



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 01:48 PM UTC

PDB ID : 8PEK / pdb_00008pek
BMRB ID : 34826
Title : Structure of the dimeric, periplasmic domain of ExbD
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Deposited on : 2023-06-14

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

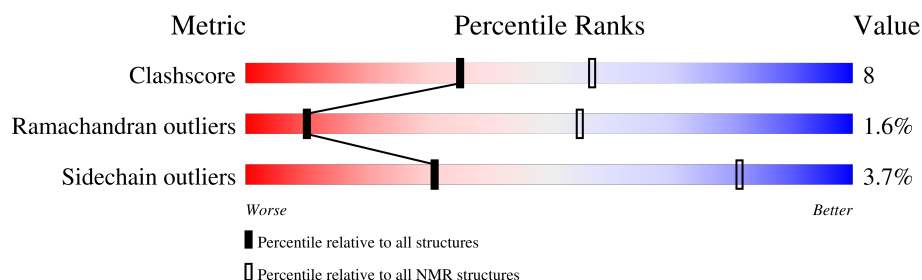
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 47%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	99	
1	B	99	

2 Ensemble composition and analysis

This entry contains 10 models. Model 7 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:43-A:137, B:43-B:137 (190)	0.46	7

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

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

The models can be grouped into 2 clusters and 1 single-model cluster was found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3056 atoms, of which 1544 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Biopolymer transport protein ExbD.

Mol	Chain	Residues	Atoms						Trace
1	A	98	Total	C	H	N	O	S	0
			1528	476	772	128	149	3	
1	B	98	Total	C	H	N	O	S	0
			1528	476	772	128	149	3	

There are 2 discrepancies between the modelled and reference sequences:

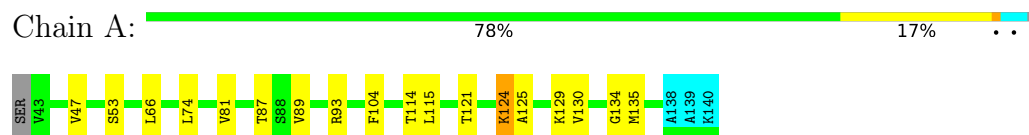
Chain	Residue	Modelled	Actual	Comment	Reference
A	42	SER	-	expression tag	UNP V5YUQ0
B	42	SER	-	expression tag	UNP V5YUQ0

4 Residue-property plots

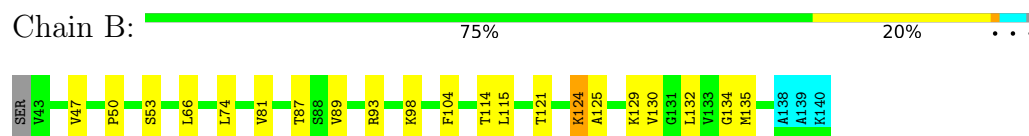
4.1 Average score per residue in the NMR ensemble

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: Biopolymer transport protein ExbD



- Molecule 1: Biopolymer transport protein ExbD

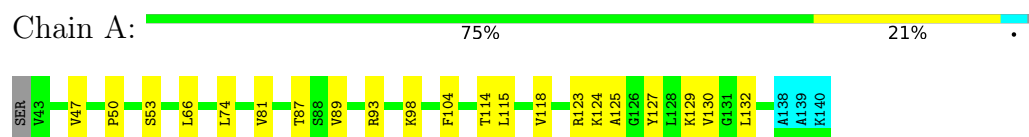


4.2 Scores per residue for each member of the ensemble

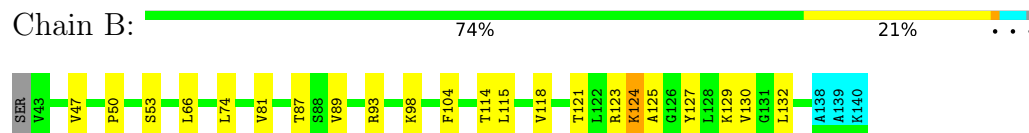
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Biopolymer transport protein ExbD

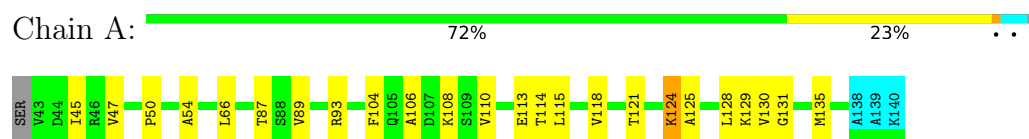


- Molecule 1: Biopolymer transport protein ExbD

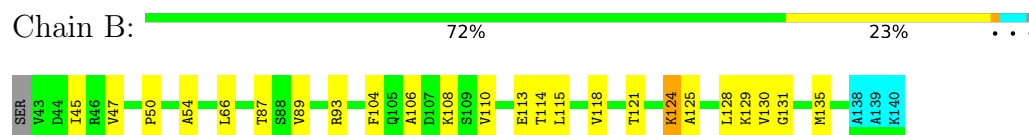


4.2.2 Score per residue for model 2

- Molecule 1: Biopolymer transport protein ExbD

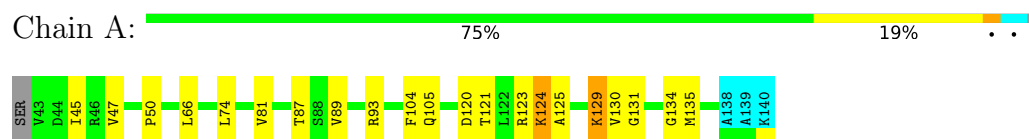


- Molecule 1: Biopolymer transport protein ExbD

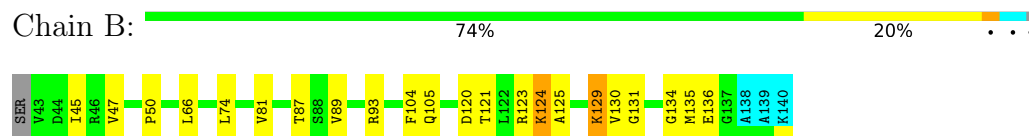


4.2.3 Score per residue for model 3

- Molecule 1: Biopolymer transport protein ExbD

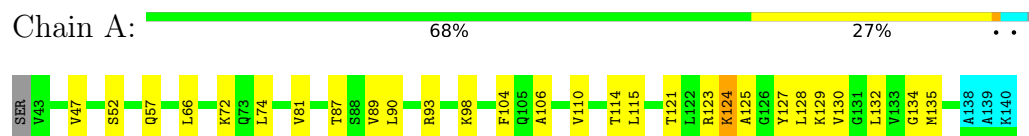


- Molecule 1: Biopolymer transport protein ExbD

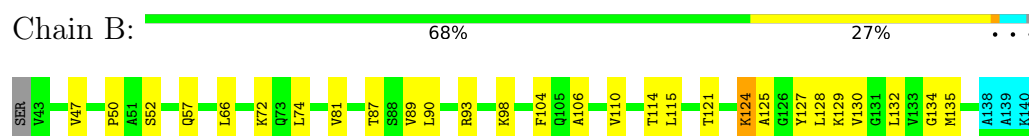


4.2.4 Score per residue for model 4

- Molecule 1: Biopolymer transport protein ExbD

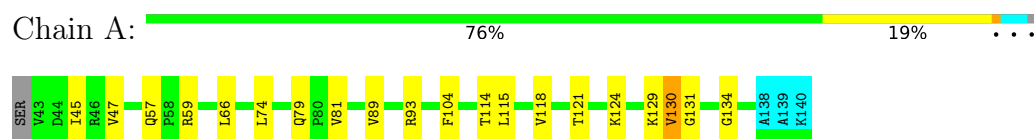


- Molecule 1: Biopolymer transport protein ExbD

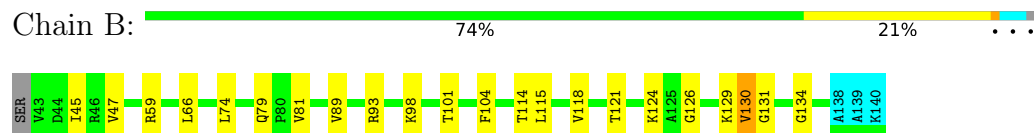


4.2.5 Score per residue for model 5

- Molecule 1: Biopolymer transport protein ExbD

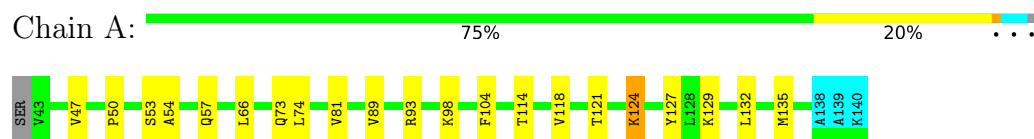


- Molecule 1: Biopolymer transport protein ExbD

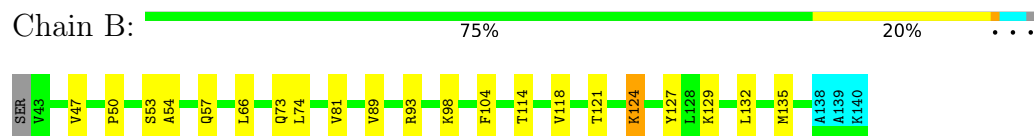


4.2.6 Score per residue for model 6

- Molecule 1: Biopolymer transport protein ExbD

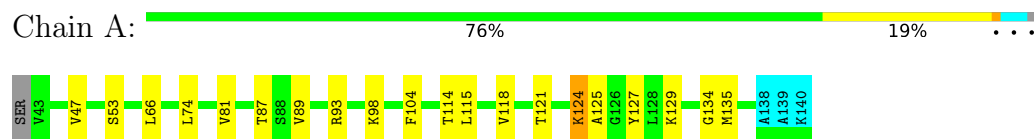


- Molecule 1: Biopolymer transport protein ExbD

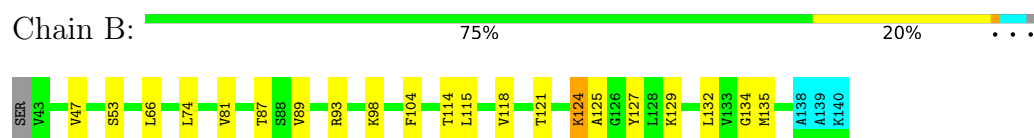


4.2.7 Score per residue for model 7 (medoid)

- Molecule 1: Biopolymer transport protein ExbD



- Molecule 1: Biopolymer transport protein ExbD



4.2.8 Score per residue for model 8

- Molecule 1: Biopolymer transport protein ExbD

Chain A: 



- Molecule 1: Biopolymer transport protein ExbD

Chain B: 



4.2.9 Score per residue for model 9

- Molecule 1: Biopolymer transport protein ExbD

Chain A: 



- Molecule 1: Biopolymer transport protein ExbD

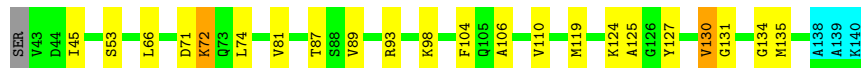
Chain B: 



4.2.10 Score per residue for model 10

- Molecule 1: Biopolymer transport protein ExbD

Chain A: 



- Molecule 1: Biopolymer transport protein ExbD

Chain B: 



5 Refinement protocol and experimental data overview

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

Of the 50 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
CNS	structure calculation	1.2
ARIA	structure calculation	2.3.3

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	1234
Number of shifts mapped to atoms	1234
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	47%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	736	749	748	14±2
1	B	736	749	748	14±2
All	All	14720	14980	14960	233

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 8.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:129:LYS:HA	1:B:47:VAL:O	0.60	1.96	9	9
1:A:47:VAL:O	1:B:129:LYS:HA	0.60	1.96	9	9
1:B:74:LEU:HB2	1:B:81:VAL:O	0.58	1.99	7	9
1:A:74:LEU:HB2	1:A:81:VAL:O	0.57	1.99	7	9
1:A:66:LEU:O	1:A:104:PHE:HA	0.56	2.00	7	10
1:B:66:LEU:O	1:B:104:PHE:HA	0.56	2.01	7	10
1:A:121:THR:O	1:A:124:LYS:HG3	0.56	2.00	5	8
1:B:121:THR:O	1:B:124:LYS:HG3	0.55	2.01	5	9
1:A:104:PHE:CE2	1:A:115:LEU:HD11	0.54	2.38	4	3
1:B:104:PHE:CE2	1:B:115:LEU:HD11	0.54	2.38	4	3
1:B:89:VAL:O	1:B:93:ARG:HG2	0.53	2.04	1	10
1:A:47:VAL:HG22	1:B:47:VAL:HG13	0.51	1.82	2	2
1:A:89:VAL:O	1:A:93:ARG:HG2	0.51	2.04	1	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:98:LYS:O	1:A:127:TYR:HA	0.50	2.06	4	5
1:B:98:LYS:O	1:B:127:TYR:HA	0.50	2.07	4	5
1:A:47:VAL:HG13	1:B:47:VAL:HG22	0.49	1.83	2	2
1:B:104:PHE:CE1	1:B:115:LEU:HD11	0.49	2.43	1	3
1:A:104:PHE:CE1	1:A:115:LEU:HD11	0.49	2.43	1	3
1:A:106:ALA:HB1	1:A:110:VAL:HG21	0.48	1.85	2	3
1:B:114:THR:O	1:B:118:VAL:HG23	0.48	2.08	5	5
1:A:114:THR:O	1:A:118:VAL:HG23	0.47	2.08	5	5
1:A:135:MET:SD	1:B:113:GLU:HA	0.47	2.49	2	1
1:A:50:PRO:HB2	1:A:54:ALA:HB3	0.46	1.87	9	3
1:A:131:GLY:HA2	1:B:45:ILE:O	0.46	2.11	2	5
1:B:50:PRO:HB2	1:B:54:ALA:HB3	0.46	1.87	2	3
1:B:106:ALA:HB1	1:B:110:VAL:HG21	0.46	1.85	2	3
1:A:113:GLU:HA	1:B:135:MET:SD	0.46	2.51	2	1
1:A:87:THR:CG2	1:A:125:ALA:HB2	0.45	2.42	1	8
1:B:87:THR:CG2	1:B:125:ALA:HB2	0.44	2.42	1	8
1:A:123:ARG:HG3	1:B:50:PRO:O	0.44	2.11	3	1
1:A:130:VAL:HG12	1:B:47:VAL:HB	0.44	1.89	8	3
1:A:74:LEU:HD12	1:A:74:LEU:N	0.44	2.28	7	7
1:A:128:LEU:C	1:A:129:LYS:HD2	0.44	2.38	2	2
1:B:104:PHE:CZ	1:B:132:LEU:HD23	0.43	2.47	4	3
1:B:128:LEU:C	1:B:129:LYS:HD2	0.43	2.38	2	2
1:A:104:PHE:CZ	1:A:132:LEU:HD23	0.43	2.47	4	3
1:A:45:ILE:O	1:B:131:GLY:HA2	0.43	2.13	2	5
1:A:123:ARG:HD2	1:B:50:PRO:O	0.43	2.14	1	2
1:B:74:LEU:N	1:B:74:LEU:HD12	0.42	2.28	7	5
1:A:47:VAL:HB	1:B:130:VAL:HG12	0.42	1.90	8	3
1:A:50:PRO:O	1:B:123:ARG:HG3	0.42	2.14	3	1
1:A:50:PRO:O	1:B:123:ARG:HD2	0.42	2.14	1	1
1:A:120:ASP:O	1:A:123:ARG:HB3	0.42	2.14	3	1
1:A:57:GLN:HA	1:A:57:GLN:OE1	0.42	2.15	4	3
1:B:57:GLN:HA	1:B:57:GLN:OE1	0.42	2.15	4	1
1:B:71:ASP:O	1:B:72:LYS:HB2	0.41	2.15	10	1
1:B:136:GLU:O	1:B:136:GLU:HG2	0.41	2.16	3	1
1:B:72:LYS:HD2	1:B:114:THR:HG21	0.41	1.92	4	1
1:B:93:ARG:HA	1:B:93:ARG:CZ	0.41	2.45	8	2
1:A:119:MET:SD	1:A:130:VAL:HG21	0.41	2.55	10	1
1:A:62:LYS:O	1:A:100:THR:HG21	0.41	2.15	9	1
1:B:62:LYS:O	1:B:100:THR:HG21	0.41	2.15	9	1
1:A:72:LYS:HD2	1:A:114:THR:HG21	0.41	1.91	4	1
1:A:93:ARG:CZ	1:A:93:ARG:HA	0.41	2.46	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:128:LEU:O	1:B:48:ASP:HA	0.41	2.16	8	1
1:A:71:ASP:O	1:A:72:LYS:HB2	0.41	2.15	10	1
1:A:132:LEU:O	1:A:132:LEU:HG	0.41	2.15	6	1
1:B:57:GLN:OE1	1:B:57:GLN:HA	0.41	2.16	6	1
1:B:132:LEU:HG	1:B:132:LEU:O	0.41	2.16	6	1
1:B:132:LEU:H	1:B:132:LEU:HD23	0.41	1.76	7	1
1:A:48:ASP:HA	1:B:128:LEU:O	0.41	2.16	8	1
1:B:119:MET:SD	1:B:130:VAL:HG21	0.41	2.55	10	1
1:A:74:LEU:N	1:A:74:LEU:HD12	0.40	2.32	10	2
1:A:93:ARG:NE	1:A:93:ARG:HA	0.40	2.31	5	1
1:B:90:LEU:HB3	1:B:127:TYR:OH	0.40	2.16	10	1
1:B:74:LEU:HD12	1:B:74:LEU:N	0.40	2.30	5	1
1:B:120:ASP:O	1:B:123:ARG:HB3	0.40	2.16	3	1
1:B:98:LYS:HB3	1:B:126:GLY:O	0.40	2.16	5	1
1:B:101:THR:HA	1:B:129:LYS:O	0.40	2.17	5	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	94/99 (95%)	88±1 (93±1%)	5±2 (5±2%)	2±1 (2±1%)	10	55
1	B	94/99 (95%)	88±1 (93±1%)	5±2 (5±2%)	2±1 (2±1%)	10	55
All	All	1880/1980 (95%)	1750 (93%)	100 (5%)	30 (2%)	10	55

All 8 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	134	GLY	7
1	B	134	GLY	7
1	A	53	SER	6
1	B	53	SER	6
1	A	52	SER	1
1	B	52	SER	1

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Mol	Chain	Res	Type	Models (Total)
1	A	59	ARG	1
1	B	59	ARG	1

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	83/85 (98%)	80±1 (96±2%)	3±1 (4±2%)	31	81
1	B	83/85 (98%)	80±1 (96±2%)	3±1 (4±2%)	31	81
All	All	1660/1700 (98%)	1598 (96%)	62 (4%)	31	81

All 20 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	124	LYS	9
1	B	124	LYS	9
1	A	135	MET	7
1	B	135	MET	7
1	A	130	VAL	6
1	B	130	VAL	6
1	A	129	LYS	2
1	B	129	LYS	2
1	A	90	LEU	2
1	B	90	LEU	2
1	A	108	LYS	1
1	B	108	LYS	1
1	A	79	GLN	1
1	B	79	GLN	1
1	A	73	GLN	1
1	B	73	GLN	1
1	A	132	LEU	1
1	B	132	LEU	1
1	A	72	LYS	1
1	B	72	LYS	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

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 47% for the well-defined parts and 47% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list*

7.1.1 Bookkeeping

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	1234
Number of shifts mapped to atoms	1234
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

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	-0.17 ± 0.12	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	92	0.53 ± 0.19	Should be checked
$^{13}\text{C}'$	97	-0.03 ± 0.12	None needed (< 0.5 ppm)
^{15}N	90	-0.91 ± 0.36	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 47%, i.e. 1199 atoms were assigned a chemical shift out of a possible 2572. 0 out of 40 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	459/936 (49%)	184/378 (49%)	188/380 (49%)	87/178 (49%)
Sidechain	686/1522 (45%)	466/988 (47%)	211/476 (44%)	9/58 (16%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	54/114 (47%)	27/54 (50%)	27/60 (45%)	0/0 (—%)
Overall	1199/2572 (47%)	677/1420 (48%)	426/916 (47%)	96/236 (41%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 47%, i.e. 1234 atoms were assigned a chemical shift out of a possible 2644. 0 out of 40 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	474/966 (49%)	190/390 (49%)	194/392 (49%)	90/184 (49%)
Sidechain	706/1564 (45%)	480/1016 (47%)	217/488 (44%)	9/60 (15%)
Aromatic	54/114 (47%)	27/54 (50%)	27/60 (45%)	0/0 (—%)
Overall	1234/2644 (47%)	697/1460 (48%)	438/940 (47%)	99/244 (41%)

7.1.4 Statistically unusual chemical shifts ⓘ

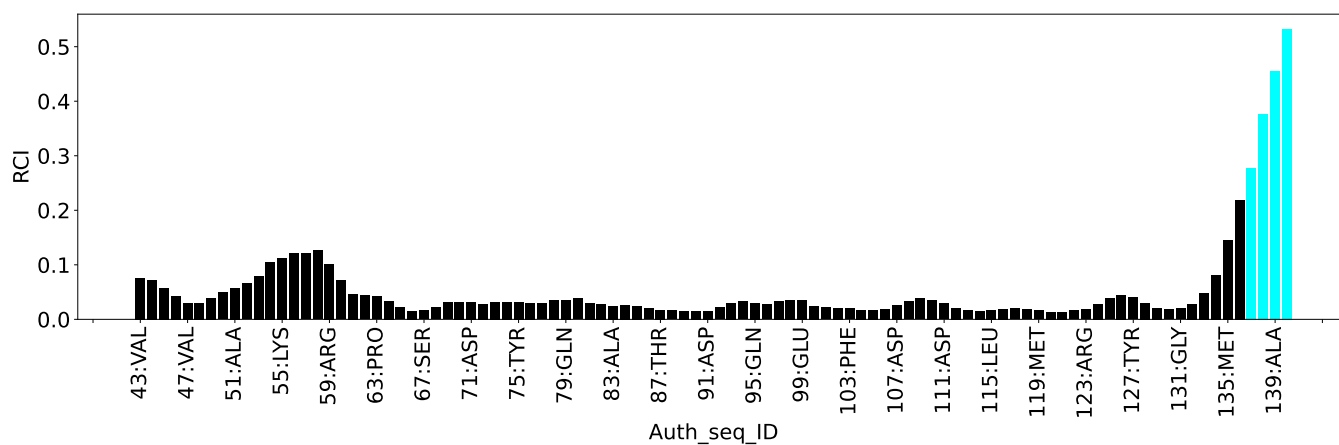
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	101	THR	HG21	0.01	0.08 – 2.19	-5.3
1	A	101	THR	HG22	0.01	0.08 – 2.19	-5.3
1	A	101	THR	HG23	0.01	0.08 – 2.19	-5.3

7.1.5 Random Coil Index (RCI) plots ⓘ

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	9092
Intra-residue ($ i-j =0$)	1774
Sequential ($ i-j =1$)	1764
Medium range ($ i-j >1$ and $ i-j <5$)	1888
Long range ($ i-j \geq 5$)	2772
Inter-chain	892
Hydrogen bond restraints	2
Disulfide bond restraints	0
Total dihedral-angle restraints	320
Number of unmapped restraints	0
Number of restraints per residue	47.5
Number of long range restraints per residue ¹	14.0

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)	121.9	0.2
0.2-0.5 (Medium)	251.0	0.5
>0.5 (Large)	477.5	3.69

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)	13.1	3.54
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

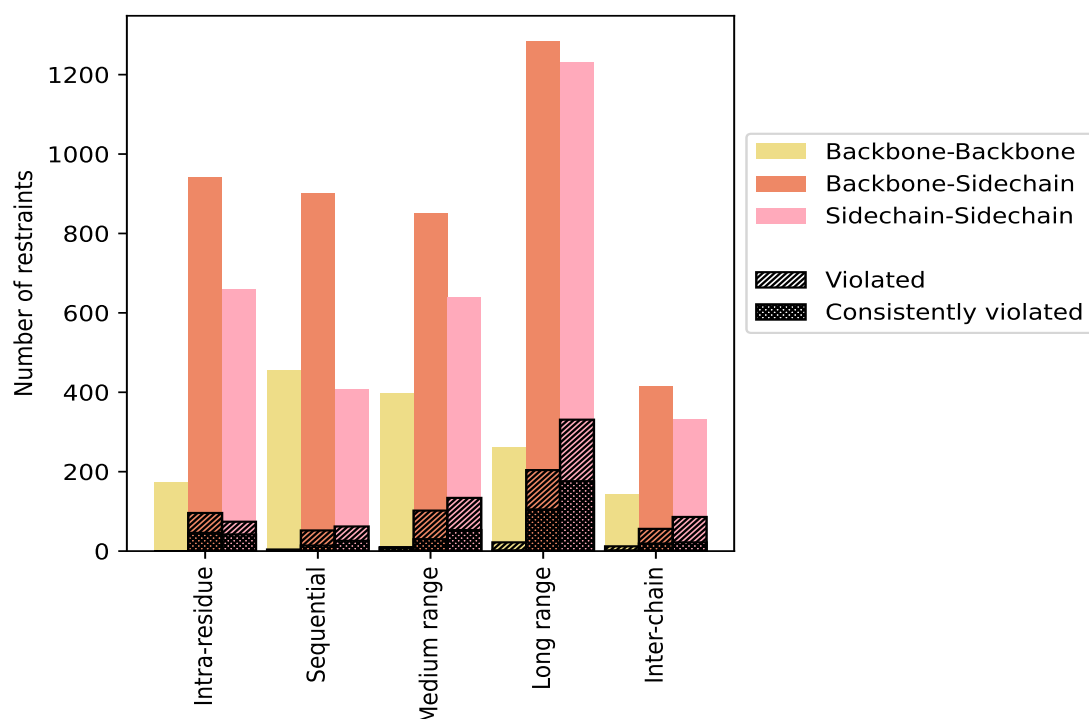
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue (i-j =0)	1774	19.5	170	9.6	1.9	88	5.0	1.0
Backbone-Backbone	174	1.9	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	940	10.3	96	10.2	1.1	46	4.9	0.5
Sidechain-Sidechain	660	7.3	74	11.2	0.8	42	6.4	0.5
Sequential (i-j =1)	1764	19.4	118	6.7	1.3	40	2.3	0.4
Backbone-Backbone	456	5.0	4	0.9	0.0	0	0.0	0.0
Backbone-Sidechain	900	9.9	52	5.8	0.6	14	1.6	0.2
Sidechain-Sidechain	408	4.5	62	15.2	0.7	26	6.4	0.3
Medium range (i-j >1 & i-j <5)	1888	20.8	246	13.0	2.7	91	4.8	1.0
Backbone-Backbone	398	4.4	10	2.5	0.1	8	2.0	0.1
Backbone-Sidechain	850	9.3	102	12.0	1.1	30	3.5	0.3
Sidechain-Sidechain	640	7.0	134	20.9	1.5	53	8.3	0.6
Long range (i-j ≥5)	2772	30.5	557	20.1	6.1	283	10.2	3.1
Backbone-Backbone	260	2.9	22	8.5	0.2	2	0.8	0.0
Backbone-Sidechain	1282	14.1	204	15.9	2.2	105	8.2	1.2
Sidechain-Sidechain	1230	13.5	331	26.9	3.6	176	14.3	1.9
Inter-chain	892	9.8	154	17.3	1.7	43	4.8	0.5
Backbone-Backbone	144	1.6	12	8.3	0.1	2	1.4	0.0
Backbone-Sidechain	416	4.6	56	13.5	0.6	19	4.6	0.2
Sidechain-Sidechain	332	3.7	86	25.9	0.9	22	6.6	0.2
Hydrogen bond	2	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	9092	100.0	1245	13.7	13.7	545	6.0	6.0
Backbone-Backbone	1432	15.8	48	3.4	0.5	12	0.8	0.1
Backbone-Sidechain	4390	48.3	510	11.6	5.6	214	4.9	2.4
Sidechain-Sidechain	3270	36.0	687	21.0	7.6	319	9.8	3.5

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

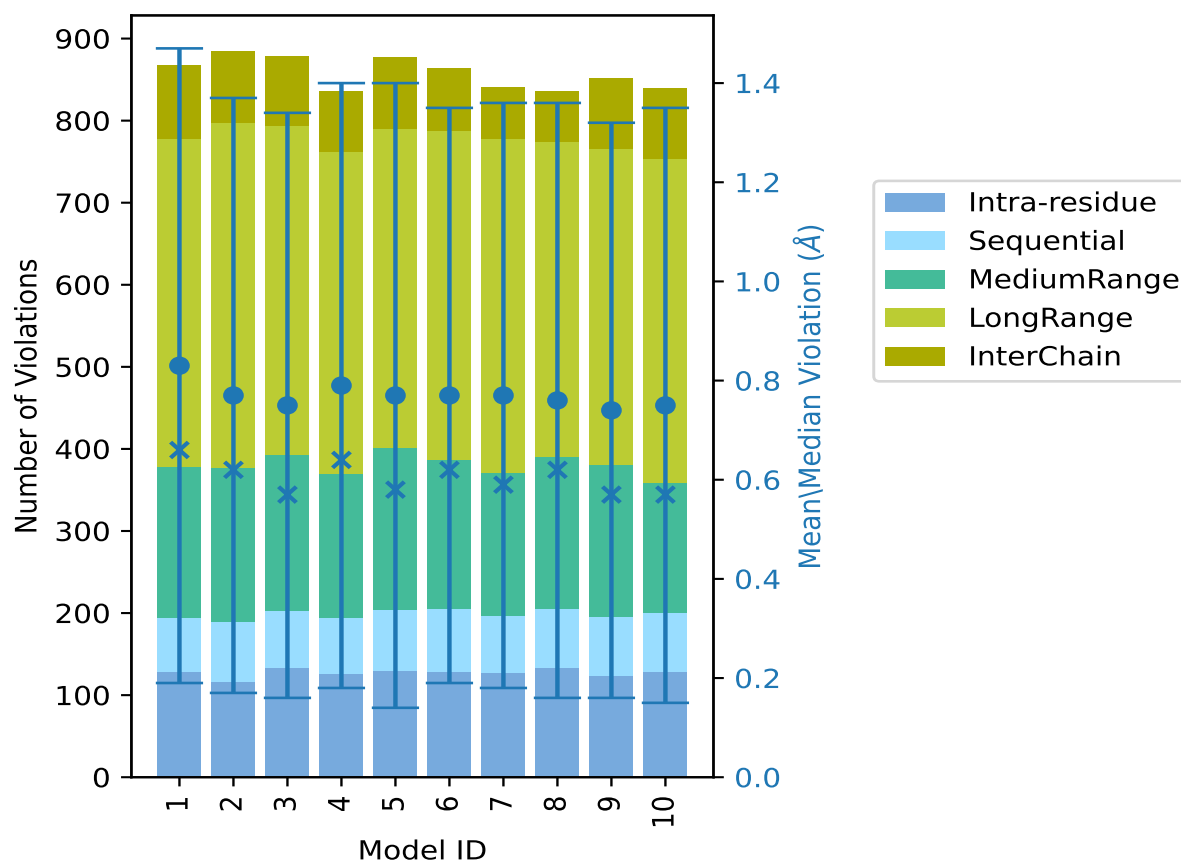
9.2 Distance violation statistics for each model [i](#)

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	128	67	183	400	90	868	0.83	3.45	0.64	0.66
2	116	74	187	420	87	884	0.77	3.08	0.6	0.62
3	133	70	190	401	85	879	0.75	3.53	0.59	0.57
4	126	68	176	392	74	836	0.79	3.37	0.61	0.64
5	130	74	198	388	87	877	0.77	3.58	0.63	0.58
6	129	76	182	401	76	864	0.77	3.25	0.58	0.62
7	127	70	174	407	63	841	0.77	3.53	0.59	0.59
8	134	71	186	383	62	836	0.76	3.69	0.6	0.62
9	124	72	184	386	86	852	0.74	3.11	0.58	0.57
10	129	71	159	395	86	840	0.75	3.27	0.6	0.57

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, 7845(IR:1604, SQ:1646, MR:1642, LR:2215, IC:738) 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	%
18	16	26	59	30	149	1	10.0
12	14	22	28	22	98	2	20.0
4	9	12	28	16	69	3	30.0

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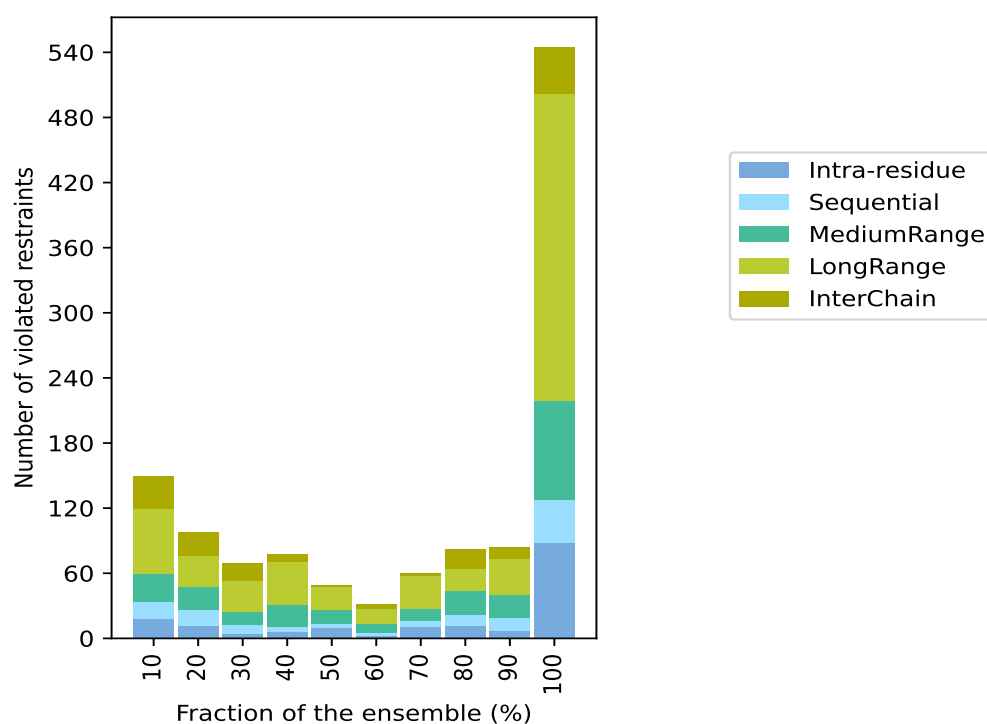
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
6	5	20	40	7	78	4	40.0
10	4	12	22	1	49	5	50.0
3	2	9	13	4	31	6	60.0
11	5	11	31	2	60	7	70.0
11	11	22	20	18	82	8	80.0
7	12	21	33	11	84	9	90.0
88	40	91	283	43	545	10	100.0

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

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

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

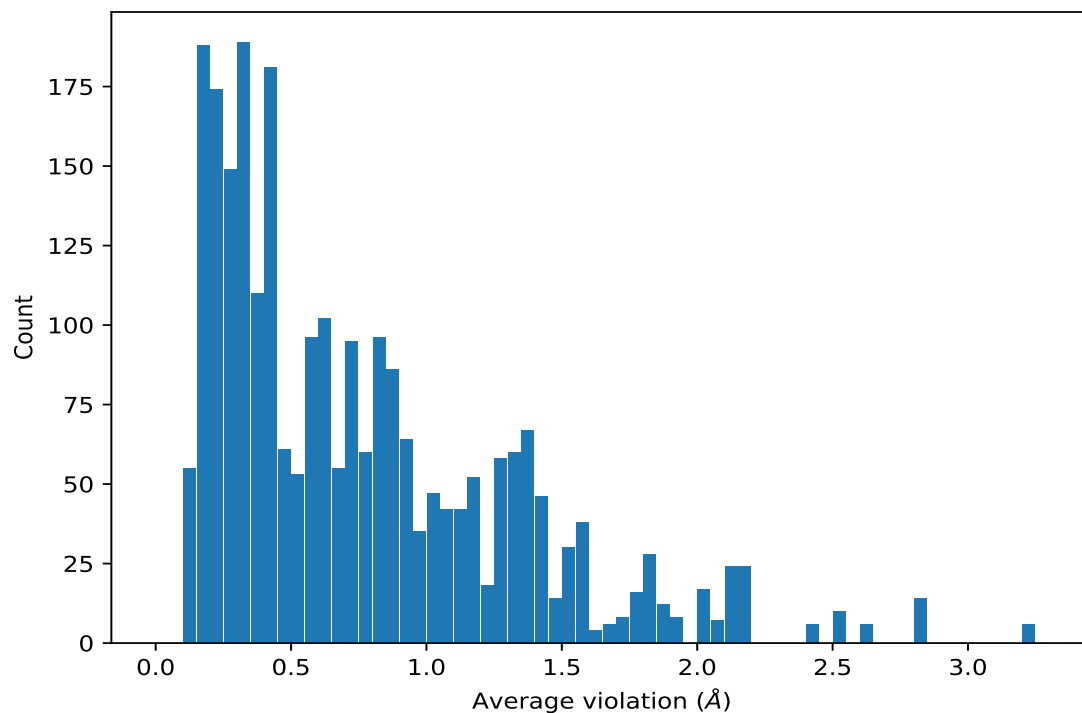


9.4 Most violated distance restraints in the ensemble [i](#)

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

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

in the ensemble



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,5301)	1:106:A:ALA:HB2	1:112:A:TYR:HB3	10	3.24	0.25	3.26
(1,5301)	1:106:A:ALA:HB1	1:112:A:TYR:HB3	10	3.24	0.25	3.26
(1,5301)	1:106:A:ALA:HB3	1:112:A:TYR:HB3	10	3.24	0.25	3.26
(1,5302)	1:106:B:ALA:HB2	1:112:B:TYR:HB3	10	3.24	0.25	3.26
(1,5302)	1:106:B:ALA:HB1	1:112:B:TYR:HB3	10	3.24	0.25	3.26
(1,5302)	1:106:B:ALA:HB3	1:112:B:TYR:HB3	10	3.24	0.25	3.26
(3,295)	1:94:A:THR:HG21	1:86:A:LEU:H	10	2.83	0.13	2.84
(3,295)	1:94:A:THR:HG22	1:86:A:LEU:H	10	2.83	0.13	2.84
(3,295)	1:94:A:THR:HG23	1:86:A:LEU:H	10	2.83	0.13	2.84
(3,296)	1:94:B:THR:HG21	1:86:B:LEU:H	10	2.83	0.13	2.84
(3,296)	1:94:B:THR:HG22	1:86:B:LEU:H	10	2.83	0.13	2.84
(3,296)	1:94:B:THR:HG23	1:86:B:LEU:H	10	2.83	0.13	2.84
(3,2062)	1:85:B:GLN:HG2	1:124:B:LYS:HD3	10	2.82	0.22	2.88
(3,2062)	1:85:B:GLN:HG3	1:124:B:LYS:HD3	10	2.82	0.22	2.88
(3,2062)	1:85:B:GLN:HG3	1:124:B:LYS:HG2	10	2.82	0.22	2.88

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,2062)	1:85:B:GLN:HG2	1:124:B:LYS:HG2	10	2.82	0.22	2.88
(3,2061)	1:85:A:GLN:HG2	1:124:A:LYS:HD3	10	2.81	0.21	2.88
(3,2061)	1:85:A:GLN:HG3	1:124:A:LYS:HD3	10	2.81	0.21	2.88
(3,2061)	1:85:A:GLN:HG3	1:124:A:LYS:HG2	10	2.81	0.21	2.88
(3,2061)	1:85:A:GLN:HG2	1:124:A:LYS:HG2	10	2.81	0.21	2.88
(3,933)	1:45:A:ILE:HG23	1:129:A:LYS:HB2	10	2.64	0.15	2.62
(3,933)	1:45:A:ILE:HG21	1:129:A:LYS:HB2	10	2.64	0.15	2.62
(3,933)	1:45:A:ILE:HG22	1:129:A:LYS:HB2	10	2.64	0.15	2.62
(3,934)	1:45:B:ILE:HG23	1:129:B:LYS:HB2	10	2.64	0.15	2.62
(3,934)	1:45:B:ILE:HG21	1:129:B:LYS:HB2	10	2.64	0.15	2.62
(3,934)	1:45:B:ILE:HG22	1:129:B:LYS:HB2	10	2.64	0.15	2.62
(1,5332)	1:108:B:LYS:HA	1:112:B:TYR:HB3	10	2.54	0.29	2.58
(1,5331)	1:108:A:LYS:HA	1:112:A:TYR:HB3	10	2.54	0.29	2.58
(1,3024)	1:57:B:GLN:HG2	1:60:B:PRO:HG2	10	2.5	0.55	2.82
(1,4563)	1:87:A:THR:HG22	1:98:A:LYS:HE3	10	2.5	0.72	2.12
(1,4563)	1:87:A:THR:HG21	1:98:A:LYS:HE3	10	2.5	0.72	2.12
(1,4563)	1:87:A:THR:HG23	1:98:A:LYS:HE3	10	2.5	0.72	2.12
(1,3023)	1:57:A:GLN:HG2	1:60:A:PRO:HG2	10	2.5	0.55	2.82
(1,4564)	1:87:B:THR:HG22	1:98:B:LYS:HE3	10	2.5	0.71	2.12
(1,4564)	1:87:B:THR:HG21	1:98:B:LYS:HE3	10	2.5	0.71	2.12
(1,4564)	1:87:B:THR:HG23	1:98:B:LYS:HE3	10	2.5	0.71	2.12
(3,2865)	1:121:A:THR:HG23	1:116:A:MET:HA	10	2.43	0.1	2.42
(3,2865)	1:121:A:THR:HG22	1:116:A:MET:HA	10	2.43	0.1	2.42
(3,2865)	1:121:A:THR:HG21	1:116:A:MET:HA	10	2.43	0.1	2.42
(3,2866)	1:121:B:THR:HG23	1:116:B:MET:HA	10	2.43	0.1	2.42
(3,2866)	1:121:B:THR:HG22	1:116:B:MET:HA	10	2.43	0.1	2.42
(3,2866)	1:121:B:THR:HG21	1:116:B:MET:HA	10	2.43	0.1	2.42
(3,3078)	1:104:B:PHE:HD1	1:138:B:ALA:HB1	10	2.17	0.6	2.42
(3,3078)	1:104:B:PHE:HD1	1:129:B:LYS:HG3	10	2.17	0.6	2.42
(3,3078)	1:104:B:PHE:HD1	1:139:B:ALA:HB1	10	2.17	0.6	2.42
(3,3078)	1:104:B:PHE:HD2	1:138:B:ALA:HB1	10	2.17	0.6	2.42
(3,3078)	1:104:B:PHE:HD2	1:138:B:ALA:HB3	10	2.17	0.6	2.42
(3,3078)	1:104:B:PHE:HD1	1:138:B:ALA:HB3	10	2.17	0.6	2.42
(3,3078)	1:104:B:PHE:HD2	1:139:B:ALA:HB2	10	2.17	0.6	2.42
(3,3077)	1:104:A:PHE:HD1	1:138:A:ALA:HB1	10	2.17	0.6	2.41
(3,3077)	1:104:A:PHE:HD1	1:129:A:LYS:HG3	10	2.17	0.6	2.41
(3,3077)	1:104:A:PHE:HD1	1:139:A:ALA:HB1	10	2.17	0.6	2.41
(3,3077)	1:104:A:PHE:HD2	1:138:A:ALA:HB1	10	2.17	0.6	2.41
(3,3077)	1:104:A:PHE:HD2	1:138:A:ALA:HB3	10	2.17	0.6	2.41
(3,3077)	1:104:A:PHE:HD1	1:138:A:ALA:HB3	10	2.17	0.6	2.41
(3,3077)	1:104:A:PHE:HD2	1:139:A:ALA:HB2	10	2.17	0.6	2.41
(3,1515)	1:55:A:LYS:HA	1:63:A:PRO:HB2	10	2.17	0.26	2.17

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,1515)	1:55:A:LYS:HA	1:129:A:LYS:HB2	10	2.17	0.26	2.17
(3,1516)	1:55:B:LYS:HA	1:63:B:PRO:HB2	10	2.17	0.27	2.17
(3,1516)	1:55:B:LYS:HA	1:129:B:LYS:HB2	10	2.17	0.27	2.17
(1,4958)	1:100:B:THR:HG22	1:129:B:LYS:HD2	10	2.17	0.54	2.31
(1,4958)	1:100:B:THR:HG23	1:129:B:LYS:HD2	10	2.17	0.54	2.31
(1,4958)	1:100:B:THR:HG21	1:129:B:LYS:HD2	10	2.17	0.54	2.31
(1,4957)	1:100:A:THR:HG22	1:129:A:LYS:HD2	10	2.16	0.53	2.3
(1,4957)	1:100:A:THR:HG23	1:129:A:LYS:HD2	10	2.16	0.53	2.3
(1,4957)	1:100:A:THR:HG21	1:129:A:LYS:HD2	10	2.16	0.53	2.3
(3,655)	1:45:A:ILE:HD13	1:125:A:ALA:H	10	2.13	0.32	2.17
(3,655)	1:45:A:ILE:HD11	1:125:A:ALA:H	10	2.13	0.32	2.17
(3,655)	1:45:A:ILE:HD12	1:125:A:ALA:H	10	2.13	0.32	2.17
(3,656)	1:45:B:ILE:HD13	1:125:B:ALA:H	10	2.13	0.33	2.17
(3,656)	1:45:B:ILE:HD11	1:125:B:ALA:H	10	2.13	0.33	2.17
(3,656)	1:45:B:ILE:HD12	1:125:B:ALA:H	10	2.13	0.33	2.17
(1,4575)	1:87:A:THR:HG22	1:102:A:ILE:HD12	10	2.13	0.25	2.19
(1,4575)	1:87:A:THR:HG21	1:102:A:ILE:HD11	10	2.13	0.25	2.19
(1,4575)	1:87:A:THR:HG23	1:102:A:ILE:HD13	10	2.13	0.25	2.19
(1,4575)	1:87:A:THR:HG21	1:102:A:ILE:HD12	10	2.13	0.25	2.19
(1,4575)	1:87:A:THR:HG22	1:102:A:ILE:HD11	10	2.13	0.25	2.19
(1,4575)	1:87:A:THR:HG21	1:102:A:ILE:HD13	10	2.13	0.25	2.19
(1,4576)	1:87:B:THR:HG22	1:102:B:ILE:HD12	10	2.12	0.25	2.19
(1,4576)	1:87:B:THR:HG21	1:102:B:ILE:HD11	10	2.12	0.25	2.19
(1,4576)	1:87:B:THR:HG23	1:102:B:ILE:HD13	10	2.12	0.25	2.19
(1,4576)	1:87:B:THR:HG21	1:102:B:ILE:HD12	10	2.12	0.25	2.19
(1,4576)	1:87:B:THR:HG22	1:102:B:ILE:HD11	10	2.12	0.25	2.19
(1,4576)	1:87:B:THR:HG21	1:102:B:ILE:HD13	10	2.12	0.25	2.19
(3,311)	1:94:A:THR:HG21	1:87:A:THR:H	10	2.12	0.13	2.1
(3,311)	1:94:A:THR:HG22	1:87:A:THR:H	10	2.12	0.13	2.1
(3,311)	1:94:A:THR:HG23	1:87:A:THR:H	10	2.12	0.13	2.1
(3,312)	1:94:B:THR:HG21	1:87:B:THR:H	10	2.12	0.13	2.1
(3,312)	1:94:B:THR:HG22	1:87:B:THR:H	10	2.12	0.13	2.1
(3,312)	1:94:B:THR:HG23	1:87:B:THR:H	10	2.12	0.13	2.1
(3,2848)	1:119:B:MET:HE3	1:75:B:TYR:HD2	10	2.05	0.26	1.99
(3,2848)	1:51:B:ALA:HB1	1:127:A:TYR:HE1	10	2.05	0.26	1.99
(3,2848)	1:51:B:ALA:HB3	1:127:A:TYR:HE1	10	2.05	0.26	1.99
(3,2848)	1:119:B:MET:HE2	1:75:B:TYR:HD2	10	2.05	0.26	1.99
(3,2848)	1:119:B:MET:HE1	1:75:B:TYR:HD1	10	2.05	0.26	1.99
(3,2848)	1:119:B:MET:HE2	1:75:B:TYR:HD1	10	2.05	0.26	1.99
(3,2848)	1:51:B:ALA:HB2	1:127:A:TYR:HE1	10	2.05	0.26	1.99
(3,2847)	1:119:A:MET:HE3	1:75:A:TYR:HD2	10	2.04	0.26	1.98
(3,2847)	1:51:A:ALA:HB1	1:127:B:TYR:HE1	10	2.04	0.26	1.98

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,2847)	1:51:A:ALA:HB3	1:127:B:TYR:HE1	10	2.04	0.26	1.98
(3,2847)	1:119:A:MET:HE2	1:75:A:TYR:HD2	10	2.04	0.26	1.98
(3,2847)	1:119:A:MET:HE1	1:75:A:TYR:HD1	10	2.04	0.26	1.98
(3,2847)	1:119:A:MET:HE2	1:75:A:TYR:HD1	10	2.04	0.26	1.98
(3,2847)	1:51:A:ALA:HB2	1:127:B:TYR:HE1	10	2.04	0.26	1.98
(1,4407)	1:83:A:ALA:HB3	1:120:A:ASP:HB2	10	2.01	0.2	1.99
(1,4407)	1:83:A:ALA:HB1	1:120:A:ASP:HB2	10	2.01	0.2	1.99
(1,4407)	1:83:A:ALA:HB2	1:120:A:ASP:HB2	10	2.01	0.2	1.99
(1,4408)	1:83:B:ALA:HB3	1:120:B:ASP:HB2	10	2.01	0.19	1.99
(1,4408)	1:83:B:ALA:HB1	1:120:B:ASP:HB2	10	2.01	0.19	1.99
(1,4408)	1:83:B:ALA:HB2	1:120:B:ASP:HB2	10	2.01	0.19	1.99
(1,5891)	1:65:A:PHE:HD1	1:93:A:ARG:HG2	10	2.0	0.15	2.02
(1,5891)	1:65:A:PHE:HD2	1:93:A:ARG:HG2	10	2.0	0.15	2.02
(1,5892)	1:65:B:PHE:HD1	1:93:B:ARG:HG2	10	2.0	0.15	2.02
(1,5892)	1:65:B:PHE:HD2	1:93:B:ARG:HG2	10	2.0	0.15	2.02
(3,765)	1:65:A:PHE:H	1:106:A:ALA:H	10	1.91	0.05	1.92
(1,4863)	1:98:A:LYS:HD3	1:125:A:ALA:HB3	10	1.91	0.22	1.9
(1,4863)	1:98:A:LYS:HD3	1:125:A:ALA:HB2	10	1.91	0.22	1.9
(1,4863)	1:98:A:LYS:HD3	1:125:A:ALA:HB1	10	1.91	0.22	1.9
(1,4864)	1:98:B:LYS:HD3	1:125:B:ALA:HB3	10	1.91	0.22	1.9
(1,4864)	1:98:B:LYS:HD3	1:125:B:ALA:HB2	10	1.91	0.22	1.9
(1,4864)	1:98:B:LYS:HD3	1:125:B:ALA:HB1	10	1.91	0.22	1.9
(3,766)	1:65:B:PHE:H	1:106:B:ALA:H	10	1.91	0.05	1.92
(3,1190)	1:108:B:LYS:HG2	1:114:B:THR:HG22	10	1.89	0.34	1.84
(3,1190)	1:108:B:LYS:HG3	1:114:B:THR:HG23	10	1.89	0.34	1.84
(3,1190)	1:108:B:LYS:HG3	1:114:B:THR:HG22	10	1.89	0.34	1.84
(3,1190)	1:108:B:LYS:HG3	1:114:B:THR:HG21	10	1.89	0.34	1.84
(3,1190)	1:108:B:LYS:HG2	1:114:B:THR:HG21	10	1.89	0.34	1.84
(3,1189)	1:108:A:LYS:HG2	1:114:A:THR:HG22	10	1.89	0.34	1.85
(3,1189)	1:108:A:LYS:HG3	1:114:A:THR:HG23	10	1.89	0.34	1.85
(3,1189)	1:108:A:LYS:HG3	1:114:A:THR:HG22	10	1.89	0.34	1.85
(3,1189)	1:108:A:LYS:HG3	1:114:A:THR:HG21	10	1.89	0.34	1.85
(3,1189)	1:108:A:LYS:HG2	1:114:A:THR:HG21	10	1.89	0.34	1.85
(1,4855)	1:98:A:LYS:HD3	1:126:A:GLY:HA2	10	1.85	0.24	1.83
(1,4856)	1:98:B:LYS:HD3	1:126:B:GLY:HA2	10	1.85	0.24	1.83
(1,5221)	1:116:A:MET:HB3	1:114:A:THR:HG21	10	1.82	0.04	1.83
(1,5221)	1:116:A:MET:HB3	1:114:A:THR:HG22	10	1.82	0.04	1.83
(1,5221)	1:116:A:MET:HB3	1:114:A:THR:HG23	10	1.82	0.04	1.83
(1,5222)	1:116:B:MET:HB3	1:114:B:THR:HG21	10	1.82	0.04	1.82
(1,5222)	1:116:B:MET:HB3	1:114:B:THR:HG22	10	1.82	0.04	1.82
(1,5222)	1:116:B:MET:HB3	1:114:B:THR:HG23	10	1.82	0.04	1.82
(3,2239)	1:94:A:THR:HG23	1:129:A:LYS:HE3	10	1.81	0.36	1.88

