(1,340)	1:142:A:ASN:HB3	1:141:A:VAL:HG11	4	4.16
(2,148)	1:199:A:LEU:HD12	1:207:A:MET:HB2	10	3.57
(2,166)	1:188:A:VAL:HG21	1:191:A:TYR:HB3	3	3.22
(1,1037)	1:165:A:HIS:H	1:217:A:VAL:HG23	5	3.19
(2,189)	1:217:A:VAL:HG22	1:165:A:HIS:HB3	5	3.15
(1,536)	1:192:A:ILE:HG13	1:188:A:VAL:HG11	3	3.07
(1,548)	1:173:A:LEU:HD11	1:187:A:VAL:HG11	10	2.95
(1,570)	1:188:A:VAL:HG22	1:187:A:VAL:HG11	2	2.93
(1,569)	1:173:A:LEU:HD11	1:188:A:VAL:HG21	1	2.77
(1,569)	1:173:A:LEU:HD12	1:188:A:VAL:HG21	2	2.76
(1,569)	1:173:A:LEU:HD12	1:188:A:VAL:HG21	10	2.76
(1,148)	1:189:A:ASP:HA	1:188:A:VAL:HG12	3	2.75
(1,548)	1:173:A:LEU:HD11	1:187:A:VAL:HG11	9	2.7
(1,569)	1:173:A:LEU:HD12	1:188:A:VAL:HG22	9	2.66
(1,607)	1:159:A:LEU:HD21	1:217:A:VAL:HA	9	2.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,607)	1:159:A:LEU:HD21	1:217:A:VAL:HA	8	2.58
(1,165)	1:164:A:ASN:HA	1:217:A:VAL:HG23	5	2.57
(1,633)	1:166:A:VAL:HG12	1:215:A:GLY:H	6	2.55
(1,569)	1:173:A:LEU:HD11	1:188:A:VAL:HG22	3	2.49
(1,709)	1:209:A:GLU:HG2	1:217:A:VAL:HG13	5	2.48
(1,561)	1:188:A:VAL:HG23	1:177:A:TRP:HE3	3	2.38
(2,147)	1:204:A:ARG:HB2	1:199:A:LEU:HD13	10	2.27
(1,564)	1:188:A:VAL:HG23	1:177:A:TRP:HZ3	3	2.27
(1,696)	1:187:A:VAL:HG12	1:188:A:VAL:HA	2	2.25
(1,548)	1:173:A:LEU:HD13	1:187:A:VAL:HG11	1	2.24
(2,166)	1:188:A:VAL:HG23	1:177:A:TRP:HB3	10	2.18
(2,166)	1:188:A:VAL:HG23	1:191:A:TYR:HB3	2	2.17
(2,166)	1:188:A:VAL:HG23	1:177:A:TRP:HB3	1	2.13
(1,649)	1:190:A:VAL:HB	1:187:A:VAL:HG23	2	2.13
(1,699)	1:144:A:ALA:HB3	1:141:A:VAL:HG13	4	2.12
(2,166)	1:188:A:VAL:HG21	1:177:A:TRP:HB3	8	2.1
(2,166)	1:188:A:VAL:HG21	1:177:A:TRP:HB3	9	2.1
(2,166)	1:188:A:VAL:HG23	1:177:A:TRP:HB3	5	2.08
(2,86)	1:145:A:GLU:HG3	1:138:A:LYS:HE3	7	2.08
(1,565)	1:188:A:VAL:HG23	1:173:A:LEU:HA	3	2.07
(1,596)	1:167:A:MET:HG2	1:159:A:LEU:HD21	8	2.06
(2,106)	1:190:A:VAL:HB	1:187:A:VAL:HG23	2	2.0
(2,166)	1:188:A:VAL:HG22	1:177:A:TRP:HB3	6	1.96
(2,166)	1:188:A:VAL:HG22	1:177:A:TRP:HB3	4	1.95
(1,340)	1:142:A:ASN:HB3	1:141:A:VAL:HG13	6	1.95
(1,340)	1:142:A:ASN:HB3	1:141:A:VAL:HG12	2	1.92
(1,340)	1:142:A:ASN:HB3	1:141:A:VAL:HG11	5	1.91
(1,340)	1:142:A:ASN:HB3	1:141:A:VAL:HG13	9	1.91
(2,88)	1:184:A:GLU:HG2	1:183:A:VAL:HG12	8	1.86
(2,88)	1:184:A:GLU:HG2	1:183:A:VAL:HG12	1	1.84
(1,1035)	1:217:A:VAL:HG21	1:218:A:ILE:H	5	1.84
(2,172)	1:199:A:LEU:HD22	1:202:A:TYR:HD2	10	1.83
(2,122)	1:147:A:GLU:HB2	1:146:A:ILE:HG23	9	1.82
(2,166)	1:188:A:VAL:HG21	1:177:A:TRP:HB3	7	1.79
(1,697)	1:177:A:TRP:HB2	1:183:A:VAL:HG21	2	1.79
(1,697)	1:177:A:TRP:HB2	1:183:A:VAL:HG23	10	1.79
(2,197)	1:187:A:VAL:HG13	1:177:A:TRP:HH2	2	1.77
(1,742)	1:207:A:MET:HE3	1:218:A:ILE:HG13	6	1.77
(1,697)	1:177:A:TRP:HB2	1:183:A:VAL:HG22	9	1.77
(1,702)	1:217:A:VAL:HG12	1:217:A:VAL:H	5	1.76
(1,340)	1:142:A:ASN:HB3	1:141:A:VAL:HG11	3	1.76
(2,78)	1:197:A:ASN:HB3	1:198:A:LYS:HB3	7	1.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,697)	1:177:A:TRP:HB2	1:183:A:VAL:HG23	7	1.73
(2,124)	1:171:A:GLN:HB3	1:172:A:ILE:HG12	2	1.72
(1,697)	1:177:A:TRP:HB2	1:183:A:VAL:HG21	1	1.71
(1,697)	1:177:A:TRP:HB2	1:183:A:VAL:HG23	5	1.71
(2,86)	1:145:A:GLU:HG3	1:138:A:LYS:HE3	4	1.7
(1,697)	1:177:A:TRP:HB2	1:183:A:VAL:HG21	4	1.7
(1,678)	1:187:A:VAL:HG11	1:188:A:VAL:H	2	1.7
(2,190)	1:141:A:VAL:HG23	1:142:A:ASN:HB3	4	1.69
(2,88)	1:184:A:GLU:HG2	1:183:A:VAL:HG13	3	1.68
(1,742)	1:207:A:MET:HE1	1:218:A:ILE:HG13	3	1.68
(1,697)	1:177:A:TRP:HB2	1:183:A:VAL:HG21	8	1.68
(1,568)	1:188:A:VAL:HG23	1:173:A:LEU:HB2	3	1.68
(1,608)	1:199:A:LEU:HD22	1:199:A:LEU:HA	10	1.67
(1,742)	1:207:A:MET:HE3	1:218:A:ILE:HG13	9	1.64
(1,654)	1:141:A:VAL:HG12	1:202:A:TYR:HE2	4	1.64
(1,49)	1:181:A:SER:HB3	1:177:A:TRP:HB2	2	1.64
(1,29)	1:190:A:VAL:HA	1:189:A:ASP:HB3	9	1.64
(1,26)	1:190:A:VAL:HA	1:193:A:ARG:HB3	6	1.64
(1,613)	1:190:A:VAL:HG23	1:189:A:ASP:HB3	9	1.63
(1,742)	1:207:A:MET:HE1	1:218:A:ILE:HG13	1	1.61
(1,742)	1:207:A:MET:HE2	1:218:A:ILE:HG13	2	1.61
(1,596)	1:167:A:MET:HG2	1:159:A:LEU:HD21	9	1.61
(2,205)	1:172:A:ILE:HG23	1:158:A:LEU:HD12	6	1.59
(1,742)	1:207:A:MET:HE2	1:218:A:ILE:HG13	10	1.59
(1,742)	1:207:A:MET:HE1	1:218:A:ILE:HG13	7	1.58
(1,643)	1:166:A:VAL:HG13	1:167:A:MET:H	6	1.58
(1,635)	1:187:A:VAL:HG23	1:191:A:TYR:HD1	2	1.57
(1,339)	1:128:A:ASN:HB3	1:207:A:MET:HG2	7	1.57
(2,241)	1:216:A:TYR:HB2	1:217:A:VAL:HB	7	1.56
(1,742)	1:207:A:MET:HE3	1:218:A:ILE:HG13	8	1.55
(1,742)	1:207:A:MET:HE1	1:218:A:ILE:HG13	4	1.54
(1,742)	1:207:A:MET:HE2	1:218:A:ILE:HG13	5	1.54
(2,241)	1:216:A:TYR:HB2	1:217:A:VAL:HB	4	1.52
(2,241)	1:216:A:TYR:HB2	1:159:A:LEU:HB3	5	1.52
(2,205)	1:172:A:ILE:HG21	1:158:A:LEU:HD11	2	1.52
(2,148)	1:199:A:LEU:HD11	1:207:A:MET:HB2	7	1.52
(1,1031)	1:166:A:VAL:H	1:166:A:VAL:HG23	6	1.51
(1,746)	1:207:A:MET:HG3	1:218:A:ILE:HG23	3	1.51
(1,645)	1:187:A:VAL:HG22	1:191:A:TYR:HE1	2	1.51
(1,26)	1:190:A:VAL:HA	1:193:A:ARG:HB3	3	1.51
(1,26)	1:190:A:VAL:HA	1:193:A:ARG:HB3	1	1.5
(1,751)	1:167:A:MET:HE3	1:158:A:LEU:HB2	5	1.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,697)	1:177:A:TRP:HB2	1:183:A:VAL:HG23	6	1.47
(2,205)	1:172:A:ILE:HG23	1:158:A:LEU:HD11	3	1.46
(1,746)	1:207:A:MET:HG3	1:218:A:ILE:HG21	1	1.46
(1,194)	1:215:A:GLY:HA2	1:169:A:ARG:HB2	8	1.46
(1,751)	1:167:A:MET:HE3	1:158:A:LEU:HB2	4	1.45
(2,241)	1:216:A:TYR:HB2	1:217:A:VAL:HB	8	1.44
(1,532)	1:173:A:LEU:HD21	1:174:A:ASN:H	9	1.44
(1,255)	1:159:A:LEU:HB2	1:218:A:ILE:HG12	4	1.44
(2,301)	1:207:A:MET:H	1:208:A:ILE:HD12	10	1.43
(1,751)	1:167:A:MET:HE3	1:158:A:LEU:HB2	3	1.43
(1,746)	1:207:A:MET:HG3	1:218:A:ILE:HG22	6	1.43
(1,697)	1:177:A:TRP:HB2	1:183:A:VAL:HG23	3	1.43
(2,241)	1:216:A:TYR:HB2	1:159:A:LEU:HB3	9	1.42
(1,751)	1:167:A:MET:HE3	1:158:A:LEU:HB2	2	1.42
(1,751)	1:167:A:MET:HE3	1:158:A:LEU:HB2	10	1.42
(2,105)	1:207:A:MET:HG3	1:218:A:ILE:HG22	6	1.41
(1,532)	1:173:A:LEU:HD22	1:174:A:ASN:H	1	1.41
(1,26)	1:190:A:VAL:HA	1:193:A:ARG:HB3	7	1.41
(1,751)	1:167:A:MET:HE2	1:158:A:LEU:HB2	7	1.4
(1,746)	1:207:A:MET:HG3	1:218:A:ILE:HG23	4	1.4
(1,751)	1:167:A:MET:HE2	1:158:A:LEU:HB2	9	1.39
(1,101)	1:170:A:GLU:HA	1:173:A:LEU:HD22	2	1.39
(1,751)	1:167:A:MET:HE1	1:158:A:LEU:HB2	6	1.38
(1,542)	1:173:A:LEU:HD12	1:177:A:TRP:HE3	9	1.38
(1,399)	1:167:A:MET:HB3	1:172:A:ILE:HG13	5	1.38
(1,154)	1:205:A:ASP:HA	1:199:A:LEU:HD12	10	1.38
(2,205)	1:172:A:ILE:HG22	1:158:A:LEU:HD12	1	1.37
(2,105)	1:207:A:MET:HG3	1:130:A:ILE:HD11	1	1.37
(1,751)	1:167:A:MET:HE3	1:158:A:LEU:HB2	1	1.37
(1,532)	1:173:A:LEU:HD23	1:174:A:ASN:H	2	1.37
(1,255)	1:159:A:LEU:HB2	1:218:A:ILE:HG12	7	1.37
(2,205)	1:172:A:ILE:HG22	1:158:A:LEU:HD12	10	1.36
(1,300)	1:202:A:TYR:HB2	1:141:A:VAL:HB	7	1.36
(2,9)	1:210:A:THR:HA	1:216:A:TYR:HB2	6	1.35
(1,751)	1:167:A:MET:HE1	1:158:A:LEU:HB2	8	1.34
(1,746)	1:207:A:MET:HG3	1:218:A:ILE:HG21	2	1.34
(2,241)	1:216:A:TYR:HB2	1:159:A:LEU:HB3	3	1.33
(2,205)	1:172:A:ILE:HG21	1:158:A:LEU:HD12	4	1.33
(1,746)	1:207:A:MET:HG3	1:218:A:ILE:HG21	8	1.33
(1,570)	1:188:A:VAL:HG22	1:187:A:VAL:HG13	3	1.33
(1,542)	1:173:A:LEU:HD11	1:177:A:TRP:HE3	1	1.32
(1,26)	1:190:A:VAL:HA	1:193:A:ARG:HB3	2	1.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,105)	1:207:A:MET:HG3	1:218:A:ILE:HG21	8	1.31
(1,194)	1:215:A:GLY:HA2	1:169:A:ARG:HB2	6	1.31
(2,215)	1:167:A:MET:HE2	1:162:A:ASN:HB3	6	1.3
(2,205)	1:172:A:ILE:HG23	1:158:A:LEU:HD13	5	1.3
(2,124)	1:171:A:GLN:HB3	1:167:A:MET:HE1	7	1.3
(2,122)	1:147:A:GLU:HB2	1:146:A:ILE:HG21	10	1.3
(1,440)	1:184:A:GLU:HB2	1:186:A:ASN:HB3	3	1.3
(2,88)	1:182:A:GLU:HG3	1:183:A:VAL:HG21	6	1.29
(1,746)	1:207:A:MET:HG3	1:218:A:ILE:HG23	5	1.29
(1,532)	1:173:A:LEU:HD22	1:174:A:ASN:H	10	1.29
(1,746)	1:207:A:MET:HG3	1:218:A:ILE:HG23	10	1.28
(1,49)	1:181:A:SER:HB3	1:177:A:TRP:HB2	10	1.28
(2,205)	1:172:A:ILE:HG23	1:158:A:LEU:HD11	7	1.27
(2,105)	1:207:A:MET:HG3	1:218:A:ILE:HG23	5	1.27
(2,78)	1:197:A:ASN:HB3	1:198:A:LYS:HB3	9	1.27
(1,386)	1:183:A:VAL:HB	1:187:A:VAL:HG13	2	1.27
(1,49)	1:181:A:SER:HB3	1:177:A:TRP:HB2	7	1.27
(2,205)	1:172:A:ILE:HG22	1:158:A:LEU:HD13	8	1.26
(2,105)	1:207:A:MET:HG3	1:218:A:ILE:HG23	10	1.26
(1,194)	1:215:A:GLY:HA2	1:169:A:ARG:HB2	1	1.26
(2,88)	1:182:A:GLU:HG3	1:183:A:VAL:HG22	2	1.25
(1,776)	1:204:A:ARG:HB2	1:130:A:ILE:HD13	4	1.25
(1,456)	1:134:A:LYS:HD3	1:157:A:TYR:HE1	10	1.25
(1,49)	1:181:A:SER:HB3	1:177:A:TRP:HB2	5	1.25
(2,9)	1:210:A:THR:HA	1:216:A:TYR:HB2	2	1.24
(1,398)	1:167:A:MET:HB3	1:172:A:ILE:HD11	5	1.24
(1,613)	1:190:A:VAL:HG21	1:189:A:ASP:HB3	10	1.23
(1,440)	1:184:A:GLU:HB2	1:186:A:ASN:HB3	8	1.23
(2,221)	1:130:A:ILE:HD13	1:127:A:VAL:H	1	1.22
(2,221)	1:130:A:ILE:HD12	1:127:A:VAL:H	5	1.22
(2,88)	1:182:A:GLU:HG3	1:183:A:VAL:HG21	5	1.22
(2,55)	1:200:A:LYS:HE3	1:196:A:ARG:HB2	8	1.21
(2,1)	1:131:A:THR:HB	1:139:A:VAL:HG11	10	1.21
(1,613)	1:190:A:VAL:HG21	1:189:A:ASP:HB3	5	1.21
(1,286)	1:205:A:ASP:HB2	1:196:A:ARG:HB2	8	1.21
(2,78)	1:197:A:ASN:HB3	1:200:A:LYS:HD2	4	1.2
(1,652)	1:141:A:VAL:HG12	1:146:A:ILE:HG12	4	1.2
(2,287)	1:159:A:LEU:H	1:156:A:LEU:HD13	8	1.19
(2,205)	1:172:A:ILE:HG22	1:158:A:LEU:HD12	9	1.19
(2,105)	1:207:A:MET:HG3	1:130:A:ILE:HD13	2	1.19
(1,613)	1:190:A:VAL:HG23	1:189:A:ASP:HB3	1	1.19
(1,300)	1:202:A:TYR:HB2	1:141:A:VAL:HB	6	1.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,300)	1:202:A:TYR:HB2	1:141:A:VAL:HB	10	1.19
(1,255)	1:159:A:LEU:HB2	1:218:A:ILE:HG12	8	1.18
(1,49)	1:181:A:SER:HB3	1:177:A:TRP:HB2	4	1.18
(2,241)	1:216:A:TYR:HB2	1:159:A:LEU:HB3	1	1.17
(1,613)	1:190:A:VAL:HG23	1:189:A:ASP:HB3	6	1.17
(1,613)	1:190:A:VAL:HG23	1:189:A:ASP:HB3	8	1.17
(1,542)	1:173:A:LEU:HD12	1:177:A:TRP:HE3	10	1.17
(1,49)	1:181:A:SER:HB3	1:177:A:TRP:HB2	3	1.17
(1,49)	1:181:A:SER:HB3	1:177:A:TRP:HB2	6	1.17
(2,87)	1:182:A:GLU:HG3	1:183:A:VAL:HG21	5	1.16
(2,86)	1:145:A:GLU:HG3	1:138:A:LYS:HE3	8	1.16
(1,613)	1:190:A:VAL:HG23	1:189:A:ASP:HB3	3	1.16
(1,101)	1:170:A:GLU:HA	1:173:A:LEU:HD21	10	1.15
(2,288)	1:208:A:ILE:HG21	1:208:A:ILE:H	9	1.14
(2,282)	1:157:A:TYR:H	1:132:A:ILE:HG12	3	1.14
(2,282)	1:157:A:TYR:H	1:148:A:LEU:HD11	7	1.14
(1,542)	1:173:A:LEU:HD12	1:177:A:TRP:HE3	2	1.14
(2,105)	1:207:A:MET:HG3	1:130:A:ILE:HD11	3	1.13
(1,408)	1:167:A:MET:HG2	1:172:A:ILE:HD12	10	1.13
(1,300)	1:202:A:TYR:HB2	1:141:A:VAL:HB	3	1.13
(2,288)	1:208:A:ILE:HG21	1:208:A:ILE:H	6	1.12
(2,241)	1:216:A:TYR:HB2	1:159:A:LEU:HB3	2	1.12
(2,1)	1:131:A:THR:HB	1:124:A:ILE:HG21	5	1.12
(2,288)	1:208:A:ILE:HG21	1:208:A:ILE:H	1	1.11
(2,288)	1:208:A:ILE:HG23	1:208:A:ILE:H	4	1.11
(2,288)	1:208:A:ILE:HG22	1:208:A:ILE:H	10	1.11
(1,440)	1:184:A:GLU:HB2	1:186:A:ASN:HB3	5	1.11
(1,408)	1:167:A:MET:HG2	1:172:A:ILE:HD12	8	1.11
(1,50)	1:181:A:SER:HB2	1:177:A:TRP:HB2	1	1.11
(2,143)	1:199:A:LEU:HD13	1:196:A:ARG:HD2	3	1.1
(2,78)	1:197:A:ASN:HB3	1:200:A:LYS:HD2	5	1.1
(1,665)	1:211:A:VAL:HA	1:211:A:VAL:HG22	9	1.1
(1,408)	1:167:A:MET:HG2	1:172:A:ILE:HD11	9	1.1
(2,224)	1:130:A:ILE:HD11	1:130:A:ILE:HB	10	1.09
(2,182)	1:166:A:VAL:HG23	1:167:A:MET:H	4	1.09
(1,456)	1:134:A:LYS:HD3	1:157:A:TYR:HE1	7	1.09
(1,300)	1:202:A:TYR:HB2	1:141:A:VAL:HB	1	1.09
(2,288)	1:208:A:ILE:HG23	1:208:A:ILE:H	3	1.08
(2,215)	1:167:A:MET:HE1	1:175:A:HIS:HB2	10	1.08
(2,183)	1:140:A:THR:HG23	1:138:A:LYS:HD2	3	1.08
(1,802)	1:124:A:ILE:HD12	1:133:A:ASP:HB2	1	1.08
(1,624)	1:149:A:THR:HG21	1:152:A:GLU:HB3	7	1.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,219)	1:216:A:TYR:HB3	1:159:A:LEU:HD22	8	1.08
(2,241)	1:216:A:TYR:HB2	1:159:A:LEU:HB3	6	1.07
(2,241)	1:216:A:TYR:HB2	1:159:A:LEU:HB3	10	1.07
(1,16)	1:188:A:VAL:HA	1:191:A:TYR:HB3	8	1.07
(2,282)	1:157:A:TYR:H	1:132:A:ILE:HG21	6	1.06
(2,215)	1:167:A:MET:HE1	1:175:A:HIS:HB2	1	1.06
(1,300)	1:202:A:TYR:HB2	1:141:A:VAL:HB	2	1.06
(1,219)	1:216:A:TYR:HB3	1:159:A:LEU:HD22	9	1.06
(2,288)	1:208:A:ILE:H	1:199:A:LEU:HD11	2	1.05
(2,229)	1:192:A:ILE:HD11	1:216:A:TYR:HD2	9	1.05
(2,219)	1:172:A:ILE:HD13	1:172:A:ILE:HA	10	1.05
(2,78)	1:197:A:ASN:HB3	1:200:A:LYS:HD2	2	1.05
(1,739)	1:207:A:MET:HG3	1:207:A:MET:HE3	8	1.05
(1,408)	1:167:A:MET:HG2	1:172:A:ILE:HD12	6	1.05
(2,100)	1:204:A:ARG:HB2	1:130:A:ILE:HD12	9	1.04
(1,739)	1:207:A:MET:HG3	1:207:A:MET:HE3	1	1.04
(1,513)	1:156:A:LEU:HB3	1:156:A:LEU:HD21	1	1.04
(1,16)	1:188:A:VAL:HA	1:191:A:TYR:HB3	10	1.04
(2,287)	1:159:A:LEU:H	1:156:A:LEU:HD11	1	1.03
(2,282)	1:157:A:TYR:H	1:148:A:LEU:HD12	9	1.03
(2,229)	1:192:A:ILE:HD11	1:216:A:TYR:HD2	7	1.03
(2,216)	1:192:A:ILE:HG23	1:192:A:ILE:H	5	1.03
(2,207)	1:208:A:ILE:HG21	1:208:A:ILE:H	5	1.03
(2,207)	1:208:A:ILE:HG21	1:208:A:ILE:H	9	1.03
(2,182)	1:214:A:VAL:HG13	1:168:A:GLN:H	3	1.03
(1,739)	1:207:A:MET:HG3	1:207:A:MET:HE3	4	1.03
(1,604)	1:185:A:THR:HG21	1:173:A:LEU:HD21	1	1.03
(1,513)	1:156:A:LEU:HB3	1:156:A:LEU:HD23	2	1.03
(1,513)	1:156:A:LEU:HB3	1:156:A:LEU:HD23	9	1.03
(1,408)	1:167:A:MET:HG2	1:172:A:ILE:HD12	1	1.03
(1,300)	1:202:A:TYR:HB2	1:141:A:VAL:HB	8	1.03
(2,286)	1:158:A:LEU:H	1:158:A:LEU:HD22	7	1.02
(2,282)	1:157:A:TYR:H	1:132:A:ILE:HG12	2	1.02
(2,219)	1:172:A:ILE:HD11	1:215:A:GLY:HA2	1	1.02
(2,207)	1:208:A:ILE:HG21	1:208:A:ILE:H	6	1.02
(2,207)	1:208:A:ILE:HG21	1:208:A:ILE:H	7	1.02
(2,207)	1:208:A:ILE:HG22	1:208:A:ILE:H	8	1.02
(1,739)	1:207:A:MET:HG3	1:207:A:MET:HE1	5	1.02
(1,739)	1:207:A:MET:HG3	1:207:A:MET:HE2	10	1.02
(1,513)	1:156:A:LEU:HB3	1:156:A:LEU:HD22	3	1.02
(1,513)	1:156:A:LEU:HB3	1:156:A:LEU:HD22	4	1.02
(1,513)	1:156:A:LEU:HB3	1:156:A:LEU:HD23	6	1.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,513)	1:156:A:LEU:HB3	1:156:A:LEU:HD23	10	1.02
(2,229)	1:192:A:ILE:HD11	1:216:A:TYR:HD2	5	1.01
(2,216)	1:192:A:ILE:HG21	1:192:A:ILE:H	8	1.01
(2,216)	1:192:A:ILE:HG23	1:192:A:ILE:H	9	1.01
(2,207)	1:208:A:ILE:HG21	1:208:A:ILE:H	2	1.01
(2,156)	1:195:A:LEU:HD13	1:152:A:GLU:HG3	2	1.01
(2,151)	1:155:A:LEU:HD12	1:153:A:TYR:H	3	1.01
(1,750)	1:167:A:MET:HG2	1:167:A:MET:HE3	1	1.01
(1,750)	1:167:A:MET:HG2	1:167:A:MET:HE2	9	1.01
(1,750)	1:167:A:MET:HG2	1:167:A:MET:HE3	10	1.01
(1,604)	1:185:A:THR:HG21	1:173:A:LEU:HD22	2	1.01
(1,513)	1:156:A:LEU:HB3	1:156:A:LEU:HD21	5	1.01
(1,513)	1:156:A:LEU:HB3	1:156:A:LEU:HD23	7	1.01
(1,513)	1:156:A:LEU:HB3	1:156:A:LEU:HD23	8	1.01
(1,101)	1:170:A:GLU:HA	1:173:A:LEU:HD23	9	1.01
(2,216)	1:192:A:ILE:HG22	1:192:A:ILE:H	7	1.0
(2,209)	1:207:A:MET:HE2	1:207:A:MET:HA	2	1.0
(2,209)	1:207:A:MET:HE2	1:207:A:MET:HA	10	1.0
(2,207)	1:208:A:ILE:HG21	1:208:A:ILE:H	1	1.0
(2,207)	1:208:A:ILE:HG23	1:208:A:ILE:H	4	1.0
(2,207)	1:208:A:ILE:HG22	1:208:A:ILE:H	10	1.0
(2,167)	1:151:A:THR:HG21	1:177:A:TRP:HE3	2	1.0
(2,151)	1:155:A:LEU:HD13	1:153:A:TYR:H	8	1.0
(2,88)	1:182:A:GLU:HG3	1:183:A:VAL:HG21	7	1.0
(2,1)	1:131:A:THR:HB	1:124:A:ILE:HG23	4	1.0
(2,1)	1:131:A:THR:HB	1:139:A:VAL:HG13	9	1.0
(1,750)	1:167:A:MET:HG2	1:167:A:MET:HE2	2	1.0
(1,739)	1:207:A:MET:HG3	1:207:A:MET:HE1	3	1.0
(1,739)	1:207:A:MET:HG3	1:207:A:MET:HE3	6	1.0
(1,101)	1:170:A:GLU:HA	1:173:A:LEU:HD21	1	1.0
(1,49)	1:181:A:SER:HB3	1:177:A:TRP:HB2	1	1.0
(1,49)	1:181:A:SER:HB3	1:177:A:TRP:HB2	8	1.0
(2,216)	1:192:A:ILE:HG22	1:192:A:ILE:H	4	0.99
(2,122)	1:147:A:GLU:HB2	1:146:A:ILE:HG22	2	0.99
(1,750)	1:167:A:MET:HG2	1:167:A:MET:HE1	6	0.99
(1,385)	1:207:A:MET:HB3	1:218:A:ILE:HG22	7	0.99
(1,16)	1:188:A:VAL:HA	1:191:A:TYR:HB3	5	0.99
(2,286)	1:158:A:LEU:H	1:158:A:LEU:HD22	3	0.98
(2,282)	1:157:A:TYR:H	1:132:A:ILE:HG12	5	0.98
(2,221)	1:130:A:ILE:HD12	1:127:A:VAL:H	3	0.98
(2,216)	1:192:A:ILE:HG23	1:192:A:ILE:H	1	0.98
(2,216)	1:192:A:ILE:HG22	1:192:A:ILE:H	10	0.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,167)	1:151:A:THR:HG22	1:151:A:THR:H	1	0.98
(2,167)	1:151:A:THR:HG21	1:151:A:THR:H	5	0.98
(2,167)	1:151:A:THR:HG23	1:151:A:THR:H	7	0.98
(2,151)	1:195:A:LEU:HD11	1:196:A:ARG:H	9	0.98
(2,92)	1:171:A:GLN:HG3	1:167:A:MET:HA	5	0.98
(1,223)	1:219:A:ARG:HD2	1:219:A:ARG:HB2	2	0.98
(2,287)	1:159:A:LEU:H	1:156:A:LEU:HD11	6	0.97
(2,221)	1:130:A:ILE:HD13	1:127:A:VAL:H	9	0.97
(2,216)	1:192:A:ILE:HG23	1:192:A:ILE:H	2	0.97
(2,216)	1:192:A:ILE:HG22	1:192:A:ILE:H	3	0.97
(2,216)	1:192:A:ILE:HG22	1:192:A:ILE:H	6	0.97
(2,215)	1:167:A:MET:HE1	1:162:A:ASN:HB3	4	0.97
(2,207)	1:208:A:ILE:HG23	1:208:A:ILE:H	3	0.97
(2,189)	1:217:A:VAL:HG23	1:165:A:HIS:HB2	1	0.97
(2,167)	1:151:A:THR:HG21	1:151:A:THR:H	3	0.97
(2,167)	1:151:A:THR:HG22	1:151:A:THR:H	4	0.97
(2,167)	1:151:A:THR:HG21	1:151:A:THR:H	6	0.97
(2,167)	1:151:A:THR:HG23	1:151:A:THR:H	9	0.97
(2,156)	1:195:A:LEU:HD13	1:152:A:GLU:HB2	3	0.97
(2,151)	1:155:A:LEU:HD12	1:153:A:TYR:H	4	0.97
(2,1)	1:131:A:THR:HB	1:124:A:ILE:HG21	2	0.97
(1,739)	1:207:A:MET:HG3	1:207:A:MET:HE2	2	0.97
(1,398)	1:167:A:MET:HB3	1:172:A:ILE:HD11	7	0.97
(1,223)	1:219:A:ARG:HD2	1:219:A:ARG:HB2	4	0.97
(1,194)	1:215:A:GLY:HA2	1:169:A:ARG:HB2	10	0.97
(2,203)	1:217:A:VAL:HG11	1:219:A:ARG:HG2	5	0.96
(2,189)	1:217:A:VAL:HG22	1:165:A:HIS:HB3	6	0.96
(2,167)	1:151:A:THR:HG21	1:151:A:THR:H	8	0.96
(2,167)	1:151:A:THR:HG22	1:151:A:THR:H	10	0.96
(2,151)	1:155:A:LEU:HD11	1:153:A:TYR:H	7	0.96
(1,560)	1:188:A:VAL:HG23	1:173:A:LEU:H	3	0.96
(1,223)	1:219:A:ARG:HD2	1:219:A:ARG:HB2	7	0.96
(1,223)	1:219:A:ARG:HD2	1:219:A:ARG:HB2	8	0.96
(2,215)	1:167:A:MET:HE3	1:175:A:HIS:HB2	9	0.95
(2,213)	1:167:A:MET:HE2	1:168:A:GLN:H	5	0.95
(2,209)	1:207:A:MET:HE3	1:207:A:MET:HA	3	0.95
(2,180)	1:149:A:THR:HG21	1:148:A:LEU:HD23	7	0.95
(1,750)	1:167:A:MET:HG2	1:167:A:MET:HE1	8	0.95
(1,223)	1:219:A:ARG:HD2	1:219:A:ARG:HB2	1	0.95
(1,223)	1:219:A:ARG:HD2	1:219:A:ARG:HB2	5	0.95
(1,223)	1:219:A:ARG:HD2	1:219:A:ARG:HB2	9	0.95
(1,111)	1:152:A:GLU:HA	1:155:A:LEU:HB3	5	0.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,221)	1:130:A:ILE:HD11	1:127:A:VAL:H	2	0.94
(2,189)	1:217:A:VAL:HG21	1:165:A:HIS:HB2	3	0.94
(2,180)	1:149:A:THR:HG21	1:148:A:LEU:HD23	3	0.94
(2,165)	1:188:A:VAL:HG22	1:186:A:ASN:H	3	0.94
(2,151)	1:155:A:LEU:HD13	1:153:A:TYR:H	10	0.94
(1,750)	1:167:A:MET:HG2	1:167:A:MET:HE3	3	0.94
(1,604)	1:185:A:THR:HG23	1:173:A:LEU:HD23	10	0.94
(1,300)	1:202:A:TYR:HB2	1:141:A:VAL:HB	5	0.94
(1,111)	1:152:A:GLU:HA	1:155:A:LEU:HB3	2	0.94
(2,209)	1:207:A:MET:HE3	1:207:A:MET:HA	4	0.93
(2,151)	1:155:A:LEU:HD11	1:153:A:TYR:H	2	0.93
(2,151)	1:155:A:LEU:HD13	1:153:A:TYR:H	5	0.93
(1,750)	1:167:A:MET:HG2	1:167:A:MET:HE3	4	0.93
(1,566)	1:188:A:VAL:HA	1:188:A:VAL:HG21	3	0.93
(1,16)	1:188:A:VAL:HA	1:191:A:TYR:HB3	1	0.93
(2,286)	1:158:A:LEU:H	1:158:A:LEU:HD23	4	0.92
(2,282)	1:157:A:TYR:H	1:148:A:LEU:HD11	1	0.92
(2,282)	1:157:A:TYR:H	1:148:A:LEU:HD12	4	0.92
(2,180)	1:149:A:THR:HG21	1:148:A:LEU:HD22	2	0.92
(2,151)	1:155:A:LEU:HD11	1:153:A:TYR:H	1	0.92
(1,408)	1:167:A:MET:HG2	1:172:A:ILE:HD12	4	0.92
(1,223)	1:219:A:ARG:HD2	1:219:A:ARG:HB2	3	0.92
(1,223)	1:219:A:ARG:HD2	1:219:A:ARG:HB2	6	0.92
(1,16)	1:188:A:VAL:HA	1:191:A:TYR:HB3	3	0.92
(2,286)	1:176:A:VAL:HG21	1:158:A:LEU:H	2	0.91
(2,282)	1:157:A:TYR:H	1:148:A:LEU:HD13	10	0.91
(2,198)	1:187:A:VAL:HG11	1:188:A:VAL:HB	8	0.91
(2,189)	1:217:A:VAL:HG23	1:165:A:HIS:HB3	2	0.91
(2,179)	1:146:A:ILE:HB	1:139:A:VAL:HG11	9	0.91
(2,145)	1:192:A:ILE:HG12	1:195:A:LEU:HD22	7	0.91
(2,86)	1:145:A:GLU:HG3	1:138:A:LYS:HE2	6	0.91
(2,1)	1:131:A:THR:HB	1:124:A:ILE:HG23	1	0.91
(1,624)	1:149:A:THR:HG21	1:152:A:GLU:HB3	2	0.91
(1,617)	1:159:A:LEU:HD22	1:159:A:LEU:HB2	6	0.91
(2,198)	1:187:A:VAL:HG13	1:188:A:VAL:HB	4	0.9
(2,198)	1:187:A:VAL:HG13	1:188:A:VAL:HB	5	0.9
(1,617)	1:159:A:LEU:HD22	1:159:A:LEU:HB2	5	0.9
(1,408)	1:167:A:MET:HG2	1:172:A:ILE:HD12	3	0.9
(2,301)	1:207:A:MET:H	1:199:A:LEU:HD11	9	0.89
(2,287)	1:159:A:LEU:H	1:158:A:LEU:HD21	10	0.89
(2,286)	1:176:A:VAL:HG21	1:158:A:LEU:H	5	0.89
(2,209)	1:207:A:MET:HE3	1:207:A:MET:HA	7	0.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,209)	1:207:A:MET:HE3	1:208:A:ILE:HA	9	0.89
(2,182)	1:214:A:VAL:HG12	1:168:A:GLN:H	8	0.89
(2,145)	1:192:A:ILE:HG12	1:172:A:ILE:HD13	3	0.89
(2,105)	1:207:A:MET:HG3	1:130:A:ILE:HD13	4	0.89
(2,86)	1:145:A:GLU:HG3	1:138:A:LYS:HE3	2	0.89
(1,111)	1:152:A:GLU:HA	1:155:A:LEU:HB3	9	0.89
(2,278)	1:172:A:ILE:HG22	1:172:A:ILE:H	2	0.88
(2,219)	1:172:A:ILE:HD13	1:215:A:GLY:HA2	5	0.88
(2,219)	1:172:A:ILE:HD11	1:215:A:GLY:HA2	6	0.88
(2,180)	1:149:A:THR:HG22	1:148:A:LEU:HD23	10	0.88
(2,179)	1:146:A:ILE:HB	1:139:A:VAL:HG13	4	0.88
(2,151)	1:155:A:LEU:HD12	1:153:A:TYR:H	6	0.88
(2,1)	1:131:A:THR:HB	1:124:A:ILE:HG21	3	0.88
(1,617)	1:159:A:LEU:HD21	1:159:A:LEU:HB2	1	0.88
(1,617)	1:159:A:LEU:HD23	1:159:A:LEU:HB2	3	0.88
(1,51)	1:181:A:SER:HB3	1:183:A:VAL:HG22	9	0.88
(1,46)	1:185:A:THR:HA	1:173:A:LEU:HD11	10	0.88
(2,278)	1:172:A:ILE:HG21	1:172:A:ILE:H	7	0.87
(2,189)	1:141:A:VAL:HG12	1:204:A:ARG:HD3	9	0.87
(2,180)	1:149:A:THR:HG21	1:148:A:LEU:HD22	1	0.87
(2,139)	1:155:A:LEU:HD21	1:155:A:LEU:H	4	0.87
(1,802)	1:124:A:ILE:HD12	1:133:A:ASP:HB2	2	0.87
(1,617)	1:159:A:LEU:HD23	1:159:A:LEU:HB2	2	0.87
(1,617)	1:159:A:LEU:HD23	1:159:A:LEU:HB2	10	0.87
(1,111)	1:152:A:GLU:HA	1:155:A:LEU:HB3	7	0.87
(2,174)	1:173:A:LEU:HG	1:177:A:TRP:HB2	9	0.86
(1,754)	1:158:A:LEU:HD13	1:167:A:MET:HE2	2	0.86
(1,527)	1:159:A:LEU:HD13	1:216:A:TYR:HB2	7	0.86
(1,300)	1:202:A:TYR:HB2	1:141:A:VAL:HB	9	0.86
(1,194)	1:215:A:GLY:HA2	1:169:A:ARG:HB2	4	0.86
(1,111)	1:152:A:GLU:HA	1:155:A:LEU:HB3	4	0.86
(1,111)	1:152:A:GLU:HA	1:155:A:LEU:HB3	6	0.86
(1,111)	1:152:A:GLU:HA	1:155:A:LEU:HB3	10	0.86
(1,46)	1:185:A:THR:HA	1:173:A:LEU:HD11	2	0.86
(1,16)	1:188:A:VAL:HA	1:191:A:TYR:HB3	7	0.86
(2,286)	1:158:A:LEU:H	1:158:A:LEU:HD21	6	0.85
(2,286)	1:158:A:LEU:H	1:158:A:LEU:HD22	9	0.85
(2,278)	1:172:A:ILE:HG21	1:172:A:ILE:H	5	0.85
(2,278)	1:172:A:ILE:HG23	1:172:A:ILE:H	10	0.85
(2,209)	1:207:A:MET:HE2	1:207:A:MET:HA	8	0.85
(2,204)	1:172:A:ILE:HG22	1:158:A:LEU:HB2	8	0.85
(2,198)	1:187:A:VAL:HG13	1:190:A:VAL:HB	10	0.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,183)	1:140:A:THR:HG23	1:138:A:LYS:HB3	9	0.85
(2,172)	1:199:A:LEU:HD21	1:202:A:TYR:HD2	4	0.85
(2,156)	1:195:A:LEU:HD12	1:152:A:GLU:HG3	5	0.85
(2,156)	1:195:A:LEU:HD13	1:152:A:GLU:HG3	9	0.85
(2,139)	1:155:A:LEU:HD22	1:155:A:LEU:H	6	0.85
(1,754)	1:158:A:LEU:HD12	1:167:A:MET:HE3	5	0.85
(1,440)	1:184:A:GLU:HB2	1:186:A:ASN:HB3	7	0.85
(1,440)	1:184:A:GLU:HB2	1:186:A:ASN:HB3	9	0.85
(2,286)	1:158:A:LEU:H	1:158:A:LEU:HD22	10	0.84
(2,282)	1:157:A:TYR:H	1:132:A:ILE:HG21	8	0.84
(2,268)	1:170:A:GLU:H	1:168:A:GLN:HB2	1	0.84
(2,183)	1:140:A:THR:HG21	1:138:A:LYS:HD2	4	0.84
(2,88)	1:182:A:GLU:HG2	1:183:A:VAL:HG22	4	0.84
(2,1)	1:131:A:THR:HB	1:124:A:ILE:HG22	7	0.84
(1,1039)	1:159:A:LEU:H	1:159:A:LEU:HD11	4	0.84
(1,987)	1:147:A:GLU:HB3	1:147:A:GLU:H	10	0.84
(1,648)	1:166:A:VAL:HA	1:166:A:VAL:HG13	6	0.84
(1,111)	1:152:A:GLU:HA	1:155:A:LEU:HB3	3	0.84
(2,227)	1:218:A:ILE:HD13	1:160:A:ALA:HB3	1	0.83
(2,209)	1:207:A:MET:HE1	1:207:A:MET:HA	5	0.83
(2,206)	1:160:A:ALA:HB2	1:161:A:GLU:HB2	5	0.83
(2,204)	1:172:A:ILE:HG23	1:155:A:LEU:HG	3	0.83
(2,198)	1:187:A:VAL:HG12	1:188:A:VAL:HB	6	0.83
(2,182)	1:214:A:VAL:HG12	1:168:A:GLN:H	10	0.83
(2,171)	1:188:A:VAL:HG11	1:188:A:VAL:H	2	0.83
(2,171)	1:173:A:LEU:HG	1:178:A:GLY:H	8	0.83
(2,171)	1:188:A:VAL:HG13	1:188:A:VAL:H	9	0.83
(2,145)	1:192:A:ILE:HG12	1:195:A:LEU:HD22	4	0.83
(2,1)	1:131:A:THR:HB	1:124:A:ILE:HG22	8	0.83
(1,748)	1:167:A:MET:HE1	1:167:A:MET:HA	7	0.83
(1,111)	1:152:A:GLU:HA	1:155:A:LEU:HB3	8	0.83
(2,294)	1:183:A:VAL:HG12	1:187:A:VAL:H	1	0.82
(2,286)	1:158:A:LEU:H	1:158:A:LEU:HD22	1	0.82
(2,278)	1:172:A:ILE:HG22	1:172:A:ILE:H	4	0.82
(2,278)	1:172:A:ILE:HG21	1:172:A:ILE:H	6	0.82
(2,219)	1:172:A:ILE:HD13	1:215:A:GLY:HA2	7	0.82
(2,204)	1:172:A:ILE:HG23	1:158:A:LEU:HB2	5	0.82
(2,198)	1:187:A:VAL:HG11	1:188:A:VAL:HB	1	0.82
(2,180)	1:149:A:THR:HG23	1:148:A:LEU:HD21	5	0.82
(2,180)	1:149:A:THR:HG23	1:148:A:LEU:HD21	9	0.82
(2,174)	1:173:A:LEU:HG	1:177:A:TRP:HB2	2	0.82
(2,171)	1:188:A:VAL:HG13	1:188:A:VAL:H	1	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,171)	1:188:A:VAL:HG11	1:188:A:VAL:H	10	0.82
(2,145)	1:192:A:ILE:HG12	1:195:A:LEU:HD22	6	0.82
(2,139)	1:155:A:LEU:HD23	1:155:A:LEU:H	1	0.82
(1,1086)	1:151:A:THR:H	1:149:A:THR:HG23	6	0.82
(1,987)	1:147:A:GLU:HB3	1:147:A:GLU:H	5	0.82
(1,633)	1:166:A:VAL:HG12	1:215:A:GLY:H	9	0.82
(1,255)	1:159:A:LEU:HB2	1:218:A:ILE:HG12	9	0.82
(2,219)	1:172:A:ILE:HD11	1:215:A:GLY:HA2	8	0.81
(2,198)	1:187:A:VAL:HG11	1:188:A:VAL:HB	7	0.81
(2,145)	1:192:A:ILE:HG12	1:195:A:LEU:HD22	5	0.81
(2,129)	1:148:A:LEU:HD11	1:149:A:THR:H	9	0.81
(1,802)	1:124:A:ILE:HD11	1:133:A:ASP:HB2	6	0.81
(1,647)	1:187:A:VAL:HA	1:187:A:VAL:HG21	2	0.81
(1,461)	1:212:A:ARG:HB3	1:210:A:THR:HG23	3	0.81
(1,448)	1:212:A:ARG:HD3	1:212:A:ARG:HB2	4	0.81
(1,286)	1:205:A:ASP:HB2	1:196:A:ARG:HB2	7	0.81
(1,46)	1:185:A:THR:HA	1:173:A:LEU:HD13	1	0.81
(2,288)	1:208:A:ILE:H	1:199:A:LEU:HD13	5	0.8
(2,288)	1:208:A:ILE:H	1:199:A:LEU:HD12	7	0.8
(2,219)	1:172:A:ILE:HD11	1:215:A:GLY:HA2	4	0.8
(2,209)	1:207:A:MET:HE3	1:207:A:MET:HA	1	0.8
(2,204)	1:172:A:ILE:HG21	1:158:A:LEU:HB2	2	0.8
(2,198)	1:187:A:VAL:HG11	1:188:A:VAL:HB	9	0.8
(2,129)	1:148:A:LEU:HD11	1:149:A:THR:H	3	0.8
(2,100)	1:204:A:ARG:HB2	1:130:A:ILE:HD13	5	0.8
(1,987)	1:147:A:GLU:HB3	1:147:A:GLU:H	6	0.8
(1,987)	1:147:A:GLU:HB3	1:147:A:GLU:H	7	0.8
(1,982)	1:170:A:GLU:HB2	1:171:A:GLN:H	1	0.8
(1,399)	1:167:A:MET:HB3	1:172:A:ILE:HG13	7	0.8
(1,16)	1:188:A:VAL:HA	1:191:A:TYR:HB3	9	0.8
(2,300)	1:172:A:ILE:HG23	1:174:A:ASN:H	9	0.79
(2,278)	1:172:A:ILE:HG23	1:172:A:ILE:H	8	0.79
(2,204)	1:172:A:ILE:HG23	1:158:A:LEU:HB2	7	0.79
(2,129)	1:148:A:LEU:HD13	1:149:A:THR:H	5	0.79
(2,117)	1:165:A:HIS:HB3	1:162:A:ASN:HB2	5	0.79
(1,987)	1:147:A:GLU:HB3	1:147:A:GLU:H	2	0.79
(1,987)	1:147:A:GLU:HB3	1:147:A:GLU:H	4	0.79
(1,820)	1:151:A:THR:HB	1:176:A:VAL:HG12	5	0.79
(1,448)	1:212:A:ARG:HD3	1:212:A:ARG:HB2	7	0.79
(1,255)	1:159:A:LEU:HB2	1:218:A:ILE:HG12	1	0.79
(1,194)	1:215:A:GLY:HA2	1:169:A:ARG:HB2	2	0.79
(1,165)	1:164:A:ASN:HA	1:217:A:VAL:HG23	10	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,26)	1:190:A:VAL:HA	1:193:A:ARG:HB3	9	0.79
(2,300)	1:172:A:ILE:HG22	1:174:A:ASN:H	2	0.78
(2,278)	1:172:A:ILE:HG21	1:172:A:ILE:H	3	0.78
(2,224)	1:207:A:MET:HE1	1:130:A:ILE:HD13	6	0.78
(2,142)	1:173:A:LEU:HD22	1:184:A:GLU:HA	3	0.78
(2,129)	1:148:A:LEU:HD12	1:149:A:THR:H	10	0.78
(1,1086)	1:151:A:THR:H	1:149:A:THR:HG23	7	0.78
(1,1039)	1:159:A:LEU:H	1:159:A:LEU:HD11	7	0.78
(1,987)	1:147:A:GLU:HB3	1:147:A:GLU:H	3	0.78
(1,111)	1:152:A:GLU:HA	1:155:A:LEU:HB3	1	0.78
(2,278)	1:172:A:ILE:H	1:188:A:VAL:HG12	1	0.77
(2,219)	1:172:A:ILE:HD11	1:215:A:GLY:HA2	3	0.77
(2,209)	1:207:A:MET:HE2	1:207:A:MET:HA	6	0.77
(2,174)	1:173:A:LEU:HG	1:177:A:TRP:HB2	10	0.77
(2,100)	1:167:A:MET:HG2	1:159:A:LEU:HD21	4	0.77
(2,55)	1:198:A:LYS:HE3	1:152:A:GLU:HB3	7	0.77
(1,1086)	1:151:A:THR:H	1:149:A:THR:HG23	1	0.77
(1,1086)	1:151:A:THR:H	1:149:A:THR:HG21	8	0.77
(1,1042)	1:176:A:VAL:HG12	1:176:A:VAL:H	7	0.77
(1,849)	1:173:A:LEU:HD12	1:173:A:LEU:H	9	0.77
(1,754)	1:158:A:LEU:HD13	1:167:A:MET:HE1	3	0.77
(1,750)	1:167:A:MET:HG2	1:167:A:MET:HE2	5	0.77
(1,596)	1:167:A:MET:HG2	1:159:A:LEU:HD21	5	0.77
(1,448)	1:212:A:ARG:HD3	1:212:A:ARG:HB3	6	0.77
(1,26)	1:190:A:VAL:HA	1:193:A:ARG:HB3	4	0.77
(2,300)	1:172:A:ILE:HG23	1:174:A:ASN:H	1	0.76
(2,227)	1:218:A:ILE:HD13	1:160:A:ALA:HB1	3	0.76
(2,171)	1:173:A:LEU:HG	1:178:A:GLY:H	7	0.76
(2,165)	1:188:A:VAL:HG22	1:186:A:ASN:H	2	0.76
(2,129)	1:148:A:LEU:HD12	1:149:A:THR:H	2	0.76
(1,1086)	1:151:A:THR:H	1:149:A:THR:HG22	5	0.76
(1,849)	1:173:A:LEU:HD12	1:173:A:LEU:H	2	0.76
(1,849)	1:173:A:LEU:HD12	1:173:A:LEU:H	10	0.76
(2,287)	1:159:A:LEU:H	1:158:A:LEU:HD22	4	0.75
(2,230)	1:216:A:TYR:HB3	1:192:A:ILE:HD11	3	0.75
(2,227)	1:218:A:ILE:HD11	1:160:A:ALA:HB1	2	0.75
(2,179)	1:146:A:ILE:HB	1:139:A:VAL:HG13	5	0.75
(2,165)	1:188:A:VAL:HG22	1:172:A:ILE:H	9	0.75
(2,145)	1:192:A:ILE:HG12	1:195:A:LEU:HD23	1	0.75
(2,143)	1:199:A:LEU:HD12	1:196:A:ARG:HD2	7	0.75
(2,1)	1:131:A:THR:HB	1:124:A:ILE:HG22	6	0.75
(1,1042)	1:176:A:VAL:HG11	1:176:A:VAL:H	3	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,633)	1:166:A:VAL:HG12	1:215:A:GLY:H	5	0.75
(1,46)	1:185:A:THR:HA	1:173:A:LEU:HD11	9	0.75
(2,294)	1:183:A:VAL:HG12	1:187:A:VAL:H	9	0.74
(2,219)	1:172:A:ILE:HD13	1:215:A:GLY:HA2	9	0.74
(2,204)	1:172:A:ILE:HG21	1:155:A:LEU:HG	4	0.74
(2,184)	1:183:A:VAL:HG13	1:177:A:TRP:HD1	1	0.74
(2,184)	1:187:A:VAL:HG21	1:177:A:TRP:HD1	4	0.74
(2,182)	1:214:A:VAL:HG11	1:168:A:GLN:H	1	0.74
(2,171)	1:173:A:LEU:HG	1:178:A:GLY:H	6	0.74
(2,145)	1:192:A:ILE:HG12	1:195:A:LEU:HD22	10	0.74
(2,139)	1:155:A:LEU:HD22	1:155:A:LEU:H	3	0.74
(2,139)	1:155:A:LEU:HD22	1:155:A:LEU:H	10	0.74
(1,1086)	1:151:A:THR:H	1:149:A:THR:HG23	4	0.74
(1,1042)	1:176:A:VAL:HG11	1:176:A:VAL:H	1	0.74
(1,1042)	1:176:A:VAL:HG13	1:176:A:VAL:H	2	0.74
(1,1042)	1:176:A:VAL:HG12	1:176:A:VAL:H	4	0.74
(1,1042)	1:176:A:VAL:HG11	1:176:A:VAL:H	6	0.74
(1,987)	1:147:A:GLU:HB3	1:147:A:GLU:H	1	0.74
(1,849)	1:173:A:LEU:HD11	1:173:A:LEU:H	1	0.74
(1,624)	1:149:A:THR:HG21	1:152:A:GLU:HB3	3	0.74
(1,133)	1:159:A:LEU:HA	1:162:A:ASN:HB2	5	0.74
(1,16)	1:188:A:VAL:HA	1:191:A:TYR:HB3	2	0.74
(1,16)	1:188:A:VAL:HA	1:191:A:TYR:HB3	6	0.74
(2,262)	1:193:A:ARG:H	1:193:A:ARG:HD3	4	0.73
(2,233)	1:207:A:MET:HE1	1:160:A:ALA:HA	6	0.73
(2,227)	1:218:A:ILE:HD11	1:160:A:ALA:HB2	6	0.73
(2,206)	1:160:A:ALA:HB3	1:161:A:GLU:HB2	4	0.73
(2,206)	1:160:A:ALA:HB2	1:161:A:GLU:HB2	7	0.73
(2,190)	1:141:A:VAL:HG23	1:142:A:ASN:HB3	9	0.73
(2,182)	1:214:A:VAL:HG13	1:168:A:GLN:H	7	0.73
(2,75)	1:128:A:ASN:HB3	1:218:A:ILE:HG23	3	0.73
(2,55)	1:163:A:LYS:HE3	1:161:A:GLU:HG2	9	0.73
(1,1086)	1:151:A:THR:H	1:149:A:THR:HG23	2	0.73
(1,1086)	1:151:A:THR:H	1:149:A:THR:HG21	10	0.73
(1,1042)	1:176:A:VAL:HG11	1:176:A:VAL:H	10	0.73
(1,633)	1:166:A:VAL:HG13	1:215:A:GLY:H	4	0.73
(1,527)	1:159:A:LEU:HD13	1:216:A:TYR:HB2	4	0.73
(1,286)	1:205:A:ASP:HB2	1:196:A:ARG:HB2	2	0.73
(1,194)	1:215:A:GLY:HA2	1:169:A:ARG:HB2	5	0.73
(2,300)	1:174:A:ASN:H	1:173:A:LEU:HG	10	0.72
(2,230)	1:216:A:TYR:HB3	1:192:A:ILE:HD13	7	0.72
(2,227)	1:218:A:ILE:HD13	1:160:A:ALA:HB3	9	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,219)	1:172:A:ILE:HD11	1:215:A:GLY:HA2	2	0.72
(2,198)	1:187:A:VAL:HG12	1:188:A:VAL:HB	3	0.72
(2,196)	1:136:A:ALA:HB3	1:135:A:ASN:H	1	0.72
(2,196)	1:136:A:ALA:HB2	1:135:A:ASN:H	2	0.72
(2,190)	1:141:A:VAL:HG23	1:142:A:ASN:HB3	5	0.72
(2,145)	1:192:A:ILE:HG12	1:195:A:LEU:HD22	8	0.72
(2,129)	1:148:A:LEU:HD11	1:149:A:THR:H	4	0.72
(1,1042)	1:176:A:VAL:HG13	1:176:A:VAL:H	9	0.72
(1,987)	1:147:A:GLU:HB3	1:147:A:GLU:H	8	0.72
(1,775)	1:130:A:ILE:HD11	1:130:A:ILE:HA	5	0.72
(1,578)	1:151:A:THR:HG21	1:191:A:TYR:HB2	9	0.72
(1,509)	1:199:A:LEU:HG	1:199:A:LEU:H	10	0.72
(1,255)	1:159:A:LEU:HB2	1:218:A:ILE:HG12	10	0.72
(2,290)	1:124:A:ILE:H	1:124:A:ILE:HG22	1	0.71
(2,287)	1:159:A:LEU:H	1:158:A:LEU:HD21	9	0.71
(2,278)	1:172:A:ILE:H	1:188:A:VAL:HG11	9	0.71
(2,206)	1:160:A:ALA:HB3	1:161:A:GLU:HB2	3	0.71
(2,182)	1:214:A:VAL:HG11	1:168:A:GLN:H	9	0.71
(2,75)	1:128:A:ASN:HB3	1:218:A:ILE:HG23	4	0.71
(1,1003)	1:159:A:LEU:HB3	1:159:A:LEU:H	1	0.71
(1,1003)	1:159:A:LEU:HB3	1:159:A:LEU:H	3	0.71
(1,1003)	1:159:A:LEU:HB3	1:159:A:LEU:H	6	0.71
(1,972)	1:169:A:ARG:H	1:168:A:GLN:HB2	1	0.71
(1,784)	1:218:A:ILE:HD12	1:218:A:ILE:HA	7	0.71
(1,604)	1:185:A:THR:HG21	1:173:A:LEU:HD22	9	0.71
(1,538)	1:199:A:LEU:HB3	1:199:A:LEU:HD12	10	0.71
(2,294)	1:183:A:VAL:HG13	1:187:A:VAL:H	3	0.7
(2,229)	1:192:A:ILE:HD12	1:216:A:TYR:HD1	6	0.7
(2,223)	1:208:A:ILE:HD12	1:196:A:ARG:HA	8	0.7
(2,206)	1:160:A:ALA:HB2	1:161:A:GLU:HB2	9	0.7
(2,182)	1:214:A:VAL:HG13	1:168:A:GLN:H	2	0.7
(2,182)	1:214:A:VAL:HG11	1:168:A:GLN:H	5	0.7
(2,180)	1:149:A:THR:HG22	1:148:A:LEU:HD21	8	0.7
(2,145)	1:192:A:ILE:HG12	1:172:A:ILE:HD13	2	0.7
(2,139)	1:155:A:LEU:HD23	1:155:A:LEU:H	8	0.7
(1,1057)	1:131:A:THR:HG22	1:131:A:THR:H	5	0.7
(1,1042)	1:176:A:VAL:HG11	1:176:A:VAL:H	5	0.7
(1,1042)	1:176:A:VAL:HG13	1:176:A:VAL:H	8	0.7
(1,1003)	1:159:A:LEU:HB3	1:159:A:LEU:H	2	0.7
(1,1003)	1:159:A:LEU:HB3	1:159:A:LEU:H	5	0.7
(1,1003)	1:159:A:LEU:HB3	1:159:A:LEU:H	10	0.7
(1,768)	1:216:A:TYR:HB3	1:172:A:ILE:HD11	5	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,753)	1:158:A:LEU:HD23	1:167:A:MET:HE3	2	0.7
(2,301)	1:207:A:MET:H	1:199:A:LEU:HD13	6	0.69
(2,287)	1:159:A:LEU:H	1:158:A:LEU:HD23	5	0.69
(2,262)	1:193:A:ARG:H	1:193:A:ARG:HD2	5	0.69
(2,228)	1:218:A:ILE:HD12	1:128:A:ASN:HB2	10	0.69
(2,204)	1:172:A:ILE:HG22	1:158:A:LEU:HB2	9	0.69
(2,191)	1:211:A:VAL:HG21	1:217:A:VAL:H	6	0.69
(2,156)	1:195:A:LEU:HD13	1:152:A:GLU:HG3	4	0.69
(2,139)	1:155:A:LEU:HD21	1:155:A:LEU:H	7	0.69
(2,139)	1:155:A:LEU:HD23	1:155:A:LEU:H	9	0.69
(2,129)	1:148:A:LEU:HD11	1:149:A:THR:H	1	0.69
(2,78)	1:197:A:ASN:HB3	1:200:A:LYS:HD2	1	0.69
(2,27)	1:154:A:ASP:HA	1:176:A:VAL:HG21	9	0.69
(1,1086)	1:151:A:THR:H	1:149:A:THR:HG22	9	0.69
(1,1047)	1:207:A:MET:HG3	1:207:A:MET:H	7	0.69
(2,297)	1:205:A:ASP:H	1:199:A:LEU:HD11	9	0.68
(2,288)	1:208:A:ILE:H	1:199:A:LEU:HD11	8	0.68
(2,287)	1:159:A:LEU:H	1:158:A:LEU:HD21	3	0.68
(2,227)	1:218:A:ILE:HD11	1:160:A:ALA:HB3	7	0.68
(2,206)	1:160:A:ALA:HB2	1:161:A:GLU:HB2	10	0.68
(2,165)	1:188:A:VAL:HG21	1:186:A:ASN:H	6	0.68
(2,156)	1:195:A:LEU:HD11	1:152:A:GLU:HG3	6	0.68
(2,139)	1:155:A:LEU:HD23	1:155:A:LEU:H	5	0.68
(2,129)	1:148:A:LEU:HD12	1:149:A:THR:H	6	0.68
(1,1057)	1:131:A:THR:HG22	1:131:A:THR:H	8	0.68
(1,986)	1:147:A:GLU:HB2	1:148:A:LEU:H	8	0.68
(1,834)	1:173:A:LEU:HD22	1:173:A:LEU:H	8	0.68
(1,784)	1:218:A:ILE:HD13	1:218:A:ILE:HA	6	0.68
(1,784)	1:218:A:ILE:HD12	1:218:A:ILE:HA	8	0.68
(1,754)	1:158:A:LEU:HD13	1:167:A:MET:HE1	7	0.68
(1,658)	1:163:A:LYS:HE3	1:127:A:VAL:HG13	7	0.68
(1,633)	1:166:A:VAL:HG12	1:215:A:GLY:H	7	0.68
(1,578)	1:151:A:THR:HG21	1:191:A:TYR:HB2	6	0.68
(1,398)	1:167:A:MET:HB3	1:172:A:ILE:HD12	2	0.68
(2,284)	1:132:A:ILE:H	1:125:A:ILE:HG21	4	0.67
(2,224)	1:207:A:MET:HE1	1:130:A:ILE:HD12	8	0.67
(2,206)	1:160:A:ALA:HB3	1:161:A:GLU:HB2	2	0.67
(2,196)	1:136:A:ALA:HB1	1:135:A:ASN:H	6	0.67
(2,189)	1:141:A:VAL:HG11	1:204:A:ARG:HD3	10	0.67
(2,180)	1:149:A:THR:HG21	1:148:A:LEU:HD22	6	0.67
(2,179)	1:146:A:ILE:HB	1:139:A:VAL:HG11	8	0.67
(2,165)	1:188:A:VAL:HG21	1:186:A:ASN:H	4	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,148)	1:199:A:LEU:HD12	1:207:A:MET:HB2	3	0.67
(2,129)	1:148:A:LEU:HD13	1:149:A:THR:H	7	0.67
(2,78)	1:197:A:ASN:HB3	1:200:A:LYS:HD2	10	0.67
(2,75)	1:128:A:ASN:HB3	1:218:A:ILE:HG21	8	0.67
(2,27)	1:154:A:ASP:HA	1:176:A:VAL:HG23	3	0.67
(1,1057)	1:131:A:THR:HG21	1:131:A:THR:H	1	0.67
(1,1003)	1:159:A:LEU:HB3	1:159:A:LEU:H	8	0.67
(1,793)	1:146:A:ILE:HD13	1:202:A:TYR:HD2	7	0.67
(1,784)	1:218:A:ILE:HD12	1:218:A:ILE:HA	1	0.67
(1,784)	1:218:A:ILE:HD13	1:218:A:ILE:HA	2	0.67
(1,658)	1:163:A:LYS:HE2	1:127:A:VAL:HG11	4	0.67
(2,221)	1:130:A:ILE:HD11	1:131:A:THR:H	7	0.66
(2,174)	1:173:A:LEU:HG	1:177:A:TRP:HB2	1	0.66
(2,171)	1:173:A:LEU:HG	1:178:A:GLY:H	5	0.66
(2,122)	1:147:A:GLU:HB2	1:146:A:ILE:HG22	1	0.66
(2,92)	1:171:A:GLN:HG3	1:167:A:MET:HA	8	0.66
(1,1003)	1:159:A:LEU:HB3	1:159:A:LEU:H	9	0.66
(1,972)	1:169:A:ARG:H	1:168:A:GLN:HB2	9	0.66
(1,834)	1:173:A:LEU:HD23	1:173:A:LEU:H	5	0.66
(1,784)	1:218:A:ILE:HD13	1:218:A:ILE:HA	5	0.66
(1,784)	1:218:A:ILE:HD12	1:218:A:ILE:HA	10	0.66
(1,775)	1:130:A:ILE:HD12	1:130:A:ILE:HA	1	0.66
(1,768)	1:216:A:TYR:HB3	1:172:A:ILE:HD12	1	0.66
(1,768)	1:216:A:TYR:HB3	1:172:A:ILE:HD11	9	0.66
(1,633)	1:166:A:VAL:HG11	1:215:A:GLY:H	2	0.66
(1,578)	1:151:A:THR:HG22	1:191:A:TYR:HB2	1	0.66
(1,29)	1:190:A:VAL:HA	1:189:A:ASP:HB3	10	0.66
(2,230)	1:216:A:TYR:HB3	1:192:A:ILE:HD11	8	0.65
(2,223)	1:208:A:ILE:HD12	1:192:A:ILE:HA	3	0.65
(2,221)	1:130:A:ILE:HD11	1:127:A:VAL:H	4	0.65
(2,196)	1:136:A:ALA:HB3	1:135:A:ASN:H	9	0.65
(2,184)	1:183:A:VAL:HG11	1:177:A:TRP:HD1	6	0.65
(2,180)	1:149:A:THR:HG21	1:148:A:LEU:HD21	4	0.65
(1,1057)	1:131:A:THR:HG23	1:131:A:THR:H	2	0.65
(1,1040)	1:190:A:VAL:HG12	1:190:A:VAL:H	2	0.65
(1,972)	1:169:A:ARG:H	1:168:A:GLN:HB2	4	0.65
(1,834)	1:173:A:LEU:HD23	1:173:A:LEU:H	4	0.65
(1,834)	1:173:A:LEU:HD23	1:173:A:LEU:H	7	0.65
(1,578)	1:151:A:THR:HG23	1:191:A:TYR:HB2	4	0.65
(1,456)	1:134:A:LYS:HD3	1:157:A:TYR:HE2	4	0.65
(1,286)	1:205:A:ASP:HB2	1:196:A:ARG:HB2	5	0.65