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,2239)	1:94:A:THR:HG23	1:129:A:LYS:HE2	10	1.81	0.36	1.88
(3,2239)	1:94:A:THR:HG21	1:129:A:LYS:HE3	10	1.81	0.36	1.88
(3,2239)	1:94:A:THR:HG22	1:129:A:LYS:HE2	10	1.81	0.36	1.88
(3,2239)	1:94:A:THR:HG22	1:129:A:LYS:HE3	10	1.81	0.36	1.88
(3,2239)	1:94:A:THR:HG21	1:129:A:LYS:HE2	10	1.81	0.36	1.88
(3,2240)	1:94:B:THR:HG23	1:129:B:LYS:HE3	10	1.81	0.36	1.87
(3,2240)	1:94:B:THR:HG23	1:129:B:LYS:HE2	10	1.81	0.36	1.87
(3,2240)	1:94:B:THR:HG21	1:129:B:LYS:HE3	10	1.81	0.36	1.87
(3,2240)	1:94:B:THR:HG22	1:129:B:LYS:HE2	10	1.81	0.36	1.87
(3,2240)	1:94:B:THR:HG22	1:129:B:LYS:HE3	10	1.81	0.36	1.87
(3,2240)	1:94:B:THR:HG21	1:129:B:LYS:HE2	10	1.81	0.36	1.87
(3,2869)	1:87:A:THR:HG22	1:98:A:LYS:HE3	10	1.8	0.24	1.87
(3,2869)	1:87:A:THR:HG21	1:98:A:LYS:HE3	10	1.8	0.24	1.87
(3,2869)	1:87:A:THR:HG23	1:98:A:LYS:HE2	10	1.8	0.24	1.87
(3,2869)	1:87:A:THR:HG23	1:98:A:LYS:HE3	10	1.8	0.24	1.87
(3,2869)	1:87:A:THR:HG21	1:98:A:LYS:HE2	10	1.8	0.24	1.87
(3,2870)	1:87:B:THR:HG22	1:98:B:LYS:HE3	10	1.8	0.24	1.88
(3,2870)	1:87:B:THR:HG21	1:98:B:LYS:HE3	10	1.8	0.24	1.88
(3,2870)	1:87:B:THR:HG23	1:98:B:LYS:HE2	10	1.8	0.24	1.88
(3,2870)	1:87:B:THR:HG23	1:98:B:LYS:HE3	10	1.8	0.24	1.88
(3,2870)	1:87:B:THR:HG21	1:98:B:LYS:HE2	10	1.8	0.24	1.88
(3,2457)	1:100:A:THR:HG22	1:66:A:LEU:HB3	10	1.79	0.15	1.78
(3,2457)	1:100:A:THR:HG23	1:66:A:LEU:HB3	10	1.79	0.15	1.78
(3,2457)	1:100:A:THR:HG21	1:66:A:LEU:HB3	10	1.79	0.15	1.78
(3,2457)	1:94:A:THR:HG21	1:66:A:LEU:HB3	10	1.79	0.15	1.78
(3,2458)	1:100:B:THR:HG22	1:66:B:LEU:HB3	10	1.79	0.15	1.78
(3,2458)	1:100:B:THR:HG23	1:66:B:LEU:HB3	10	1.79	0.15	1.78
(3,2458)	1:100:B:THR:HG21	1:66:B:LEU:HB3	10	1.79	0.15	1.78
(3,2458)	1:94:B:THR:HG21	1:66:B:LEU:HB3	10	1.79	0.15	1.78
(1,3140)	1:98:B:LYS:HE2	1:96:B:ALA:HB1	10	1.78	0.25	1.88
(1,3140)	1:98:B:LYS:HE2	1:96:B:ALA:HB2	10	1.78	0.25	1.88
(1,3140)	1:98:B:LYS:HE2	1:96:B:ALA:HB3	10	1.78	0.25	1.88
(1,3139)	1:98:A:LYS:HE2	1:96:A:ALA:HB1	10	1.78	0.25	1.87
(1,3139)	1:98:A:LYS:HE2	1:96:A:ALA:HB2	10	1.78	0.25	1.87
(1,3139)	1:98:A:LYS:HE2	1:96:A:ALA:HB3	10	1.78	0.25	1.87
(1,5800)	1:134:B:GLY:HA2	1:137:B:GLY:HA2	10	1.76	0.32	1.78
(1,5799)	1:134:A:GLY:HA2	1:137:A:GLY:HA2	10	1.76	0.32	1.78
(3,879)	1:69:A:LYS:HB2	1:140:A:LYS:HE3	10	1.74	1.07	1.33
(3,879)	1:69:A:LYS:HB2	1:140:A:LYS:HE2	10	1.74	1.07	1.33
(3,880)	1:69:B:LYS:HB2	1:140:B:LYS:HE3	10	1.73	1.07	1.32
(3,880)	1:69:B:LYS:HB2	1:140:B:LYS:HE2	10	1.73	1.07	1.32
(3,345)	1:106:A:ALA:HB2	1:114:A:THR:H	10	1.69	0.2	1.69

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,345)	1:106:A:ALA:HB1	1:114:A:THR:H	10	1.69	0.2	1.69
(3,345)	1:106:A:ALA:HB3	1:114:A:THR:H	10	1.69	0.2	1.69
(3,346)	1:106:B:ALA:HB2	1:114:B:THR:H	10	1.69	0.2	1.69
(3,346)	1:106:B:ALA:HB1	1:114:B:THR:H	10	1.69	0.2	1.69
(3,346)	1:106:B:ALA:HB3	1:114:B:THR:H	10	1.69	0.2	1.69
(3,1759)	1:69:A:LYS:HE2	1:73:A:GLN:HG2	10	1.61	0.5	1.74
(3,1759)	1:69:A:LYS:HE3	1:73:A:GLN:HB2	10	1.61	0.5	1.74
(3,1760)	1:69:B:LYS:HE2	1:73:B:GLN:HG2	10	1.61	0.5	1.74
(3,1760)	1:69:B:LYS:HE3	1:73:B:GLN:HB2	10	1.61	0.5	1.74
(3,181)	1:115:A:LEU:HD11	1:66:A:LEU:H	10	1.58	0.14	1.58
(3,181)	1:115:A:LEU:HD12	1:66:A:LEU:H	10	1.58	0.14	1.58
(3,181)	1:115:A:LEU:HD13	1:66:A:LEU:H	10	1.58	0.14	1.58
(3,182)	1:115:B:LEU:HD11	1:66:B:LEU:H	10	1.58	0.13	1.58
(3,182)	1:115:B:LEU:HD12	1:66:B:LEU:H	10	1.58	0.13	1.58
(3,182)	1:115:B:LEU:HD13	1:66:B:LEU:H	10	1.58	0.13	1.58
(3,2545)	1:102:A:ILE:HD12	1:128:A:LEU:HG	10	1.57	0.09	1.54
(3,2545)	1:102:A:ILE:HD11	1:128:A:LEU:HG	10	1.57	0.09	1.54
(3,2545)	1:102:A:ILE:HD13	1:128:A:LEU:HG	10	1.57	0.09	1.54
(3,2546)	1:102:B:ILE:HD12	1:128:B:LEU:HG	10	1.57	0.09	1.54
(3,2546)	1:102:B:ILE:HD11	1:128:B:LEU:HG	10	1.57	0.09	1.54
(3,2546)	1:102:B:ILE:HD13	1:128:B:LEU:HG	10	1.57	0.09	1.54
(1,4711)	1:92:A:GLN:HG2	1:79:A:GLN:HB3	10	1.56	0.2	1.58
(1,4712)	1:92:B:GLN:HG2	1:79:B:GLN:HB3	10	1.56	0.2	1.58
(1,4113)	1:74:A:LEU:HA	1:115:A:LEU:HD13	10	1.56	0.24	1.48
(1,4113)	1:74:A:LEU:HA	1:115:A:LEU:HD11	10	1.56	0.24	1.48
(1,4113)	1:74:A:LEU:HA	1:115:A:LEU:HD12	10	1.56	0.24	1.48
(1,4114)	1:74:B:LEU:HA	1:115:B:LEU:HD13	10	1.56	0.24	1.48
(1,4114)	1:74:B:LEU:HA	1:115:B:LEU:HD11	10	1.56	0.24	1.48
(1,4114)	1:74:B:LEU:HA	1:115:B:LEU:HD12	10	1.56	0.24	1.48
(1,3593)	1:115:A:LEU:HD13	1:75:A:TYR:HB3	10	1.55	0.28	1.47
(1,3593)	1:115:A:LEU:HD11	1:75:A:TYR:HB3	10	1.55	0.28	1.47
(1,3593)	1:115:A:LEU:HD12	1:75:A:TYR:HB3	10	1.55	0.28	1.47
(1,3594)	1:115:B:LEU:HD13	1:75:B:TYR:HB3	10	1.55	0.28	1.47
(1,3594)	1:115:B:LEU:HD11	1:75:B:TYR:HB3	10	1.55	0.28	1.47
(1,3594)	1:115:B:LEU:HD12	1:75:B:TYR:HB3	10	1.55	0.28	1.47
(3,3071)	1:104:A:PHE:HE1	1:72:A:LYS:HG3	10	1.55	0.24	1.52
(3,3071)	1:104:A:PHE:HE1	1:129:A:LYS:HG3	10	1.55	0.24	1.52
(3,3071)	1:104:A:PHE:HE1	1:139:A:ALA:HB1	10	1.55	0.24	1.52
(3,3071)	1:104:A:PHE:HE2	1:72:A:LYS:HG3	10	1.55	0.24	1.52
(3,3071)	1:104:A:PHE:HE2	1:129:A:LYS:HG3	10	1.55	0.24	1.52
(3,3072)	1:104:B:PHE:HE1	1:72:B:LYS:HG3	10	1.55	0.24	1.52
(3,3072)	1:104:B:PHE:HE1	1:129:B:LYS:HG3	10	1.55	0.24	1.52

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,3072)	1:104:B:PHE:HE1	1:139:B:ALA:HB1	10	1.55	0.24	1.52
(3,3072)	1:104:B:PHE:HE2	1:72:B:LYS:HG3	10	1.55	0.24	1.52
(3,3072)	1:104:B:PHE:HE2	1:129:B:LYS:HG3	10	1.55	0.24	1.52
(3,1608)	1:65:B:PHE:HB2	1:60:B:PRO:HG2	10	1.55	0.29	1.58
(3,1608)	1:65:B:PHE:HB2	1:136:B:GLU:HG3	10	1.55	0.29	1.58
(3,1607)	1:65:A:PHE:HB2	1:60:A:PRO:HG2	10	1.54	0.29	1.58
(3,1607)	1:65:A:PHE:HB2	1:136:A:GLU:HG3	10	1.54	0.29	1.58
(1,5404)	1:110:B:VAL:HG23	1:115:B:LEU:HB3	10	1.53	0.12	1.54
(1,5404)	1:110:B:VAL:HG21	1:115:B:LEU:HB3	10	1.53	0.12	1.54
(1,5404)	1:110:B:VAL:HG22	1:115:B:LEU:HB3	10	1.53	0.12	1.54
(1,5403)	1:110:A:VAL:HG23	1:115:A:LEU:HB3	10	1.53	0.12	1.54
(1,5403)	1:110:A:VAL:HG21	1:115:A:LEU:HB3	10	1.53	0.12	1.54
(1,5403)	1:110:A:VAL:HG22	1:115:A:LEU:HB3	10	1.53	0.12	1.54
(3,2925)	1:126:A:GLY:HA3	1:50:B:PRO:HG3	10	1.53	0.48	1.5
(1,3580)	1:115:B:LEU:HD13	1:75:B:TYR:HA	10	1.52	0.2	1.5
(1,3580)	1:115:B:LEU:HD11	1:75:B:TYR:HA	10	1.52	0.2	1.5
(1,3580)	1:115:B:LEU:HD12	1:75:B:TYR:HA	10	1.52	0.2	1.5
(1,3579)	1:115:A:LEU:HD13	1:75:A:TYR:HA	10	1.52	0.2	1.5
(1,3579)	1:115:A:LEU:HD11	1:75:A:TYR:HA	10	1.52	0.2	1.5
(1,3579)	1:115:A:LEU:HD12	1:75:A:TYR:HA	10	1.52	0.2	1.5
(3,2926)	1:126:B:GLY:HA3	1:50:A:PRO:HG3	10	1.52	0.48	1.52
(3,1403)	1:122:A:LEU:HA	1:49:B:LEU:HB3	10	1.51	0.27	1.6
(3,1403)	1:122:A:LEU:HA	1:98:A:LYS:HG3	10	1.51	0.27	1.6
(3,1404)	1:122:B:LEU:HA	1:49:A:LEU:HB3	10	1.51	0.27	1.6
(3,1404)	1:122:B:LEU:HA	1:98:B:LYS:HG3	10	1.51	0.27	1.6
(1,5797)	1:134:A:GLY:HA2	1:137:A:GLY:HA3	10	1.5	0.25	1.48
(1,5798)	1:134:B:GLY:HA2	1:137:B:GLY:HA3	10	1.5	0.25	1.48
(1,4321)	1:127:A:TYR:HA	1:49:B:LEU:HB3	10	1.5	0.2	1.45
(1,4322)	1:127:B:TYR:HA	1:49:A:LEU:HB3	10	1.5	0.21	1.42
(1,1119)	1:93:A:ARG:HG3	1:90:A:LEU:H	10	1.5	0.09	1.54
(1,1120)	1:93:B:ARG:HG3	1:90:B:LEU:H	10	1.5	0.09	1.54
(3,1829)	1:58:A:PRO:HG2	1:55:A:LYS:HE2	10	1.48	0.43	1.36
(3,1829)	1:108:A:LYS:HE2	1:135:A:MET:HE2	10	1.48	0.43	1.36
(3,1829)	1:58:A:PRO:HG2	1:55:A:LYS:HE3	10	1.48	0.43	1.36
(3,1829)	1:108:A:LYS:HE2	1:135:A:MET:HE1	10	1.48	0.43	1.36
(3,1830)	1:58:B:PRO:HG2	1:55:B:LYS:HE2	10	1.48	0.43	1.36
(3,1830)	1:108:B:LYS:HE2	1:135:B:MET:HE2	10	1.48	0.43	1.36
(3,1830)	1:58:B:PRO:HG2	1:55:B:LYS:HE3	10	1.48	0.43	1.36
(3,1830)	1:108:B:LYS:HE2	1:135:B:MET:HE1	10	1.48	0.43	1.36
(1,2871)	1:129:A:LYS:HB3	1:49:B:LEU:HB3	10	1.48	0.05	1.44
(1,2872)	1:129:B:LYS:HB3	1:49:A:LEU:HB3	10	1.47	0.06	1.44
(3,847)	1:44:A:ASP:HA	1:46:A:ARG:HG2	10	1.46	0.26	1.53

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,847)	1:44:A:ASP:HA	1:123:A:ARG:HG3	10	1.46	0.26	1.53
(3,848)	1:44:B:ASP:HA	1:46:B:ARG:HG2	10	1.46	0.26	1.52
(3,848)	1:44:B:ASP:HA	1:123:B:ARG:HG3	10	1.46	0.26	1.52
(3,2681)	1:108:A:LYS:HB2	1:112:A:TYR:HB3	10	1.44	0.31	1.49
(3,2682)	1:108:B:LYS:HB2	1:112:B:TYR:HB3	10	1.44	0.31	1.48
(3,303)	1:124:A:LYS:HG2	1:86:A:LEU:H	10	1.43	0.18	1.42
(3,304)	1:124:B:LYS:HG2	1:86:B:LEU:H	10	1.43	0.18	1.42
(3,691)	1:45:A:ILE:HG23	1:128:A:LEU:H	10	1.42	0.12	1.38
(3,691)	1:45:A:ILE:HG21	1:128:A:LEU:H	10	1.42	0.12	1.38
(3,691)	1:45:A:ILE:HG22	1:128:A:LEU:H	10	1.42	0.12	1.38
(1,5311)	1:106:A:ALA:HB2	1:114:A:THR:HG21	10	1.42	0.22	1.38
(1,5311)	1:106:A:ALA:HB1	1:114:A:THR:HG22	10	1.42	0.22	1.38
(1,5311)	1:106:A:ALA:HB3	1:114:A:THR:HG21	10	1.42	0.22	1.38
(1,5311)	1:106:A:ALA:HB1	1:114:A:THR:HG23	10	1.42	0.22	1.38
(1,5311)	1:106:A:ALA:HB2	1:114:A:THR:HG23	10	1.42	0.22	1.38
(1,5311)	1:106:A:ALA:HB1	1:114:A:THR:HG21	10	1.42	0.22	1.38
(1,5311)	1:106:A:ALA:HB2	1:114:A:THR:HG22	10	1.42	0.22	1.38
(3,692)	1:45:B:ILE:HG23	1:128:B:LEU:H	10	1.42	0.12	1.38
(3,692)	1:45:B:ILE:HG21	1:128:B:LEU:H	10	1.42	0.12	1.38
(3,692)	1:45:B:ILE:HG22	1:128:B:LEU:H	10	1.42	0.12	1.38
(1,5312)	1:106:B:ALA:HB2	1:114:B:THR:HG21	10	1.42	0.22	1.38
(1,5312)	1:106:B:ALA:HB1	1:114:B:THR:HG22	10	1.42	0.22	1.38
(1,5312)	1:106:B:ALA:HB3	1:114:B:THR:HG21	10	1.42	0.22	1.38
(1,5312)	1:106:B:ALA:HB1	1:114:B:THR:HG23	10	1.42	0.22	1.38
(1,5312)	1:106:B:ALA:HB2	1:114:B:THR:HG23	10	1.42	0.22	1.38
(1,5312)	1:106:B:ALA:HB1	1:114:B:THR:HG21	10	1.42	0.22	1.38
(1,5312)	1:106:B:ALA:HB2	1:114:B:THR:HG22	10	1.42	0.22	1.38
(3,1667)	1:67:A:SER:HA	1:115:A:LEU:HD11	10	1.41	0.11	1.4
(3,1667)	1:115:A:LEU:HD12	1:104:A:PHE:HA	10	1.41	0.11	1.4
(3,1667)	1:115:A:LEU:HD13	1:104:A:PHE:HA	10	1.41	0.11	1.4
(3,1667)	1:115:A:LEU:HD11	1:104:A:PHE:HA	10	1.41	0.11	1.4
(3,1667)	1:67:A:SER:HA	1:115:A:LEU:HD13	10	1.41	0.11	1.4
(3,1667)	1:67:A:SER:HA	1:115:A:LEU:HD12	10	1.41	0.11	1.4
(3,1668)	1:67:B:SER:HA	1:115:B:LEU:HD11	10	1.41	0.11	1.4
(3,1668)	1:115:B:LEU:HD12	1:104:B:PHE:HA	10	1.41	0.11	1.4
(3,1668)	1:115:B:LEU:HD13	1:104:B:PHE:HA	10	1.41	0.11	1.4
(3,1668)	1:115:B:LEU:HD11	1:104:B:PHE:HA	10	1.41	0.11	1.4
(3,1668)	1:67:B:SER:HA	1:115:B:LEU:HD13	10	1.41	0.11	1.4
(3,1668)	1:67:B:SER:HA	1:115:B:LEU:HD12	10	1.41	0.11	1.4
(3,2298)	1:90:B:LEU:HA	1:96:B:ALA:HB3	10	1.4	0.47	1.62
(3,2298)	1:90:B:LEU:HA	1:96:B:ALA:HB1	10	1.4	0.47	1.62
(3,2298)	1:90:B:LEU:HA	1:96:B:ALA:HB2	10	1.4	0.47	1.62

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,2297)	1:90:A:LEU:HA	1:96:A:ALA:HB3	10	1.4	0.48	1.62
(3,2297)	1:90:A:LEU:HA	1:96:A:ALA:HB1	10	1.4	0.48	1.62
(3,2297)	1:90:A:LEU:HA	1:96:A:ALA:HB2	10	1.4	0.48	1.62
(1,4122)	1:74:B:LEU:HB2	1:110:B:VAL:HG12	10	1.4	0.07	1.42
(1,4122)	1:74:B:LEU:HB2	1:110:B:VAL:HG13	10	1.4	0.07	1.42
(1,4122)	1:74:B:LEU:HB2	1:110:B:VAL:HG11	10	1.4	0.07	1.42
(1,4681)	1:91:A:ASP:HA	1:96:A:ALA:HB3	10	1.39	0.53	1.66
(1,4681)	1:91:A:ASP:HA	1:96:A:ALA:HB1	10	1.39	0.53	1.66
(1,4681)	1:91:A:ASP:HA	1:96:A:ALA:HB2	10	1.39	0.53	1.66
(1,4682)	1:91:B:ASP:HA	1:96:B:ALA:HB3	10	1.39	0.53	1.65
(1,4682)	1:91:B:ASP:HA	1:96:B:ALA:HB1	10	1.39	0.53	1.65
(1,4682)	1:91:B:ASP:HA	1:96:B:ALA:HB2	10	1.39	0.53	1.65
(1,4121)	1:74:A:LEU:HB2	1:110:A:VAL:HG12	10	1.39	0.07	1.42
(1,4121)	1:74:A:LEU:HB2	1:110:A:VAL:HG13	10	1.39	0.07	1.42
(1,4121)	1:74:A:LEU:HB2	1:110:A:VAL:HG11	10	1.39	0.07	1.42
(3,912)	1:45:B:ILE:HD11	1:46:B:ARG:HD3	10	1.39	0.47	1.62
(3,912)	1:45:B:ILE:HD13	1:46:B:ARG:HD2	10	1.39	0.47	1.62
(3,912)	1:45:B:ILE:HD13	1:46:B:ARG:HD3	10	1.39	0.47	1.62
(3,912)	1:45:B:ILE:HD11	1:46:B:ARG:HD2	10	1.39	0.47	1.62
(3,911)	1:45:A:ILE:HD11	1:46:A:ARG:HD3	10	1.39	0.46	1.61
(3,911)	1:45:A:ILE:HD13	1:46:A:ARG:HD2	10	1.39	0.46	1.61
(3,911)	1:45:A:ILE:HD13	1:46:A:ARG:HD3	10	1.39	0.46	1.61
(3,911)	1:45:A:ILE:HD11	1:46:A:ARG:HD2	10	1.39	0.46	1.61
(1,5625)	1:87:A:THR:HG22	1:126:A:GLY:HA3	10	1.39	0.05	1.38
(1,5625)	1:87:A:THR:HG21	1:126:A:GLY:HA3	10	1.39	0.05	1.38
(1,5625)	1:87:A:THR:HG23	1:126:A:GLY:HA3	10	1.39	0.05	1.38
(1,5626)	1:87:B:THR:HG22	1:126:B:GLY:HA3	10	1.38	0.05	1.37
(1,5626)	1:87:B:THR:HG21	1:126:B:GLY:HA3	10	1.38	0.05	1.37
(1,5626)	1:87:B:THR:HG23	1:126:B:GLY:HA3	10	1.38	0.05	1.37
(1,5386)	1:104:B:PHE:HZ	1:110:B:VAL:HG22	10	1.38	0.16	1.43
(1,5386)	1:104:B:PHE:HZ	1:110:B:VAL:HG23	10	1.38	0.16	1.43
(1,5386)	1:104:B:PHE:HZ	1:110:B:VAL:HG21	10	1.38	0.16	1.43
(1,5385)	1:104:A:PHE:HZ	1:110:A:VAL:HG22	10	1.38	0.16	1.43
(1,5385)	1:104:A:PHE:HZ	1:110:A:VAL:HG23	10	1.38	0.16	1.43
(1,5385)	1:104:A:PHE:HZ	1:110:A:VAL:HG21	10	1.38	0.16	1.43
(3,2846)	1:51:B:ALA:HB1	1:127:A:TYR:HD2	10	1.37	0.33	1.4
(3,2846)	1:51:B:ALA:HB1	1:127:A:TYR:HD1	10	1.37	0.33	1.4
(3,2846)	1:51:B:ALA:HB3	1:127:A:TYR:HD1	10	1.37	0.33	1.4
(3,2846)	1:51:B:ALA:HB2	1:127:A:TYR:HD2	10	1.37	0.33	1.4
(3,2846)	1:51:B:ALA:HB2	1:127:A:TYR:HD1	10	1.37	0.33	1.4
(1,3948)	1:91:B:ASP:HB2	1:96:B:ALA:HB3	10	1.37	0.37	1.48
(1,3948)	1:91:B:ASP:HB2	1:96:B:ALA:HB1	10	1.37	0.37	1.48

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3948)	1:91:B:ASP:HB2	1:96:B:ALA:HB2	10	1.37	0.37	1.48
(1,3947)	1:91:A:ASP:HB2	1:96:A:ALA:HB3	10	1.37	0.38	1.47
(1,3947)	1:91:A:ASP:HB2	1:96:A:ALA:HB1	10	1.37	0.38	1.47
(1,3947)	1:91:A:ASP:HB2	1:96:A:ALA:HB2	10	1.37	0.38	1.47
(3,2845)	1:51:A:ALA:HB1	1:127:B:TYR:HD2	10	1.37	0.33	1.4
(3,2845)	1:51:A:ALA:HB1	1:127:B:TYR:HD1	10	1.37	0.33	1.4
(3,2845)	1:51:A:ALA:HB3	1:127:B:TYR:HD1	10	1.37	0.33	1.4
(3,2845)	1:51:A:ALA:HB2	1:127:B:TYR:HD2	10	1.37	0.33	1.4
(3,2845)	1:51:A:ALA:HB2	1:127:B:TYR:HD1	10	1.37	0.33	1.4
(3,2873)	1:87:A:THR:HG23	1:124:A:LYS:HB2	10	1.36	0.12	1.35
(3,2873)	1:87:A:THR:HG22	1:124:A:LYS:HB2	10	1.36	0.12	1.35
(3,2873)	1:87:A:THR:HG21	1:124:A:LYS:HB2	10	1.36	0.12	1.35
(3,2873)	1:121:A:THR:HG21	1:124:A:LYS:HB3	10	1.36	0.12	1.35
(3,2873)	1:121:A:THR:HG23	1:124:A:LYS:HB3	10	1.36	0.12	1.35
(3,2874)	1:87:B:THR:HG23	1:124:B:LYS:HB2	10	1.36	0.12	1.35
(3,2874)	1:87:B:THR:HG22	1:124:B:LYS:HB2	10	1.36	0.12	1.35
(3,2874)	1:87:B:THR:HG21	1:124:B:LYS:HB2	10	1.36	0.12	1.35
(3,2874)	1:121:B:THR:HG21	1:124:B:LYS:HB3	10	1.36	0.12	1.35
(3,2874)	1:121:B:THR:HG23	1:124:B:LYS:HB3	10	1.36	0.12	1.35
(3,1823)	1:129:A:LYS:HD2	1:45:A:ILE:HG23	10	1.36	0.85	1.0
(3,1823)	1:129:A:LYS:HD2	1:45:A:ILE:HG21	10	1.36	0.85	1.0
(3,1823)	1:129:A:LYS:HD2	1:45:A:ILE:HG22	10	1.36	0.85	1.0
(3,1824)	1:129:B:LYS:HD2	1:45:B:ILE:HG23	10	1.35	0.85	1.0
(3,1824)	1:129:B:LYS:HD2	1:45:B:ILE:HG21	10	1.35	0.85	1.0
(3,1824)	1:129:B:LYS:HD2	1:45:B:ILE:HG22	10	1.35	0.85	1.0
(3,551)	1:90:A:LEU:HB3	1:103:A:PHE:H	10	1.34	0.11	1.39
(3,552)	1:90:B:LEU:HB3	1:103:B:PHE:H	10	1.34	0.11	1.39
(3,1122)	1:54:B:ALA:HB1	1:57:B:GLN:HG2	10	1.33	0.18	1.3
(3,1122)	1:54:B:ALA:HB2	1:57:B:GLN:HG2	10	1.33	0.18	1.3
(3,1122)	1:54:B:ALA:HB3	1:57:B:GLN:HG2	10	1.33	0.18	1.3
(3,1122)	1:54:B:ALA:HB2	1:57:B:GLN:HG3	10	1.33	0.18	1.3
(3,2534)	1:102:B:ILE:HG21	1:133:B:VAL:HB	10	1.33	0.19	1.36
(3,2534)	1:102:B:ILE:HG23	1:133:B:VAL:HB	10	1.33	0.19	1.36
(3,2534)	1:102:B:ILE:HG21	1:119:B:MET:HB2	10	1.33	0.19	1.36
(3,2534)	1:102:B:ILE:HG22	1:119:B:MET:HB2	10	1.33	0.19	1.36
(3,2534)	1:102:B:ILE:HG23	1:119:B:MET:HB2	10	1.33	0.19	1.36
(3,1121)	1:54:A:ALA:HB1	1:57:A:GLN:HG2	10	1.33	0.18	1.3
(3,1121)	1:54:A:ALA:HB2	1:57:A:GLN:HG2	10	1.33	0.18	1.3
(3,1121)	1:54:A:ALA:HB3	1:57:A:GLN:HG2	10	1.33	0.18	1.3
(3,1121)	1:54:A:ALA:HB2	1:57:A:GLN:HG3	10	1.33	0.18	1.3
(3,2533)	1:102:A:ILE:HG21	1:133:A:VAL:HB	10	1.33	0.19	1.35
(3,2533)	1:102:A:ILE:HG23	1:133:A:VAL:HB	10	1.33	0.19	1.35

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,2533)	1:102:A:ILE:HG21	1:119:A:MET:HB2	10	1.33	0.19	1.35
(3,2533)	1:102:A:ILE:HG22	1:119:A:MET:HB2	10	1.33	0.19	1.35
(3,2533)	1:102:A:ILE:HG23	1:119:A:MET:HB2	10	1.33	0.19	1.35
(3,575)	1:115:A:LEU:HD22	1:115:A:LEU:H	10	1.32	0.03	1.33
(3,575)	1:115:A:LEU:HD23	1:115:A:LEU:H	10	1.32	0.03	1.33
(3,575)	1:115:A:LEU:HD21	1:115:A:LEU:H	10	1.32	0.03	1.33
(3,576)	1:115:B:LEU:HD22	1:115:B:LEU:H	10	1.32	0.03	1.33
(3,576)	1:115:B:LEU:HD23	1:115:B:LEU:H	10	1.32	0.03	1.33
(3,576)	1:115:B:LEU:HD21	1:115:B:LEU:H	10	1.32	0.03	1.33
(3,171)	1:46:A:ARG:HB2	1:64:B:VAL:H	10	1.32	0.26	1.27
(3,1522)	1:45:B:ILE:HG23	1:129:B:LYS:HB2	10	1.32	0.14	1.29
(3,1522)	1:45:B:ILE:HG21	1:129:B:LYS:HB2	10	1.32	0.14	1.29
(3,1522)	1:45:B:ILE:HG22	1:129:B:LYS:HB2	10	1.32	0.14	1.29
(3,1522)	1:129:B:LYS:HB2	1:45:A:ILE:HG21	10	1.32	0.14	1.29
(3,1521)	1:45:A:ILE:HG23	1:129:A:LYS:HB2	10	1.32	0.14	1.29
(3,1521)	1:45:A:ILE:HG21	1:129:A:LYS:HB2	10	1.32	0.14	1.29
(3,1521)	1:45:A:ILE:HG22	1:129:A:LYS:HB2	10	1.32	0.14	1.29
(3,1521)	1:129:A:LYS:HB2	1:45:B:ILE:HG21	10	1.32	0.14	1.29
(3,172)	1:46:B:ARG:HB2	1:64:A:VAL:H	10	1.31	0.26	1.27
(3,2006)	1:81:B:VAL:HB	1:66:B:LEU:HG	10	1.3	0.19	1.27
(3,2006)	1:81:B:VAL:HB	1:93:B:ARG:HG3	10	1.3	0.19	1.27
(3,2005)	1:81:A:VAL:HB	1:66:A:LEU:HG	10	1.3	0.19	1.27
(3,2005)	1:81:A:VAL:HB	1:93:A:ARG:HG3	10	1.3	0.19	1.27
(1,5557)	1:116:A:MET:HE2	1:119:A:MET:HE2	10	1.3	0.26	1.18
(1,5557)	1:116:A:MET:HE2	1:119:A:MET:HE1	10	1.3	0.26	1.18
(1,5557)	1:116:A:MET:HE3	1:119:A:MET:HE3	10	1.3	0.26	1.18
(1,5557)	1:116:A:MET:HE1	1:119:A:MET:HE2	10	1.3	0.26	1.18
(1,5557)	1:116:A:MET:HE1	1:119:A:MET:HE3	10	1.3	0.26	1.18
(1,5557)	1:116:A:MET:HE3	1:119:A:MET:HE1	10	1.3	0.26	1.18
(1,5557)	1:116:A:MET:HE2	1:119:A:MET:HE3	10	1.3	0.26	1.18
(1,5557)	1:116:A:MET:HE3	1:119:A:MET:HE2	10	1.3	0.26	1.18
(1,5558)	1:116:B:MET:HE2	1:119:B:MET:HE2	10	1.3	0.26	1.17
(1,5558)	1:116:B:MET:HE2	1:119:B:MET:HE1	10	1.3	0.26	1.17
(1,5558)	1:116:B:MET:HE3	1:119:B:MET:HE3	10	1.3	0.26	1.17
(1,5558)	1:116:B:MET:HE1	1:119:B:MET:HE2	10	1.3	0.26	1.17
(1,5558)	1:116:B:MET:HE1	1:119:B:MET:HE3	10	1.3	0.26	1.17
(1,5558)	1:116:B:MET:HE3	1:119:B:MET:HE1	10	1.3	0.26	1.17
(1,5558)	1:116:B:MET:HE3	1:119:B:MET:HE2	10	1.3	0.26	1.17
(3,351)	1:98:A:LYS:HG2	1:90:A:LEU:H	10	1.29	0.26	1.35
(3,352)	1:98:B:LYS:HG2	1:90:B:LEU:H	10	1.29	0.26	1.35
(1,5503)	1:114:A:THR:HG21	1:104:A:PHE:HZ	10	1.29	0.16	1.26
(1,5503)	1:114:A:THR:HG22	1:104:A:PHE:HZ	10	1.29	0.16	1.26

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,5503)	1:114:A:THR:HG23	1:104:A:PHE:HZ	10	1.29	0.16	1.26
(1,5504)	1:114:B:THR:HG21	1:104:B:PHE:HZ	10	1.29	0.16	1.27
(1,5504)	1:114:B:THR:HG22	1:104:B:PHE:HZ	10	1.29	0.16	1.27
(1,5504)	1:114:B:THR:HG23	1:104:B:PHE:HZ	10	1.29	0.16	1.27
(1,2320)	1:57:B:GLN:HG2	1:57:B:GLN:HE22	10	1.29	0.12	1.34
(1,2319)	1:57:A:GLN:HG2	1:57:A:GLN:HE22	10	1.29	0.12	1.34
(1,3239)	1:99:A:GLU:HG2	1:49:B:LEU:HB3	10	1.28	0.45	1.25
(1,5419)	1:110:A:VAL:HG11	1:114:A:THR:HG22	10	1.28	0.41	1.31
(1,5419)	1:110:A:VAL:HG12	1:114:A:THR:HG23	10	1.28	0.41	1.31
(1,5419)	1:110:A:VAL:HG13	1:114:A:THR:HG22	10	1.28	0.41	1.31
(1,5419)	1:110:A:VAL:HG12	1:114:A:THR:HG21	10	1.28	0.41	1.31
(1,5419)	1:110:A:VAL:HG13	1:114:A:THR:HG21	10	1.28	0.41	1.31
(1,5419)	1:110:A:VAL:HG12	1:114:A:THR:HG22	10	1.28	0.41	1.31
(1,5419)	1:110:A:VAL:HG11	1:114:A:THR:HG23	10	1.28	0.41	1.31
(1,5420)	1:110:B:VAL:HG11	1:114:B:THR:HG22	10	1.28	0.41	1.31
(1,5420)	1:110:B:VAL:HG12	1:114:B:THR:HG23	10	1.28	0.41	1.31
(1,5420)	1:110:B:VAL:HG13	1:114:B:THR:HG22	10	1.28	0.41	1.31
(1,5420)	1:110:B:VAL:HG12	1:114:B:THR:HG21	10	1.28	0.41	1.31
(1,5420)	1:110:B:VAL:HG13	1:114:B:THR:HG21	10	1.28	0.41	1.31
(1,5420)	1:110:B:VAL:HG12	1:114:B:THR:HG22	10	1.28	0.41	1.31
(1,5420)	1:110:B:VAL:HG11	1:114:B:THR:HG23	10	1.28	0.41	1.31
(1,3240)	1:99:B:GLU:HG2	1:49:A:LEU:HB3	10	1.28	0.46	1.25
(1,2819)	1:54:A:ALA:HB1	1:44:B:ASP:HB2	10	1.27	0.49	1.4
(1,2819)	1:54:A:ALA:HB2	1:44:B:ASP:HB2	10	1.27	0.49	1.4
(1,5314)	1:106:B:ALA:HB3	1:115:B:LEU:HD22	10	1.27	0.2	1.27
(1,5314)	1:106:B:ALA:HB2	1:115:B:LEU:HD21	10	1.27	0.2	1.27
(1,5314)	1:106:B:ALA:HB1	1:115:B:LEU:HD21	10	1.27	0.2	1.27
(1,5314)	1:106:B:ALA:HB2	1:115:B:LEU:HD23	10	1.27	0.2	1.27
(1,5314)	1:106:B:ALA:HB1	1:115:B:LEU:HD22	10	1.27	0.2	1.27
(1,5314)	1:106:B:ALA:HB3	1:115:B:LEU:HD21	10	1.27	0.2	1.27
(1,5314)	1:106:B:ALA:HB2	1:115:B:LEU:HD22	10	1.27	0.2	1.27
(1,5313)	1:106:A:ALA:HB3	1:115:A:LEU:HD22	10	1.27	0.2	1.27
(1,5313)	1:106:A:ALA:HB2	1:115:A:LEU:HD21	10	1.27	0.2	1.27
(1,5313)	1:106:A:ALA:HB1	1:115:A:LEU:HD21	10	1.27	0.2	1.27
(1,5313)	1:106:A:ALA:HB2	1:115:A:LEU:HD23	10	1.27	0.2	1.27
(1,5313)	1:106:A:ALA:HB1	1:115:A:LEU:HD22	10	1.27	0.2	1.27
(1,5313)	1:106:A:ALA:HB3	1:115:A:LEU:HD21	10	1.27	0.2	1.27
(1,5313)	1:106:A:ALA:HB2	1:115:A:LEU:HD22	10	1.27	0.2	1.27
(1,2820)	1:54:B:ALA:HB1	1:44:A:ASP:HB2	10	1.27	0.49	1.36
(1,2820)	1:54:B:ALA:HB2	1:44:A:ASP:HB2	10	1.27	0.49	1.36
(3,2334)	1:98:B:LYS:HG2	1:101:B:THR:HA	10	1.26	0.11	1.29
(3,2333)	1:98:A:LYS:HG2	1:101:A:THR:HA	10	1.26	0.12	1.28

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,1441)	1:61:A:GLU:HG2	1:62:A:LYS:HB3	10	1.25	0.13	1.18
(3,1441)	1:113:A:GLU:HG3	1:116:A:MET:HB3	10	1.25	0.13	1.18
(3,1442)	1:61:B:GLU:HG2	1:62:B:LYS:HB3	10	1.25	0.13	1.18
(3,1442)	1:113:B:GLU:HG3	1:116:B:MET:HB3	10	1.25	0.13	1.18
(3,919)	1:45:A:ILE:HD11	1:46:B:ARG:HG2	10	1.24	0.18	1.18
(3,919)	1:45:A:ILE:HD11	1:46:A:ARG:HG3	10	1.24	0.18	1.18
(3,919)	1:45:A:ILE:HD13	1:46:A:ARG:HG3	10	1.24	0.18	1.18
(3,919)	1:45:A:ILE:HD13	1:46:B:ARG:HG2	10	1.24	0.18	1.18
(3,920)	1:45:B:ILE:HD11	1:46:A:ARG:HG2	10	1.24	0.19	1.18
(3,920)	1:45:B:ILE:HD11	1:46:B:ARG:HG3	10	1.24	0.19	1.18
(3,920)	1:45:B:ILE:HD13	1:46:B:ARG:HG3	10	1.24	0.19	1.18
(3,920)	1:45:B:ILE:HD13	1:46:A:ARG:HG2	10	1.24	0.19	1.18
(3,3091)	1:127:A:TYR:HE1	1:104:A:PHE:HB3	10	1.21	0.12	1.23
(3,3091)	1:127:A:TYR:HE2	1:104:A:PHE:HB3	10	1.21	0.12	1.23
(3,3092)	1:127:B:TYR:HE1	1:104:B:PHE:HB3	10	1.21	0.12	1.23
(3,3092)	1:127:B:TYR:HE2	1:104:B:PHE:HB3	10	1.21	0.12	1.23
(1,3589)	1:115:A:LEU:HD12	1:112:A:TYR:HB3	10	1.19	0.16	1.14
(1,3589)	1:115:A:LEU:HD13	1:112:A:TYR:HB3	10	1.19	0.16	1.14
(1,3589)	1:115:A:LEU:HD11	1:112:A:TYR:HB3	10	1.19	0.16	1.14
(1,3590)	1:115:B:LEU:HD12	1:112:B:TYR:HB3	10	1.19	0.16	1.14
(1,3590)	1:115:B:LEU:HD13	1:112:B:TYR:HB3	10	1.19	0.16	1.14
(1,3590)	1:115:B:LEU:HD11	1:112:B:TYR:HB3	10	1.19	0.16	1.14
(3,2835)	1:116:A:MET:HE2	1:120:A:ASP:HA	10	1.19	0.17	1.15
(3,2835)	1:116:A:MET:HE3	1:120:A:ASP:HA	10	1.19	0.17	1.15
(3,2835)	1:116:A:MET:HE1	1:120:A:ASP:HA	10	1.19	0.17	1.15
(3,2836)	1:116:B:MET:HE2	1:120:B:ASP:HA	10	1.19	0.17	1.15
(3,2836)	1:116:B:MET:HE3	1:120:B:ASP:HA	10	1.19	0.17	1.15
(3,2836)	1:116:B:MET:HE1	1:120:B:ASP:HA	10	1.19	0.17	1.15
(1,4443)	1:79:A:GLN:HB2	1:65:A:PHE:HB3	10	1.18	0.37	1.17
(1,4444)	1:79:B:GLN:HB2	1:65:B:PHE:HB3	10	1.18	0.37	1.17
(3,1291)	1:119:A:MET:HB2	1:123:A:ARG:HA	10	1.18	0.13	1.19
(3,1291)	1:119:A:MET:HB2	1:121:A:THR:HA	10	1.18	0.13	1.19
(3,1292)	1:119:B:MET:HB2	1:123:B:ARG:HA	10	1.18	0.13	1.19
(3,1292)	1:119:B:MET:HB2	1:121:B:THR:HA	10	1.18	0.13	1.19
(3,1849)	1:136:A:GLU:HB2	1:140:A:LYS:HE3	10	1.18	0.45	1.4
(3,1849)	1:85:A:GLN:HB2	1:124:A:LYS:HE2	10	1.18	0.45	1.4
(3,1849)	1:73:A:GLN:HB3	1:140:A:LYS:HE2	10	1.18	0.45	1.4
(3,1849)	1:85:A:GLN:HB2	1:124:A:LYS:HE3	10	1.18	0.45	1.4
(3,1850)	1:136:B:GLU:HB2	1:140:B:LYS:HE3	10	1.17	0.45	1.4
(3,1850)	1:85:B:GLN:HB2	1:124:B:LYS:HE2	10	1.17	0.45	1.4
(3,1850)	1:73:B:GLN:HB3	1:140:B:LYS:HE2	10	1.17	0.45	1.4
(3,1850)	1:85:B:GLN:HB2	1:124:B:LYS:HE3	10	1.17	0.45	1.4

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1859)	1:110:A:VAL:HG22	1:118:A:VAL:H	10	1.17	0.12	1.19
(1,1859)	1:110:A:VAL:HG23	1:118:A:VAL:H	10	1.17	0.12	1.19
(1,1859)	1:110:A:VAL:HG21	1:118:A:VAL:H	10	1.17	0.12	1.19
(1,1860)	1:110:B:VAL:HG22	1:118:B:VAL:H	10	1.17	0.12	1.19
(1,1860)	1:110:B:VAL:HG23	1:118:B:VAL:H	10	1.17	0.12	1.19
(1,1860)	1:110:B:VAL:HG21	1:118:B:VAL:H	10	1.17	0.12	1.19
(3,693)	1:45:A:ILE:HG23	1:128:A:LEU:H	10	1.17	0.12	1.12
(3,693)	1:45:A:ILE:HG21	1:128:A:LEU:H	10	1.17	0.12	1.12
(3,693)	1:45:A:ILE:HG22	1:128:A:LEU:H	10	1.17	0.12	1.12
(1,5528)	1:115:B:LEU:HD22	1:68:B:VAL:HA	10	1.16	0.15	1.17
(1,5528)	1:115:B:LEU:HD21	1:68:B:VAL:HA	10	1.16	0.15	1.17
(1,5528)	1:115:B:LEU:HD23	1:68:B:VAL:HA	10	1.16	0.15	1.17
(3,694)	1:45:B:ILE:HG23	1:128:B:LEU:H	10	1.16	0.12	1.12
(3,694)	1:45:B:ILE:HG21	1:128:B:LEU:H	10	1.16	0.12	1.12
(3,694)	1:45:B:ILE:HG22	1:128:B:LEU:H	10	1.16	0.12	1.12
(1,5527)	1:115:A:LEU:HD22	1:68:A:VAL:HA	10	1.16	0.15	1.17
(1,5527)	1:115:A:LEU:HD21	1:68:A:VAL:HA	10	1.16	0.15	1.17
(1,5527)	1:115:A:LEU:HD23	1:68:A:VAL:HA	10	1.16	0.15	1.17
(1,2027)	1:98:A:LYS:HD3	1:125:A:ALA:H	10	1.15	0.22	1.19
(1,2028)	1:98:B:LYS:HD3	1:125:B:ALA:H	10	1.15	0.23	1.19
(3,2488)	1:101:B:THR:HB	1:98:B:LYS:HB2	10	1.14	0.06	1.12
(3,2488)	1:101:B:THR:HB	1:50:B:PRO:HG2	10	1.14	0.06	1.12
(3,2487)	1:101:A:THR:HB	1:98:A:LYS:HB2	10	1.14	0.06	1.13
(3,2487)	1:101:A:THR:HB	1:50:A:PRO:HG2	10	1.14	0.06	1.13
(3,471)	1:90:A:LEU:HB3	1:102:A:ILE:H	10	1.13	0.09	1.12
(3,472)	1:90:B:LEU:HB3	1:102:B:ILE:H	10	1.13	0.09	1.12
(1,5675)	1:125:A:ALA:HB1	1:102:A:ILE:HD12	10	1.12	0.09	1.09
(1,5675)	1:125:A:ALA:HB3	1:102:A:ILE:HD11	10	1.12	0.09	1.09
(1,5675)	1:125:A:ALA:HB2	1:102:A:ILE:HD13	10	1.12	0.09	1.09
(1,5675)	1:125:A:ALA:HB3	1:102:A:ILE:HD13	10	1.12	0.09	1.09
(1,5675)	1:125:A:ALA:HB1	1:102:A:ILE:HD11	10	1.12	0.09	1.09
(1,5675)	1:125:A:ALA:HB1	1:102:A:ILE:HD13	10	1.12	0.09	1.09
(1,5676)	1:125:B:ALA:HB1	1:102:B:ILE:HD12	10	1.12	0.09	1.1
(1,5676)	1:125:B:ALA:HB3	1:102:B:ILE:HD11	10	1.12	0.09	1.1
(1,5676)	1:125:B:ALA:HB2	1:102:B:ILE:HD13	10	1.12	0.09	1.1
(1,5676)	1:125:B:ALA:HB3	1:102:B:ILE:HD13	10	1.12	0.09	1.1
(1,5676)	1:125:B:ALA:HB1	1:102:B:ILE:HD11	10	1.12	0.09	1.1
(1,5676)	1:125:B:ALA:HB1	1:102:B:ILE:HD13	10	1.12	0.09	1.1
(3,952)	1:46:B:ARG:HB2	1:48:A:ASP:HB2	10	1.12	0.41	1.15
(3,952)	1:123:B:ARG:HB2	1:127:B:TYR:HB2	10	1.12	0.41	1.15
(1,3431)	1:64:A:VAL:HA	1:93:A:ARG:HG2	10	1.12	0.13	1.14
(1,3432)	1:64:B:VAL:HA	1:93:B:ARG:HG2	10	1.12	0.13	1.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,951)	1:46:A:ARG:HB2	1:48:B:ASP:HB2	10	1.12	0.41	1.15
(3,951)	1:123:A:ARG:HB2	1:127:A:TYR:HB2	10	1.12	0.41	1.15
(3,1079)	1:56:A:PRO:HG2	1:50:A:PRO:HD2	10	1.11	0.21	1.12
(3,1079)	1:56:A:PRO:HG3	1:50:A:PRO:HD2	10	1.11	0.21	1.12
(3,1080)	1:56:B:PRO:HG2	1:50:B:PRO:HD2	10	1.11	0.21	1.12
(3,1080)	1:56:B:PRO:HG3	1:50:B:PRO:HD2	10	1.11	0.21	1.12
(1,4810)	1:96:B:ALA:HB2	1:100:B:THR:HB	10	1.1	0.14	1.09
(1,4810)	1:96:B:ALA:HB3	1:100:B:THR:HB	10	1.1	0.14	1.09
(1,4810)	1:96:B:ALA:HB1	1:100:B:THR:HB	10	1.1	0.14	1.09
(1,4809)	1:96:A:ALA:HB2	1:100:A:THR:HB	10	1.1	0.15	1.09
(1,4809)	1:96:A:ALA:HB3	1:100:A:THR:HB	10	1.1	0.15	1.09
(1,4809)	1:96:A:ALA:HB1	1:100:A:THR:HB	10	1.1	0.15	1.09
(1,796)	1:115:B:LEU:HD13	1:75:B:TYR:H	10	1.09	0.21	1.04
(1,796)	1:115:B:LEU:HD11	1:75:B:TYR:H	10	1.09	0.21	1.04
(1,796)	1:115:B:LEU:HD12	1:75:B:TYR:H	10	1.09	0.21	1.04
(1,795)	1:115:A:LEU:HD13	1:75:A:TYR:H	10	1.09	0.21	1.04
(1,795)	1:115:A:LEU:HD11	1:75:A:TYR:H	10	1.09	0.21	1.04
(1,795)	1:115:A:LEU:HD12	1:75:A:TYR:H	10	1.09	0.21	1.04
(3,2903)	1:105:A:GLN:HB2	1:69:A:LYS:HD3	10	1.08	0.23	1.14
(3,2903)	1:87:A:THR:HG21	1:124:A:LYS:HB2	10	1.08	0.23	1.14
(3,2903)	1:87:A:THR:HG22	1:124:A:LYS:HB2	10	1.08	0.23	1.14
(3,2904)	1:105:B:GLN:HB2	1:69:B:LYS:HD3	10	1.08	0.23	1.14
(3,2904)	1:87:B:THR:HG22	1:124:B:LYS:HB2	10	1.08	0.23	1.14
(3,2904)	1:87:B:THR:HG21	1:124:B:LYS:HB2	10	1.08	0.23	1.14
(1,4134)	1:74:B:LEU:HB3	1:110:B:VAL:HG12	10	1.08	0.09	1.1
(1,4134)	1:74:B:LEU:HB3	1:110:B:VAL:HG13	10	1.08	0.09	1.1
(1,4134)	1:74:B:LEU:HB3	1:110:B:VAL:HG11	10	1.08	0.09	1.1
(1,4133)	1:74:A:LEU:HB3	1:110:A:VAL:HG12	10	1.08	0.09	1.1
(1,4133)	1:74:A:LEU:HB3	1:110:A:VAL:HG13	10	1.08	0.09	1.1
(1,4133)	1:74:A:LEU:HB3	1:110:A:VAL:HG11	10	1.08	0.09	1.1
(3,159)	1:58:A:PRO:HB2	1:62:A:LYS:H	10	1.07	0.31	1.12
(3,159)	1:129:A:LYS:HB3	1:62:A:LYS:H	10	1.07	0.31	1.12
(3,160)	1:58:B:PRO:HB2	1:62:B:LYS:H	10	1.07	0.31	1.12
(3,160)	1:129:B:LYS:HB3	1:62:B:LYS:H	10	1.07	0.31	1.12
(1,2823)	1:54:A:ALA:HB1	1:55:A:LYS:HB2	10	1.07	0.04	1.08
(1,2823)	1:54:A:ALA:HB3	1:55:A:LYS:HB2	10	1.07	0.04	1.08
(1,2823)	1:54:A:ALA:HB2	1:55:A:LYS:HB2	10	1.07	0.04	1.08
(1,2824)	1:54:B:ALA:HB1	1:55:B:LYS:HB2	10	1.07	0.04	1.08
(1,2824)	1:54:B:ALA:HB3	1:55:B:LYS:HB2	10	1.07	0.04	1.08
(1,2824)	1:54:B:ALA:HB2	1:55:B:LYS:HB2	10	1.07	0.04	1.08
(3,2853)	1:119:A:MET:HE2	1:121:A:THR:HB	10	1.05	0.33	1.1
(3,2853)	1:119:A:MET:HE3	1:121:A:THR:HB	10	1.05	0.33	1.1