(2,294)	1:183:A:VAL:HG13	1:187:A:VAL:H	10	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,233)	1:207:A:MET:HE3	1:160:A:ALA:HA	5	0.64
(2,230)	1:216:A:TYR:HB3	1:192:A:ILE:HD12	4	0.64
(2,204)	1:172:A:ILE:HG22	1:158:A:LEU:HB2	10	0.64
(2,190)	1:141:A:VAL:HG23	1:142:A:ASN:HB3	2	0.64
(2,184)	1:183:A:VAL:HG12	1:177:A:TRP:HD1	5	0.64
(2,148)	1:199:A:LEU:HD11	1:207:A:MET:HE1	9	0.64
(2,102)	1:167:A:MET:HG3	1:167:A:MET:HA	2	0.64
(1,1040)	1:190:A:VAL:HG11	1:190:A:VAL:H	1	0.64
(1,1040)	1:190:A:VAL:HG11	1:190:A:VAL:H	3	0.64
(1,1040)	1:190:A:VAL:HG12	1:190:A:VAL:H	10	0.64
(1,820)	1:151:A:THR:HB	1:176:A:VAL:HG12	10	0.64
(1,784)	1:218:A:ILE:HD12	1:218:A:ILE:HA	3	0.64
(1,768)	1:216:A:TYR:HB3	1:172:A:ILE:HD12	6	0.64
(1,633)	1:166:A:VAL:HG11	1:215:A:GLY:H	3	0.64
(2,297)	1:205:A:ASP:H	1:199:A:LEU:HD13	6	0.63
(2,284)	1:132:A:ILE:H	1:125:A:ILE:HG21	8	0.63
(2,230)	1:216:A:TYR:HB3	1:192:A:ILE:HD12	2	0.63
(2,165)	1:188:A:VAL:HG23	1:186:A:ASN:H	8	0.63
(2,156)	1:195:A:LEU:HD13	1:152:A:GLU:HG3	7	0.63
(2,75)	1:128:A:ASN:HB3	1:218:A:ILE:HG21	1	0.63
(2,40)	1:204:A:ARG:HD2	1:204:A:ARG:HB2	3	0.63
(2,9)	1:210:A:THR:HA	1:209:A:GLU:HG2	1	0.63
(1,1086)	1:151:A:THR:H	1:149:A:THR:HG23	3	0.63
(1,834)	1:173:A:LEU:HD21	1:173:A:LEU:H	3	0.63
(1,834)	1:173:A:LEU:HD21	1:173:A:LEU:H	6	0.63
(1,784)	1:218:A:ILE:HD11	1:218:A:ILE:HA	4	0.63
(1,784)	1:218:A:ILE:HD12	1:218:A:ILE:HA	9	0.63
(1,541)	1:134:A:LYS:HG3	1:134:A:LYS:H	5	0.63
(1,248)	1:133:A:ASP:HB3	1:138:A:LYS:H	10	0.63
(2,228)	1:218:A:ILE:HD12	1:128:A:ASN:HB2	1	0.62
(2,204)	1:172:A:ILE:HG22	1:155:A:LEU:HG	6	0.62
(2,179)	1:146:A:ILE:HB	1:139:A:VAL:HG13	7	0.62
(2,109)	1:187:A:VAL:HB	1:187:A:VAL:H	2	0.62
(2,40)	1:204:A:ARG:HD2	1:204:A:ARG:HB2	2	0.62
(1,1040)	1:190:A:VAL:HG13	1:190:A:VAL:H	5	0.62
(1,1040)	1:190:A:VAL:HG12	1:190:A:VAL:H	8	0.62
(1,986)	1:147:A:GLU:HB2	1:148:A:LEU:H	4	0.62
(1,633)	1:166:A:VAL:HG11	1:215:A:GLY:H	1	0.62
(1,624)	1:149:A:THR:HG22	1:152:A:GLU:HB3	10	0.62
(1,541)	1:134:A:LYS:HG3	1:134:A:LYS:H	2	0.62
(1,530)	1:159:A:LEU:HB2	1:159:A:LEU:HD11	8	0.62
(1,255)	1:159:A:LEU:HB2	1:218:A:ILE:HG12	5	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,223)	1:208:A:ILE:HD12	1:196:A:ARG:HA	7	0.61
(2,196)	1:136:A:ALA:HB2	1:135:A:ASN:H	8	0.61
(2,184)	1:187:A:VAL:HG21	1:177:A:TRP:HD1	8	0.61
(2,178)	1:149:A:THR:HG21	1:148:A:LEU:HB3	7	0.61
(2,78)	1:197:A:ASN:HB3	1:198:A:LYS:HB3	3	0.61
(2,40)	1:204:A:ARG:HD2	1:204:A:ARG:HB2	1	0.61
(2,40)	1:204:A:ARG:HD2	1:204:A:ARG:HB2	5	0.61
(1,1057)	1:131:A:THR:HG23	1:131:A:THR:H	4	0.61
(1,1004)	1:207:A:MET:H	1:206:A:LYS:HB3	9	0.61
(1,986)	1:147:A:GLU:HB2	1:148:A:LEU:H	2	0.61
(1,820)	1:151:A:THR:HB	1:176:A:VAL:HG12	3	0.61
(1,596)	1:167:A:MET:HG2	1:159:A:LEU:HD21	4	0.61
(1,541)	1:134:A:LYS:HG3	1:134:A:LYS:H	3	0.61
(1,541)	1:134:A:LYS:HG3	1:134:A:LYS:H	8	0.61
(1,530)	1:159:A:LEU:HB2	1:159:A:LEU:HD11	9	0.61
(1,303)	1:202:A:TYR:HB3	1:141:A:VAL:HG12	4	0.61
(1,165)	1:164:A:ASN:HA	1:217:A:VAL:HG23	8	0.61
(1,29)	1:190:A:VAL:HA	1:189:A:ASP:HB3	6	0.61
(1,16)	1:188:A:VAL:HA	1:191:A:TYR:HB3	4	0.61
(2,287)	1:159:A:LEU:H	1:158:A:LEU:HD23	2	0.6
(2,287)	1:159:A:LEU:H	1:158:A:LEU:HD21	7	0.6
(2,281)	1:148:A:LEU:HD11	1:153:A:TYR:H	4	0.6
(2,263)	1:166:A:VAL:H	1:165:A:HIS:HB2	5	0.6
(2,230)	1:216:A:TYR:HB3	1:192:A:ILE:HD12	10	0.6
(2,206)	1:160:A:ALA:HB1	1:161:A:GLU:HB2	6	0.6
(2,196)	1:136:A:ALA:HB3	1:135:A:ASN:H	5	0.6
(2,196)	1:136:A:ALA:HB2	1:135:A:ASN:H	7	0.6
(2,165)	1:188:A:VAL:HG23	1:186:A:ASN:H	7	0.6
(2,139)	1:155:A:LEU:HD21	1:155:A:LEU:H	2	0.6
(2,129)	1:132:A:ILE:HG12	1:140:A:THR:H	8	0.6
(2,87)	1:209:A:GLU:HG3	1:217:A:VAL:HG12	6	0.6
(2,75)	1:128:A:ASN:HB3	1:218:A:ILE:HG23	10	0.6
(2,60)	1:159:A:LEU:HB2	1:159:A:LEU:HD11	4	0.6
(1,1057)	1:131:A:THR:HG23	1:131:A:THR:H	7	0.6
(1,1040)	1:190:A:VAL:HG11	1:190:A:VAL:H	4	0.6
(1,1040)	1:190:A:VAL:HG13	1:190:A:VAL:H	6	0.6
(1,1040)	1:190:A:VAL:HG13	1:190:A:VAL:H	7	0.6
(1,1039)	1:159:A:LEU:H	1:159:A:LEU:HD13	9	0.6
(1,849)	1:173:A:LEU:HD13	1:173:A:LEU:H	7	0.6
(1,820)	1:151:A:THR:HB	1:176:A:VAL:HG12	1	0.6
(1,820)	1:151:A:THR:HB	1:176:A:VAL:HG13	4	0.6
(1,658)	1:163:A:LYS:HE2	1:127:A:VAL:HG13	5	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,633)	1:166:A:VAL:HG11	1:215:A:GLY:H	8	0.6
(1,579)	1:151:A:THR:HG21	1:154:A:ASP:HB3	8	0.6
(1,578)	1:151:A:THR:HG22	1:191:A:TYR:HB2	3	0.6
(1,547)	1:173:A:LEU:HD12	1:173:A:LEU:HB2	1	0.6
(1,547)	1:173:A:LEU:HD13	1:173:A:LEU:HB2	10	0.6
(1,527)	1:159:A:LEU:HD11	1:216:A:TYR:HB2	3	0.6
(2,301)	1:207:A:MET:H	1:199:A:LEU:HD13	5	0.59
(2,196)	1:136:A:ALA:HB2	1:135:A:ASN:H	4	0.59
(2,156)	1:195:A:LEU:HD12	1:152:A:GLU:HG3	10	0.59
(2,145)	1:192:A:ILE:HG12	1:172:A:ILE:HD12	9	0.59
(2,39)	1:219:A:ARG:HD3	1:217:A:VAL:HG11	5	0.59
(1,1057)	1:131:A:THR:HG22	1:131:A:THR:H	3	0.59
(1,1057)	1:131:A:THR:HG23	1:131:A:THR:H	6	0.59
(1,1040)	1:190:A:VAL:HG11	1:190:A:VAL:H	9	0.59
(1,1000)	1:169:A:ARG:HB2	1:169:A:ARG:H	6	0.59
(1,820)	1:151:A:THR:HB	1:176:A:VAL:HG11	7	0.59
(1,578)	1:151:A:THR:HG23	1:191:A:TYR:HB2	10	0.59
(1,547)	1:173:A:LEU:HD13	1:173:A:LEU:HB2	2	0.59
(1,547)	1:173:A:LEU:HD13	1:173:A:LEU:HB2	9	0.59
(1,541)	1:134:A:LYS:HG2	1:134:A:LYS:H	4	0.59
(1,541)	1:134:A:LYS:HG3	1:134:A:LYS:H	9	0.59
(2,297)	1:205:A:ASP:H	1:199:A:LEU:HD22	10	0.58
(2,286)	1:158:A:LEU:H	1:158:A:LEU:HD22	8	0.58
(2,281)	1:148:A:LEU:HD13	1:153:A:TYR:H	5	0.58
(2,223)	1:208:A:ILE:HD11	1:196:A:ARG:HA	4	0.58
(2,191)	1:211:A:VAL:HG22	1:217:A:VAL:H	3	0.58
(2,190)	1:141:A:VAL:HG21	1:142:A:ASN:HB3	6	0.58
(2,165)	1:188:A:VAL:HG22	1:186:A:ASN:H	10	0.58
(2,148)	1:199:A:LEU:HD12	1:207:A:MET:HB2	5	0.58
(2,60)	1:159:A:LEU:HB2	1:159:A:LEU:HD11	7	0.58
(2,9)	1:210:A:THR:HA	1:209:A:GLU:HG2	4	0.58
(1,1085)	1:151:A:THR:HG22	1:151:A:THR:H	2	0.58
(1,986)	1:147:A:GLU:HB2	1:148:A:LEU:H	7	0.58
(1,658)	1:163:A:LYS:HE2	1:127:A:VAL:HG13	10	0.58
(1,579)	1:151:A:THR:HG21	1:154:A:ASP:HB3	3	0.58
(1,541)	1:134:A:LYS:HG3	1:134:A:LYS:H	7	0.58
(1,255)	1:159:A:LEU:HB2	1:218:A:ILE:HG12	2	0.58
(1,81)	1:169:A:ARG:HA	1:169:A:ARG:HG3	6	0.58
(2,301)	1:207:A:MET:H	1:199:A:LEU:HD12	3	0.57
(2,228)	1:218:A:ILE:HD11	1:128:A:ASN:HB2	4	0.57
(2,227)	1:160:A:ALA:HB2	1:125:A:ILE:HD12	10	0.57
(2,196)	1:136:A:ALA:HB2	1:135:A:ASN:H	10	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,191)	1:211:A:VAL:HG21	1:217:A:VAL:H	1	0.57
(2,178)	1:149:A:THR:HG21	1:148:A:LEU:HB3	3	0.57
(2,163)	1:154:A:ASP:HA	1:176:A:VAL:HG21	6	0.57
(2,156)	1:195:A:LEU:HD12	1:152:A:GLU:HG3	8	0.57
(2,42)	1:204:A:ARG:HD3	1:130:A:ILE:HD13	10	0.57
(2,30)	1:205:A:ASP:HA	1:199:A:LEU:HG	4	0.57
(1,1057)	1:131:A:THR:HG22	1:131:A:THR:H	9	0.57
(1,1000)	1:169:A:ARG:HB2	1:169:A:ARG:H	9	0.57
(1,29)	1:190:A:VAL:HA	1:189:A:ASP:HB3	1	0.57
(2,284)	1:132:A:ILE:H	1:125:A:ILE:HG23	7	0.56
(2,233)	1:207:A:MET:HE2	1:160:A:ALA:HA	3	0.56
(2,229)	1:192:A:ILE:HD13	1:216:A:TYR:HD1	1	0.56
(2,222)	1:205:A:ASP:HA	1:208:A:ILE:HD12	7	0.56
(2,196)	1:136:A:ALA:HB3	1:135:A:ASN:H	3	0.56
(2,191)	1:211:A:VAL:HG22	1:217:A:VAL:H	7	0.56
(2,179)	1:146:A:ILE:HB	1:139:A:VAL:HG11	2	0.56
(2,165)	1:188:A:VAL:HG21	1:172:A:ILE:H	1	0.56
(2,163)	1:154:A:ASP:HA	1:176:A:VAL:HG21	4	0.56
(2,113)	1:200:A:LYS:HB2	1:200:A:LYS:HE2	3	0.56
(1,1085)	1:151:A:THR:HG21	1:151:A:THR:H	5	0.56
(1,1004)	1:207:A:MET:H	1:206:A:LYS:HB3	3	0.56
(1,1004)	1:207:A:MET:H	1:206:A:LYS:HB3	10	0.56
(1,986)	1:147:A:GLU:HB2	1:148:A:LEU:H	1	0.56
(1,986)	1:147:A:GLU:HB2	1:148:A:LEU:H	6	0.56
(1,972)	1:169:A:ARG:H	1:168:A:GLN:HB2	2	0.56
(1,972)	1:169:A:ARG:H	1:168:A:GLN:HB2	6	0.56
(1,754)	1:158:A:LEU:HD12	1:167:A:MET:HE2	8	0.56
(1,658)	1:163:A:LYS:HE2	1:127:A:VAL:HG13	6	0.56
(1,255)	1:159:A:LEU:HB2	1:218:A:ILE:HG12	3	0.56
(1,29)	1:190:A:VAL:HA	1:189:A:ASP:HB3	3	0.56
(2,307)	1:211:A:VAL:H	1:216:A:TYR:HD1	9	0.55
(2,281)	1:148:A:LEU:HD11	1:153:A:TYR:H	1	0.55
(2,281)	1:148:A:LEU:HD12	1:153:A:TYR:H	6	0.55
(2,230)	1:216:A:TYR:HB3	1:192:A:ILE:HD13	9	0.55
(2,229)	1:192:A:ILE:HD13	1:216:A:TYR:HD2	10	0.55
(2,215)	1:167:A:MET:HE1	1:162:A:ASN:HB3	3	0.55
(2,179)	1:146:A:ILE:HB	1:139:A:VAL:HG12	6	0.55
(2,172)	1:199:A:LEU:HD22	1:202:A:TYR:HD2	8	0.55
(2,153)	1:173:A:LEU:HD12	1:177:A:TRP:H	9	0.55
(2,100)	1:167:A:MET:HG2	1:159:A:LEU:HD22	3	0.55
(2,47)	1:204:A:ARG:HD2	1:199:A:LEU:HD22	4	0.55
(2,27)	1:207:A:MET:HA	1:218:A:ILE:HG22	6	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,9)	1:210:A:THR:HA	1:209:A:GLU:HG3	5	0.55
(1,1085)	1:151:A:THR:HG22	1:151:A:THR:H	1	0.55
(1,1085)	1:151:A:THR:HG21	1:151:A:THR:H	3	0.55
(1,1085)	1:151:A:THR:HG23	1:151:A:THR:H	7	0.55
(1,1085)	1:151:A:THR:HG23	1:151:A:THR:H	9	0.55
(1,1039)	1:159:A:LEU:H	1:159:A:LEU:HD13	8	0.55
(1,1011)	1:151:A:THR:H	1:150:A:LYS:HB2	2	0.55
(1,1000)	1:169:A:ARG:HB2	1:169:A:ARG:H	1	0.55
(1,849)	1:173:A:LEU:HD11	1:173:A:LEU:H	4	0.55
(1,81)	1:169:A:ARG:HA	1:169:A:ARG:HG2	2	0.55
(2,307)	1:211:A:VAL:H	1:216:A:TYR:HD1	5	0.54
(2,301)	1:207:A:MET:H	1:199:A:LEU:HD11	1	0.54
(2,284)	1:132:A:ILE:H	1:125:A:ILE:HG21	10	0.54
(2,228)	1:218:A:ILE:HD12	1:128:A:ASN:HB2	8	0.54
(2,213)	1:167:A:MET:HE2	1:168:A:GLN:H	3	0.54
(2,190)	1:141:A:VAL:HG23	1:142:A:ASN:HB3	3	0.54
(2,184)	1:187:A:VAL:HG21	1:177:A:TRP:HD1	3	0.54
(2,163)	1:154:A:ASP:HA	1:176:A:VAL:HG21	9	0.54
(2,127)	1:132:A:ILE:HG12	1:157:A:TYR:HB2	8	0.54
(2,75)	1:128:A:ASN:HB3	1:218:A:ILE:HG23	5	0.54
(2,31)	1:205:A:ASP:HA	1:196:A:ARG:HD2	7	0.54
(1,1085)	1:151:A:THR:HG22	1:151:A:THR:H	4	0.54
(1,1085)	1:151:A:THR:HG21	1:151:A:THR:H	6	0.54
(1,1085)	1:151:A:THR:HG21	1:151:A:THR:H	8	0.54
(1,1057)	1:131:A:THR:HG23	1:131:A:THR:H	10	0.54
(1,849)	1:173:A:LEU:HD11	1:173:A:LEU:H	6	0.54
(1,820)	1:151:A:THR:HB	1:176:A:VAL:HG11	9	0.54
(1,793)	1:146:A:ILE:HD11	1:202:A:TYR:HD1	6	0.54
(1,768)	1:216:A:TYR:HB3	1:172:A:ILE:HD12	4	0.54
(1,527)	1:159:A:LEU:HD13	1:216:A:TYR:HB2	5	0.54
(1,81)	1:169:A:ARG:HA	1:169:A:ARG:HG3	1	0.54
(1,26)	1:190:A:VAL:HA	1:193:A:ARG:HB3	10	0.54
(2,215)	1:167:A:MET:HE2	1:175:A:HIS:HB2	8	0.53
(2,178)	1:149:A:THR:HG21	1:148:A:LEU:HB3	2	0.53
(2,156)	1:195:A:LEU:HD12	1:152:A:GLU:HG3	1	0.53
(2,148)	1:199:A:LEU:HD13	1:207:A:MET:HB2	6	0.53
(2,122)	1:170:A:GLU:HB3	1:173:A:LEU:HD22	8	0.53
(2,27)	1:207:A:MET:HA	1:218:A:ILE:HG22	7	0.53
(2,9)	1:210:A:THR:HA	1:209:A:GLU:HG3	8	0.53
(2,9)	1:210:A:THR:HA	1:209:A:GLU:HG2	10	0.53
(1,1085)	1:151:A:THR:HG22	1:151:A:THR:H	10	0.53
(1,1011)	1:151:A:THR:H	1:150:A:LYS:HB2	6	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1004)	1:207:A:MET:H	1:206:A:LYS:HB3	1	0.53
(1,1004)	1:207:A:MET:H	1:206:A:LYS:HB3	2	0.53
(1,1000)	1:169:A:ARG:HB2	1:169:A:ARG:H	2	0.53
(1,1000)	1:169:A:ARG:HB2	1:169:A:ARG:H	10	0.53
(1,972)	1:169:A:ARG:H	1:168:A:GLN:HB2	10	0.53
(1,768)	1:216:A:TYR:HB3	1:172:A:ILE:HD12	2	0.53
(1,681)	1:136:A:ALA:HB2	1:133:A:ASP:HB3	10	0.53
(1,643)	1:166:A:VAL:HG13	1:167:A:MET:H	10	0.53
(1,578)	1:151:A:THR:HG22	1:191:A:TYR:HB2	5	0.53
(1,578)	1:151:A:THR:HG23	1:191:A:TYR:HB2	7	0.53
(1,492)	1:130:A:ILE:HG13	1:130:A:ILE:H	7	0.53
(1,29)	1:190:A:VAL:HA	1:189:A:ASP:HB3	5	0.53
(2,263)	1:166:A:VAL:H	1:165:A:HIS:HB2	6	0.52
(2,229)	1:192:A:ILE:HD12	1:216:A:TYR:HD1	8	0.52
(2,228)	1:218:A:ILE:HD12	1:128:A:ASN:HB2	3	0.52
(2,227)	1:160:A:ALA:HB3	1:125:A:ILE:HD11	4	0.52
(2,204)	1:172:A:ILE:HG23	1:155:A:LEU:HG	1	0.52
(2,163)	1:154:A:ASP:HA	1:176:A:VAL:HG23	1	0.52
(2,163)	1:154:A:ASP:HA	1:176:A:VAL:HG23	3	0.52
(2,127)	1:132:A:ILE:HG12	1:157:A:TYR:HB2	6	0.52
(2,86)	1:145:A:GLU:HG3	1:138:A:LYS:HE2	9	0.52
(2,9)	1:210:A:THR:HA	1:209:A:GLU:HG3	3	0.52
(1,1000)	1:169:A:ARG:HB2	1:169:A:ARG:H	8	0.52
(1,972)	1:169:A:ARG:H	1:168:A:GLN:HB2	7	0.52
(1,849)	1:173:A:LEU:HD12	1:173:A:LEU:H	3	0.52
(1,820)	1:151:A:THR:HB	1:176:A:VAL:HG12	6	0.52
(1,801)	1:124:A:ILE:HD11	1:124:A:ILE:H	1	0.52
(1,776)	1:204:A:ARG:HB2	1:130:A:ILE:HD12	9	0.52
(1,768)	1:216:A:TYR:HB3	1:172:A:ILE:HD12	3	0.52
(1,768)	1:216:A:TYR:HB3	1:172:A:ILE:HD12	10	0.52
(1,753)	1:158:A:LEU:HD23	1:167:A:MET:HE1	7	0.52
(1,633)	1:166:A:VAL:HG13	1:215:A:GLY:H	10	0.52
(1,579)	1:151:A:THR:HG23	1:154:A:ASP:HB3	9	0.52
(1,522)	1:191:A:TYR:HB2	1:155:A:LEU:HD23	4	0.52
(1,95)	1:170:A:GLU:HA	1:170:A:GLU:HG2	5	0.52
(1,81)	1:169:A:ARG:HA	1:169:A:ARG:HG3	9	0.52
(2,284)	1:132:A:ILE:H	1:125:A:ILE:HG21	5	0.51
(2,206)	1:160:A:ALA:HB2	1:161:A:GLU:HB2	1	0.51
(2,178)	1:149:A:THR:HG21	1:148:A:LEU:HB3	1	0.51
(2,163)	1:154:A:ASP:HA	1:176:A:VAL:HG22	10	0.51
(2,30)	1:205:A:ASP:HA	1:196:A:ARG:HB3	1	0.51
(2,30)	1:205:A:ASP:HA	1:196:A:ARG:HB3	3	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1000)	1:169:A:ARG:HB2	1:169:A:ARG:H	5	0.51
(1,986)	1:147:A:GLU:HB2	1:148:A:LEU:H	10	0.51
(1,849)	1:173:A:LEU:HD11	1:173:A:LEU:H	5	0.51
(1,834)	1:173:A:LEU:HD22	1:173:A:LEU:H	10	0.51
(1,776)	1:204:A:ARG:HB2	1:130:A:ILE:HD11	1	0.51
(1,597)	1:170:A:GLU:HG2	1:185:A:THR:HG21	1	0.51
(1,579)	1:151:A:THR:HG21	1:154:A:ASP:HB3	2	0.51
(1,541)	1:134:A:LYS:HG3	1:134:A:LYS:H	1	0.51
(1,522)	1:191:A:TYR:HB2	1:155:A:LEU:HD21	6	0.51
(1,165)	1:164:A:ASN:HA	1:217:A:VAL:HG21	1	0.51
(1,29)	1:190:A:VAL:HA	1:189:A:ASP:HB3	8	0.51
(2,294)	1:183:A:VAL:HG12	1:187:A:VAL:H	8	0.5
(2,284)	1:132:A:ILE:H	1:125:A:ILE:HG22	3	0.5
(2,229)	1:192:A:ILE:HD12	1:216:A:TYR:HD2	3	0.5
(2,223)	1:208:A:ILE:HD13	1:196:A:ARG:HA	6	0.5
(2,148)	1:199:A:LEU:HD13	1:207:A:MET:HB2	2	0.5
(2,127)	1:132:A:ILE:HG12	1:157:A:TYR:HB2	10	0.5
(2,27)	1:207:A:MET:HA	1:218:A:ILE:HG21	2	0.5
(1,1004)	1:207:A:MET:H	1:206:A:LYS:HB3	8	0.5
(1,986)	1:147:A:GLU:HB2	1:148:A:LEU:H	3	0.5
(1,849)	1:173:A:LEU:HD12	1:173:A:LEU:H	8	0.5
(1,832)	1:153:A:TYR:HB3	1:148:A:LEU:HD12	4	0.5
(1,748)	1:167:A:MET:HE2	1:167:A:MET:HA	5	0.5
(1,530)	1:159:A:LEU:HB2	1:159:A:LEU:HD11	4	0.5
(1,81)	1:169:A:ARG:HA	1:169:A:ARG:HG2	5	0.5
(2,314)	1:204:A:ARG:H	1:199:A:LEU:HD23	8	0.49
(2,301)	1:207:A:MET:H	1:199:A:LEU:HD13	8	0.49
(2,290)	1:124:A:ILE:HD11	1:124:A:ILE:H	4	0.49
(2,284)	1:132:A:ILE:H	1:125:A:ILE:HG22	1	0.49
(2,281)	1:148:A:LEU:HD11	1:153:A:TYR:H	8	0.49
(2,199)	1:136:A:ALA:HB2	1:138:A:LYS:HB3	10	0.49
(2,191)	1:211:A:VAL:HG23	1:217:A:VAL:H	10	0.49
(2,163)	1:154:A:ASP:HA	1:176:A:VAL:HG21	2	0.49
(2,163)	1:154:A:ASP:HA	1:176:A:VAL:HG21	7	0.49
(2,92)	1:171:A:GLN:HG3	1:167:A:MET:HA	9	0.49
(2,86)	1:147:A:GLU:HG2	1:138:A:LYS:HE2	3	0.49
(2,78)	1:197:A:ASN:HB3	1:198:A:LYS:HB3	8	0.49
(2,27)	1:207:A:MET:HA	1:218:A:ILE:HG21	1	0.49
(1,1080)	1:169:A:ARG:H	1:169:A:ARG:HD2	1	0.49
(1,1000)	1:169:A:ARG:HB2	1:169:A:ARG:H	4	0.49
(1,834)	1:173:A:LEU:HD22	1:173:A:LEU:H	2	0.49
(1,773)	1:130:A:ILE:HD13	1:130:A:ILE:H	1	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,652)	1:141:A:VAL:HG13	1:146:A:ILE:HG12	5	0.49
(1,596)	1:167:A:MET:HG2	1:159:A:LEU:HD22	10	0.49
(1,530)	1:159:A:LEU:HB2	1:159:A:LEU:HD11	7	0.49
(1,225)	1:204:A:ARG:HD3	1:204:A:ARG:HB2	4	0.49
(2,316)	1:176:A:VAL:HG21	1:154:A:ASP:H	4	0.48
(2,284)	1:132:A:ILE:H	1:125:A:ILE:HG21	2	0.48
(2,262)	1:193:A:ARG:H	1:193:A:ARG:HD2	10	0.48
(2,233)	1:207:A:MET:HE2	1:160:A:ALA:HA	4	0.48
(2,213)	1:167:A:MET:HE3	1:168:A:GLN:H	8	0.48
(2,206)	1:160:A:ALA:HB1	1:161:A:GLU:HB2	8	0.48
(2,148)	1:199:A:LEU:HD11	1:207:A:MET:HB2	1	0.48
(2,127)	1:132:A:ILE:HG12	1:157:A:TYR:HB2	1	0.48
(2,92)	1:171:A:GLN:HG3	1:167:A:MET:HA	4	0.48
(2,60)	1:159:A:LEU:HB2	1:218:A:ILE:HD11	8	0.48
(2,44)	1:196:A:ARG:HD2	1:195:A:LEU:HB3	1	0.48
(2,44)	1:196:A:ARG:HD2	1:195:A:LEU:HB3	9	0.48
(2,27)	1:207:A:MET:HA	1:218:A:ILE:HG23	4	0.48
(1,834)	1:173:A:LEU:HD23	1:173:A:LEU:H	9	0.48
(1,823)	1:124:A:ILE:HD11	1:133:A:ASP:HB3	9	0.48
(1,820)	1:151:A:THR:HB	1:176:A:VAL:HG11	8	0.48
(1,793)	1:146:A:ILE:HD11	1:202:A:TYR:HD2	8	0.48
(1,768)	1:216:A:TYR:HB3	1:172:A:ILE:HD12	8	0.48
(1,754)	1:158:A:LEU:HD11	1:167:A:MET:HE1	4	0.48
(1,579)	1:151:A:THR:HG21	1:154:A:ASP:HB3	1	0.48
(1,342)	1:170:A:GLU:HG3	1:170:A:GLU:HB3	7	0.48
(1,165)	1:164:A:ASN:HA	1:217:A:VAL:HG21	6	0.48
(1,81)	1:169:A:ARG:HA	1:169:A:ARG:HG2	10	0.48
(2,297)	1:205:A:ASP:H	1:199:A:LEU:HD13	5	0.47
(2,284)	1:132:A:ILE:H	1:125:A:ILE:HG23	9	0.47
(2,213)	1:167:A:MET:HE1	1:168:A:GLN:H	9	0.47
(2,191)	1:211:A:VAL:HG23	1:217:A:VAL:H	2	0.47
(2,172)	1:199:A:LEU:HD21	1:202:A:TYR:HD1	5	0.47
(2,165)	1:188:A:VAL:HG22	1:186:A:ASN:H	5	0.47
(2,163)	1:154:A:ASP:HA	1:176:A:VAL:HG21	5	0.47
(2,148)	1:199:A:LEU:HD13	1:207:A:MET:HB2	8	0.47
(2,122)	1:170:A:GLU:HB3	1:173:A:LEU:HD21	6	0.47
(1,972)	1:169:A:ARG:H	1:168:A:GLN:HB2	3	0.47
(1,834)	1:173:A:LEU:HD22	1:173:A:LEU:H	1	0.47
(1,832)	1:153:A:TYR:HB3	1:148:A:LEU:HD13	2	0.47
(1,832)	1:153:A:TYR:HB3	1:148:A:LEU:HD11	5	0.47
(1,823)	1:124:A:ILE:HD11	1:133:A:ASP:HB3	4	0.47
(1,823)	1:124:A:ILE:HD13	1:133:A:ASP:HB3	7	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,793)	1:146:A:ILE:HD13	1:202:A:TYR:HD1	3	0.47
(1,768)	1:216:A:TYR:HB3	1:172:A:ILE:HD11	7	0.47
(1,643)	1:166:A:VAL:HG11	1:167:A:MET:H	9	0.47
(1,579)	1:151:A:THR:HG21	1:154:A:ASP:HB3	5	0.47
(1,579)	1:151:A:THR:HG22	1:154:A:ASP:HB3	10	0.47
(1,527)	1:159:A:LEU:HD12	1:216:A:TYR:HB2	2	0.47
(1,429)	1:219:A:ARG:HB3	1:219:A:ARG:HD3	10	0.47
(1,413)	1:188:A:VAL:HB	1:188:A:VAL:H	3	0.47
(1,342)	1:170:A:GLU:HG3	1:170:A:GLU:HB3	2	0.47
(1,342)	1:170:A:GLU:HG3	1:170:A:GLU:HB3	3	0.47
(1,342)	1:170:A:GLU:HG3	1:170:A:GLU:HB3	4	0.47
(1,342)	1:170:A:GLU:HG3	1:170:A:GLU:HB3	8	0.47
(1,342)	1:170:A:GLU:HG3	1:170:A:GLU:HB3	10	0.47
(1,330)	1:197:A:ASN:HB3	1:197:A:ASN:H	7	0.47
(1,81)	1:169:A:ARG:HA	1:169:A:ARG:HG2	8	0.47
(2,301)	1:207:A:MET:H	1:199:A:LEU:HD13	2	0.46
(2,291)	1:199:A:LEU:HD22	1:199:A:LEU:H	9	0.46
(2,223)	1:208:A:ILE:HD13	1:196:A:ARG:HA	2	0.46
(2,213)	1:167:A:MET:HE2	1:168:A:GLN:H	4	0.46
(2,213)	1:167:A:MET:HE2	1:168:A:GLN:H	10	0.46
(2,191)	1:211:A:VAL:HG23	1:217:A:VAL:H	9	0.46
(2,184)	1:183:A:VAL:HG11	1:177:A:TRP:HD1	7	0.46
(2,148)	1:199:A:LEU:HD12	1:207:A:MET:HB2	4	0.46
(2,127)	1:132:A:ILE:HG12	1:157:A:TYR:HB2	4	0.46
(1,1068)	1:181:A:SER:H	1:180:A:ASN:HB2	6	0.46
(1,1010)	1:135:A:ASN:H	1:134:A:LYS:HB2	6	0.46
(1,832)	1:153:A:TYR:HB3	1:148:A:LEU:HD13	10	0.46
(1,820)	1:151:A:THR:HB	1:176:A:VAL:HG11	2	0.46
(1,563)	1:188:A:VAL:HG22	1:189:A:ASP:H	2	0.46
(1,492)	1:130:A:ILE:HG13	1:130:A:ILE:H	10	0.46
(1,444)	1:177:A:TRP:HB3	1:177:A:TRP:HE3	1	0.46
(1,342)	1:170:A:GLU:HG3	1:170:A:GLU:HB3	6	0.46
(1,342)	1:170:A:GLU:HG3	1:170:A:GLU:HB3	9	0.46
(1,280)	1:203:A:ASP:HB2	1:203:A:ASP:H	10	0.46
(1,255)	1:159:A:LEU:HB2	1:218:A:ILE:HG12	6	0.46
(1,233)	1:155:A:LEU:HB3	1:155:A:LEU:H	1	0.46
(1,233)	1:155:A:LEU:HB3	1:155:A:LEU:H	7	0.46
(1,233)	1:155:A:LEU:HB3	1:155:A:LEU:H	8	0.46
(1,233)	1:155:A:LEU:HB3	1:155:A:LEU:H	10	0.46
(1,225)	1:204:A:ARG:HD3	1:204:A:ARG:HB2	9	0.46
(1,81)	1:169:A:ARG:HA	1:169:A:ARG:HG2	4	0.46
(2,230)	1:216:A:TYR:HB3	1:192:A:ILE:HD12	1	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,227)	1:160:A:ALA:HB1	1:125:A:ILE:HD13	8	0.45
(2,226)	1:159:A:LEU:HB3	1:218:A:ILE:HD13	1	0.45
(2,178)	1:149:A:THR:HG22	1:148:A:LEU:HB3	10	0.45
(2,163)	1:154:A:ASP:HA	1:176:A:VAL:HG22	8	0.45
(2,100)	1:167:A:MET:HG2	1:159:A:LEU:HD23	1	0.45
(1,1030)	1:195:A:LEU:HD22	1:195:A:LEU:H	5	0.45
(1,1030)	1:195:A:LEU:HD22	1:195:A:LEU:H	8	0.45
(1,1004)	1:207:A:MET:H	1:206:A:LYS:HB3	7	0.45
(1,965)	1:189:A:ASP:HB2	1:189:A:ASP:H	9	0.45
(1,754)	1:158:A:LEU:HD11	1:167:A:MET:HE1	1	0.45
(1,748)	1:167:A:MET:HE2	1:167:A:MET:HA	2	0.45
(1,579)	1:151:A:THR:HG23	1:154:A:ASP:HB3	6	0.45
(1,563)	1:188:A:VAL:HG23	1:189:A:ASP:H	9	0.45
(1,446)	1:168:A:GLN:HB3	1:168:A:GLN:H	3	0.45
(1,446)	1:168:A:GLN:HB3	1:168:A:GLN:H	5	0.45
(1,446)	1:168:A:GLN:HB3	1:168:A:GLN:H	10	0.45
(1,444)	1:177:A:TRP:HB3	1:177:A:TRP:HE3	6	0.45
(1,444)	1:177:A:TRP:HB3	1:177:A:TRP:HE3	8	0.45
(1,342)	1:170:A:GLU:HG3	1:170:A:GLU:HB3	1	0.45
(1,280)	1:203:A:ASP:HB2	1:203:A:ASP:H	1	0.45
(1,233)	1:155:A:LEU:HB3	1:155:A:LEU:H	2	0.45
(1,233)	1:155:A:LEU:HB3	1:155:A:LEU:H	3	0.45
(1,233)	1:155:A:LEU:HB3	1:155:A:LEU:H	5	0.45
(1,121)	1:140:A:THR:HA	1:141:A:VAL:HG13	4	0.45
(2,297)	1:205:A:ASP:H	1:199:A:LEU:HD13	8	0.44
(2,233)	1:207:A:MET:HE2	1:160:A:ALA:HA	1	0.44
(2,178)	1:149:A:THR:HG21	1:148:A:LEU:HB3	6	0.44
(2,127)	1:132:A:ILE:HG12	1:157:A:TYR:HB2	3	0.44
(1,1072)	1:195:A:LEU:HD12	1:196:A:ARG:H	2	0.44
(1,1072)	1:195:A:LEU:HD11	1:196:A:ARG:H	8	0.44
(1,1068)	1:181:A:SER:H	1:180:A:ASN:HB2	2	0.44
(1,794)	1:146:A:ILE:HD13	1:202:A:TYR:HE2	10	0.44
(1,689)	1:214:A:VAL:HG21	1:215:A:GLY:H	7	0.44
(1,689)	1:214:A:VAL:HG21	1:215:A:GLY:H	8	0.44
(1,652)	1:141:A:VAL:HG12	1:146:A:ILE:HG12	9	0.44
(1,651)	1:127:A:VAL:HG13	1:163:A:LYS:HG3	7	0.44
(1,581)	1:185:A:THR:HG22	1:173:A:LEU:HD11	3	0.44
(1,579)	1:151:A:THR:HG22	1:154:A:ASP:HB3	7	0.44
(1,492)	1:130:A:ILE:HG13	1:130:A:ILE:H	6	0.44
(1,446)	1:168:A:GLN:HB3	1:168:A:GLN:H	8	0.44
(1,444)	1:177:A:TRP:HB3	1:177:A:TRP:HE3	4	0.44
(1,280)	1:203:A:ASP:HB2	1:203:A:ASP:H	9	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,233)	1:155:A:LEU:HB3	1:155:A:LEU:H	9	0.44
(2,294)	1:183:A:VAL:HG13	1:187:A:VAL:H	7	0.43
(2,281)	1:148:A:LEU:HD12	1:153:A:TYR:H	10	0.43
(2,189)	1:141:A:VAL:HG13	1:204:A:ARG:HD3	7	0.43
(2,127)	1:132:A:ILE:HG12	1:157:A:TYR:HB2	2	0.43
(2,127)	1:132:A:ILE:HG12	1:157:A:TYR:HB2	7	0.43
(2,89)	1:137:A:PHE:HB3	1:137:A:PHE:H	7	0.43
(2,74)	1:153:A:TYR:HB2	1:148:A:LEU:HD12	4	0.43
(2,36)	1:193:A:ARG:HA	1:196:A:ARG:HD3	7	0.43
(2,30)	1:205:A:ASP:HA	1:196:A:ARG:HB3	6	0.43
(1,1072)	1:195:A:LEU:HD12	1:196:A:ARG:H	4	0.43
(1,1030)	1:195:A:LEU:HD23	1:195:A:LEU:H	1	0.43
(1,844)	1:200:A:LYS:HD3	1:200:A:LYS:H	6	0.43
(1,774)	1:208:A:ILE:HD11	1:208:A:ILE:H	1	0.43
(1,765)	1:172:A:ILE:HD13	1:172:A:ILE:H	5	0.43
(1,754)	1:158:A:LEU:HD11	1:167:A:MET:HE1	10	0.43
(1,689)	1:214:A:VAL:HG23	1:215:A:GLY:H	5	0.43
(1,643)	1:166:A:VAL:HG13	1:167:A:MET:H	1	0.43
(1,563)	1:188:A:VAL:HG23	1:189:A:ASP:H	8	0.43
(1,508)	1:156:A:LEU:HD21	1:156:A:LEU:H	1	0.43
(1,508)	1:156:A:LEU:HD23	1:156:A:LEU:H	2	0.43
(1,508)	1:156:A:LEU:HD23	1:156:A:LEU:H	9	0.43
(1,456)	1:134:A:LYS:HD3	1:157:A:TYR:HE1	3	0.43
(1,446)	1:168:A:GLN:HB3	1:168:A:GLN:H	6	0.43
(1,446)	1:168:A:GLN:HB3	1:168:A:GLN:H	9	0.43
(1,444)	1:177:A:TRP:HB3	1:177:A:TRP:HE3	7	0.43
(1,444)	1:177:A:TRP:HB3	1:177:A:TRP:HE3	9	0.43
(1,233)	1:155:A:LEU:HB3	1:155:A:LEU:H	4	0.43
(1,233)	1:155:A:LEU:HB3	1:155:A:LEU:H	6	0.43
(1,194)	1:215:A:GLY:HA2	1:169:A:ARG:HB2	9	0.43
(1,96)	1:170:A:GLU:HA	1:170:A:GLU:HB3	1	0.43
(2,317)	1:172:A:ILE:H	1:168:A:GLN:HB2	5	0.42
(2,314)	1:204:A:ARG:H	1:199:A:LEU:HD22	5	0.42
(2,297)	1:205:A:ASP:H	1:199:A:LEU:HD11	7	0.42
(2,227)	1:218:A:ILE:HD11	1:160:A:ALA:HB3	5	0.42
(2,226)	1:125:A:ILE:HD13	1:132:A:ILE:HB	5	0.42
(2,191)	1:211:A:VAL:HG22	1:217:A:VAL:H	8	0.42
(2,122)	1:170:A:GLU:HB3	1:173:A:LEU:HD21	3	0.42
(2,122)	1:170:A:GLU:HB3	1:173:A:LEU:HD23	4	0.42
(2,89)	1:137:A:PHE:HB3	1:137:A:PHE:H	10	0.42
(2,88)	1:182:A:GLU:HG3	1:183:A:VAL:HG21	10	0.42
(2,9)	1:210:A:THR:HA	1:209:A:GLU:HG3	9	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1030)	1:195:A:LEU:HD22	1:195:A:LEU:H	2	0.42
(1,1030)	1:195:A:LEU:HD21	1:195:A:LEU:H	3	0.42
(1,1011)	1:151:A:THR:H	1:150:A:LYS:HB2	8	0.42
(1,1011)	1:151:A:THR:H	1:150:A:LYS:HB2	10	0.42
(1,832)	1:153:A:TYR:HB3	1:148:A:LEU:HD11	7	0.42
(1,793)	1:146:A:ILE:HD11	1:202:A:TYR:HD2	1	0.42
(1,774)	1:208:A:ILE:HD12	1:208:A:ILE:H	7	0.42
(1,774)	1:208:A:ILE:HD12	1:208:A:ILE:H	8	0.42
(1,773)	1:130:A:ILE:HD12	1:130:A:ILE:H	5	0.42
(1,765)	1:172:A:ILE:HD11	1:172:A:ILE:H	2	0.42
(1,754)	1:158:A:LEU:HD11	1:167:A:MET:HE3	9	0.42
(1,730)	1:216:A:TYR:HB2	1:208:A:ILE:HG23	5	0.42
(1,689)	1:214:A:VAL:HG22	1:215:A:GLY:H	1	0.42
(1,689)	1:214:A:VAL:HG21	1:215:A:GLY:H	3	0.42
(1,689)	1:214:A:VAL:HG22	1:215:A:GLY:H	6	0.42
(1,651)	1:127:A:VAL:HG11	1:163:A:LYS:HG2	5	0.42
(1,522)	1:191:A:TYR:HB2	1:155:A:LEU:HD22	8	0.42
(1,492)	1:130:A:ILE:HG13	1:130:A:ILE:H	8	0.42
(1,446)	1:168:A:GLN:HB3	1:168:A:GLN:H	2	0.42
(1,446)	1:168:A:GLN:HB3	1:168:A:GLN:H	4	0.42
(1,446)	1:168:A:GLN:HB3	1:168:A:GLN:H	7	0.42
(1,444)	1:177:A:TRP:HB3	1:177:A:TRP:HE3	3	0.42
(1,444)	1:177:A:TRP:HB3	1:177:A:TRP:HE3	5	0.42
(1,50)	1:181:A:SER:HB2	1:177:A:TRP:HB2	5	0.42
(2,316)	1:176:A:VAL:HG21	1:154:A:ASP:H	9	0.41
(2,306)	1:190:A:VAL:HG23	1:191:A:TYR:H	7	0.41
(2,228)	1:218:A:ILE:HD13	1:128:A:ASN:HB2	5	0.41
(2,213)	1:167:A:MET:HE3	1:168:A:GLN:H	6	0.41
(2,197)	1:187:A:VAL:HG11	1:177:A:TRP:HH2	8	0.41
(2,178)	1:149:A:THR:HG22	1:148:A:LEU:HB3	8	0.41
(2,153)	1:173:A:LEU:HD11	1:177:A:TRP:H	1	0.41
(2,142)	1:173:A:LEU:HD21	1:184:A:GLU:HA	7	0.41
(2,113)	1:200:A:LYS:HB3	1:200:A:LYS:HE2	1	0.41
(2,113)	1:200:A:LYS:HB3	1:200:A:LYS:HE2	4	0.41
(2,113)	1:200:A:LYS:HB2	1:200:A:LYS:HE2	5	0.41
(2,89)	1:137:A:PHE:HB3	1:137:A:PHE:H	3	0.41
(2,89)	1:137:A:PHE:HB3	1:137:A:PHE:H	6	0.41
(2,44)	1:196:A:ARG:HD2	1:195:A:LEU:HB3	4	0.41
(2,44)	1:196:A:ARG:HD2	1:195:A:LEU:HB3	6	0.41
(2,9)	1:210:A:THR:HA	1:209:A:GLU:HG3	7	0.41
(1,1072)	1:195:A:LEU:HD11	1:196:A:ARG:H	1	0.41
(1,1072)	1:195:A:LEU:HD12	1:196:A:ARG:H	6	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1030)	1:195:A:LEU:HD22	1:195:A:LEU:H	4	0.41
(1,1030)	1:195:A:LEU:HD22	1:195:A:LEU:H	7	0.41
(1,1010)	1:135:A:ASN:H	1:134:A:LYS:HB3	10	0.41
(1,793)	1:146:A:ILE:HD12	1:202:A:TYR:HD2	2	0.41
(1,774)	1:208:A:ILE:HD11	1:208:A:ILE:H	4	0.41
(1,774)	1:208:A:ILE:HD13	1:208:A:ILE:H	6	0.41
(1,774)	1:208:A:ILE:HD13	1:208:A:ILE:H	9	0.41
(1,765)	1:172:A:ILE:HD13	1:172:A:ILE:H	7	0.41
(1,765)	1:172:A:ILE:HD11	1:172:A:ILE:H	8	0.41
(1,689)	1:214:A:VAL:HG23	1:215:A:GLY:H	2	0.41
(1,522)	1:191:A:TYR:HB2	1:155:A:LEU:HD22	9	0.41
(1,444)	1:177:A:TRP:HB3	1:177:A:TRP:HE3	2	0.41
(1,444)	1:177:A:TRP:HB3	1:177:A:TRP:HE3	10	0.41
(1,252)	1:138:A:LYS:HE2	1:138:A:LYS:HG2	2	0.41
(2,316)	1:176:A:VAL:HG23	1:154:A:ASP:H	1	0.4
(2,295)	1:177:A:TRP:HE1	1:187:A:VAL:HG13	2	0.4
(2,214)	1:167:A:MET:HE1	1:158:A:LEU:HA	8	0.4
(2,213)	1:167:A:MET:HE2	1:168:A:GLN:H	1	0.4
(2,188)	1:141:A:VAL:HG22	1:202:A:TYR:HB3	4	0.4
(2,127)	1:132:A:ILE:HG12	1:157:A:TYR:HB2	9	0.4
(2,89)	1:137:A:PHE:HB3	1:137:A:PHE:H	8	0.4
(2,44)	1:196:A:ARG:HD3	1:195:A:LEU:HB3	7	0.4
(2,39)	1:219:A:ARG:HD3	1:217:A:VAL:HG21	2	0.4
(2,27)	1:207:A:MET:HA	1:218:A:ILE:HG23	5	0.4
(1,1072)	1:195:A:LEU:HD11	1:196:A:ARG:H	5	0.4
(1,1030)	1:195:A:LEU:HD22	1:195:A:LEU:H	6	0.4
(1,1030)	1:195:A:LEU:HD21	1:195:A:LEU:H	9	0.4
(1,1030)	1:195:A:LEU:HD22	1:195:A:LEU:H	10	0.4
(1,972)	1:169:A:ARG:H	1:168:A:GLN:HB2	5	0.4
(1,774)	1:208:A:ILE:HD13	1:208:A:ILE:H	3	0.4
(1,765)	1:172:A:ILE:HD11	1:172:A:ILE:H	4	0.4
(1,765)	1:172:A:ILE:HD13	1:172:A:ILE:H	9	0.4
(1,754)	1:158:A:LEU:HD11	1:167:A:MET:HE2	6	0.4
(1,753)	1:158:A:LEU:HD23	1:167:A:MET:HE2	3	0.4
(1,689)	1:214:A:VAL:HG21	1:215:A:GLY:H	4	0.4
(1,664)	1:217:A:VAL:HG22	1:217:A:VAL:HA	5	0.4
(1,581)	1:185:A:THR:HG21	1:173:A:LEU:HD13	6	0.4
(1,563)	1:188:A:VAL:HG22	1:189:A:ASP:H	5	0.4
(1,532)	1:173:A:LEU:HD23	1:174:A:ASN:H	5	0.4
(1,508)	1:156:A:LEU:HD23	1:156:A:LEU:H	7	0.4
(1,508)	1:156:A:LEU:HD23	1:156:A:LEU:H	10	0.4
(1,446)	1:168:A:GLN:HB3	1:168:A:GLN:H	1	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,263)	1:166:A:VAL:H	1:165:A:HIS:HB3	2	0.39
(2,263)	1:166:A:VAL:H	1:165:A:HIS:HB2	4	0.39
(2,222)	1:205:A:ASP:HA	1:208:A:ILE:HD12	8	0.39
(2,164)	1:176:A:VAL:HG22	1:155:A:LEU:H	4	0.39
(2,162)	1:148:A:LEU:HD21	1:149:A:THR:H	9	0.39
(2,127)	1:132:A:ILE:HG12	1:157:A:TYR:HB2	5	0.39
(2,113)	1:200:A:LYS:HB3	1:200:A:LYS:HE3	7	0.39
(2,89)	1:137:A:PHE:HB3	1:137:A:PHE:H	1	0.39
(2,89)	1:137:A:PHE:HB3	1:137:A:PHE:H	5	0.39
(2,89)	1:137:A:PHE:HB3	1:137:A:PHE:H	9	0.39
(2,75)	1:128:A:ASN:HB3	1:218:A:ILE:HG21	2	0.39
(2,74)	1:128:A:ASN:HB2	1:218:A:ILE:HG23	2	0.39
(2,62)	1:125:A:ILE:HB	1:126:A:ASP:H	7	0.39
(2,27)	1:207:A:MET:HA	1:218:A:ILE:HG23	10	0.39
(1,1072)	1:195:A:LEU:HD12	1:196:A:ARG:H	3	0.39
(1,984)	1:188:A:VAL:HB	1:189:A:ASP:H	3	0.39
(1,774)	1:208:A:ILE:HD13	1:208:A:ILE:H	2	0.39
(1,765)	1:172:A:ILE:HD11	1:172:A:ILE:H	3	0.39
(1,765)	1:172:A:ILE:HD11	1:172:A:ILE:H	6	0.39
(1,757)	1:192:A:ILE:HG22	1:196:A:ARG:H	7	0.39
(1,689)	1:214:A:VAL:HG21	1:215:A:GLY:H	9	0.39
(1,652)	1:141:A:VAL:HG12	1:146:A:ILE:HG12	7	0.39
(1,643)	1:166:A:VAL:HG13	1:167:A:MET:H	4	0.39
(1,642)	1:183:A:VAL:HG11	1:187:A:VAL:HG11	3	0.39
(1,596)	1:167:A:MET:HG2	1:159:A:LEU:HD22	3	0.39
(1,581)	1:185:A:THR:HG22	1:173:A:LEU:HD13	4	0.39
(1,581)	1:185:A:THR:HG23	1:173:A:LEU:HD13	5	0.39
(1,581)	1:185:A:THR:HG23	1:173:A:LEU:HD11	8	0.39
(1,578)	1:151:A:THR:HG23	1:191:A:TYR:HB2	8	0.39
(1,449)	1:161:A:GLU:HB2	1:125:A:ILE:HG22	5	0.39
(2,316)	1:176:A:VAL:HG22	1:154:A:ASP:H	10	0.38
(2,301)	1:207:A:MET:H	1:199:A:LEU:HD12	4	0.38
(2,294)	1:183:A:VAL:HG13	1:187:A:VAL:H	6	0.38
(2,223)	1:208:A:ILE:HD13	1:196:A:ARG:HA	9	0.38
(2,199)	1:136:A:ALA:HB3	1:138:A:LYS:HB3	1	0.38
(2,172)	1:199:A:LEU:HD22	1:202:A:TYR:HD2	9	0.38
(2,162)	1:148:A:LEU:HD21	1:149:A:THR:H	5	0.38
(2,124)	1:171:A:GLN:HB3	1:167:A:MET:HE2	5	0.38
(2,122)	1:170:A:GLU:HB3	1:173:A:LEU:HD23	5	0.38
(2,113)	1:200:A:LYS:HB2	1:200:A:LYS:HE3	10	0.38
(2,94)	1:171:A:GLN:HG3	1:171:A:GLN:HA	3	0.38
(2,89)	1:137:A:PHE:HB3	1:137:A:PHE:H	2	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,62)	1:125:A:ILE:HB	1:126:A:ASP:H	2	0.38
(1,1076)	1:154:A:ASP:H	1:155:A:LEU:HD13	9	0.38
(1,1072)	1:195:A:LEU:HD11	1:196:A:ARG:H	10	0.38
(1,1037)	1:165:A:HIS:H	1:217:A:VAL:HG21	8	0.38
(1,986)	1:147:A:GLU:HB2	1:148:A:LEU:H	5	0.38
(1,972)	1:169:A:ARG:H	1:168:A:GLN:HB2	8	0.38
(1,832)	1:153:A:TYR:HB3	1:148:A:LEU:HD12	8	0.38
(1,793)	1:146:A:ILE:HD13	1:202:A:TYR:HD2	10	0.38
(1,765)	1:172:A:ILE:HD11	1:172:A:ILE:H	1	0.38
(1,757)	1:192:A:ILE:HG23	1:196:A:ARG:H	1	0.38
(1,757)	1:192:A:ILE:HG22	1:196:A:ARG:H	10	0.38
(1,709)	1:209:A:GLU:HG3	1:217:A:VAL:HG12	6	0.38
(1,689)	1:214:A:VAL:HG22	1:215:A:GLY:H	10	0.38
(1,682)	1:136:A:ALA:HB1	1:135:A:ASN:HB3	1	0.38
(1,651)	1:127:A:VAL:HG13	1:163:A:LYS:HG3	6	0.38
(1,643)	1:166:A:VAL:HG13	1:167:A:MET:H	5	0.38
(1,643)	1:166:A:VAL:HG13	1:167:A:MET:H	8	0.38
(1,583)	1:139:A:VAL:HG22	1:133:A:ASP:H	7	0.38
(1,563)	1:188:A:VAL:HG22	1:189:A:ASP:H	1	0.38
(1,463)	1:172:A:ILE:HG12	1:172:A:ILE:H	6	0.38
(1,352)	1:147:A:GLU:HG3	1:147:A:GLU:H	8	0.38
(2,316)	1:176:A:VAL:HG21	1:154:A:ASP:H	5	0.37
(2,316)	1:176:A:VAL:HG21	1:154:A:ASP:H	6	0.37
(2,284)	1:132:A:ILE:H	1:125:A:ILE:HG21	6	0.37
(2,143)	1:199:A:LEU:HD13	1:196:A:ARG:HD2	5	0.37
(2,42)	1:204:A:ARG:HD3	1:130:A:ILE:HD13	6	0.37
(1,1078)	1:165:A:HIS:H	1:163:A:LYS:HG3	8	0.37
(1,1076)	1:154:A:ASP:H	1:155:A:LEU:HD13	5	0.37
(1,1072)	1:195:A:LEU:HD11	1:196:A:ARG:H	7	0.37
(1,832)	1:153:A:TYR:HB3	1:148:A:LEU:HD12	9	0.37
(1,796)	1:146:A:ILE:HA	1:146:A:ILE:HD11	5	0.37
(1,796)	1:146:A:ILE:HA	1:146:A:ILE:HD11	9	0.37
(1,774)	1:208:A:ILE:HD12	1:208:A:ILE:H	10	0.37
(1,757)	1:192:A:ILE:HG22	1:196:A:ARG:H	6	0.37
(1,581)	1:185:A:THR:HG23	1:173:A:LEU:HD12	7	0.37
(1,579)	1:151:A:THR:HG21	1:154:A:ASP:HB3	4	0.37
(1,563)	1:188:A:VAL:HG22	1:189:A:ASP:H	10	0.37
(1,544)	1:173:A:LEU:HD12	1:173:A:LEU:HA	2	0.37
(1,544)	1:173:A:LEU:HD12	1:173:A:LEU:HA	10	0.37
(1,532)	1:173:A:LEU:HD23	1:174:A:ASN:H	7	0.37
(1,522)	1:191:A:TYR:HB2	1:155:A:LEU:HD22	5	0.37
(1,508)	1:156:A:LEU:HD22	1:156:A:LEU:H	3	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,508)	1:156:A:LEU:HD22	1:156:A:LEU:H	4	0.37
(1,508)	1:156:A:LEU:HD23	1:156:A:LEU:H	6	0.37
(1,463)	1:172:A:ILE:HG12	1:172:A:ILE:H	8	0.37
(1,461)	1:212:A:ARG:HB2	1:210:A:THR:HG23	1	0.37
(1,427)	1:219:A:ARG:HB3	1:219:A:ARG:H	6	0.37
(1,211)	1:216:A:TYR:HB2	1:217:A:VAL:H	5	0.37
(2,306)	1:190:A:VAL:HG21	1:191:A:TYR:H	4	0.36
(2,306)	1:190:A:VAL:HG23	1:191:A:TYR:H	6	0.36
(2,297)	1:205:A:ASP:H	1:199:A:LEU:HD12	3	0.36
(2,232)	1:192:A:ILE:HD13	1:208:A:ILE:HG23	9	0.36
(2,229)	1:192:A:ILE:HD13	1:216:A:TYR:HD2	2	0.36
(2,214)	1:167:A:MET:HE1	1:159:A:LEU:HA	6	0.36
(2,183)	1:140:A:THR:HG21	1:138:A:LYS:HD2	1	0.36
(2,178)	1:149:A:THR:HG21	1:148:A:LEU:HB3	4	0.36
(2,100)	1:204:A:ARG:HB2	1:130:A:ILE:HD13	6	0.36
(2,87)	1:209:A:GLU:HG3	1:217:A:VAL:HG13	8	0.36
(2,62)	1:125:A:ILE:HB	1:126:A:ASP:H	6	0.36
(2,62)	1:125:A:ILE:HB	1:126:A:ASP:H	10	0.36
(2,47)	1:204:A:ARG:HD2	1:199:A:LEU:HD23	9	0.36
(1,796)	1:146:A:ILE:HA	1:146:A:ILE:HD12	4	0.36
(1,796)	1:146:A:ILE:HA	1:146:A:ILE:HD12	10	0.36
(1,765)	1:172:A:ILE:HD11	1:172:A:ILE:H	10	0.36
(1,733)	1:130:A:ILE:HG21	1:131:A:THR:H	6	0.36
(1,730)	1:216:A:TYR:HB2	1:208:A:ILE:HG21	1	0.36
(1,652)	1:141:A:VAL:HG12	1:146:A:ILE:HG12	8	0.36
(1,643)	1:166:A:VAL:HG11	1:167:A:MET:H	3	0.36
(1,532)	1:173:A:LEU:HD21	1:174:A:ASN:H	3	0.36
(1,531)	1:192:A:ILE:HG13	1:192:A:ILE:H	3	0.36
(1,522)	1:191:A:TYR:HB2	1:155:A:LEU:HD22	1	0.36
(1,463)	1:172:A:ILE:HG12	1:172:A:ILE:H	3	0.36
(1,171)	1:186:A:ASN:HA	1:186:A:ASN:HB2	7	0.36
(1,144)	1:189:A:ASP:HA	1:189:A:ASP:HB2	5	0.36
(1,144)	1:189:A:ASP:HA	1:189:A:ASP:HB2	6	0.36
(1,144)	1:189:A:ASP:HA	1:189:A:ASP:HB2	8	0.36
(1,50)	1:181:A:SER:HB2	1:177:A:TRP:HB2	2	0.36
(2,318)	1:175:A:HIS:H	1:176:A:VAL:HG23	6	0.35
(2,316)	1:176:A:VAL:HG23	1:154:A:ASP:H	3	0.35
(2,297)	1:205:A:ASP:H	1:199:A:LEU:HD13	2	0.35
(2,281)	1:148:A:LEU:HD12	1:153:A:TYR:H	2	0.35
(2,233)	1:207:A:MET:HE3	1:160:A:ALA:HA	10	0.35
(2,232)	1:192:A:ILE:HD12	1:208:A:ILE:HG23	2	0.35
(2,228)	1:218:A:ILE:HD13	1:128:A:ASN:HB2	2	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,223)	1:208:A:ILE:HD13	1:196:A:ARG:HA	5	0.35
(2,203)	1:217:A:VAL:HG11	1:219:A:ARG:HG3	10	0.35
(2,184)	1:183:A:VAL:HG13	1:177:A:TRP:HD1	9	0.35
(2,184)	1:183:A:VAL:HG11	1:177:A:TRP:HD1	10	0.35
(2,179)	1:146:A:ILE:HB	1:139:A:VAL:HG13	3	0.35
(2,178)	1:149:A:THR:HG23	1:148:A:LEU:HB3	5	0.35
(2,178)	1:149:A:THR:HG23	1:148:A:LEU:HB3	9	0.35
(2,173)	1:210:A:THR:HG22	1:216:A:TYR:HE1	9	0.35
(2,97)	1:127:A:VAL:HB	1:163:A:LYS:HB3	10	0.35
(1,1080)	1:169:A:ARG:H	1:169:A:ARG:HD2	5	0.35
(1,1076)	1:154:A:ASP:H	1:155:A:LEU:HD13	8	0.35
(1,1045)	1:192:A:ILE:HG23	1:192:A:ILE:H	5	0.35
(1,1002)	1:187:A:VAL:HB	1:187:A:VAL:H	2	0.35
(1,978)	1:126:A:ASP:HB2	1:126:A:ASP:H	3	0.35
(1,823)	1:124:A:ILE:HD12	1:133:A:ASP:HB3	3	0.35
(1,805)	1:192:A:ILE:HD12	1:192:A:ILE:H	9	0.35
(1,757)	1:192:A:ILE:HG23	1:196:A:ARG:H	2	0.35
(1,757)	1:192:A:ILE:HG22	1:196:A:ARG:H	3	0.35
(1,735)	1:125:A:ILE:HG21	1:126:A:ASP:H	2	0.35
(1,733)	1:130:A:ILE:HG23	1:131:A:THR:H	10	0.35
(1,730)	1:216:A:TYR:HB2	1:208:A:ILE:HG23	3	0.35
(1,649)	1:190:A:VAL:HB	1:187:A:VAL:HG22	6	0.35
(1,575)	1:151:A:THR:HG22	1:177:A:TRP:HH2	5	0.35
(1,531)	1:192:A:ILE:HG13	1:192:A:ILE:H	2	0.35
(1,304)	1:174:A:ASN:HB3	1:174:A:ASN:H	8	0.35
(1,252)	1:138:A:LYS:HE2	1:138:A:LYS:HG2	4	0.35
(1,252)	1:138:A:LYS:HE3	1:138:A:LYS:HG2	5	0.35
(1,171)	1:186:A:ASN:HA	1:186:A:ASN:HB2	5	0.35
(1,171)	1:186:A:ASN:HA	1:186:A:ASN:HB2	8	0.35
(1,171)	1:186:A:ASN:HA	1:186:A:ASN:HB2	9	0.35
(1,144)	1:189:A:ASP:HA	1:189:A:ASP:HB2	1	0.35
(1,144)	1:189:A:ASP:HA	1:189:A:ASP:HB2	3	0.35
(1,144)	1:189:A:ASP:HA	1:189:A:ASP:HB2	10	0.35
(2,306)	1:190:A:VAL:HG23	1:191:A:TYR:H	8	0.34
(2,294)	1:183:A:VAL:HG11	1:187:A:VAL:H	5	0.34
(2,280)	1:148:A:LEU:H	1:148:A:LEU:HD23	9	0.34
(2,232)	1:192:A:ILE:HD12	1:208:A:ILE:HG23	10	0.34
(2,228)	1:218:A:ILE:HD13	1:128:A:ASN:HB2	6	0.34
(2,228)	1:218:A:ILE:HD12	1:128:A:ASN:HB2	9	0.34
(2,223)	1:208:A:ILE:HD12	1:196:A:ARG:HA	10	0.34
(2,214)	1:167:A:MET:HE3	1:159:A:LEU:HA	1	0.34
(2,212)	1:207:A:MET:HE2	1:130:A:ILE:HD13	7	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,185)	1:187:A:VAL:HB	1:183:A:VAL:HG12	1	0.34
(2,170)	1:159:A:LEU:HD22	1:159:A:LEU:H	10	0.34
(2,62)	1:125:A:ILE:HB	1:126:A:ASP:H	5	0.34
(2,62)	1:125:A:ILE:HB	1:126:A:ASP:H	8	0.34
(2,42)	1:204:A:ARG:HD3	1:130:A:ILE:HD11	1	0.34
(2,42)	1:204:A:ARG:HD3	1:130:A:ILE:HD13	5	0.34
(2,42)	1:204:A:ARG:HD3	1:130:A:ILE:HD12	7	0.34
(1,1076)	1:154:A:ASP:H	1:155:A:LEU:HD11	2	0.34
(1,1045)	1:192:A:ILE:HG23	1:192:A:ILE:H	9	0.34
(1,1037)	1:165:A:HIS:H	1:217:A:VAL:HG21	9	0.34
(1,1011)	1:151:A:THR:H	1:150:A:LYS:HB2	5	0.34
(1,978)	1:126:A:ASP:HB2	1:126:A:ASP:H	2	0.34
(1,774)	1:208:A:ILE:HD13	1:208:A:ILE:H	5	0.34
(1,738)	1:128:A:ASN:HB3	1:207:A:MET:HE2	9	0.34
(1,662)	1:176:A:VAL:HG13	1:177:A:TRP:HE3	9	0.34
(1,658)	1:163:A:LYS:HE2	1:127:A:VAL:HG12	2	0.34
(1,651)	1:127:A:VAL:HG11	1:163:A:LYS:HG3	9	0.34
(1,563)	1:188:A:VAL:HG21	1:189:A:ASP:H	4	0.34
(1,563)	1:188:A:VAL:HG21	1:189:A:ASP:H	6	0.34