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,2853)	1:119:A:MET:HE1	1:121:A:THR:HB	10	1.05	0.33	1.1
(3,2854)	1:119:B:MET:HE2	1:121:B:THR:HB	10	1.05	0.32	1.1
(3,2854)	1:119:B:MET:HE3	1:121:B:THR:HB	10	1.05	0.32	1.1
(3,2854)	1:119:B:MET:HE1	1:121:B:THR:HB	10	1.05	0.32	1.1
(3,2220)	1:93:B:ARG:HD2	1:66:B:LEU:HB3	10	1.04	0.22	1.0
(3,2220)	1:93:B:ARG:HD3	1:66:B:LEU:HB3	10	1.04	0.22	1.0
(3,2219)	1:93:A:ARG:HD2	1:66:A:LEU:HB3	10	1.04	0.22	1.01
(3,2219)	1:93:A:ARG:HD3	1:66:A:LEU:HB3	10	1.04	0.22	1.01
(3,2632)	1:105:B:GLN:HG3	1:110:B:VAL:HG22	10	1.03	0.2	0.97
(3,2632)	1:105:B:GLN:HG3	1:110:B:VAL:HG23	10	1.03	0.2	0.97
(3,2632)	1:105:B:GLN:HG3	1:110:B:VAL:HG21	10	1.03	0.2	0.97
(3,2631)	1:105:A:GLN:HG3	1:110:A:VAL:HG22	10	1.03	0.2	0.97
(3,2631)	1:105:A:GLN:HG3	1:110:A:VAL:HG23	10	1.03	0.2	0.97
(3,2631)	1:105:A:GLN:HG3	1:110:A:VAL:HG21	10	1.03	0.2	0.97
(3,2642)	1:115:B:LEU:HD13	1:116:B:MET:HG2	10	1.02	0.4	1.27
(3,2642)	1:115:B:LEU:HD11	1:116:B:MET:HG2	10	1.02	0.4	1.27
(3,2642)	1:116:B:MET:HG2	1:45:B:ILE:HD12	10	1.02	0.4	1.27
(3,2642)	1:115:B:LEU:HD12	1:116:B:MET:HG2	10	1.02	0.4	1.27
(3,2642)	1:116:B:MET:HG2	1:45:B:ILE:HD11	10	1.02	0.4	1.27
(3,2641)	1:115:A:LEU:HD13	1:116:A:MET:HG2	10	1.02	0.4	1.27
(3,2641)	1:115:A:LEU:HD11	1:116:A:MET:HG2	10	1.02	0.4	1.27
(3,2641)	1:116:A:MET:HG2	1:45:A:ILE:HD12	10	1.02	0.4	1.27
(3,2641)	1:115:A:LEU:HD12	1:116:A:MET:HG2	10	1.02	0.4	1.27
(3,2641)	1:116:A:MET:HG2	1:45:A:ILE:HD11	10	1.02	0.4	1.27
(1,4808)	1:96:B:ALA:HB1	1:127:B:TYR:HA	10	1.01	0.2	1.05
(1,4808)	1:96:B:ALA:HB2	1:127:B:TYR:HA	10	1.01	0.2	1.05
(1,4808)	1:96:B:ALA:HB3	1:127:B:TYR:HA	10	1.01	0.2	1.05
(1,4807)	1:96:A:ALA:HB1	1:127:A:TYR:HA	10	1.01	0.21	1.05
(1,4807)	1:96:A:ALA:HB2	1:127:A:TYR:HA	10	1.01	0.21	1.05
(1,4807)	1:96:A:ALA:HB3	1:127:A:TYR:HA	10	1.01	0.21	1.05
(1,2816)	1:54:B:ALA:HB2	1:50:B:PRO:HD2	10	1.01	0.19	1.05
(1,2816)	1:54:B:ALA:HB1	1:50:B:PRO:HD2	10	1.01	0.19	1.05
(1,2816)	1:54:B:ALA:HB3	1:50:B:PRO:HD2	10	1.01	0.19	1.05
(1,2815)	1:54:A:ALA:HB2	1:50:A:PRO:HD2	10	1.01	0.19	1.06
(1,2815)	1:54:A:ALA:HB1	1:50:A:PRO:HD2	10	1.01	0.19	1.06
(1,2815)	1:54:A:ALA:HB3	1:50:A:PRO:HD2	10	1.01	0.19	1.06
(3,2111)	1:87:A:THR:HG23	1:124:A:LYS:HB2	10	1.0	0.12	0.98
(3,2111)	1:87:A:THR:HG22	1:124:A:LYS:HB2	10	1.0	0.12	0.98
(3,2111)	1:87:A:THR:HG21	1:124:A:LYS:HB2	10	1.0	0.12	0.98
(3,2112)	1:87:B:THR:HG23	1:124:B:LYS:HB2	10	0.99	0.12	0.98
(3,2112)	1:87:B:THR:HG22	1:124:B:LYS:HB2	10	0.99	0.12	0.98
(3,2112)	1:87:B:THR:HG21	1:124:B:LYS:HB2	10	0.99	0.12	0.98

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,853)	1:88:A:SER:HA	1:124:A:LYS:HE3	10	0.99	0.42	0.94
(1,5552)	1:116:B:MET:HE2	1:113:B:GLU:HA	10	0.99	0.29	0.9
(1,5552)	1:116:B:MET:HE3	1:113:B:GLU:HA	10	0.99	0.29	0.9
(1,5552)	1:116:B:MET:HE1	1:113:B:GLU:HA	10	0.99	0.29	0.9
(3,854)	1:88:B:SER:HA	1:124:B:LYS:HE3	10	0.99	0.42	0.95
(1,5551)	1:116:A:MET:HE2	1:113:A:GLU:HA	10	0.99	0.29	0.9
(1,5551)	1:116:A:MET:HE3	1:113:A:GLU:HA	10	0.99	0.29	0.9
(1,5551)	1:116:A:MET:HE1	1:113:A:GLU:HA	10	0.99	0.29	0.9
(3,2109)	1:87:A:THR:HG21	1:89:A:VAL:HB	10	0.98	0.39	0.86
(3,2109)	1:87:A:THR:HG23	1:89:A:VAL:HB	10	0.98	0.39	0.86
(3,2109)	1:87:A:THR:HG22	1:89:A:VAL:HB	10	0.98	0.39	0.86
(1,3235)	1:61:A:GLU:HB3	1:62:A:LYS:HG2	10	0.98	0.59	0.88
(3,2110)	1:87:B:THR:HG21	1:89:B:VAL:HB	10	0.98	0.39	0.86
(3,2110)	1:87:B:THR:HG23	1:89:B:VAL:HB	10	0.98	0.39	0.86
(3,2110)	1:87:B:THR:HG22	1:89:B:VAL:HB	10	0.98	0.39	0.86
(1,3236)	1:61:B:GLU:HB3	1:62:B:LYS:HG2	10	0.98	0.59	0.87
(1,3506)	1:120:B:ASP:HB3	1:116:B:MET:HB2	10	0.98	0.21	0.92
(1,3505)	1:120:A:ASP:HB3	1:116:A:MET:HB2	10	0.98	0.21	0.91
(1,1996)	1:49:B:LEU:HB2	1:123:A:ARG:H	10	0.97	0.25	0.92
(1,1995)	1:49:A:LEU:HB2	1:123:B:ARG:H	10	0.97	0.25	0.92
(1,5810)	1:134:B:GLY:HA3	1:116:A:MET:HE2	10	0.96	0.25	0.97
(1,5810)	1:134:B:GLY:HA3	1:116:A:MET:HE3	10	0.96	0.25	0.97
(1,5810)	1:134:B:GLY:HA3	1:116:A:MET:HE1	10	0.96	0.25	0.97
(1,5809)	1:134:A:GLY:HA3	1:116:B:MET:HE2	10	0.96	0.25	0.97
(1,5809)	1:134:A:GLY:HA3	1:116:B:MET:HE3	10	0.96	0.25	0.97
(1,5809)	1:134:A:GLY:HA3	1:116:B:MET:HE1	10	0.96	0.25	0.97
(1,4717)	1:92:A:GLN:HG2	1:102:A:ILE:HG13	10	0.95	0.11	0.98
(1,4718)	1:92:B:GLN:HG2	1:102:B:ILE:HG13	10	0.95	0.11	0.98
(3,462)	1:102:B:ILE:HG23	1:101:B:THR:H	10	0.94	0.07	0.93
(3,462)	1:102:B:ILE:HG22	1:101:B:THR:H	10	0.94	0.07	0.93
(3,462)	1:102:B:ILE:HG21	1:101:B:THR:H	10	0.94	0.07	0.93
(3,461)	1:102:A:ILE:HG23	1:101:A:THR:H	10	0.94	0.07	0.94
(3,461)	1:102:A:ILE:HG22	1:101:A:THR:H	10	0.94	0.07	0.94
(3,461)	1:102:A:ILE:HG21	1:101:A:THR:H	10	0.94	0.07	0.94
(1,5581)	1:118:A:VAL:HB	1:83:A:ALA:HB2	10	0.94	0.25	1.06
(1,5581)	1:118:A:VAL:HB	1:83:A:ALA:HB3	10	0.94	0.25	1.06
(1,5581)	1:118:A:VAL:HB	1:83:A:ALA:HB1	10	0.94	0.25	1.06
(1,5582)	1:118:B:VAL:HB	1:83:B:ALA:HB2	10	0.94	0.25	1.06
(1,5582)	1:118:B:VAL:HB	1:83:B:ALA:HB3	10	0.94	0.25	1.06
(1,5582)	1:118:B:VAL:HB	1:83:B:ALA:HB1	10	0.94	0.25	1.06
(3,1805)	1:98:A:LYS:HE2	1:124:A:LYS:HD2	10	0.94	0.19	0.95
(3,1806)	1:98:B:LYS:HE2	1:124:B:LYS:HD2	10	0.93	0.19	0.94

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,2937)	1:127:A:TYR:HB2	1:45:A:ILE:HD11	10	0.92	0.37	0.86
(3,2937)	1:127:A:TYR:HB2	1:45:A:ILE:HD13	10	0.92	0.37	0.86
(3,2938)	1:127:B:TYR:HB2	1:45:B:ILE:HD11	10	0.92	0.37	0.86
(3,2938)	1:127:B:TYR:HB2	1:45:B:ILE:HD13	10	0.92	0.37	0.86
(3,2913)	1:86:A:LEU:HB3	1:125:A:ALA:HA	10	0.92	0.13	0.88
(3,2914)	1:86:B:LEU:HB3	1:125:B:ALA:HA	10	0.92	0.13	0.87
(1,3596)	1:115:B:LEU:HD11	1:119:B:MET:HG3	10	0.91	0.29	1.02
(1,3596)	1:115:B:LEU:HD12	1:119:B:MET:HG3	10	0.91	0.29	1.02
(1,3596)	1:115:B:LEU:HD13	1:119:B:MET:HG3	10	0.91	0.29	1.02
(1,3595)	1:115:A:LEU:HD11	1:119:A:MET:HG3	10	0.91	0.29	1.02
(1,3595)	1:115:A:LEU:HD12	1:119:A:MET:HG3	10	0.91	0.29	1.02
(1,3595)	1:115:A:LEU:HD13	1:119:A:MET:HG3	10	0.91	0.29	1.02
(1,3603)	1:115:A:LEU:HD13	1:116:A:MET:HE2	10	0.91	0.17	0.98
(1,3603)	1:115:A:LEU:HD11	1:116:A:MET:HE2	10	0.91	0.17	0.98
(1,3603)	1:115:A:LEU:HD12	1:116:A:MET:HE3	10	0.91	0.17	0.98
(1,3603)	1:115:A:LEU:HD11	1:116:A:MET:HE3	10	0.91	0.17	0.98
(1,3603)	1:115:A:LEU:HD13	1:116:A:MET:HE1	10	0.91	0.17	0.98
(1,3604)	1:115:B:LEU:HD13	1:116:B:MET:HE2	10	0.91	0.17	0.98
(1,3604)	1:115:B:LEU:HD11	1:116:B:MET:HE2	10	0.91	0.17	0.98
(1,3604)	1:115:B:LEU:HD12	1:116:B:MET:HE3	10	0.91	0.17	0.98
(1,3604)	1:115:B:LEU:HD11	1:116:B:MET:HE3	10	0.91	0.17	0.98
(1,3604)	1:115:B:LEU:HD13	1:116:B:MET:HE1	10	0.91	0.17	0.98
(3,2843)	1:102:A:ILE:HG22	1:118:A:VAL:HA	10	0.9	0.12	0.93
(3,2843)	1:115:A:LEU:HD22	1:118:A:VAL:HA	10	0.9	0.12	0.93
(3,2843)	1:102:A:ILE:HG21	1:118:A:VAL:HA	10	0.9	0.12	0.93
(3,2843)	1:115:A:LEU:HD21	1:118:A:VAL:HA	10	0.9	0.12	0.93
(3,2843)	1:102:A:ILE:HG23	1:118:A:VAL:HA	10	0.9	0.12	0.93
(3,2844)	1:102:B:ILE:HG22	1:118:B:VAL:HA	10	0.9	0.12	0.93
(3,2844)	1:115:B:LEU:HD22	1:118:B:VAL:HA	10	0.9	0.12	0.93
(3,2844)	1:102:B:ILE:HG21	1:118:B:VAL:HA	10	0.9	0.12	0.93
(3,2844)	1:115:B:LEU:HD21	1:118:B:VAL:HA	10	0.9	0.12	0.93
(3,2844)	1:102:B:ILE:HG23	1:118:B:VAL:HA	10	0.9	0.12	0.93
(3,1953)	1:79:A:GLN:HG2	1:88:A:SER:HB3	10	0.89	0.81	0.65
(3,1953)	1:79:A:GLN:HG2	1:88:A:SER:HB2	10	0.89	0.81	0.65
(3,1954)	1:79:B:GLN:HG2	1:88:B:SER:HB3	10	0.89	0.81	0.64
(3,1954)	1:79:B:GLN:HG2	1:88:B:SER:HB2	10	0.89	0.81	0.64
(1,2085)	1:98:A:LYS:HD3	1:127:A:TYR:H	10	0.88	0.29	0.94
(1,2086)	1:98:B:LYS:HD3	1:127:B:TYR:H	10	0.88	0.29	0.94
(3,1873)	1:105:A:GLN:HG3	1:119:A:MET:HE3	10	0.87	0.31	0.97
(3,1873)	1:73:A:GLN:HG2	1:69:A:LYS:HD2	10	0.87	0.31	0.97
(3,1873)	1:105:A:GLN:HG3	1:119:A:MET:HE1	10	0.87	0.31	0.97
(3,1873)	1:105:A:GLN:HG3	1:119:A:MET:HE2	10	0.87	0.31	0.97

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,5405)	1:110:A:VAL:HG12	1:104:A:PHE:HZ	10	0.87	0.16	0.9
(1,5405)	1:110:A:VAL:HG13	1:104:A:PHE:HZ	10	0.87	0.16	0.9
(1,5405)	1:110:A:VAL:HG11	1:104:A:PHE:HZ	10	0.87	0.16	0.9
(1,5406)	1:110:B:VAL:HG12	1:104:B:PHE:HZ	10	0.87	0.16	0.9
(1,5406)	1:110:B:VAL:HG13	1:104:B:PHE:HZ	10	0.87	0.16	0.9
(1,5406)	1:110:B:VAL:HG11	1:104:B:PHE:HZ	10	0.87	0.16	0.9
(3,2353)	1:98:A:LYS:HG2	1:96:A:ALA:HB1	10	0.87	0.18	0.92
(3,2353)	1:98:A:LYS:HG2	1:96:A:ALA:HB2	10	0.87	0.18	0.92
(3,2353)	1:98:A:LYS:HG2	1:96:A:ALA:HB3	10	0.87	0.18	0.92
(3,1874)	1:105:B:GLN:HG3	1:119:B:MET:HE3	10	0.87	0.31	0.97
(3,1874)	1:73:B:GLN:HG2	1:69:B:LYS:HD2	10	0.87	0.31	0.97
(3,1874)	1:105:B:GLN:HG3	1:119:B:MET:HE1	10	0.87	0.31	0.97
(3,1874)	1:105:B:GLN:HG3	1:119:B:MET:HE2	10	0.87	0.31	0.97
(3,604)	1:87:B:THR:H	1:119:B:MET:H	10	0.87	0.13	0.89
(3,2354)	1:98:B:LYS:HG2	1:96:B:ALA:HB1	10	0.87	0.17	0.92
(3,2354)	1:98:B:LYS:HG2	1:96:B:ALA:HB2	10	0.87	0.17	0.92
(3,2354)	1:98:B:LYS:HG2	1:96:B:ALA:HB3	10	0.87	0.17	0.92
(3,603)	1:87:A:THR:H	1:119:A:MET:H	10	0.87	0.12	0.89
(1,5238)	1:105:B:GLN:HB2	1:101:B:THR:HG22	10	0.85	0.17	0.88
(1,5238)	1:105:B:GLN:HB2	1:101:B:THR:HG21	10	0.85	0.17	0.88
(1,5238)	1:105:B:GLN:HB2	1:101:B:THR:HG23	10	0.85	0.17	0.88
(3,286)	1:124:B:LYS:HG2	1:84:B:ASP:H	10	0.85	0.17	0.81
(1,5237)	1:105:A:GLN:HB2	1:101:A:THR:HG22	10	0.85	0.16	0.88
(1,5237)	1:105:A:GLN:HB2	1:101:A:THR:HG21	10	0.85	0.16	0.88
(1,5237)	1:105:A:GLN:HB2	1:101:A:THR:HG23	10	0.85	0.16	0.88
(3,285)	1:124:A:LYS:HG2	1:84:A:ASP:H	10	0.85	0.16	0.8
(3,2453)	1:94:A:THR:HG22	1:64:A:VAL:HB	10	0.85	0.16	0.8
(3,2453)	1:64:A:VAL:HB	1:100:A:THR:HG23	10	0.85	0.16	0.8
(3,2453)	1:94:A:THR:HG23	1:64:A:VAL:HB	10	0.85	0.16	0.8
(3,2453)	1:94:A:THR:HG21	1:64:A:VAL:HB	10	0.85	0.16	0.8
(3,2454)	1:94:B:THR:HG22	1:64:B:VAL:HB	10	0.85	0.16	0.8
(3,2454)	1:64:B:VAL:HB	1:100:B:THR:HG23	10	0.85	0.16	0.8
(3,2454)	1:94:B:THR:HG23	1:64:B:VAL:HB	10	0.85	0.16	0.8
(3,2454)	1:94:B:THR:HG21	1:64:B:VAL:HB	10	0.85	0.16	0.8
(1,2496)	1:45:B:ILE:HA	1:54:A:ALA:HB2	10	0.83	0.28	0.9
(1,2496)	1:45:B:ILE:HA	1:54:A:ALA:HB1	10	0.83	0.28	0.9
(1,2496)	1:45:B:ILE:HA	1:54:A:ALA:HB3	10	0.83	0.28	0.9
(1,2495)	1:45:A:ILE:HA	1:54:B:ALA:HB2	10	0.83	0.28	0.88
(1,2495)	1:45:A:ILE:HA	1:54:B:ALA:HB1	10	0.83	0.28	0.88
(1,2495)	1:45:A:ILE:HA	1:54:B:ALA:HB3	10	0.83	0.28	0.88
(1,5621)	1:119:A:MET:HE2	1:121:A:THR:HB	10	0.82	0.33	0.86
(1,5621)	1:119:A:MET:HE3	1:121:A:THR:HB	10	0.82	0.33	0.86

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,5621)	1:119:A:MET:HE1	1:121:A:THR:HB	10	0.82	0.33	0.86
(1,5622)	1:119:B:MET:HE2	1:121:B:THR:HB	10	0.82	0.33	0.86
(1,5622)	1:119:B:MET:HE3	1:121:B:THR:HB	10	0.82	0.33	0.86
(1,5622)	1:119:B:MET:HE1	1:121:B:THR:HB	10	0.82	0.33	0.86
(3,2199)	1:92:A:GLN:HG2	1:87:A:THR:HG22	10	0.82	0.08	0.8
(3,2199)	1:92:A:GLN:HG2	1:87:A:THR:HG21	10	0.82	0.08	0.8
(3,2199)	1:92:A:GLN:HG2	1:87:A:THR:HG23	10	0.82	0.08	0.8
(3,1955)	1:79:A:GLN:HG2	1:91:A:ASP:HB3	10	0.82	0.67	0.6
(3,1955)	1:79:A:GLN:HG3	1:91:A:ASP:HB3	10	0.82	0.67	0.6
(3,1956)	1:79:B:GLN:HG2	1:91:B:ASP:HB3	10	0.82	0.67	0.59
(3,1956)	1:79:B:GLN:HG3	1:91:B:ASP:HB3	10	0.82	0.67	0.59
(1,1764)	1:118:B:VAL:HG13	1:115:B:LEU:H	10	0.82	0.06	0.83
(1,1764)	1:118:B:VAL:HG11	1:115:B:LEU:H	10	0.82	0.06	0.83
(1,1764)	1:118:B:VAL:HG12	1:115:B:LEU:H	10	0.82	0.06	0.83
(3,2464)	1:100:B:THR:HG22	1:102:B:ILE:HG23	10	0.82	0.11	0.8
(3,2464)	1:100:B:THR:HG23	1:102:B:ILE:HG22	10	0.82	0.11	0.8
(3,2464)	1:100:B:THR:HG22	1:102:B:ILE:HG22	10	0.82	0.11	0.8
(3,2464)	1:100:B:THR:HG21	1:102:B:ILE:HG22	10	0.82	0.11	0.8
(3,2464)	1:100:B:THR:HG23	1:102:B:ILE:HG23	10	0.82	0.11	0.8
(3,2464)	1:100:B:THR:HG21	1:102:B:ILE:HG21	10	0.82	0.11	0.8
(3,2464)	1:100:B:THR:HG21	1:102:B:ILE:HG23	10	0.82	0.11	0.8
(3,2464)	1:94:B:THR:HG21	1:102:B:ILE:HG22	10	0.82	0.11	0.8
(3,2200)	1:92:B:GLN:HG2	1:87:B:THR:HG22	10	0.81	0.08	0.8
(3,2200)	1:92:B:GLN:HG2	1:87:B:THR:HG21	10	0.81	0.08	0.8
(3,2200)	1:92:B:GLN:HG2	1:87:B:THR:HG23	10	0.81	0.08	0.8
(1,1763)	1:118:A:VAL:HG13	1:115:A:LEU:H	10	0.81	0.06	0.83
(1,1763)	1:118:A:VAL:HG11	1:115:A:LEU:H	10	0.81	0.06	0.83
(1,1763)	1:118:A:VAL:HG12	1:115:A:LEU:H	10	0.81	0.06	0.83
(3,2463)	1:100:A:THR:HG22	1:102:A:ILE:HG23	10	0.81	0.11	0.8
(3,2463)	1:100:A:THR:HG23	1:102:A:ILE:HG22	10	0.81	0.11	0.8
(3,2463)	1:100:A:THR:HG22	1:102:A:ILE:HG22	10	0.81	0.11	0.8
(3,2463)	1:100:A:THR:HG21	1:102:A:ILE:HG22	10	0.81	0.11	0.8
(3,2463)	1:100:A:THR:HG23	1:102:A:ILE:HG23	10	0.81	0.11	0.8
(3,2463)	1:100:A:THR:HG21	1:102:A:ILE:HG21	10	0.81	0.11	0.8
(3,2463)	1:100:A:THR:HG21	1:102:A:ILE:HG23	10	0.81	0.11	0.8
(3,2463)	1:94:A:THR:HG21	1:102:A:ILE:HG22	10	0.81	0.11	0.8
(1,4771)	1:94:A:THR:HG22	1:102:A:ILE:HG23	10	0.81	0.11	0.8
(1,4771)	1:94:A:THR:HG21	1:102:A:ILE:HG22	10	0.81	0.11	0.8
(1,4771)	1:94:A:THR:HG22	1:102:A:ILE:HG22	10	0.81	0.11	0.8
(1,4771)	1:94:A:THR:HG23	1:102:A:ILE:HG22	10	0.81	0.11	0.8
(1,4771)	1:94:A:THR:HG21	1:102:A:ILE:HG23	10	0.81	0.11	0.8
(1,4771)	1:94:A:THR:HG21	1:102:A:ILE:HG21	10	0.81	0.11	0.8

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,4771)	1:94:A:THR:HG23	1:102:A:ILE:HG23	10	0.81	0.11	0.8
(3,2943)	1:128:A:LEU:HA	1:125:A:ALA:HB1	10	0.81	0.11	0.83
(3,2943)	1:128:A:LEU:HA	1:125:A:ALA:HB3	10	0.81	0.11	0.83
(3,2943)	1:128:A:LEU:HA	1:125:A:ALA:HB2	10	0.81	0.11	0.83
(3,2944)	1:128:B:LEU:HA	1:125:B:ALA:HB1	10	0.81	0.11	0.82
(3,2944)	1:128:B:LEU:HA	1:125:B:ALA:HB3	10	0.81	0.11	0.82
(3,2944)	1:128:B:LEU:HA	1:125:B:ALA:HB2	10	0.81	0.11	0.82
(1,4772)	1:94:B:THR:HG22	1:102:B:ILE:HG23	10	0.81	0.11	0.8
(1,4772)	1:94:B:THR:HG21	1:102:B:ILE:HG22	10	0.81	0.11	0.8
(1,4772)	1:94:B:THR:HG22	1:102:B:ILE:HG22	10	0.81	0.11	0.8
(1,4772)	1:94:B:THR:HG23	1:102:B:ILE:HG22	10	0.81	0.11	0.8
(1,4772)	1:94:B:THR:HG21	1:102:B:ILE:HG23	10	0.81	0.11	0.8
(1,4772)	1:94:B:THR:HG21	1:102:B:ILE:HG21	10	0.81	0.11	0.8
(1,4772)	1:94:B:THR:HG23	1:102:B:ILE:HG23	10	0.81	0.11	0.8
(3,845)	1:44:A:ASP:HA	1:105:B:GLN:HB3	10	0.8	0.35	0.9
(3,845)	1:44:A:ASP:HA	1:116:A:MET:HG3	10	0.8	0.35	0.9
(1,532)	1:102:B:ILE:HG23	1:65:B:PHE:H	10	0.8	0.12	0.78
(1,532)	1:102:B:ILE:HG22	1:65:B:PHE:H	10	0.8	0.12	0.78
(1,532)	1:102:B:ILE:HG21	1:65:B:PHE:H	10	0.8	0.12	0.78
(1,531)	1:102:A:ILE:HG23	1:65:A:PHE:H	10	0.79	0.12	0.78
(1,531)	1:102:A:ILE:HG22	1:65:A:PHE:H	10	0.79	0.12	0.78
(1,531)	1:102:A:ILE:HG21	1:65:A:PHE:H	10	0.79	0.12	0.78
(1,5066)	1:115:B:LEU:HD13	1:119:B:MET:HA	10	0.79	0.2	0.84
(1,5066)	1:115:B:LEU:HD11	1:119:B:MET:HA	10	0.79	0.2	0.84
(1,5066)	1:115:B:LEU:HD12	1:119:B:MET:HA	10	0.79	0.2	0.84
(1,5065)	1:115:A:LEU:HD13	1:119:A:MET:HA	10	0.79	0.2	0.84
(1,5065)	1:115:A:LEU:HD11	1:119:A:MET:HA	10	0.79	0.2	0.84
(1,5065)	1:115:A:LEU:HD12	1:119:A:MET:HA	10	0.79	0.2	0.84
(3,1878)	1:105:B:GLN:HG3	1:110:B:VAL:HG12	10	0.78	0.16	0.82
(3,1878)	1:105:B:GLN:HG3	1:110:B:VAL:HG13	10	0.78	0.16	0.82
(3,1878)	1:105:B:GLN:HG3	1:110:B:VAL:HG11	10	0.78	0.16	0.82
(3,1877)	1:105:A:GLN:HG3	1:110:A:VAL:HG12	10	0.78	0.16	0.82
(3,1877)	1:105:A:GLN:HG3	1:110:A:VAL:HG13	10	0.78	0.16	0.82
(3,1877)	1:105:A:GLN:HG3	1:110:A:VAL:HG11	10	0.78	0.16	0.82
(1,1861)	1:110:A:VAL:HG12	1:118:A:VAL:H	10	0.78	0.16	0.84
(1,1861)	1:110:A:VAL:HG13	1:118:A:VAL:H	10	0.78	0.16	0.84
(1,1861)	1:110:A:VAL:HG11	1:118:A:VAL:H	10	0.78	0.16	0.84
(1,1862)	1:110:B:VAL:HG12	1:118:B:VAL:H	10	0.78	0.16	0.84
(1,1862)	1:110:B:VAL:HG13	1:118:B:VAL:H	10	0.78	0.16	0.84
(1,1862)	1:110:B:VAL:HG11	1:118:B:VAL:H	10	0.78	0.16	0.84
(1,5125)	1:102:A:ILE:HG21	1:66:A:LEU:HG	10	0.77	0.08	0.74
(1,5125)	1:102:A:ILE:HG23	1:66:A:LEU:HG	10	0.77	0.08	0.74

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,5125)	1:102:A:ILE:HG22	1:66:A:LEU:HG	10	0.77	0.08	0.74
(1,5126)	1:102:B:ILE:HG21	1:66:B:LEU:HG	10	0.77	0.08	0.74
(1,5126)	1:102:B:ILE:HG23	1:66:B:LEU:HG	10	0.77	0.08	0.74
(1,5126)	1:102:B:ILE:HG22	1:66:B:LEU:HG	10	0.77	0.08	0.74
(1,5421)	1:110:A:VAL:HG12	1:115:A:LEU:HD12	10	0.77	0.24	0.7
(1,5421)	1:110:A:VAL:HG13	1:115:A:LEU:HD13	10	0.77	0.24	0.7
(1,5421)	1:110:A:VAL:HG11	1:115:A:LEU:HD12	10	0.77	0.24	0.7
(1,5421)	1:110:A:VAL:HG13	1:115:A:LEU:HD11	10	0.77	0.24	0.7
(1,5421)	1:110:A:VAL:HG13	1:115:A:LEU:HD12	10	0.77	0.24	0.7
(1,5421)	1:110:A:VAL:HG11	1:115:A:LEU:HD11	10	0.77	0.24	0.7
(1,5421)	1:110:A:VAL:HG11	1:115:A:LEU:HD13	10	0.77	0.24	0.7
(1,5422)	1:110:B:VAL:HG12	1:115:B:LEU:HD12	10	0.77	0.24	0.7
(1,5422)	1:110:B:VAL:HG13	1:115:B:LEU:HD13	10	0.77	0.24	0.7
(1,5422)	1:110:B:VAL:HG11	1:115:B:LEU:HD12	10	0.77	0.24	0.7
(1,5422)	1:110:B:VAL:HG13	1:115:B:LEU:HD11	10	0.77	0.24	0.7
(1,5422)	1:110:B:VAL:HG13	1:115:B:LEU:HD12	10	0.77	0.24	0.7
(1,5422)	1:110:B:VAL:HG11	1:115:B:LEU:HD11	10	0.77	0.24	0.7
(1,5422)	1:110:B:VAL:HG11	1:115:B:LEU:HD13	10	0.77	0.24	0.7
(3,2821)	1:113:A:GLU:HG2	1:115:A:LEU:HD21	10	0.77	0.22	0.84
(3,2821)	1:113:A:GLU:HG2	1:115:A:LEU:HD23	10	0.77	0.22	0.84
(3,2821)	1:113:A:GLU:HG2	1:115:A:LEU:HD22	10	0.77	0.22	0.84
(3,2822)	1:113:B:GLU:HG2	1:115:B:LEU:HD21	10	0.77	0.21	0.83
(3,2822)	1:113:B:GLU:HG2	1:115:B:LEU:HD23	10	0.77	0.21	0.83
(3,2822)	1:113:B:GLU:HG2	1:115:B:LEU:HD22	10	0.77	0.21	0.83
(1,3022)	1:56:B:PRO:HD2	1:57:B:GLN:HG3	10	0.74	0.17	0.72
(1,5929)	1:112:A:TYR:HE1	1:110:B:VAL:HG13	10	0.74	0.14	0.8
(1,5929)	1:112:A:TYR:HE2	1:110:B:VAL:HG11	10	0.74	0.14	0.8
(1,5929)	1:112:A:TYR:HE2	1:110:B:VAL:HG12	10	0.74	0.14	0.8
(1,5929)	1:112:A:TYR:HE1	1:110:B:VAL:HG12	10	0.74	0.14	0.8
(1,5929)	1:112:A:TYR:HE2	1:110:B:VAL:HG13	10	0.74	0.14	0.8
(1,5930)	1:112:B:TYR:HE1	1:110:A:VAL:HG13	10	0.74	0.13	0.8
(1,5930)	1:112:B:TYR:HE2	1:110:A:VAL:HG11	10	0.74	0.13	0.8
(1,5930)	1:112:B:TYR:HE2	1:110:A:VAL:HG12	10	0.74	0.13	0.8
(1,5930)	1:112:B:TYR:HE1	1:110:A:VAL:HG12	10	0.74	0.13	0.8
(1,5930)	1:112:B:TYR:HE2	1:110:A:VAL:HG13	10	0.74	0.13	0.8
(1,3021)	1:56:A:PRO:HD2	1:57:A:GLN:HG3	10	0.74	0.17	0.71
(1,1557)	1:115:A:LEU:HD11	1:105:A:GLN:H	10	0.74	0.18	0.71
(1,1557)	1:115:A:LEU:HD12	1:105:A:GLN:H	10	0.74	0.18	0.71
(1,1557)	1:115:A:LEU:HD13	1:105:A:GLN:H	10	0.74	0.18	0.71
(1,1558)	1:115:B:LEU:HD11	1:105:B:GLN:H	10	0.73	0.18	0.71
(1,1558)	1:115:B:LEU:HD12	1:105:B:GLN:H	10	0.73	0.18	0.71
(1,1558)	1:115:B:LEU:HD13	1:105:B:GLN:H	10	0.73	0.18	0.71

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,4751)	1:94:A:THR:HG21	1:96:A:ALA:HA	10	0.73	0.22	0.8
(1,4751)	1:94:A:THR:HG23	1:96:A:ALA:HA	10	0.73	0.22	0.8
(1,4751)	1:94:A:THR:HG22	1:96:A:ALA:HA	10	0.73	0.22	0.8
(1,4752)	1:94:B:THR:HG21	1:96:B:ALA:HA	10	0.72	0.22	0.8
(1,4752)	1:94:B:THR:HG23	1:96:B:ALA:HA	10	0.72	0.22	0.8
(1,4752)	1:94:B:THR:HG22	1:96:B:ALA:HA	10	0.72	0.22	0.8
(1,4277)	1:93:A:ARG:HG2	1:65:A:PHE:HB3	10	0.72	0.14	0.72
(1,4278)	1:93:B:ARG:HG2	1:65:B:PHE:HB3	10	0.72	0.14	0.72
(1,4204)	1:107:B:ASP:HB2	1:110:B:VAL:HG13	10	0.72	0.06	0.73
(1,4204)	1:107:B:ASP:HB2	1:110:B:VAL:HG11	10	0.72	0.06	0.73
(1,4204)	1:107:B:ASP:HB2	1:110:B:VAL:HG12	10	0.72	0.06	0.73
(1,3577)	1:66:A:LEU:HA	1:115:A:LEU:HD13	10	0.72	0.11	0.72
(1,3577)	1:66:A:LEU:HA	1:115:A:LEU:HD12	10	0.72	0.11	0.72
(1,3577)	1:66:A:LEU:HA	1:115:A:LEU:HD11	10	0.72	0.11	0.72
(1,4203)	1:107:A:ASP:HB2	1:110:A:VAL:HG13	10	0.72	0.06	0.73
(1,4203)	1:107:A:ASP:HB2	1:110:A:VAL:HG11	10	0.72	0.06	0.73
(1,4203)	1:107:A:ASP:HB2	1:110:A:VAL:HG12	10	0.72	0.06	0.73
(1,3578)	1:66:B:LEU:HA	1:115:B:LEU:HD13	10	0.71	0.11	0.72
(1,3578)	1:66:B:LEU:HA	1:115:B:LEU:HD12	10	0.71	0.11	0.72
(1,3578)	1:66:B:LEU:HA	1:115:B:LEU:HD11	10	0.71	0.11	0.72
(1,5056)	1:119:B:MET:HA	1:122:B:LEU:HB3	10	0.71	0.08	0.72
(1,5055)	1:119:A:MET:HA	1:122:A:LEU:HB3	10	0.71	0.08	0.72
(1,3542)	1:66:B:LEU:HB2	1:106:B:ALA:HB1	10	0.71	0.11	0.71
(1,3542)	1:66:B:LEU:HB2	1:106:B:ALA:HB3	10	0.71	0.11	0.71
(1,3542)	1:66:B:LEU:HB2	1:106:B:ALA:HB2	10	0.71	0.11	0.71
(1,3541)	1:66:A:LEU:HB2	1:106:A:ALA:HB1	10	0.71	0.11	0.71
(1,3541)	1:66:A:LEU:HB2	1:106:A:ALA:HB3	10	0.71	0.11	0.71
(1,3541)	1:66:A:LEU:HB2	1:106:A:ALA:HB2	10	0.71	0.11	0.71
(3,2851)	1:49:A:LEU:HA	1:51:A:ALA:HB1	10	0.7	0.12	0.68
(3,2851)	1:119:A:MET:HE3	1:114:A:THR:HB	10	0.7	0.12	0.68
(3,2851)	1:49:A:LEU:HA	1:51:A:ALA:HB2	10	0.7	0.12	0.68
(3,2851)	1:49:A:LEU:HA	1:51:A:ALA:HB3	10	0.7	0.12	0.68
(3,2852)	1:49:B:LEU:HA	1:51:B:ALA:HB1	10	0.7	0.12	0.68
(3,2852)	1:119:B:MET:HE3	1:114:B:THR:HB	10	0.7	0.12	0.68
(3,2852)	1:49:B:LEU:HA	1:51:B:ALA:HB2	10	0.7	0.12	0.68
(3,2852)	1:49:B:LEU:HA	1:51:B:ALA:HB3	10	0.7	0.12	0.68
(1,4495)	1:115:A:LEU:HB3	1:106:A:ALA:HB2	10	0.7	0.15	0.7
(1,4495)	1:115:A:LEU:HB3	1:106:A:ALA:HB1	10	0.7	0.15	0.7
(1,4495)	1:115:A:LEU:HB3	1:106:A:ALA:HB3	10	0.7	0.15	0.7
(1,4496)	1:115:B:LEU:HB3	1:106:B:ALA:HB2	10	0.7	0.15	0.7
(1,4496)	1:115:B:LEU:HB3	1:106:B:ALA:HB1	10	0.7	0.15	0.7
(1,4496)	1:115:B:LEU:HB3	1:106:B:ALA:HB3	10	0.7	0.15	0.7

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,2729)	1:110:A:VAL:HG22	1:119:A:MET:HE1	10	0.7	0.14	0.76
(3,2729)	1:110:A:VAL:HG23	1:119:A:MET:HE3	10	0.7	0.14	0.76
(3,2729)	1:110:A:VAL:HG22	1:119:A:MET:HE3	10	0.7	0.14	0.76
(3,2729)	1:110:A:VAL:HG21	1:119:A:MET:HE3	10	0.7	0.14	0.76
(3,2729)	1:110:A:VAL:HG23	1:119:A:MET:HE1	10	0.7	0.14	0.76
(3,2729)	1:110:A:VAL:HG22	1:119:A:MET:HE2	10	0.7	0.14	0.76
(3,2730)	1:110:B:VAL:HG22	1:119:B:MET:HE1	10	0.7	0.14	0.76
(3,2730)	1:110:B:VAL:HG23	1:119:B:MET:HE3	10	0.7	0.14	0.76
(3,2730)	1:110:B:VAL:HG22	1:119:B:MET:HE3	10	0.7	0.14	0.76
(3,2730)	1:110:B:VAL:HG21	1:119:B:MET:HE3	10	0.7	0.14	0.76
(3,2730)	1:110:B:VAL:HG23	1:119:B:MET:HE1	10	0.7	0.14	0.76
(3,2730)	1:110:B:VAL:HG22	1:119:B:MET:HE2	10	0.7	0.14	0.76
(1,98)	1:106:B:ALA:HB2	1:107:B:ASP:H	10	0.7	0.11	0.69
(1,98)	1:106:B:ALA:HB1	1:107:B:ASP:H	10	0.7	0.11	0.69
(1,98)	1:106:B:ALA:HB3	1:107:B:ASP:H	10	0.7	0.11	0.69
(1,97)	1:106:A:ALA:HB2	1:107:A:ASP:H	10	0.69	0.11	0.69
(1,97)	1:106:A:ALA:HB1	1:107:A:ASP:H	10	0.69	0.11	0.69
(1,97)	1:106:A:ALA:HB3	1:107:A:ASP:H	10	0.69	0.11	0.69
(1,3777)	1:68:A:VAL:HB	1:114:A:THR:HG21	10	0.69	0.23	0.62
(1,3777)	1:68:A:VAL:HB	1:114:A:THR:HG22	10	0.69	0.23	0.62
(1,3777)	1:68:A:VAL:HB	1:114:A:THR:HG23	10	0.69	0.23	0.62
(1,1125)	1:90:A:LEU:HG	1:90:A:LEU:H	10	0.69	0.06	0.68
(1,3778)	1:68:B:VAL:HB	1:114:B:THR:HG21	10	0.69	0.23	0.62
(1,3778)	1:68:B:VAL:HB	1:114:B:THR:HG22	10	0.69	0.23	0.62
(1,3778)	1:68:B:VAL:HB	1:114:B:THR:HG23	10	0.69	0.23	0.62
(1,1126)	1:90:B:LEU:HG	1:90:B:LEU:H	10	0.69	0.06	0.68
(1,3781)	1:115:A:LEU:HD12	1:68:A:VAL:HB	10	0.68	0.17	0.64
(1,3781)	1:115:A:LEU:HD13	1:68:A:VAL:HB	10	0.68	0.17	0.64
(1,3781)	1:115:A:LEU:HD11	1:68:A:VAL:HB	10	0.68	0.17	0.64
(1,3782)	1:115:B:LEU:HD12	1:68:B:VAL:HB	10	0.67	0.17	0.64
(1,3782)	1:115:B:LEU:HD13	1:68:B:VAL:HB	10	0.67	0.17	0.64
(1,3782)	1:115:B:LEU:HD11	1:68:B:VAL:HB	10	0.67	0.17	0.64
(1,4518)	1:86:B:LEU:HG	1:90:B:LEU:HG	10	0.67	0.15	0.7
(1,4517)	1:86:A:LEU:HG	1:90:A:LEU:HG	10	0.66	0.15	0.69
(1,4132)	1:74:B:LEU:HB3	1:119:B:MET:HE3	10	0.66	0.22	0.57
(1,4132)	1:74:B:LEU:HB3	1:119:B:MET:HE2	10	0.66	0.22	0.57
(1,4132)	1:74:B:LEU:HB3	1:119:B:MET:HE1	10	0.66	0.22	0.57
(1,4131)	1:74:A:LEU:HB3	1:119:A:MET:HE3	10	0.65	0.22	0.56
(1,4131)	1:74:A:LEU:HB3	1:119:A:MET:HE2	10	0.65	0.22	0.56
(1,4131)	1:74:A:LEU:HB3	1:119:A:MET:HE1	10	0.65	0.22	0.56
(1,2559)	1:45:A:ILE:HG23	1:54:B:ALA:HB2	10	0.64	0.25	0.58
(1,2559)	1:45:A:ILE:HG21	1:54:B:ALA:HB1	10	0.64	0.25	0.58

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2559)	1:45:A:ILE:HG23	1:54:B:ALA:HB3	10	0.64	0.25	0.58
(1,2559)	1:45:A:ILE:HG22	1:54:B:ALA:HB2	10	0.64	0.25	0.58
(1,2559)	1:45:A:ILE:HG22	1:54:B:ALA:HB1	10	0.64	0.25	0.58
(1,2559)	1:45:A:ILE:HG22	1:54:B:ALA:HB3	10	0.64	0.25	0.58
(1,2559)	1:45:A:ILE:HG21	1:54:B:ALA:HB2	10	0.64	0.25	0.58
(1,2560)	1:45:B:ILE:HG23	1:54:A:ALA:HB2	10	0.64	0.25	0.58
(1,2560)	1:45:B:ILE:HG21	1:54:A:ALA:HB1	10	0.64	0.25	0.58
(1,2560)	1:45:B:ILE:HG23	1:54:A:ALA:HB3	10	0.64	0.25	0.58
(1,2560)	1:45:B:ILE:HG22	1:54:A:ALA:HB2	10	0.64	0.25	0.58
(1,2560)	1:45:B:ILE:HG22	1:54:A:ALA:HB1	10	0.64	0.25	0.58
(1,2560)	1:45:B:ILE:HG22	1:54:A:ALA:HB3	10	0.64	0.25	0.58
(1,2560)	1:45:B:ILE:HG21	1:54:A:ALA:HB2	10	0.64	0.25	0.58
(3,3059)	1:65:A:PHE:HE1	1:93:A:ARG:HB2	10	0.64	0.23	0.58
(3,3059)	1:65:A:PHE:HE2	1:93:A:ARG:HB2	10	0.64	0.23	0.58
(1,3783)	1:68:A:VAL:HB	1:106:A:ALA:HB2	10	0.64	0.16	0.6
(1,3783)	1:68:A:VAL:HB	1:106:A:ALA:HB1	10	0.64	0.16	0.6
(1,3783)	1:68:A:VAL:HB	1:106:A:ALA:HB3	10	0.64	0.16	0.6
(1,3784)	1:68:B:VAL:HB	1:106:B:ALA:HB2	10	0.64	0.17	0.6
(1,3784)	1:68:B:VAL:HB	1:106:B:ALA:HB1	10	0.64	0.17	0.6
(1,3784)	1:68:B:VAL:HB	1:106:B:ALA:HB3	10	0.64	0.17	0.6
(3,3060)	1:65:B:PHE:HE1	1:93:B:ARG:HB2	10	0.64	0.23	0.58
(3,3060)	1:65:B:PHE:HE2	1:93:B:ARG:HB2	10	0.64	0.23	0.58
(3,2295)	1:96:A:ALA:HA	1:100:A:THR:HG23	10	0.63	0.19	0.67
(3,2295)	1:96:A:ALA:HA	1:100:A:THR:HG21	10	0.63	0.19	0.67
(3,2295)	1:96:A:ALA:HA	1:100:A:THR:HG22	10	0.63	0.19	0.67
(3,2296)	1:96:B:ALA:HA	1:100:B:THR:HG23	10	0.63	0.18	0.67
(3,2296)	1:96:B:ALA:HA	1:100:B:THR:HG21	10	0.63	0.18	0.67
(3,2296)	1:96:B:ALA:HA	1:100:B:THR:HG22	10	0.63	0.18	0.67
(1,3968)	1:72:B:LYS:HB2	1:114:B:THR:HG22	10	0.63	0.31	0.62
(1,3968)	1:72:B:LYS:HB2	1:114:B:THR:HG23	10	0.63	0.31	0.62
(1,3968)	1:72:B:LYS:HB2	1:114:B:THR:HG21	10	0.63	0.31	0.62
(1,3967)	1:72:A:LYS:HB2	1:114:A:THR:HG22	10	0.63	0.31	0.62
(1,3967)	1:72:A:LYS:HB2	1:114:A:THR:HG23	10	0.63	0.31	0.62
(1,3967)	1:72:A:LYS:HB2	1:114:A:THR:HG21	10	0.63	0.31	0.62
(1,4803)	1:96:A:ALA:HB1	1:127:A:TYR:HE1	10	0.63	0.27	0.75
(1,4803)	1:96:A:ALA:HB2	1:127:A:TYR:HE2	10	0.63	0.27	0.75
(1,4803)	1:96:A:ALA:HB3	1:127:A:TYR:HE2	10	0.63	0.27	0.75
(1,4803)	1:96:A:ALA:HB1	1:127:A:TYR:HE2	10	0.63	0.27	0.75
(1,4803)	1:96:A:ALA:HB3	1:127:A:TYR:HE1	10	0.63	0.27	0.75
(1,4804)	1:96:B:ALA:HB1	1:127:B:TYR:HE1	10	0.63	0.26	0.74
(1,4804)	1:96:B:ALA:HB2	1:127:B:TYR:HE2	10	0.63	0.26	0.74
(1,4804)	1:96:B:ALA:HB3	1:127:B:TYR:HE2	10	0.63	0.26	0.74

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,4804)	1:96:B:ALA:HB1	1:127:B:TYR:HE2	10	0.63	0.26	0.74
(1,4804)	1:96:B:ALA:HB3	1:127:B:TYR:HE1	10	0.63	0.26	0.74
(1,2357)	1:82:A:ASN:HB2	1:82:A:ASN:HD22	10	0.63	0.14	0.72
(1,2358)	1:82:B:ASN:HB2	1:82:B:ASN:HD22	10	0.62	0.14	0.72
(1,5603)	1:119:A:MET:HE3	1:130:A:VAL:HA	10	0.62	0.24	0.67
(1,5603)	1:119:A:MET:HE2	1:130:A:VAL:HA	10	0.62	0.24	0.67
(1,5603)	1:119:A:MET:HE1	1:130:A:VAL:HA	10	0.62	0.24	0.67
(1,5604)	1:119:B:MET:HE3	1:130:B:VAL:HA	10	0.62	0.24	0.67
(1,5604)	1:119:B:MET:HE2	1:130:B:VAL:HA	10	0.62	0.24	0.67
(1,5604)	1:119:B:MET:HE1	1:130:B:VAL:HA	10	0.62	0.24	0.67
(3,275)	1:73:A:GLN:HG2	1:79:A:GLN:H	10	0.62	0.45	0.54
(3,276)	1:73:B:GLN:HG2	1:79:B:GLN:H	10	0.62	0.45	0.55
(1,4861)	1:98:A:LYS:HD3	1:127:A:TYR:HB2	10	0.61	0.31	0.74
(1,4862)	1:98:B:LYS:HD3	1:127:B:TYR:HB2	10	0.61	0.31	0.74
(1,3779)	1:68:A:VAL:HB	1:110:A:VAL:HG22	10	0.61	0.12	0.56
(1,3779)	1:68:A:VAL:HB	1:110:A:VAL:HG23	10	0.61	0.12	0.56
(1,3779)	1:68:A:VAL:HB	1:110:A:VAL:HG21	10	0.61	0.12	0.56
(1,3780)	1:68:B:VAL:HB	1:110:B:VAL:HG22	10	0.61	0.12	0.56
(1,3780)	1:68:B:VAL:HB	1:110:B:VAL:HG23	10	0.61	0.12	0.56
(1,3780)	1:68:B:VAL:HB	1:110:B:VAL:HG21	10	0.61	0.12	0.56
(3,2127)	1:87:A:THR:HG21	1:88:A:SER:HB2	10	0.61	0.18	0.58
(3,2127)	1:87:A:THR:HG23	1:88:A:SER:HB2	10	0.61	0.18	0.58
(3,2127)	1:87:A:THR:HG22	1:88:A:SER:HB2	10	0.61	0.18	0.58
(1,2643)	1:125:A:ALA:HA	1:98:A:LYS:HD3	10	0.6	0.2	0.65
(3,2128)	1:87:B:THR:HG21	1:88:B:SER:HB2	10	0.6	0.18	0.56
(3,2128)	1:87:B:THR:HG23	1:88:B:SER:HB2	10	0.6	0.18	0.56
(3,2128)	1:87:B:THR:HG22	1:88:B:SER:HB2	10	0.6	0.18	0.56
(1,2644)	1:125:B:ALA:HA	1:98:B:LYS:HD3	10	0.6	0.2	0.64
(3,2237)	1:90:A:LEU:HA	1:94:A:THR:HG21	10	0.59	0.15	0.56
(3,2237)	1:90:A:LEU:HA	1:94:A:THR:HG22	10	0.59	0.15	0.56
(3,2237)	1:90:A:LEU:HA	1:94:A:THR:HG23	10	0.59	0.15	0.56
(3,2238)	1:90:B:LEU:HA	1:94:B:THR:HG21	10	0.59	0.15	0.56
(3,2238)	1:90:B:LEU:HA	1:94:B:THR:HG22	10	0.59	0.15	0.56
(3,2238)	1:90:B:LEU:HA	1:94:B:THR:HG23	10	0.59	0.15	0.56
(3,1490)	1:129:B:LYS:HG2	1:46:A:ARG:HB3	10	0.58	0.18	0.58
(3,1490)	1:129:B:LYS:HG3	1:46:A:ARG:HB2	10	0.58	0.18	0.58
(3,1490)	1:129:B:LYS:HG3	1:46:A:ARG:HB3	10	0.58	0.18	0.58
(3,1279)	1:57:A:GLN:HG2	1:60:A:PRO:HG3	10	0.58	0.28	0.72
(3,1278)	1:57:B:GLN:HG2	1:50:B:PRO:HD2	10	0.57	0.37	0.52
(3,1278)	1:57:B:GLN:HG3	1:50:B:PRO:HD2	10	0.57	0.37	0.52
(3,1277)	1:57:A:GLN:HG2	1:50:A:PRO:HD2	10	0.57	0.36	0.52
(3,1277)	1:57:A:GLN:HG3	1:50:A:PRO:HD2	10	0.57	0.36	0.52

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,1489)	1:129:A:LYS:HG2	1:46:B:ARG:HB3	10	0.57	0.18	0.59
(3,1489)	1:129:A:LYS:HG3	1:46:B:ARG:HB2	10	0.57	0.18	0.59
(3,1489)	1:129:A:LYS:HG3	1:46:B:ARG:HB3	10	0.57	0.18	0.59
(1,3966)	1:72:B:LYS:HA	1:110:B:VAL:HG11	10	0.57	0.28	0.47
(1,3966)	1:72:B:LYS:HA	1:110:B:VAL:HG12	10	0.57	0.28	0.47
(1,3966)	1:72:B:LYS:HA	1:110:B:VAL:HG13	10	0.57	0.28	0.47
(1,3965)	1:72:A:LYS:HA	1:110:A:VAL:HG11	10	0.57	0.28	0.47
(1,3965)	1:72:A:LYS:HA	1:110:A:VAL:HG12	10	0.57	0.28	0.47
(1,3965)	1:72:A:LYS:HA	1:110:A:VAL:HG13	10	0.57	0.28	0.47
(3,1280)	1:57:B:GLN:HG2	1:60:B:PRO:HG3	10	0.57	0.28	0.72
(1,2044)	1:98:B:LYS:HD3	1:126:B:GLY:H	10	0.56	0.27	0.64
(1,2043)	1:98:A:LYS:HD3	1:126:A:GLY:H	10	0.55	0.27	0.63
(3,2963)	1:129:A:LYS:HG3	1:45:A:ILE:HG23	10	0.53	0.24	0.5
(3,2963)	1:129:A:LYS:HG3	1:45:A:ILE:HG21	10	0.53	0.24	0.5
(3,2963)	1:129:A:LYS:HG3	1:45:A:ILE:HG22	10	0.53	0.24	0.5
(3,2964)	1:129:B:LYS:HG3	1:45:B:ILE:HG23	10	0.53	0.24	0.5
(3,2964)	1:129:B:LYS:HG3	1:45:B:ILE:HG21	10	0.53	0.24	0.5
(3,2964)	1:129:B:LYS:HG3	1:45:B:ILE:HG22	10	0.53	0.24	0.5
(3,2456)	1:100:B:THR:HG22	1:129:B:LYS:HB3	10	0.53	0.2	0.54
(3,2456)	1:100:B:THR:HG23	1:129:B:LYS:HB3	10	0.53	0.2	0.54
(3,2456)	1:100:B:THR:HG21	1:129:B:LYS:HB3	10	0.53	0.2	0.54
(3,995)	1:47:A:VAL:HB	1:128:B:LEU:HG	10	0.53	0.19	0.5
(3,996)	1:47:B:VAL:HB	1:128:A:LEU:HG	10	0.53	0.19	0.48
(3,2455)	1:100:A:THR:HG22	1:129:A:LYS:HB3	10	0.53	0.2	0.54
(3,2455)	1:100:A:THR:HG23	1:129:A:LYS:HB3	10	0.53	0.2	0.54
(3,2455)	1:100:A:THR:HG21	1:129:A:LYS:HB3	10	0.53	0.2	0.54
(1,3855)	1:69:A:LYS:HD3	1:65:A:PHE:HB2	10	0.52	0.25	0.45
(1,3856)	1:69:B:LYS:HD3	1:65:B:PHE:HB2	10	0.52	0.25	0.45
(1,5607)	1:51:A:ALA:HB2	1:124:B:LYS:HA	10	0.52	0.34	0.48
(1,5607)	1:51:A:ALA:HB1	1:124:B:LYS:HA	10	0.52	0.34	0.48
(1,5607)	1:51:A:ALA:HB3	1:124:B:LYS:HA	10	0.52	0.34	0.48
(1,5608)	1:51:B:ALA:HB2	1:124:A:LYS:HA	10	0.52	0.33	0.5
(1,5608)	1:51:B:ALA:HB1	1:124:A:LYS:HA	10	0.52	0.33	0.5
(1,5608)	1:51:B:ALA:HB3	1:124:A:LYS:HA	10	0.52	0.33	0.5
(1,2507)	1:122:A:LEU:HB2	1:130:A:VAL:HB	10	0.52	0.1	0.5
(1,2508)	1:122:B:LEU:HB2	1:130:B:VAL:HB	10	0.52	0.1	0.5
(1,2663)	1:49:A:LEU:HB2	1:50:A:PRO:HD3	10	0.51	0.1	0.51
(1,2664)	1:49:B:LEU:HB2	1:50:B:PRO:HD3	10	0.51	0.1	0.51
(1,5212)	1:104:B:PHE:HB2	1:115:B:LEU:HD11	10	0.5	0.1	0.48
(1,5212)	1:104:B:PHE:HB2	1:115:B:LEU:HD12	10	0.5	0.1	0.48
(1,5212)	1:104:B:PHE:HB2	1:115:B:LEU:HD13	10	0.5	0.1	0.48
(1,5211)	1:104:A:PHE:HB2	1:115:A:LEU:HD11	10	0.49	0.1	0.48