(1,531)	1:192:A:ILE:HG13	1:192:A:ILE:H	6	0.34
(1,463)	1:172:A:ILE:HG12	1:172:A:ILE:H	4	0.34
(1,375)	1:141:A:VAL:HB	1:141:A:VAL:H	4	0.34
(1,337)	1:197:A:ASN:HB2	1:197:A:ASN:HA	7	0.34
(1,252)	1:138:A:LYS:HE2	1:138:A:LYS:HG2	6	0.34
(1,26)	1:190:A:VAL:HA	1:193:A:ARG:HB3	8	0.34
(2,233)	1:207:A:MET:HE2	1:160:A:ALA:HA	9	0.33
(2,187)	1:127:A:VAL:HG22	1:126:A:ASP:HA	1	0.33
(2,113)	1:205:A:ASP:HB3	1:200:A:LYS:HB2	2	0.33
(2,102)	1:167:A:MET:HG3	1:167:A:MET:HA	5	0.33
(2,62)	1:125:A:ILE:HB	1:126:A:ASP:H	4	0.33
(1,1080)	1:169:A:ARG:H	1:169:A:ARG:HD2	8	0.33
(1,1068)	1:181:A:SER:H	1:180:A:ASN:HB2	9	0.33
(1,1045)	1:192:A:ILE:HG21	1:192:A:ILE:H	8	0.33
(1,978)	1:126:A:ASP:HB2	1:126:A:ASP:H	8	0.33
(1,757)	1:192:A:ILE:HG22	1:196:A:ARG:H	4	0.33
(1,746)	1:207:A:MET:HG3	1:218:A:ILE:HG23	9	0.33
(1,730)	1:216:A:TYR:HB2	1:208:A:ILE:HG22	7	0.33
(1,730)	1:216:A:TYR:HB2	1:208:A:ILE:HG22	9	0.33
(1,662)	1:176:A:VAL:HG11	1:177:A:TRP:HE3	6	0.33
(1,651)	1:127:A:VAL:HG12	1:163:A:LYS:HG2	4	0.33
(1,624)	1:149:A:THR:HG23	1:152:A:GLU:HB3	5	0.33
(1,624)	1:149:A:THR:HG23	1:152:A:GLU:HB3	9	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,578)	1:151:A:THR:HG23	1:191:A:TYR:HB2	2	0.33
(1,544)	1:173:A:LEU:HD11	1:173:A:LEU:HA	1	0.33
(1,544)	1:173:A:LEU:HD12	1:173:A:LEU:HA	9	0.33
(1,531)	1:192:A:ILE:HG13	1:192:A:ILE:H	4	0.33
(1,531)	1:192:A:ILE:HG13	1:192:A:ILE:H	7	0.33
(1,527)	1:159:A:LEU:HD13	1:216:A:TYR:HB2	1	0.33
(1,479)	1:193:A:ARG:HG3	1:193:A:ARG:HA	2	0.33
(1,427)	1:219:A:ARG:HB3	1:219:A:ARG:H	2	0.33
(1,427)	1:219:A:ARG:HB3	1:219:A:ARG:H	5	0.33
(1,70)	1:192:A:ILE:HA	1:192:A:ILE:HG13	5	0.33
(1,70)	1:192:A:ILE:HA	1:192:A:ILE:HG13	8	0.33
(1,70)	1:192:A:ILE:HA	1:192:A:ILE:HG13	9	0.33
(2,309)	1:140:A:THR:H	1:132:A:ILE:HG13	9	0.32
(2,309)	1:140:A:THR:H	1:132:A:ILE:HG13	10	0.32
(2,232)	1:192:A:ILE:HD11	1:208:A:ILE:HG23	8	0.32
(2,213)	1:167:A:MET:HE3	1:167:A:MET:H	7	0.32
(2,171)	1:173:A:LEU:HG	1:178:A:GLY:H	4	0.32
(2,153)	1:173:A:LEU:HD12	1:177:A:TRP:H	10	0.32
(2,97)	1:127:A:VAL:HB	1:163:A:LYS:HB3	9	0.32
(2,79)	1:152:A:GLU:HG3	1:155:A:LEU:HD12	3	0.32
(2,62)	1:125:A:ILE:HB	1:126:A:ASP:H	9	0.32
(2,48)	1:173:A:LEU:HB2	1:174:A:ASN:H	1	0.32
(2,48)	1:173:A:LEU:HB2	1:174:A:ASN:H	2	0.32
(1,1076)	1:154:A:ASP:H	1:155:A:LEU:HD12	3	0.32
(1,1076)	1:154:A:ASP:H	1:155:A:LEU:HD11	7	0.32
(1,1045)	1:192:A:ILE:HG22	1:192:A:ILE:H	7	0.32
(1,832)	1:153:A:TYR:HB3	1:148:A:LEU:HD12	3	0.32
(1,823)	1:124:A:ILE:HD13	1:133:A:ASP:HB3	5	0.32
(1,793)	1:146:A:ILE:HD12	1:202:A:TYR:HD1	5	0.32
(1,793)	1:146:A:ILE:HD12	1:202:A:TYR:HD2	9	0.32
(1,757)	1:192:A:ILE:HG21	1:196:A:ARG:H	8	0.32
(1,749)	1:167:A:MET:HE3	1:167:A:MET:HG3	7	0.32
(1,736)	1:207:A:MET:HE2	1:130:A:ILE:H	4	0.32
(1,682)	1:136:A:ALA:HB3	1:135:A:ASN:HB2	2	0.32
(1,662)	1:176:A:VAL:HG12	1:177:A:TRP:HE3	4	0.32
(1,662)	1:176:A:VAL:HG11	1:177:A:TRP:HE3	10	0.32
(1,651)	1:127:A:VAL:HG12	1:163:A:LYS:HG2	3	0.32
(1,585)	1:139:A:VAL:HG22	1:153:A:TYR:HE1	7	0.32
(1,583)	1:139:A:VAL:HG23	1:133:A:ASP:H	2	0.32
(1,532)	1:173:A:LEU:HD21	1:174:A:ASN:H	6	0.32
(1,532)	1:173:A:LEU:HD22	1:174:A:ASN:H	8	0.32
(1,531)	1:192:A:ILE:HG13	1:192:A:ILE:H	1	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,531)	1:192:A:ILE:HG13	1:192:A:ILE:H	10	0.32
(1,508)	1:156:A:LEU:HD21	1:156:A:LEU:H	5	0.32
(1,449)	1:161:A:GLU:HB2	1:125:A:ILE:HG23	3	0.32
(1,449)	1:161:A:GLU:HB2	1:125:A:ILE:HG21	7	0.32
(1,355)	1:184:A:GLU:HG2	1:184:A:GLU:H	7	0.32
(1,220)	1:216:A:TYR:HB3	1:192:A:ILE:HD11	3	0.32
(1,171)	1:186:A:ASN:HA	1:186:A:ASN:HB2	3	0.32
(2,317)	1:172:A:ILE:H	1:168:A:GLN:HB2	7	0.31
(2,316)	1:176:A:VAL:HG22	1:154:A:ASP:H	8	0.31
(2,262)	1:193:A:ARG:H	1:193:A:ARG:HD3	8	0.31
(2,232)	1:192:A:ILE:HD12	1:208:A:ILE:HG23	1	0.31
(2,226)	1:159:A:LEU:HB3	1:218:A:ILE:HD11	6	0.31
(2,221)	1:130:A:ILE:HD11	1:131:A:THR:H	8	0.31
(2,199)	1:136:A:ALA:HB3	1:138:A:LYS:HB2	9	0.31
(2,193)	1:176:A:VAL:HG11	1:177:A:TRP:HZ3	2	0.31
(2,43)	1:196:A:ARG:HA	1:195:A:LEU:HB3	9	0.31
(1,1076)	1:154:A:ASP:H	1:155:A:LEU:HD11	1	0.31
(1,1076)	1:154:A:ASP:H	1:155:A:LEU:HD12	6	0.31
(1,1048)	1:207:A:MET:H	1:206:A:LYS:HG3	9	0.31
(1,1045)	1:192:A:ILE:HG23	1:192:A:ILE:H	1	0.31
(1,1045)	1:192:A:ILE:HG22	1:192:A:ILE:H	4	0.31
(1,998)	1:217:A:VAL:HB	1:167:A:MET:H	5	0.31
(1,978)	1:126:A:ASP:HB2	1:126:A:ASP:H	9	0.31
(1,832)	1:153:A:TYR:HB3	1:148:A:LEU:HD12	1	0.31
(1,823)	1:124:A:ILE:HD11	1:133:A:ASP:HB3	8	0.31
(1,793)	1:146:A:ILE:HD13	1:202:A:TYR:HD2	4	0.31
(1,735)	1:125:A:ILE:HG22	1:126:A:ASP:H	7	0.31
(1,735)	1:125:A:ILE:HG21	1:126:A:ASP:H	10	0.31
(1,724)	1:132:A:ILE:HG22	1:139:A:VAL:HA	2	0.31
(1,652)	1:141:A:VAL:HG13	1:146:A:ILE:HG12	2	0.31
(1,624)	1:149:A:THR:HG22	1:152:A:GLU:HB3	8	0.31
(1,596)	1:167:A:MET:HG2	1:159:A:LEU:HD22	7	0.31
(1,532)	1:173:A:LEU:HD23	1:174:A:ASN:H	4	0.31
(1,531)	1:192:A:ILE:HG13	1:192:A:ILE:H	5	0.31
(1,522)	1:191:A:TYR:HB2	1:155:A:LEU:HD23	2	0.31
(1,467)	1:171:A:GLN:HB3	1:171:A:GLN:H	5	0.31
(1,467)	1:171:A:GLN:HB3	1:171:A:GLN:H	8	0.31
(1,449)	1:161:A:GLU:HB2	1:125:A:ILE:HG22	4	0.31
(1,443)	1:177:A:TRP:HB3	1:177:A:TRP:H	1	0.31
(1,443)	1:177:A:TRP:HB3	1:177:A:TRP:H	9	0.31
(1,443)	1:177:A:TRP:HB3	1:177:A:TRP:H	10	0.31
(1,430)	1:211:A:VAL:HB	1:211:A:VAL:H	9	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,427)	1:219:A:ARG:HB3	1:219:A:ARG:H	8	0.31
(1,355)	1:184:A:GLU:HG2	1:184:A:GLU:H	10	0.31
(1,265)	1:189:A:ASP:HB3	1:190:A:VAL:H	9	0.31
(1,226)	1:169:A:ARG:HD2	1:169:A:ARG:HB2	10	0.31
(1,225)	1:204:A:ARG:HD3	1:204:A:ARG:HB2	3	0.31
(1,221)	1:219:A:ARG:HD2	1:219:A:ARG:H	5	0.31
(2,307)	1:211:A:VAL:H	1:216:A:TYR:HD1	7	0.3
(2,232)	1:192:A:ILE:HD12	1:208:A:ILE:HG22	6	0.3
(2,232)	1:192:A:ILE:HD13	1:208:A:ILE:HG23	7	0.3
(2,229)	1:192:A:ILE:HD13	1:216:A:TYR:HD2	4	0.3
(2,212)	1:207:A:MET:HE2	1:218:A:ILE:HG23	8	0.3
(2,173)	1:210:A:THR:HG22	1:216:A:TYR:HE1	3	0.3
(2,162)	1:148:A:LEU:HD22	1:149:A:THR:H	1	0.3
(2,162)	1:148:A:LEU:HD23	1:149:A:THR:H	10	0.3
(2,153)	1:173:A:LEU:HD12	1:177:A:TRP:H	2	0.3
(2,122)	1:170:A:GLU:HB3	1:173:A:LEU:HD23	7	0.3
(2,105)	1:207:A:MET:HG3	1:218:A:ILE:HG23	9	0.3
(2,92)	1:171:A:GLN:HG3	1:167:A:MET:HA	3	0.3
(2,62)	1:125:A:ILE:HB	1:126:A:ASP:H	3	0.3
(2,55)	1:198:A:LYS:HE2	1:152:A:GLU:HB3	6	0.3
(2,48)	1:173:A:LEU:HB2	1:174:A:ASN:H	9	0.3
(2,48)	1:173:A:LEU:HB2	1:174:A:ASN:H	10	0.3
(2,47)	1:204:A:ARG:HD2	1:141:A:VAL:HG22	5	0.3
(2,26)	1:219:A:ARG:HA	1:219:A:ARG:HG2	6	0.3
(1,1084)	1:124:A:ILE:H	1:124:A:ILE:HG13	4	0.3
(1,1076)	1:154:A:ASP:H	1:155:A:LEU:HD12	4	0.3
(1,1076)	1:154:A:ASP:H	1:155:A:LEU:HD13	10	0.3
(1,1045)	1:192:A:ILE:HG23	1:192:A:ILE:H	2	0.3
(1,1045)	1:192:A:ILE:HG22	1:192:A:ILE:H	10	0.3
(1,844)	1:200:A:LYS:HD3	1:200:A:LYS:H	9	0.3
(1,810)	1:124:A:ILE:HG13	1:124:A:ILE:HA	6	0.3
(1,805)	1:192:A:ILE:HD11	1:192:A:ILE:H	2	0.3
(1,762)	1:192:A:ILE:HG22	1:208:A:ILE:HD12	9	0.3
(1,724)	1:132:A:ILE:HG22	1:139:A:VAL:HA	3	0.3
(1,705)	1:217:A:VAL:HG13	1:217:A:VAL:HA	9	0.3
(1,705)	1:217:A:VAL:HG12	1:217:A:VAL:HA	10	0.3
(1,682)	1:136:A:ALA:HB1	1:135:A:ASN:HB2	5	0.3
(1,682)	1:136:A:ALA:HB3	1:135:A:ASN:HB2	10	0.3
(1,662)	1:176:A:VAL:HG13	1:177:A:TRP:HE3	8	0.3
(1,634)	1:183:A:VAL:HG12	1:187:A:VAL:H	1	0.3
(1,619)	1:159:A:LEU:HD23	1:192:A:ILE:HD13	6	0.3
(1,596)	1:167:A:MET:HG2	1:159:A:LEU:HD21	6	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,583)	1:139:A:VAL:HG23	1:133:A:ASP:H	8	0.3
(1,575)	1:151:A:THR:HG22	1:177:A:TRP:HH2	8	0.3
(1,555)	1:175:A:HIS:HB2	1:176:A:VAL:HG22	1	0.3
(1,531)	1:192:A:ILE:HG13	1:192:A:ILE:H	8	0.3
(1,479)	1:193:A:ARG:HG3	1:193:A:ARG:HA	3	0.3
(1,479)	1:193:A:ARG:HG3	1:193:A:ARG:HA	7	0.3
(1,449)	1:161:A:GLU:HB2	1:125:A:ILE:HG22	8	0.3
(1,443)	1:177:A:TRP:HB3	1:177:A:TRP:H	5	0.3
(1,427)	1:219:A:ARG:HB3	1:219:A:ARG:H	9	0.3
(1,399)	1:167:A:MET:HB3	1:172:A:ILE:HG13	2	0.3
(1,70)	1:192:A:ILE:HA	1:192:A:ILE:HG13	2	0.3
(1,70)	1:192:A:ILE:HA	1:192:A:ILE:HG13	4	0.3
(1,70)	1:192:A:ILE:HA	1:192:A:ILE:HG13	7	0.3
(2,318)	1:175:A:HIS:H	1:176:A:VAL:HG23	4	0.29
(2,314)	1:204:A:ARG:H	1:199:A:LEU:HD23	2	0.29
(2,306)	1:190:A:VAL:HG23	1:191:A:TYR:H	3	0.29
(2,291)	1:199:A:LEU:HD21	1:199:A:LEU:H	6	0.29
(2,290)	1:124:A:ILE:HD11	1:124:A:ILE:H	9	0.29
(2,230)	1:216:A:TYR:HB3	1:192:A:ILE:HD12	6	0.29
(2,221)	1:130:A:ILE:HD11	1:131:A:THR:H	10	0.29
(2,199)	1:136:A:ALA:HB2	1:138:A:LYS:HB3	2	0.29
(2,199)	1:136:A:ALA:HB1	1:138:A:LYS:HB3	6	0.29
(2,197)	1:187:A:VAL:HG12	1:177:A:TRP:HH2	3	0.29
(2,197)	1:187:A:VAL:HG12	1:177:A:TRP:HH2	4	0.29
(2,179)	1:146:A:ILE:HB	1:139:A:VAL:HG13	1	0.29
(2,126)	1:132:A:ILE:HG13	1:139:A:VAL:HA	6	0.29
(2,104)	1:167:A:MET:HB2	1:167:A:MET:HG2	7	0.29
(2,74)	1:153:A:TYR:HB2	1:148:A:LEU:HD12	8	0.29
(2,44)	1:196:A:ARG:HD2	1:195:A:LEU:HB3	10	0.29
(1,1072)	1:195:A:LEU:HD11	1:196:A:ARG:H	9	0.29
(1,1048)	1:207:A:MET:H	1:206:A:LYS:HG2	5	0.29
(1,1048)	1:207:A:MET:H	1:206:A:LYS:HG2	6	0.29
(1,1048)	1:207:A:MET:H	1:206:A:LYS:HG3	10	0.29
(1,1045)	1:192:A:ILE:HG22	1:192:A:ILE:H	3	0.29
(1,1045)	1:192:A:ILE:HG22	1:192:A:ILE:H	6	0.29
(1,781)	1:130:A:ILE:HG12	1:130:A:ILE:HD13	8	0.29
(1,772)	1:132:A:ILE:HD12	1:157:A:TYR:H	9	0.29
(1,766)	1:172:A:ILE:HD13	1:216:A:TYR:HD2	9	0.29
(1,733)	1:130:A:ILE:HG22	1:131:A:THR:H	7	0.29
(1,724)	1:132:A:ILE:HG21	1:139:A:VAL:HA	1	0.29
(1,716)	1:160:A:ALA:HB2	1:156:A:LEU:HD13	8	0.29
(1,705)	1:217:A:VAL:HG12	1:217:A:VAL:HA	8	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,661)	1:190:A:VAL:HG11	1:191:A:TYR:H	9	0.29
(1,652)	1:141:A:VAL:HG11	1:146:A:ILE:HG12	10	0.29
(1,651)	1:127:A:VAL:HG13	1:163:A:LYS:HG2	2	0.29
(1,651)	1:127:A:VAL:HG13	1:163:A:LYS:HG3	10	0.29
(1,596)	1:167:A:MET:HG2	1:159:A:LEU:HD23	1	0.29
(1,583)	1:139:A:VAL:HG21	1:133:A:ASP:H	3	0.29
(1,583)	1:139:A:VAL:HG23	1:133:A:ASP:H	6	0.29
(1,531)	1:192:A:ILE:HG13	1:192:A:ILE:H	9	0.29
(1,449)	1:161:A:GLU:HB2	1:125:A:ILE:HG23	1	0.29
(1,443)	1:177:A:TRP:HB3	1:177:A:TRP:H	3	0.29
(1,443)	1:177:A:TRP:HB3	1:177:A:TRP:H	4	0.29
(1,443)	1:177:A:TRP:HB3	1:177:A:TRP:H	6	0.29
(1,443)	1:177:A:TRP:HB3	1:177:A:TRP:H	7	0.29
(1,443)	1:177:A:TRP:HB3	1:177:A:TRP:H	8	0.29
(1,252)	1:138:A:LYS:HE2	1:138:A:LYS:HG2	3	0.29
(1,225)	1:204:A:ARG:HD3	1:204:A:ARG:HB2	2	0.29
(1,220)	1:216:A:TYR:HB3	1:192:A:ILE:HD13	7	0.29
(1,158)	1:184:A:GLU:HA	1:184:A:GLU:HG3	3	0.29
(1,70)	1:192:A:ILE:HA	1:192:A:ILE:HG13	1	0.29
(1,70)	1:192:A:ILE:HA	1:192:A:ILE:HG13	3	0.29
(1,70)	1:192:A:ILE:HA	1:192:A:ILE:HG13	10	0.29
(2,316)	1:176:A:VAL:HG21	1:154:A:ASP:H	7	0.28
(2,306)	1:190:A:VAL:HG23	1:191:A:TYR:H	9	0.28
(2,280)	1:148:A:LEU:H	1:148:A:LEU:HD23	5	0.28
(2,279)	1:140:A:THR:H	1:140:A:THR:HG21	6	0.28
(2,232)	1:208:A:ILE:HD12	1:192:A:ILE:HD11	3	0.28
(2,213)	1:167:A:MET:HE2	1:167:A:MET:H	2	0.28
(2,200)	1:187:A:VAL:HG13	1:187:A:VAL:HG22	2	0.28
(2,187)	1:127:A:VAL:HG23	1:126:A:ASP:HA	9	0.28
(2,183)	1:140:A:THR:HG22	1:138:A:LYS:HD2	8	0.28
(2,164)	1:176:A:VAL:HG22	1:155:A:LEU:H	9	0.28
(2,162)	1:148:A:LEU:HD23	1:149:A:THR:H	3	0.28
(2,142)	1:173:A:LEU:HD21	1:184:A:GLU:HA	4	0.28
(2,104)	1:167:A:MET:HB2	1:167:A:MET:HG2	5	0.28
(2,97)	1:127:A:VAL:HB	1:163:A:LYS:HB3	6	0.28
(2,82)	1:138:A:LYS:HB3	1:133:A:ASP:HB3	10	0.28
(2,56)	1:133:A:ASP:HB2	1:138:A:LYS:HB3	10	0.28
(2,44)	1:196:A:ARG:HD3	1:195:A:LEU:HB3	3	0.28
(1,844)	1:200:A:LYS:HD2	1:200:A:LYS:H	3	0.28
(1,781)	1:130:A:ILE:HG12	1:130:A:ILE:HD13	7	0.28
(1,757)	1:192:A:ILE:HG23	1:196:A:ARG:H	5	0.28
(1,736)	1:207:A:MET:HE3	1:130:A:ILE:H	2	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,724)	1:132:A:ILE:HG22	1:139:A:VAL:HA	6	0.28
(1,705)	1:217:A:VAL:HG12	1:217:A:VAL:HA	3	0.28
(1,705)	1:217:A:VAL:HG11	1:217:A:VAL:HA	7	0.28
(1,682)	1:136:A:ALA:HB1	1:135:A:ASN:HB3	9	0.28
(1,649)	1:190:A:VAL:HB	1:187:A:VAL:HG23	7	0.28
(1,649)	1:190:A:VAL:HB	1:187:A:VAL:HG21	9	0.28
(1,618)	1:190:A:VAL:HG21	1:190:A:VAL:HG13	2	0.28
(1,583)	1:139:A:VAL:HG21	1:133:A:ASP:H	5	0.28
(1,583)	1:139:A:VAL:HG23	1:133:A:ASP:H	9	0.28
(1,467)	1:171:A:GLN:HB3	1:171:A:GLN:H	9	0.28
(1,355)	1:184:A:GLU:HG2	1:184:A:GLU:H	6	0.28
(1,291)	1:191:A:TYR:HB3	1:191:A:TYR:H	10	0.28
(1,147)	1:219:A:ARG:HA	1:219:A:ARG:HB2	1	0.28
(1,147)	1:219:A:ARG:HA	1:219:A:ARG:HB2	2	0.28
(1,147)	1:219:A:ARG:HA	1:219:A:ARG:HB2	4	0.28
(1,147)	1:219:A:ARG:HA	1:219:A:ARG:HB2	8	0.28
(1,147)	1:219:A:ARG:HA	1:219:A:ARG:HB2	9	0.28
(1,70)	1:192:A:ILE:HA	1:192:A:ILE:HG13	6	0.28
(2,233)	1:207:A:MET:HE3	1:160:A:ALA:HA	2	0.27
(2,226)	1:159:A:LEU:HB3	1:218:A:ILE:HD13	3	0.27
(2,113)	1:205:A:ASP:HB3	1:200:A:LYS:HB2	8	0.27
(2,87)	1:209:A:GLU:HG3	1:217:A:VAL:HG12	2	0.27
(2,71)	1:202:A:TYR:HB3	1:141:A:VAL:HB	2	0.27
(2,62)	1:125:A:ILE:HB	1:126:A:ASP:H	1	0.27
(2,40)	1:204:A:ARG:HD2	1:204:A:ARG:HB2	6	0.27
(2,27)	1:207:A:MET:HA	1:218:A:ILE:HG21	8	0.27
(1,1080)	1:169:A:ARG:H	1:169:A:ARG:HD3	3	0.27
(1,1037)	1:165:A:HIS:H	1:217:A:VAL:HG23	7	0.27
(1,829)	1:147:A:GLU:HB2	1:147:A:GLU:HA	3	0.27
(1,829)	1:147:A:GLU:HB2	1:147:A:GLU:HA	4	0.27
(1,829)	1:147:A:GLU:HB2	1:147:A:GLU:HA	5	0.27
(1,829)	1:147:A:GLU:HB2	1:147:A:GLU:HA	6	0.27
(1,829)	1:147:A:GLU:HB2	1:147:A:GLU:HA	7	0.27
(1,829)	1:147:A:GLU:HB2	1:147:A:GLU:HA	10	0.27
(1,810)	1:124:A:ILE:HG13	1:124:A:ILE:HA	8	0.27
(1,781)	1:130:A:ILE:HG12	1:130:A:ILE:HD12	1	0.27
(1,781)	1:130:A:ILE:HG12	1:130:A:ILE:HD11	6	0.27
(1,781)	1:130:A:ILE:HG12	1:130:A:ILE:HD12	9	0.27
(1,781)	1:130:A:ILE:HG12	1:130:A:ILE:HD11	10	0.27
(1,776)	1:204:A:ARG:HB2	1:130:A:ILE:HD13	5	0.27
(1,762)	1:192:A:ILE:HG21	1:208:A:ILE:HD11	7	0.27
(1,736)	1:207:A:MET:HE2	1:130:A:ILE:H	9	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,724)	1:132:A:ILE:HG21	1:139:A:VAL:HA	4	0.27
(1,724)	1:132:A:ILE:HG23	1:139:A:VAL:HA	9	0.27
(1,716)	1:160:A:ALA:HB3	1:156:A:LEU:HD11	5	0.27
(1,705)	1:217:A:VAL:HG12	1:217:A:VAL:HA	1	0.27
(1,705)	1:217:A:VAL:HG12	1:217:A:VAL:HA	2	0.27
(1,705)	1:217:A:VAL:HG11	1:217:A:VAL:HA	4	0.27
(1,705)	1:217:A:VAL:HG12	1:217:A:VAL:HA	6	0.27
(1,682)	1:136:A:ALA:HB3	1:135:A:ASN:HB3	4	0.27
(1,661)	1:190:A:VAL:HG12	1:191:A:TYR:H	2	0.27
(1,658)	1:163:A:LYS:HE3	1:127:A:VAL:HG12	8	0.27
(1,652)	1:141:A:VAL:HG11	1:146:A:ILE:HG12	6	0.27
(1,624)	1:149:A:THR:HG21	1:152:A:GLU:HB3	4	0.27
(1,618)	1:190:A:VAL:HG22	1:190:A:VAL:HG11	6	0.27
(1,618)	1:190:A:VAL:HG22	1:190:A:VAL:HG11	7	0.27
(1,614)	1:216:A:TYR:HB2	1:159:A:LEU:HD22	8	0.27
(1,605)	1:210:A:THR:HG22	1:211:A:VAL:H	4	0.27
(1,605)	1:210:A:THR:HG22	1:211:A:VAL:H	10	0.27
(1,583)	1:139:A:VAL:HG23	1:133:A:ASP:H	1	0.27
(1,583)	1:139:A:VAL:HG21	1:133:A:ASP:H	4	0.27
(1,583)	1:139:A:VAL:HG22	1:133:A:ASP:H	10	0.27
(1,563)	1:188:A:VAL:HG23	1:189:A:ASP:H	7	0.27
(1,555)	1:175:A:HIS:HB2	1:176:A:VAL:HG23	5	0.27
(1,522)	1:191:A:TYR:HB2	1:155:A:LEU:HD23	7	0.27
(1,479)	1:193:A:ARG:HG3	1:193:A:ARG:HA	1	0.27
(1,467)	1:171:A:GLN:HB3	1:171:A:GLN:H	1	0.27
(1,467)	1:171:A:GLN:HB3	1:171:A:GLN:H	2	0.27
(1,467)	1:171:A:GLN:HB3	1:171:A:GLN:H	3	0.27
(1,467)	1:171:A:GLN:HB3	1:171:A:GLN:H	4	0.27
(1,467)	1:171:A:GLN:HB3	1:171:A:GLN:H	10	0.27
(1,449)	1:161:A:GLU:HB2	1:125:A:ILE:HG22	10	0.27
(1,443)	1:177:A:TRP:HB3	1:177:A:TRP:H	2	0.27
(1,427)	1:219:A:ARG:HB3	1:219:A:ARG:H	3	0.27
(1,291)	1:191:A:TYR:HB3	1:191:A:TYR:H	1	0.27
(1,291)	1:191:A:TYR:HB3	1:191:A:TYR:H	3	0.27
(1,291)	1:191:A:TYR:HB3	1:191:A:TYR:H	8	0.27
(1,291)	1:191:A:TYR:HB3	1:191:A:TYR:H	9	0.27
(1,147)	1:219:A:ARG:HA	1:219:A:ARG:HB2	3	0.27
(1,147)	1:219:A:ARG:HA	1:219:A:ARG:HB2	5	0.27
(1,147)	1:219:A:ARG:HA	1:219:A:ARG:HB2	6	0.27
(1,147)	1:219:A:ARG:HA	1:219:A:ARG:HB2	7	0.27
(1,54)	1:166:A:VAL:HA	1:217:A:VAL:HB	5	0.27
(2,318)	1:175:A:HIS:H	1:176:A:VAL:HG23	5	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,317)	1:172:A:ILE:H	1:168:A:GLN:HB2	2	0.26
(2,317)	1:172:A:ILE:H	1:168:A:GLN:HB2	8	0.26
(2,309)	1:140:A:THR:H	1:132:A:ILE:HG13	3	0.26
(2,306)	1:190:A:VAL:HG22	1:191:A:TYR:H	2	0.26
(2,306)	1:190:A:VAL:HG21	1:191:A:TYR:H	5	0.26
(2,303)	1:219:A:ARG:HG3	1:219:A:ARG:H	10	0.26
(2,281)	1:148:A:LEU:HD13	1:153:A:TYR:H	7	0.26
(2,279)	1:140:A:THR:H	1:140:A:THR:HG23	3	0.26
(2,187)	1:127:A:VAL:HG21	1:126:A:ASP:HA	3	0.26
(2,184)	1:183:A:VAL:HG12	1:177:A:TRP:HD1	2	0.26
(2,97)	1:127:A:VAL:HB	1:163:A:LYS:HB3	1	0.26
(2,92)	1:171:A:GLN:HG3	1:167:A:MET:HA	6	0.26
(2,71)	1:202:A:TYR:HB3	1:141:A:VAL:HB	3	0.26
(2,48)	1:173:A:LEU:HB2	1:174:A:ASN:H	7	0.26
(2,42)	1:204:A:ARG:HD3	1:130:A:ILE:HD13	4	0.26
(1,1084)	1:124:A:ILE:H	1:124:A:ILE:HG13	9	0.26
(1,1078)	1:165:A:HIS:H	1:163:A:LYS:HG3	1	0.26
(1,1024)	1:146:A:ILE:HG12	1:146:A:ILE:H	4	0.26
(1,1024)	1:146:A:ILE:HG12	1:146:A:ILE:H	6	0.26
(1,975)	1:158:A:LEU:H	1:157:A:TYR:HB2	6	0.26
(1,832)	1:153:A:TYR:HB3	1:148:A:LEU:HD13	6	0.26
(1,829)	1:147:A:GLU:HB2	1:147:A:GLU:HA	1	0.26
(1,829)	1:147:A:GLU:HB2	1:147:A:GLU:HA	2	0.26
(1,818)	1:149:A:THR:HG22	1:149:A:THR:HB	1	0.26
(1,818)	1:149:A:THR:HG23	1:149:A:THR:HB	4	0.26
(1,818)	1:149:A:THR:HG22	1:149:A:THR:HB	6	0.26
(1,818)	1:149:A:THR:HG23	1:149:A:THR:HB	10	0.26
(1,810)	1:124:A:ILE:HG13	1:124:A:ILE:HA	2	0.26
(1,810)	1:124:A:ILE:HG13	1:124:A:ILE:HA	3	0.26
(1,810)	1:124:A:ILE:HG13	1:124:A:ILE:HA	4	0.26
(1,810)	1:124:A:ILE:HG13	1:124:A:ILE:HA	10	0.26
(1,781)	1:130:A:ILE:HG12	1:130:A:ILE:HD11	3	0.26
(1,781)	1:130:A:ILE:HG12	1:130:A:ILE:HD11	5	0.26
(1,766)	1:172:A:ILE:HD13	1:216:A:TYR:HD2	5	0.26
(1,757)	1:192:A:ILE:HG23	1:196:A:ARG:H	9	0.26
(1,733)	1:130:A:ILE:HG21	1:131:A:THR:H	9	0.26
(1,661)	1:190:A:VAL:HG12	1:191:A:TYR:H	10	0.26
(1,652)	1:141:A:VAL:HG11	1:146:A:ILE:HG12	1	0.26
(1,634)	1:183:A:VAL:HG11	1:187:A:VAL:H	2	0.26
(1,624)	1:149:A:THR:HG21	1:152:A:GLU:HB3	1	0.26
(1,618)	1:190:A:VAL:HG22	1:190:A:VAL:HG12	3	0.26
(1,618)	1:190:A:VAL:HG22	1:190:A:VAL:HG13	8	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,618)	1:190:A:VAL:HG21	1:190:A:VAL:HG13	9	0.26
(1,618)	1:190:A:VAL:HG23	1:190:A:VAL:HG13	10	0.26
(1,607)	1:159:A:LEU:HD23	1:217:A:VAL:HA	7	0.26
(1,574)	1:151:A:THR:HG23	1:191:A:TYR:HE2	1	0.26
(1,522)	1:191:A:TYR:HB2	1:155:A:LEU:HD21	10	0.26
(1,467)	1:171:A:GLN:HB3	1:171:A:GLN:H	6	0.26
(1,461)	1:212:A:ARG:HB3	1:210:A:THR:HG23	5	0.26
(1,449)	1:161:A:GLU:HB2	1:125:A:ILE:HG21	9	0.26
(1,448)	1:212:A:ARG:HD3	1:212:A:ARG:HB2	10	0.26
(1,427)	1:219:A:ARG:HB3	1:219:A:ARG:H	1	0.26
(1,355)	1:184:A:GLU:HG2	1:184:A:GLU:H	4	0.26
(1,291)	1:191:A:TYR:HB3	1:191:A:TYR:H	2	0.26
(1,291)	1:191:A:TYR:HB3	1:191:A:TYR:H	5	0.26
(1,291)	1:191:A:TYR:HB3	1:191:A:TYR:H	7	0.26
(1,225)	1:204:A:ARG:HD3	1:204:A:ARG:HB2	1	0.26
(1,219)	1:216:A:TYR:HB3	1:159:A:LEU:HD22	5	0.26
(1,158)	1:184:A:GLU:HA	1:184:A:GLU:HG3	5	0.26
(1,158)	1:184:A:GLU:HA	1:184:A:GLU:HG3	7	0.26
(2,318)	1:175:A:HIS:H	1:176:A:VAL:HG22	3	0.25
(2,279)	1:140:A:THR:H	1:140:A:THR:HG23	2	0.25
(2,211)	1:125:A:ILE:HB	1:125:A:ILE:HG21	2	0.25
(2,187)	1:127:A:VAL:HG21	1:126:A:ASP:HA	10	0.25
(2,170)	1:199:A:LEU:HD21	1:199:A:LEU:H	1	0.25
(2,162)	1:148:A:LEU:HD22	1:149:A:THR:H	2	0.25
(2,162)	1:148:A:LEU:HD21	1:149:A:THR:H	4	0.25
(2,126)	1:132:A:ILE:HG13	1:139:A:VAL:HA	1	0.25
(2,92)	1:171:A:GLN:HG3	1:167:A:MET:HA	1	0.25
(2,74)	1:128:A:ASN:HB2	1:218:A:ILE:HG23	10	0.25
(2,30)	1:205:A:ASP:HA	1:196:A:ARG:HB3	9	0.25
(2,26)	1:219:A:ARG:HA	1:219:A:ARG:HG2	3	0.25
(1,1080)	1:169:A:ARG:H	1:169:A:ARG:HD3	9	0.25
(1,1056)	1:179:A:TYR:HB2	1:179:A:TYR:H	2	0.25
(1,1037)	1:165:A:HIS:H	1:217:A:VAL:HG23	4	0.25
(1,829)	1:147:A:GLU:HB2	1:147:A:GLU:HA	8	0.25
(1,818)	1:149:A:THR:HG22	1:149:A:THR:HB	2	0.25
(1,818)	1:149:A:THR:HG22	1:149:A:THR:HB	3	0.25
(1,818)	1:149:A:THR:HG22	1:149:A:THR:HB	7	0.25
(1,805)	1:192:A:ILE:HD11	1:192:A:ILE:H	10	0.25
(1,745)	1:160:A:ALA:HA	1:218:A:ILE:HG22	9	0.25
(1,735)	1:125:A:ILE:HG21	1:126:A:ASP:H	4	0.25
(1,735)	1:125:A:ILE:HG23	1:126:A:ASP:H	6	0.25
(1,733)	1:130:A:ILE:HG21	1:131:A:THR:H	3	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,724)	1:132:A:ILE:HG21	1:139:A:VAL:HA	10	0.25
(1,662)	1:176:A:VAL:HG13	1:177:A:TRP:HE3	2	0.25
(1,661)	1:190:A:VAL:HG11	1:191:A:TYR:H	4	0.25
(1,661)	1:190:A:VAL:HG12	1:191:A:TYR:H	8	0.25
(1,659)	1:202:A:TYR:HB2	1:141:A:VAL:HG12	4	0.25
(1,651)	1:127:A:VAL:HG12	1:163:A:LYS:HG2	1	0.25
(1,651)	1:127:A:VAL:HG13	1:163:A:LYS:HG2	8	0.25
(1,642)	1:183:A:VAL:HG12	1:187:A:VAL:HG13	2	0.25
(1,641)	1:166:A:VAL:HB	1:166:A:VAL:HG21	4	0.25
(1,641)	1:166:A:VAL:HB	1:166:A:VAL:HG22	5	0.25
(1,641)	1:166:A:VAL:HB	1:166:A:VAL:HG23	9	0.25
(1,618)	1:190:A:VAL:HG23	1:190:A:VAL:HG12	4	0.25
(1,605)	1:210:A:THR:HG23	1:211:A:VAL:H	9	0.25
(1,587)	1:139:A:VAL:HG21	1:138:A:LYS:HA	7	0.25
(1,585)	1:139:A:VAL:HG23	1:153:A:TYR:HE1	8	0.25
(1,574)	1:151:A:THR:HG23	1:191:A:TYR:HE2	3	0.25
(1,527)	1:159:A:LEU:HD13	1:216:A:TYR:HB2	10	0.25
(1,467)	1:171:A:GLN:HB3	1:171:A:GLN:H	7	0.25
(1,466)	1:193:A:ARG:HB3	1:193:A:ARG:H	2	0.25
(1,466)	1:193:A:ARG:HB3	1:193:A:ARG:H	7	0.25
(1,463)	1:172:A:ILE:HG12	1:172:A:ILE:H	1	0.25
(1,463)	1:172:A:ILE:HG12	1:172:A:ILE:H	9	0.25
(1,396)	1:167:A:MET:HG2	1:167:A:MET:HB3	3	0.25
(1,360)	1:147:A:GLU:HG3	1:147:A:GLU:HA	6	0.25
(1,355)	1:184:A:GLU:HG2	1:184:A:GLU:H	5	0.25
(1,355)	1:184:A:GLU:HG2	1:184:A:GLU:H	9	0.25
(1,340)	1:142:A:ASN:HB3	1:141:A:VAL:HG13	1	0.25
(1,340)	1:142:A:ASN:HB3	1:141:A:VAL:HG11	7	0.25
(1,225)	1:204:A:ARG:HD3	1:204:A:ARG:HB2	5	0.25
(1,158)	1:184:A:GLU:HA	1:184:A:GLU:HG3	1	0.25
(1,158)	1:184:A:GLU:HA	1:184:A:GLU:HG3	9	0.25
(2,317)	1:172:A:ILE:H	1:171:A:GLN:HG2	1	0.24
(2,316)	1:176:A:VAL:HG21	1:154:A:ASP:H	2	0.24
(2,314)	1:204:A:ARG:H	1:199:A:LEU:HD21	3	0.24
(2,306)	1:190:A:VAL:HG23	1:191:A:TYR:H	1	0.24
(2,297)	1:205:A:ASP:H	1:199:A:LEU:HD11	1	0.24
(2,232)	1:192:A:ILE:HD12	1:208:A:ILE:HG21	4	0.24
(2,185)	1:187:A:VAL:HB	1:183:A:VAL:HG11	6	0.24
(2,142)	1:173:A:LEU:HD21	1:184:A:GLU:HA	8	0.24
(2,102)	1:167:A:MET:HG3	1:167:A:MET:HA	8	0.24
(2,71)	1:202:A:TYR:HB3	1:141:A:VAL:HB	1	0.24
(2,71)	1:202:A:TYR:HB3	1:141:A:VAL:HB	6	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,48)	1:173:A:LEU:HB2	1:174:A:ASN:H	5	0.24
(2,43)	1:195:A:LEU:HB3	1:192:A:ILE:HA	6	0.24
(2,43)	1:195:A:LEU:HB3	1:192:A:ILE:HA	10	0.24
(2,35)	1:216:A:TYR:HB2	1:159:A:LEU:HD22	8	0.24
(2,30)	1:205:A:ASP:HA	1:196:A:ARG:HB3	7	0.24
(1,1048)	1:207:A:MET:H	1:206:A:LYS:HG3	7	0.24
(1,818)	1:149:A:THR:HG22	1:149:A:THR:HB	5	0.24
(1,818)	1:149:A:THR:HG21	1:149:A:THR:HB	8	0.24
(1,818)	1:149:A:THR:HG22	1:149:A:THR:HB	9	0.24
(1,810)	1:124:A:ILE:HG13	1:124:A:ILE:HA	5	0.24
(1,810)	1:124:A:ILE:HG13	1:124:A:ILE:HA	9	0.24
(1,796)	1:146:A:ILE:HA	1:146:A:ILE:HD13	8	0.24
(1,781)	1:130:A:ILE:HG12	1:130:A:ILE:HD13	2	0.24
(1,762)	1:192:A:ILE:HG23	1:208:A:ILE:HD11	8	0.24
(1,724)	1:132:A:ILE:HG22	1:139:A:VAL:HA	5	0.24
(1,724)	1:132:A:ILE:HG22	1:139:A:VAL:HA	7	0.24
(1,686)	1:144:A:ALA:HB3	1:145:A:GLU:H	7	0.24
(1,662)	1:176:A:VAL:HG13	1:177:A:TRP:HE3	7	0.24
(1,661)	1:190:A:VAL:HG11	1:191:A:TYR:H	1	0.24
(1,661)	1:190:A:VAL:HG13	1:191:A:TYR:H	6	0.24
(1,661)	1:190:A:VAL:HG13	1:191:A:TYR:H	7	0.24
(1,643)	1:166:A:VAL:HG13	1:167:A:MET:H	2	0.24
(1,641)	1:166:A:VAL:HB	1:166:A:VAL:HG21	1	0.24
(1,641)	1:166:A:VAL:HB	1:166:A:VAL:HG21	2	0.24
(1,641)	1:166:A:VAL:HB	1:166:A:VAL:HG21	3	0.24
(1,641)	1:166:A:VAL:HB	1:166:A:VAL:HG22	6	0.24
(1,641)	1:166:A:VAL:HB	1:166:A:VAL:HG22	10	0.24
(1,624)	1:149:A:THR:HG21	1:152:A:GLU:HB3	6	0.24
(1,621)	1:131:A:THR:HG22	1:126:A:ASP:HA	4	0.24
(1,618)	1:190:A:VAL:HG22	1:190:A:VAL:HG12	1	0.24
(1,618)	1:190:A:VAL:HG23	1:190:A:VAL:HG11	5	0.24
(1,607)	1:159:A:LEU:HD22	1:217:A:VAL:HA	4	0.24
(1,607)	1:159:A:LEU:HD23	1:217:A:VAL:HA	10	0.24
(1,522)	1:191:A:TYR:HB2	1:155:A:LEU:HD21	3	0.24
(1,514)	1:156:A:LEU:HD21	1:156:A:LEU:HG	1	0.24
(1,514)	1:156:A:LEU:HD22	1:156:A:LEU:HG	2	0.24
(1,514)	1:156:A:LEU:HD22	1:156:A:LEU:HG	6	0.24
(1,514)	1:156:A:LEU:HD22	1:156:A:LEU:HG	8	0.24
(1,514)	1:156:A:LEU:HD22	1:156:A:LEU:HG	9	0.24
(1,492)	1:130:A:ILE:HG13	1:130:A:ILE:H	9	0.24
(1,466)	1:193:A:ARG:HB3	1:193:A:ARG:H	1	0.24
(1,466)	1:193:A:ARG:HB3	1:193:A:ARG:H	3	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,463)	1:172:A:ILE:HG12	1:172:A:ILE:H	10	0.24
(1,427)	1:219:A:ARG:HB3	1:219:A:ARG:H	4	0.24
(1,396)	1:167:A:MET:HG2	1:167:A:MET:HB3	1	0.24
(1,396)	1:167:A:MET:HG2	1:167:A:MET:HB3	4	0.24
(1,396)	1:167:A:MET:HG2	1:167:A:MET:HB3	6	0.24
(1,396)	1:167:A:MET:HG2	1:167:A:MET:HB3	9	0.24
(1,396)	1:167:A:MET:HG2	1:167:A:MET:HB3	10	0.24
(1,360)	1:147:A:GLU:HG3	1:147:A:GLU:HA	3	0.24
(1,340)	1:142:A:ASN:HB3	1:141:A:VAL:HG11	8	0.24
(1,291)	1:191:A:TYR:HB3	1:191:A:TYR:H	6	0.24
(1,158)	1:184:A:GLU:HA	1:184:A:GLU:HG3	2	0.24
(1,158)	1:184:A:GLU:HA	1:184:A:GLU:HG3	8	0.24
(1,147)	1:219:A:ARG:HA	1:219:A:ARG:HB2	10	0.24
(1,48)	1:181:A:SER:HB2	1:181:A:SER:HA	2	0.24
(1,48)	1:181:A:SER:HB2	1:181:A:SER:HA	3	0.24
(1,48)	1:181:A:SER:HB2	1:181:A:SER:HA	4	0.24
(1,48)	1:181:A:SER:HB2	1:181:A:SER:HA	5	0.24
(1,48)	1:181:A:SER:HB2	1:181:A:SER:HA	6	0.24
(1,48)	1:181:A:SER:HB2	1:181:A:SER:HA	8	0.24
(1,48)	1:181:A:SER:HB2	1:181:A:SER:HA	10	0.24
(1,36)	1:187:A:VAL:HA	1:190:A:VAL:HG22	9	0.24
(2,317)	1:172:A:ILE:H	1:168:A:GLN:HB2	6	0.23
(2,309)	1:140:A:THR:H	1:132:A:ILE:HG13	1	0.23
(2,294)	1:183:A:VAL:HG12	1:187:A:VAL:H	4	0.23
(2,290)	1:124:A:ILE:HD12	1:124:A:ILE:H	10	0.23
(2,289)	1:214:A:VAL:HG13	1:215:A:GLY:H	3	0.23
(2,228)	1:218:A:ILE:HD12	1:128:A:ASN:HB2	7	0.23
(2,212)	1:207:A:MET:HE1	1:218:A:ILE:HG22	10	0.23
(2,185)	1:166:A:VAL:HG13	1:217:A:VAL:HB	7	0.23
(2,183)	1:140:A:THR:HG23	1:138:A:LYS:HD2	10	0.23
(2,102)	1:167:A:MET:HG3	1:167:A:MET:HA	4	0.23
(2,74)	1:153:A:TYR:HB2	1:148:A:LEU:HD12	1	0.23
(2,71)	1:202:A:TYR:HB3	1:141:A:VAL:HB	5	0.23
(2,30)	1:205:A:ASP:HA	1:196:A:ARG:HB3	10	0.23
(1,810)	1:124:A:ILE:HG13	1:124:A:ILE:HA	7	0.23
(1,789)	1:125:A:ILE:HD13	1:161:A:GLU:H	9	0.23
(1,781)	1:130:A:ILE:HG12	1:130:A:ILE:HD13	4	0.23
(1,762)	1:192:A:ILE:HG22	1:208:A:ILE:HD12	5	0.23
(1,736)	1:207:A:MET:HE2	1:130:A:ILE:H	3	0.23
(1,735)	1:125:A:ILE:HG23	1:126:A:ASP:H	5	0.23
(1,730)	1:216:A:TYR:HB2	1:208:A:ILE:HG21	8	0.23
(1,686)	1:144:A:ALA:HB3	1:145:A:GLU:H	5	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,662)	1:176:A:VAL:HG11	1:177:A:TRP:HE3	1	0.23
(1,662)	1:176:A:VAL:HG11	1:177:A:TRP:HE3	3	0.23
(1,641)	1:166:A:VAL:HB	1:166:A:VAL:HG22	7	0.23
(1,641)	1:166:A:VAL:HB	1:166:A:VAL:HG22	8	0.23
(1,585)	1:139:A:VAL:HG21	1:153:A:TYR:HE1	3	0.23
(1,514)	1:156:A:LEU:HD21	1:156:A:LEU:HG	3	0.23
(1,514)	1:156:A:LEU:HD22	1:156:A:LEU:HG	7	0.23
(1,514)	1:156:A:LEU:HD22	1:156:A:LEU:HG	10	0.23
(1,463)	1:172:A:ILE:HG12	1:172:A:ILE:H	7	0.23
(1,449)	1:161:A:GLU:HB2	1:125:A:ILE:HG22	6	0.23
(1,177)	1:126:A:ASP:HA	1:125:A:ILE:HG23	7	0.23
(1,80)	1:169:A:ARG:HA	1:169:A:ARG:HB2	7	0.23
(1,48)	1:181:A:SER:HB2	1:181:A:SER:HA	7	0.23
(2,318)	1:175:A:HIS:H	1:176:A:VAL:HG23	7	0.22
(2,291)	1:199:A:LEU:HD23	1:199:A:LEU:H	3	0.22
(2,279)	1:140:A:THR:H	1:140:A:THR:HG21	1	0.22
(2,233)	1:207:A:MET:HE1	1:160:A:ALA:HA	8	0.22
(2,232)	1:192:A:ILE:HD13	1:208:A:ILE:HG22	5	0.22
(2,211)	1:125:A:ILE:HB	1:125:A:ILE:HG21	4	0.22
(2,211)	1:125:A:ILE:HB	1:125:A:ILE:HG21	6	0.22
(2,211)	1:125:A:ILE:HB	1:125:A:ILE:HG23	9	0.22
(2,211)	1:125:A:ILE:HB	1:125:A:ILE:HG21	10	0.22
(2,197)	1:187:A:VAL:HG13	1:177:A:TRP:HH2	1	0.22
(2,197)	1:187:A:VAL:HG11	1:177:A:TRP:HH2	6	0.22
(2,193)	1:176:A:VAL:HG11	1:177:A:TRP:HZ3	9	0.22
(2,193)	1:176:A:VAL:HG12	1:177:A:TRP:HZ3	10	0.22
(2,162)	1:148:A:LEU:HD21	1:149:A:THR:H	8	0.22
(2,106)	1:190:A:VAL:HB	1:187:A:VAL:HG22	6	0.22
(2,102)	1:167:A:MET:HG3	1:217:A:VAL:HA	3	0.22
(2,55)	1:200:A:LYS:HE2	1:196:A:ARG:HB2	5	0.22
(2,39)	1:219:A:ARG:HD3	1:217:A:VAL:HG12	1	0.22
(2,30)	1:205:A:ASP:HA	1:199:A:LEU:HG	2	0.22
(1,1080)	1:169:A:ARG:H	1:169:A:ARG:HD3	6	0.22
(1,1078)	1:165:A:HIS:H	1:163:A:LYS:HG2	6	0.22
(1,1024)	1:146:A:ILE:HG12	1:146:A:ILE:H	1	0.22
(1,844)	1:200:A:LYS:HD2	1:200:A:LYS:H	8	0.22
(1,812)	1:192:A:ILE:HD13	1:208:A:ILE:HG23	9	0.22
(1,805)	1:192:A:ILE:HD13	1:192:A:ILE:H	8	0.22
(1,796)	1:146:A:ILE:HA	1:146:A:ILE:HD12	7	0.22
(1,772)	1:132:A:ILE:HD13	1:157:A:TYR:H	4	0.22
(1,745)	1:160:A:ALA:HA	1:218:A:ILE:HG22	5	0.22
(1,686)	1:144:A:ALA:HB1	1:145:A:GLU:H	8	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,634)	1:183:A:VAL:HG12	1:187:A:VAL:H	9	0.22
(1,607)	1:159:A:LEU:HD23	1:217:A:VAL:HA	3	0.22
(1,514)	1:156:A:LEU:HD21	1:156:A:LEU:HG	4	0.22
(1,514)	1:156:A:LEU:HD23	1:156:A:LEU:HG	5	0.22
(1,419)	1:187:A:VAL:HB	1:188:A:VAL:H	3	0.22
(1,396)	1:167:A:MET:HG2	1:167:A:MET:HB3	2	0.22
(1,396)	1:167:A:MET:HG2	1:167:A:MET:HB3	8	0.22
(1,266)	1:189:A:ASP:HB3	1:189:A:ASP:H	3	0.22
(1,266)	1:189:A:ASP:HB3	1:189:A:ASP:H	5	0.22
(1,266)	1:189:A:ASP:HB3	1:189:A:ASP:H	8	0.22
(1,225)	1:204:A:ARG:HD3	1:204:A:ARG:HB2	6	0.22
(1,220)	1:216:A:TYR:HB3	1:192:A:ILE:HD11	8	0.22
(2,318)	1:175:A:HIS:H	1:158:A:LEU:HD21	2	0.21
(2,317)	1:172:A:ILE:H	1:168:A:GLN:HB2	9	0.21
(2,306)	1:190:A:VAL:HG21	1:191:A:TYR:H	10	0.21
(2,281)	1:148:A:LEU:HD11	1:153:A:TYR:H	3	0.21
(2,279)	1:140:A:THR:H	1:140:A:THR:HG21	7	0.21
(2,279)	1:140:A:THR:H	1:140:A:THR:HG23	10	0.21
(2,217)	1:192:A:ILE:HG23	1:216:A:TYR:HE1	3	0.21
(2,212)	1:207:A:MET:HE3	1:218:A:ILE:HG21	1	0.21
(2,211)	1:125:A:ILE:HB	1:125:A:ILE:HG22	1	0.21
(2,211)	1:125:A:ILE:HB	1:125:A:ILE:HG23	7	0.21
(2,170)	1:159:A:LEU:HD21	1:159:A:LEU:H	6	0.21
(2,102)	1:167:A:MET:HG3	1:167:A:MET:HA	7	0.21
(2,87)	1:209:A:GLU:HG2	1:217:A:VAL:HG12	10	0.21
(2,82)	1:138:A:LYS:HB3	1:133:A:ASP:HB3	1	0.21
(2,48)	1:173:A:LEU:HB2	1:174:A:ASN:H	6	0.21
(2,48)	1:173:A:LEU:HB2	1:174:A:ASN:H	8	0.21
(2,47)	1:204:A:ARG:HD2	1:141:A:VAL:HG21	10	0.21
(2,43)	1:196:A:ARG:HA	1:195:A:LEU:HB3	7	0.21
(2,30)	1:205:A:ASP:HA	1:199:A:LEU:HG	5	0.21
(1,1084)	1:124:A:ILE:H	1:124:A:ILE:HG13	10	0.21
(1,1078)	1:165:A:HIS:H	1:163:A:LYS:HG2	10	0.21
(1,1039)	1:159:A:LEU:H	1:159:A:LEU:HD13	3	0.21
(1,1024)	1:146:A:ILE:HG12	1:146:A:ILE:H	3	0.21
(1,990)	1:145:A:GLU:HB3	1:146:A:ILE:H	7	0.21
(1,990)	1:145:A:GLU:HB3	1:146:A:ILE:H	8	0.21
(1,812)	1:192:A:ILE:HD12	1:208:A:ILE:HG23	2	0.21
(1,686)	1:144:A:ALA:HB3	1:145:A:GLU:H	2	0.21
(1,686)	1:144:A:ALA:HB1	1:145:A:GLU:H	3	0.21
(1,683)	1:136:A:ALA:HB3	1:133:A:ASP:HB2	3	0.21
(1,661)	1:190:A:VAL:HG11	1:191:A:TYR:H	3	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,661)	1:190:A:VAL:HG13	1:191:A:TYR:H	5	0.21
(1,637)	1:187:A:VAL:HG22	1:177:A:TRP:HZ2	10	0.21
(1,573)	1:151:A:THR:HG21	1:152:A:GLU:H	9	0.21
(1,550)	1:150:A:LYS:HG3	1:149:A:THR:HB	3	0.21
(1,521)	1:191:A:TYR:HB3	1:155:A:LEU:HD23	3	0.21
(1,519)	1:192:A:ILE:HA	1:155:A:LEU:HD21	8	0.21
(1,516)	1:155:A:LEU:HD23	1:192:A:ILE:H	6	0.21
(1,463)	1:172:A:ILE:HG12	1:172:A:ILE:H	2	0.21
(1,461)	1:212:A:ARG:HB2	1:210:A:THR:HG21	2	0.21
(1,427)	1:219:A:ARG:HB3	1:219:A:ARG:H	7	0.21
(1,419)	1:187:A:VAL:HB	1:188:A:VAL:H	8	0.21
(1,419)	1:187:A:VAL:HB	1:188:A:VAL:H	10	0.21
(1,266)	1:189:A:ASP:HB3	1:189:A:ASP:H	1	0.21
(1,266)	1:189:A:ASP:HB3	1:189:A:ASP:H	6	0.21
(1,219)	1:216:A:TYR:HB3	1:159:A:LEU:HD22	6	0.21
(1,177)	1:126:A:ASP:HA	1:125:A:ILE:HG23	9	0.21
(1,158)	1:184:A:GLU:HA	1:184:A:GLU:HG3	4	0.21
(1,158)	1:184:A:GLU:HA	1:184:A:GLU:HG3	10	0.21
(1,26)	1:190:A:VAL:HA	1:193:A:ARG:HB3	5	0.21
(2,314)	1:204:A:ARG:H	1:199:A:LEU:HD22	6	0.2
(2,280)	1:148:A:LEU:H	1:148:A:LEU:HD22	3	0.2
(2,280)	1:148:A:LEU:H	1:148:A:LEU:HD22	10	0.2
(2,223)	1:208:A:ILE:HD11	1:196:A:ARG:HA	1	0.2
(2,211)	1:125:A:ILE:HB	1:125:A:ILE:HG22	3	0.2
(2,211)	1:125:A:ILE:HB	1:125:A:ILE:HG21	8	0.2
(2,208)	1:130:A:ILE:HG23	1:131:A:THR:HA	10	0.2
(2,199)	1:136:A:ALA:HB2	1:138:A:LYS:HB3	8	0.2
(2,164)	1:176:A:VAL:HG21	1:155:A:LEU:H	3	0.2
(2,126)	1:132:A:ILE:HG13	1:139:A:VAL:HA	3	0.2
(2,97)	1:127:A:VAL:HB	1:163:A:LYS:HB3	3	0.2
(2,71)	1:202:A:TYR:HB3	1:141:A:VAL:HB	9	0.2
(1,1084)	1:124:A:ILE:H	1:124:A:ILE:HG13	6	0.2
(1,1080)	1:169:A:ARG:H	1:169:A:ARG:HD2	7	0.2
(1,1048)	1:207:A:MET:H	1:206:A:LYS:HG3	3	0.2
(1,1039)	1:159:A:LEU:H	1:159:A:LEU:HD12	6	0.2
(1,1024)	1:146:A:ILE:HG12	1:146:A:ILE:H	2	0.2
(1,1024)	1:146:A:ILE:HG12	1:146:A:ILE:H	10	0.2
(1,983)	1:207:A:MET:H	1:207:A:MET:HB2	9	0.2
(1,975)	1:158:A:LEU:H	1:157:A:TYR:HB2	10	0.2
(1,812)	1:192:A:ILE:HD12	1:208:A:ILE:HG23	10	0.2
(1,782)	1:208:A:ILE:HD12	1:192:A:ILE:HD13	9	0.2
(1,762)	1:192:A:ILE:HG21	1:208:A:ILE:HD11	10	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,726)	1:132:A:ILE:HG23	1:134:A:LYS:HA	8	0.2
(1,724)	1:132:A:ILE:HG22	1:139:A:VAL:HA	8	0.2
(1,683)	1:136:A:ALA:HB3	1:133:A:ASP:HB2	5	0.2
(1,682)	1:136:A:ALA:HB3	1:135:A:ASN:HB3	8	0.2
(1,632)	1:140:A:THR:HG21	1:141:A:VAL:H	9	0.2
(1,587)	1:139:A:VAL:HG22	1:138:A:LYS:HA	9	0.2
(1,587)	1:139:A:VAL:HG21	1:138:A:LYS:HA	10	0.2
(1,528)	1:159:A:LEU:HB3	1:159:A:LEU:HD12	7	0.2
(1,521)	1:191:A:TYR:HB3	1:155:A:LEU:HD22	8	0.2
(1,521)	1:191:A:TYR:HB3	1:155:A:LEU:HD23	10	0.2
(1,519)	1:192:A:ILE:HA	1:155:A:LEU:HD22	2	0.2
(1,419)	1:187:A:VAL:HB	1:188:A:VAL:H	4	0.2
(1,419)	1:187:A:VAL:HB	1:188:A:VAL:H	9	0.2
(1,360)	1:147:A:GLU:HG3	1:147:A:GLU:HA	4	0.2
(1,355)	1:184:A:GLU:HG2	1:184:A:GLU:H	2	0.2
(1,220)	1:216:A:TYR:HB3	1:192:A:ILE:HD12	2	0.2
(1,220)	1:216:A:TYR:HB3	1:192:A:ILE:HD12	4	0.2
(1,69)	1:153:A:TYR:HA	1:156:A:LEU:HB2	6	0.2
(1,28)	1:172:A:ILE:HA	1:175:A:HIS:HB3	3	0.2
(2,318)	1:175:A:HIS:H	1:158:A:LEU:HD23	9	0.19
(2,291)	1:199:A:LEU:HD21	1:199:A:LEU:H	1	0.19
(2,279)	1:140:A:THR:H	1:140:A:THR:HG22	8	0.19
(2,238)	1:128:A:ASN:HB2	1:128:A:ASN:HA	1	0.19
(2,238)	1:128:A:ASN:HB2	1:128:A:ASN:HA	8	0.19
(2,222)	1:205:A:ASP:HA	1:208:A:ILE:HD12	10	0.19
(2,211)	1:125:A:ILE:HB	1:125:A:ILE:HG21	5	0.19
(2,199)	1:136:A:ALA:HB2	1:138:A:LYS:HB3	4	0.19
(2,162)	1:148:A:LEU:HD22	1:149:A:THR:H	6	0.19
(2,102)	1:167:A:MET:HG3	1:167:A:MET:HA	6	0.19
(2,97)	1:127:A:VAL:HB	1:163:A:LYS:HB3	8	0.19
(2,74)	1:128:A:ASN:HB2	1:218:A:ILE:HG22	5	0.19
(2,71)	1:202:A:TYR:HB3	1:141:A:VAL:HB	7	0.19
(2,48)	1:173:A:LEU:HB2	1:174:A:ASN:H	4	0.19
(2,30)	1:205:A:ASP:HA	1:199:A:LEU:HG	8	0.19
(2,26)	1:219:A:ARG:HA	1:219:A:ARG:HG2	8	0.19
(2,2)	1:185:A:THR:HB	1:169:A:ARG:HB2	3	0.19
(1,1068)	1:181:A:SER:H	1:180:A:ASN:HB2	5	0.19
(1,1024)	1:146:A:ILE:HG12	1:146:A:ILE:H	8	0.19
(1,812)	1:192:A:ILE:HD11	1:208:A:ILE:HG22	3	0.19
(1,776)	1:204:A:ARG:HB2	1:130:A:ILE:HD13	2	0.19
(1,707)	1:166:A:VAL:HA	1:217:A:VAL:HG12	7	0.19
(1,686)	1:144:A:ALA:HB2	1:145:A:GLU:H	4	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,682)	1:136:A:ALA:HB1	1:135:A:ASN:HB3	3	0.19
(1,682)	1:136:A:ALA:HB3	1:135:A:ASN:HB3	7	0.19
(1,659)	1:202:A:TYR:HB2	1:141:A:VAL:HG12	9	0.19
(1,642)	1:183:A:VAL:HG13	1:187:A:VAL:HG12	1	0.19
(1,632)	1:140:A:THR:HG22	1:141:A:VAL:H	1	0.19
(1,632)	1:140:A:THR:HG21	1:141:A:VAL:H	3	0.19
(1,632)	1:140:A:THR:HG22	1:141:A:VAL:H	7	0.19
(1,621)	1:131:A:THR:HG21	1:126:A:ASP:HA	9	0.19
(1,589)	1:185:A:THR:HG21	1:184:A:GLU:HA	4	0.19
(1,589)	1:185:A:THR:HG22	1:184:A:GLU:HA	5	0.19
(1,587)	1:139:A:VAL:HG22	1:138:A:LYS:HA	1	0.19
(1,548)	1:173:A:LEU:HD12	1:187:A:VAL:HG12	7	0.19
(1,521)	1:191:A:TYR:HB3	1:155:A:LEU:HD22	7	0.19
(1,519)	1:192:A:ILE:HA	1:155:A:LEU:HD22	4	0.19
(1,519)	1:192:A:ILE:HA	1:155:A:LEU:HD21	5	0.19
(1,519)	1:192:A:ILE:HA	1:155:A:LEU:HD22	7	0.19
(1,508)	1:156:A:LEU:HD23	1:156:A:LEU:H	8	0.19
(1,496)	1:130:A:ILE:HG12	1:130:A:ILE:HA	7	0.19
(1,466)	1:193:A:ARG:HB3	1:193:A:ARG:H	6	0.19
(1,431)	1:211:A:VAL:HB	1:215:A:GLY:H	9	0.19
(1,419)	1:187:A:VAL:HB	1:188:A:VAL:H	1	0.19
(1,419)	1:187:A:VAL:HB	1:188:A:VAL:H	5	0.19
(1,352)	1:147:A:GLU:HG3	1:147:A:GLU:H	4	0.19
(1,340)	1:142:A:ASN:HB3	1:141:A:VAL:HG12	10	0.19
(1,286)	1:205:A:ASP:HB2	1:196:A:ARG:HB2	4	0.19
(1,266)	1:189:A:ASP:HB3	1:189:A:ASP:H	10	0.19
(1,211)	1:216:A:TYR:HB2	1:217:A:VAL:H	1	0.19
(1,182)	1:201:A:PRO:HD2	1:200:A:LYS:HB3	6	0.19
(1,177)	1:126:A:ASP:HA	1:125:A:ILE:HG21	5	0.19
(1,98)	1:170:A:GLU:HA	1:173:A:LEU:HB2	5	0.19
(1,36)	1:187:A:VAL:HA	1:190:A:VAL:HG23	6	0.19
(1,36)	1:187:A:VAL:HA	1:190:A:VAL:HG23	7	0.19
(2,317)	1:172:A:ILE:H	1:168:A:GLN:HB2	10	0.18
(2,277)	1:172:A:ILE:HG23	1:173:A:LEU:H	9	0.18
(2,239)	1:153:A:TYR:HB3	1:148:A:LEU:HB3	9	0.18
(2,218)	1:196:A:ARG:HD3	1:192:A:ILE:HG22	3	0.18
(2,217)	1:192:A:ILE:HG23	1:216:A:TYR:HE1	4	0.18
(2,200)	1:187:A:VAL:HG11	1:187:A:VAL:HG21	4	0.18
(2,200)	1:187:A:VAL:HG12	1:187:A:VAL:HG22	9	0.18
(2,164)	1:176:A:VAL:HG22	1:155:A:LEU:H	6	0.18