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,5211)	1:104:A:PHE:HB2	1:115:A:LEU:HD12	10	0.49	0.1	0.48
(1,5211)	1:104:A:PHE:HB2	1:115:A:LEU:HD13	10	0.49	0.1	0.48
(3,2507)	1:86:A:LEU:HG	1:119:A:MET:HA	10	0.49	0.13	0.43
(3,2508)	1:86:B:LEU:HG	1:119:B:MET:HA	10	0.49	0.13	0.43
(1,3549)	1:66:A:LEU:HB3	1:122:A:LEU:HG	10	0.49	0.19	0.43
(1,3550)	1:66:B:LEU:HB3	1:122:B:LEU:HG	10	0.49	0.19	0.42
(1,2689)	1:93:A:ARG:HG3	1:92:A:GLN:HB3	10	0.48	0.13	0.44
(1,2690)	1:93:B:ARG:HG3	1:92:B:GLN:HB3	10	0.48	0.13	0.45
(3,802)	1:79:B:GLN:HG2	1:79:B:GLN:HE22	10	0.47	0.01	0.47
(3,802)	1:79:B:GLN:HG3	1:79:B:GLN:HE22	10	0.47	0.01	0.47
(3,801)	1:79:A:GLN:HG2	1:79:A:GLN:HE22	10	0.47	0.01	0.46
(3,801)	1:79:A:GLN:HG3	1:79:A:GLN:HE22	10	0.47	0.01	0.46
(1,2973)	1:56:A:PRO:HD2	1:50:A:PRO:HD2	10	0.45	0.23	0.44
(1,2974)	1:56:B:PRO:HD2	1:50:B:PRO:HD2	10	0.45	0.23	0.44
(3,414)	1:93:B:ARG:HA	1:97:B:ASN:H	10	0.45	0.1	0.48
(3,413)	1:93:A:ARG:HA	1:97:A:ASN:H	10	0.45	0.09	0.47
(3,2114)	1:87:B:THR:HG23	1:124:B:LYS:HD3	10	0.44	0.15	0.37
(3,2114)	1:87:B:THR:HG22	1:124:B:LYS:HD3	10	0.44	0.15	0.37
(3,2114)	1:87:B:THR:HG21	1:124:B:LYS:HD3	10	0.44	0.15	0.37
(3,2113)	1:87:A:THR:HG23	1:124:A:LYS:HD3	10	0.44	0.15	0.37
(3,2113)	1:87:A:THR:HG22	1:124:A:LYS:HD3	10	0.44	0.15	0.37
(3,2113)	1:87:A:THR:HG21	1:124:A:LYS:HD3	10	0.44	0.15	0.37
(1,5128)	1:100:B:THR:HG22	1:102:B:ILE:HG23	10	0.44	0.11	0.42
(1,5128)	1:100:B:THR:HG23	1:102:B:ILE:HG22	10	0.44	0.11	0.42
(1,5128)	1:100:B:THR:HG22	1:102:B:ILE:HG22	10	0.44	0.11	0.42
(1,5128)	1:100:B:THR:HG21	1:102:B:ILE:HG22	10	0.44	0.11	0.42
(1,5128)	1:100:B:THR:HG23	1:102:B:ILE:HG23	10	0.44	0.11	0.42
(1,5128)	1:100:B:THR:HG21	1:102:B:ILE:HG21	10	0.44	0.11	0.42
(1,5128)	1:100:B:THR:HG21	1:102:B:ILE:HG23	10	0.44	0.11	0.42
(1,5127)	1:100:A:THR:HG22	1:102:A:ILE:HG23	10	0.44	0.12	0.42
(1,5127)	1:100:A:THR:HG23	1:102:A:ILE:HG22	10	0.44	0.12	0.42
(1,5127)	1:100:A:THR:HG22	1:102:A:ILE:HG22	10	0.44	0.12	0.42
(1,5127)	1:100:A:THR:HG21	1:102:A:ILE:HG22	10	0.44	0.12	0.42
(1,5127)	1:100:A:THR:HG23	1:102:A:ILE:HG23	10	0.44	0.12	0.42
(1,5127)	1:100:A:THR:HG21	1:102:A:ILE:HG21	10	0.44	0.12	0.42
(1,5127)	1:100:A:THR:HG21	1:102:A:ILE:HG23	10	0.44	0.12	0.42
(1,3606)	1:115:B:LEU:HD13	1:119:B:MET:HE2	10	0.43	0.06	0.46
(1,3606)	1:115:B:LEU:HD12	1:119:B:MET:HE1	10	0.43	0.06	0.46
(1,3606)	1:115:B:LEU:HD13	1:119:B:MET:HE3	10	0.43	0.06	0.46
(1,3606)	1:115:B:LEU:HD12	1:119:B:MET:HE3	10	0.43	0.06	0.46
(1,3606)	1:115:B:LEU:HD11	1:119:B:MET:HE2	10	0.43	0.06	0.46
(1,5413)	1:68:A:VAL:HB	1:110:A:VAL:HG12	10	0.43	0.13	0.39

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,5413)	1:68:A:VAL:HB	1:110:A:VAL:HG13	10	0.43	0.13	0.39
(1,5413)	1:68:A:VAL:HB	1:110:A:VAL:HG11	10	0.43	0.13	0.39
(1,5414)	1:68:B:VAL:HB	1:110:B:VAL:HG12	10	0.43	0.13	0.39
(1,5414)	1:68:B:VAL:HB	1:110:B:VAL:HG13	10	0.43	0.13	0.39
(1,5414)	1:68:B:VAL:HB	1:110:B:VAL:HG11	10	0.43	0.13	0.39
(1,3605)	1:115:A:LEU:HD13	1:119:A:MET:HE2	10	0.43	0.06	0.46
(1,3605)	1:115:A:LEU:HD12	1:119:A:MET:HE1	10	0.43	0.06	0.46
(1,3605)	1:115:A:LEU:HD13	1:119:A:MET:HE3	10	0.43	0.06	0.46
(1,3605)	1:115:A:LEU:HD12	1:119:A:MET:HE3	10	0.43	0.06	0.46
(1,3605)	1:115:A:LEU:HD11	1:119:A:MET:HE2	10	0.43	0.06	0.46
(1,3221)	1:122:A:LEU:HA	1:125:A:ALA:HB1	10	0.43	0.16	0.41
(1,3221)	1:122:A:LEU:HA	1:125:A:ALA:HB3	10	0.43	0.16	0.41
(1,3221)	1:122:A:LEU:HA	1:125:A:ALA:HB2	10	0.43	0.16	0.41
(1,3222)	1:122:B:LEU:HA	1:125:B:ALA:HB1	10	0.43	0.16	0.42
(1,3222)	1:122:B:LEU:HA	1:125:B:ALA:HB3	10	0.43	0.16	0.42
(1,3222)	1:122:B:LEU:HA	1:125:B:ALA:HB2	10	0.43	0.16	0.42
(1,405)	1:58:A:PRO:HB3	1:59:A:ARG:H	10	0.43	0.07	0.44
(1,406)	1:58:B:PRO:HB3	1:59:B:ARG:H	10	0.43	0.07	0.44
(1,3609)	1:115:A:LEU:HD12	1:110:A:VAL:HG22	10	0.42	0.2	0.34
(1,3609)	1:115:A:LEU:HD13	1:110:A:VAL:HG22	10	0.42	0.2	0.34
(1,3609)	1:115:A:LEU:HD12	1:110:A:VAL:HG23	10	0.42	0.2	0.34
(1,3609)	1:115:A:LEU:HD11	1:110:A:VAL:HG22	10	0.42	0.2	0.34
(1,3609)	1:115:A:LEU:HD11	1:110:A:VAL:HG21	10	0.42	0.2	0.34
(1,3609)	1:115:A:LEU:HD13	1:110:A:VAL:HG23	10	0.42	0.2	0.34
(1,3610)	1:115:B:LEU:HD12	1:110:B:VAL:HG22	10	0.42	0.2	0.34
(1,3610)	1:115:B:LEU:HD13	1:110:B:VAL:HG22	10	0.42	0.2	0.34
(1,3610)	1:115:B:LEU:HD12	1:110:B:VAL:HG23	10	0.42	0.2	0.34
(1,3610)	1:115:B:LEU:HD11	1:110:B:VAL:HG22	10	0.42	0.2	0.34
(1,3610)	1:115:B:LEU:HD11	1:110:B:VAL:HG21	10	0.42	0.2	0.34
(1,3610)	1:115:B:LEU:HD13	1:110:B:VAL:HG23	10	0.42	0.2	0.34
(3,1639)	1:115:A:LEU:HD11	1:131:A:GLY:HA3	10	0.42	0.14	0.44
(3,1639)	1:115:A:LEU:HD12	1:131:A:GLY:HA3	10	0.42	0.14	0.44
(3,1639)	1:115:A:LEU:HD11	1:131:A:GLY:HA2	10	0.42	0.14	0.44
(3,1639)	1:115:A:LEU:HD13	1:131:A:GLY:HA3	10	0.42	0.14	0.44
(3,1639)	1:115:A:LEU:HD13	1:131:A:GLY:HA2	10	0.42	0.14	0.44
(3,1640)	1:115:B:LEU:HD11	1:131:B:GLY:HA3	10	0.42	0.14	0.45
(3,1640)	1:115:B:LEU:HD12	1:131:B:GLY:HA3	10	0.42	0.14	0.45
(3,1640)	1:115:B:LEU:HD11	1:131:B:GLY:HA2	10	0.42	0.14	0.45
(3,1640)	1:115:B:LEU:HD13	1:131:B:GLY:HA3	10	0.42	0.14	0.45
(3,1640)	1:115:B:LEU:HD13	1:131:B:GLY:HA2	10	0.42	0.14	0.45
(3,2351)	1:98:A:LYS:HG3	1:125:A:ALA:HB3	10	0.42	0.17	0.42
(3,2351)	1:98:A:LYS:HG3	1:125:A:ALA:HB2	10	0.42	0.17	0.42

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,2351)	1:98:A:LYS:HG3	1:125:A:ALA:HB1	10	0.42	0.17	0.42
(3,2107)	1:87:A:THR:HG21	1:88:A:SER:HB2	10	0.42	0.07	0.42
(3,2107)	1:87:A:THR:HG22	1:124:A:LYS:HA	10	0.42	0.07	0.42
(3,2107)	1:87:A:THR:HG22	1:88:A:SER:HB2	10	0.42	0.07	0.42
(3,2107)	1:87:A:THR:HG21	1:124:A:LYS:HA	10	0.42	0.07	0.42
(3,2107)	1:87:A:THR:HG23	1:124:A:LYS:HA	10	0.42	0.07	0.42
(3,2107)	1:87:A:THR:HG23	1:88:A:SER:HB2	10	0.42	0.07	0.42
(3,2108)	1:87:B:THR:HG21	1:88:B:SER:HB2	10	0.42	0.07	0.42
(3,2108)	1:87:B:THR:HG22	1:124:B:LYS:HA	10	0.42	0.07	0.42
(3,2108)	1:87:B:THR:HG22	1:88:B:SER:HB2	10	0.42	0.07	0.42
(3,2108)	1:87:B:THR:HG21	1:124:B:LYS:HA	10	0.42	0.07	0.42
(3,2108)	1:87:B:THR:HG23	1:124:B:LYS:HA	10	0.42	0.07	0.42
(3,2108)	1:87:B:THR:HG23	1:88:B:SER:HB2	10	0.42	0.07	0.42
(3,2352)	1:98:B:LYS:HG3	1:125:B:ALA:HB3	10	0.42	0.17	0.41
(3,2352)	1:98:B:LYS:HG3	1:125:B:ALA:HB2	10	0.42	0.17	0.41
(3,2352)	1:98:B:LYS:HG3	1:125:B:ALA:HB1	10	0.42	0.17	0.41
(1,3440)	1:64:B:VAL:HA	1:102:B:ILE:HG23	10	0.41	0.07	0.4
(1,3440)	1:64:B:VAL:HA	1:102:B:ILE:HG22	10	0.41	0.07	0.4
(1,3440)	1:64:B:VAL:HA	1:102:B:ILE:HG21	10	0.41	0.07	0.4
(1,99)	1:110:A:VAL:HG13	1:107:A:ASP:H	10	0.41	0.06	0.4
(1,99)	1:110:A:VAL:HG11	1:107:A:ASP:H	10	0.41	0.06	0.4
(1,99)	1:110:A:VAL:HG12	1:107:A:ASP:H	10	0.41	0.06	0.4
(1,100)	1:110:B:VAL:HG13	1:107:B:ASP:H	10	0.41	0.06	0.4
(1,100)	1:110:B:VAL:HG11	1:107:B:ASP:H	10	0.41	0.06	0.4
(1,100)	1:110:B:VAL:HG12	1:107:B:ASP:H	10	0.41	0.06	0.4
(1,23)	1:92:A:GLN:HG2	1:92:A:GLN:HE22	10	0.41	0.0	0.41
(1,24)	1:92:B:GLN:HG2	1:92:B:GLN:HE22	10	0.41	0.0	0.41
(1,3439)	1:64:A:VAL:HA	1:102:A:ILE:HG23	10	0.41	0.07	0.39
(1,3439)	1:64:A:VAL:HA	1:102:A:ILE:HG22	10	0.41	0.07	0.39
(1,3439)	1:64:A:VAL:HA	1:102:A:ILE:HG21	10	0.41	0.07	0.39
(1,4396)	1:83:B:ALA:HA	1:83:B:ALA:HB3	10	0.4	0.01	0.4
(1,4396)	1:83:B:ALA:HA	1:83:B:ALA:HB1	10	0.4	0.01	0.4
(1,4396)	1:83:B:ALA:HA	1:83:B:ALA:HB2	10	0.4	0.01	0.4
(1,1226)	1:93:B:ARG:HG3	1:93:B:ARG:H	10	0.4	0.08	0.39
(1,1225)	1:93:A:ARG:HG3	1:93:A:ARG:H	10	0.4	0.08	0.38
(1,4812)	1:96:B:ALA:HA	1:96:B:ALA:HB1	10	0.4	0.01	0.4
(1,4812)	1:96:B:ALA:HA	1:96:B:ALA:HB2	10	0.4	0.01	0.4
(1,4812)	1:96:B:ALA:HA	1:96:B:ALA:HB3	10	0.4	0.01	0.4
(1,930)	1:83:B:ALA:HB2	1:83:B:ALA:H	10	0.4	0.03	0.4
(1,930)	1:83:B:ALA:HB3	1:83:B:ALA:H	10	0.4	0.03	0.4
(1,930)	1:83:B:ALA:HB1	1:83:B:ALA:H	10	0.4	0.03	0.4
(1,4811)	1:96:A:ALA:HA	1:96:A:ALA:HB1	10	0.4	0.01	0.4

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,4811)	1:96:A:ALA:HA	1:96:A:ALA:HB2	10	0.4	0.01	0.4
(1,4811)	1:96:A:ALA:HA	1:96:A:ALA:HB3	10	0.4	0.01	0.4
(1,929)	1:83:A:ALA:HB2	1:83:A:ALA:H	10	0.4	0.03	0.4
(1,929)	1:83:A:ALA:HB3	1:83:A:ALA:H	10	0.4	0.03	0.4
(1,929)	1:83:A:ALA:HB1	1:83:A:ALA:H	10	0.4	0.03	0.4
(3,2556)	1:103:B:PHE:HA	1:45:A:ILE:HG21	10	0.4	0.22	0.4
(3,2556)	1:103:B:PHE:HA	1:45:A:ILE:HG22	10	0.4	0.22	0.4
(3,2556)	1:103:B:PHE:HA	1:115:B:LEU:HD11	10	0.4	0.22	0.4
(3,2556)	1:103:B:PHE:HA	1:45:A:ILE:HG23	10	0.4	0.22	0.4
(3,2556)	1:103:B:PHE:HA	1:115:B:LEU:HD13	10	0.4	0.22	0.4
(1,4395)	1:83:A:ALA:HA	1:83:A:ALA:HB3	10	0.4	0.01	0.4
(1,4395)	1:83:A:ALA:HA	1:83:A:ALA:HB1	10	0.4	0.01	0.4
(1,4395)	1:83:A:ALA:HA	1:83:A:ALA:HB2	10	0.4	0.01	0.4
(3,2877)	1:83:A:ALA:HB3	1:121:A:THR:HG23	10	0.39	0.1	0.38
(3,2877)	1:86:A:LEU:HB3	1:121:A:THR:HG22	10	0.39	0.1	0.38
(3,2877)	1:83:A:ALA:HB1	1:121:A:THR:HG22	10	0.39	0.1	0.38
(3,2877)	1:83:A:ALA:HB3	1:121:A:THR:HG22	10	0.39	0.1	0.38
(3,2877)	1:83:A:ALA:HB2	1:121:A:THR:HG21	10	0.39	0.1	0.38
(3,2877)	1:83:A:ALA:HB2	1:121:A:THR:HG22	10	0.39	0.1	0.38
(3,2878)	1:83:B:ALA:HB3	1:121:B:THR:HG23	10	0.39	0.1	0.38
(3,2878)	1:86:B:LEU:HB3	1:121:B:THR:HG22	10	0.39	0.1	0.38
(3,2878)	1:83:B:ALA:HB1	1:121:B:THR:HG22	10	0.39	0.1	0.38
(3,2878)	1:83:B:ALA:HB3	1:121:B:THR:HG22	10	0.39	0.1	0.38
(3,2878)	1:83:B:ALA:HB2	1:121:B:THR:HG21	10	0.39	0.1	0.38
(3,2878)	1:83:B:ALA:HB2	1:121:B:THR:HG22	10	0.39	0.1	0.38
(3,1099)	1:138:A:ALA:HA	1:138:A:ALA:HB3	10	0.38	0.01	0.38
(3,1099)	1:139:A:ALA:HA	1:139:A:ALA:HB1	10	0.38	0.01	0.38
(3,1099)	1:139:A:ALA:HA	1:139:A:ALA:HB2	10	0.38	0.01	0.38
(3,1099)	1:139:A:ALA:HA	1:139:A:ALA:HB3	10	0.38	0.01	0.38
(3,1099)	1:138:A:ALA:HA	1:138:A:ALA:HB1	10	0.38	0.01	0.38
(3,1100)	1:139:B:ALA:HA	1:139:B:ALA:HB1	10	0.38	0.01	0.38
(3,1100)	1:139:B:ALA:HA	1:139:B:ALA:HB2	10	0.38	0.01	0.38
(3,1100)	1:138:B:ALA:HA	1:138:B:ALA:HB1	10	0.38	0.01	0.38
(3,1100)	1:139:B:ALA:HA	1:139:B:ALA:HB3	10	0.38	0.01	0.38
(3,73)	1:46:A:ARG:HG2	1:46:A:ARG:H	10	0.35	0.11	0.32
(3,479)	1:115:A:LEU:HD11	1:104:A:PHE:H	10	0.35	0.11	0.35
(3,479)	1:115:A:LEU:HD12	1:104:A:PHE:H	10	0.35	0.11	0.35
(3,479)	1:115:A:LEU:HD13	1:104:A:PHE:H	10	0.35	0.11	0.35
(3,74)	1:46:B:ARG:HG2	1:46:B:ARG:H	10	0.35	0.11	0.32
(3,480)	1:115:B:LEU:HD11	1:104:B:PHE:H	10	0.35	0.1	0.35
(3,480)	1:115:B:LEU:HD12	1:104:B:PHE:H	10	0.35	0.1	0.35
(3,480)	1:115:B:LEU:HD13	1:104:B:PHE:H	10	0.35	0.1	0.35

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,4567)	1:87:A:THR:HG23	1:124:A:LYS:HD2	10	0.35	0.19	0.32
(1,4567)	1:87:A:THR:HG22	1:124:A:LYS:HD2	10	0.35	0.19	0.32
(1,4567)	1:87:A:THR:HG21	1:124:A:LYS:HD2	10	0.35	0.19	0.32
(1,4568)	1:87:B:THR:HG23	1:124:B:LYS:HD2	10	0.35	0.19	0.32
(1,4568)	1:87:B:THR:HG22	1:124:B:LYS:HD2	10	0.35	0.19	0.32
(1,4568)	1:87:B:THR:HG21	1:124:B:LYS:HD2	10	0.35	0.19	0.32
(1,2779)	1:51:A:ALA:HB1	1:51:A:ALA:HA	10	0.35	0.0	0.35
(1,2779)	1:51:A:ALA:HB3	1:51:A:ALA:HA	10	0.35	0.0	0.35
(1,2779)	1:51:A:ALA:HB2	1:51:A:ALA:HA	10	0.35	0.0	0.35
(1,2780)	1:51:B:ALA:HB1	1:51:B:ALA:HA	10	0.35	0.0	0.35
(1,2780)	1:51:B:ALA:HB3	1:51:B:ALA:HA	10	0.35	0.0	0.35
(1,2780)	1:51:B:ALA:HB2	1:51:B:ALA:HA	10	0.35	0.0	0.35
(3,2442)	1:94:B:THR:HG23	1:100:B:THR:HB	10	0.35	0.08	0.39
(3,2442)	1:100:B:THR:HB	1:100:B:THR:HG23	10	0.35	0.08	0.39
(3,2442)	1:100:B:THR:HB	1:100:B:THR:HG22	10	0.35	0.08	0.39
(3,2442)	1:94:B:THR:HG22	1:100:B:THR:HB	10	0.35	0.08	0.39
(3,2442)	1:100:B:THR:HB	1:100:B:THR:HG21	10	0.35	0.08	0.39
(3,2442)	1:94:B:THR:HG21	1:100:B:THR:HB	10	0.35	0.08	0.39
(1,1197)	1:92:A:GLN:HG2	1:92:A:GLN:H	10	0.35	0.06	0.36
(3,2441)	1:94:A:THR:HG23	1:100:A:THR:HB	10	0.35	0.09	0.39
(3,2441)	1:100:A:THR:HB	1:100:A:THR:HG23	10	0.35	0.09	0.39
(3,2441)	1:100:A:THR:HB	1:100:A:THR:HG22	10	0.35	0.09	0.39
(3,2441)	1:94:A:THR:HG22	1:100:A:THR:HB	10	0.35	0.09	0.39
(3,2441)	1:100:A:THR:HB	1:100:A:THR:HG21	10	0.35	0.09	0.39
(3,2441)	1:94:A:THR:HG21	1:100:A:THR:HB	10	0.35	0.09	0.39
(1,1198)	1:92:B:GLN:HG2	1:92:B:GLN:H	10	0.35	0.06	0.35
(1,5305)	1:106:A:ALA:HB2	1:110:A:VAL:HB	10	0.34	0.06	0.33
(1,5305)	1:106:A:ALA:HB1	1:110:A:VAL:HB	10	0.34	0.06	0.33
(1,5305)	1:106:A:ALA:HB3	1:110:A:VAL:HB	10	0.34	0.06	0.33
(1,5306)	1:106:B:ALA:HB2	1:110:B:VAL:HB	10	0.34	0.06	0.32
(1,5306)	1:106:B:ALA:HB1	1:110:B:VAL:HB	10	0.34	0.06	0.32
(1,5306)	1:106:B:ALA:HB3	1:110:B:VAL:HB	10	0.34	0.06	0.32
(1,3607)	1:115:A:LEU:HD13	1:115:A:LEU:HG	10	0.33	0.01	0.34
(1,3607)	1:115:A:LEU:HD11	1:115:A:LEU:HG	10	0.33	0.01	0.34
(1,3607)	1:115:A:LEU:HD12	1:115:A:LEU:HG	10	0.33	0.01	0.34
(1,3608)	1:115:B:LEU:HD13	1:115:B:LEU:HG	10	0.33	0.01	0.34
(1,3608)	1:115:B:LEU:HD11	1:115:B:LEU:HG	10	0.33	0.01	0.34
(1,3608)	1:115:B:LEU:HD12	1:115:B:LEU:HG	10	0.33	0.01	0.34
(3,580)	1:108:B:LYS:HG3	1:116:A:MET:H	10	0.33	0.11	0.34
(1,2811)	1:54:A:ALA:HA	1:54:A:ALA:HB3	10	0.33	0.02	0.32
(1,2811)	1:54:A:ALA:HA	1:54:A:ALA:HB2	10	0.33	0.02	0.32
(1,2811)	1:54:A:ALA:HA	1:54:A:ALA:HB1	10	0.33	0.02	0.32

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2812)	1:54:B:ALA:HA	1:54:B:ALA:HB3	10	0.33	0.02	0.32
(1,2812)	1:54:B:ALA:HA	1:54:B:ALA:HB2	10	0.33	0.02	0.32
(1,2812)	1:54:B:ALA:HA	1:54:B:ALA:HB1	10	0.33	0.02	0.32
(1,5370)	1:110:B:VAL:HA	1:110:B:VAL:HG23	10	0.33	0.02	0.33
(1,5370)	1:110:B:VAL:HA	1:110:B:VAL:HG21	10	0.33	0.02	0.33
(1,5370)	1:110:B:VAL:HA	1:110:B:VAL:HG22	10	0.33	0.02	0.33
(3,579)	1:108:A:LYS:HG2	1:116:B:MET:H	10	0.33	0.11	0.36
(3,579)	1:108:A:LYS:HG3	1:116:B:MET:H	10	0.33	0.11	0.36
(1,5369)	1:110:A:VAL:HA	1:110:A:VAL:HG23	10	0.32	0.02	0.33
(1,5369)	1:110:A:VAL:HA	1:110:A:VAL:HG21	10	0.32	0.02	0.33
(1,5369)	1:110:A:VAL:HA	1:110:A:VAL:HG22	10	0.32	0.02	0.33
(1,3750)	1:68:B:VAL:HA	1:110:B:VAL:HG12	10	0.32	0.05	0.32
(1,3750)	1:68:B:VAL:HA	1:110:B:VAL:HG13	10	0.32	0.05	0.32
(1,3750)	1:68:B:VAL:HA	1:110:B:VAL:HG11	10	0.32	0.05	0.32
(1,3749)	1:68:A:VAL:HA	1:110:A:VAL:HG12	10	0.32	0.05	0.32
(1,3749)	1:68:A:VAL:HA	1:110:A:VAL:HG13	10	0.32	0.05	0.32
(1,3749)	1:68:A:VAL:HA	1:110:A:VAL:HG11	10	0.32	0.05	0.32
(1,253)	1:45:A:ILE:HG21	1:47:A:VAL:H	10	0.32	0.13	0.31
(1,253)	1:45:A:ILE:HG22	1:47:A:VAL:H	10	0.32	0.13	0.31
(1,253)	1:45:A:ILE:HG23	1:47:A:VAL:H	10	0.32	0.13	0.31
(1,254)	1:45:B:ILE:HG21	1:47:B:VAL:H	10	0.32	0.13	0.31
(1,254)	1:45:B:ILE:HG22	1:47:B:VAL:H	10	0.32	0.13	0.31
(1,254)	1:45:B:ILE:HG23	1:47:B:VAL:H	10	0.32	0.13	0.31
(1,2272)	1:139:B:ALA:HB2	1:139:B:ALA:H	10	0.31	0.09	0.25
(1,2272)	1:139:B:ALA:HB3	1:139:B:ALA:H	10	0.31	0.09	0.25
(1,2272)	1:139:B:ALA:HB1	1:139:B:ALA:H	10	0.31	0.09	0.25
(3,257)	1:81:A:VAL:HA	1:77:A:GLY:H	10	0.31	0.1	0.35
(1,2271)	1:139:A:ALA:HB2	1:139:A:ALA:H	10	0.31	0.09	0.25
(1,2271)	1:139:A:ALA:HB3	1:139:A:ALA:H	10	0.31	0.09	0.25
(1,2271)	1:139:A:ALA:HB1	1:139:A:ALA:H	10	0.31	0.09	0.25
(3,258)	1:81:B:VAL:HA	1:77:B:GLY:H	10	0.31	0.1	0.35
(3,107)	1:49:A:LEU:HG	1:51:A:ALA:H	10	0.3	0.07	0.31
(3,108)	1:49:B:LEU:HG	1:51:B:ALA:H	10	0.3	0.07	0.31
(1,5106)	1:102:B:ILE:HG23	1:127:B:TYR:HE1	10	0.3	0.08	0.3
(1,5106)	1:102:B:ILE:HG22	1:127:B:TYR:HE2	10	0.3	0.08	0.3
(1,5106)	1:102:B:ILE:HG22	1:127:B:TYR:HE1	10	0.3	0.08	0.3
(1,5106)	1:102:B:ILE:HG21	1:127:B:TYR:HE2	10	0.3	0.08	0.3
(1,5106)	1:102:B:ILE:HG23	1:127:B:TYR:HE2	10	0.3	0.08	0.3
(1,5105)	1:102:A:ILE:HG23	1:127:A:TYR:HE1	10	0.3	0.09	0.3
(1,5105)	1:102:A:ILE:HG22	1:127:A:TYR:HE2	10	0.3	0.09	0.3
(1,5105)	1:102:A:ILE:HG22	1:127:A:TYR:HE1	10	0.3	0.09	0.3
(1,5105)	1:102:A:ILE:HG21	1:127:A:TYR:HE2	10	0.3	0.09	0.3

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,5105)	1:102:A:ILE:HG23	1:127:A:TYR:HE2	10	0.3	0.09	0.3
(1,3031)	1:119:A:MET:HG2	1:119:A:MET:HE2	10	0.3	0.02	0.3
(1,3031)	1:119:A:MET:HG2	1:119:A:MET:HE3	10	0.3	0.02	0.3
(1,3031)	1:119:A:MET:HG2	1:119:A:MET:HE1	10	0.3	0.02	0.3
(1,3032)	1:119:B:MET:HG2	1:119:B:MET:HE2	10	0.29	0.02	0.29
(1,3032)	1:119:B:MET:HG2	1:119:B:MET:HE3	10	0.29	0.02	0.29
(1,3032)	1:119:B:MET:HG2	1:119:B:MET:HE1	10	0.29	0.02	0.29
(1,5507)	1:114:A:THR:HB	1:114:A:THR:HG22	10	0.29	0.02	0.29
(1,5507)	1:114:A:THR:HB	1:114:A:THR:HG23	10	0.29	0.02	0.29
(1,5507)	1:114:A:THR:HB	1:114:A:THR:HG21	10	0.29	0.02	0.29
(1,5519)	1:115:A:LEU:HG	1:116:A:MET:HE2	10	0.29	0.06	0.28
(1,5519)	1:115:A:LEU:HG	1:116:A:MET:HE3	10	0.29	0.06	0.28
(1,5519)	1:115:A:LEU:HG	1:116:A:MET:HE1	10	0.29	0.06	0.28
(1,5508)	1:114:B:THR:HB	1:114:B:THR:HG22	10	0.28	0.02	0.29
(1,5508)	1:114:B:THR:HB	1:114:B:THR:HG23	10	0.28	0.02	0.29
(1,5508)	1:114:B:THR:HB	1:114:B:THR:HG21	10	0.28	0.02	0.29
(1,5520)	1:115:B:LEU:HG	1:116:B:MET:HE2	10	0.28	0.06	0.28
(1,5520)	1:115:B:LEU:HG	1:116:B:MET:HE3	10	0.28	0.06	0.28
(1,5520)	1:115:B:LEU:HG	1:116:B:MET:HE1	10	0.28	0.06	0.28
(1,1964)	1:121:B:THR:HG22	1:121:B:THR:H	10	0.28	0.02	0.28
(1,1964)	1:121:B:THR:HG21	1:121:B:THR:H	10	0.28	0.02	0.28
(1,1964)	1:121:B:THR:HG23	1:121:B:THR:H	10	0.28	0.02	0.28
(1,1963)	1:121:A:THR:HG22	1:121:A:THR:H	10	0.28	0.03	0.28
(1,1963)	1:121:A:THR:HG21	1:121:A:THR:H	10	0.28	0.03	0.28
(1,1963)	1:121:A:THR:HG23	1:121:A:THR:H	10	0.28	0.03	0.28
(3,1892)	1:74:B:LEU:HB3	1:86:B:LEU:HB3	10	0.27	0.15	0.25
(3,1891)	1:74:A:LEU:HB3	1:86:A:LEU:HB3	10	0.27	0.15	0.25
(1,5539)	1:115:A:LEU:HG	1:115:A:LEU:HD23	10	0.27	0.02	0.28
(1,5539)	1:115:A:LEU:HG	1:115:A:LEU:HD22	10	0.27	0.02	0.28
(1,5539)	1:115:A:LEU:HG	1:115:A:LEU:HD21	10	0.27	0.02	0.28
(1,5540)	1:115:B:LEU:HG	1:115:B:LEU:HD23	10	0.27	0.02	0.28
(1,5540)	1:115:B:LEU:HG	1:115:B:LEU:HD22	10	0.27	0.02	0.28
(1,5540)	1:115:B:LEU:HG	1:115:B:LEU:HD21	10	0.27	0.02	0.28
(1,3540)	1:66:B:LEU:HB2	1:102:B:ILE:HG21	10	0.26	0.11	0.23
(1,3540)	1:66:B:LEU:HB2	1:102:B:ILE:HG23	10	0.26	0.11	0.23
(1,3540)	1:66:B:LEU:HB2	1:102:B:ILE:HG22	10	0.26	0.11	0.23
(1,3539)	1:66:A:LEU:HB2	1:102:A:ILE:HG21	10	0.26	0.11	0.23
(1,3539)	1:66:A:LEU:HB2	1:102:A:ILE:HG23	10	0.26	0.11	0.23
(1,3539)	1:66:A:LEU:HB2	1:102:A:ILE:HG22	10	0.26	0.11	0.23
(1,5589)	1:119:A:MET:HG3	1:119:A:MET:HE1	10	0.26	0.07	0.24
(1,5589)	1:119:A:MET:HG3	1:119:A:MET:HE2	10	0.26	0.07	0.24
(1,5589)	1:119:A:MET:HG3	1:119:A:MET:HE3	10	0.26	0.07	0.24

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,5590)	1:119:B:MET:HG3	1:119:B:MET:HE1	10	0.26	0.07	0.24
(1,5590)	1:119:B:MET:HG3	1:119:B:MET:HE2	10	0.26	0.07	0.24
(1,5590)	1:119:B:MET:HG3	1:119:B:MET:HE3	10	0.26	0.07	0.24
(1,5378)	1:110:B:VAL:HB	1:110:B:VAL:HG22	10	0.25	0.01	0.25
(1,5378)	1:110:B:VAL:HB	1:110:B:VAL:HG23	10	0.25	0.01	0.25
(1,5378)	1:110:B:VAL:HB	1:110:B:VAL:HG21	10	0.25	0.01	0.25
(1,5377)	1:110:A:VAL:HB	1:110:A:VAL:HG22	10	0.25	0.01	0.25
(1,5377)	1:110:A:VAL:HB	1:110:A:VAL:HG23	10	0.25	0.01	0.25
(1,5377)	1:110:A:VAL:HB	1:110:A:VAL:HG21	10	0.25	0.01	0.25
(1,2784)	1:70:B:ALA:HB1	1:70:B:ALA:HA	10	0.24	0.0	0.24
(1,2784)	1:70:B:ALA:HB3	1:70:B:ALA:HA	10	0.24	0.0	0.24
(1,2784)	1:70:B:ALA:HB2	1:70:B:ALA:HA	10	0.24	0.0	0.24
(1,4552)	1:87:B:THR:HB	1:87:B:THR:HG22	10	0.24	0.01	0.24
(1,4552)	1:87:B:THR:HB	1:87:B:THR:HG21	10	0.24	0.01	0.24
(1,4552)	1:87:B:THR:HB	1:87:B:THR:HG23	10	0.24	0.01	0.24
(1,2783)	1:70:A:ALA:HB1	1:70:A:ALA:HA	10	0.24	0.01	0.24
(1,2783)	1:70:A:ALA:HB3	1:70:A:ALA:HA	10	0.24	0.01	0.24
(1,2783)	1:70:A:ALA:HB2	1:70:A:ALA:HA	10	0.24	0.01	0.24
(1,4551)	1:87:A:THR:HB	1:87:A:THR:HG22	10	0.24	0.01	0.24
(1,4551)	1:87:A:THR:HB	1:87:A:THR:HG21	10	0.24	0.01	0.24
(1,4551)	1:87:A:THR:HB	1:87:A:THR:HG23	10	0.24	0.01	0.24
(1,4111)	1:74:A:LEU:HA	1:110:A:VAL:HG12	10	0.24	0.07	0.24
(1,4111)	1:74:A:LEU:HA	1:110:A:VAL:HG13	10	0.24	0.07	0.24
(1,4111)	1:74:A:LEU:HA	1:110:A:VAL:HG11	10	0.24	0.07	0.24
(1,4112)	1:74:B:LEU:HA	1:110:B:VAL:HG12	10	0.24	0.07	0.24
(1,4112)	1:74:B:LEU:HA	1:110:B:VAL:HG13	10	0.24	0.07	0.24
(1,4112)	1:74:B:LEU:HA	1:110:B:VAL:HG11	10	0.24	0.07	0.24
(3,2465)	1:100:A:THR:HG22	1:102:A:ILE:HD13	10	0.23	0.08	0.24
(3,2465)	1:100:A:THR:HG23	1:102:A:ILE:HD12	10	0.23	0.08	0.24
(3,2465)	1:100:A:THR:HG22	1:102:A:ILE:HD11	10	0.23	0.08	0.24
(3,2465)	1:100:A:THR:HG23	1:102:A:ILE:HD11	10	0.23	0.08	0.24
(3,2465)	1:100:A:THR:HG21	1:102:A:ILE:HD13	10	0.23	0.08	0.24
(3,2465)	1:94:A:THR:HG23	1:102:A:ILE:HD11	10	0.23	0.08	0.24
(3,2465)	1:100:A:THR:HG21	1:102:A:ILE:HD11	10	0.23	0.08	0.24
(3,2465)	1:94:A:THR:HG21	1:102:A:ILE:HD13	10	0.23	0.08	0.24
(3,695)	1:129:A:LYS:HB3	1:128:A:LEU:H	10	0.23	0.06	0.24
(3,696)	1:129:B:LYS:HB3	1:128:B:LEU:H	10	0.23	0.06	0.24
(3,749)	1:135:A:MET:HB2	1:136:A:GLU:H	10	0.21	0.04	0.2
(3,749)	1:135:A:MET:HB3	1:136:A:GLU:H	10	0.21	0.04	0.2
(3,750)	1:135:B:MET:HB2	1:136:B:GLU:H	10	0.21	0.04	0.2
(3,750)	1:135:B:MET:HB3	1:136:B:GLU:H	10	0.21	0.04	0.2
(1,3248)	1:99:B:GLU:HG2	1:99:B:GLU:HB2	10	0.2	0.01	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3247)	1:99:A:GLU:HG2	1:99:A:GLU:HB2	10	0.2	0.01	0.2
(1,5151)	1:102:A:ILE:HG23	1:102:A:ILE:HD11	10	0.2	0.02	0.2
(1,5151)	1:102:A:ILE:HG22	1:102:A:ILE:HD13	10	0.2	0.02	0.2
(1,5151)	1:102:A:ILE:HG22	1:102:A:ILE:HD12	10	0.2	0.02	0.2
(1,5151)	1:102:A:ILE:HG22	1:102:A:ILE:HD11	10	0.2	0.02	0.2
(1,5151)	1:102:A:ILE:HG23	1:102:A:ILE:HD13	10	0.2	0.02	0.2
(1,5151)	1:102:A:ILE:HG21	1:102:A:ILE:HD13	10	0.2	0.02	0.2
(1,5151)	1:102:A:ILE:HG23	1:102:A:ILE:HD12	10	0.2	0.02	0.2
(1,5152)	1:102:B:ILE:HG23	1:102:B:ILE:HD11	10	0.2	0.02	0.2
(1,5152)	1:102:B:ILE:HG22	1:102:B:ILE:HD13	10	0.2	0.02	0.2
(1,5152)	1:102:B:ILE:HG22	1:102:B:ILE:HD12	10	0.2	0.02	0.2
(1,5152)	1:102:B:ILE:HG22	1:102:B:ILE:HD11	10	0.2	0.02	0.2
(1,5152)	1:102:B:ILE:HG23	1:102:B:ILE:HD13	10	0.2	0.02	0.2
(1,5152)	1:102:B:ILE:HG21	1:102:B:ILE:HD13	10	0.2	0.02	0.2
(1,5152)	1:102:B:ILE:HG23	1:102:B:ILE:HD12	10	0.2	0.02	0.2
(1,5379)	1:110:A:VAL:HB	1:110:A:VAL:HG11	10	0.2	0.01	0.2
(1,5379)	1:110:A:VAL:HB	1:110:A:VAL:HG12	10	0.2	0.01	0.2
(1,5379)	1:110:A:VAL:HB	1:110:A:VAL:HG13	10	0.2	0.01	0.2
(1,5380)	1:110:B:VAL:HB	1:110:B:VAL:HG11	10	0.2	0.01	0.2
(1,5380)	1:110:B:VAL:HB	1:110:B:VAL:HG12	10	0.2	0.01	0.2
(1,5380)	1:110:B:VAL:HB	1:110:B:VAL:HG13	10	0.2	0.01	0.2
(1,5662)	1:125:B:ALA:HA	1:125:B:ALA:HB2	10	0.19	0.02	0.19
(1,5662)	1:125:B:ALA:HA	1:125:B:ALA:HB1	10	0.19	0.02	0.19
(1,5662)	1:125:B:ALA:HA	1:125:B:ALA:HB3	10	0.19	0.02	0.19
(1,5661)	1:125:A:ALA:HA	1:125:A:ALA:HB2	10	0.19	0.02	0.19
(1,5661)	1:125:A:ALA:HA	1:125:A:ALA:HB1	10	0.19	0.02	0.19
(1,5661)	1:125:A:ALA:HA	1:125:A:ALA:HB3	10	0.19	0.02	0.19
(1,2466)	1:88:B:SER:HA	1:87:B:THR:HG21	10	0.18	0.04	0.19
(1,2466)	1:88:B:SER:HA	1:87:B:THR:HG23	10	0.18	0.04	0.19
(1,2466)	1:88:B:SER:HA	1:87:B:THR:HG22	10	0.18	0.04	0.19
(1,1479)	1:122:A:LEU:HB3	1:122:A:LEU:H	10	0.18	0.01	0.18
(1,2465)	1:88:A:SER:HA	1:87:A:THR:HG21	10	0.18	0.04	0.19
(1,2465)	1:88:A:SER:HA	1:87:A:THR:HG23	10	0.18	0.04	0.19
(1,2465)	1:88:A:SER:HA	1:87:A:THR:HG22	10	0.18	0.04	0.19
(1,1480)	1:122:B:LEU:HB3	1:122:B:LEU:H	10	0.18	0.0	0.18
(1,5623)	1:121:A:THR:HB	1:121:A:THR:HG23	10	0.18	0.01	0.18
(1,5623)	1:121:A:THR:HB	1:121:A:THR:HG21	10	0.18	0.01	0.18
(1,5623)	1:121:A:THR:HB	1:121:A:THR:HG22	10	0.18	0.01	0.18
(1,5624)	1:121:B:THR:HB	1:121:B:THR:HG23	10	0.18	0.01	0.18
(1,5624)	1:121:B:THR:HB	1:121:B:THR:HG21	10	0.18	0.01	0.18
(1,5624)	1:121:B:THR:HB	1:121:B:THR:HG22	10	0.18	0.01	0.18
(1,4533)	1:87:A:THR:HA	1:87:A:THR:HG22	10	0.18	0.02	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,4533)	1:87:A:THR:HA	1:87:A:THR:HG21	10	0.18	0.02	0.18
(1,4533)	1:87:A:THR:HA	1:87:A:THR:HG23	10	0.18	0.02	0.18
(1,4534)	1:87:B:THR:HA	1:87:B:THR:HG22	10	0.18	0.02	0.18
(1,4534)	1:87:B:THR:HA	1:87:B:THR:HG21	10	0.18	0.02	0.18
(1,4534)	1:87:B:THR:HA	1:87:B:THR:HG23	10	0.18	0.02	0.18
(3,2868)	1:121:B:THR:HA	1:121:B:THR:HG21	10	0.18	0.03	0.18
(3,2868)	1:121:B:THR:HA	1:121:B:THR:HG23	10	0.18	0.03	0.18
(3,2868)	1:121:B:THR:HA	1:121:B:THR:HG22	10	0.18	0.03	0.18
(1,1474)	1:122:B:LEU:HD12	1:122:B:LEU:H	10	0.17	0.03	0.18
(1,1474)	1:122:B:LEU:HD13	1:122:B:LEU:H	10	0.17	0.03	0.18
(1,1474)	1:122:B:LEU:HD11	1:122:B:LEU:H	10	0.17	0.03	0.18
(1,1473)	1:122:A:LEU:HD12	1:122:A:LEU:H	10	0.17	0.03	0.18
(1,1473)	1:122:A:LEU:HD13	1:122:A:LEU:H	10	0.17	0.03	0.18
(1,1473)	1:122:A:LEU:HD11	1:122:A:LEU:H	10	0.17	0.03	0.18
(1,964)	1:83:B:ALA:HB1	1:84:B:ASP:H	10	0.17	0.02	0.18
(1,964)	1:83:B:ALA:HB2	1:84:B:ASP:H	10	0.17	0.02	0.18
(1,964)	1:83:B:ALA:HB3	1:84:B:ASP:H	10	0.17	0.02	0.18
(3,2867)	1:121:A:THR:HA	1:121:A:THR:HG21	10	0.17	0.03	0.16
(3,2867)	1:121:A:THR:HA	1:121:A:THR:HG23	10	0.17	0.03	0.16
(3,2867)	1:121:A:THR:HA	1:121:A:THR:HG22	10	0.17	0.03	0.16
(1,963)	1:83:A:ALA:HB1	1:84:A:ASP:H	10	0.17	0.02	0.18
(1,963)	1:83:A:ALA:HB2	1:84:A:ASP:H	10	0.17	0.02	0.18
(1,963)	1:83:A:ALA:HB3	1:84:A:ASP:H	10	0.17	0.02	0.18
(1,5129)	1:102:A:ILE:HG22	1:102:A:ILE:HG13	10	0.17	0.01	0.17
(1,5129)	1:102:A:ILE:HG21	1:102:A:ILE:HG13	10	0.17	0.01	0.17
(1,5129)	1:102:A:ILE:HG23	1:102:A:ILE:HG13	10	0.17	0.01	0.17
(1,5130)	1:102:B:ILE:HG22	1:102:B:ILE:HG13	10	0.17	0.01	0.17
(1,5130)	1:102:B:ILE:HG21	1:102:B:ILE:HG13	10	0.17	0.01	0.17
(1,5130)	1:102:B:ILE:HG23	1:102:B:ILE:HG13	10	0.17	0.01	0.17
(1,2897)	1:55:A:LYS:HB2	1:55:A:LYS:HG2	10	0.16	0.0	0.16
(1,2898)	1:55:B:LYS:HB2	1:55:B:LYS:HG2	10	0.16	0.0	0.16
(1,5514)	1:115:B:LEU:HB2	1:115:B:LEU:HG	10	0.16	0.0	0.16
(1,5513)	1:115:A:LEU:HB2	1:115:A:LEU:HG	10	0.16	0.0	0.16
(1,5099)	1:102:A:ILE:HG13	1:102:A:ILE:HD12	10	0.15	0.0	0.15
(1,5099)	1:102:A:ILE:HG13	1:102:A:ILE:HD11	10	0.15	0.0	0.15
(1,5099)	1:102:A:ILE:HG13	1:102:A:ILE:HD13	10	0.15	0.0	0.15
(1,5100)	1:102:B:ILE:HG13	1:102:B:ILE:HD12	10	0.15	0.0	0.15
(1,5100)	1:102:B:ILE:HG13	1:102:B:ILE:HD11	10	0.15	0.0	0.15
(1,5100)	1:102:B:ILE:HG13	1:102:B:ILE:HD13	10	0.15	0.0	0.15
(3,2079)	1:115:A:LEU:HA	1:115:A:LEU:HB3	10	0.15	0.0	0.15
(3,2080)	1:115:B:LEU:HA	1:115:B:LEU:HB3	10	0.15	0.0	0.15
(1,5289)	1:106:A:ALA:HA	1:106:A:ALA:HB1	10	0.15	0.0	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,5289)	1:106:A:ALA:HA	1:106:A:ALA:HB3	10	0.15	0.0	0.15
(1,5289)	1:106:A:ALA:HA	1:106:A:ALA:HB2	10	0.15	0.0	0.15
(1,5290)	1:106:B:ALA:HA	1:106:B:ALA:HB1	10	0.15	0.0	0.15
(1,5290)	1:106:B:ALA:HA	1:106:B:ALA:HB3	10	0.15	0.0	0.15
(1,5290)	1:106:B:ALA:HA	1:106:B:ALA:HB2	10	0.15	0.0	0.15
(1,4938)	1:100:B:THR:HB	1:100:B:THR:HG22	10	0.15	0.01	0.15
(1,4938)	1:100:B:THR:HB	1:100:B:THR:HG23	10	0.15	0.01	0.15
(1,4938)	1:100:B:THR:HB	1:100:B:THR:HG21	10	0.15	0.01	0.15
(1,4937)	1:100:A:THR:HB	1:100:A:THR:HG22	10	0.15	0.01	0.15
(1,4937)	1:100:A:THR:HB	1:100:A:THR:HG23	10	0.15	0.01	0.15
(1,4937)	1:100:A:THR:HB	1:100:A:THR:HG21	10	0.15	0.01	0.15
(1,974)	1:85:B:GLN:HB3	1:85:B:GLN:H	10	0.14	0.02	0.14
(1,973)	1:85:A:GLN:HB3	1:85:A:GLN:H	10	0.14	0.02	0.14
(1,4513)	1:86:A:LEU:HG	1:86:A:LEU:HB2	10	0.13	0.0	0.13
(1,4514)	1:86:B:LEU:HG	1:86:B:LEU:HB2	10	0.12	0.01	0.12
(1,2851)	1:55:A:LYS:HA	1:55:A:LYS:HG3	10	0.12	0.02	0.11
(1,2852)	1:55:B:LYS:HA	1:55:B:LYS:HG3	10	0.12	0.02	0.11
(3,815)	1:88:A:SER:HB3	1:79:A:GLN:HE22	9	1.51	0.67	1.51
(3,815)	1:88:A:SER:HB2	1:79:A:GLN:HE22	9	1.51	0.67	1.51
(3,816)	1:88:B:SER:HB3	1:79:B:GLN:HE22	9	1.51	0.67	1.48
(3,816)	1:88:B:SER:HB2	1:79:B:GLN:HE22	9	1.51	0.67	1.48
(1,4853)	1:98:A:LYS:HD3	1:51:B:ALA:HA	9	1.39	0.53	1.41
(1,4854)	1:98:B:LYS:HD3	1:51:A:ALA:HA	9	1.38	0.54	1.44
(1,5925)	1:112:A:TYR:HE2	1:113:A:GLU:HB3	9	1.22	0.31	1.14
(1,5925)	1:112:A:TYR:HE1	1:113:A:GLU:HB3	9	1.22	0.31	1.14
(1,5926)	1:112:B:TYR:HE2	1:113:B:GLU:HB3	9	1.22	0.3	1.13
(1,5926)	1:112:B:TYR:HE1	1:113:B:GLU:HB3	9	1.22	0.3	1.13
(3,2175)	1:108:A:LYS:HA	1:139:A:ALA:HB3	9	1.16	0.55	1.17
(3,2175)	1:108:A:LYS:HA	1:139:A:ALA:HB2	9	1.16	0.55	1.17
(3,2175)	1:108:A:LYS:HA	1:139:A:ALA:HB1	9	1.16	0.55	1.17
(3,2176)	1:108:B:LYS:HA	1:139:B:ALA:HB3	9	1.16	0.55	1.16
(3,2176)	1:108:B:LYS:HA	1:139:B:ALA:HB2	9	1.16	0.55	1.16
(3,2176)	1:108:B:LYS:HA	1:139:B:ALA:HB1	9	1.16	0.55	1.16
(3,977)	1:104:A:PHE:HB2	1:131:A:GLY:HA3	9	1.12	0.14	1.1
(3,978)	1:104:B:PHE:HB2	1:131:B:GLY:HA3	9	1.12	0.14	1.1
(1,5483)	1:124:A:LYS:HA	1:123:A:ARG:HB2	9	1.1	0.03	1.1
(1,5484)	1:124:B:LYS:HA	1:123:B:ARG:HB2	9	1.1	0.03	1.09
(1,4721)	1:93:A:ARG:HA	1:77:A:GLY:HA2	9	1.01	0.54	1.11
(1,4722)	1:93:B:ARG:HA	1:77:B:GLY:HA2	9	1.01	0.53	1.11
(1,3351)	1:124:A:LYS:HG2	1:84:A:ASP:HB3	9	1.0	0.26	1.02
(1,1209)	1:89:A:VAL:HG23	1:93:A:ARG:H	9	1.0	0.18	0.99
(1,1209)	1:89:A:VAL:HG22	1:93:A:ARG:H	9	1.0	0.18	0.99

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1209)	1:89:A:VAL:HG21	1:93:A:ARG:H	9	1.0	0.18	0.99
(1,3352)	1:124:B:LYS:HG2	1:84:B:ASP:HB3	9	1.0	0.26	1.01
(1,1210)	1:89:B:VAL:HG23	1:93:B:ARG:H	9	1.0	0.19	1.0
(1,1210)	1:89:B:VAL:HG22	1:93:B:ARG:H	9	1.0	0.19	1.0
(1,1210)	1:89:B:VAL:HG21	1:93:B:ARG:H	9	1.0	0.19	1.0
(1,2910)	1:55:B:LYS:HG3	1:58:B:PRO:HG2	9	0.94	0.54	0.72
(1,2909)	1:55:A:LYS:HG3	1:58:A:PRO:HG2	9	0.94	0.54	0.72
(1,45)	1:89:A:VAL:HG13	1:85:A:GLN:H	9	0.89	0.09	0.89
(1,45)	1:89:A:VAL:HG12	1:85:A:GLN:H	9	0.89	0.09	0.89
(1,45)	1:89:A:VAL:HG11	1:85:A:GLN:H	9	0.89	0.09	0.89
(1,46)	1:89:B:VAL:HG13	1:85:B:GLN:H	9	0.89	0.09	0.89
(1,46)	1:89:B:VAL:HG12	1:85:B:GLN:H	9	0.89	0.09	0.89
(1,46)	1:89:B:VAL:HG11	1:85:B:GLN:H	9	0.89	0.09	0.89
(3,846)	1:44:B:ASP:HA	1:105:A:GLN:HB3	9	0.88	0.27	0.92
(3,846)	1:44:B:ASP:HA	1:116:B:MET:HG3	9	0.88	0.27	0.92
(1,5646)	1:124:B:LYS:HG3	1:124:B:LYS:HE3	9	0.86	0.02	0.86
(1,5645)	1:124:A:LYS:HG3	1:124:A:LYS:HE3	9	0.86	0.02	0.86
(3,2288)	1:95:B:GLN:HG2	1:63:B:PRO:HB2	9	0.86	0.56	0.65
(3,2287)	1:95:A:GLN:HG2	1:63:A:PRO:HB2	9	0.86	0.56	0.65
(3,149)	1:58:A:PRO:HB2	1:61:A:GLU:H	9	0.79	0.21	0.81
(3,150)	1:58:B:PRO:HB2	1:61:B:GLU:H	9	0.79	0.21	0.79
(1,2772)	1:60:B:PRO:HD3	1:63:B:PRO:HB2	9	0.68	0.04	0.67
(1,2771)	1:60:A:PRO:HD3	1:63:A:PRO:HB2	9	0.68	0.04	0.67
(3,459)	1:49:A:LEU:HB2	1:122:B:LEU:H	9	0.66	0.23	0.68
(3,460)	1:49:B:LEU:HB2	1:122:A:LEU:H	9	0.66	0.23	0.66
(3,903)	1:45:A:ILE:HB	1:49:B:LEU:HB3	9	0.6	0.17	0.66
(3,903)	1:122:A:LEU:HB2	1:49:B:LEU:HB3	9	0.6	0.17	0.66
(3,904)	1:45:B:ILE:HB	1:49:A:LEU:HB3	9	0.6	0.17	0.66
(3,904)	1:122:B:LEU:HB2	1:49:A:LEU:HB3	9	0.6	0.17	0.66
(1,1067)	1:89:A:VAL:HG12	1:88:A:SER:H	9	0.59	0.08	0.56
(1,1067)	1:89:A:VAL:HG11	1:88:A:SER:H	9	0.59	0.08	0.56
(1,1067)	1:89:A:VAL:HG13	1:88:A:SER:H	9	0.59	0.08	0.56
(1,1068)	1:89:B:VAL:HG12	1:88:B:SER:H	9	0.58	0.08	0.56
(1,1068)	1:89:B:VAL:HG11	1:88:B:SER:H	9	0.58	0.08	0.56
(1,1068)	1:89:B:VAL:HG13	1:88:B:SER:H	9	0.58	0.08	0.56
(1,1003)	1:89:A:VAL:HG13	1:86:A:LEU:H	9	0.55	0.1	0.57
(1,1003)	1:89:A:VAL:HG12	1:86:A:LEU:H	9	0.55	0.1	0.57
(1,1003)	1:89:A:VAL:HG11	1:86:A:LEU:H	9	0.55	0.1	0.57
(1,1004)	1:89:B:VAL:HG13	1:86:B:LEU:H	9	0.55	0.1	0.57
(1,1004)	1:89:B:VAL:HG12	1:86:B:LEU:H	9	0.55	0.1	0.57
(1,1004)	1:89:B:VAL:HG11	1:86:B:LEU:H	9	0.55	0.1	0.57
(3,263)	1:92:A:GLN:HG3	1:79:A:GLN:H	9	0.55	0.19	0.51

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,263)	1:85:A:GLN:HG3	1:79:A:GLN:H	9	0.55	0.19	0.51
(1,2734)	1:50:B:PRO:HG2	1:54:B:ALA:HB2	9	0.55	0.18	0.53
(1,2734)	1:50:B:PRO:HG2	1:54:B:ALA:HB1	9	0.55	0.18	0.53
(1,2734)	1:50:B:PRO:HG2	1:54:B:ALA:HB3	9	0.55	0.18	0.53
(1,2733)	1:50:A:PRO:HG2	1:54:A:ALA:HB2	9	0.55	0.18	0.53
(1,2733)	1:50:A:PRO:HG2	1:54:A:ALA:HB1	9	0.55	0.18	0.53
(1,2733)	1:50:A:PRO:HG2	1:54:A:ALA:HB3	9	0.55	0.18	0.53
(3,264)	1:92:B:GLN:HG3	1:79:B:GLN:H	9	0.55	0.19	0.51
(3,264)	1:85:B:GLN:HG3	1:79:B:GLN:H	9	0.55	0.19	0.51
(3,974)	1:46:B:ARG:HD3	1:46:B:ARG:HA	9	0.51	0.03	0.52
(3,974)	1:46:B:ARG:HD2	1:46:B:ARG:HA	9	0.51	0.03	0.52
(3,973)	1:46:A:ARG:HD3	1:46:A:ARG:HA	9	0.51	0.03	0.52
(3,973)	1:46:A:ARG:HD2	1:46:A:ARG:HA	9	0.51	0.03	0.52
(3,2555)	1:103:A:PHE:HA	1:45:B:ILE:HG21	9	0.43	0.21	0.45
(3,2555)	1:103:A:PHE:HA	1:115:A:LEU:HD11	9	0.43	0.21	0.45
(3,2555)	1:103:A:PHE:HA	1:45:B:ILE:HG23	9	0.43	0.21	0.45
(3,2555)	1:103:A:PHE:HA	1:115:A:LEU:HD13	9	0.43	0.21	0.45
(3,2555)	1:103:A:PHE:HA	1:45:B:ILE:HG22	9	0.43	0.21	0.45
(1,5690)	1:126:B:GLY:HA3	1:98:B:LYS:HD3	9	0.39	0.23	0.34
(1,5689)	1:126:A:GLY:HA3	1:98:A:LYS:HD3	9	0.39	0.23	0.33
(1,382)	1:55:B:LYS:HB3	1:57:B:GLN:H	9	0.37	0.16	0.35
(1,381)	1:55:A:LYS:HB3	1:57:A:GLN:H	9	0.37	0.15	0.36
(3,2323)	1:127:A:TYR:HE1	1:98:A:LYS:HG2	9	0.36	0.13	0.37
(3,2323)	1:127:A:TYR:HE2	1:98:A:LYS:HG2	9	0.36	0.13	0.37
(3,2324)	1:127:B:TYR:HE1	1:98:B:LYS:HG2	9	0.36	0.13	0.37
(3,2324)	1:127:B:TYR:HE2	1:98:B:LYS:HG2	9	0.36	0.13	0.37
(3,1539)	1:46:A:ARG:HG2	1:128:B:LEU:HB3	9	0.35	0.17	0.33
(3,3073)	1:104:A:PHE:HD1	1:65:A:PHE:HB2	9	0.35	0.07	0.33
(3,3073)	1:104:A:PHE:HD2	1:65:A:PHE:HB2	9	0.35	0.07	0.33
(3,3074)	1:104:B:PHE:HD1	1:65:B:PHE:HB2	9	0.35	0.07	0.33
(3,3074)	1:104:B:PHE:HD2	1:65:B:PHE:HB2	9	0.35	0.07	0.33
(3,1540)	1:46:B:ARG:HG2	1:128:A:LEU:HB3	9	0.35	0.16	0.31
(3,1997)	1:81:A:VAL:HA	1:66:A:LEU:HB2	9	0.34	0.12	0.33
(3,1998)	1:81:B:VAL:HA	1:66:B:LEU:HB2	9	0.34	0.12	0.33
(3,1894)	1:123:B:ARG:HG2	1:124:B:LYS:HE2	9	0.32	0.22	0.27
(3,1894)	1:123:B:ARG:HG2	1:124:B:LYS:HE3	9	0.32	0.22	0.27
(1,5667)	1:87:A:THR:HA	1:125:A:ALA:HB2	9	0.32	0.14	0.28
(1,5667)	1:87:A:THR:HA	1:125:A:ALA:HB1	9	0.32	0.14	0.28
(1,5667)	1:87:A:THR:HA	1:125:A:ALA:HB3	9	0.32	0.14	0.28
(1,5668)	1:87:B:THR:HA	1:125:B:ALA:HB2	9	0.32	0.14	0.28
(1,5668)	1:87:B:THR:HA	1:125:B:ALA:HB1	9	0.32	0.14	0.28
(1,5668)	1:87:B:THR:HA	1:125:B:ALA:HB3	9	0.32	0.14	0.28

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,1893)	1:123:A:ARG:HG2	1:124:A:LYS:HE2	9	0.32	0.22	0.26
(3,1893)	1:123:A:ARG:HG2	1:124:A:LYS:HE3	9	0.32	0.22	0.26
(1,3354)	1:122:B:LEU:HG	1:119:B:MET:HB2	9	0.31	0.13	0.25
(1,3353)	1:122:A:LEU:HG	1:119:A:MET:HB2	9	0.31	0.13	0.25
(3,1887)	1:74:A:LEU:HB2	1:83:A:ALA:HB3	9	0.31	0.13	0.29
(3,1887)	1:74:A:LEU:HB2	1:86:A:LEU:HB3	9	0.31	0.13	0.29
(3,1887)	1:74:A:LEU:HB2	1:83:A:ALA:HB2	9	0.31	0.13	0.29
(3,1887)	1:74:A:LEU:HB2	1:83:A:ALA:HB1	9	0.31	0.13	0.29
(3,1888)	1:74:B:LEU:HB2	1:83:B:ALA:HB3	9	0.31	0.13	0.29
(3,1888)	1:74:B:LEU:HB2	1:86:B:LEU:HB3	9	0.31	0.13	0.29
(3,1888)	1:74:B:LEU:HB2	1:83:B:ALA:HB2	9	0.31	0.13	0.29
(3,1888)	1:74:B:LEU:HB2	1:83:B:ALA:HB1	9	0.31	0.13	0.29
(1,5751)	1:86:A:LEU:HG	1:102:A:ILE:HD11	9	0.3	0.06	0.3
(1,5751)	1:86:A:LEU:HG	1:102:A:ILE:HD13	9	0.3	0.06	0.3
(1,5751)	1:86:A:LEU:HG	1:102:A:ILE:HD12	9	0.3	0.06	0.3
(1,5752)	1:86:B:LEU:HG	1:102:B:ILE:HD11	9	0.3	0.06	0.3
(1,5752)	1:86:B:LEU:HG	1:102:B:ILE:HD13	9	0.3	0.06	0.3
(1,5752)	1:86:B:LEU:HG	1:102:B:ILE:HD12	9	0.3	0.06	0.3
(3,2249)	1:94:A:THR:HG22	1:64:A:VAL:HB	9	0.3	0.13	0.25
(3,2249)	1:94:A:THR:HG23	1:64:A:VAL:HB	9	0.3	0.13	0.25
(3,2249)	1:94:A:THR:HG21	1:64:A:VAL:HB	9	0.3	0.13	0.25
(3,2249)	1:94:A:THR:HG21	1:93:A:ARG:HB3	9	0.3	0.13	0.25
(3,2249)	1:94:A:THR:HG22	1:93:A:ARG:HB3	9	0.3	0.13	0.25
(3,2250)	1:94:B:THR:HG22	1:64:B:VAL:HB	9	0.3	0.13	0.25
(3,2250)	1:94:B:THR:HG23	1:64:B:VAL:HB	9	0.3	0.13	0.25
(3,2250)	1:94:B:THR:HG21	1:64:B:VAL:HB	9	0.3	0.13	0.25
(3,2250)	1:94:B:THR:HG21	1:93:B:ARG:HB3	9	0.3	0.13	0.25
(3,2250)	1:94:B:THR:HG22	1:93:B:ARG:HB3	9	0.3	0.13	0.25
(3,2823)	1:115:A:LEU:HD23	1:116:B:MET:HG2	9	0.29	0.13	0.26
(3,2823)	1:115:A:LEU:HD21	1:116:B:MET:HG2	9	0.29	0.13	0.26
(3,2823)	1:115:A:LEU:HD23	1:116:A:MET:HG3	9	0.29	0.13	0.26
(3,2823)	1:115:A:LEU:HD21	1:116:A:MET:HG3	9	0.29	0.13	0.26
(3,2823)	1:115:A:LEU:HD22	1:116:B:MET:HG2	9	0.29	0.13	0.26
(3,2824)	1:115:B:LEU:HD23	1:116:A:MET:HG2	9	0.29	0.13	0.26
(3,2824)	1:115:B:LEU:HD21	1:116:A:MET:HG2	9	0.29	0.13	0.26
(3,2824)	1:115:B:LEU:HD23	1:116:B:MET:HG3	9	0.29	0.13	0.26
(3,2824)	1:115:B:LEU:HD21	1:116:B:MET:HG3	9	0.29	0.13	0.26
(3,2824)	1:115:B:LEU:HD22	1:116:A:MET:HG2	9	0.29	0.13	0.26
(1,5553)	1:116:A:MET:HE2	1:114:A:THR:HA	9	0.28	0.13	0.26
(1,5553)	1:116:A:MET:HE3	1:114:A:THR:HA	9	0.28	0.13	0.26
(1,5553)	1:116:A:MET:HE1	1:114:A:THR:HA	9	0.28	0.13	0.26
(1,5554)	1:116:B:MET:HE2	1:114:B:THR:HA	9	0.28	0.13	0.27

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,5554)	1:116:B:MET:HE3	1:114:B:THR:HA	9	0.28	0.13	0.27
(1,5554)	1:116:B:MET:HE1	1:114:B:THR:HA	9	0.28	0.13	0.27
(3,2466)	1:100:B:THR:HG22	1:102:B:ILE:HD13	9	0.25	0.07	0.25
(3,2466)	1:100:B:THR:HG23	1:102:B:ILE:HD12	9	0.25	0.07	0.25
(3,2466)	1:100:B:THR:HG22	1:102:B:ILE:HD11	9	0.25	0.07	0.25
(3,2466)	1:100:B:THR:HG23	1:102:B:ILE:HD11	9	0.25	0.07	0.25
(3,2466)	1:94:B:THR:HG23	1:102:B:ILE:HD11	9	0.25	0.07	0.25
(3,2466)	1:100:B:THR:HG21	1:102:B:ILE:HD11	9	0.25	0.07	0.25
(3,2466)	1:94:B:THR:HG21	1:102:B:ILE:HD13	9	0.25	0.07	0.25
(1,1525)	1:66:A:LEU:HB2	1:104:A:PHE:H	9	0.24	0.09	0.23
(1,1526)	1:66:B:LEU:HB2	1:104:B:PHE:H	9	0.24	0.09	0.23
(1,1842)	1:118:B:VAL:HG12	1:117:B:SER:H	9	0.21	0.04	0.21
(1,1842)	1:118:B:VAL:HG13	1:117:B:SER:H	9	0.21	0.04	0.21
(1,1842)	1:118:B:VAL:HG11	1:117:B:SER:H	9	0.21	0.04	0.21
(1,1841)	1:118:A:VAL:HG12	1:117:A:SER:H	9	0.21	0.04	0.21
(1,1841)	1:118:A:VAL:HG13	1:117:A:SER:H	9	0.21	0.04	0.21
(1,1841)	1:118:A:VAL:HG11	1:117:A:SER:H	9	0.21	0.04	0.21
(1,2576)	1:98:B:LYS:HB2	1:98:B:LYS:HD3	9	0.17	0.01	0.17
(1,2575)	1:98:A:LYS:HB2	1:98:A:LYS:HD3	9	0.17	0.01	0.17
(1,4565)	1:87:A:THR:HG23	1:125:A:ALA:HB2	9	0.17	0.04	0.15
(1,4565)	1:87:A:THR:HG22	1:125:A:ALA:HB1	9	0.17	0.04	0.15
(1,4565)	1:87:A:THR:HG21	1:125:A:ALA:HB3	9	0.17	0.04	0.15
(1,4565)	1:87:A:THR:HG21	1:125:A:ALA:HB1	9	0.17	0.04	0.15
(1,4565)	1:87:A:THR:HG23	1:125:A:ALA:HB1	9	0.17	0.04	0.15
(1,4565)	1:87:A:THR:HG22	1:125:A:ALA:HB2	9	0.17	0.04	0.15
(1,4565)	1:87:A:THR:HG21	1:125:A:ALA:HB2	9	0.17	0.04	0.15
(1,4566)	1:87:B:THR:HG23	1:125:B:ALA:HB2	9	0.17	0.04	0.15
(1,4566)	1:87:B:THR:HG22	1:125:B:ALA:HB1	9	0.17	0.04	0.15
(1,4566)	1:87:B:THR:HG21	1:125:B:ALA:HB3	9	0.17	0.04	0.15
(1,4566)	1:87:B:THR:HG21	1:125:B:ALA:HB1	9	0.17	0.04	0.15
(1,4566)	1:87:B:THR:HG23	1:125:B:ALA:HB1	9	0.17	0.04	0.15
(1,4566)	1:87:B:THR:HG22	1:125:B:ALA:HB2	9	0.17	0.04	0.15
(1,4566)	1:87:B:THR:HG21	1:125:B:ALA:HB2	9	0.17	0.04	0.15
(1,434)	1:61:B:GLU:HB2	1:61:B:GLU:H	9	0.11	0.01	0.11
(1,2343)	1:89:A:VAL:HB	1:79:A:GLN:HE22	8	1.27	0.49	1.17
(1,2344)	1:89:B:VAL:HB	1:79:B:GLN:HE22	8	1.27	0.49	1.16
(3,582)	1:49:B:LEU:HG	1:116:A:MET:H	8	1.25	0.25	1.32
(3,582)	1:72:B:LYS:HD3	1:116:B:MET:H	8	1.25	0.25	1.32
(3,581)	1:49:A:LEU:HG	1:116:B:MET:H	8	1.25	0.25	1.31
(3,581)	1:72:A:LYS:HD3	1:116:A:MET:H	8	1.25	0.25	1.31
(1,2782)	1:51:B:ALA:HB1	1:126:A:GLY:HA3	8	0.92	0.43	0.86
(1,2782)	1:51:B:ALA:HB2	1:126:A:GLY:HA3	8	0.92	0.43	0.86

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2782)	1:51:B:ALA:HB3	1:126:A:GLY:HA3	8	0.92	0.43	0.86
(1,2781)	1:51:A:ALA:HB1	1:126:B:GLY:HA3	8	0.91	0.42	0.87
(1,2781)	1:51:A:ALA:HB2	1:126:B:GLY:HA3	8	0.91	0.42	0.87
(1,2781)	1:51:A:ALA:HB3	1:126:B:GLY:HA3	8	0.91	0.42	0.87
(1,4049)	1:85:A:GLN:HB2	1:88:A:SER:HB2	8	0.91	0.12	0.92
(1,4050)	1:85:B:GLN:HB2	1:88:B:SER:HB2	8	0.9	0.11	0.91
(3,1285)	1:57:A:GLN:HG3	1:129:A:LYS:HD2	8	0.89	0.29	0.8
(3,1286)	1:57:B:GLN:HG3	1:129:B:LYS:HD2	8	0.89	0.29	0.8
(3,3100)	1:127:B:TYR:HE1	1:93:B:ARG:HG3	8	0.88	0.27	0.88
(3,3100)	1:75:B:TYR:HE2	1:140:B:LYS:HD2	8	0.88	0.27	0.88
(3,3100)	1:127:B:TYR:HE2	1:129:B:LYS:HD2	8	0.88	0.27	0.88
(3,3100)	1:75:B:TYR:HE1	1:140:B:LYS:HD2	8	0.88	0.27	0.88
(3,3100)	1:75:B:TYR:HE1	1:140:B:LYS:HD3	8	0.88	0.27	0.88
(3,3100)	1:75:B:TYR:HE2	1:140:B:LYS:HD3	8	0.88	0.27	0.88
(3,3099)	1:127:A:TYR:HE1	1:93:A:ARG:HG3	8	0.87	0.27	0.87
(3,3099)	1:75:A:TYR:HE2	1:140:A:LYS:HD2	8	0.87	0.27	0.87
(3,3099)	1:127:A:TYR:HE2	1:129:A:LYS:HD2	8	0.87	0.27	0.87
(3,3099)	1:75:A:TYR:HE1	1:140:A:LYS:HD2	8	0.87	0.27	0.87
(3,3099)	1:75:A:TYR:HE1	1:140:A:LYS:HD3	8	0.87	0.27	0.87
(3,3099)	1:75:A:TYR:HE2	1:140:A:LYS:HD3	8	0.87	0.27	0.87
(1,4363)	1:82:A:ASN:HB3	1:85:A:GLN:HG2	8	0.86	0.69	0.48
(1,4364)	1:82:B:ASN:HB3	1:85:B:GLN:HG2	8	0.86	0.69	0.49
(3,2514)	1:129:B:LYS:HD2	1:102:B:ILE:HG13	8	0.76	0.27	0.89
(3,2513)	1:129:A:LYS:HD2	1:102:A:ILE:HG13	8	0.76	0.27	0.88
(3,1295)	1:58:A:PRO:HG2	1:55:A:LYS:HE2	8	0.72	1.01	0.26
(3,1295)	1:58:A:PRO:HG2	1:55:A:LYS:HE3	8	0.72	1.01	0.26
(3,1296)	1:58:B:PRO:HG2	1:55:B:LYS:HE2	8	0.72	1.01	0.26
(3,1296)	1:58:B:PRO:HG2	1:55:B:LYS:HE3	8	0.72	1.01	0.26
(1,2562)	1:45:B:ILE:HG22	1:49:A:LEU:HD13	8	0.67	0.1	0.67
(1,2562)	1:45:B:ILE:HG23	1:49:A:LEU:HD11	8	0.67	0.1	0.67
(1,2562)	1:45:B:ILE:HG22	1:49:A:LEU:HD12	8	0.67	0.1	0.67
(1,2562)	1:45:B:ILE:HG21	1:49:A:LEU:HD11	8	0.67	0.1	0.67
(1,2562)	1:45:B:ILE:HG21	1:49:A:LEU:HD13	8	0.67	0.1	0.67
(1,2562)	1:45:B:ILE:HG21	1:49:A:LEU:HD12	8	0.67	0.1	0.67
(1,2561)	1:45:A:ILE:HG22	1:49:B:LEU:HD13	8	0.66	0.09	0.66
(1,2561)	1:45:A:ILE:HG23	1:49:B:LEU:HD11	8	0.66	0.09	0.66
(1,2561)	1:45:A:ILE:HG22	1:49:B:LEU:HD12	8	0.66	0.09	0.66
(1,2561)	1:45:A:ILE:HG21	1:49:B:LEU:HD11	8	0.66	0.09	0.66
(1,2561)	1:45:A:ILE:HG21	1:49:B:LEU:HD13	8	0.66	0.09	0.66
(1,2561)	1:45:A:ILE:HG21	1:49:B:LEU:HD12	8	0.66	0.09	0.66
(1,4795)	1:96:A:ALA:HA	1:90:A:LEU:HB2	8	0.59	0.25	0.63
(1,4796)	1:96:B:ALA:HA	1:90:B:LEU:HB2	8	0.59	0.25	0.62

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,4504)	1:86:B:LEU:HB2	1:121:B:THR:HG23	8	0.56	0.32	0.5
(1,4504)	1:86:B:LEU:HB2	1:121:B:THR:HG22	8	0.56	0.32	0.5
(1,4504)	1:86:B:LEU:HB2	1:121:B:THR:HG21	8	0.56	0.32	0.5
(1,4503)	1:86:A:LEU:HB2	1:121:A:THR:HG23	8	0.56	0.32	0.5
(1,4503)	1:86:A:LEU:HB2	1:121:A:THR:HG22	8	0.56	0.32	0.5
(1,4503)	1:86:A:LEU:HB2	1:121:A:THR:HG21	8	0.56	0.32	0.5
(3,232)	1:72:B:LYS:HG2	1:72:B:LYS:H	8	0.56	0.05	0.55
(3,232)	1:70:B:ALA:HB1	1:72:B:LYS:H	8	0.56	0.05	0.55
(3,231)	1:72:A:LYS:HG2	1:72:A:LYS:H	8	0.55	0.05	0.55
(3,231)	1:70:A:ALA:HB1	1:72:A:LYS:H	8	0.55	0.05	0.55
(1,3367)	1:123:A:ARG:HG2	1:50:B:PRO:HD3	8	0.54	0.27	0.44
(1,3368)	1:123:B:ARG:HG2	1:50:A:PRO:HD3	8	0.53	0.29	0.43
(3,2532)	1:102:B:ILE:HG21	1:133:B:VAL:HB	8	0.51	0.28	0.43
(3,2532)	1:102:B:ILE:HG23	1:133:B:VAL:HB	8	0.51	0.28	0.43
(3,2532)	1:102:B:ILE:HG22	1:133:B:VAL:HB	8	0.51	0.28	0.43
(3,2531)	1:102:A:ILE:HG21	1:133:A:VAL:HB	8	0.51	0.29	0.43
(3,2531)	1:102:A:ILE:HG23	1:133:A:VAL:HB	8	0.51	0.29	0.43
(3,2531)	1:102:A:ILE:HG22	1:133:A:VAL:HB	8	0.51	0.29	0.43
(3,608)	1:134:B:GLY:HA3	1:119:A:MET:H	8	0.49	0.34	0.42
(3,607)	1:134:A:GLY:HA3	1:119:B:MET:H	8	0.49	0.35	0.41
(3,437)	1:87:A:THR:HG22	1:100:A:THR:H	8	0.48	0.09	0.52
(3,437)	1:87:A:THR:HG21	1:100:A:THR:H	8	0.48	0.09	0.52
(3,437)	1:87:A:THR:HG23	1:100:A:THR:H	8	0.48	0.09	0.52
(3,438)	1:87:B:THR:HG22	1:100:B:THR:H	8	0.48	0.09	0.52
(3,438)	1:87:B:THR:HG21	1:100:B:THR:H	8	0.48	0.09	0.52
(3,438)	1:87:B:THR:HG23	1:100:B:THR:H	8	0.48	0.09	0.52
(3,1768)	1:70:B:ALA:HA	1:74:B:LEU:HG	8	0.48	0.18	0.48
(3,1768)	1:70:B:ALA:HA	1:105:B:GLN:HB3	8	0.48	0.18	0.48
(3,1767)	1:70:A:ALA:HA	1:74:A:LEU:HG	8	0.48	0.19	0.48
(3,1767)	1:70:A:ALA:HA	1:105:A:GLN:HB3	8	0.48	0.19	0.48
(3,1833)	1:72:A:LYS:HE2	1:110:A:VAL:HG23	8	0.45	0.61	0.16
(3,1833)	1:72:A:LYS:HE2	1:110:A:VAL:HG21	8	0.45	0.61	0.16
(3,1834)	1:72:B:LYS:HE2	1:110:B:VAL:HG23	8	0.45	0.61	0.16
(3,1834)	1:72:B:LYS:HE2	1:110:B:VAL:HG21	8	0.45	0.61	0.16
(1,4759)	1:94:A:THR:HG23	1:99:A:GLU:HG3	8	0.44	0.16	0.43
(1,4759)	1:94:A:THR:HG21	1:99:A:GLU:HG3	8	0.44	0.16	0.43
(1,4759)	1:94:A:THR:HG22	1:99:A:GLU:HG3	8	0.44	0.16	0.43
(1,4760)	1:94:B:THR:HG23	1:99:B:GLU:HG3	8	0.44	0.16	0.43
(1,4760)	1:94:B:THR:HG21	1:99:B:GLU:HG3	8	0.44	0.16	0.43
(1,4760)	1:94:B:THR:HG22	1:99:B:GLU:HG3	8	0.44	0.16	0.43
(3,1728)	1:69:B:LYS:HB3	1:66:B:LEU:HG	8	0.42	0.06	0.42
(3,1727)	1:69:A:LYS:HB3	1:66:A:LEU:HG	8	0.41	0.07	0.42

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,1106)	1:51:B:ALA:HA	1:124:A:LYS:HB3	8	0.41	0.2	0.34
(3,1105)	1:51:A:ALA:HA	1:124:B:LYS:HB3	8	0.41	0.19	0.36
(1,3973)	1:72:A:LYS:HB3	1:72:A:LYS:HD3	8	0.41	0.04	0.4
(1,3974)	1:72:B:LYS:HB3	1:72:B:LYS:HD3	8	0.41	0.04	0.4
(3,2974)	1:130:B:VAL:HB	1:119:B:MET:HE1	8	0.38	0.22	0.32
(3,2974)	1:130:B:VAL:HB	1:119:B:MET:HE3	8	0.38	0.22	0.32
(3,2974)	1:130:B:VAL:HB	1:119:B:MET:HE2	8	0.38	0.22	0.32
(3,2973)	1:130:A:VAL:HB	1:119:A:MET:HE1	8	0.38	0.22	0.31
(3,2973)	1:130:A:VAL:HB	1:119:A:MET:HE3	8	0.38	0.22	0.31
(3,2973)	1:130:A:VAL:HB	1:119:A:MET:HE2	8	0.38	0.22	0.31
(1,1122)	1:110:B:VAL:HG23	1:114:B:THR:H	8	0.35	0.16	0.36
(1,1122)	1:110:B:VAL:HG21	1:114:B:THR:H	8	0.35	0.16	0.36
(1,1122)	1:110:B:VAL:HG22	1:114:B:THR:H	8	0.35	0.16	0.36
(1,1121)	1:110:A:VAL:HG23	1:114:A:THR:H	8	0.35	0.16	0.36
(1,1121)	1:110:A:VAL:HG21	1:114:A:THR:H	8	0.35	0.16	0.36
(1,1121)	1:110:A:VAL:HG22	1:114:A:THR:H	8	0.35	0.16	0.36
(1,5356)	1:107:B:ASP:HB2	1:109:B:SER:HB3	8	0.35	0.05	0.33
(1,5355)	1:107:A:ASP:HB2	1:109:A:SER:HB3	8	0.35	0.06	0.33
(3,1642)	1:115:B:LEU:HD11	1:131:B:GLY:HA3	8	0.34	0.12	0.35
(3,1642)	1:115:B:LEU:HD13	1:131:B:GLY:HA3	8	0.34	0.12	0.35
(3,1642)	1:115:B:LEU:HD11	1:131:B:GLY:HA2	8	0.34	0.12	0.35
(3,1642)	1:115:B:LEU:HD13	1:131:B:GLY:HA2	8	0.34	0.12	0.35
(3,1642)	1:115:B:LEU:HD12	1:131:B:GLY:HA3	8	0.34	0.12	0.35
(3,1642)	1:115:B:LEU:HD13	1:120:B:ASP:HB3	8	0.34	0.12	0.35
(3,1641)	1:115:A:LEU:HD11	1:131:A:GLY:HA3	8	0.33	0.12	0.34
(3,1641)	1:115:A:LEU:HD13	1:131:A:GLY:HA3	8	0.33	0.12	0.34
(3,1641)	1:115:A:LEU:HD11	1:131:A:GLY:HA2	8	0.33	0.12	0.34
(3,1641)	1:115:A:LEU:HD13	1:131:A:GLY:HA2	8	0.33	0.12	0.34
(3,1641)	1:115:A:LEU:HD12	1:131:A:GLY:HA3	8	0.33	0.12	0.34
(3,1641)	1:115:A:LEU:HD13	1:120:A:ASP:HB3	8	0.33	0.12	0.34
(1,4573)	1:87:A:THR:HG22	1:90:A:LEU:HG	8	0.33	0.13	0.32
(1,4573)	1:87:A:THR:HG21	1:90:A:LEU:HG	8	0.33	0.13	0.32
(1,4573)	1:87:A:THR:HG23	1:90:A:LEU:HG	8	0.33	0.13	0.32
(1,4574)	1:87:B:THR:HG22	1:90:B:LEU:HG	8	0.33	0.13	0.31
(1,4574)	1:87:B:THR:HG21	1:90:B:LEU:HG	8	0.33	0.13	0.31
(1,4574)	1:87:B:THR:HG23	1:90:B:LEU:HG	8	0.33	0.13	0.31
(1,4816)	1:92:B:GLN:HG3	1:96:B:ALA:HB3	8	0.32	0.06	0.32
(1,4816)	1:92:B:GLN:HG3	1:96:B:ALA:HB1	8	0.32	0.06	0.32
(1,4816)	1:92:B:GLN:HG3	1:96:B:ALA:HB2	8	0.32	0.06	0.32
(1,4815)	1:92:A:GLN:HG3	1:96:A:ALA:HB3	8	0.32	0.05	0.31
(1,4815)	1:92:A:GLN:HG3	1:96:A:ALA:HB1	8	0.32	0.05	0.31
(1,4815)	1:92:A:GLN:HG3	1:96:A:ALA:HB2	8	0.32	0.05	0.31

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,1895)	1:123:A:ARG:HG2	1:50:B:PRO:HB3	8	0.32	0.15	0.26
(3,1896)	1:123:B:ARG:HG2	1:50:A:PRO:HB3	8	0.32	0.16	0.26
(1,2241)	1:136:A:GLU:HB3	1:136:A:GLU:H	8	0.31	0.02	0.32
(1,2242)	1:136:B:GLU:HB3	1:136:B:GLU:H	8	0.31	0.02	0.32
(3,77)	1:46:A:ARG:HD2	1:47:A:VAL:H	8	0.31	0.1	0.29
(3,78)	1:46:B:ARG:HD2	1:47:B:VAL:H	8	0.31	0.11	0.29
(3,2317)	1:123:A:ARG:HB2	1:124:A:LYS:HG3	8	0.3	0.09	0.3
(3,2318)	1:123:B:ARG:HB2	1:124:B:LYS:HG3	8	0.3	0.09	0.3
(3,2849)	1:119:A:MET:HE1	1:103:A:PHE:HA	8	0.26	0.11	0.26
(3,2849)	1:119:A:MET:HE2	1:103:A:PHE:HA	8	0.26	0.11	0.26
(3,2849)	1:119:A:MET:HE3	1:103:A:PHE:HA	8	0.26	0.11	0.26
(3,2850)	1:119:B:MET:HE1	1:103:B:PHE:HA	8	0.26	0.11	0.26
(3,2850)	1:119:B:MET:HE2	1:103:B:PHE:HA	8	0.26	0.11	0.26
(3,2850)	1:119:B:MET:HE3	1:103:B:PHE:HA	8	0.26	0.11	0.26
(1,5762)	1:129:B:LYS:HG2	1:129:B:LYS:HA	8	0.26	0.02	0.26
(1,5761)	1:129:A:LYS:HG2	1:129:A:LYS:HA	8	0.26	0.02	0.26
(1,5394)	1:110:B:VAL:HG23	1:112:B:TYR:HB3	8	0.26	0.07	0.26
(1,5394)	1:110:B:VAL:HG21	1:112:B:TYR:HB3	8	0.26	0.07	0.26
(1,5394)	1:110:B:VAL:HG22	1:112:B:TYR:HB3	8	0.26	0.07	0.26
(1,5393)	1:110:A:VAL:HG23	1:112:A:TYR:HB3	8	0.26	0.07	0.26
(1,5393)	1:110:A:VAL:HG21	1:112:A:TYR:HB3	8	0.26	0.07	0.26
(1,5393)	1:110:A:VAL:HG22	1:112:A:TYR:HB3	8	0.26	0.07	0.26
(1,5149)	1:100:A:THR:HG22	1:102:A:ILE:HD13	8	0.23	0.08	0.22
(1,5149)	1:100:A:THR:HG22	1:102:A:ILE:HD11	8	0.23	0.08	0.22
(1,5149)	1:100:A:THR:HG23	1:102:A:ILE:HD11	8	0.23	0.08	0.22
(1,5149)	1:100:A:THR:HG23	1:102:A:ILE:HD12	8	0.23	0.08	0.22
(1,5149)	1:100:A:THR:HG21	1:102:A:ILE:HD12	8	0.23	0.08	0.22
(1,5149)	1:100:A:THR:HG21	1:102:A:ILE:HD11	8	0.23	0.08	0.22
(1,5149)	1:100:A:THR:HG22	1:102:A:ILE:HD12	8	0.23	0.08	0.22
(1,5150)	1:100:B:THR:HG22	1:102:B:ILE:HD13	8	0.23	0.08	0.21
(1,5150)	1:100:B:THR:HG22	1:102:B:ILE:HD11	8	0.23	0.08	0.21
(1,5150)	1:100:B:THR:HG23	1:102:B:ILE:HD11	8	0.23	0.08	0.21
(1,5150)	1:100:B:THR:HG23	1:102:B:ILE:HD12	8	0.23	0.08	0.21
(1,5150)	1:100:B:THR:HG21	1:102:B:ILE:HD12	8	0.23	0.08	0.21
(1,5150)	1:100:B:THR:HG21	1:102:B:ILE:HD11	8	0.23	0.08	0.21
(1,5150)	1:100:B:THR:HG22	1:102:B:ILE:HD12	8	0.23	0.08	0.21
(1,1688)	1:139:B:ALA:HA	1:140:B:LYS:H	8	0.22	0.09	0.22
(1,3972)	1:72:B:LYS:HB3	1:72:B:LYS:HD2	8	0.22	0.16	0.18
(1,1687)	1:139:A:ALA:HA	1:140:A:LYS:H	8	0.22	0.09	0.23
(1,3971)	1:72:A:LYS:HB3	1:72:A:LYS:HD2	8	0.22	0.16	0.17
(1,349)	1:54:A:ALA:HA	1:55:A:LYS:H	8	0.21	0.05	0.2
(1,350)	1:54:B:ALA:HA	1:55:B:LYS:H	8	0.2	0.05	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1066)	1:87:B:THR:HG21	1:88:B:SER:H	8	0.19	0.07	0.16
(1,1066)	1:87:B:THR:HG23	1:88:B:SER:H	8	0.19	0.07	0.16
(1,1066)	1:87:B:THR:HG22	1:88:B:SER:H	8	0.19	0.07	0.16
(1,433)	1:61:A:GLU:HB2	1:61:A:GLU:H	8	0.12	0.01	0.12
(1,933)	1:82:A:ASN:HD22	1:84:A:ASP:H	7	1.4	0.09	1.39
(1,934)	1:82:B:ASN:HD22	1:84:B:ASP:H	7	1.39	0.09	1.39
(3,994)	1:47:B:VAL:HB	1:60:A:PRO:HG3	7	1.35	0.53	1.63
(3,994)	1:47:B:VAL:HB	1:99:A:GLU:HG2	7	1.35	0.53	1.63
(3,994)	1:47:B:VAL:HB	1:116:A:MET:HG3	7	1.35	0.53	1.63
(3,993)	1:47:A:VAL:HB	1:60:B:PRO:HG3	7	1.33	0.53	1.61
(3,993)	1:47:A:VAL:HB	1:99:B:GLU:HG2	7	1.33	0.53	1.61
(3,993)	1:47:A:VAL:HB	1:116:B:MET:HG3	7	1.33	0.53	1.61
(1,3274)	1:61:B:GLU:HG2	1:62:B:LYS:HG2	7	1.32	0.74	1.69
(1,3273)	1:61:A:GLU:HG2	1:62:A:LYS:HG2	7	1.32	0.73	1.69
(1,2353)	1:85:A:GLN:HE22	1:82:A:ASN:HD22	7	1.26	0.71	1.28
(1,2354)	1:85:B:GLN:HE22	1:82:B:ASN:HD22	7	1.26	0.72	1.3
(1,4011)	1:72:A:LYS:HD3	1:110:A:VAL:HG11	7	1.06	0.08	1.02
(1,4011)	1:72:A:LYS:HD3	1:110:A:VAL:HG13	7	1.06	0.08	1.02
(1,4011)	1:72:A:LYS:HD3	1:110:A:VAL:HG12	7	1.06	0.08	1.02
(1,4012)	1:72:B:LYS:HD3	1:110:B:VAL:HG11	7	1.06	0.09	1.02
(1,4012)	1:72:B:LYS:HD3	1:110:B:VAL:HG13	7	1.06	0.09	1.02
(1,4012)	1:72:B:LYS:HD3	1:110:B:VAL:HG12	7	1.06	0.09	1.02
(1,4005)	1:72:A:LYS:HD3	1:107:A:ASP:HB3	7	0.89	0.13	0.89
(1,4006)	1:72:B:LYS:HD3	1:107:B:ASP:HB3	7	0.89	0.13	0.89
(1,5307)	1:106:A:ALA:HB1	1:116:A:MET:HE2	7	0.87	0.26	0.95
(1,5307)	1:106:A:ALA:HB3	1:116:A:MET:HE2	7	0.87	0.26	0.95
(1,5307)	1:106:A:ALA:HB2	1:116:A:MET:HE2	7	0.87	0.26	0.95
(1,5307)	1:106:A:ALA:HB3	1:116:A:MET:HE3	7	0.87	0.26	0.95
(1,5307)	1:106:A:ALA:HB2	1:116:A:MET:HE3	7	0.87	0.26	0.95
(1,5308)	1:106:B:ALA:HB1	1:116:B:MET:HE2	7	0.87	0.26	0.95
(1,5308)	1:106:B:ALA:HB3	1:116:B:MET:HE2	7	0.87	0.26	0.95
(1,5308)	1:106:B:ALA:HB2	1:116:B:MET:HE2	7	0.87	0.26	0.95
(1,5308)	1:106:B:ALA:HB3	1:116:B:MET:HE3	7	0.87	0.26	0.95
(1,5308)	1:106:B:ALA:HB2	1:116:B:MET:HE3	7	0.87	0.26	0.95
(3,3005)	1:106:A:ALA:HB3	1:135:A:MET:HG2	7	0.8	0.63	0.73
(3,3005)	1:106:A:ALA:HB2	1:135:A:MET:HG2	7	0.8	0.63	0.73
(3,3005)	1:106:A:ALA:HB1	1:135:A:MET:HG2	7	0.8	0.63	0.73
(3,3006)	1:106:B:ALA:HB3	1:135:B:MET:HG2	7	0.8	0.63	0.73
(3,3006)	1:106:B:ALA:HB2	1:135:B:MET:HG2	7	0.8	0.63	0.73
(3,3006)	1:106:B:ALA:HB1	1:135:B:MET:HG2	7	0.8	0.63	0.73
(1,4004)	1:72:B:LYS:HD3	1:110:B:VAL:HA	7	0.77	0.21	0.66
(1,4003)	1:72:A:LYS:HD3	1:110:A:VAL:HA	7	0.77	0.21	0.65

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,2474)	1:101:B:THR:HA	1:45:A:ILE:HG21	7	0.71	0.31	0.82
(3,2474)	1:53:B:SER:HB2	1:45:A:ILE:HD13	7	0.71	0.31	0.82
(3,2474)	1:101:B:THR:HA	1:45:A:ILE:HG23	7	0.71	0.31	0.82
(3,2473)	1:101:A:THR:HA	1:45:B:ILE:HG21	7	0.71	0.3	0.8
(3,2473)	1:53:A:SER:HB2	1:45:B:ILE:HD13	7	0.71	0.3	0.8
(3,2473)	1:101:A:THR:HA	1:45:B:ILE:HG23	7	0.71	0.3	0.8
(1,4010)	1:72:B:LYS:HD3	1:110:B:VAL:HG23	7	0.59	0.17	0.54
(1,4010)	1:72:B:LYS:HD3	1:110:B:VAL:HG21	7	0.59	0.17	0.54
(1,4010)	1:72:B:LYS:HD3	1:110:B:VAL:HG22	7	0.59	0.17	0.54
(1,4009)	1:72:A:LYS:HD3	1:110:A:VAL:HG23	7	0.59	0.17	0.54
(1,4009)	1:72:A:LYS:HD3	1:110:A:VAL:HG21	7	0.59	0.17	0.54
(1,4009)	1:72:A:LYS:HD3	1:110:A:VAL:HG22	7	0.59	0.17	0.54
(1,4349)	1:82:A:ASN:HB2	1:82:A:ASN:HA	7	0.57	0.0	0.57
(1,4350)	1:82:B:ASN:HB2	1:82:B:ASN:HA	7	0.57	0.0	0.57
(1,3960)	1:72:B:LYS:HA	1:72:B:LYS:HD3	7	0.55	0.06	0.54
(1,3959)	1:72:A:LYS:HA	1:72:A:LYS:HD3	7	0.55	0.05	0.54
(3,2692)	1:108:B:LYS:HE2	1:109:B:SER:HB3	7	0.5	0.37	0.44
(3,2692)	1:108:B:LYS:HE3	1:109:B:SER:HB3	7	0.5	0.37	0.44
(1,1689)	1:140:A:LYS:HB2	1:140:A:LYS:H	7	0.49	0.03	0.5
(1,1690)	1:140:B:LYS:HB2	1:140:B:LYS:H	7	0.49	0.02	0.5
(3,2691)	1:108:A:LYS:HE2	1:109:A:SER:HB3	7	0.49	0.38	0.42
(3,2691)	1:108:A:LYS:HE3	1:109:A:SER:HB3	7	0.49	0.38	0.42
(1,3343)	1:129:A:LYS:HB2	1:101:A:THR:HG21	7	0.47	0.12	0.48
(1,3343)	1:129:A:LYS:HB2	1:101:A:THR:HG23	7	0.47	0.12	0.48
(1,3343)	1:129:A:LYS:HB2	1:101:A:THR:HG22	7	0.47	0.12	0.48
(1,3344)	1:129:B:LYS:HB2	1:101:B:THR:HG21	7	0.47	0.12	0.47
(1,3344)	1:129:B:LYS:HB2	1:101:B:THR:HG23	7	0.47	0.12	0.47
(1,3344)	1:129:B:LYS:HB2	1:101:B:THR:HG22	7	0.47	0.12	0.47
(1,4007)	1:72:A:LYS:HD3	1:114:A:THR:HG22	7	0.41	0.12	0.42
(1,4007)	1:72:A:LYS:HD3	1:114:A:THR:HG21	7	0.41	0.12	0.42
(1,4008)	1:72:B:LYS:HD3	1:114:B:THR:HG22	7	0.41	0.12	0.42
(1,4008)	1:72:B:LYS:HD3	1:114:B:THR:HG21	7	0.41	0.12	0.42
(1,3729)	1:67:A:SER:HB3	1:115:A:LEU:HD12	7	0.39	0.19	0.43
(1,3729)	1:67:A:SER:HB3	1:115:A:LEU:HD13	7	0.39	0.19	0.43
(1,3729)	1:67:A:SER:HB3	1:115:A:LEU:HD11	7	0.39	0.19	0.43
(3,383)	1:98:A:LYS:H	1:93:A:ARG:H	7	0.36	0.12	0.34
(1,943)	1:121:A:THR:HB	1:84:A:ASP:H	7	0.36	0.13	0.35
(1,944)	1:121:B:THR:HB	1:84:B:ASP:H	7	0.36	0.13	0.35
(3,384)	1:98:B:LYS:H	1:93:B:ARG:H	7	0.36	0.12	0.34
(1,5613)	1:121:A:THR:HA	1:124:A:LYS:HE3	7	0.35	0.2	0.37
(1,5614)	1:121:B:THR:HA	1:124:B:LYS:HE3	7	0.35	0.2	0.37
(3,2499)	1:101:A:THR:HG22	1:50:A:PRO:HB3	7	0.33	0.21	0.23

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,2499)	1:101:A:THR:HG23	1:50:A:PRO:HB3	7	0.33	0.21	0.23
(3,2499)	1:101:A:THR:HG21	1:50:A:PRO:HB3	7	0.33	0.21	0.23
(3,2500)	1:101:B:THR:HG22	1:50:B:PRO:HB3	7	0.33	0.21	0.23
(3,2500)	1:101:B:THR:HG23	1:50:B:PRO:HB3	7	0.33	0.21	0.23
(3,2500)	1:101:B:THR:HG21	1:50:B:PRO:HB3	7	0.33	0.21	0.23
(1,5907)	1:65:A:PHE:HE1	1:100:A:THR:HG23	7	0.32	0.15	0.36
(1,5907)	1:65:A:PHE:HE1	1:100:A:THR:HG21	7	0.32	0.15	0.36
(1,5907)	1:65:A:PHE:HE2	1:100:A:THR:HG22	7	0.32	0.15	0.36
(1,5907)	1:65:A:PHE:HE2	1:100:A:THR:HG21	7	0.32	0.15	0.36
(1,5908)	1:65:B:PHE:HE1	1:100:B:THR:HG23	7	0.32	0.15	0.36
(1,5908)	1:65:B:PHE:HE1	1:100:B:THR:HG21	7	0.32	0.15	0.36
(1,5908)	1:65:B:PHE:HE2	1:100:B:THR:HG22	7	0.32	0.15	0.36
(1,5908)	1:65:B:PHE:HE2	1:100:B:THR:HG21	7	0.32	0.15	0.36
(3,2905)	1:124:A:LYS:HD2	1:121:A:THR:HA	7	0.29	0.13	0.28
(3,1385)	1:60:A:PRO:HG2	1:129:A:LYS:HB3	7	0.29	0.11	0.27
(3,1386)	1:60:B:PRO:HG2	1:129:B:LYS:HB3	7	0.29	0.11	0.27
(3,2738)	1:108:B:LYS:HD3	1:110:B:VAL:HG11	7	0.28	0.06	0.27
(3,2738)	1:108:B:LYS:HD3	1:110:B:VAL:HG12	7	0.28	0.06	0.27
(3,2738)	1:108:B:LYS:HD2	1:110:B:VAL:HG11	7	0.28	0.06	0.27
(3,2738)	1:108:B:LYS:HD3	1:110:B:VAL:HG13	7	0.28	0.06	0.27
(3,2737)	1:108:A:LYS:HD3	1:110:A:VAL:HG11	7	0.28	0.06	0.26
(3,2737)	1:108:A:LYS:HD3	1:110:A:VAL:HG12	7	0.28	0.06	0.26
(3,2737)	1:108:A:LYS:HD2	1:110:A:VAL:HG11	7	0.28	0.06	0.26
(3,2737)	1:108:A:LYS:HD3	1:110:A:VAL:HG13	7	0.28	0.06	0.26
(1,915)	1:82:A:ASN:HB3	1:82:A:ASN:H	7	0.27	0.02	0.27
(1,916)	1:82:B:ASN:HB3	1:82:B:ASN:H	7	0.26	0.02	0.27
(1,2267)	1:138:A:ALA:HB1	1:138:A:ALA:H	7	0.24	0.14	0.16
(1,2267)	1:138:A:ALA:HB3	1:138:A:ALA:H	7	0.24	0.14	0.16
(1,2267)	1:138:A:ALA:HB2	1:138:A:ALA:H	7	0.24	0.14	0.16
(1,2268)	1:138:B:ALA:HB1	1:138:B:ALA:H	7	0.24	0.14	0.16
(1,2268)	1:138:B:ALA:HB3	1:138:B:ALA:H	7	0.24	0.14	0.16
(1,2268)	1:138:B:ALA:HB2	1:138:B:ALA:H	7	0.24	0.14	0.16
(1,1065)	1:87:A:THR:HG23	1:88:A:SER:H	7	0.19	0.07	0.15
(1,1065)	1:87:A:THR:HG22	1:88:A:SER:H	7	0.19	0.07	0.15
(1,1065)	1:87:A:THR:HG21	1:88:A:SER:H	7	0.19	0.07	0.15
(1,4481)	1:86:A:LEU:HA	1:90:A:LEU:HG	7	0.19	0.06	0.17
(1,4482)	1:86:B:LEU:HA	1:90:B:LEU:HG	7	0.19	0.06	0.17
(1,4636)	1:90:B:LEU:HB2	1:64:B:VAL:HB	7	0.17	0.04	0.15
(1,4635)	1:90:A:LEU:HB2	1:64:A:VAL:HB	7	0.17	0.04	0.15
(1,5084)	1:102:B:ILE:HB	1:102:B:ILE:HG21	7	0.1	0.0	0.1
(1,5084)	1:102:B:ILE:HB	1:102:B:ILE:HG23	7	0.1	0.0	0.1
(3,1724)	1:135:B:MET:HG2	1:115:B:LEU:HD23	6	0.91	0.6	0.9