(2,164)	1:176:A:VAL:HG23	1:155:A:LEU:H	8	0.18
(2,164)	1:176:A:VAL:HG22	1:155:A:LEU:H	10	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,147)	1:204:A:ARG:HB2	1:199:A:LEU:HD11	7	0.18
(2,102)	1:167:A:MET:HG3	1:167:A:MET:HA	10	0.18
(2,43)	1:195:A:LEU:HB3	1:192:A:ILE:HA	3	0.18
(2,26)	1:219:A:ARG:HA	1:219:A:ARG:HG2	9	0.18
(2,10)	1:157:A:TYR:HA	1:156:A:LEU:HB3	1	0.18
(2,10)	1:157:A:TYR:HA	1:156:A:LEU:HB3	6	0.18
(2,10)	1:157:A:TYR:HA	1:156:A:LEU:HB3	8	0.18
(1,1084)	1:124:A:ILE:H	1:124:A:ILE:HG13	8	0.18
(1,1048)	1:207:A:MET:H	1:206:A:LYS:HG3	2	0.18
(1,1029)	1:130:A:ILE:HG12	1:130:A:ILE:H	2	0.18
(1,1029)	1:130:A:ILE:HG12	1:130:A:ILE:H	3	0.18
(1,1003)	1:159:A:LEU:HB3	1:159:A:LEU:H	7	0.18
(1,993)	1:194:A:TYR:H	1:193:A:ARG:HB2	5	0.18
(1,975)	1:158:A:LEU:H	1:157:A:TYR:HB2	4	0.18
(1,812)	1:192:A:ILE:HD11	1:208:A:ILE:HG23	8	0.18
(1,794)	1:146:A:ILE:HD12	1:202:A:TYR:HE2	9	0.18
(1,730)	1:216:A:TYR:HB2	1:208:A:ILE:HG22	4	0.18
(1,730)	1:216:A:TYR:HB2	1:208:A:ILE:HG23	6	0.18
(1,717)	1:160:A:ALA:HB2	1:132:A:ILE:HD13	10	0.18
(1,686)	1:144:A:ALA:HB1	1:145:A:GLU:H	9	0.18
(1,683)	1:136:A:ALA:HB2	1:133:A:ASP:HB2	4	0.18
(1,683)	1:136:A:ALA:HB2	1:133:A:ASP:HB2	7	0.18
(1,683)	1:136:A:ALA:HB2	1:133:A:ASP:HB2	8	0.18
(1,665)	1:211:A:VAL:HA	1:211:A:VAL:HG21	10	0.18
(1,649)	1:190:A:VAL:HB	1:187:A:VAL:HG23	3	0.18
(1,632)	1:140:A:THR:HG21	1:141:A:VAL:H	2	0.18
(1,632)	1:140:A:THR:HG22	1:141:A:VAL:H	4	0.18
(1,632)	1:140:A:THR:HG23	1:141:A:VAL:H	8	0.18
(1,621)	1:131:A:THR:HG22	1:126:A:ASP:HA	10	0.18
(1,607)	1:159:A:LEU:HD23	1:217:A:VAL:HA	2	0.18
(1,589)	1:185:A:THR:HG22	1:184:A:GLU:HA	7	0.18
(1,576)	1:151:A:THR:HG23	1:177:A:TRP:HZ2	8	0.18
(1,521)	1:191:A:TYR:HB3	1:155:A:LEU:HD21	9	0.18
(1,519)	1:192:A:ILE:HA	1:155:A:LEU:HD23	6	0.18
(1,492)	1:130:A:ILE:HG13	1:130:A:ILE:H	3	0.18
(1,461)	1:212:A:ARG:HB2	1:210:A:THR:HG22	8	0.18
(1,291)	1:191:A:TYR:HB3	1:191:A:TYR:H	4	0.18
(1,246)	1:133:A:ASP:HB3	1:133:A:ASP:H	6	0.18
(1,211)	1:216:A:TYR:HB2	1:217:A:VAL:H	9	0.18
(1,182)	1:201:A:PRO:HD2	1:200:A:LYS:HB3	9	0.18
(1,177)	1:126:A:ASP:HA	1:125:A:ILE:HG21	4	0.18
(1,148)	1:189:A:ASP:HA	1:188:A:VAL:HG13	8	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,41)	1:185:A:THR:HA	1:173:A:LEU:HB3	5	0.18
(2,309)	1:140:A:THR:H	1:132:A:ILE:HG13	6	0.17
(2,301)	1:207:A:MET:H	1:199:A:LEU:HD11	7	0.17
(2,279)	1:140:A:THR:H	1:140:A:THR:HG21	5	0.17
(2,238)	1:128:A:ASN:HB2	1:128:A:ASN:HA	7	0.17
(2,222)	1:205:A:ASP:HA	1:208:A:ILE:HD13	6	0.17
(2,221)	1:130:A:ILE:HD11	1:131:A:THR:H	6	0.17
(2,200)	1:187:A:VAL:HG13	1:187:A:VAL:HG21	6	0.17
(2,102)	1:167:A:MET:HG3	1:167:A:MET:HA	1	0.17
(2,102)	1:167:A:MET:HG3	1:167:A:MET:HA	9	0.17
(2,100)	1:204:A:ARG:HB2	1:130:A:ILE:HD12	7	0.17
(2,91)	1:171:A:GLN:HG3	1:168:A:GLN:H	4	0.17
(2,75)	1:128:A:ASN:HB3	1:218:A:ILE:HG23	9	0.17
(2,48)	1:173:A:LEU:HB2	1:174:A:ASN:H	3	0.17
(2,2)	1:185:A:THR:HB	1:173:A:LEU:HB3	9	0.17
(2,2)	1:185:A:THR:HB	1:173:A:LEU:HB3	10	0.17
(1,1037)	1:165:A:HIS:H	1:217:A:VAL:HG22	10	0.17
(1,1029)	1:130:A:ILE:HG12	1:130:A:ILE:H	9	0.17
(1,1024)	1:146:A:ILE:HG12	1:146:A:ILE:H	5	0.17
(1,1024)	1:146:A:ILE:HG12	1:146:A:ILE:H	7	0.17
(1,990)	1:145:A:GLU:HB3	1:146:A:ILE:H	2	0.17
(1,990)	1:145:A:GLU:HB3	1:146:A:ILE:H	5	0.17
(1,975)	1:158:A:LEU:H	1:157:A:TYR:HB2	1	0.17
(1,975)	1:158:A:LEU:H	1:157:A:TYR:HB2	7	0.17
(1,812)	1:192:A:ILE:HD12	1:208:A:ILE:HG23	1	0.17
(1,805)	1:192:A:ILE:HD11	1:192:A:ILE:H	1	0.17
(1,805)	1:192:A:ILE:HD11	1:192:A:ILE:H	4	0.17
(1,800)	1:146:A:ILE:HD11	1:139:A:VAL:HG13	7	0.17
(1,745)	1:160:A:ALA:HA	1:218:A:ILE:HG21	6	0.17
(1,745)	1:160:A:ALA:HA	1:218:A:ILE:HG21	7	0.17
(1,709)	1:209:A:GLU:HG3	1:217:A:VAL:HG11	9	0.17
(1,686)	1:144:A:ALA:HB2	1:145:A:GLU:H	6	0.17
(1,652)	1:141:A:VAL:HG12	1:146:A:ILE:HG12	3	0.17
(1,636)	1:141:A:VAL:HG12	1:202:A:TYR:HD2	4	0.17
(1,634)	1:183:A:VAL:HG13	1:187:A:VAL:H	3	0.17
(1,632)	1:140:A:THR:HG22	1:141:A:VAL:H	5	0.17
(1,632)	1:140:A:THR:HG22	1:141:A:VAL:H	6	0.17
(1,621)	1:131:A:THR:HG22	1:126:A:ASP:HA	8	0.17
(1,605)	1:210:A:THR:HG22	1:211:A:VAL:H	6	0.17
(1,521)	1:191:A:TYR:HB3	1:155:A:LEU:HD23	6	0.17
(1,516)	1:155:A:LEU:HD21	1:192:A:ILE:H	8	0.17
(1,482)	1:148:A:LEU:HD11	1:153:A:TYR:H	4	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,419)	1:187:A:VAL:HB	1:188:A:VAL:H	6	0.17
(1,367)	1:171:A:GLN:HG3	1:171:A:GLN:H	7	0.17
(1,342)	1:170:A:GLU:HG3	1:170:A:GLU:HB3	5	0.17
(1,333)	1:197:A:ASN:HB2	1:198:A:LYS:H	6	0.17
(1,220)	1:216:A:TYR:HB3	1:192:A:ILE:HD12	10	0.17
(1,177)	1:126:A:ASP:HA	1:125:A:ILE:HG21	10	0.17
(1,148)	1:189:A:ASP:HA	1:188:A:VAL:HG12	5	0.17
(1,41)	1:185:A:THR:HA	1:173:A:LEU:HB3	7	0.17
(2,279)	1:140:A:THR:H	1:140:A:THR:HG21	4	0.16
(2,238)	1:128:A:ASN:HB2	1:128:A:ASN:HA	10	0.16
(2,214)	1:167:A:MET:HE2	1:159:A:LEU:HA	9	0.16
(2,203)	1:217:A:VAL:HG12	1:219:A:ARG:HG2	3	0.16
(2,200)	1:187:A:VAL:HG12	1:187:A:VAL:HG21	1	0.16
(2,200)	1:187:A:VAL:HG13	1:187:A:VAL:HG21	8	0.16
(2,197)	1:187:A:VAL:HG12	1:177:A:TRP:HH2	5	0.16
(2,193)	1:176:A:VAL:HG12	1:177:A:TRP:HZ3	6	0.16
(2,193)	1:176:A:VAL:HG11	1:177:A:TRP:HZ3	8	0.16
(2,187)	1:127:A:VAL:HG23	1:126:A:ASP:HA	8	0.16
(2,185)	1:187:A:VAL:HB	1:183:A:VAL:HG11	5	0.16
(2,100)	1:167:A:MET:HG2	1:159:A:LEU:HD22	2	0.16
(2,91)	1:171:A:GLN:HG3	1:168:A:GLN:H	9	0.16
(2,74)	1:153:A:TYR:HB2	1:148:A:LEU:HD12	3	0.16
(2,36)	1:205:A:ASP:HA	1:196:A:ARG:HD2	3	0.16
(2,31)	1:205:A:ASP:HA	1:196:A:ARG:HD2	8	0.16
(2,26)	1:219:A:ARG:HA	1:219:A:ARG:HG2	4	0.16
(2,15)	1:152:A:GLU:HA	1:152:A:GLU:HB2	3	0.16
(2,10)	1:157:A:TYR:HA	1:156:A:LEU:HB3	4	0.16
(2,10)	1:157:A:TYR:HA	1:156:A:LEU:HB3	10	0.16
(1,1039)	1:159:A:LEU:H	1:159:A:LEU:HD12	5	0.16
(1,1032)	1:219:A:ARG:H	1:218:A:ILE:HG23	5	0.16
(1,1003)	1:159:A:LEU:HB3	1:159:A:LEU:H	4	0.16
(1,1001)	1:159:A:LEU:HB3	1:160:A:ALA:H	5	0.16
(1,990)	1:145:A:GLU:HB3	1:146:A:ILE:H	3	0.16
(1,979)	1:175:A:HIS:H	1:174:A:ASN:HB2	6	0.16
(1,975)	1:158:A:LEU:H	1:157:A:TYR:HB2	8	0.16
(1,968)	1:175:A:HIS:H	1:174:A:ASN:HB3	8	0.16
(1,812)	1:192:A:ILE:HD12	1:208:A:ILE:HG22	6	0.16
(1,812)	1:192:A:ILE:HD13	1:208:A:ILE:HG23	7	0.16
(1,805)	1:192:A:ILE:HD12	1:192:A:ILE:H	5	0.16
(1,805)	1:192:A:ILE:HD11	1:192:A:ILE:H	6	0.16
(1,805)	1:192:A:ILE:HD12	1:192:A:ILE:H	7	0.16
(1,800)	1:146:A:ILE:HD12	1:139:A:VAL:HG11	8	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,745)	1:160:A:ALA:HA	1:218:A:ILE:HG23	1	0.16
(1,745)	1:160:A:ALA:HA	1:218:A:ILE:HG23	8	0.16
(1,700)	1:172:A:ILE:HG22	1:177:A:TRP:HE3	2	0.16
(1,686)	1:144:A:ALA:HB2	1:145:A:GLU:H	1	0.16
(1,683)	1:136:A:ALA:HB3	1:133:A:ASP:HB2	9	0.16
(1,665)	1:211:A:VAL:HA	1:211:A:VAL:HG21	4	0.16
(1,665)	1:211:A:VAL:HA	1:211:A:VAL:HG22	6	0.16
(1,665)	1:211:A:VAL:HA	1:211:A:VAL:HG23	7	0.16
(1,665)	1:211:A:VAL:HA	1:211:A:VAL:HG23	8	0.16
(1,632)	1:140:A:THR:HG21	1:141:A:VAL:H	10	0.16
(1,619)	1:159:A:LEU:HD21	1:192:A:ILE:HD13	10	0.16
(1,591)	1:159:A:LEU:HA	1:159:A:LEU:HD22	7	0.16
(1,587)	1:139:A:VAL:HG22	1:138:A:LYS:HA	8	0.16
(1,585)	1:139:A:VAL:HG22	1:153:A:TYR:HE1	10	0.16
(1,574)	1:151:A:THR:HG23	1:191:A:TYR:HE2	4	0.16
(1,573)	1:151:A:THR:HG22	1:152:A:GLU:H	8	0.16
(1,528)	1:159:A:LEU:HB3	1:159:A:LEU:HD12	4	0.16
(1,521)	1:191:A:TYR:HB3	1:155:A:LEU:HD23	2	0.16
(1,448)	1:212:A:ARG:HD3	1:212:A:ARG:HB3	8	0.16
(1,445)	1:177:A:TRP:HB2	1:177:A:TRP:HD1	2	0.16
(1,445)	1:177:A:TRP:HB2	1:177:A:TRP:HD1	10	0.16
(1,427)	1:219:A:ARG:HB3	1:219:A:ARG:H	10	0.16
(1,419)	1:187:A:VAL:HB	1:188:A:VAL:H	7	0.16
(1,390)	1:204:A:ARG:HB3	1:204:A:ARG:H	6	0.16
(1,367)	1:171:A:GLN:HG3	1:171:A:GLN:H	1	0.16
(1,356)	1:194:A:TYR:HB3	1:194:A:TYR:H	2	0.16
(1,356)	1:194:A:TYR:HB3	1:194:A:TYR:H	3	0.16
(1,356)	1:194:A:TYR:HB3	1:194:A:TYR:H	7	0.16
(1,222)	1:219:A:ARG:HA	1:219:A:ARG:HD3	10	0.16
(1,168)	1:160:A:ALA:HA	1:127:A:VAL:HB	2	0.16
(1,153)	1:206:A:LYS:HA	1:206:A:LYS:HG2	8	0.16
(1,121)	1:140:A:THR:HA	1:141:A:VAL:HG11	6	0.16
(2,289)	1:214:A:VAL:HG11	1:215:A:GLY:H	9	0.15
(2,277)	1:172:A:ILE:HG23	1:173:A:LEU:H	1	0.15
(2,277)	1:172:A:ILE:HG23	1:173:A:LEU:H	10	0.15
(2,239)	1:153:A:TYR:HB3	1:148:A:LEU:HB3	2	0.15
(2,217)	1:192:A:ILE:HG21	1:216:A:TYR:HE2	1	0.15
(2,214)	1:167:A:MET:HE3	1:159:A:LEU:HA	10	0.15
(2,212)	1:207:A:MET:HE2	1:130:A:ILE:HD11	4	0.15
(2,200)	1:183:A:VAL:HG12	1:187:A:VAL:HG11	5	0.15
(2,172)	1:199:A:LEU:HD22	1:202:A:TYR:HD2	2	0.15
(2,162)	1:148:A:LEU:HD23	1:149:A:THR:H	7	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,117)	1:165:A:HIS:HB2	1:162:A:ASN:HB2	8	0.15
(2,106)	1:190:A:VAL:HB	1:187:A:VAL:HG23	7	0.15
(2,106)	1:190:A:VAL:HB	1:187:A:VAL:HG21	9	0.15
(2,92)	1:171:A:GLN:HG3	1:167:A:MET:HA	7	0.15
(2,79)	1:152:A:GLU:HG3	1:155:A:LEU:HD11	2	0.15
(2,71)	1:202:A:TYR:HB3	1:141:A:VAL:HB	10	0.15
(2,55)	1:200:A:LYS:HE3	1:196:A:ARG:HB2	4	0.15
(2,26)	1:219:A:ARG:HA	1:219:A:ARG:HG2	1	0.15
(2,26)	1:219:A:ARG:HA	1:219:A:ARG:HG2	2	0.15
(2,15)	1:152:A:GLU:HA	1:152:A:GLU:HG3	2	0.15
(2,14)	1:196:A:ARG:HA	1:196:A:ARG:HD3	7	0.15
(2,10)	1:157:A:TYR:HA	1:156:A:LEU:HB3	2	0.15
(2,10)	1:157:A:TYR:HA	1:156:A:LEU:HB3	9	0.15
(1,1075)	1:147:A:GLU:H	1:146:A:ILE:HB	3	0.15
(1,1029)	1:130:A:ILE:HG12	1:130:A:ILE:H	4	0.15
(1,979)	1:175:A:HIS:H	1:174:A:ASN:HB2	4	0.15
(1,975)	1:158:A:LEU:H	1:157:A:TYR:HB2	9	0.15
(1,800)	1:146:A:ILE:HD13	1:139:A:VAL:HG11	9	0.15
(1,785)	1:125:A:ILE:HD12	1:161:A:GLU:HA	8	0.15
(1,734)	1:146:A:ILE:HG21	1:147:A:GLU:H	10	0.15
(1,730)	1:216:A:TYR:HB2	1:208:A:ILE:HG21	10	0.15
(1,665)	1:211:A:VAL:HA	1:211:A:VAL:HG22	1	0.15
(1,623)	1:149:A:THR:HG22	1:149:A:THR:HA	6	0.15
(1,607)	1:159:A:LEU:HD21	1:217:A:VAL:HA	1	0.15
(1,605)	1:210:A:THR:HG23	1:211:A:VAL:H	5	0.15
(1,594)	1:156:A:LEU:HA	1:156:A:LEU:HD12	2	0.15
(1,589)	1:185:A:THR:HG22	1:184:A:GLU:HA	8	0.15
(1,550)	1:150:A:LYS:HG2	1:149:A:THR:HB	7	0.15
(1,492)	1:130:A:ILE:HG13	1:130:A:ILE:H	4	0.15
(1,482)	1:148:A:LEU:HD13	1:153:A:TYR:H	5	0.15
(1,445)	1:177:A:TRP:HB2	1:177:A:TRP:HD1	3	0.15
(1,445)	1:177:A:TRP:HB2	1:177:A:TRP:HD1	5	0.15
(1,445)	1:177:A:TRP:HB2	1:177:A:TRP:HD1	7	0.15
(1,445)	1:177:A:TRP:HB2	1:177:A:TRP:HD1	9	0.15
(1,356)	1:194:A:TYR:HB3	1:194:A:TYR:H	4	0.15
(1,356)	1:194:A:TYR:HB3	1:194:A:TYR:H	6	0.15
(1,356)	1:194:A:TYR:HB3	1:194:A:TYR:H	9	0.15
(1,356)	1:194:A:TYR:HB3	1:194:A:TYR:H	10	0.15
(1,333)	1:197:A:ASN:HB2	1:198:A:LYS:H	3	0.15
(1,333)	1:197:A:ASN:HB2	1:198:A:LYS:H	8	0.15
(1,282)	1:203:A:ASP:HB3	1:203:A:ASP:HA	8	0.15
(1,247)	1:133:A:ASP:HB2	1:133:A:ASP:H	10	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,246)	1:133:A:ASP:HB3	1:133:A:ASP:H	1	0.15
(1,211)	1:216:A:TYR:HB2	1:217:A:VAL:H	10	0.15
(1,195)	1:215:A:GLY:HA2	1:169:A:ARG:HG2	10	0.15
(1,182)	1:201:A:PRO:HD2	1:200:A:LYS:HB2	3	0.15
(1,168)	1:160:A:ALA:HA	1:127:A:VAL:HB	4	0.15
(1,168)	1:160:A:ALA:HA	1:127:A:VAL:HB	5	0.15
(1,121)	1:140:A:THR:HA	1:141:A:VAL:HG13	2	0.15
(1,121)	1:140:A:THR:HA	1:141:A:VAL:HG12	3	0.15
(1,121)	1:140:A:THR:HA	1:141:A:VAL:HG12	8	0.15
(1,69)	1:153:A:TYR:HA	1:156:A:LEU:HB2	2	0.15
(2,318)	1:175:A:HIS:H	1:158:A:LEU:HD23	1	0.14
(2,307)	1:211:A:VAL:H	1:216:A:TYR:HD2	8	0.14
(2,296)	1:139:A:VAL:H	1:146:A:ILE:HB	10	0.14
(2,280)	1:148:A:LEU:H	1:148:A:LEU:HD21	2	0.14
(2,239)	1:153:A:TYR:HB3	1:148:A:LEU:HB3	5	0.14
(2,234)	1:214:A:VAL:HG11	1:214:A:VAL:HA	8	0.14
(2,222)	1:205:A:ASP:HA	1:208:A:ILE:HD13	9	0.14
(2,212)	1:207:A:MET:HE1	1:218:A:ILE:HG23	5	0.14
(2,208)	1:130:A:ILE:HG21	1:131:A:THR:HA	6	0.14
(2,200)	1:187:A:VAL:HG11	1:187:A:VAL:HG21	3	0.14
(2,43)	1:195:A:LEU:HB3	1:192:A:ILE:HA	2	0.14
(2,43)	1:195:A:LEU:HB3	1:192:A:ILE:HA	4	0.14
(2,42)	1:204:A:ARG:HD3	1:130:A:ILE:HD11	9	0.14
(2,31)	1:205:A:ASP:HA	1:196:A:ARG:HD2	5	0.14
(2,11)	1:169:A:ARG:HA	1:172:A:ILE:HD11	3	0.14
(2,6)	1:191:A:TYR:HA	1:192:A:ILE:H	5	0.14
(2,6)	1:191:A:TYR:HA	1:192:A:ILE:H	9	0.14
(1,1068)	1:181:A:SER:H	1:180:A:ASN:HB2	7	0.14
(1,1024)	1:146:A:ILE:HG12	1:146:A:ILE:H	9	0.14
(1,979)	1:175:A:HIS:H	1:174:A:ASN:HB2	7	0.14
(1,979)	1:175:A:HIS:H	1:174:A:ASN:HB2	9	0.14
(1,745)	1:160:A:ALA:HA	1:218:A:ILE:HG22	3	0.14
(1,738)	1:128:A:ASN:HB3	1:207:A:MET:HE1	10	0.14
(1,734)	1:146:A:ILE:HG23	1:147:A:GLU:H	4	0.14
(1,730)	1:216:A:TYR:HB2	1:208:A:ILE:HG21	2	0.14
(1,717)	1:160:A:ALA:HB2	1:132:A:ILE:HD13	9	0.14
(1,709)	1:209:A:GLU:HG3	1:217:A:VAL:HG13	8	0.14
(1,665)	1:211:A:VAL:HA	1:211:A:VAL:HG21	2	0.14
(1,665)	1:211:A:VAL:HA	1:211:A:VAL:HG23	3	0.14
(1,665)	1:211:A:VAL:HA	1:211:A:VAL:HG23	5	0.14
(1,642)	1:183:A:VAL:HG13	1:187:A:VAL:HG13	8	0.14
(1,616)	1:199:A:LEU:HG	1:199:A:LEU:HD22	2	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,616)	1:199:A:LEU:HG	1:199:A:LEU:HD21	5	0.14
(1,616)	1:199:A:LEU:HG	1:199:A:LEU:HD22	8	0.14
(1,594)	1:156:A:LEU:HA	1:156:A:LEU:HD13	9	0.14
(1,573)	1:151:A:THR:HG22	1:152:A:GLU:H	2	0.14
(1,573)	1:151:A:THR:HG22	1:152:A:GLU:H	3	0.14
(1,573)	1:151:A:THR:HG23	1:152:A:GLU:H	10	0.14
(1,519)	1:192:A:ILE:HA	1:155:A:LEU:HD21	1	0.14
(1,519)	1:192:A:ILE:HA	1:155:A:LEU:HD23	3	0.14
(1,445)	1:177:A:TRP:HB2	1:177:A:TRP:HD1	6	0.14
(1,388)	1:167:A:MET:HG3	1:167:A:MET:H	9	0.14
(1,377)	1:183:A:VAL:HB	1:184:A:GLU:H	2	0.14
(1,367)	1:171:A:GLN:HG3	1:171:A:GLN:H	2	0.14
(1,367)	1:171:A:GLN:HG3	1:171:A:GLN:H	9	0.14
(1,360)	1:147:A:GLU:HG3	1:147:A:GLU:HA	9	0.14
(1,356)	1:194:A:TYR:HB3	1:194:A:TYR:H	1	0.14
(1,333)	1:197:A:ASN:HB2	1:198:A:LYS:H	5	0.14
(1,333)	1:197:A:ASN:HB2	1:198:A:LYS:H	10	0.14
(1,300)	1:202:A:TYR:HB2	1:141:A:VAL:HB	4	0.14
(1,282)	1:203:A:ASP:HB3	1:203:A:ASP:HA	4	0.14
(1,282)	1:203:A:ASP:HB3	1:203:A:ASP:HA	5	0.14
(1,282)	1:203:A:ASP:HB3	1:203:A:ASP:HA	6	0.14
(1,282)	1:203:A:ASP:HB3	1:203:A:ASP:HA	7	0.14
(1,246)	1:133:A:ASP:HB3	1:133:A:ASP:H	2	0.14
(1,195)	1:215:A:GLY:HA2	1:169:A:ARG:HG2	8	0.14
(1,177)	1:126:A:ASP:HA	1:125:A:ILE:HG22	1	0.14
(1,169)	1:160:A:ALA:HA	1:218:A:ILE:HB	7	0.14
(1,153)	1:206:A:LYS:HA	1:206:A:LYS:HG2	1	0.14
(1,148)	1:189:A:ASP:HA	1:188:A:VAL:HG11	4	0.14
(1,121)	1:140:A:THR:HA	1:141:A:VAL:HG11	1	0.14
(1,98)	1:170:A:GLU:HA	1:173:A:LEU:HB2	4	0.14
(1,41)	1:185:A:THR:HA	1:173:A:LEU:HB3	4	0.14
(1,41)	1:185:A:THR:HA	1:173:A:LEU:HB3	8	0.14
(2,309)	1:140:A:THR:H	1:132:A:ILE:HG13	2	0.13
(2,309)	1:140:A:THR:H	1:132:A:ILE:HG13	7	0.13
(2,307)	1:211:A:VAL:H	1:216:A:TYR:HD2	1	0.13
(2,280)	1:148:A:LEU:H	1:148:A:LEU:HD23	8	0.13
(2,277)	1:172:A:ILE:HG22	1:173:A:LEU:H	2	0.13
(2,222)	1:205:A:ASP:HA	1:208:A:ILE:HD13	3	0.13
(2,170)	1:159:A:LEU:HD22	1:159:A:LEU:H	3	0.13
(2,168)	1:151:A:THR:HB	1:151:A:THR:HG22	1	0.13
(2,168)	1:151:A:THR:HB	1:151:A:THR:HG22	5	0.13
(2,168)	1:151:A:THR:HB	1:151:A:THR:HG21	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,168)	1:151:A:THR:HB	1:151:A:THR:HG23	7	0.13
(2,168)	1:151:A:THR:HB	1:151:A:THR:HG21	10	0.13
(2,164)	1:176:A:VAL:HG21	1:155:A:LEU:H	1	0.13
(2,158)	1:195:A:LEU:HG	1:195:A:LEU:HD12	1	0.13
(2,158)	1:195:A:LEU:HG	1:195:A:LEU:HD21	2	0.13
(2,158)	1:195:A:LEU:HG	1:195:A:LEU:HD21	4	0.13
(2,158)	1:195:A:LEU:HG	1:195:A:LEU:HD12	5	0.13
(2,158)	1:195:A:LEU:HG	1:195:A:LEU:HD21	6	0.13
(2,158)	1:195:A:LEU:HG	1:195:A:LEU:HD13	7	0.13
(2,158)	1:195:A:LEU:HG	1:195:A:LEU:HD12	8	0.13
(2,158)	1:195:A:LEU:HG	1:195:A:LEU:HD13	9	0.13
(2,126)	1:132:A:ILE:HG13	1:139:A:VAL:HA	8	0.13
(2,97)	1:127:A:VAL:HB	1:163:A:LYS:HB3	2	0.13
(2,87)	1:209:A:GLU:HG3	1:217:A:VAL:HG13	3	0.13
(2,75)	1:128:A:ASN:HB3	1:218:A:ILE:HG22	7	0.13
(2,10)	1:157:A:TYR:HA	1:156:A:LEU:HB3	5	0.13
(2,6)	1:191:A:TYR:HA	1:192:A:ILE:H	1	0.13
(2,6)	1:191:A:TYR:HA	1:192:A:ILE:H	2	0.13
(2,6)	1:191:A:TYR:HA	1:192:A:ILE:H	7	0.13
(2,6)	1:191:A:TYR:HA	1:192:A:ILE:H	8	0.13
(1,1084)	1:124:A:ILE:H	1:124:A:ILE:HG13	2	0.13
(1,1068)	1:181:A:SER:H	1:180:A:ASN:HB2	8	0.13
(1,1039)	1:159:A:LEU:H	1:159:A:LEU:HD12	1	0.13
(1,1001)	1:159:A:LEU:HB3	1:160:A:ALA:H	2	0.13
(1,975)	1:158:A:LEU:H	1:157:A:TYR:HB2	2	0.13
(1,898)	1:154:A:ASP:H	1:153:A:TYR:HD2	9	0.13
(1,800)	1:146:A:ILE:HD12	1:139:A:VAL:HG13	1	0.13
(1,800)	1:146:A:ILE:HD13	1:139:A:VAL:HG11	2	0.13
(1,704)	1:172:A:ILE:HG22	1:177:A:TRP:HZ3	2	0.13
(1,643)	1:166:A:VAL:HG11	1:167:A:MET:H	7	0.13
(1,623)	1:149:A:THR:HG22	1:149:A:THR:HA	3	0.13
(1,616)	1:199:A:LEU:HG	1:199:A:LEU:HD21	1	0.13
(1,616)	1:199:A:LEU:HG	1:199:A:LEU:HD23	3	0.13
(1,616)	1:199:A:LEU:HG	1:199:A:LEU:HD21	6	0.13
(1,616)	1:199:A:LEU:HG	1:199:A:LEU:HD22	7	0.13
(1,594)	1:156:A:LEU:HA	1:156:A:LEU:HD12	4	0.13
(1,587)	1:139:A:VAL:HG23	1:138:A:LYS:HA	3	0.13
(1,554)	1:148:A:LEU:HB3	1:148:A:LEU:HD22	1	0.13
(1,554)	1:148:A:LEU:HB3	1:148:A:LEU:HD23	3	0.13
(1,554)	1:148:A:LEU:HB3	1:148:A:LEU:HD21	5	0.13
(1,554)	1:148:A:LEU:HB3	1:148:A:LEU:HD22	6	0.13
(1,550)	1:150:A:LYS:HG3	1:149:A:THR:HB	4	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,519)	1:192:A:ILE:HA	1:155:A:LEU:HD21	9	0.13
(1,519)	1:192:A:ILE:HA	1:155:A:LEU:HD23	10	0.13
(1,482)	1:148:A:LEU:HD11	1:153:A:TYR:H	1	0.13
(1,482)	1:148:A:LEU:HD12	1:153:A:TYR:H	6	0.13
(1,479)	1:193:A:ARG:HG3	1:193:A:ARG:HA	4	0.13
(1,445)	1:177:A:TRP:HB2	1:177:A:TRP:HD1	4	0.13
(1,445)	1:177:A:TRP:HB2	1:177:A:TRP:HD1	8	0.13
(1,388)	1:167:A:MET:HG3	1:167:A:MET:H	1	0.13
(1,377)	1:183:A:VAL:HB	1:184:A:GLU:H	3	0.13
(1,377)	1:183:A:VAL:HB	1:184:A:GLU:H	6	0.13
(1,367)	1:171:A:GLN:HG3	1:171:A:GLN:H	4	0.13
(1,367)	1:171:A:GLN:HG3	1:171:A:GLN:H	10	0.13
(1,356)	1:194:A:TYR:HB3	1:194:A:TYR:H	5	0.13
(1,356)	1:194:A:TYR:HB3	1:194:A:TYR:H	8	0.13
(1,339)	1:128:A:ASN:HB3	1:207:A:MET:HG2	9	0.13
(1,333)	1:197:A:ASN:HB2	1:198:A:LYS:H	1	0.13
(1,323)	1:128:A:ASN:HB2	1:128:A:ASN:HA	2	0.13
(1,286)	1:205:A:ASP:HB2	1:196:A:ARG:HB2	6	0.13
(1,282)	1:203:A:ASP:HB3	1:203:A:ASP:HA	2	0.13
(1,211)	1:216:A:TYR:HB2	1:217:A:VAL:H	8	0.13
(1,182)	1:201:A:PRO:HD2	1:200:A:LYS:HB2	2	0.13
(1,177)	1:126:A:ASP:HA	1:125:A:ILE:HG21	6	0.13
(1,177)	1:126:A:ASP:HA	1:125:A:ILE:HG21	8	0.13
(1,168)	1:160:A:ALA:HA	1:127:A:VAL:HB	7	0.13
(1,148)	1:189:A:ASP:HA	1:188:A:VAL:HG12	2	0.13
(1,98)	1:170:A:GLU:HA	1:173:A:LEU:HB2	3	0.13
(1,51)	1:181:A:SER:HB3	1:183:A:VAL:HG21	1	0.13
(1,29)	1:190:A:VAL:HA	1:189:A:ASP:HB3	7	0.13
(2,289)	1:214:A:VAL:HG12	1:215:A:GLY:H	10	0.12
(2,280)	1:148:A:LEU:H	1:148:A:LEU:HD21	1	0.12