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,1724)	1:135:B:MET:HG2	1:115:B:LEU:HD21	6	0.91	0.6	0.9
(3,1724)	1:135:B:MET:HG2	1:115:B:LEU:HD22	6	0.91	0.6	0.9
(3,1723)	1:135:A:MET:HG2	1:115:A:LEU:HD23	6	0.91	0.6	0.9
(3,1723)	1:135:A:MET:HG2	1:115:A:LEU:HD21	6	0.91	0.6	0.9
(3,1723)	1:135:A:MET:HG2	1:115:A:LEU:HD22	6	0.91	0.6	0.9
(1,4077)	1:105:A:GLN:HG3	1:137:A:GLY:HA3	6	0.74	0.32	0.73
(1,4078)	1:105:B:GLN:HG3	1:137:B:GLY:HA3	6	0.74	0.32	0.73
(1,4000)	1:72:B:LYS:HG2	1:114:B:THR:HG22	6	0.64	0.51	0.38
(1,4000)	1:72:B:LYS:HG2	1:114:B:THR:HG23	6	0.64	0.51	0.38
(1,4000)	1:72:B:LYS:HG2	1:114:B:THR:HG21	6	0.64	0.51	0.38
(1,3999)	1:72:A:LYS:HG2	1:114:A:THR:HG22	6	0.64	0.51	0.38
(1,3999)	1:72:A:LYS:HG2	1:114:A:THR:HG23	6	0.64	0.51	0.38
(1,3999)	1:72:A:LYS:HG2	1:114:A:THR:HG21	6	0.64	0.51	0.38
(3,489)	1:132:A:LEU:HG	1:105:A:GLN:H	6	0.64	0.21	0.74
(3,489)	1:122:A:LEU:HG	1:105:A:GLN:H	6	0.64	0.21	0.74
(3,489)	1:116:A:MET:HE3	1:105:A:GLN:H	6	0.64	0.21	0.74
(3,490)	1:132:B:LEU:HG	1:105:B:GLN:H	6	0.64	0.22	0.75
(3,490)	1:122:B:LEU:HG	1:105:B:GLN:H	6	0.64	0.22	0.75
(3,490)	1:116:B:MET:HE3	1:105:B:GLN:H	6	0.64	0.22	0.75
(3,3023)	1:129:A:LYS:HA	1:97:A:ASN:HB2	6	0.49	0.3	0.36
(3,3024)	1:129:B:LYS:HA	1:97:B:ASN:HB2	6	0.49	0.31	0.35
(1,3730)	1:67:B:SER:HB3	1:115:B:LEU:HD12	6	0.44	0.17	0.45
(1,3730)	1:67:B:SER:HB3	1:115:B:LEU:HD13	6	0.44	0.17	0.45
(1,3730)	1:67:B:SER:HB3	1:115:B:LEU:HD11	6	0.44	0.17	0.45
(1,1744)	1:139:B:ALA:HB1	1:140:B:LYS:H	6	0.33	0.07	0.34
(1,1744)	1:139:B:ALA:HB2	1:140:B:LYS:H	6	0.33	0.07	0.34
(1,1744)	1:139:B:ALA:HB3	1:140:B:LYS:H	6	0.33	0.07	0.34
(1,1743)	1:139:A:ALA:HB1	1:140:A:LYS:H	6	0.33	0.07	0.32
(1,1743)	1:139:A:ALA:HB2	1:140:A:LYS:H	6	0.33	0.07	0.32
(1,1743)	1:139:A:ALA:HB3	1:140:A:LYS:H	6	0.33	0.07	0.32
(3,2906)	1:124:B:LYS:HD2	1:121:B:THR:HA	6	0.32	0.12	0.29
(1,4516)	1:128:B:LEU:HG	1:49:A:LEU:HB3	6	0.3	0.08	0.32
(1,4515)	1:128:A:LEU:HG	1:49:B:LEU:HB3	6	0.3	0.08	0.3
(3,1067)	1:50:A:PRO:HA	1:54:A:ALA:HB2	6	0.29	0.2	0.2
(3,1067)	1:50:A:PRO:HA	1:54:A:ALA:HB1	6	0.29	0.2	0.2
(3,1067)	1:50:A:PRO:HA	1:54:A:ALA:HB3	6	0.29	0.2	0.2
(3,1068)	1:50:B:PRO:HA	1:54:B:ALA:HB2	6	0.29	0.2	0.19
(3,1068)	1:50:B:PRO:HA	1:54:B:ALA:HB1	6	0.29	0.2	0.19
(3,1068)	1:50:B:PRO:HA	1:54:B:ALA:HB3	6	0.29	0.2	0.19
(1,5731)	1:128:A:LEU:HA	1:49:B:LEU:HB3	6	0.29	0.06	0.3
(1,5732)	1:128:B:LEU:HA	1:49:A:LEU:HB3	6	0.28	0.07	0.31
(1,3598)	1:115:B:LEU:HD13	1:119:B:MET:HG2	6	0.27	0.09	0.24

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3598)	1:115:B:LEU:HD12	1:119:B:MET:HG2	6	0.27	0.09	0.24
(1,3597)	1:115:A:LEU:HD13	1:119:A:MET:HG2	6	0.27	0.09	0.24
(1,3597)	1:115:A:LEU:HD12	1:119:A:MET:HG2	6	0.27	0.09	0.24
(1,4182)	1:98:B:LYS:HE2	1:96:B:ALA:HA	6	0.26	0.09	0.24
(1,4181)	1:98:A:LYS:HE2	1:96:A:ALA:HA	6	0.26	0.09	0.24
(1,61)	1:85:A:GLN:HB3	1:82:A:ASN:H	6	0.2	0.08	0.18
(1,62)	1:85:B:GLN:HB3	1:82:B:ASN:H	6	0.2	0.08	0.17
(1,3611)	1:115:A:LEU:HD12	1:106:A:ALA:HB1	6	0.18	0.07	0.18
(1,3611)	1:115:A:LEU:HD12	1:106:A:ALA:HB2	6	0.18	0.07	0.18
(1,3611)	1:115:A:LEU:HD11	1:106:A:ALA:HB3	6	0.18	0.07	0.18
(1,3611)	1:115:A:LEU:HD12	1:106:A:ALA:HB3	6	0.18	0.07	0.18
(1,3611)	1:115:A:LEU:HD11	1:106:A:ALA:HB2	6	0.18	0.07	0.18
(1,3612)	1:115:B:LEU:HD12	1:106:B:ALA:HB1	6	0.18	0.07	0.18
(1,3612)	1:115:B:LEU:HD12	1:106:B:ALA:HB2	6	0.18	0.07	0.18
(1,3612)	1:115:B:LEU:HD11	1:106:B:ALA:HB3	6	0.18	0.07	0.18
(1,3612)	1:115:B:LEU:HD12	1:106:B:ALA:HB3	6	0.18	0.07	0.18
(1,3612)	1:115:B:LEU:HD11	1:106:B:ALA:HB2	6	0.18	0.07	0.18
(1,1405)	1:99:A:GLU:HB3	1:99:A:GLU:H	6	0.11	0.01	0.11
(1,5083)	1:102:A:ILE:HB	1:102:A:ILE:HG21	6	0.1	0.0	0.11
(1,5083)	1:102:A:ILE:HB	1:102:A:ILE:HG23	6	0.1	0.0	0.11
(3,1191)	1:108:A:LYS:HE3	1:108:A:LYS:HD2	6	0.1	0.0	0.11
(3,1191)	1:108:A:LYS:HE2	1:108:A:LYS:HD3	6	0.1	0.0	0.11
(3,1191)	1:108:A:LYS:HE3	1:108:A:LYS:HD3	6	0.1	0.0	0.11
(1,2352)	1:85:B:GLN:HE22	1:82:B:ASN:HD21	5	0.78	0.46	0.76
(1,2351)	1:85:A:GLN:HE22	1:82:A:ASN:HD21	5	0.78	0.46	0.77
(3,861)	1:43:A:VAL:HA	1:138:B:ALA:HB2	5	0.68	0.21	0.72
(3,861)	1:117:A:SER:HA	1:115:A:LEU:HG	5	0.68	0.21	0.72
(3,861)	1:88:A:SER:HA	1:96:A:ALA:HB3	5	0.68	0.21	0.72
(3,862)	1:43:B:VAL:HA	1:138:A:ALA:HB2	5	0.67	0.24	0.75
(3,862)	1:117:B:SER:HA	1:115:B:LEU:HG	5	0.67	0.24	0.75
(3,862)	1:88:B:SER:HA	1:96:B:ALA:HB3	5	0.67	0.24	0.75
(3,1526)	1:132:B:LEU:HG	1:106:B:ALA:HB3	5	0.59	0.2	0.53
(3,1526)	1:132:B:LEU:HG	1:106:B:ALA:HB2	5	0.59	0.2	0.53
(3,1526)	1:132:B:LEU:HG	1:106:B:ALA:HB1	5	0.59	0.2	0.53
(3,1525)	1:132:A:LEU:HG	1:106:A:ALA:HB3	5	0.59	0.2	0.52
(3,1525)	1:132:A:LEU:HG	1:106:A:ALA:HB2	5	0.59	0.2	0.52
(3,1525)	1:132:A:LEU:HG	1:106:A:ALA:HB1	5	0.59	0.2	0.52
(1,2368)	1:84:B:ASP:HB2	1:85:B:GLN:HE22	5	0.57	0.26	0.5
(1,2367)	1:84:A:ASP:HB2	1:85:A:GLN:HE22	5	0.57	0.26	0.51
(3,1359)	1:79:A:GLN:HG3	1:86:A:LEU:HB3	5	0.53	0.63	0.22
(3,1360)	1:79:B:GLN:HG3	1:86:B:LEU:HB3	5	0.53	0.63	0.23
(1,4912)	1:100:B:THR:HA	1:129:B:LYS:HD2	5	0.48	0.15	0.5

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,4911)	1:100:A:THR:HA	1:129:A:LYS:HD2	5	0.48	0.15	0.5
(3,2387)	1:99:A:GLU:HG3	1:129:A:LYS:HE2	5	0.43	0.15	0.42
(3,2388)	1:99:B:GLU:HG3	1:129:B:LYS:HE2	5	0.43	0.15	0.42
(1,4472)	1:86:B:LEU:HA	1:89:B:VAL:HB	5	0.37	0.48	0.12
(1,4471)	1:86:A:LEU:HA	1:89:A:VAL:HB	5	0.36	0.48	0.11
(1,2813)	1:54:A:ALA:HB1	1:53:A:SER:HB2	5	0.34	0.1	0.27
(1,2813)	1:54:A:ALA:HB3	1:53:A:SER:HB2	5	0.34	0.1	0.27
(1,2813)	1:54:A:ALA:HB2	1:53:A:SER:HB2	5	0.34	0.1	0.27
(1,2814)	1:54:B:ALA:HB1	1:53:B:SER:HB2	5	0.34	0.1	0.27
(1,2814)	1:54:B:ALA:HB3	1:53:B:SER:HB2	5	0.34	0.1	0.27
(1,2814)	1:54:B:ALA:HB2	1:53:B:SER:HB2	5	0.34	0.1	0.27
(1,3676)	1:67:B:SER:HB2	1:105:B:GLN:HG2	5	0.31	0.13	0.24
(1,3675)	1:67:A:SER:HB2	1:105:A:GLN:HG2	5	0.31	0.13	0.24
(1,5258)	1:105:B:GLN:HG2	1:65:B:PHE:HB2	5	0.29	0.18	0.19
(1,5257)	1:105:A:GLN:HG2	1:65:A:PHE:HB2	5	0.29	0.18	0.19
(1,5402)	1:110:B:VAL:HG23	1:116:B:MET:HE1	5	0.29	0.16	0.25
(1,5402)	1:110:B:VAL:HG23	1:116:B:MET:HE2	5	0.29	0.16	0.25
(1,5402)	1:110:B:VAL:HG22	1:116:B:MET:HE2	5	0.29	0.16	0.25
(1,5402)	1:110:B:VAL:HG21	1:116:B:MET:HE2	5	0.29	0.16	0.25
(1,5401)	1:110:A:VAL:HG23	1:116:A:MET:HE1	5	0.29	0.16	0.24
(1,5401)	1:110:A:VAL:HG23	1:116:A:MET:HE2	5	0.29	0.16	0.24
(1,5401)	1:110:A:VAL:HG22	1:116:A:MET:HE2	5	0.29	0.16	0.24
(1,5401)	1:110:A:VAL:HG21	1:116:A:MET:HE2	5	0.29	0.16	0.24
(1,4535)	1:87:A:THR:HA	1:90:A:LEU:HG	5	0.26	0.03	0.26
(1,4536)	1:87:B:THR:HA	1:90:B:LEU:HG	5	0.26	0.03	0.25
(3,918)	1:45:B:ILE:HB	1:45:B:ILE:HD12	5	0.24	0.01	0.24
(3,918)	1:45:B:ILE:HB	1:45:B:ILE:HD11	5	0.24	0.01	0.24
(3,917)	1:45:A:ILE:HB	1:45:A:ILE:HD12	5	0.24	0.01	0.24
(3,917)	1:45:A:ILE:HB	1:45:A:ILE:HD11	5	0.24	0.01	0.24
(3,2449)	1:100:A:THR:HG21	1:129:A:LYS:HE3	5	0.23	0.06	0.24
(3,2449)	1:100:A:THR:HG22	1:129:A:LYS:HE2	5	0.23	0.06	0.24
(3,2449)	1:100:A:THR:HG23	1:129:A:LYS:HE2	5	0.23	0.06	0.24
(3,2450)	1:100:B:THR:HG22	1:129:B:LYS:HE3	5	0.23	0.06	0.24
(3,2450)	1:100:B:THR:HG22	1:129:B:LYS:HE2	5	0.23	0.06	0.24
(3,2450)	1:100:B:THR:HG21	1:129:B:LYS:HE3	5	0.23	0.06	0.24
(3,2450)	1:100:B:THR:HG23	1:129:B:LYS:HE2	5	0.23	0.06	0.24
(1,824)	1:79:B:GLN:HB2	1:76:B:VAL:H	5	0.23	0.06	0.26
(1,823)	1:79:A:GLN:HB2	1:76:A:VAL:H	5	0.22	0.06	0.25
(3,1553)	1:64:A:VAL:HA	1:61:A:GLU:HG2	5	0.22	0.11	0.2
(3,2542)	1:102:B:ILE:HD12	1:61:B:GLU:HG3	5	0.22	0.14	0.16
(3,2542)	1:102:B:ILE:HD11	1:61:B:GLU:HG3	5	0.22	0.14	0.16
(3,2542)	1:102:B:ILE:HD12	1:95:B:GLN:HG2	5	0.22	0.14	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,2542)	1:102:B:ILE:HD11	1:95:B:GLN:HG2	5	0.22	0.14	0.16
(1,761)	1:110:A:VAL:HG13	1:74:A:LEU:H	5	0.19	0.08	0.16
(1,761)	1:110:A:VAL:HG11	1:74:A:LEU:H	5	0.19	0.08	0.16
(1,761)	1:110:A:VAL:HG12	1:74:A:LEU:H	5	0.19	0.08	0.16
(1,2919)	1:56:A:PRO:HA	1:45:B:ILE:HA	5	0.19	0.12	0.11
(1,762)	1:110:B:VAL:HG13	1:74:B:LEU:H	5	0.19	0.08	0.16
(1,762)	1:110:B:VAL:HG11	1:74:B:LEU:H	5	0.19	0.08	0.16
(1,762)	1:110:B:VAL:HG12	1:74:B:LEU:H	5	0.19	0.08	0.16
(1,2)	1:57:B:GLN:HG3	1:57:B:GLN:H	5	0.18	0.03	0.15
(1,1)	1:57:A:GLN:HG3	1:57:A:GLN:H	5	0.17	0.03	0.15
(1,1274)	1:94:B:THR:HG21	1:94:B:THR:H	5	0.16	0.01	0.16
(1,1274)	1:94:B:THR:HG22	1:94:B:THR:H	5	0.16	0.01	0.16
(1,5375)	1:110:A:VAL:HB	1:112:A:TYR:HB3	5	0.16	0.04	0.17
(1,5376)	1:110:B:VAL:HB	1:112:B:TYR:HB3	5	0.16	0.04	0.17
(1,1273)	1:94:A:THR:HG21	1:94:A:THR:H	5	0.16	0.01	0.16
(1,1273)	1:94:A:THR:HG22	1:94:A:THR:H	5	0.16	0.01	0.16
(1,1403)	1:99:A:GLU:HG2	1:99:A:GLU:H	5	0.15	0.03	0.13
(1,1404)	1:99:B:GLU:HG2	1:99:B:GLU:H	5	0.15	0.03	0.14
(1,1649)	1:110:A:VAL:HG23	1:115:A:LEU:H	5	0.14	0.04	0.15
(1,1649)	1:110:A:VAL:HG21	1:115:A:LEU:H	5	0.14	0.04	0.15
(1,1649)	1:110:A:VAL:HG22	1:115:A:LEU:H	5	0.14	0.04	0.15
(1,1650)	1:110:B:VAL:HG23	1:115:B:LEU:H	5	0.14	0.04	0.15
(1,1650)	1:110:B:VAL:HG21	1:115:B:LEU:H	5	0.14	0.04	0.15
(1,1650)	1:110:B:VAL:HG22	1:115:B:LEU:H	5	0.14	0.04	0.15
(1,1406)	1:99:B:GLU:HB3	1:99:B:GLU:H	5	0.11	0.0	0.11
(3,1192)	1:108:B:LYS:HE3	1:108:B:LYS:HD2	5	0.11	0.0	0.11
(3,1192)	1:108:B:LYS:HE2	1:108:B:LYS:HD3	5	0.11	0.0	0.11
(3,1192)	1:108:B:LYS:HE3	1:108:B:LYS:HD3	5	0.11	0.0	0.11
(1,5418)	1:72:B:LYS:HG3	1:110:B:VAL:HG13	4	1.13	0.69	1.13
(1,5418)	1:72:B:LYS:HG3	1:110:B:VAL:HG12	4	1.13	0.69	1.13
(1,5417)	1:72:A:LYS:HG3	1:110:A:VAL:HG13	4	1.13	0.69	1.13
(1,5417)	1:72:A:LYS:HG3	1:110:A:VAL:HG12	4	1.13	0.69	1.13
(3,1645)	1:115:A:LEU:HD12	1:116:A:MET:HG2	4	0.97	0.07	0.94
(3,1645)	1:115:A:LEU:HD13	1:116:A:MET:HG2	4	0.97	0.07	0.94
(3,1646)	1:115:B:LEU:HD12	1:116:B:MET:HG2	4	0.97	0.07	0.94
(3,1646)	1:115:B:LEU:HD13	1:116:B:MET:HG2	4	0.97	0.07	0.94
(3,2833)	1:112:A:TYR:HE1	1:116:A:MET:HE3	4	0.83	0.08	0.85
(3,2833)	1:112:A:TYR:HE1	1:116:A:MET:HE1	4	0.83	0.08	0.85
(3,2833)	1:112:A:TYR:HE1	1:116:A:MET:HE2	4	0.83	0.08	0.85
(3,2834)	1:112:B:TYR:HE1	1:116:B:MET:HE3	4	0.83	0.08	0.85
(3,2834)	1:112:B:TYR:HE1	1:116:B:MET:HE1	4	0.83	0.08	0.85
(3,2834)	1:112:B:TYR:HE1	1:116:B:MET:HE2	4	0.83	0.08	0.85

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,3083)	1:112:A:TYR:HE1	1:116:A:MET:HE3	4	0.83	0.08	0.85
(3,3083)	1:112:A:TYR:HE1	1:116:A:MET:HE1	4	0.83	0.08	0.85
(3,3083)	1:112:A:TYR:HE1	1:116:A:MET:HE2	4	0.83	0.08	0.85
(3,3084)	1:112:B:TYR:HE1	1:116:B:MET:HE3	4	0.83	0.08	0.85
(3,3084)	1:112:B:TYR:HE1	1:116:B:MET:HE1	4	0.83	0.08	0.85
(3,3084)	1:112:B:TYR:HE1	1:116:B:MET:HE2	4	0.83	0.08	0.85
(1,5830)	1:135:B:MET:HE3	1:108:B:LYS:HA	4	0.8	0.92	0.31
(1,5830)	1:135:B:MET:HE2	1:108:B:LYS:HA	4	0.8	0.92	0.31
(1,5830)	1:135:B:MET:HE1	1:108:B:LYS:HA	4	0.8	0.92	0.31
(3,1776)	1:71:B:ASP:HA	1:111:B:ASP:HB2	4	0.8	0.08	0.8
(3,1775)	1:71:A:ASP:HA	1:111:A:ASP:HB2	4	0.8	0.08	0.8
(1,5829)	1:135:A:MET:HE3	1:108:A:LYS:HA	4	0.79	0.92	0.31
(1,5829)	1:135:A:MET:HE2	1:108:A:LYS:HA	4	0.79	0.92	0.31
(1,5829)	1:135:A:MET:HE1	1:108:A:LYS:HA	4	0.79	0.92	0.31
(3,2640)	1:116:B:MET:HG2	1:110:A:VAL:HA	4	0.77	0.1	0.75
(3,2639)	1:116:A:MET:HG2	1:110:B:VAL:HA	4	0.76	0.11	0.74
(3,3001)	1:135:A:MET:HA	1:116:B:MET:HE2	4	0.72	0.26	0.84
(3,3001)	1:135:A:MET:HA	1:116:B:MET:HE3	4	0.72	0.26	0.84
(3,3001)	1:135:A:MET:HA	1:116:B:MET:HE1	4	0.72	0.26	0.84
(3,3002)	1:135:B:MET:HA	1:116:A:MET:HE3	4	0.7	0.25	0.81
(3,3002)	1:135:B:MET:HA	1:116:A:MET:HE2	4	0.7	0.25	0.81
(3,3002)	1:135:B:MET:HA	1:116:A:MET:HE1	4	0.7	0.25	0.81
(3,1630)	1:66:B:LEU:HB3	1:140:B:LYS:HG2	4	0.66	0.25	0.69
(3,1630)	1:66:B:LEU:HB3	1:140:B:LYS:HG3	4	0.66	0.25	0.69
(3,1629)	1:66:A:LEU:HB3	1:140:A:LYS:HG2	4	0.66	0.25	0.68
(3,1629)	1:66:A:LEU:HB3	1:140:A:LYS:HG3	4	0.66	0.25	0.68
(3,2373)	1:98:A:LYS:HG2	1:98:A:LYS:HE2	4	0.57	0.02	0.58
(3,2374)	1:98:B:LYS:HG2	1:98:B:LYS:HE2	4	0.57	0.03	0.58
(3,1563)	1:110:A:VAL:HB	1:72:A:LYS:HG2	4	0.56	0.05	0.54
(3,1564)	1:110:B:VAL:HB	1:72:B:LYS:HG2	4	0.56	0.04	0.54
(3,2371)	1:98:A:LYS:HE2	1:126:A:GLY:HA2	4	0.51	0.12	0.48
(3,2372)	1:98:B:LYS:HE2	1:126:B:GLY:HA2	4	0.51	0.12	0.48
(1,4154)	1:123:B:ARG:HG2	1:49:A:LEU:HB3	4	0.5	0.46	0.31
(1,4153)	1:123:A:ARG:HG2	1:49:B:LEU:HB3	4	0.5	0.46	0.31
(3,1104)	1:139:B:ALA:HA	1:136:B:GLU:HB2	4	0.45	0.24	0.45
(3,1104)	1:51:B:ALA:HA	1:43:A:VAL:HB	4	0.45	0.24	0.45
(3,615)	1:49:A:LEU:HA	1:120:B:ASP:H	4	0.44	0.24	0.34
(3,1103)	1:139:A:ALA:HA	1:136:A:GLU:HB2	4	0.44	0.24	0.44
(3,1103)	1:51:A:ALA:HA	1:43:B:VAL:HB	4	0.44	0.24	0.44
(3,616)	1:49:B:LEU:HA	1:120:A:ASP:H	4	0.43	0.24	0.32
(3,2713)	1:109:A:SER:HB3	1:72:A:LYS:HE3	4	0.41	0.24	0.4
(3,2713)	1:109:A:SER:HB3	1:72:A:LYS:HE2	4	0.41	0.24	0.4

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,5529)	1:115:A:LEU:HD22	1:135:A:MET:HA	4	0.41	0.28	0.31
(1,5529)	1:115:A:LEU:HD21	1:135:A:MET:HA	4	0.41	0.28	0.31
(1,5530)	1:115:B:LEU:HD22	1:135:B:MET:HA	4	0.41	0.28	0.31
(1,5530)	1:115:B:LEU:HD21	1:135:B:MET:HA	4	0.41	0.28	0.31
(1,3137)	1:98:A:LYS:HE3	1:125:A:ALA:HB3	4	0.41	0.14	0.39
(1,3137)	1:98:A:LYS:HE3	1:125:A:ALA:HB2	4	0.41	0.14	0.39
(1,3137)	1:98:A:LYS:HE3	1:125:A:ALA:HB1	4	0.41	0.14	0.39
(1,3138)	1:98:B:LYS:HE3	1:125:B:ALA:HB3	4	0.41	0.14	0.39
(1,3138)	1:98:B:LYS:HE3	1:125:B:ALA:HB2	4	0.41	0.14	0.39
(1,3138)	1:98:B:LYS:HE3	1:125:B:ALA:HB1	4	0.41	0.14	0.39
(1,763)	1:73:A:GLN:HG2	1:74:A:LEU:H	4	0.39	0.04	0.4
(1,764)	1:73:B:GLN:HG2	1:74:B:LEU:H	4	0.39	0.04	0.4
(3,111)	1:98:A:LYS:HB3	1:51:B:ALA:H	4	0.39	0.15	0.39
(3,112)	1:98:B:LYS:HB3	1:51:A:ALA:H	4	0.36	0.18	0.38
(1,2552)	1:45:B:ILE:HG23	1:56:A:PRO:HB3	4	0.34	0.14	0.35
(1,2552)	1:45:B:ILE:HG22	1:56:A:PRO:HB3	4	0.34	0.14	0.35
(1,2552)	1:45:B:ILE:HG21	1:56:A:PRO:HB3	4	0.34	0.14	0.35
(1,2551)	1:45:A:ILE:HG23	1:56:B:PRO:HB3	4	0.34	0.13	0.34
(1,2551)	1:45:A:ILE:HG22	1:56:B:PRO:HB3	4	0.34	0.13	0.34
(1,2551)	1:45:A:ILE:HG21	1:56:B:PRO:HB3	4	0.34	0.13	0.34
(3,2117)	1:88:A:SER:HB2	1:96:A:ALA:HA	4	0.3	0.11	0.3
(3,2118)	1:88:B:SER:HB2	1:96:B:ALA:HA	4	0.3	0.11	0.3
(1,5416)	1:110:B:VAL:HG13	1:70:B:ALA:HB3	4	0.3	0.06	0.29
(1,5416)	1:110:B:VAL:HG13	1:70:B:ALA:HB2	4	0.3	0.06	0.29
(1,5416)	1:110:B:VAL:HG12	1:70:B:ALA:HB1	4	0.3	0.06	0.29
(1,5416)	1:110:B:VAL:HG11	1:70:B:ALA:HB1	4	0.3	0.06	0.29
(1,5415)	1:110:A:VAL:HG13	1:70:A:ALA:HB3	4	0.3	0.06	0.29
(1,5415)	1:110:A:VAL:HG13	1:70:A:ALA:HB2	4	0.3	0.06	0.29
(1,5415)	1:110:A:VAL:HG12	1:70:A:ALA:HB1	4	0.3	0.06	0.29
(1,5415)	1:110:A:VAL:HG11	1:70:A:ALA:HB1	4	0.3	0.06	0.29
(3,1554)	1:64:B:VAL:HA	1:61:B:GLU:HG2	4	0.26	0.11	0.2
(1,5259)	1:116:A:MET:HG2	1:116:A:MET:HE3	4	0.24	0.02	0.24
(1,5259)	1:116:A:MET:HG2	1:116:A:MET:HE1	4	0.24	0.02	0.24
(1,5259)	1:116:A:MET:HG2	1:116:A:MET:HE2	4	0.24	0.02	0.24
(1,5260)	1:116:B:MET:HG2	1:116:B:MET:HE3	4	0.24	0.02	0.24
(1,5260)	1:116:B:MET:HG2	1:116:B:MET:HE1	4	0.24	0.02	0.24
(1,5260)	1:116:B:MET:HG2	1:116:B:MET:HE2	4	0.24	0.02	0.24
(3,2541)	1:102:A:ILE:HD12	1:61:A:GLU:HG3	4	0.24	0.14	0.2
(3,2541)	1:102:A:ILE:HD11	1:61:A:GLU:HG3	4	0.24	0.14	0.2
(3,2541)	1:102:A:ILE:HD12	1:95:A:GLN:HG2	4	0.24	0.14	0.2
(3,2541)	1:102:A:ILE:HD11	1:95:A:GLN:HG2	4	0.24	0.14	0.2
(1,1069)	1:90:A:LEU:HB3	1:88:A:SER:H	4	0.24	0.1	0.21

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1070)	1:90:B:LEU:HB3	1:88:B:SER:H	4	0.24	0.1	0.21
(3,619)	1:124:A:LYS:HE2	1:120:A:ASP:H	4	0.22	0.08	0.22
(3,619)	1:124:A:LYS:HE3	1:120:A:ASP:H	4	0.22	0.08	0.22
(3,2930)	1:126:B:GLY:HA2	1:91:B:ASP:HA	4	0.22	0.17	0.14
(3,620)	1:124:B:LYS:HE2	1:120:B:ASP:H	4	0.22	0.08	0.22
(3,620)	1:124:B:LYS:HE3	1:120:B:ASP:H	4	0.22	0.08	0.22
(1,3837)	1:69:A:LYS:HG3	1:115:A:LEU:HD13	4	0.22	0.09	0.18
(1,3837)	1:69:A:LYS:HG3	1:115:A:LEU:HD11	4	0.22	0.09	0.18
(1,3838)	1:69:B:LYS:HG3	1:115:B:LEU:HD13	4	0.22	0.09	0.18
(1,3838)	1:69:B:LYS:HG3	1:115:B:LEU:HD11	4	0.22	0.09	0.18
(1,4769)	1:94:A:THR:HG22	1:102:A:ILE:HG13	4	0.21	0.06	0.21
(1,4769)	1:94:A:THR:HG21	1:102:A:ILE:HG13	4	0.21	0.06	0.21
(1,4769)	1:94:A:THR:HG23	1:102:A:ILE:HG13	4	0.21	0.06	0.21
(1,4770)	1:94:B:THR:HG22	1:102:B:ILE:HG13	4	0.21	0.06	0.21
(1,4770)	1:94:B:THR:HG21	1:102:B:ILE:HG13	4	0.21	0.06	0.21
(1,4770)	1:94:B:THR:HG23	1:102:B:ILE:HG13	4	0.21	0.06	0.21
(1,4326)	1:127:B:TYR:HA	1:90:B:LEU:HG	4	0.2	0.09	0.18
(3,2158)	1:127:B:TYR:HA	1:90:B:LEU:HG	4	0.2	0.09	0.18
(1,4325)	1:127:A:TYR:HA	1:90:A:LEU:HG	4	0.2	0.08	0.18
(3,2157)	1:127:A:TYR:HA	1:90:A:LEU:HG	4	0.2	0.08	0.18
(1,3210)	1:122:B:LEU:HA	1:87:B:THR:HB	4	0.19	0.05	0.18
(1,3209)	1:122:A:LEU:HA	1:87:A:THR:HB	4	0.19	0.05	0.17
(3,2241)	1:98:A:LYS:HE3	1:94:A:THR:HG23	4	0.19	0.11	0.13
(3,2241)	1:98:A:LYS:HE3	1:94:A:THR:HG22	4	0.19	0.11	0.13
(1,3459)	1:64:A:VAL:HB	1:102:A:ILE:HG23	4	0.18	0.03	0.19
(1,3459)	1:64:A:VAL:HB	1:102:A:ILE:HG22	4	0.18	0.03	0.19
(1,3459)	1:64:A:VAL:HB	1:102:A:ILE:HG21	4	0.18	0.03	0.19
(1,3460)	1:64:B:VAL:HB	1:102:B:ILE:HG23	4	0.18	0.03	0.19
(1,3460)	1:64:B:VAL:HB	1:102:B:ILE:HG22	4	0.18	0.03	0.19
(1,3460)	1:64:B:VAL:HB	1:102:B:ILE:HG21	4	0.18	0.03	0.19
(3,2242)	1:98:B:LYS:HE3	1:94:B:THR:HG23	4	0.18	0.11	0.12
(3,2242)	1:98:B:LYS:HE3	1:94:B:THR:HG22	4	0.18	0.11	0.12
(1,2355)	1:82:A:ASN:HB3	1:82:A:ASN:HD22	4	0.14	0.01	0.15
(1,2356)	1:82:B:ASN:HB3	1:82:B:ASN:HD22	4	0.14	0.0	0.14
(1,2680)	1:93:B:ARG:HG3	1:90:B:LEU:HA	4	0.14	0.03	0.14
(3,736)	1:132:B:LEU:HG	1:134:B:GLY:H	4	0.14	0.05	0.12
(1,2679)	1:93:A:ARG:HG3	1:90:A:LEU:HA	4	0.14	0.03	0.14
(3,2049)	1:119:A:MET:HG2	1:72:A:LYS:HA	4	0.13	0.0	0.13
(3,2050)	1:119:B:MET:HG2	1:72:B:LYS:HA	4	0.13	0.01	0.13
(1,1077)	1:88:A:SER:HB2	1:89:A:VAL:H	4	0.12	0.02	0.12
(1,1078)	1:88:B:SER:HB2	1:89:B:VAL:H	4	0.12	0.02	0.12
(1,1467)	1:100:A:THR:HG23	1:101:A:THR:H	4	0.12	0.02	0.11

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1467)	1:100:A:THR:HG21	1:101:A:THR:H	4	0.12	0.02	0.11
(1,1467)	1:100:A:THR:HG22	1:101:A:THR:H	4	0.12	0.02	0.11
(1,193)	1:43:A:VAL:HB	1:44:A:ASP:H	3	0.72	0.05	0.75
(1,194)	1:43:B:VAL:HB	1:44:B:ASP:H	3	0.72	0.05	0.75
(1,2841)	1:57:A:GLN:HA	1:60:A:PRO:HB3	3	0.67	0.2	0.62
(1,2842)	1:57:B:GLN:HA	1:60:B:PRO:HB3	3	0.67	0.19	0.62
(3,869)	1:43:A:VAL:HB	1:56:B:PRO:HD3	3	0.63	0.17	0.54
(3,870)	1:43:B:VAL:HB	1:56:A:PRO:HD3	3	0.62	0.16	0.56
(1,3991)	1:72:A:LYS:HG3	1:72:A:LYS:HE2	3	0.62	0.09	0.68
(1,3992)	1:72:B:LYS:HG3	1:72:B:LYS:HE2	3	0.62	0.09	0.68
(3,810)	1:86:B:LEU:HA	1:79:B:GLN:HE21	3	0.6	0.12	0.54
(3,810)	1:89:B:VAL:HA	1:79:B:GLN:HE21	3	0.6	0.12	0.54
(1,3726)	1:67:B:SER:HB3	1:114:B:THR:HG23	3	0.59	0.04	0.6
(1,3726)	1:67:B:SER:HB3	1:114:B:THR:HG21	3	0.59	0.04	0.6
(3,809)	1:86:A:LEU:HA	1:79:A:GLN:HE21	3	0.59	0.13	0.53
(3,809)	1:89:A:VAL:HA	1:79:A:GLN:HE21	3	0.59	0.13	0.53
(1,3725)	1:67:A:SER:HB3	1:114:A:THR:HG23	3	0.59	0.05	0.6
(1,3725)	1:67:A:SER:HB3	1:114:A:THR:HG21	3	0.59	0.05	0.6
(3,812)	1:89:B:VAL:HA	1:79:B:GLN:HE22	3	0.56	0.08	0.57
(3,811)	1:89:A:VAL:HA	1:79:A:GLN:HE22	3	0.56	0.08	0.57
(3,2714)	1:109:B:SER:HB3	1:72:B:LYS:HE2	3	0.52	0.18	0.47
(3,2714)	1:109:B:SER:HB3	1:72:B:LYS:HE3	3	0.52	0.18	0.47
(3,1736)	1:69:B:LYS:HD2	1:108:B:LYS:HE2	3	0.45	0.23	0.54
(3,1736)	1:69:B:LYS:HD2	1:72:B:LYS:HE2	3	0.45	0.23	0.54
(3,1735)	1:69:A:LYS:HD2	1:108:A:LYS:HE2	3	0.45	0.23	0.53
(3,1735)	1:69:A:LYS:HD2	1:72:A:LYS:HE2	3	0.45	0.23	0.53
(3,1010)	1:48:B:ASP:HB3	1:57:B:GLN:HB3	3	0.43	0.24	0.4
(3,1010)	1:44:B:ASP:HB2	1:105:A:GLN:HG2	3	0.43	0.24	0.4
(3,1009)	1:48:A:ASP:HB3	1:57:A:GLN:HB3	3	0.4	0.21	0.41
(3,1009)	1:44:A:ASP:HB2	1:105:B:GLN:HG2	3	0.4	0.21	0.41
(3,1043)	1:49:A:LEU:HB2	1:56:A:PRO:HG3	3	0.4	0.06	0.43
(3,1044)	1:49:B:LEU:HB2	1:56:B:PRO:HG3	3	0.4	0.06	0.43
(1,2682)	1:93:B:ARG:HG3	1:91:B:ASP:HB3	3	0.38	0.04	0.37
(1,2681)	1:93:A:ARG:HG3	1:91:A:ASP:HB3	3	0.37	0.04	0.37
(3,1813)	1:72:A:LYS:HB3	1:72:A:LYS:HD3	3	0.36	0.02	0.36
(3,1813)	1:62:A:LYS:HD2	1:95:A:GLN:HB2	3	0.36	0.02	0.36
(3,1814)	1:72:B:LYS:HB3	1:72:B:LYS:HD3	3	0.36	0.02	0.36
(3,1814)	1:62:B:LYS:HD2	1:95:B:GLN:HB2	3	0.36	0.02	0.36
(3,1535)	1:123:A:ARG:HG2	1:50:B:PRO:HD2	3	0.35	0.27	0.19
(3,1535)	1:63:A:PRO:HG2	1:60:A:PRO:HD2	3	0.35	0.27	0.19
(3,3039)	1:112:A:TYR:HD1	1:109:B:SER:HB2	3	0.34	0.23	0.23
(3,3039)	1:112:A:TYR:HD2	1:109:B:SER:HB2	3	0.34	0.23	0.23

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,3040)	1:112:B:TYR:HD1	1:109:A:SER:HB2	3	0.32	0.23	0.21
(3,3040)	1:112:B:TYR:HD2	1:109:A:SER:HB2	3	0.32	0.23	0.21
(3,2923)	1:126:A:GLY:HA3	1:120:A:ASP:HA	3	0.31	0.14	0.35
(3,2924)	1:126:B:GLY:HA3	1:120:B:ASP:HA	3	0.31	0.14	0.35
(3,2060)	1:119:B:MET:HG2	1:49:A:LEU:HG	3	0.3	0.08	0.33
(3,2059)	1:119:A:MET:HG2	1:49:B:LEU:HG	3	0.29	0.07	0.3
(1,4753)	1:94:A:THR:HG23	1:97:A:ASN:HB3	3	0.27	0.11	0.34
(1,4754)	1:94:B:THR:HG23	1:97:B:ASN:HB3	3	0.27	0.11	0.34
(3,2929)	1:126:A:GLY:HA2	1:91:A:ASP:HA	3	0.26	0.18	0.16
(1,2212)	1:45:B:ILE:H	1:135:A:MET:H	3	0.25	0.11	0.24
(1,2920)	1:56:B:PRO:HA	1:45:A:ILE:HA	3	0.24	0.12	0.22
(1,4609)	1:90:A:LEU:HB3	1:99:A:GLU:HA	3	0.23	0.04	0.26
(1,4610)	1:90:B:LEU:HB3	1:99:B:GLU:HA	3	0.23	0.04	0.25
(1,4152)	1:123:B:ARG:HG2	1:51:A:ALA:HB2	3	0.23	0.09	0.19
(1,4152)	1:123:B:ARG:HG2	1:51:A:ALA:HB1	3	0.23	0.09	0.19
(1,4673)	1:91:A:ASP:HA	1:96:A:ALA:HA	3	0.23	0.1	0.18
(1,4674)	1:91:B:ASP:HA	1:96:B:ALA:HA	3	0.23	0.1	0.18
(1,4151)	1:123:A:ARG:HG2	1:51:B:ALA:HB2	3	0.21	0.09	0.18
(1,4151)	1:123:A:ARG:HG2	1:51:B:ALA:HB1	3	0.21	0.09	0.18
(3,2832)	1:112:B:TYR:HD1	1:116:B:MET:HE1	3	0.21	0.02	0.2
(3,2832)	1:112:B:TYR:HD1	1:116:B:MET:HE3	3	0.21	0.02	0.2
(3,2832)	1:116:B:MET:HE3	1:112:A:TYR:HD1	3	0.21	0.02	0.2
(3,2831)	1:112:A:TYR:HD1	1:116:A:MET:HE1	3	0.2	0.03	0.2
(3,2831)	1:112:A:TYR:HD1	1:116:A:MET:HE3	3	0.2	0.03	0.2
(3,2831)	1:116:A:MET:HE3	1:112:B:TYR:HD1	3	0.2	0.03	0.2
(1,4358)	1:82:B:ASN:HB2	1:83:B:ALA:HB2	3	0.2	0.04	0.21
(3,361)	1:102:A:ILE:HA	1:91:A:ASP:H	3	0.2	0.08	0.17
(1,4357)	1:82:A:ASN:HB2	1:83:A:ALA:HB2	3	0.2	0.04	0.2
(3,362)	1:102:B:ILE:HA	1:91:B:ASP:H	3	0.2	0.08	0.16
(1,2514)	1:45:B:ILE:HD11	1:49:A:LEU:HA	3	0.18	0.08	0.13
(1,2514)	1:45:B:ILE:HD13	1:49:A:LEU:HA	3	0.18	0.08	0.13
(1,4051)	1:93:A:ARG:HB3	1:64:A:VAL:HA	3	0.18	0.03	0.18
(3,125)	1:56:A:PRO:HG2	1:57:A:GLN:H	3	0.18	0.04	0.18
(1,4052)	1:93:B:ARG:HB3	1:64:B:VAL:HA	3	0.18	0.04	0.18
(1,5537)	1:115:A:LEU:HD23	1:116:A:MET:HE1	3	0.18	0.03	0.16
(1,5537)	1:115:A:LEU:HD21	1:116:A:MET:HE1	3	0.18	0.03	0.16
(1,5537)	1:115:A:LEU:HD22	1:116:A:MET:HE2	3	0.18	0.03	0.16
(1,5538)	1:115:B:LEU:HD23	1:116:B:MET:HE1	3	0.18	0.03	0.16
(1,5538)	1:115:B:LEU:HD21	1:116:B:MET:HE1	3	0.18	0.03	0.16
(1,5538)	1:115:B:LEU:HD22	1:116:B:MET:HE2	3	0.18	0.03	0.16
(3,126)	1:56:B:PRO:HG2	1:57:B:GLN:H	3	0.18	0.04	0.17
(1,2513)	1:45:A:ILE:HD11	1:49:B:LEU:HA	3	0.17	0.08	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2513)	1:45:A:ILE:HD13	1:49:B:LEU:HA	3	0.17	0.08	0.14
(1,5919)	1:104:A:PHE:HD1	1:115:A:LEU:HD12	3	0.17	0.04	0.17
(1,5919)	1:104:A:PHE:HD2	1:115:A:LEU:HD12	3	0.17	0.04	0.17
(1,5919)	1:104:A:PHE:HD2	1:115:A:LEU:HD13	3	0.17	0.04	0.17
(1,5920)	1:104:B:PHE:HD1	1:115:B:LEU:HD12	3	0.17	0.04	0.17
(1,5920)	1:104:B:PHE:HD2	1:115:B:LEU:HD12	3	0.17	0.04	0.17
(1,5920)	1:104:B:PHE:HD2	1:115:B:LEU:HD13	3	0.17	0.04	0.17
(1,3461)	1:64:A:VAL:HB	1:102:A:ILE:HD13	3	0.16	0.05	0.14
(1,3461)	1:64:A:VAL:HB	1:102:A:ILE:HD11	3	0.16	0.05	0.14
(1,3462)	1:64:B:VAL:HB	1:102:B:ILE:HD13	3	0.16	0.05	0.14
(1,3462)	1:64:B:VAL:HB	1:102:B:ILE:HD11	3	0.16	0.05	0.14
(1,3689)	1:67:A:SER:HB2	1:115:A:LEU:HD13	3	0.16	0.01	0.16
(1,3689)	1:67:A:SER:HB2	1:115:A:LEU:HD11	3	0.16	0.01	0.16
(1,3689)	1:67:A:SER:HB2	1:115:A:LEU:HD12	3	0.16	0.01	0.16
(1,3690)	1:67:B:SER:HB2	1:115:B:LEU:HD13	3	0.16	0.01	0.16
(1,3690)	1:67:B:SER:HB2	1:115:B:LEU:HD11	3	0.16	0.01	0.16
(1,3690)	1:67:B:SER:HB2	1:115:B:LEU:HD12	3	0.16	0.01	0.16
(1,4397)	1:83:A:ALA:HA	1:121:A:THR:HG22	3	0.16	0.06	0.14
(1,4397)	1:83:A:ALA:HA	1:121:A:THR:HG23	3	0.16	0.06	0.14
(1,4398)	1:83:B:ALA:HA	1:121:B:THR:HG22	3	0.16	0.06	0.14
(1,4398)	1:83:B:ALA:HA	1:121:B:THR:HG23	3	0.16	0.06	0.14
(3,735)	1:132:A:LEU:HG	1:134:A:GLY:H	3	0.16	0.04	0.15
(1,1036)	1:89:B:VAL:HG11	1:87:B:THR:H	3	0.16	0.0	0.16
(1,1036)	1:89:B:VAL:HG13	1:87:B:THR:H	3	0.16	0.0	0.16
(1,1036)	1:89:B:VAL:HG12	1:87:B:THR:H	3	0.16	0.0	0.16
(1,1035)	1:89:A:VAL:HG11	1:87:A:THR:H	3	0.15	0.01	0.16
(1,1035)	1:89:A:VAL:HG13	1:87:A:THR:H	3	0.15	0.01	0.16
(1,1035)	1:89:A:VAL:HG12	1:87:A:THR:H	3	0.15	0.01	0.16
(1,1468)	1:100:B:THR:HG21	1:101:B:THR:H	3	0.13	0.02	0.13
(1,1468)	1:100:B:THR:HG23	1:101:B:THR:H	3	0.13	0.02	0.13
(1,1468)	1:100:B:THR:HG22	1:101:B:THR:H	3	0.13	0.02	0.13
(3,1450)	1:61:B:GLU:HG2	1:62:B:LYS:HG2	2	1.7	0.04	1.7
(3,1450)	1:136:B:GLU:HG2	1:139:B:ALA:HB3	2	1.7	0.04	1.7
(3,1449)	1:61:A:GLU:HG2	1:62:A:LYS:HG2	2	1.7	0.03	1.7
(3,1449)	1:136:A:GLU:HG2	1:139:A:ALA:HB3	2	1.7	0.03	1.7
(1,3271)	1:140:A:LYS:HG3	1:67:A:SER:HB3	2	1.21	0.11	1.21
(1,3272)	1:140:B:LYS:HG3	1:67:B:SER:HB3	2	1.21	0.12	1.21
(1,4876)	1:99:B:GLU:HA	1:129:B:LYS:HD3	2	1.06	0.06	1.06
(1,4875)	1:99:A:GLU:HA	1:129:A:LYS:HD3	2	1.06	0.06	1.06
(3,2393)	1:99:A:GLU:HG3	1:129:A:LYS:HD3	2	1.04	0.03	1.04
(3,2394)	1:99:B:GLU:HG3	1:129:B:LYS:HD3	2	1.04	0.03	1.04
(3,1670)	1:67:B:SER:HB2	1:80:B:PRO:HD3	2	0.91	0.23	0.91

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,1669)	1:67:A:SER:HB2	1:80:A:PRO:HD3	2	0.9	0.23	0.9
(3,1102)	1:138:B:ALA:HA	1:136:B:GLU:HG3	2	0.87	0.05	0.87
(3,1101)	1:138:A:ALA:HA	1:136:A:GLU:HG3	2	0.86	0.05	0.86
(1,2125)	1:129:A:LYS:HD3	1:129:A:LYS:H	2	0.81	0.04	0.81
(1,2126)	1:129:B:LYS:HD3	1:129:B:LYS:H	2	0.81	0.04	0.81
(1,2239)	1:136:A:GLU:HB2	1:136:A:GLU:H	2	0.81	0.0	0.81
(1,2240)	1:136:B:GLU:HB2	1:136:B:GLU:H	2	0.81	0.0	0.81
(1,2587)	1:46:A:ARG:HG2	1:129:B:LYS:HG3	2	0.66	0.2	0.66
(1,2588)	1:46:B:ARG:HG2	1:129:A:LYS:HG3	2	0.65	0.2	0.65
(3,2896)	1:123:B:ARG:HD3	1:51:A:ALA:HB1	2	0.64	0.09	0.64
(3,2896)	1:123:B:ARG:HD2	1:54:A:ALA:HB3	2	0.64	0.09	0.64
(3,2895)	1:123:A:ARG:HD3	1:51:B:ALA:HB1	2	0.6	0.1	0.6
(3,2895)	1:123:A:ARG:HD2	1:54:B:ALA:HB3	2	0.6	0.1	0.6
(1,5825)	1:135:A:MET:HE3	1:112:B:TYR:HD1	2	0.6	0.41	0.6
(1,5825)	1:135:A:MET:HE2	1:112:B:TYR:HD2	2	0.6	0.41	0.6
(1,5826)	1:135:B:MET:HE3	1:112:A:TYR:HD1	2	0.6	0.43	0.6
(1,5826)	1:135:B:MET:HE2	1:112:A:TYR:HD2	2	0.6	0.43	0.6
(3,2391)	1:136:A:GLU:HG3	1:140:A:LYS:HB3	2	0.57	0.02	0.57
(3,2392)	1:136:B:GLU:HG3	1:140:B:LYS:HB3	2	0.57	0.02	0.57
(1,2471)	1:43:A:VAL:HB	1:46:A:ARG:HA	2	0.57	0.24	0.57
(1,2472)	1:43:B:VAL:HB	1:46:B:ARG:HA	2	0.57	0.24	0.57
(1,3961)	1:72:A:LYS:HA	1:72:A:LYS:HG3	2	0.56	0.01	0.56
(1,3962)	1:72:B:LYS:HA	1:72:B:LYS:HG3	2	0.56	0.01	0.56
(3,997)	1:47:A:VAL:HB	1:129:B:LYS:HG3	2	0.52	0.02	0.52
(3,998)	1:47:B:VAL:HB	1:129:A:LYS:HG3	2	0.51	0.0	0.51
(1,2902)	1:55:B:LYS:HB2	1:45:A:ILE:HG12	2	0.49	0.1	0.49
(1,2901)	1:55:A:LYS:HB2	1:45:B:ILE:HG12	2	0.48	0.08	0.48
(1,3996)	1:72:B:LYS:HG3	1:114:B:THR:HG23	2	0.46	0.05	0.46
(1,3996)	1:72:B:LYS:HG3	1:114:B:THR:HG21	2	0.46	0.05	0.46
(3,1536)	1:123:B:ARG:HG2	1:50:A:PRO:HD2	2	0.46	0.27	0.46
(3,1536)	1:63:B:PRO:HG2	1:60:B:PRO:HD2	2	0.46	0.27	0.46
(1,3995)	1:72:A:LYS:HG3	1:114:A:THR:HG23	2	0.46	0.05	0.46
(1,3995)	1:72:A:LYS:HG3	1:114:A:THR:HG21	2	0.46	0.05	0.46
(3,1488)	1:61:B:GLU:HB2	1:62:B:LYS:HG2	2	0.44	0.05	0.44
(1,5805)	1:134:A:GLY:HA3	1:116:B:MET:HB2	2	0.44	0.11	0.44
(3,1487)	1:61:A:GLU:HB2	1:62:A:LYS:HG2	2	0.44	0.06	0.44
(1,5806)	1:134:B:GLY:HA3	1:116:A:MET:HB2	2	0.43	0.08	0.43
(3,1055)	1:49:A:LEU:HG	1:45:B:ILE:HA	2	0.42	0.02	0.42
(1,2105)	1:129:A:LYS:HD3	1:128:A:LEU:H	2	0.42	0.05	0.42
(1,2106)	1:129:B:LYS:HD3	1:128:B:LEU:H	2	0.41	0.05	0.41
(1,2624)	1:48:B:ASP:HB3	1:46:A:ARG:HB2	2	0.41	0.27	0.41
(3,1056)	1:49:B:LEU:HG	1:45:A:ILE:HA	2	0.41	0.01	0.41

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2623)	1:48:A:ASP:HB3	1:46:B:ARG:HB2	2	0.4	0.24	0.4
(3,743)	1:116:A:MET:HE1	1:135:B:MET:H	2	0.35	0.05	0.35
(3,743)	1:116:A:MET:HE2	1:135:B:MET:H	2	0.35	0.05	0.35
(3,744)	1:116:B:MET:HE1	1:135:A:MET:H	2	0.35	0.06	0.35
(3,744)	1:116:B:MET:HE2	1:135:A:MET:H	2	0.35	0.06	0.35
(1,2211)	1:45:A:ILE:H	1:135:B:MET:H	2	0.3	0.08	0.3
(3,1753)	1:69:A:LYS:HE3	1:71:A:ASP:HB2	2	0.3	0.16	0.3
(3,1754)	1:69:B:LYS:HE3	1:71:B:ASP:HB2	2	0.3	0.16	0.3
(3,1031)	1:46:A:ARG:HG3	1:48:A:ASP:HB2	2	0.29	0.0	0.29
(3,1032)	1:46:B:ARG:HG3	1:48:B:ASP:HB2	2	0.29	0.0	0.29
(3,1545)	1:63:A:PRO:HD2	1:93:A:ARG:HD3	2	0.28	0.12	0.28
(3,1546)	1:63:B:PRO:HD2	1:93:B:ARG:HD3	2	0.28	0.12	0.28
(1,3419)	1:64:A:VAL:HA	1:67:A:SER:HB2	2	0.27	0.01	0.27
(1,3420)	1:64:B:VAL:HA	1:67:B:SER:HB2	2	0.27	0.01	0.27
(3,1109)	1:139:A:ALA:HA	1:140:A:LYS:HD3	2	0.27	0.15	0.27
(3,1109)	1:139:A:ALA:HA	1:140:A:LYS:HD2	2	0.27	0.15	0.27
(1,2924)	1:56:B:PRO:HA	1:50:B:PRO:HD2	2	0.26	0.1	0.26
(1,3507)	1:65:A:PHE:HB2	1:140:A:LYS:HB2	2	0.26	0.03	0.26
(3,1110)	1:139:B:ALA:HA	1:140:B:LYS:HD3	2	0.26	0.16	0.26
(3,1110)	1:139:B:ALA:HA	1:140:B:LYS:HD2	2	0.26	0.16	0.26
(3,2789)	1:136:A:GLU:HG3	1:136:A:GLU:HA	2	0.26	0.02	0.26
(1,2923)	1:56:A:PRO:HA	1:50:A:PRO:HD2	2	0.26	0.11	0.26
(1,3508)	1:65:B:PHE:HB2	1:140:B:LYS:HB2	2	0.26	0.03	0.26
(3,2790)	1:136:B:GLU:HG3	1:136:B:GLU:HA	2	0.26	0.02	0.26
(1,3458)	1:110:B:VAL:HB	1:114:B:THR:HG23	2	0.25	0.07	0.25
(1,3458)	1:110:B:VAL:HB	1:114:B:THR:HG22	2	0.25	0.07	0.25
(1,5471)	1:112:A:TYR:HB3	1:115:A:LEU:HD23	2	0.25	0.04	0.25
(1,5472)	1:112:B:TYR:HB3	1:115:B:LEU:HD23	2	0.25	0.04	0.25
(1,3457)	1:110:A:VAL:HB	1:114:A:THR:HG23	2	0.24	0.06	0.24
(1,3457)	1:110:A:VAL:HB	1:114:A:THR:HG22	2	0.24	0.06	0.24
(1,4428)	1:84:B:ASP:HB2	1:85:B:GLN:HG2	2	0.24	0.03	0.24
(1,4427)	1:84:A:ASP:HB2	1:85:A:GLN:HG2	2	0.23	0.03	0.23
(3,2875)	1:121:A:THR:HG21	1:124:A:LYS:HG2	2	0.23	0.11	0.23
(3,2875)	1:87:A:THR:HG21	1:124:A:LYS:HD3	2	0.23	0.11	0.23
(3,2876)	1:121:B:THR:HG21	1:124:B:LYS:HG2	2	0.22	0.12	0.22
(3,2876)	1:87:B:THR:HG21	1:124:B:LYS:HD3	2	0.22	0.12	0.22
(3,734)	1:120:B:ASP:HA	1:134:A:GLY:H	2	0.22	0.02	0.22
(3,2953)	1:128:A:LEU:HB3	1:122:A:LEU:HB2	2	0.22	0.09	0.22
(3,2954)	1:128:B:LEU:HB3	1:122:B:LEU:HB2	2	0.22	0.09	0.22
(1,4704)	1:108:B:LYS:HA	1:115:B:LEU:HD13	2	0.22	0.02	0.22
(3,733)	1:120:A:ASP:HA	1:134:B:GLY:H	2	0.22	0.07	0.22
(3,1053)	1:93:A:ARG:HG3	1:94:A:THR:HA	2	0.22	0.02	0.22