(2,234)	1:214:A:VAL:HG12	1:214:A:VAL:HA	2	0.12
(2,234)	1:214:A:VAL:HG12	1:214:A:VAL:HA	7	0.12
(2,226)	1:125:A:ILE:HD13	1:132:A:ILE:HB	10	0.12
(2,185)	1:187:A:VAL:HB	1:183:A:VAL:HG13	10	0.12
(2,183)	1:140:A:THR:HG21	1:138:A:LYS:HD2	5	0.12
(2,168)	1:151:A:THR:HA	1:151:A:THR:HG21	3	0.12
(2,168)	1:151:A:THR:HB	1:151:A:THR:HG23	4	0.12
(2,168)	1:151:A:THR:HB	1:151:A:THR:HG22	9	0.12
(2,164)	1:176:A:VAL:HG21	1:155:A:LEU:H	2	0.12
(2,160)	1:134:A:LYS:HG2	1:134:A:LYS:HD3	1	0.12
(2,158)	1:195:A:LEU:HG	1:195:A:LEU:HD13	3	0.12
(2,158)	1:195:A:LEU:HG	1:195:A:LEU:HD12	10	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,137)	1:124:A:ILE:HG13	1:124:A:ILE:HD12	7	0.12
(2,137)	1:156:A:LEU:HG	1:156:A:LEU:HD12	10	0.12
(2,91)	1:171:A:GLN:HG3	1:168:A:GLN:H	5	0.12
(2,91)	1:171:A:GLN:HG3	1:168:A:GLN:H	6	0.12
(2,87)	1:209:A:GLU:HG2	1:217:A:VAL:HG11	4	0.12
(2,10)	1:157:A:TYR:HA	1:156:A:LEU:HB3	3	0.12
(2,10)	1:157:A:TYR:HA	1:156:A:LEU:HB3	7	0.12
(2,6)	1:191:A:TYR:HA	1:192:A:ILE:H	3	0.12
(2,6)	1:191:A:TYR:HA	1:192:A:ILE:H	4	0.12
(2,6)	1:191:A:TYR:HA	1:192:A:ILE:H	10	0.12
(2,5)	1:166:A:VAL:HA	1:217:A:VAL:HG22	6	0.12
(1,1084)	1:124:A:ILE:H	1:124:A:ILE:HG13	5	0.12
(1,1084)	1:124:A:ILE:H	1:124:A:ILE:HG13	7	0.12
(1,1075)	1:147:A:GLU:H	1:146:A:ILE:HB	4	0.12
(1,1075)	1:147:A:GLU:H	1:146:A:ILE:HB	5	0.12
(1,1075)	1:147:A:GLU:H	1:146:A:ILE:HB	10	0.12
(1,993)	1:194:A:TYR:H	1:193:A:ARG:HB2	10	0.12
(1,990)	1:145:A:GLU:HB3	1:146:A:ILE:H	1	0.12
(1,975)	1:158:A:LEU:H	1:157:A:TYR:HB2	3	0.12
(1,898)	1:154:A:ASP:H	1:153:A:TYR:HD2	5	0.12
(1,848)	1:150:A:LYS:HG2	1:150:A:LYS:HA	2	0.12
(1,844)	1:200:A:LYS:HD2	1:200:A:LYS:H	4	0.12
(1,844)	1:200:A:LYS:HD2	1:200:A:LYS:H	10	0.12
(1,817)	1:140:A:THR:HB	1:141:A:VAL:H	7	0.12
(1,800)	1:146:A:ILE:HD11	1:139:A:VAL:HG13	3	0.12
(1,755)	1:193:A:ARG:HA	1:192:A:ILE:HG21	8	0.12
(1,735)	1:125:A:ILE:HG23	1:126:A:ASP:H	8	0.12
(1,734)	1:146:A:ILE:HG21	1:147:A:GLU:H	5	0.12
(1,726)	1:132:A:ILE:HG23	1:134:A:LYS:HA	5	0.12
(1,707)	1:166:A:VAL:HA	1:217:A:VAL:HG11	2	0.12
(1,662)	1:176:A:VAL:HG11	1:177:A:TRP:HE3	5	0.12
(1,634)	1:183:A:VAL:HG13	1:187:A:VAL:H	10	0.12
(1,623)	1:149:A:THR:HG21	1:149:A:THR:HA	5	0.12
(1,616)	1:199:A:LEU:HG	1:199:A:LEU:HD22	9	0.12
(1,616)	1:199:A:LEU:HG	1:199:A:LEU:HD22	10	0.12
(1,605)	1:210:A:THR:HG23	1:211:A:VAL:H	3	0.12
(1,589)	1:185:A:THR:HG21	1:184:A:GLU:HA	3	0.12
(1,589)	1:185:A:THR:HG23	1:184:A:GLU:HA	6	0.12
(1,554)	1:148:A:LEU:HB3	1:148:A:LEU:HD21	8	0.12
(1,554)	1:148:A:LEU:HB3	1:148:A:LEU:HD21	9	0.12
(1,516)	1:155:A:LEU:HD22	1:192:A:ILE:H	4	0.12
(1,482)	1:148:A:LEU:HD11	1:153:A:TYR:H	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,445)	1:177:A:TRP:HB2	1:177:A:TRP:HD1	1	0.12
(1,433)	1:184:A:GLU:HB3	1:184:A:GLU:H	5	0.12
(1,433)	1:184:A:GLU:HB3	1:184:A:GLU:H	10	0.12
(1,390)	1:204:A:ARG:HB3	1:204:A:ARG:H	4	0.12
(1,390)	1:204:A:ARG:HB3	1:204:A:ARG:H	5	0.12
(1,377)	1:183:A:VAL:HB	1:184:A:GLU:H	7	0.12
(1,367)	1:171:A:GLN:HG3	1:171:A:GLN:H	3	0.12
(1,333)	1:197:A:ASN:HB2	1:198:A:LYS:H	4	0.12
(1,323)	1:128:A:ASN:HB2	1:128:A:ASN:HA	1	0.12
(1,323)	1:128:A:ASN:HB2	1:128:A:ASN:HA	4	0.12
(1,323)	1:128:A:ASN:HB2	1:128:A:ASN:HA	5	0.12
(1,323)	1:128:A:ASN:HB2	1:128:A:ASN:HA	6	0.12
(1,323)	1:128:A:ASN:HB2	1:128:A:ASN:HA	8	0.12
(1,323)	1:128:A:ASN:HB2	1:128:A:ASN:HA	9	0.12
(1,286)	1:205:A:ASP:HB2	1:196:A:ARG:HB2	1	0.12
(1,223)	1:219:A:ARG:HD3	1:219:A:ARG:HB2	10	0.12
(1,220)	1:216:A:TYR:HB3	1:192:A:ILE:HD13	9	0.12
(1,185)	1:201:A:PRO:HD3	1:201:A:PRO:HB2	3	0.12
(1,185)	1:201:A:PRO:HD3	1:201:A:PRO:HB2	9	0.12
(1,182)	1:201:A:PRO:HD2	1:200:A:LYS:HB2	1	0.12
(1,182)	1:201:A:PRO:HD2	1:200:A:LYS:HB2	5	0.12
(1,177)	1:126:A:ASP:HA	1:125:A:ILE:HG22	3	0.12
(1,161)	1:174:A:ASN:HA	1:178:A:GLY:H	9	0.12
(1,158)	1:184:A:GLU:HA	1:184:A:GLU:HG3	6	0.12
(1,98)	1:170:A:GLU:HA	1:173:A:LEU:HB2	6	0.12
(1,98)	1:170:A:GLU:HA	1:173:A:LEU:HB2	7	0.12
(1,98)	1:170:A:GLU:HA	1:173:A:LEU:HB2	8	0.12
(1,41)	1:185:A:THR:HA	1:173:A:LEU:HB3	6	0.12
(1,29)	1:190:A:VAL:HA	1:189:A:ASP:HB3	2	0.12
(2,289)	1:214:A:VAL:HG12	1:215:A:GLY:H	8	0.11
(2,280)	1:148:A:LEU:H	1:148:A:LEU:HD23	4	0.11
(2,280)	1:148:A:LEU:H	1:148:A:LEU:HD22	7	0.11
(2,234)	1:214:A:VAL:HG13	1:214:A:VAL:HA	1	0.11
(2,168)	1:151:A:THR:HB	1:151:A:THR:HG23	8	0.11
(2,160)	1:138:A:LYS:HB2	1:138:A:LYS:HG3	4	0.11
(2,137)	1:156:A:LEU:HG	1:156:A:LEU:HD13	2	0.11
(2,137)	1:156:A:LEU:HG	1:156:A:LEU:HD12	3	0.11
(2,137)	1:156:A:LEU:HG	1:156:A:LEU:HD12	5	0.11
(2,137)	1:156:A:LEU:HG	1:156:A:LEU:HD12	6	0.11
(2,136)	1:130:A:ILE:HG12	1:130:A:ILE:HD13	7	0.11
(2,97)	1:127:A:VAL:HB	1:163:A:LYS:HB3	4	0.11
(2,90)	1:214:A:VAL:HB	1:214:A:VAL:HG11	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,47)	1:204:A:ARG:HD2	1:141:A:VAL:HG22	7	0.11
(2,43)	1:195:A:LEU:HB3	1:192:A:ILE:HA	1	0.11
(2,31)	1:205:A:ASP:HA	1:196:A:ARG:HD2	2	0.11
(2,26)	1:219:A:ARG:HA	1:219:A:ARG:HG2	7	0.11
(2,6)	1:191:A:TYR:HA	1:192:A:ILE:H	6	0.11
(1,1037)	1:165:A:HIS:H	1:217:A:VAL:HG21	3	0.11
(1,975)	1:158:A:LEU:H	1:157:A:TYR:HB2	5	0.11
(1,950)	1:181:A:SER:HB2	1:181:A:SER:H	1	0.11
(1,928)	1:180:A:ASN:H	1:179:A:TYR:HA	4	0.11
(1,928)	1:180:A:ASN:H	1:179:A:TYR:HA	6	0.11
(1,898)	1:154:A:ASP:H	1:153:A:TYR:HD2	4	0.11
(1,801)	1:124:A:ILE:HD11	1:124:A:ILE:H	4	0.11
(1,800)	1:146:A:ILE:HD11	1:139:A:VAL:HG13	4	0.11
(1,800)	1:146:A:ILE:HD13	1:139:A:VAL:HG13	5	0.11
(1,800)	1:146:A:ILE:HD12	1:139:A:VAL:HG12	6	0.11
(1,762)	1:192:A:ILE:HG22	1:208:A:ILE:HD12	2	0.11
(1,716)	1:160:A:ALA:HB3	1:156:A:LEU:HD12	7	0.11
(1,616)	1:199:A:LEU:HG	1:199:A:LEU:HD21	4	0.11
(1,612)	1:190:A:VAL:HA	1:190:A:VAL:HG21	9	0.11
(1,594)	1:156:A:LEU:HA	1:156:A:LEU:HD11	5	0.11
(1,587)	1:139:A:VAL:HG23	1:138:A:LYS:HA	4	0.11
(1,576)	1:151:A:THR:HG23	1:177:A:TRP:HZ2	5	0.11
(1,554)	1:148:A:LEU:HB3	1:148:A:LEU:HD21	4	0.11
(1,528)	1:159:A:LEU:HB3	1:159:A:LEU:HD13	2	0.11
(1,461)	1:212:A:ARG:HB3	1:210:A:THR:HG22	6	0.11
(1,449)	1:161:A:GLU:HB2	1:125:A:ILE:HG22	2	0.11
(1,433)	1:184:A:GLU:HB3	1:184:A:GLU:H	7	0.11
(1,390)	1:204:A:ARG:HB3	1:204:A:ARG:H	3	0.11
(1,388)	1:167:A:MET:HG3	1:167:A:MET:H	6	0.11
(1,377)	1:183:A:VAL:HB	1:184:A:GLU:H	4	0.11
(1,333)	1:197:A:ASN:HB2	1:198:A:LYS:H	2	0.11
(1,286)	1:205:A:ASP:HB2	1:196:A:ARG:HB2	9	0.11
(1,195)	1:215:A:GLY:HA2	1:169:A:ARG:HG2	1	0.11
(1,185)	1:201:A:PRO:HD3	1:201:A:PRO:HB2	1	0.11
(1,185)	1:201:A:PRO:HD3	1:201:A:PRO:HB2	2	0.11
(1,185)	1:201:A:PRO:HD3	1:201:A:PRO:HB2	5	0.11
(1,185)	1:201:A:PRO:HD3	1:201:A:PRO:HB2	6	0.11
(1,185)	1:201:A:PRO:HD3	1:201:A:PRO:HB2	7	0.11
(1,182)	1:201:A:PRO:HD2	1:200:A:LYS:HB2	4	0.11
(1,182)	1:201:A:PRO:HD2	1:200:A:LYS:HB2	8	0.11
(1,177)	1:126:A:ASP:HA	1:125:A:ILE:HG21	2	0.11
(1,168)	1:160:A:ALA:HA	1:127:A:VAL:HB	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,121)	1:140:A:THR:HA	1:141:A:VAL:HG12	7	0.11
(2,289)	1:214:A:VAL:HG11	1:215:A:GLY:H	4	0.1
(2,185)	1:166:A:VAL:HG12	1:217:A:VAL:HB	2	0.1
(2,164)	1:176:A:VAL:HG21	1:155:A:LEU:H	7	0.1
(2,160)	1:134:A:LYS:HG2	1:134:A:LYS:HD3	3	0.1
(2,137)	1:124:A:ILE:HG13	1:124:A:ILE:HD13	4	0.1
(2,137)	1:156:A:LEU:HG	1:156:A:LEU:HD11	9	0.1
(2,90)	1:214:A:VAL:HB	1:214:A:VAL:HG21	3	0.1
(2,90)	1:214:A:VAL:HB	1:214:A:VAL:HG21	7	0.1
(2,90)	1:214:A:VAL:HB	1:214:A:VAL:HG11	9	0.1
(2,56)	1:133:A:ASP:HB2	1:138:A:LYS:HB2	9	0.1
(2,41)	1:193:A:ARG:HD3	1:193:A:ARG:HG2	2	0.1
(2,36)	1:193:A:ARG:HA	1:196:A:ARG:HD3	8	0.1
(1,1075)	1:147:A:GLU:H	1:146:A:ILE:HB	2	0.1
(1,1039)	1:159:A:LEU:H	1:159:A:LEU:HD12	10	0.1
(1,979)	1:175:A:HIS:H	1:174:A:ASN:HB2	2	0.1
(1,796)	1:146:A:ILE:HA	1:146:A:ILE:HD13	6	0.1
(1,794)	1:146:A:ILE:HD12	1:202:A:TYR:HE1	5	0.1
(1,778)	1:130:A:ILE:HG13	1:130:A:ILE:HD12	7	0.1
(1,778)	1:130:A:ILE:HG13	1:130:A:ILE:HD12	8	0.1
(1,772)	1:132:A:ILE:HD13	1:157:A:TYR:H	2	0.1
(1,707)	1:166:A:VAL:HA	1:217:A:VAL:HG12	4	0.1
(1,675)	1:176:A:VAL:HG22	1:176:A:VAL:HG13	4	0.1
(1,610)	1:210:A:THR:HB	1:210:A:THR:HG22	8	0.1
(1,594)	1:156:A:LEU:HA	1:156:A:LEU:HD11	3	0.1
(1,587)	1:139:A:VAL:HG22	1:138:A:LYS:HA	6	0.1
(1,521)	1:191:A:TYR:HB3	1:155:A:LEU:HD21	1	0.1
(1,496)	1:130:A:ILE:HG12	1:130:A:ILE:HA	2	0.1
(1,456)	1:134:A:LYS:HD3	1:157:A:TYR:HE1	5	0.1
(1,433)	1:184:A:GLU:HB3	1:184:A:GLU:H	4	0.1
(1,395)	1:167:A:MET:HB2	1:167:A:MET:HG2	7	0.1
(1,390)	1:204:A:ARG:HB3	1:204:A:ARG:H	2	0.1
(1,377)	1:183:A:VAL:HB	1:184:A:GLU:H	1	0.1
(1,375)	1:141:A:VAL:HB	1:141:A:VAL:H	3	0.1
(1,360)	1:147:A:GLU:HG3	1:147:A:GLU:HA	8	0.1
(1,323)	1:128:A:ASN:HB2	1:128:A:ASN:HA	7	0.1
(1,195)	1:215:A:GLY:HA2	1:169:A:ARG:HG2	2	0.1
(1,185)	1:201:A:PRO:HD3	1:201:A:PRO:HB2	4	0.1
(1,185)	1:201:A:PRO:HD3	1:201:A:PRO:HB2	8	0.1
(1,185)	1:201:A:PRO:HD3	1:201:A:PRO:HB2	10	0.1
(1,169)	1:160:A:ALA:HA	1:218:A:ILE:HB	3	0.1
(1,133)	1:159:A:LEU:HA	1:162:A:ASN:HB2	2	0.1

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

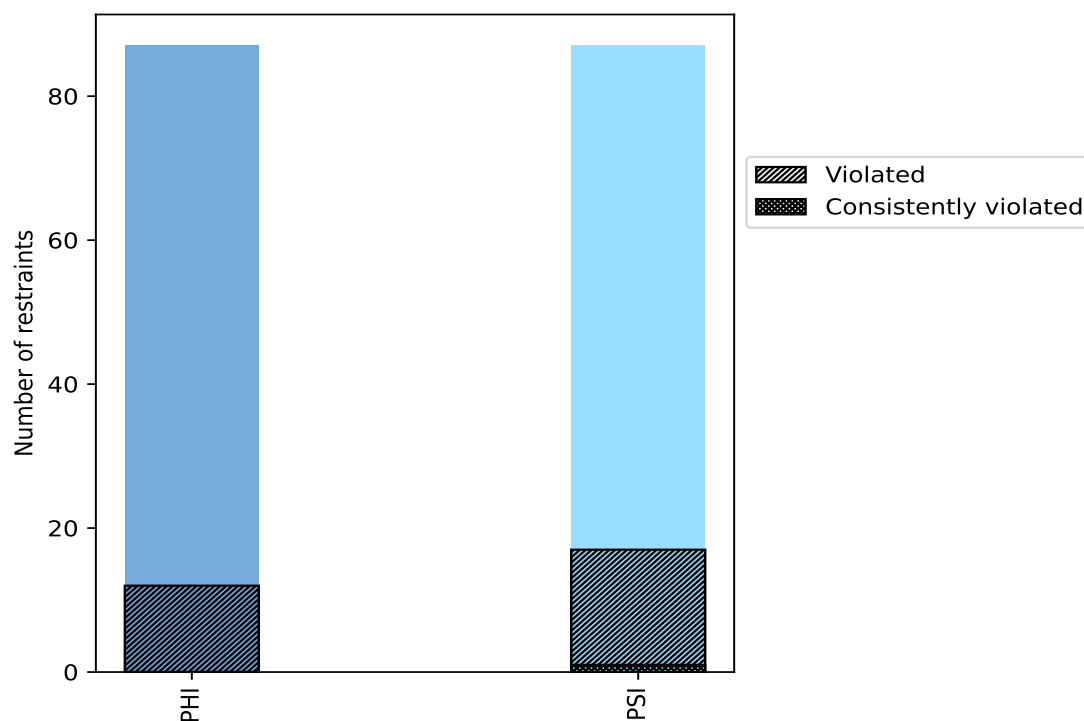
10.1 Summary of dihedral-angle violations [i](#)

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	87	50.0	12	13.8	6.9	0	0.0	0.0
PSI	87	50.0	17	19.5	9.8	1	1.1	0.6
Total	174	100.0	29	16.7	16.7	1	0.6	0.6

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](#)



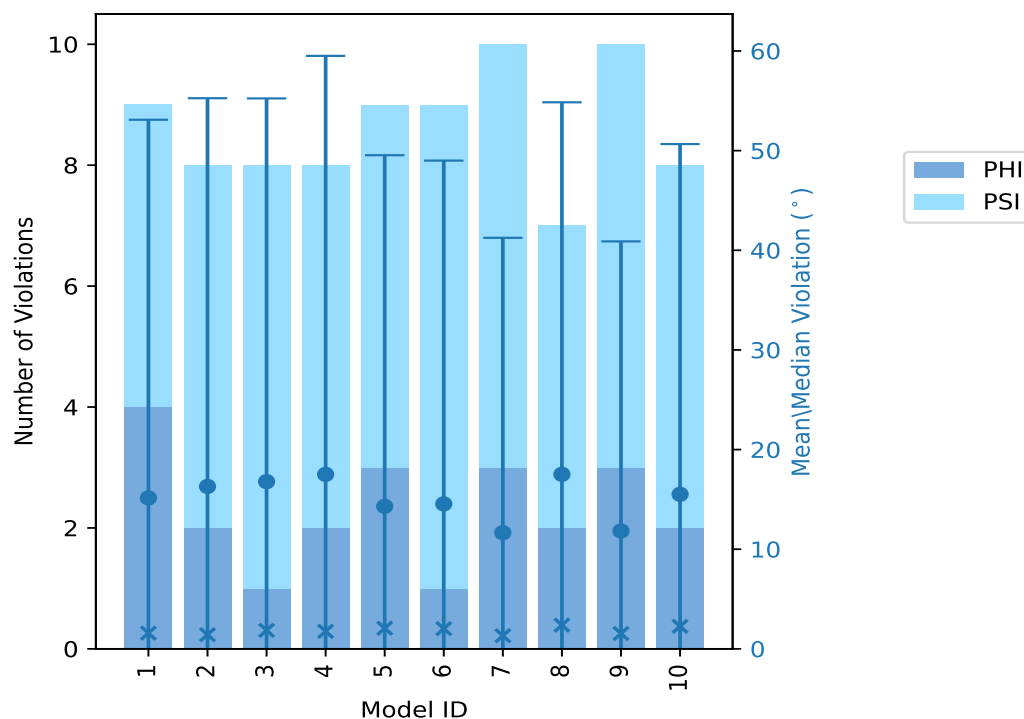
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model [i](#)

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	4	5	9	15.15	122.48	37.95	1.58
2	2	6	8	16.3	119.37	38.96	1.42
3	1	7	8	16.78	118.48	38.46	1.86
4	2	6	8	17.51	128.62	42.0	1.76
5	3	6	9	14.3	113.95	35.24	2.07
6	1	8	9	14.55	111.93	34.45	2.03
7	3	7	10	11.66	100.35	29.59	1.32
8	2	5	7	17.52	108.94	37.33	2.38
9	3	7	10	11.83	98.97	29.06	1.54
10	2	6	8	15.51	108.49	35.15	2.26

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

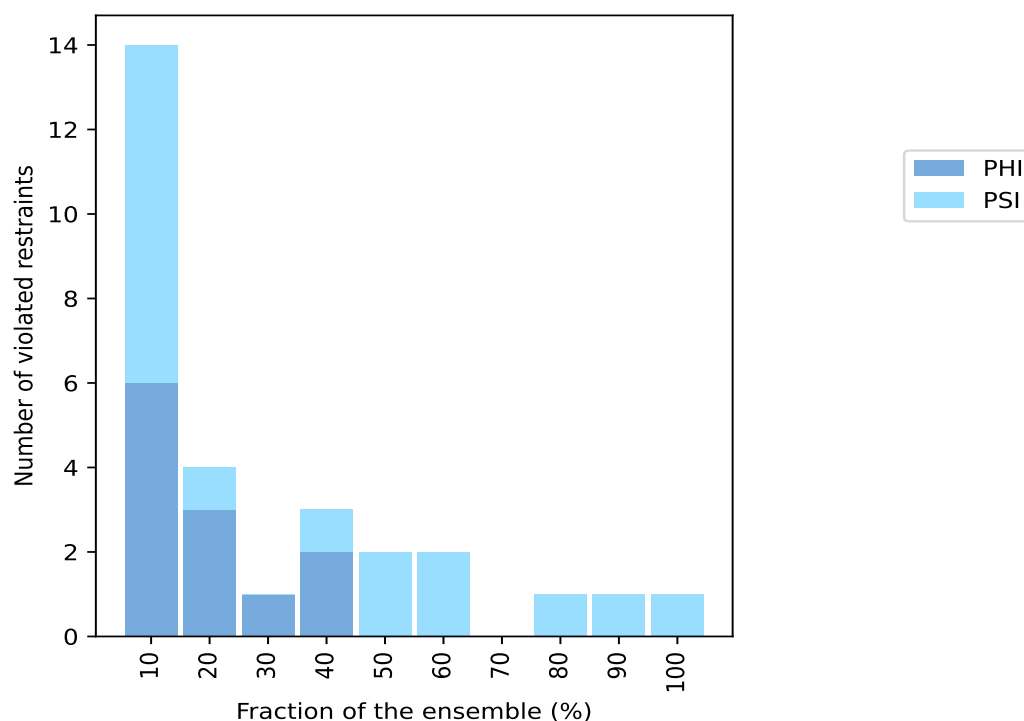
10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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	%
6	8	14	1	10.0
3	1	4	2	20.0
1	0	1	3	30.0
2	1	3	4	40.0
0	2	2	5	50.0
0	2	2	6	60.0
0	0	0	7	70.0
0	1	1	8	80.0
0	1	1	9	90.0
0	1	1	10	100.0

¹ Number of models with violations

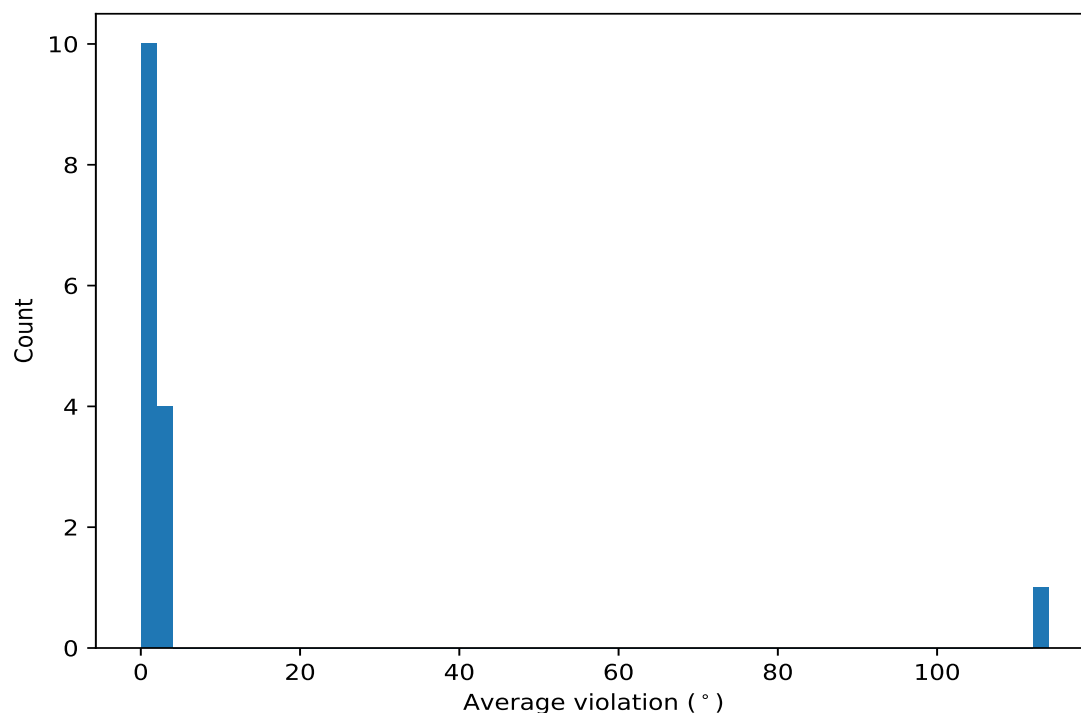
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,148)	1:204:A:ARG:N	1:204:A:ARG:CA	1:204:A:ARG:C	1:205:A:ASP:N	10	113.16	8.94	112.94
(1,154)	1:207:A:MET:N	1:207:A:MET:CA	1:207:A:MET:C	1:208:A:ILE:N	9	2.29	1.29	1.93
(1,156)	1:208:A:ILE:N	1:208:A:ILE:CA	1:208:A:ILE:C	1:209:A:GLU:N	8	1.7	0.63	1.68
(1,110)	1:183:A:VAL:N	1:183:A:VAL:CA	1:183:A:VAL:C	1:184:A:GLU:N	6	2.71	1.59	2.01
(1,114)	1:185:A:THR:N	1:185:A:THR:CA	1:185:A:THR:C	1:186:A:ASN:N	6	1.95	0.59	1.96
(1,78)	1:162:A:ASN:N	1:162:A:ASN:CA	1:162:A:ASN:C	1:163:A:LYS:N	5	2.72	0.98	3.3
(1,16)	1:131:A:THR:N	1:131:A:THR:CA	1:131:A:THR:C	1:132:A:ILE:N	5	1.64	0.74	1.39
(1,13)	1:129:A:GLY:C	1:130:A:ILE:N	1:130:A:ILE:CA	1:130:A:ILE:C	4	2.55	0.52	2.52
(1,153)	1:206:A:LYS:C	1:207:A:MET:N	1:207:A:MET:CA	1:207:A:MET:C	4	1.99	0.25	2.04
(1,106)	1:177:A:TRP:N	1:177:A:TRP:CA	1:177:A:TRP:C	1:178:A:GLY:N	4	1.55	0.26	1.54
(1,1)	1:123:A:ASP:C	1:124:A:ILE:N	1:124:A:ILE:CA	1:124:A:ILE:C	3	1.26	0.04	1.25
(1,91)	1:169:A:ARG:C	1:170:A:GLU:N	1:170:A:GLU:CA	1:170:A:GLU:C	2	1.52	0.17	1.52
(1,116)	1:186:A:ASN:N	1:186:A:ASN:CA	1:186:A:ASN:C	1:187:A:VAL:N	2	1.38	0.09	1.38

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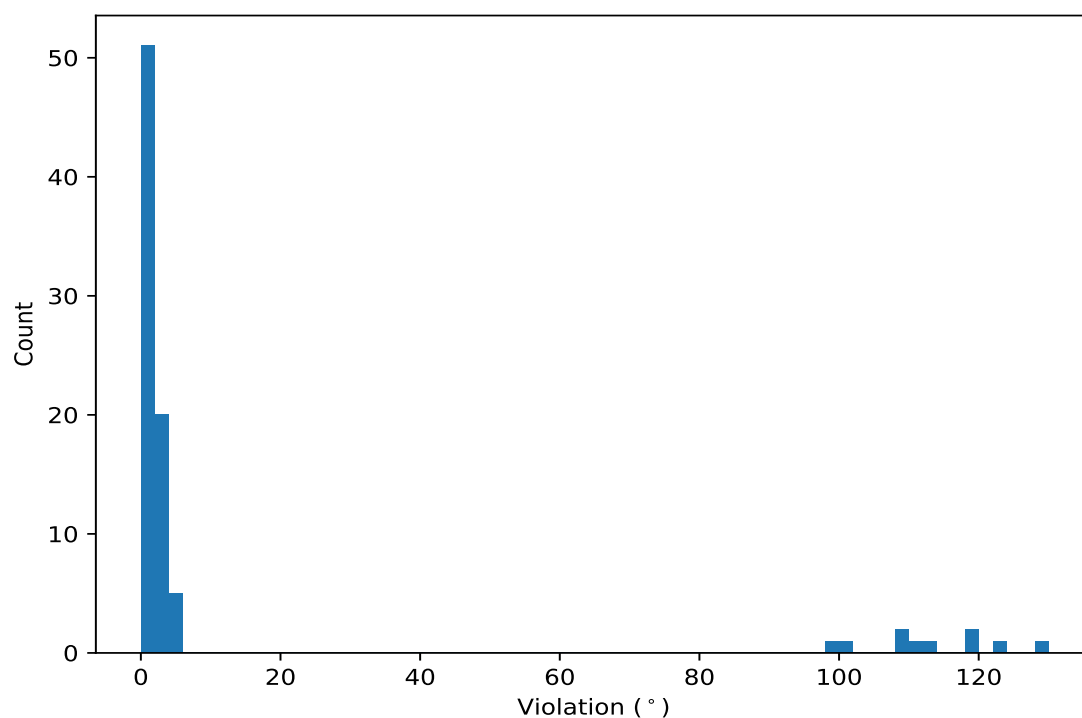
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,5)	1:125:A:ILE:C	1:126:A:ASP:N	1:126:A:ASP:CA	1:126:A:ASP:C	2	1.27	0.19	1.27
(1,23)	1:134:A:LYS:C	1:135:A:ASN:N	1:135:A:ASN:CA	1:135:A:ASN:C	2	1.23	0.1	1.23

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 (°)
(1,148)	1:204:A:ARG:N	1:204:A:ARG:CA	1:204:A:ARG:C	1:205:A:ASP:N	4	128.62
(1,148)	1:204:A:ARG:N	1:204:A:ARG:CA	1:204:A:ARG:C	1:205:A:ASP:N	1	122.48
(1,148)	1:204:A:ARG:N	1:204:A:ARG:CA	1:204:A:ARG:C	1:205:A:ASP:N	2	119.37
(1,148)	1:204:A:ARG:N	1:204:A:ARG:CA	1:204:A:ARG:C	1:205:A:ASP:N	3	118.48
(1,148)	1:204:A:ARG:N	1:204:A:ARG:CA	1:204:A:ARG:C	1:205:A:ASP:N	5	113.95

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,148)	1:204:A:ARG:N	1:204:A:ARG:CA	1:204:A:ARG:C	1:205:A:ASP:N	6	111.93
(1,148)	1:204:A:ARG:N	1:204:A:ARG:CA	1:204:A:ARG:C	1:205:A:ASP:N	8	108.94
(1,148)	1:204:A:ARG:N	1:204:A:ARG:CA	1:204:A:ARG:C	1:205:A:ASP:N	10	108.49
(1,148)	1:204:A:ARG:N	1:204:A:ARG:CA	1:204:A:ARG:C	1:205:A:ASP:N	7	100.35
(1,148)	1:204:A:ARG:N	1:204:A:ARG:CA	1:204:A:ARG:C	1:205:A:ASP:N	9	98.97
(1,154)	1:207:A:MET:N	1:207:A:MET:CA	1:207:A:MET:C	1:208:A:ILE:N	7	5.41
(1,110)	1:183:A:VAL:N	1:183:A:VAL:CA	1:183:A:VAL:C	1:184:A:GLU:N	3	4.95
(1,110)	1:183:A:VAL:N	1:183:A:VAL:CA	1:183:A:VAL:C	1:184:A:GLU:N	6	4.84
(1,168)	1:215:A:GLY:N	1:215:A:GLY:CA	1:215:A:GLY:C	1:216:A:TYR:N	9	4.47
(1,79)	1:163:A:LYS:C	1:164:A:ASN:N	1:164:A:ASN:CA	1:164:A:ASN:C	8	4.03
(1,78)	1:162:A:ASN:N	1:162:A:ASN:CA	1:162:A:ASN:C	1:163:A:LYS:N	6	3.82
(1,78)	1:162:A:ASN:N	1:162:A:ASN:CA	1:162:A:ASN:C	1:163:A:LYS:N	1	3.38
(1,78)	1:162:A:ASN:N	1:162:A:ASN:CA	1:162:A:ASN:C	1:163:A:LYS:N	10	3.3
(1,174)	1:218:A:ILE:N	1:218:A:ILE:CA	1:218:A:ILE:C	1:219:A:ARG:N	5	3.29
(1,13)	1:129:A:GLY:C	1:130:A:ILE:N	1:130:A:ILE:CA	1:130:A:ILE:C	9	3.19
(1,156)	1:208:A:ILE:N	1:208:A:ILE:CA	1:208:A:ILE:C	1:209:A:GLU:N	9	3.11
(1,16)	1:131:A:THR:N	1:131:A:THR:CA	1:131:A:THR:C	1:132:A:ILE:N	6	3.1
(1,154)	1:207:A:MET:N	1:207:A:MET:CA	1:207:A:MET:C	1:208:A:ILE:N	8	3.08
(1,114)	1:185:A:THR:N	1:185:A:THR:CA	1:185:A:THR:C	1:186:A:ASN:N	2	3.02
(1,13)	1:129:A:GLY:C	1:130:A:ILE:N	1:130:A:ILE:CA	1:130:A:ILE:C	3	2.94
(1,154)	1:207:A:MET:N	1:207:A:MET:CA	1:207:A:MET:C	1:208:A:ILE:N	10	2.79
(1,110)	1:183:A:VAL:N	1:183:A:VAL:CA	1:183:A:VAL:C	1:184:A:GLU:N	8	2.38
(1,47)	1:146:A:ILE:C	1:147:A:GLU:N	1:147:A:GLU:CA	1:147:A:GLU:C	10	2.35
(1,154)	1:207:A:MET:N	1:207:A:MET:CA	1:207:A:MET:C	1:208:A:ILE:N	5	2.29
(1,153)	1:206:A:LYS:C	1:207:A:MET:N	1:207:A:MET:CA	1:207:A:MET:C	5	2.29
(1,114)	1:185:A:THR:N	1:185:A:THR:CA	1:185:A:THR:C	1:186:A:ASN:N	10	2.16
(1,13)	1:129:A:GLY:C	1:130:A:ILE:N	1:130:A:ILE:CA	1:130:A:ILE:C	7	2.1
(1,153)	1:206:A:LYS:C	1:207:A:MET:N	1:207:A:MET:CA	1:207:A:MET:C	8	2.09
(1,114)	1:185:A:THR:N	1:185:A:THR:CA	1:185:A:THR:C	1:186:A:ASN:N	5	2.07
(1,156)	1:208:A:ILE:N	1:208:A:ILE:CA	1:208:A:ILE:C	1:209:A:GLU:N	6	2.03
(1,153)	1:206:A:LYS:C	1:207:A:MET:N	1:207:A:MET:CA	1:207:A:MET:C	1	1.98
(1,101)	1:174:A:ASN:C	1:175:A:HIS:N	1:175:A:HIS:CA	1:175:A:HIS:C	1	1.98
(1,13)	1:129:A:GLY:C	1:130:A:ILE:N	1:130:A:ILE:CA	1:130:A:ILE:C	4	1.98
(1,154)	1:207:A:MET:N	1:207:A:MET:CA	1:207:A:MET:C	1:208:A:ILE:N	4	1.93
(1,106)	1:177:A:TRP:N	1:177:A:TRP:CA	1:177:A:TRP:C	1:178:A:GLY:N	3	1.91
(1,114)	1:185:A:THR:N	1:185:A:THR:CA	1:185:A:THR:C	1:186:A:ASN:N	4	1.86
(1,156)	1:208:A:ILE:N	1:208:A:ILE:CA	1:208:A:ILE:C	1:209:A:GLU:N	3	1.81
(1,171)	1:216:A:TYR:C	1:217:A:VAL:N	1:217:A:VAL:CA	1:217:A:VAL:C	2	1.79
(1,156)	1:208:A:ILE:N	1:208:A:ILE:CA	1:208:A:ILE:C	1:209:A:GLU:N	10	1.77
(1,78)	1:162:A:ASN:N	1:162:A:ASN:CA	1:162:A:ASN:C	1:163:A:LYS:N	7	1.7
(1,91)	1:169:A:ARG:C	1:170:A:GLU:N	1:170:A:GLU:CA	1:170:A:GLU:C	10	1.69
(1,110)	1:183:A:VAL:N	1:183:A:VAL:CA	1:183:A:VAL:C	1:184:A:GLU:N	4	1.65
(1,106)	1:177:A:TRP:N	1:177:A:TRP:CA	1:177:A:TRP:C	1:178:A:GLY:N	9	1.61
(1,153)	1:206:A:LYS:C	1:207:A:MET:N	1:207:A:MET:CA	1:207:A:MET:C	4	1.59
(1,156)	1:208:A:ILE:N	1:208:A:ILE:CA	1:208:A:ILE:C	1:209:A:GLU:N	1	1.58
(1,50)	1:148:A:LEU:N	1:148:A:LEU:CA	1:148:A:LEU:C	1:149:A:THR:N	10	1.54
(1,154)	1:207:A:MET:N	1:207:A:MET:CA	1:207:A:MET:C	1:208:A:ILE:N	3	1.47
(1,116)	1:186:A:ASN:N	1:186:A:ASN:CA	1:186:A:ASN:C	1:187:A:VAL:N	9	1.47
(1,5)	1:125:A:ILE:C	1:126:A:ASP:N	1:126:A:ASP:CA	1:126:A:ASP:C	6	1.47
(1,106)	1:177:A:TRP:N	1:177:A:TRP:CA	1:177:A:TRP:C	1:178:A:GLY:N	2	1.46
(1,16)	1:131:A:THR:N	1:131:A:THR:CA	1:131:A:THR:C	1:132:A:ILE:N	9	1.46

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,154)	1:207:A:MET:N	1:207:A:MET:CA	1:207:A:MET:C	1:208:A:ILE:N	1	1.43
(1,110)	1:183:A:VAL:N	1:183:A:VAL:CA	1:183:A:VAL:C	1:184:A:GLU:N	7	1.39
(1,16)	1:131:A:THR:N	1:131:A:THR:CA	1:131:A:THR:C	1:132:A:ILE:N	3	1.39
(1,12)	1:129:A:GLY:N	1:129:A:GLY:CA	1:129:A:GLY:C	1:130:A:ILE:N	2	1.39
(1,78)	1:162:A:ASN:N	1:162:A:ASN:CA	1:162:A:ASN:C	1:163:A:LYS:N	5	1.38
(1,114)	1:185:A:THR:N	1:185:A:THR:CA	1:185:A:THR:C	1:186:A:ASN:N	9	1.35
(1,91)	1:169:A:ARG:C	1:170:A:GLU:N	1:170:A:GLU:CA	1:170:A:GLU:C	9	1.34
(1,90)	1:169:A:ARG:N	1:169:A:ARG:CA	1:169:A:ARG:C	1:170:A:GLU:N	6	1.33
(1,23)	1:134:A:LYS:C	1:135:A:ASN:N	1:135:A:ASN:CA	1:135:A:ASN:C	9	1.33
(1,1)	1:123:A:ASP:C	1:124:A:ILE:N	1:124:A:ILE:CA	1:124:A:ILE:C	2	1.31
(1,116)	1:186:A:ASN:N	1:186:A:ASN:CA	1:186:A:ASN:C	1:187:A:VAL:N	3	1.29
(1,114)	1:185:A:THR:N	1:185:A:THR:CA	1:185:A:THR:C	1:186:A:ASN:N	7	1.25
(1,20)	1:133:A:ASP:N	1:133:A:ASP:CA	1:133:A:ASP:C	1:134:A:LYS:N	6	1.25
(1,1)	1:123:A:ASP:C	1:124:A:ILE:N	1:124:A:ILE:CA	1:124:A:ILE:C	5	1.25
(1,6)	1:126:A:ASP:N	1:126:A:ASP:CA	1:126:A:ASP:C	1:127:A:VAL:N	4	1.24
(1,1)	1:123:A:ASP:C	1:124:A:ILE:N	1:124:A:ILE:CA	1:124:A:ILE:C	1	1.21
(1,156)	1:208:A:ILE:N	1:208:A:ILE:CA	1:208:A:ILE:C	1:209:A:GLU:N	4	1.2
(1,106)	1:177:A:TRP:N	1:177:A:TRP:CA	1:177:A:TRP:C	1:178:A:GLY:N	7	1.2
(1,55)	1:150:A:LYS:C	1:151:A:THR:N	1:151:A:THR:CA	1:151:A:THR:C	1	1.19
(1,154)	1:207:A:MET:N	1:207:A:MET:CA	1:207:A:MET:C	1:208:A:ILE:N	6	1.16
(1,16)	1:131:A:THR:N	1:131:A:THR:CA	1:131:A:THR:C	1:132:A:ILE:N	8	1.13
(1,23)	1:134:A:LYS:C	1:135:A:ASN:N	1:135:A:ASN:CA	1:135:A:ASN:C	7	1.12
(1,16)	1:131:A:THR:N	1:131:A:THR:CA	1:131:A:THR:C	1:132:A:ILE:N	1	1.12
(1,156)	1:208:A:ILE:N	1:208:A:ILE:CA	1:208:A:ILE:C	1:209:A:GLU:N	7	1.11
(1,170)	1:216:A:TYR:N	1:216:A:TYR:CA	1:216:A:TYR:C	1:217:A:VAL:N	5	1.1
(1,5)	1:125:A:ILE:C	1:126:A:ASP:N	1:126:A:ASP:CA	1:126:A:ASP:C	5	1.08
(1,110)	1:183:A:VAL:N	1:183:A:VAL:CA	1:183:A:VAL:C	1:184:A:GLU:N	2	1.06
(1,154)	1:207:A:MET:N	1:207:A:MET:CA	1:207:A:MET:C	1:208:A:ILE:N	2	1.02
(1,29)	1:137:A:PHE:C	1:138:A:LYS:N	1:138:A:LYS:CA	1:138:A:LYS:C	7	1.01
(1,156)	1:208:A:ILE:N	1:208:A:ILE:CA	1:208:A:ILE:C	1:209:A:GLU:N	8	1.0