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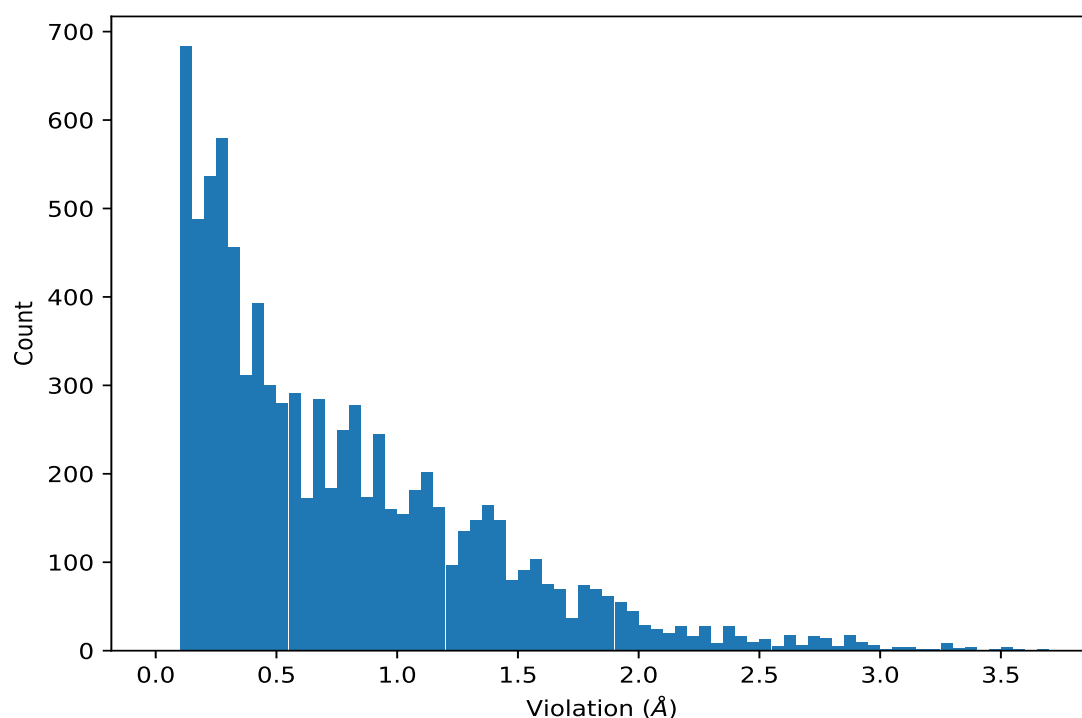
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,1054)	1:93:B:ARG:HG3	1:94:B:THR:HA	2	0.22	0.02	0.22
(1,4703)	1:108:A:LYS:HA	1:115:A:LEU:HD13	2	0.21	0.01	0.21
(1,3721)	1:67:A:SER:HB3	1:69:A:LYS:HD2	2	0.19	0.03	0.19
(3,317)	1:96:A:ALA:HA	1:88:A:SER:H	2	0.19	0.03	0.19
(3,318)	1:96:B:ALA:HA	1:88:B:SER:H	2	0.19	0.03	0.19
(3,2007)	1:82:A:ASN:HB2	1:85:A:GLN:HG2	2	0.19	0.01	0.19
(3,2008)	1:82:B:ASN:HB2	1:85:B:GLN:HG2	2	0.19	0.01	0.19
(1,3722)	1:67:B:SER:HB3	1:69:B:LYS:HD2	2	0.18	0.04	0.18
(1,5889)	1:65:A:PHE:HD2	1:101:A:THR:HB	2	0.16	0.03	0.16
(1,5890)	1:65:B:PHE:HD2	1:101:B:THR:HB	2	0.16	0.02	0.16
(1,5021)	1:101:A:THR:HG23	1:130:A:VAL:HA	2	0.14	0.02	0.14
(1,5022)	1:101:B:THR:HG23	1:130:B:VAL:HA	2	0.14	0.02	0.14
(3,2855)	1:119:A:MET:HE3	1:104:A:PHE:HB3	2	0.14	0.02	0.14
(3,2855)	1:119:A:MET:HE2	1:104:A:PHE:HB3	2	0.14	0.02	0.14
(3,2856)	1:119:B:MET:HE3	1:104:B:PHE:HB3	2	0.14	0.02	0.14
(3,2856)	1:119:B:MET:HE2	1:104:B:PHE:HB3	2	0.14	0.02	0.14
(1,927)	1:82:A:ASN:HB2	1:83:A:ALA:H	2	0.12	0.0	0.12
(1,928)	1:82:B:ASN:HB2	1:83:B:ALA:H	2	0.12	0.0	0.12
(1,20)	1:105:B:GLN:HG2	1:105:B:GLN:HE22	2	0.11	0.01	0.11
(1,4569)	1:86:A:LEU:HB3	1:87:A:THR:HG22	2	0.11	0.0	0.11
(1,4569)	1:86:A:LEU:HB3	1:87:A:THR:HG23	2	0.11	0.0	0.11
(1,19)	1:105:A:GLN:HG2	1:105:A:GLN:HE22	2	0.11	0.0	0.11
(1,4570)	1:86:B:LEU:HB3	1:87:B:THR:HG22	2	0.1	0.0	0.1
(1,4570)	1:86:B:LEU:HB3	1:87:B:THR:HG23	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)
(1,4564)	1:87:B:THR:HG21	1:98:B:LYS:HE3	8	3.69
(1,4563)	1:87:A:THR:HG21	1:98:A:LYS:HE3	8	3.69
(3,880)	1:69:B:LYS:HB2	1:140:B:LYS:HE2	5	3.58
(3,879)	1:69:A:LYS:HB2	1:140:A:LYS:HE2	5	3.58
(1,5302)	1:106:B:ALA:HB3	1:112:B:TYR:HB3	3	3.53
(1,5302)	1:106:B:ALA:HB3	1:112:B:TYR:HB3	7	3.53
(1,5301)	1:106:A:ALA:HB3	1:112:A:TYR:HB3	3	3.53
(1,5301)	1:106:A:ALA:HB3	1:112:A:TYR:HB3	7	3.52
(1,5302)	1:106:B:ALA:HB2	1:112:B:TYR:HB3	1	3.45
(1,5301)	1:106:A:ALA:HB2	1:112:A:TYR:HB3	1	3.45
(3,880)	1:69:B:LYS:HB2	1:140:B:LYS:HE3	8	3.39
(3,879)	1:69:A:LYS:HB2	1:140:A:LYS:HE3	8	3.39
(1,5302)	1:106:B:ALA:HB1	1:112:B:TYR:HB3	4	3.37
(1,5301)	1:106:A:ALA:HB1	1:112:A:TYR:HB3	4	3.37
(3,1296)	1:58:B:PRO:HG2	1:55:B:LYS:HE2	5	3.34
(3,1295)	1:58:A:PRO:HG2	1:55:A:LYS:HE2	5	3.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4563)	1:87:A:THR:HG23	1:98:A:LYS:HE3	3	3.31
(1,4564)	1:87:B:THR:HG23	1:98:B:LYS:HE3	3	3.3
(1,5301)	1:106:A:ALA:HB2	1:112:A:TYR:HB3	8	3.28
(1,5302)	1:106:B:ALA:HB2	1:112:B:TYR:HB3	8	3.27
(1,4563)	1:87:A:THR:HG23	1:98:A:LYS:HE3	10	3.27
(1,4564)	1:87:B:THR:HG23	1:98:B:LYS:HE3	10	3.26
(3,1824)	1:129:B:LYS:HD2	1:45:B:ILE:HG23	5	3.25
(3,1823)	1:129:A:LYS:HD2	1:45:A:ILE:HG23	5	3.25
(1,5302)	1:106:B:ALA:HB1	1:112:B:TYR:HB3	6	3.25
(1,5301)	1:106:A:ALA:HB1	1:112:A:TYR:HB3	6	3.25
(1,5302)	1:106:B:ALA:HB2	1:112:B:TYR:HB3	5	3.2
(1,5301)	1:106:A:ALA:HB2	1:112:A:TYR:HB3	5	3.2
(3,1954)	1:79:B:GLN:HG2	1:88:B:SER:HB3	5	3.16
(3,1953)	1:79:A:GLN:HG2	1:88:A:SER:HB3	5	3.16
(3,2062)	1:85:B:GLN:HG2	1:124:B:LYS:HD3	1	3.15
(3,2061)	1:85:A:GLN:HG2	1:124:A:LYS:HD3	1	3.14
(1,4563)	1:87:A:THR:HG21	1:98:A:LYS:HE3	9	3.11
(1,4564)	1:87:B:THR:HG21	1:98:B:LYS:HE3	9	3.1
(1,5302)	1:106:B:ALA:HB1	1:112:B:TYR:HB3	2	3.08
(1,5301)	1:106:A:ALA:HB1	1:112:A:TYR:HB3	2	3.08
(1,5302)	1:106:B:ALA:HB1	1:112:B:TYR:HB3	9	3.07
(1,5301)	1:106:A:ALA:HB1	1:112:A:TYR:HB3	9	3.07
(3,296)	1:94:B:THR:HG22	1:86:B:LEU:H	10	3.04
(3,295)	1:94:A:THR:HG22	1:86:A:LEU:H	10	3.04
(3,2062)	1:85:B:GLN:HG2	1:124:B:LYS:HD3	5	2.99
(3,2061)	1:85:A:GLN:HG2	1:124:A:LYS:HD3	5	2.99
(3,2062)	1:85:B:GLN:HG3	1:124:B:LYS:HD3	10	2.95
(3,2061)	1:85:A:GLN:HG3	1:124:A:LYS:HD3	10	2.95
(3,296)	1:94:B:THR:HG23	1:86:B:LEU:H	8	2.95
(3,295)	1:94:A:THR:HG23	1:86:A:LEU:H	8	2.95
(3,934)	1:45:B:ILE:HG23	1:129:B:LYS:HB2	5	2.93
(3,933)	1:45:A:ILE:HG23	1:129:A:LYS:HB2	5	2.93
(3,296)	1:94:B:THR:HG23	1:86:B:LEU:H	4	2.92
(3,295)	1:94:A:THR:HG23	1:86:A:LEU:H	4	2.92
(1,3024)	1:57:B:GLN:HG2	1:60:B:PRO:HG2	1	2.92
(1,3023)	1:57:A:GLN:HG2	1:60:A:PRO:HG2	1	2.92
(3,2062)	1:85:B:GLN:HG2	1:124:B:LYS:HG2	9	2.91
(3,2061)	1:85:A:GLN:HG2	1:124:A:LYS:HG2	9	2.91
(3,296)	1:94:B:THR:HG21	1:86:B:LEU:H	1	2.91
(3,295)	1:94:A:THR:HG21	1:86:A:LEU:H	1	2.91
(3,2062)	1:85:B:GLN:HG2	1:124:B:LYS:HD3	7	2.9
(1,3024)	1:57:B:GLN:HG2	1:60:B:PRO:HG2	3	2.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3023)	1:57:A:GLN:HG2	1:60:A:PRO:HG2	3	2.9
(1,3023)	1:57:A:GLN:HG2	1:60:A:PRO:HG2	6	2.9
(3,2061)	1:85:A:GLN:HG2	1:124:A:LYS:HD3	7	2.89
(1,3024)	1:57:B:GLN:HG2	1:60:B:PRO:HG2	4	2.89
(1,3024)	1:57:B:GLN:HG2	1:60:B:PRO:HG2	6	2.89
(1,3023)	1:57:A:GLN:HG2	1:60:A:PRO:HG2	4	2.89
(3,3078)	1:104:B:PHE:HD2	1:138:B:ALA:HB3	5	2.88
(3,3077)	1:104:A:PHE:HD2	1:138:A:ALA:HB3	5	2.88
(3,296)	1:94:B:THR:HG21	1:86:B:LEU:H	9	2.88
(3,295)	1:94:A:THR:HG21	1:86:A:LEU:H	9	2.88
(1,5332)	1:108:B:LYS:HA	1:112:B:TYR:HB3	7	2.88
(1,5331)	1:108:A:LYS:HA	1:112:A:TYR:HB3	7	2.87
(3,2062)	1:85:B:GLN:HG3	1:124:B:LYS:HD3	6	2.86
(3,2061)	1:85:A:GLN:HG3	1:124:A:LYS:HD3	6	2.86
(1,3024)	1:57:B:GLN:HG2	1:60:B:PRO:HG2	9	2.85
(1,3023)	1:57:A:GLN:HG2	1:60:A:PRO:HG2	9	2.84
(3,934)	1:45:B:ILE:HG23	1:129:B:LYS:HB2	3	2.81
(3,933)	1:45:A:ILE:HG23	1:129:A:LYS:HB2	3	2.81
(3,296)	1:94:B:THR:HG22	1:86:B:LEU:H	3	2.81
(3,295)	1:94:A:THR:HG22	1:86:A:LEU:H	3	2.81
(1,5332)	1:108:B:LYS:HA	1:112:B:TYR:HB3	3	2.8
(1,5332)	1:108:B:LYS:HA	1:112:B:TYR:HB3	5	2.8
(1,5331)	1:108:A:LYS:HA	1:112:A:TYR:HB3	3	2.8
(1,5331)	1:108:A:LYS:HA	1:112:A:TYR:HB3	5	2.8
(1,3024)	1:57:B:GLN:HG2	1:60:B:PRO:HG2	7	2.8
(1,3023)	1:57:A:GLN:HG2	1:60:A:PRO:HG2	7	2.8
(3,296)	1:94:B:THR:HG21	1:86:B:LEU:H	2	2.78
(3,295)	1:94:A:THR:HG21	1:86:A:LEU:H	2	2.78
(1,5332)	1:108:B:LYS:HA	1:112:B:TYR:HB3	1	2.77
(1,5331)	1:108:A:LYS:HA	1:112:A:TYR:HB3	1	2.77
(3,3078)	1:104:B:PHE:HD1	1:129:B:LYS:HG3	2	2.76
(3,3077)	1:104:A:PHE:HD1	1:129:A:LYS:HG3	2	2.76
(1,5332)	1:108:B:LYS:HA	1:112:B:TYR:HB3	4	2.76
(1,5331)	1:108:A:LYS:HA	1:112:A:TYR:HB3	4	2.76
(1,4958)	1:100:B:THR:HG23	1:129:B:LYS:HD2	10	2.74
(1,4957)	1:100:A:THR:HG23	1:129:A:LYS:HD2	10	2.74
(3,295)	1:94:A:THR:HG21	1:86:A:LEU:H	6	2.73
(1,4958)	1:100:B:THR:HG23	1:129:B:LYS:HD2	2	2.73
(1,4957)	1:100:A:THR:HG23	1:129:A:LYS:HD2	2	2.73
(3,934)	1:45:B:ILE:HG22	1:129:B:LYS:HB2	10	2.72
(3,933)	1:45:A:ILE:HG22	1:129:A:LYS:HB2	10	2.72
(3,296)	1:94:B:THR:HG21	1:86:B:LEU:H	6	2.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4958)	1:100:B:THR:HG21	1:129:B:LYS:HD2	7	2.72
(1,4957)	1:100:A:THR:HG21	1:129:A:LYS:HD2	7	2.72
(3,2062)	1:85:B:GLN:HG3	1:124:B:LYS:HG2	4	2.71
(3,2061)	1:85:A:GLN:HG3	1:124:A:LYS:HD3	2	2.71
(3,2061)	1:85:A:GLN:HG3	1:124:A:LYS:HG2	4	2.71
(1,3024)	1:57:B:GLN:HG2	1:60:B:PRO:HG2	2	2.71
(1,3023)	1:57:A:GLN:HG2	1:60:A:PRO:HG2	2	2.71
(3,2062)	1:85:B:GLN:HG3	1:124:B:LYS:HD3	2	2.7
(3,656)	1:45:B:ILE:HD12	1:125:B:ALA:H	4	2.69
(3,934)	1:45:B:ILE:HG21	1:129:B:LYS:HB2	2	2.68
(3,933)	1:45:A:ILE:HG21	1:129:A:LYS:HB2	2	2.68
(3,655)	1:45:A:ILE:HD12	1:125:A:ALA:H	4	2.68
(1,5302)	1:106:B:ALA:HB2	1:112:B:TYR:HB3	10	2.67
(1,5301)	1:106:A:ALA:HB2	1:112:A:TYR:HB3	10	2.67
(3,2865)	1:121:A:THR:HG22	1:116:A:MET:HA	8	2.65
(3,2062)	1:85:B:GLN:HG2	1:124:B:LYS:HD3	3	2.65
(3,2061)	1:85:A:GLN:HG2	1:124:A:LYS:HD3	3	2.65
(3,296)	1:94:B:THR:HG21	1:86:B:LEU:H	7	2.65
(3,2866)	1:121:B:THR:HG22	1:116:B:MET:HA	8	2.64
(3,295)	1:94:A:THR:HG21	1:86:A:LEU:H	7	2.64
(3,1516)	1:55:B:LYS:HA	1:63:B:PRO:HB2	4	2.63
(3,1515)	1:55:A:LYS:HA	1:63:A:PRO:HB2	4	2.63
(3,934)	1:45:B:ILE:HG21	1:129:B:LYS:HB2	7	2.63
(3,933)	1:45:A:ILE:HG21	1:129:A:LYS:HB2	7	2.63
(3,296)	1:94:B:THR:HG21	1:86:B:LEU:H	5	2.63
(3,295)	1:94:A:THR:HG21	1:86:A:LEU:H	5	2.63
(3,1823)	1:129:A:LYS:HD2	1:45:A:ILE:HG23	1	2.61
(3,934)	1:45:B:ILE:HG22	1:129:B:LYS:HB2	8	2.61
(3,933)	1:45:A:ILE:HG22	1:129:A:LYS:HB2	8	2.61
(3,1824)	1:129:B:LYS:HD2	1:45:B:ILE:HG23	1	2.6
(3,816)	1:88:B:SER:HB3	1:79:B:GLN:HE22	6	2.6
(3,815)	1:88:A:SER:HB3	1:79:A:GLN:HE22	6	2.6
(3,934)	1:45:B:ILE:HG22	1:129:B:LYS:HB2	4	2.59
(3,933)	1:45:A:ILE:HG22	1:129:A:LYS:HB2	4	2.59
(3,3078)	1:104:B:PHE:HD1	1:138:B:ALA:HB1	9	2.56
(3,3077)	1:104:A:PHE:HD1	1:138:A:ALA:HB1	9	2.56
(3,879)	1:69:A:LYS:HB2	1:140:A:LYS:HE2	10	2.56
(3,880)	1:69:B:LYS:HB2	1:140:B:LYS:HE2	10	2.55
(3,656)	1:45:B:ILE:HD12	1:125:B:ALA:H	5	2.55
(3,655)	1:45:A:ILE:HD12	1:125:A:ALA:H	5	2.55
(3,2866)	1:121:B:THR:HG23	1:116:B:MET:HA	5	2.54
(3,2865)	1:121:A:THR:HG23	1:116:A:MET:HA	5	2.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4575)	1:87:A:THR:HG22	1:102:A:ILE:HD12	1	2.54
(3,934)	1:45:B:ILE:HG22	1:129:B:LYS:HB2	6	2.53
(3,933)	1:45:A:ILE:HG22	1:129:A:LYS:HB2	6	2.53
(1,4576)	1:87:B:THR:HG22	1:102:B:ILE:HD12	1	2.53
(3,934)	1:45:B:ILE:HG21	1:129:B:LYS:HB2	9	2.52
(3,933)	1:45:A:ILE:HG21	1:129:A:LYS:HB2	9	2.52
(3,1830)	1:108:B:LYS:HE2	1:135:B:MET:HE1	5	2.51
(3,1829)	1:108:A:LYS:HE2	1:135:A:MET:HE1	5	2.5
(1,4958)	1:100:B:THR:HG23	1:129:B:LYS:HD2	4	2.49
(1,4957)	1:100:A:THR:HG23	1:129:A:LYS:HD2	4	2.49
(3,2848)	1:119:B:MET:HE3	1:75:B:TYR:HD2	1	2.48
(3,2847)	1:119:A:MET:HE3	1:75:A:TYR:HD2	1	2.48
(3,2866)	1:121:B:THR:HG23	1:116:B:MET:HA	1	2.47
(3,2865)	1:121:A:THR:HG23	1:116:A:MET:HA	1	2.47
(3,2866)	1:121:B:THR:HG22	1:116:B:MET:HA	2	2.46
(3,2865)	1:121:A:THR:HG22	1:116:A:MET:HA	2	2.46
(3,3078)	1:104:B:PHE:HD1	1:138:B:ALA:HB3	7	2.45
(1,4958)	1:100:B:THR:HG22	1:129:B:LYS:HD2	9	2.45
(3,3077)	1:104:A:PHE:HD1	1:138:A:ALA:HB3	7	2.44
(1,4957)	1:100:A:THR:HG22	1:129:A:LYS:HD2	9	2.44
(3,3078)	1:104:B:PHE:HD2	1:139:B:ALA:HB2	10	2.43
(3,2848)	1:51:B:ALA:HB2	1:127:A:TYR:HE1	10	2.43
(3,1516)	1:55:B:LYS:HA	1:63:B:PRO:HB2	5	2.43
(3,1515)	1:55:A:LYS:HA	1:63:A:PRO:HB2	5	2.43
(3,3077)	1:104:A:PHE:HD2	1:139:A:ALA:HB2	10	2.42
(3,2866)	1:121:B:THR:HG22	1:116:B:MET:HA	6	2.42
(3,2866)	1:121:B:THR:HG22	1:116:B:MET:HA	9	2.42
(3,2865)	1:121:A:THR:HG22	1:116:A:MET:HA	6	2.42
(3,2865)	1:121:A:THR:HG22	1:116:A:MET:HA	9	2.42
(1,4407)	1:83:A:ALA:HB3	1:120:A:ASP:HB2	4	2.42
(3,2866)	1:121:B:THR:HG22	1:116:B:MET:HA	4	2.41
(3,2865)	1:121:A:THR:HG22	1:116:A:MET:HA	4	2.41
(1,4853)	1:98:A:LYS:HD3	1:51:B:ALA:HA	1	2.41
(1,4408)	1:83:B:ALA:HB3	1:120:B:ASP:HB2	4	2.41
(3,3078)	1:104:B:PHE:HD1	1:138:B:ALA:HB1	6	2.4
(3,3077)	1:104:A:PHE:HD1	1:138:A:ALA:HB1	6	2.4
(1,2910)	1:55:B:LYS:HG3	1:58:B:PRO:HG2	5	2.4
(1,2909)	1:55:A:LYS:HG3	1:58:A:PRO:HG2	5	2.4
(3,1190)	1:108:B:LYS:HG3	1:114:B:THR:HG22	6	2.39
(3,1189)	1:108:A:LYS:HG3	1:114:A:THR:HG22	6	2.39
(3,934)	1:45:B:ILE:HG23	1:129:B:LYS:HB2	1	2.39
(3,933)	1:45:A:ILE:HG23	1:129:A:LYS:HB2	1	2.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5830)	1:135:B:MET:HE3	1:108:B:LYS:HA	1	2.39
(1,5332)	1:108:B:LYS:HA	1:112:B:TYR:HB3	2	2.39
(1,5331)	1:108:A:LYS:HA	1:112:A:TYR:HB3	2	2.39
(1,4854)	1:98:B:LYS:HD3	1:51:A:ALA:HA	1	2.39
(3,2925)	1:126:A:GLY:HA3	1:50:B:PRO:HG3	1	2.38
(3,2866)	1:121:B:THR:HG22	1:116:B:MET:HA	3	2.38
(3,2865)	1:121:A:THR:HG22	1:116:A:MET:HA	3	2.38
(3,2847)	1:51:A:ALA:HB2	1:127:B:TYR:HE1	10	2.38
(1,5800)	1:134:B:GLY:HA2	1:137:B:GLY:HA2	1	2.38
(1,5799)	1:134:A:GLY:HA2	1:137:A:GLY:HA2	1	2.38
(1,5829)	1:135:A:MET:HE3	1:108:A:LYS:HA	1	2.37
(1,5332)	1:108:B:LYS:HA	1:112:B:TYR:HB3	8	2.37
(3,2926)	1:126:B:GLY:HA3	1:50:A:PRO:HG3	1	2.36
(3,2240)	1:94:B:THR:HG23	1:129:B:LYS:HE2	7	2.36
(3,2239)	1:94:A:THR:HG23	1:129:A:LYS:HE2	7	2.36
(3,1516)	1:55:B:LYS:HA	1:63:B:PRO:HB2	3	2.36
(3,1515)	1:55:A:LYS:HA	1:63:A:PRO:HB2	3	2.36
(1,5331)	1:108:A:LYS:HA	1:112:A:TYR:HB3	8	2.36
(3,2865)	1:121:A:THR:HG22	1:116:A:MET:HA	10	2.35
(1,5331)	1:108:A:LYS:HA	1:112:A:TYR:HB3	9	2.35
(3,2866)	1:121:B:THR:HG22	1:116:B:MET:HA	10	2.34
(1,5332)	1:108:B:LYS:HA	1:112:B:TYR:HB3	9	2.34
(3,2062)	1:85:B:GLN:HG2	1:124:B:LYS:HD3	8	2.33
(3,2061)	1:85:A:GLN:HG2	1:124:A:LYS:HD3	8	2.33
(3,1190)	1:108:B:LYS:HG3	1:114:B:THR:HG23	10	2.32
(3,1189)	1:108:A:LYS:HG3	1:114:A:THR:HG23	10	2.32
(1,5332)	1:108:B:LYS:HA	1:112:B:TYR:HB3	6	2.31
(1,5331)	1:108:A:LYS:HA	1:112:A:TYR:HB3	6	2.31
(1,4863)	1:98:A:LYS:HD3	1:125:A:ALA:HB3	1	2.31
(3,2288)	1:95:B:GLN:HG2	1:63:B:PRO:HB2	2	2.3
(3,2287)	1:95:A:GLN:HG2	1:63:A:PRO:HB2	2	2.3
(1,4864)	1:98:B:LYS:HD3	1:125:B:ALA:HB3	1	2.3
(3,2240)	1:94:B:THR:HG23	1:129:B:LYS:HE2	2	2.29
(3,2239)	1:94:A:THR:HG23	1:129:A:LYS:HE2	2	2.29
(3,1760)	1:69:B:LYS:HE3	1:73:B:GLN:HB2	7	2.29
(3,1759)	1:69:A:LYS:HE3	1:73:A:GLN:HB2	7	2.29
(3,1516)	1:55:B:LYS:HA	1:63:B:PRO:HB2	1	2.29
(3,1515)	1:55:A:LYS:HA	1:63:A:PRO:HB2	1	2.29
(1,4855)	1:98:A:LYS:HD3	1:126:A:GLY:HA2	2	2.29
(3,1516)	1:55:B:LYS:HA	1:63:B:PRO:HB2	10	2.28
(3,1515)	1:55:A:LYS:HA	1:63:A:PRO:HB2	10	2.28
(3,312)	1:94:B:THR:HG22	1:87:B:THR:H	10	2.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,311)	1:94:A:THR:HG22	1:87:A:THR:H	10	2.28
(1,4856)	1:98:B:LYS:HD3	1:126:B:GLY:HA2	2	2.28
(1,5891)	1:65:A:PHE:HD1	1:93:A:ARG:HG2	10	2.27
(3,656)	1:45:B:ILE:HD11	1:125:B:ALA:H	10	2.26
(3,655)	1:45:A:ILE:HD11	1:125:A:ALA:H	10	2.26
(3,312)	1:94:B:THR:HG21	1:87:B:THR:H	1	2.26
(3,311)	1:94:A:THR:HG21	1:87:A:THR:H	1	2.26
(1,5892)	1:65:B:PHE:HD1	1:93:B:ARG:HG2	10	2.26
(3,2866)	1:121:B:THR:HG21	1:116:B:MET:HA	7	2.25
(3,312)	1:94:B:THR:HG23	1:87:B:THR:H	8	2.25
(3,311)	1:94:A:THR:HG23	1:87:A:THR:H	8	2.25
(1,4576)	1:87:B:THR:HG21	1:102:B:ILE:HD11	7	2.25
(1,4575)	1:87:A:THR:HG21	1:102:A:ILE:HD11	7	2.25
(1,4575)	1:87:A:THR:HG21	1:102:A:ILE:HD13	8	2.25
(1,4575)	1:87:A:THR:HG23	1:102:A:ILE:HD13	10	2.25
(3,2865)	1:121:A:THR:HG21	1:116:A:MET:HA	7	2.24
(3,816)	1:88:B:SER:HB3	1:79:B:GLN:HE22	3	2.24
(3,815)	1:88:A:SER:HB3	1:79:A:GLN:HE22	3	2.24
(1,4576)	1:87:B:THR:HG21	1:102:B:ILE:HD13	8	2.24
(1,4576)	1:87:B:THR:HG23	1:102:B:ILE:HD13	10	2.24
(3,1190)	1:108:B:LYS:HG3	1:114:B:THR:HG21	5	2.23
(3,1956)	1:79:B:GLN:HG2	1:91:B:ASP:HB3	3	2.21
(3,1955)	1:79:A:GLN:HG2	1:91:A:ASP:HB3	3	2.21
(3,1189)	1:108:A:LYS:HG3	1:114:A:THR:HG21	5	2.21
(3,656)	1:45:B:ILE:HD12	1:125:B:ALA:H	8	2.21
(3,655)	1:45:A:ILE:HD12	1:125:A:ALA:H	8	2.21
(3,879)	1:69:A:LYS:HB2	1:140:A:LYS:HE2	3	2.2
(3,656)	1:45:B:ILE:HD13	1:125:B:ALA:H	1	2.2
(3,655)	1:45:A:ILE:HD13	1:125:A:ALA:H	1	2.2
(1,4576)	1:87:B:THR:HG23	1:102:B:ILE:HD13	4	2.2
(1,4575)	1:87:A:THR:HG23	1:102:A:ILE:HD13	4	2.2
(3,2870)	1:87:B:THR:HG22	1:98:B:LYS:HE3	1	2.19
(3,2848)	1:119:B:MET:HE1	1:75:B:TYR:HD1	6	2.19
(3,2847)	1:119:A:MET:HE1	1:75:A:TYR:HD1	6	2.19
(3,880)	1:69:B:LYS:HB2	1:140:B:LYS:HE2	3	2.19
(3,312)	1:94:B:THR:HG23	1:87:B:THR:H	4	2.19
(3,311)	1:94:A:THR:HG23	1:87:A:THR:H	4	2.19
(1,4564)	1:87:B:THR:HG22	1:98:B:LYS:HE3	1	2.19
(3,2869)	1:87:A:THR:HG22	1:98:A:LYS:HE3	1	2.18
(3,2848)	1:119:B:MET:HE3	1:75:B:TYR:HD2	5	2.18
(3,2847)	1:119:A:MET:HE3	1:75:A:TYR:HD2	5	2.18
(1,4576)	1:87:B:THR:HG21	1:102:B:ILE:HD11	2	2.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4575)	1:87:A:THR:HG21	1:102:A:ILE:HD11	2	2.18
(1,4563)	1:87:A:THR:HG22	1:98:A:LYS:HE3	1	2.18
(1,5800)	1:134:B:GLY:HA2	1:137:B:GLY:HA2	2	2.17
(1,5799)	1:134:A:GLY:HA2	1:137:A:GLY:HA2	2	2.17
(1,4958)	1:100:B:THR:HG23	1:129:B:LYS:HD2	6	2.17
(1,4957)	1:100:A:THR:HG23	1:129:A:LYS:HD2	6	2.17
(1,4864)	1:98:B:LYS:HD3	1:125:B:ALA:HB3	7	2.17
(1,4863)	1:98:A:LYS:HD3	1:125:A:ALA:HB3	7	2.17
(1,4407)	1:83:A:ALA:HB2	1:120:A:ASP:HB2	7	2.17
(3,1760)	1:69:B:LYS:HE3	1:73:B:GLN:HB2	10	2.16
(3,1759)	1:69:A:LYS:HE3	1:73:A:GLN:HB2	10	2.16
(1,5892)	1:65:B:PHE:HD1	1:93:B:ARG:HG2	8	2.16
(1,5891)	1:65:A:PHE:HD1	1:93:A:ARG:HG2	8	2.16
(1,4408)	1:83:B:ALA:HB2	1:120:B:ASP:HB2	7	2.16
(3,3078)	1:104:B:PHE:HD1	1:138:B:ALA:HB1	1	2.15
(3,656)	1:45:B:ILE:HD12	1:125:B:ALA:H	6	2.15
(3,655)	1:45:A:ILE:HD12	1:125:A:ALA:H	6	2.15
(3,3077)	1:104:A:PHE:HD1	1:138:A:ALA:HB1	1	2.14
(3,816)	1:88:B:SER:HB3	1:79:B:GLN:HE22	8	2.14
(1,4408)	1:83:B:ALA:HB3	1:120:B:ASP:HB2	10	2.14
(1,4407)	1:83:A:ALA:HB3	1:120:A:ASP:HB2	10	2.14
(3,815)	1:88:A:SER:HB3	1:79:A:GLN:HE22	8	2.13
(1,4856)	1:98:B:LYS:HD3	1:126:B:GLY:HA2	7	2.13
(1,4855)	1:98:A:LYS:HD3	1:126:A:GLY:HA2	7	2.13
(3,2110)	1:87:B:THR:HG21	1:89:B:VAL:HB	1	2.12
(3,2109)	1:87:A:THR:HG21	1:89:A:VAL:HB	1	2.12
(3,1190)	1:108:B:LYS:HG2	1:114:B:THR:HG22	7	2.12
(1,4576)	1:87:B:THR:HG23	1:102:B:ILE:HD13	3	2.12
(1,4575)	1:87:A:THR:HG23	1:102:A:ILE:HD13	3	2.12
(1,3594)	1:115:B:LEU:HD11	1:75:B:TYR:HB3	2	2.12
(3,1189)	1:108:A:LYS:HG2	1:114:A:THR:HG22	7	2.11
(3,312)	1:94:B:THR:HG21	1:87:B:THR:H	9	2.11
(3,311)	1:94:A:THR:HG21	1:87:A:THR:H	9	2.11
(1,3593)	1:115:A:LEU:HD11	1:75:A:TYR:HB3	2	2.11
(1,4114)	1:74:B:LEU:HA	1:115:B:LEU:HD11	2	2.1
(1,4113)	1:74:A:LEU:HA	1:115:A:LEU:HD11	2	2.1
(1,2354)	1:85:B:GLN:HE22	1:82:B:ASN:HD22	3	2.1
(3,312)	1:94:B:THR:HG21	1:87:B:THR:H	2	2.09
(3,311)	1:94:A:THR:HG21	1:87:A:THR:H	2	2.09
(1,4407)	1:83:A:ALA:HB1	1:120:A:ASP:HB2	9	2.09
(1,2820)	1:54:B:ALA:HB2	1:44:A:ASP:HB2	3	2.09
(1,2353)	1:85:A:GLN:HE22	1:82:A:ASN:HD22	3	2.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,312)	1:94:B:THR:HG22	1:87:B:THR:H	3	2.08
(3,311)	1:94:A:THR:HG22	1:87:A:THR:H	3	2.08
(1,5892)	1:65:B:PHE:HD2	1:93:B:ARG:HG2	6	2.08
(1,4576)	1:87:B:THR:HG21	1:102:B:ILE:HD11	9	2.08
(1,4575)	1:87:A:THR:HG21	1:102:A:ILE:HD11	9	2.08
(1,4408)	1:83:B:ALA:HB1	1:120:B:ASP:HB2	9	2.08
(3,1516)	1:55:B:LYS:HA	1:63:B:PRO:HB2	7	2.07
(3,1515)	1:55:A:LYS:HA	1:63:A:PRO:HB2	7	2.07
(1,5891)	1:65:A:PHE:HD2	1:93:A:ARG:HG2	6	2.07
(1,4856)	1:98:B:LYS:HD3	1:126:B:GLY:HA2	6	2.07
(1,4855)	1:98:A:LYS:HD3	1:126:A:GLY:HA2	6	2.07
(1,2819)	1:54:A:ALA:HB2	1:44:B:ASP:HB2	3	2.07
(3,2870)	1:87:B:THR:HG21	1:98:B:LYS:HE3	7	2.06
(3,2869)	1:87:A:THR:HG21	1:98:A:LYS:HE3	7	2.06
(3,1516)	1:55:B:LYS:HA	1:63:B:PRO:HB2	8	2.06
(3,1515)	1:55:A:LYS:HA	1:63:A:PRO:HB2	8	2.06
(1,4864)	1:98:B:LYS:HD3	1:125:B:ALA:HB2	4	2.06
(1,4564)	1:87:B:THR:HG21	1:98:B:LYS:HE3	7	2.06
(1,4563)	1:87:A:THR:HG21	1:98:A:LYS:HE3	7	2.06
(3,3006)	1:106:B:ALA:HB3	1:135:B:MET:HG2	1	2.05
(3,3005)	1:106:A:ALA:HB3	1:135:A:MET:HG2	1	2.05
(3,1834)	1:72:B:LYS:HE2	1:110:B:VAL:HG23	10	2.05
(3,1833)	1:72:A:LYS:HE2	1:110:A:VAL:HG23	10	2.05
(3,312)	1:94:B:THR:HG21	1:87:B:THR:H	6	2.05
(3,311)	1:94:A:THR:HG21	1:87:A:THR:H	6	2.05
(1,4863)	1:98:A:LYS:HD3	1:125:A:ALA:HB2	4	2.05
(1,5892)	1:65:B:PHE:HD2	1:93:B:ARG:HG2	7	2.04
(1,5891)	1:65:A:PHE:HD1	1:93:A:ARG:HG2	2	2.04
(1,5891)	1:65:A:PHE:HD2	1:93:A:ARG:HG2	7	2.04
(3,2458)	1:94:B:THR:HG21	1:66:B:LEU:HB3	9	2.03
(3,2457)	1:94:A:THR:HG21	1:66:A:LEU:HB3	9	2.03
(1,5892)	1:65:B:PHE:HD1	1:93:B:ARG:HG2	2	2.03
(1,4863)	1:98:A:LYS:HD3	1:125:A:ALA:HB2	6	2.03
(1,3239)	1:99:A:GLU:HG2	1:49:B:LEU:HB3	8	2.03
(3,2926)	1:126:B:GLY:HA3	1:50:A:PRO:HG3	4	2.02
(1,4864)	1:98:B:LYS:HD3	1:125:B:ALA:HB2	6	2.02
(3,2925)	1:126:A:GLY:HA3	1:50:B:PRO:HG3	4	2.01
(3,312)	1:94:B:THR:HG21	1:87:B:THR:H	7	2.01
(3,311)	1:94:A:THR:HG21	1:87:A:THR:H	7	2.01
(1,5892)	1:65:B:PHE:HD1	1:93:B:ARG:HG2	3	2.01
(1,5891)	1:65:A:PHE:HD1	1:93:A:ARG:HG2	3	2.01
(1,4407)	1:83:A:ALA:HB1	1:120:A:ASP:HB2	2	2.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3240)	1:99:B:GLU:HG2	1:49:A:LEU:HB3	3	2.01
(1,3240)	1:99:B:GLU:HG2	1:49:A:LEU:HB3	8	2.01
(1,3239)	1:99:A:GLU:HG2	1:49:B:LEU:HB3	3	2.01
(3,2848)	1:51:B:ALA:HB2	1:127:A:TYR:HE1	9	2.0
(3,2847)	1:51:A:ALA:HB2	1:127:B:TYR:HE1	9	2.0
(1,4408)	1:83:B:ALA:HB1	1:120:B:ASP:HB2	2	2.0
(3,2240)	1:94:B:THR:HG22	1:129:B:LYS:HE2	4	1.99
(3,2239)	1:94:A:THR:HG22	1:129:A:LYS:HE2	4	1.99
(3,1724)	1:135:B:MET:HG2	1:115:B:LEU:HD23	1	1.99
(3,1723)	1:135:A:MET:HG2	1:115:A:LEU:HD23	1	1.99
(3,1516)	1:55:B:LYS:HA	1:63:B:PRO:HB2	2	1.99
(3,1515)	1:55:A:LYS:HA	1:63:A:PRO:HB2	2	1.99
(3,1190)	1:108:B:LYS:HG2	1:114:B:THR:HG22	1	1.99
(3,1189)	1:108:A:LYS:HG2	1:114:A:THR:HG22	1	1.99
(3,346)	1:106:B:ALA:HB1	1:114:B:THR:H	6	1.99
(3,345)	1:106:A:ALA:HB1	1:114:A:THR:H	6	1.99
(1,3140)	1:98:B:LYS:HE2	1:96:B:ALA:HB1	1	1.99
(1,3140)	1:98:B:LYS:HE2	1:96:B:ALA:HB1	4	1.99
(1,3139)	1:98:A:LYS:HE2	1:96:A:ALA:HB1	4	1.99
(1,2354)	1:85:B:GLN:HE22	1:82:B:ASN:HD22	1	1.99
(1,2353)	1:85:A:GLN:HE22	1:82:A:ASN:HD22	1	1.99
(3,2848)	1:51:B:ALA:HB1	1:127:A:TYR:HE1	2	1.98
(3,2845)	1:51:A:ALA:HB1	1:127:B:TYR:HD1	4	1.98
(3,766)	1:65:B:PHE:H	1:106:B:ALA:H	8	1.98
(3,765)	1:65:A:PHE:H	1:106:A:ALA:H	8	1.98
(1,4864)	1:98:B:LYS:HD3	1:125:B:ALA:HB3	5	1.98
(1,4863)	1:98:A:LYS:HD3	1:125:A:ALA:HB3	5	1.98
(1,4408)	1:83:B:ALA:HB1	1:120:B:ASP:HB2	3	1.98
(1,4321)	1:127:A:TYR:HA	1:49:B:LEU:HB3	1	1.98
(1,3580)	1:115:B:LEU:HD11	1:75:B:TYR:HA	2	1.98
(1,3579)	1:115:A:LEU:HD11	1:75:A:TYR:HA	2	1.98
(1,3140)	1:98:B:LYS:HE2	1:96:B:ALA:HB1	9	1.98
(1,3139)	1:98:A:LYS:HE2	1:96:A:ALA:HB1	1	1.98
(1,3139)	1:98:A:LYS:HE2	1:96:A:ALA:HB1	9	1.98
(3,2848)	1:119:B:MET:HE2	1:75:B:TYR:HD2	4	1.97
(3,2847)	1:119:A:MET:HE2	1:75:A:TYR:HD2	4	1.97
(3,2240)	1:94:B:THR:HG23	1:129:B:LYS:HE3	5	1.97
(3,2239)	1:94:A:THR:HG23	1:129:A:LYS:HE3	5	1.97
(3,766)	1:65:B:PHE:H	1:106:B:ALA:H	7	1.97
(3,765)	1:65:A:PHE:H	1:106:A:ALA:H	7	1.97
(1,4407)	1:83:A:ALA:HB1	1:120:A:ASP:HB2	3	1.97
(1,4322)	1:127:B:TYR:HA	1:49:A:LEU:HB3	1	1.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,2846)	1:51:B:ALA:HB1	1:127:A:TYR:HD1	4	1.96
(3,1760)	1:69:B:LYS:HE2	1:73:B:GLN:HG2	1	1.96
(3,1759)	1:69:A:LYS:HE2	1:73:A:GLN:HG2	1	1.96
(3,656)	1:45:B:ILE:HD13	1:125:B:ALA:H	2	1.96
(3,655)	1:45:A:ILE:HD13	1:125:A:ALA:H	2	1.96
(1,5798)	1:134:B:GLY:HA2	1:137:B:GLY:HA3	1	1.96
(1,5797)	1:134:A:GLY:HA2	1:137:A:GLY:HA3	1	1.96
(1,3140)	1:98:B:LYS:HE2	1:96:B:ALA:HB3	7	1.96
(1,3139)	1:98:A:LYS:HE2	1:96:A:ALA:HB3	7	1.96
(3,2870)	1:87:B:THR:HG21	1:98:B:LYS:HE2	8	1.95
(3,2869)	1:87:A:THR:HG21	1:98:A:LYS:HE2	8	1.95
(3,766)	1:65:B:PHE:H	1:106:B:ALA:H	10	1.95
(3,765)	1:65:A:PHE:H	1:106:A:ALA:H	10	1.95
(1,5332)	1:108:B:LYS:HA	1:112:B:TYR:HB3	10	1.95
(1,5331)	1:108:A:LYS:HA	1:112:A:TYR:HB3	10	1.95
(1,4958)	1:100:B:THR:HG21	1:129:B:LYS:HD2	8	1.95
(1,4957)	1:100:A:THR:HG21	1:129:A:LYS:HD2	8	1.95
(1,2343)	1:89:A:VAL:HB	1:79:A:GLN:HE22	6	1.95
(3,3072)	1:104:B:PHE:HE2	1:72:B:LYS:HG3	5	1.94
(3,3071)	1:104:A:PHE:HE2	1:72:A:LYS:HG3	5	1.94
(3,2458)	1:100:B:THR:HG23	1:66:B:LEU:HB3	10	1.94
(3,2457)	1:100:A:THR:HG23	1:66:A:LEU:HB3	10	1.94
(3,655)	1:45:A:ILE:HD13	1:125:A:ALA:H	9	1.94
(1,3236)	1:61:B:GLU:HB3	1:62:B:LYS:HG2	2	1.94
(1,3235)	1:61:A:GLU:HB3	1:62:A:LYS:HG2	2	1.94
(1,2344)	1:89:B:VAL:HB	1:79:B:GLN:HE22	6	1.94
(3,2847)	1:51:A:ALA:HB1	1:127:B:TYR:HE1	2	1.93
(3,1760)	1:69:B:LYS:HE3	1:73:B:GLN:HB2	9	1.93
(3,1759)	1:69:A:LYS:HE3	1:73:A:GLN:HB2	9	1.93
(3,1608)	1:65:B:PHE:HB2	1:136:B:GLU:HG3	8	1.93
(3,1607)	1:65:A:PHE:HB2	1:136:A:GLU:HG3	8	1.93
(3,766)	1:65:B:PHE:H	1:106:B:ALA:H	3	1.93
(3,766)	1:65:B:PHE:H	1:106:B:ALA:H	4	1.93
(3,765)	1:65:A:PHE:H	1:106:A:ALA:H	3	1.93
(3,656)	1:45:B:ILE:HD13	1:125:B:ALA:H	9	1.93
(1,4856)	1:98:B:LYS:HD3	1:126:B:GLY:HA2	4	1.93
(1,4855)	1:98:A:LYS:HD3	1:126:A:GLY:HA2	4	1.93
(1,4408)	1:83:B:ALA:HB3	1:120:B:ASP:HB2	6	1.93
(3,766)	1:65:B:PHE:H	1:106:B:ALA:H	2	1.92
(3,765)	1:65:A:PHE:H	1:106:A:ALA:H	2	1.92
(3,765)	1:65:A:PHE:H	1:106:A:ALA:H	4	1.92
(3,765)	1:65:A:PHE:H	1:106:A:ALA:H	5	1.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,345)	1:106:A:ALA:HB3	1:114:A:THR:H	7	1.92
(1,5892)	1:65:B:PHE:HD2	1:93:B:ARG:HG2	9	1.92
(1,4407)	1:83:A:ALA:HB3	1:120:A:ASP:HB2	6	1.92
(3,2870)	1:87:B:THR:HG23	1:98:B:LYS:HE3	4	1.91
(3,2869)	1:87:A:THR:HG23	1:98:A:LYS:HE3	4	1.91
(3,2458)	1:100:B:THR:HG23	1:66:B:LEU:HB3	6	1.91
(3,2457)	1:100:A:THR:HG23	1:66:A:LEU:HB3	6	1.91
(3,766)	1:65:B:PHE:H	1:106:B:ALA:H	5	1.91
(3,346)	1:106:B:ALA:HB3	1:114:B:THR:H	7	1.91
(3,345)	1:106:A:ALA:HB2	1:114:A:THR:H	1	1.91
(1,5891)	1:65:A:PHE:HD2	1:93:A:ARG:HG2	5	1.91
(1,5891)	1:65:A:PHE:HD2	1:93:A:ARG:HG2	9	1.91
(1,5800)	1:134:B:GLY:HA2	1:137:B:GLY:HA2	8	1.91
(1,5799)	1:134:A:GLY:HA2	1:137:A:GLY:HA2	8	1.91
(1,4682)	1:91:B:ASP:HA	1:96:B:ALA:HB3	1	1.91
(1,4681)	1:91:A:ASP:HA	1:96:A:ALA:HB3	1	1.91
(1,4564)	1:87:B:THR:HG23	1:98:B:LYS:HE3	4	1.91
(1,4563)	1:87:A:THR:HG23	1:98:A:LYS:HE3	4	1.91
(1,4364)	1:82:B:ASN:HB3	1:85:B:GLN:HG2	10	1.91
(1,4363)	1:82:A:ASN:HB3	1:85:A:GLN:HG2	10	1.91
(1,3140)	1:98:B:LYS:HE2	1:96:B:ALA:HB2	2	1.91
(1,3139)	1:98:A:LYS:HE2	1:96:A:ALA:HB2	2	1.91
(3,2870)	1:87:B:THR:HG22	1:98:B:LYS:HE3	6	1.9
(3,2869)	1:87:A:THR:HG22	1:98:A:LYS:HE3	6	1.9
(3,346)	1:106:B:ALA:HB2	1:114:B:THR:H	1	1.9
(1,5892)	1:65:B:PHE:HD2	1:93:B:ARG:HG2	5	1.9
(1,4564)	1:87:B:THR:HG22	1:98:B:LYS:HE3	6	1.9
(1,4563)	1:87:A:THR:HG22	1:98:A:LYS:HE3	6	1.9
(1,2354)	1:85:B:GLN:HE22	1:82:B:ASN:HD22	9	1.9
(1,2353)	1:85:A:GLN:HE22	1:82:A:ASN:HD22	9	1.9
(1,2344)	1:89:B:VAL:HB	1:79:B:GLN:HE22	3	1.9
(3,3078)	1:104:B:PHE:HD2	1:138:B:ALA:HB1	4	1.89
(3,3077)	1:104:A:PHE:HD2	1:138:A:ALA:HB1	4	1.89
(1,4682)	1:91:B:ASP:HA	1:96:B:ALA:HB1	2	1.89
(1,4681)	1:91:A:ASP:HA	1:96:A:ALA:HB1	2	1.89
(1,3593)	1:115:A:LEU:HD13	1:75:A:TYR:HB3	6	1.89
(1,2343)	1:89:A:VAL:HB	1:79:A:GLN:HE22	3	1.89
(3,2240)	1:94:B:THR:HG21	1:129:B:LYS:HE2	10	1.88
(3,2239)	1:94:A:THR:HG21	1:129:A:LYS:HE2	10	1.88
(3,276)	1:73:B:GLN:HG2	1:79:B:GLN:H	6	1.88
(3,275)	1:73:A:GLN:HG2	1:79:A:GLN:H	6	1.88
(1,3594)	1:115:B:LEU:HD13	1:75:B:TYR:HB3	6	1.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3274)	1:61:B:GLU:HG2	1:62:B:LYS:HG2	6	1.88
(3,2925)	1:126:A:GLY:HA3	1:50:B:PRO:HG3	10	1.87
(3,2298)	1:90:B:LEU:HA	1:96:B:ALA:HB3	1	1.87
(3,2239)	1:94:A:THR:HG23	1:129:A:LYS:HE2	9	1.87
(3,765)	1:65:A:PHE:H	1:106:A:ALA:H	9	1.87
(3,656)	1:45:B:ILE:HD11	1:125:B:ALA:H	3	1.87
(3,655)	1:45:A:ILE:HD11	1:125:A:ALA:H	3	1.87
(1,5892)	1:65:B:PHE:HD1	1:93:B:ARG:HG2	1	1.87
(1,5891)	1:65:A:PHE:HD1	1:93:A:ARG:HG2	1	1.87
(1,5800)	1:134:B:GLY:HA2	1:137:B:GLY:HA2	5	1.87
(1,5799)	1:134:A:GLY:HA2	1:137:A:GLY:HA2	5	1.87
(1,5222)	1:116:B:MET:HB3	1:114:B:THR:HG22	10	1.87
(1,5221)	1:116:A:MET:HB3	1:114:A:THR:HG21	1	1.87
(1,5221)	1:116:A:MET:HB3	1:114:A:THR:HG22	10	1.87
(1,3273)	1:61:A:GLU:HG2	1:62:A:LYS:HG2	6	1.87
(1,3236)	1:61:B:GLU:HB3	1:62:B:LYS:HG2	6	1.87
(3,2847)	1:51:A:ALA:HB3	1:127:B:TYR:HE1	3	1.86
(3,2297)	1:90:A:LEU:HA	1:96:A:ALA:HB3	1	1.86
(3,2240)	1:94:B:THR:HG23	1:129:B:LYS:HE2	9	1.86
(3,766)	1:65:B:PHE:H	1:106:B:ALA:H	9	1.86
(3,765)	1:65:A:PHE:H	1:106:A:ALA:H	1	1.86
(1,5312)	1:106:B:ALA:HB1	1:114:B:THR:HG21	6	1.86
(1,5311)	1:106:A:ALA:HB1	1:114:A:THR:HG21	6	1.86
(1,5222)	1:116:B:MET:HB3	1:114:B:THR:HG21	1	1.86
(1,4958)	1:100:B:THR:HG22	1:129:B:LYS:HD2	3	1.86
(1,4856)	1:98:B:LYS:HD3	1:126:B:GLY:HA2	5	1.86
(1,4855)	1:98:A:LYS:HD3	1:126:A:GLY:HA2	5	1.86
(1,3274)	1:61:B:GLU:HG2	1:62:B:LYS:HG2	2	1.86
(1,3235)	1:61:A:GLU:HB3	1:62:A:LYS:HG2	6	1.86
(1,3024)	1:57:B:GLN:HG2	1:60:B:PRO:HG2	8	1.86
(1,3023)	1:57:A:GLN:HG2	1:60:A:PRO:HG2	8	1.86
(3,2870)	1:87:B:THR:HG21	1:98:B:LYS:HE3	2	1.85
(3,766)	1:65:B:PHE:H	1:106:B:ALA:H	1	1.85
(3,312)	1:94:B:THR:HG21	1:87:B:THR:H	5	1.85
(3,311)	1:94:A:THR:HG21	1:87:A:THR:H	5	1.85
(1,5222)	1:116:B:MET:HB3	1:114:B:THR:HG22	2	1.85
(1,5221)	1:116:A:MET:HB3	1:114:A:THR:HG23	4	1.85
(1,4957)	1:100:A:THR:HG22	1:129:A:LYS:HD2	3	1.85
(1,4854)	1:98:B:LYS:HD3	1:51:A:ALA:HA	4	1.85
(1,4712)	1:92:B:GLN:HG2	1:79:B:GLN:HB3	4	1.85
(1,4564)	1:87:B:THR:HG21	1:98:B:LYS:HE3	2	1.85
(1,3273)	1:61:A:GLU:HG2	1:62:A:LYS:HG2	2	1.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,2869)	1:87:A:THR:HG21	1:98:A:LYS:HE3	2	1.84
(3,1515)	1:55:A:LYS:HA	1:129:A:LYS:HB2	9	1.84
(1,5222)	1:116:B:MET:HB3	1:114:B:THR:HG23	4	1.84
(1,5221)	1:116:A:MET:HB3	1:114:A:THR:HG22	2	1.84
(1,5221)	1:116:A:MET:HB3	1:114:A:THR:HG21	7	1.84
(1,4711)	1:92:A:GLN:HG2	1:79:A:GLN:HB3	4	1.84
(1,4563)	1:87:A:THR:HG21	1:98:A:LYS:HE3	2	1.84
(1,4408)	1:83:B:ALA:HB2	1:120:B:ASP:HB2	8	1.84
(1,4407)	1:83:A:ALA:HB2	1:120:A:ASP:HB2	8	1.84
(1,3140)	1:98:B:LYS:HE2	1:96:B:ALA:HB1	8	1.84
(3,2297)	1:90:A:LEU:HA	1:96:A:ALA:HB1	2	1.83
(3,1516)	1:55:B:LYS:HA	1:129:B:LYS:HB2	9	1.83
(1,5222)	1:116:B:MET:HB3	1:114:B:THR:HG21	7	1.83
(1,4853)	1:98:A:LYS:HD3	1:51:B:ALA:HA	4	1.83
(1,3139)	1:98:A:LYS:HE2	1:96:A:ALA:HB1	8	1.83
(3,2926)	1:126:B:GLY:HA3	1:50:A:PRO:HG3	10	1.82
(3,2848)	1:119:B:MET:HE2	1:75:B:TYR:HD1	7	1.82
(3,2847)	1:119:A:MET:HE2	1:75:A:TYR:HD1	7	1.82
(3,2458)	1:100:B:THR:HG23	1:66:B:LEU:HB3	4	1.82
(3,2457)	1:100:A:THR:HG23	1:66:A:LEU:HB3	4	1.82
(3,2298)	1:90:B:LEU:HA	1:96:B:ALA:HB1	2	1.82
(3,2298)	1:90:B:LEU:HA	1:96:B:ALA:HB3	4	1.82
(3,2297)	1:90:A:LEU:HA	1:96:A:ALA:HB3	4	1.82
(3,1608)	1:65:B:PHE:HB2	1:60:B:PRO:HG2	2	1.82
(3,1607)	1:65:A:PHE:HB2	1:60:A:PRO:HG2	2	1.82
(1,5420)	1:110:B:VAL:HG12	1:114:B:THR:HG22	6	1.82
(1,5419)	1:110:A:VAL:HG12	1:114:A:THR:HG22	6	1.82
(1,5419)	1:110:A:VAL:HG11	1:114:A:THR:HG23	10	1.82
(1,5418)	1:72:B:LYS:HG3	1:110:B:VAL:HG12	2	1.82
(1,5418)	1:72:B:LYS:HG3	1:110:B:VAL:HG12	4	1.82
(1,5417)	1:72:A:LYS:HG3	1:110:A:VAL:HG12	4	1.82
(1,5221)	1:116:A:MET:HB3	1:114:A:THR:HG23	5	1.82
(1,4864)	1:98:B:LYS:HD3	1:125:B:ALA:HB2	2	1.82
(1,4863)	1:98:A:LYS:HD3	1:125:A:ALA:HB2	2	1.82
(1,4682)	1:91:B:ASP:HA	1:96:B:ALA:HB3	4	1.82
(1,4681)	1:91:A:ASP:HA	1:96:A:ALA:HB3	4	1.82
(1,4575)	1:87:A:THR:HG22	1:102:A:ILE:HD11	6	1.82
(1,4408)	1:83:B:ALA:HB3	1:120:B:ASP:HB2	5	1.82
(1,4407)	1:83:A:ALA:HB3	1:120:A:ASP:HB2	5	1.82
(3,3072)	1:104:B:PHE:HE2	1:129:B:LYS:HG3	6	1.81
(3,3071)	1:104:A:PHE:HE1	1:72:A:LYS:HG3	1	1.81
(3,3071)	1:104:A:PHE:HE2	1:129:A:LYS:HG3	6	1.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,2848)	1:51:B:ALA:HB3	1:127:A:TYR:HE1	3	1.81
(3,2682)	1:108:B:LYS:HB2	1:112:B:TYR:HB3	7	1.81
(3,2681)	1:108:A:LYS:HB2	1:112:A:TYR:HB3	7	1.81
(3,2176)	1:108:B:LYS:HA	1:139:B:ALA:HB3	1	1.81
(3,766)	1:65:B:PHE:H	1:106:B:ALA:H	6	1.81
(3,765)	1:65:A:PHE:H	1:106:A:ALA:H	6	1.81
(3,346)	1:106:B:ALA:HB2	1:114:B:THR:H	5	1.81
(1,5420)	1:110:B:VAL:HG11	1:114:B:THR:HG23	10	1.81
(1,5417)	1:72:A:LYS:HG3	1:110:A:VAL:HG12	2	1.81
(1,5222)	1:116:B:MET:HB3	1:114:B:THR:HG23	5	1.81
(1,4722)	1:93:B:ARG:HA	1:77:B:GLY:HA2	1	1.81
(1,4721)	1:93:A:ARG:HA	1:77:A:GLY:HA2	1	1.81
(1,4576)	1:87:B:THR:HG22	1:102:B:ILE:HD11	6	1.81
(3,3072)	1:104:B:PHE:HE1	1:72:B:LYS:HG3	1	1.8
(3,2240)	1:94:B:THR:HG23	1:129:B:LYS:HE3	1	1.8
(3,2239)	1:94:A:THR:HG23	1:129:A:LYS:HE3	1	1.8
(3,2175)	1:108:A:LYS:HA	1:139:A:ALA:HB3	1	1.8
(3,1829)	1:108:A:LYS:HE2	1:135:A:MET:HE2	2	1.8
(3,1403)	1:122:A:LEU:HA	1:49:B:LEU:HB3	1	1.8
(3,994)	1:47:B:VAL:HB	1:99:A:GLU:HG2	9	1.8
(3,345)	1:106:A:ALA:HB2	1:114:A:THR:H	5	1.8
(1,5800)	1:134:B:GLY:HA2	1:137:B:GLY:HA2	3	1.8
(1,5799)	1:134:A:GLY:HA2	1:137:A:GLY:HA2	3	1.8
(1,5798)	1:134:B:GLY:HA2	1:137:B:GLY:HA3	2	1.8
(1,5797)	1:134:A:GLY:HA2	1:137:A:GLY:HA3	2	1.8
(1,4863)	1:98:A:LYS:HD3	1:125:A:ALA:HB3	8	1.8
(1,3274)	1:61:B:GLU:HG2	1:62:B:LYS:HG2	8	1.8
(1,3273)	1:61:A:GLU:HG2	1:62:A:LYS:HG2	8	1.8
(3,2925)	1:126:A:GLY:HA3	1:50:B:PRO:HG3	5	1.79
(3,2458)	1:100:B:THR:HG21	1:66:B:LEU:HB3	7	1.79
(3,2457)	1:100:A:THR:HG21	1:66:A:LEU:HB3	7	1.79
(3,1830)	1:108:B:LYS:HE2	1:135:B:MET:HE2	2	1.79
(3,1404)	1:122:B:LEU:HA	1:49:A:LEU:HB3	1	1.79
(3,1359)	1:79:A:GLN:HG3	1:86:A:LEU:HB3	5	1.79
(3,352)	1:98:B:LYS:HG2	1:90:B:LEU:H	5	1.79
(1,5222)	1:116:B:MET:HB3	1:114:B:THR:HG21	8	1.79
(1,4864)	1:98:B:LYS:HD3	1:125:B:ALA:HB3	8	1.79
(1,4856)	1:98:B:LYS:HD3	1:126:B:GLY:HA2	1	1.79
(1,4855)	1:98:A:LYS:HD3	1:126:A:GLY:HA2	1	1.79
(1,4682)	1:91:B:ASP:HA	1:96:B:ALA:HB2	7	1.79
(1,4681)	1:91:A:ASP:HA	1:96:A:ALA:HB2	7	1.79
(3,2682)	1:108:B:LYS:HB2	1:112:B:TYR:HB3	5	1.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,2681)	1:108:A:LYS:HB2	1:112:A:TYR:HB3	5	1.78
(3,1360)	1:79:B:GLN:HG3	1:86:B:LEU:HB3	5	1.78
(3,993)	1:47:A:VAL:HB	1:99:B:GLU:HG2	9	1.78
(3,351)	1:98:A:LYS:HG2	1:90:A:LEU:H	5	1.78
(3,181)	1:115:A:LEU:HD13	1:66:A:LEU:H	7	1.78
(1,5558)	1:116:B:MET:HE3	1:119:B:MET:HE2	9	1.78
(1,5557)	1:116:A:MET:HE3	1:119:A:MET:HE2	9	1.78
(1,5312)	1:106:B:ALA:HB2	1:114:B:THR:HG22	10	1.78
(1,5311)	1:106:A:ALA:HB2	1:114:A:THR:HG22	10	1.78
(1,5222)	1:116:B:MET:HB3	1:114:B:THR:HG23	9	1.78
(1,5221)	1:116:A:MET:HB3	1:114:A:THR:HG21	8	1.78
(1,5221)	1:116:A:MET:HB3	1:114:A:THR:HG23	9	1.78
(1,4364)	1:82:B:ASN:HB3	1:85:B:GLN:HG2	6	1.78
(1,4363)	1:82:A:ASN:HB3	1:85:A:GLN:HG2	6	1.78
(1,4114)	1:74:B:LEU:HA	1:115:B:LEU:HD12	4	1.78
(1,4113)	1:74:A:LEU:HA	1:115:A:LEU:HD12	4	1.78
(1,3139)	1:98:A:LYS:HE2	1:96:A:ALA:HB3	6	1.78
(1,2820)	1:54:B:ALA:HB1	1:44:A:ASP:HB2	4	1.78
(3,2458)	1:100:B:THR:HG23	1:66:B:LEU:HB3	2	1.77
(3,2457)	1:100:A:THR:HG23	1:66:A:LEU:HB3	2	1.77
(3,1830)	1:58:B:PRO:HG2	1:55:B:LYS:HE3	10	1.77
(3,1608)	1:65:B:PHE:HB2	1:60:B:PRO:HG2	1	1.77
(3,1404)	1:122:B:LEU:HA	1:49:A:LEU:HB3	9	1.77
(3,1403)	1:122:A:LEU:HA	1:49:B:LEU:HB3	9	1.77
(3,920)	1:45:B:ILE:HD11	1:46:B:ARG:HG3	10	1.77
(3,919)	1:45:A:ILE:HD11	1:46:A:ARG:HG3	10	1.77
(3,182)	1:115:B:LEU:HD13	1:66:B:LEU:H	7	1.77
(1,5800)	1:134:B:GLY:HA2	1:137:B:GLY:HA2	4	1.77
(1,5799)	1:134:A:GLY:HA2	1:137:A:GLY:HA2	4	1.77
(1,5222)	1:116:B:MET:HB3	1:114:B:THR:HG21	6	1.77
(1,5221)	1:116:A:MET:HB3	1:114:A:THR:HG21	6	1.77
(1,4722)	1:93:B:ARG:HA	1:77:B:GLY:HA2	4	1.77
(1,4721)	1:93:A:ARG:HA	1:77:A:GLY:HA2	4	1.77
(1,4712)	1:92:B:GLN:HG2	1:79:B:GLN:HB3	1	1.77
(1,3140)	1:98:B:LYS:HE2	1:96:B:ALA:HB3	6	1.77
(3,1829)	1:58:A:PRO:HG2	1:55:A:LYS:HE3	10	1.76
(3,1760)	1:69:B:LYS:HE3	1:73:B:GLN:HB2	4	1.76
(3,1759)	1:69:A:LYS:HE3	1:73:A:GLN:HB2	4	1.76
(3,1608)	1:65:B:PHE:HB2	1:60:B:PRO:HG2	3	1.76
(3,1607)	1:65:A:PHE:HB2	1:60:A:PRO:HG2	1	1.76
(3,182)	1:115:B:LEU:HD13	1:66:B:LEU:H	4	1.76
(3,181)	1:115:A:LEU:HD13	1:66:A:LEU:H	4	1.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5222)	1:116:B:MET:HB3	1:114:B:THR:HG21	3	1.76
(1,5221)	1:116:A:MET:HB3	1:114:A:THR:HG21	3	1.76
(1,4712)	1:92:B:GLN:HG2	1:79:B:GLN:HB3	8	1.76
(1,4711)	1:92:A:GLN:HG2	1:79:A:GLN:HB3	1	1.76
(1,4711)	1:92:A:GLN:HG2	1:79:A:GLN:HB3	8	1.76
(1,2819)	1:54:A:ALA:HB1	1:44:B:ASP:HB2	4	1.76
(3,2926)	1:126:B:GLY:HA3	1:50:A:PRO:HG3	5	1.75
(3,2458)	1:100:B:THR:HG21	1:66:B:LEU:HB3	8	1.75
(3,2457)	1:100:A:THR:HG21	1:66:A:LEU:HB3	8	1.75
(3,2176)	1:108:B:LYS:HA	1:139:B:ALA:HB3	5	1.75
(3,1608)	1:65:B:PHE:HB2	1:60:B:PRO:HG2	10	1.75
(3,1607)	1:65:A:PHE:HB2	1:60:A:PRO:HG2	3	1.75
(3,1607)	1:65:A:PHE:HB2	1:60:A:PRO:HG2	10	1.75
(1,5404)	1:110:B:VAL:HG23	1:115:B:LEU:HB3	2	1.75
(1,3948)	1:91:B:ASP:HB2	1:96:B:ALA:HB1	2	1.75
(1,3947)	1:91:A:ASP:HB2	1:96:A:ALA:HB1	2	1.75
(1,3580)	1:115:B:LEU:HD12	1:75:B:TYR:HA	4	1.75
(1,3579)	1:115:A:LEU:HD12	1:75:A:TYR:HA	4	1.75
(3,2682)	1:108:B:LYS:HB2	1:112:B:TYR:HB3	1	1.74
(3,2681)	1:108:A:LYS:HB2	1:112:A:TYR:HB3	1	1.74
(3,2175)	1:108:A:LYS:HA	1:139:A:ALA:HB3	5	1.74
(3,1450)	1:136:B:GLU:HG2	1:139:B:ALA:HB3	2	1.74
(3,848)	1:44:B:ASP:HA	1:123:B:ARG:HG3	8	1.74
(3,847)	1:44:A:ASP:HA	1:123:A:ARG:HG3	8	1.74
(1,5403)	1:110:A:VAL:HG23	1:115:A:LEU:HB3	2	1.74
(3,2458)	1:100:B:THR:HG22	1:66:B:LEU:HB3	1	1.73
(3,2457)	1:100:A:THR:HG22	1:66:A:LEU:HB3	1	1.73
(3,1516)	1:55:B:LYS:HA	1:63:B:PRO:HB2	6	1.73
(3,1515)	1:55:A:LYS:HA	1:63:A:PRO:HB2	6	1.73
(3,1449)	1:136:A:GLU:HG2	1:139:A:ALA:HB3	2	1.73
(3,854)	1:88:B:SER:HA	1:124:B:LYS:HE3	1	1.73
(3,853)	1:88:A:SER:HA	1:124:A:LYS:HE3	1	1.73
(1,4856)	1:98:B:LYS:HD3	1:126:B:GLY:HA2	8	1.73
(1,4855)	1:98:A:LYS:HD3	1:126:A:GLY:HA2	8	1.73
(1,3947)	1:91:A:ASP:HB2	1:96:A:ALA:HB3	1	1.73
(1,3594)	1:115:B:LEU:HD12	1:75:B:TYR:HB3	4	1.73
(1,3593)	1:115:A:LEU:HD12	1:75:A:TYR:HB3	4	1.73
(3,2458)	1:100:B:THR:HG22	1:66:B:LEU:HB3	3	1.72
(3,2457)	1:100:A:THR:HG22	1:66:A:LEU:HB3	3	1.72
(3,181)	1:115:A:LEU:HD11	1:66:A:LEU:H	1	1.72
(1,5892)	1:65:B:PHE:HD1	1:93:B:ARG:HG2	4	1.72
(1,5891)	1:65:A:PHE:HD1	1:93:A:ARG:HG2	4	1.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4864)	1:98:B:LYS:HD3	1:125:B:ALA:HB2	9	1.72
(1,4863)	1:98:A:LYS:HD3	1:125:A:ALA:HB2	9	1.72
(1,4322)	1:127:B:TYR:HA	1:49:A:LEU:HB3	6	1.72
(1,3948)	1:91:B:ASP:HB2	1:96:B:ALA:HB3	1	1.72
(1,3947)	1:91:A:ASP:HB2	1:96:A:ALA:HB2	7	1.72
(3,1760)	1:69:B:LYS:HE3	1:73:B:GLN:HB2	2	1.71
(3,1759)	1:69:A:LYS:HE3	1:73:A:GLN:HB2	2	1.71
(3,1189)	1:108:A:LYS:HG3	1:114:A:THR:HG23	2	1.71
(3,1121)	1:54:A:ALA:HB2	1:57:A:GLN:HG3	9	1.71
(3,692)	1:45:B:ILE:HG23	1:128:B:LEU:H	5	1.71
(3,691)	1:45:A:ILE:HG23	1:128:A:LEU:H	5	1.71
(3,182)	1:115:B:LEU:HD11	1:66:B:LEU:H	1	1.71
(1,3948)	1:91:B:ASP:HB2	1:96:B:ALA:HB2	7	1.71
(3,2870)	1:87:B:THR:HG21	1:98:B:LYS:HE3	5	1.7
(3,2869)	1:87:A:THR:HG21	1:98:A:LYS:HE3	5	1.7
(3,2546)	1:102:B:ILE:HD13	1:128:B:LEU:HG	10	1.7
(3,2545)	1:102:A:ILE:HD13	1:128:A:LEU:HG	10	1.7
(3,1190)	1:108:B:LYS:HG3	1:114:B:THR:HG23	2	1.7
(3,1122)	1:54:B:ALA:HB2	1:57:B:GLN:HG3	9	1.7
(1,4864)	1:98:B:LYS:HD3	1:125:B:ALA:HB1	3	1.7
(1,4863)	1:98:A:LYS:HD3	1:125:A:ALA:HB1	3	1.7
(1,4564)	1:87:B:THR:HG21	1:98:B:LYS:HE3	5	1.7
(1,4563)	1:87:A:THR:HG21	1:98:A:LYS:HE3	5	1.7
(1,4408)	1:83:B:ALA:HB3	1:120:B:ASP:HB2	1	1.7
(1,4407)	1:83:A:ALA:HB3	1:120:A:ASP:HB2	1	1.7
(3,1404)	1:122:B:LEU:HA	1:98:B:LYS:HG3	2	1.69
(3,1403)	1:122:A:LEU:HA	1:98:A:LYS:HG3	2	1.69
(3,994)	1:47:B:VAL:HB	1:60:A:PRO:HG3	1	1.69
(3,346)	1:106:B:ALA:HB1	1:114:B:THR:H	4	1.69
(3,346)	1:106:B:ALA:HB2	1:114:B:THR:H	10	1.69
(3,345)	1:106:A:ALA:HB1	1:114:A:THR:H	4	1.69
(3,345)	1:106:A:ALA:HB2	1:114:A:THR:H	10	1.69
(3,304)	1:124:B:LYS:HG2	1:86:B:LEU:H	1	1.69
(3,303)	1:124:A:LYS:HG2	1:86:A:LEU:H	1	1.69
(3,172)	1:46:B:ARG:HB2	1:64:A:VAL:H	6	1.69
(1,4114)	1:74:B:LEU:HA	1:115:B:LEU:HD11	9	1.69
(1,4113)	1:74:A:LEU:HA	1:115:A:LEU:HD11	9	1.69
(1,3593)	1:115:A:LEU:HD11	1:75:A:TYR:HB3	9	1.69
(1,3274)	1:61:B:GLU:HG2	1:62:B:LYS:HG2	3	1.69
(1,3273)	1:61:A:GLU:HG2	1:62:A:LYS:HG2	3	1.69
(3,2546)	1:102:B:ILE:HD12	1:128:B:LEU:HG	1	1.68
(3,2545)	1:102:A:ILE:HD12	1:128:A:LEU:HG	1	1.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,2298)	1:90:B:LEU:HA	1:96:B:ALA:HB2	7	1.68
(3,2297)	1:90:A:LEU:HA	1:96:A:ALA:HB2	7	1.68
(3,2175)	1:108:A:LYS:HA	1:139:A:ALA:HB2	4	1.68
(3,993)	1:47:A:VAL:HB	1:60:B:PRO:HG3	1	1.68
(3,912)	1:45:B:ILE:HD11	1:46:B:ARG:HD3	9	1.68
(3,848)	1:44:B:ASP:HA	1:46:B:ARG:HG2	5	1.68
(1,5558)	1:116:B:MET:HE3	1:119:B:MET:HE3	4	1.68
(1,5557)	1:116:A:MET:HE3	1:119:A:MET:HE3	4	1.68
(1,4712)	1:92:B:GLN:HG2	1:79:B:GLN:HB3	3	1.68
(1,4711)	1:92:A:GLN:HG2	1:79:A:GLN:HB3	3	1.68
(1,3594)	1:115:B:LEU:HD11	1:75:B:TYR:HB3	9	1.68
(1,2782)	1:51:B:ALA:HB1	1:126:A:GLY:HA3	1	1.68
(1,2344)	1:89:B:VAL:HB	1:79:B:GLN:HE22	8	1.68
(1,2343)	1:89:A:VAL:HB	1:79:A:GLN:HE22	8	1.68
(3,2546)	1:102:B:ILE:HD13	1:128:B:LEU:HG	4	1.67
(3,2545)	1:102:A:ILE:HD13	1:128:A:LEU:HG	4	1.67
(3,2176)	1:108:B:LYS:HA	1:139:B:ALA:HB2	4	1.67
(3,2006)	1:81:B:VAL:HB	1:66:B:LEU:HG	1	1.67
(3,2005)	1:81:A:VAL:HB	1:66:A:LEU:HG	1	1.67
(3,1450)	1:61:B:GLU:HG2	1:62:B:LYS:HG2	1	1.67
(3,1449)	1:61:A:GLU:HG2	1:62:A:LYS:HG2	1	1.67
(3,952)	1:46:B:ARG:HB2	1:48:A:ASP:HB2	8	1.67
(3,911)	1:45:A:ILE:HD11	1:46:A:ARG:HD3	9	1.67
(3,847)	1:44:A:ASP:HA	1:46:A:ARG:HG2	5	1.67
(1,4681)	1:91:A:ASP:HA	1:96:A:ALA:HB2	6	1.67
(1,4322)	1:127:B:TYR:HA	1:49:A:LEU:HB3	9	1.67
(1,4321)	1:127:A:TYR:HA	1:49:B:LEU:HB3	9	1.67
(1,3274)	1:61:B:GLU:HG2	1:62:B:LYS:HG2	1	1.67
(1,3273)	1:61:A:GLU:HG2	1:62:A:LYS:HG2	1	1.67
(1,2781)	1:51:A:ALA:HB1	1:126:B:GLY:HA3	1	1.67
(3,2874)	1:87:B:THR:HG23	1:124:B:LYS:HB2	1	1.66
(3,2873)	1:87:A:THR:HG23	1:124:A:LYS:HB2	1	1.66
(3,2846)	1:51:B:ALA:HB2	1:127:A:TYR:HD2	5	1.66
(3,951)	1:46:A:ARG:HB2	1:48:B:ASP:HB2	8	1.66
(3,912)	1:45:B:ILE:HD13	1:46:B:ARG:HD3	5	1.66
(3,911)	1:45:A:ILE:HD13	1:46:A:ARG:HD3	5	1.66
(1,5797)	1:134:A:GLY:HA2	1:137:A:GLY:HA3	8	1.66
(1,4682)	1:91:B:ASP:HA	1:96:B:ALA:HB2	6	1.66
(1,4443)	1:79:A:GLN:HB2	1:65:A:PHE:HB3	8	1.66
(1,4321)	1:127:A:TYR:HA	1:49:B:LEU:HB3	6	1.66
(3,2682)	1:108:B:LYS:HB2	1:112:B:TYR:HB3	3	1.65
(3,2681)	1:108:A:LYS:HB2	1:112:A:TYR:HB3	3	1.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,1404)	1:122:B:LEU:HA	1:98:B:LYS:HG3	6	1.65
(3,912)	1:45:B:ILE:HD11	1:46:B:ARG:HD3	3	1.65
(3,911)	1:45:A:ILE:HD11	1:46:A:ARG:HD3	3	1.65
(3,171)	1:46:A:ARG:HB2	1:64:B:VAL:H	6	1.65
(1,5798)	1:134:B:GLY:HA2	1:137:B:GLY:HA3	8	1.65
(1,5404)	1:110:B:VAL:HG21	1:115:B:LEU:HB3	9	1.65
(1,5403)	1:110:A:VAL:HG21	1:115:A:LEU:HB3	9	1.65
(1,4681)	1:91:A:ASP:HA	1:96:A:ALA:HB3	8	1.65
(1,4444)	1:79:B:GLN:HB2	1:65:B:PHE:HB3	8	1.65
(1,3140)	1:98:B:LYS:HE2	1:96:B:ALA:HB3	3	1.65
(3,2534)	1:102:B:ILE:HG21	1:133:B:VAL:HB	8	1.64
(3,2533)	1:102:A:ILE:HG21	1:133:A:VAL:HB	8	1.64
(3,1850)	1:85:B:GLN:HB2	1:124:B:LYS:HE3	5	1.64
(3,1849)	1:85:A:GLN:HB2	1:124:A:LYS:HE3	5	1.64
(3,1403)	1:122:A:LEU:HA	1:98:A:LYS:HG3	6	1.64
(3,912)	1:45:B:ILE:HD11	1:46:B:ARG:HD3	7	1.64
(3,911)	1:45:A:ILE:HD11	1:46:A:ARG:HD3	7	1.64
(3,304)	1:124:B:LYS:HG2	1:86:B:LEU:H	10	1.64
(3,303)	1:124:A:LYS:HG2	1:86:A:LEU:H	10	1.64
(1,4682)	1:91:B:ASP:HA	1:96:B:ALA:HB3	8	1.64
(1,4444)	1:79:B:GLN:HB2	1:65:B:PHE:HB3	6	1.64
(1,4443)	1:79:A:GLN:HB2	1:65:A:PHE:HB3	6	1.64
(1,3139)	1:98:A:LYS:HE2	1:96:A:ALA:HB3	3	1.64
(3,2848)	1:51:B:ALA:HB2	1:127:A:TYR:HE1	8	1.63
(3,2846)	1:51:B:ALA:HB1	1:127:A:TYR:HD2	1	1.63
(3,2297)	1:90:A:LEU:HA	1:96:A:ALA:HB2	6	1.63
(3,1668)	1:115:B:LEU:HD13	1:104:B:PHE:HA	4	1.63
(3,1667)	1:115:A:LEU:HD13	1:104:A:PHE:HA	4	1.63
(3,994)	1:47:B:VAL:HB	1:60:A:PRO:HG3	4	1.63
(3,994)	1:47:B:VAL:HB	1:99:A:GLU:HG2	10	1.63
(3,993)	1:47:A:VAL:HB	1:60:B:PRO:HG3	4	1.63
(3,912)	1:45:B:ILE:HD13	1:46:B:ARG:HD3	8	1.63
(3,911)	1:45:A:ILE:HD13	1:46:A:ARG:HD3	8	1.63
(3,815)	1:88:A:SER:HB2	1:79:A:GLN:HE22	4	1.63
(3,304)	1:124:B:LYS:HG2	1:86:B:LEU:H	6	1.63
(3,303)	1:124:A:LYS:HG2	1:86:A:LEU:H	6	1.63
(1,5798)	1:134:B:GLY:HA2	1:137:B:GLY:HA3	3	1.63
(1,5797)	1:134:A:GLY:HA2	1:137:A:GLY:HA3	3	1.63
(1,4856)	1:98:B:LYS:HD3	1:126:B:GLY:HA2	3	1.63
(1,4855)	1:98:A:LYS:HD3	1:126:A:GLY:HA2	3	1.63
(1,3024)	1:57:B:GLN:HG2	1:60:B:PRO:HG2	10	1.63
(1,3023)	1:57:A:GLN:HG2	1:60:A:PRO:HG2	10	1.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,2298)	1:90:B:LEU:HA	1:96:B:ALA:HB2	6	1.62
(3,1404)	1:122:B:LEU:HA	1:49:A:LEU:HB3	4	1.62
(3,952)	1:123:B:ARG:HB2	1:127:B:TYR:HB2	3	1.62
(3,816)	1:88:B:SER:HB2	1:79:B:GLN:HE22	4	1.62
(3,2845)	1:51:A:ALA:HB1	1:127:B:TYR:HD2	1	1.61
(3,2845)	1:51:A:ALA:HB2	1:127:B:TYR:HD2	5	1.61
(3,2298)	1:90:B:LEU:HA	1:96:B:ALA:HB3	8	1.61
(3,2297)	1:90:A:LEU:HA	1:96:A:ALA:HB3	8	1.61
(3,1956)	1:79:B:GLN:HG2	1:91:B:ASP:HB3	10	1.61
(3,1955)	1:79:A:GLN:HG2	1:91:A:ASP:HB3	10	1.61
(3,1403)	1:122:A:LEU:HA	1:49:B:LEU:HB3	4	1.61
(3,993)	1:47:A:VAL:HB	1:99:B:GLU:HG2	10	1.61
(3,951)	1:123:A:ARG:HB2	1:127:A:TYR:HB2	3	1.61
(1,5926)	1:112:B:TYR:HE2	1:113:B:GLU:HB3	2	1.61
(1,5925)	1:112:A:TYR:HE2	1:113:A:GLU:HB3	2	1.61
(3,3072)	1:104:B:PHE:HE2	1:129:B:LYS:HG3	9	1.6
(3,3071)	1:104:A:PHE:HE2	1:129:A:LYS:HG3	9	1.6
(3,2681)	1:108:A:LYS:HB2	1:112:A:TYR:HB3	4	1.6
(3,2632)	1:105:B:GLN:HG3	1:110:B:VAL:HG22	8	1.6
(3,1522)	1:129:B:LYS:HB2	1:45:A:ILE:HG21	5	1.6
(3,1403)	1:122:A:LEU:HA	1:98:A:LYS:HG3	10	1.6
(3,1190)	1:108:B:LYS:HG3	1:114:B:THR:HG22	8	1.6
(3,1190)	1:108:B:LYS:HG2	1:114:B:THR:HG21	9	1.6
(3,1189)	1:108:A:LYS:HG3	1:114:A:THR:HG22	8	1.6
(3,1189)	1:108:A:LYS:HG2	1:114:A:THR:HG21	9	1.6
(3,912)	1:45:B:ILE:HD11	1:46:B:ARG:HD3	2	1.6
(3,182)	1:115:B:LEU:HD12	1:66:B:LEU:H	2	1.6
(3,181)	1:115:A:LEU:HD12	1:66:A:LEU:H	2	1.6
(1,4711)	1:92:A:GLN:HG2	1:79:A:GLN:HB3	10	1.6
(1,4113)	1:74:A:LEU:HA	1:115:A:LEU:HD13	3	1.6
(1,2872)	1:129:B:LYS:HB3	1:49:A:LEU:HB3	6	1.6
(3,2938)	1:127:B:TYR:HB2	1:45:B:ILE:HD13	4	1.59
(3,2937)	1:127:A:TYR:HB2	1:45:A:ILE:HD13	4	1.59
(3,2847)	1:51:A:ALA:HB2	1:127:B:TYR:HE1	8	1.59
(3,2682)	1:108:B:LYS:HB2	1:112:B:TYR:HB3	4	1.59
(3,2631)	1:105:A:GLN:HG3	1:110:A:VAL:HG22	8	1.59
(3,1404)	1:122:B:LEU:HA	1:98:B:LYS:HG3	10	1.59
(3,911)	1:45:A:ILE:HD11	1:46:A:ARG:HD3	2	1.59
(3,182)	1:115:B:LEU:HD11	1:66:B:LEU:H	5	1.59
(3,181)	1:115:A:LEU:HD11	1:66:A:LEU:H	5	1.59
(3,172)	1:46:B:ARG:HB2	1:64:A:VAL:H	1	1.59
(3,172)	1:46:B:ARG:HB2	1:64:A:VAL:H	4	1.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,171)	1:46:A:ARG:HB2	1:64:B:VAL:H	1	1.59
(1,5504)	1:114:B:THR:HG22	1:104:B:PHE:HZ	10	1.59
(1,5503)	1:114:A:THR:HG22	1:104:A:PHE:HZ	10	1.59
(1,5420)	1:110:B:VAL:HG13	1:114:B:THR:HG21	5	1.59
(1,5419)	1:110:A:VAL:HG13	1:114:A:THR:HG21	5	1.59
(1,4856)	1:98:B:LYS:HD3	1:126:B:GLY:HA2	9	1.59
(1,4575)	1:87:A:THR:HG21	1:102:A:ILE:HD12	5	1.59
(1,4114)	1:74:B:LEU:HA	1:115:B:LEU:HD13	3	1.59
(1,3140)	1:98:B:LYS:HE2	1:96:B:ALA:HB1	5	1.59
(3,2869)	1:87:A:THR:HG23	1:98:A:LYS:HE2	3	1.58
(3,2546)	1:102:B:ILE:HD13	1:128:B:LEU:HG	8	1.58
(3,2545)	1:102:A:ILE:HD13	1:128:A:LEU:HG	8	1.58
(3,1521)	1:129:A:LYS:HB2	1:45:B:ILE:HG21	5	1.58
(3,848)	1:44:B:ASP:HA	1:46:B:ARG:HG2	2	1.58
(3,847)	1:44:A:ASP:HA	1:46:A:ARG:HG2	2	1.58
(3,582)	1:49:B:LEU:HG	1:116:A:MET:H	1	1.58
(3,581)	1:49:A:LEU:HG	1:116:B:MET:H	1	1.58
(3,171)	1:46:A:ARG:HB2	1:64:B:VAL:H	4	1.58
(1,5926)	1:112:B:TYR:HE2	1:113:B:GLU:HB3	7	1.58
(1,5925)	1:112:A:TYR:HE2	1:113:A:GLU:HB3	7	1.58
(1,4855)	1:98:A:LYS:HD3	1:126:A:GLY:HA2	9	1.58
(1,4853)	1:98:A:LYS:HD3	1:51:B:ALA:HA	5	1.58
(1,4712)	1:92:B:GLN:HG2	1:79:B:GLN:HB3	7	1.58
(1,4712)	1:92:B:GLN:HG2	1:79:B:GLN:HB3	10	1.58
(1,4576)	1:87:B:THR:HG21	1:102:B:ILE:HD12	5	1.58
(1,3580)	1:115:B:LEU:HD11	1:75:B:TYR:HA	9	1.58
(1,3579)	1:115:A:LEU:HD11	1:75:A:TYR:HA	9	1.58
(1,3139)	1:98:A:LYS:HE2	1:96:A:ALA:HB1	5	1.58
(1,1120)	1:93:B:ARG:HG3	1:90:B:LEU:H	9	1.58
(1,1119)	1:93:A:ARG:HG3	1:90:A:LEU:H	9	1.58
(3,2870)	1:87:B:THR:HG23	1:98:B:LYS:HE2	3	1.57
(3,1850)	1:85:B:GLN:HB2	1:124:B:LYS:HE2	10	1.57
(3,1849)	1:85:A:GLN:HB2	1:124:A:LYS:HE2	10	1.57
(1,5419)	1:110:A:VAL:HG11	1:114:A:THR:HG22	1	1.57
(1,5386)	1:104:B:PHE:HZ	1:110:B:VAL:HG23	9	1.57
(1,5385)	1:104:A:PHE:HZ	1:110:A:VAL:HG23	9	1.57
(1,4711)	1:92:A:GLN:HG2	1:79:A:GLN:HB3	7	1.57
(1,3948)	1:91:B:ASP:HB2	1:96:B:ALA:HB3	4	1.57
(1,3947)	1:91:A:ASP:HB2	1:96:A:ALA:HB3	4	1.57
(1,2352)	1:85:B:GLN:HE22	1:82:B:ASN:HD21	1	1.57
(1,2351)	1:85:A:GLN:HE22	1:82:A:ASN:HD21	1	1.57
(1,1996)	1:49:B:LEU:HB2	1:123:A:ARG:H	2	1.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1995)	1:49:A:LEU:HB2	1:123:B:ARG:H	2	1.57
(1,1120)	1:93:B:ARG:HG3	1:90:B:LEU:H	3	1.57
(1,1119)	1:93:A:ARG:HG3	1:90:A:LEU:H	3	1.57
(1,796)	1:115:B:LEU:HD11	1:75:B:TYR:H	2	1.57
(1,795)	1:115:A:LEU:HD11	1:75:A:TYR:H	2	1.57
(3,2545)	1:102:A:ILE:HD11	1:128:A:LEU:HG	6	1.56
(3,1404)	1:122:B:LEU:HA	1:49:A:LEU:HB3	7	1.56
(3,848)	1:44:B:ASP:HA	1:46:B:ARG:HG2	3	1.56
(3,847)	1:44:A:ASP:HA	1:46:A:ARG:HG2	3	1.56
(3,182)	1:115:B:LEU:HD11	1:66:B:LEU:H	3	1.56
(3,181)	1:115:A:LEU:HD11	1:66:A:LEU:H	3	1.56
(3,171)	1:46:A:ARG:HB2	1:64:B:VAL:H	8	1.56
(1,5925)	1:112:A:TYR:HE2	1:113:A:GLU:HB3	4	1.56
(1,5800)	1:134:B:GLY:HA2	1:137:B:GLY:HA2	6	1.56
(1,5799)	1:134:A:GLY:HA2	1:137:A:GLY:HA2	6	1.56
(1,5420)	1:110:B:VAL:HG11	1:114:B:THR:HG22	1	1.56
(1,5420)	1:110:B:VAL:HG12	1:114:B:THR:HG22	7	1.56
(1,5404)	1:110:B:VAL:HG23	1:115:B:LEU:HB3	4	1.56
(1,5403)	1:110:A:VAL:HG23	1:115:A:LEU:HB3	4	1.56
(1,5314)	1:106:B:ALA:HB1	1:115:B:LEU:HD22	7	1.56
(1,3594)	1:115:B:LEU:HD12	1:75:B:TYR:HB3	7	1.56
(1,3593)	1:115:A:LEU:HD12	1:75:A:TYR:HB3	7	1.56
(3,2853)	1:119:A:MET:HE3	1:121:A:THR:HB	8	1.55
(3,2546)	1:102:B:ILE:HD11	1:128:B:LEU:HG	6	1.55
(3,848)	1:44:B:ASP:HA	1:46:B:ARG:HG2	9	1.55
(3,847)	1:44:A:ASP:HA	1:46:A:ARG:HG2	9	1.55
(3,692)	1:45:B:ILE:HG22	1:128:B:LEU:H	4	1.55
(3,691)	1:45:A:ILE:HG22	1:128:A:LEU:H	4	1.55
(3,182)	1:115:B:LEU:HD13	1:66:B:LEU:H	8	1.55
(3,181)	1:115:A:LEU:HD13	1:66:A:LEU:H	8	1.55
(1,5926)	1:112:B:TYR:HE2	1:113:B:GLU:HB3	4	1.55
(1,5419)	1:110:A:VAL:HG12	1:114:A:THR:HG22	7	1.55
(1,5404)	1:110:B:VAL:HG23	1:115:B:LEU:HB3	1	1.55
(1,5404)	1:110:B:VAL:HG23	1:115:B:LEU:HB3	10	1.55
(1,5403)	1:110:A:VAL:HG23	1:115:A:LEU:HB3	1	1.55
(1,5403)	1:110:A:VAL:HG23	1:115:A:LEU:HB3	10	1.55
(1,5386)	1:104:B:PHE:HZ	1:110:B:VAL:HG21	7	1.55
(1,5385)	1:104:A:PHE:HZ	1:110:A:VAL:HG21	7	1.55
(1,5313)	1:106:A:ALA:HB1	1:115:A:LEU:HD22	7	1.55
(1,4864)	1:98:B:LYS:HD3	1:125:B:ALA:HB3	10	1.55
(1,4444)	1:79:B:GLN:HB2	1:65:B:PHE:HB3	9	1.55
(1,4443)	1:79:A:GLN:HB2	1:65:A:PHE:HB3	9	1.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2871)	1:129:A:LYS:HB3	1:49:B:LEU:HB3	6	1.55
(1,2871)	1:129:A:LYS:HB3	1:49:B:LEU:HB3	9	1.55
(1,1120)	1:93:B:ARG:HG3	1:90:B:LEU:H	2	1.55
(1,1120)	1:93:B:ARG:HG3	1:90:B:LEU:H	5	1.55
(1,1120)	1:93:B:ARG:HG3	1:90:B:LEU:H	6	1.55
(1,1119)	1:93:A:ARG:HG3	1:90:A:LEU:H	2	1.55
(1,1119)	1:93:A:ARG:HG3	1:90:A:LEU:H	5	1.55
(1,1119)	1:93:A:ARG:HG3	1:90:A:LEU:H	6	1.55
(3,2926)	1:126:B:GLY:HA3	1:50:A:PRO:HG3	6	1.54
(3,2854)	1:119:B:MET:HE3	1:121:B:THR:HB	8	1.54
(3,2546)	1:102:B:ILE:HD11	1:128:B:LEU:HG	2	1.54
(3,1849)	1:136:A:GLU:HB2	1:140:A:LYS:HE3	1	1.54
(3,1403)	1:122:A:LEU:HA	1:49:B:LEU:HB3	7	1.54
(3,172)	1:46:B:ARG:HB2	1:64:A:VAL:H	8	1.54
(1,4863)	1:98:A:LYS:HD3	1:125:A:ALA:HB3	10	1.54
(1,2872)	1:129:B:LYS:HB3	1:49:A:LEU:HB3	1	1.54
(1,2872)	1:129:B:LYS:HB3	1:49:A:LEU:HB3	9	1.54
(1,2871)	1:129:A:LYS:HB3	1:49:B:LEU:HB3	1	1.54
(1,1120)	1:93:B:ARG:HG3	1:90:B:LEU:H	4	1.54
(1,1119)	1:93:A:ARG:HG3	1:90:A:LEU:H	1	1.54
(1,1119)	1:93:A:ARG:HG3	1:90:A:LEU:H	4	1.54
(1,934)	1:82:B:ASN:HD22	1:84:B:ASP:H	7	1.54
(1,933)	1:82:A:ASN:HD22	1:84:A:ASP:H	7	1.54
(3,3072)	1:104:B:PHE:HE1	1:129:B:LYS:HG3	10	1.53
(3,3071)	1:104:A:PHE:HE1	1:129:A:LYS:HG3	10	1.53
(3,2546)	1:102:B:ILE:HD12	1:128:B:LEU:HG	5	1.53
(3,2546)	1:102:B:ILE:HD11	1:128:B:LEU:HG	7	1.53
(3,2545)	1:102:A:ILE:HD11	1:128:A:LEU:HG	2	1.53
(3,2545)	1:102:A:ILE:HD12	1:128:A:LEU:HG	5	1.53
(3,2545)	1:102:A:ILE:HD11	1:128:A:LEU:HG	7	1.53
(3,1850)	1:136:B:GLU:HB2	1:140:B:LYS:HE3	1	1.53
(3,1668)	1:115:B:LEU:HD12	1:104:B:PHE:HA	2	1.53
(3,1667)	1:115:A:LEU:HD12	1:104:A:PHE:HA	2	1.53
(3,345)	1:106:A:ALA:HB3	1:114:A:THR:H	3	1.53
(3,182)	1:115:B:LEU:HD11	1:66:B:LEU:H	10	1.53
(1,5314)	1:106:B:ALA:HB2	1:115:B:LEU:HD23	4	1.53
(1,5313)	1:106:A:ALA:HB2	1:115:A:LEU:HD23	4	1.53
(1,4854)	1:98:B:LYS:HD3	1:51:A:ALA:HA	5	1.53
(1,2871)	1:129:A:LYS:HB3	1:49:B:LEU:HB3	10	1.53
(1,1120)	1:93:B:ARG:HG3	1:90:B:LEU:H	1	1.53
(3,912)	1:45:B:ILE:HD13	1:46:B:ARG:HD3	6	1.52
(3,911)	1:45:A:ILE:HD13	1:46:A:ARG:HD3	6	1.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,346)	1:106:B:ALA:HB3	1:114:B:THR:H	3	1.52
(3,345)	1:106:A:ALA:HB2	1:114:A:THR:H	8	1.52
(3,181)	1:115:A:LEU:HD11	1:66:A:LEU:H	10	1.52
(3,159)	1:58:A:PRO:HB2	1:62:A:LYS:H	3	1.52
(1,5798)	1:134:B:GLY:HA2	1:137:B:GLY:HA3	5	1.52
(1,5797)	1:134:A:GLY:HA2	1:137:A:GLY:HA3	5	1.52
(1,5404)	1:110:B:VAL:HG22	1:115:B:LEU:HB3	7	1.52
(1,5403)	1:110:A:VAL:HG22	1:115:A:LEU:HB3	7	1.52
(1,4122)	1:74:B:LEU:HB2	1:110:B:VAL:HG13	4	1.52
(1,4121)	1:74:A:LEU:HB2	1:110:A:VAL:HG13	4	1.52
(1,3580)	1:115:B:LEU:HD13	1:75:B:TYR:HA	6	1.52
(1,3579)	1:115:A:LEU:HD13	1:75:A:TYR:HA	6	1.52
(1,3024)	1:57:B:GLN:HG2	1:60:B:PRO:HG2	5	1.52
(3,3072)	1:104:B:PHE:HE1	1:129:B:LYS:HG3	2	1.51
(3,3071)	1:104:A:PHE:HE1	1:129:A:LYS:HG3	2	1.51
(3,2926)	1:126:B:GLY:HA3	1:50:A:PRO:HG3	9	1.51
(3,2925)	1:126:A:GLY:HA3	1:50:B:PRO:HG3	9	1.51
(3,2870)	1:87:B:THR:HG23	1:98:B:LYS:HE2	10	1.51
(3,2869)	1:87:A:THR:HG23	1:98:A:LYS:HE2	10	1.51
(3,2176)	1:108:B:LYS:HA	1:139:B:ALA:HB3	9	1.51
(3,2175)	1:108:A:LYS:HA	1:139:A:ALA:HB3	9	1.51
(3,1760)	1:69:B:LYS:HE3	1:73:B:GLN:HB2	6	1.51
(3,1759)	1:69:A:LYS:HE3	1:73:A:GLN:HB2	6	1.51
(3,1189)	1:108:A:LYS:HG3	1:114:A:THR:HG21	4	1.51
(3,847)	1:44:A:ASP:HA	1:46:A:ARG:HG2	4	1.51
(3,815)	1:88:A:SER:HB3	1:79:A:GLN:HE22	7	1.51
(3,346)	1:106:B:ALA:HB2	1:114:B:THR:H	8	1.51
(3,160)	1:58:B:PRO:HB2	1:62:B:LYS:H	3	1.51
(1,5386)	1:104:B:PHE:HZ	1:110:B:VAL:HG22	2	1.51
(1,5386)	1:104:B:PHE:HZ	1:110:B:VAL:HG22	5	1.51
(1,5385)	1:104:A:PHE:HZ	1:110:A:VAL:HG22	2	1.51
(1,5385)	1:104:A:PHE:HZ	1:110:A:VAL:HG22	5	1.51
(1,4363)	1:82:A:ASN:HB3	1:85:A:GLN:HG2	4	1.51
(1,4114)	1:74:B:LEU:HA	1:115:B:LEU:HD12	7	1.51
(1,4113)	1:74:A:LEU:HA	1:115:A:LEU:HD12	7	1.51
(1,3948)	1:91:B:ASP:HB2	1:96:B:ALA:HB2	6	1.51
(1,3580)	1:115:B:LEU:HD13	1:75:B:TYR:HA	3	1.51
(1,3579)	1:115:A:LEU:HD13	1:75:A:TYR:HA	3	1.51
(1,3023)	1:57:A:GLN:HG2	1:60:A:PRO:HG2	5	1.51
(1,933)	1:82:A:ASN:HD22	1:84:A:ASP:H	4	1.51
(3,2836)	1:116:B:MET:HE2	1:120:B:ASP:HA	10	1.5
(3,2835)	1:116:A:MET:HE2	1:120:A:ASP:HA	10	1.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,1190)	1:108:B:LYS:HG3	1:114:B:THR:HG21	4	1.5
(3,848)	1:44:B:ASP:HA	1:46:B:ARG:HG2	4	1.5
(3,582)	1:72:B:LYS:HD3	1:116:B:MET:H	9	1.5
(3,581)	1:72:A:LYS:HD3	1:116:A:MET:H	9	1.5
(1,5800)	1:134:B:GLY:HA2	1:137:B:GLY:HA2	7	1.5
(1,5799)	1:134:A:GLY:HA2	1:137:A:GLY:HA2	7	1.5
(1,5404)	1:110:B:VAL:HG23	1:115:B:LEU:HB3	5	1.5
(1,4364)	1:82:B:ASN:HB3	1:85:B:GLN:HG2	4	1.5
(1,3947)	1:91:A:ASP:HB2	1:96:A:ALA:HB2	6	1.5
(1,3240)	1:99:B:GLU:HG2	1:49:A:LEU:HB3	5	1.5
(1,3240)	1:99:B:GLU:HG2	1:49:A:LEU:HB3	6	1.5
(1,3239)	1:99:A:GLU:HG2	1:49:B:LEU:HB3	5	1.5
(1,2872)	1:129:B:LYS:HB3	1:49:A:LEU:HB3	10	1.5
(1,1086)	1:89:B:VAL:HG21	1:89:B:VAL:H	1	1.5
(1,1085)	1:89:A:VAL:HG21	1:89:A:VAL:H	1	1.5
(3,2846)	1:51:B:ALA:HB2	1:127:A:TYR:HD1	10	1.49
(3,2845)	1:51:A:ALA:HB1	1:127:B:TYR:HD2	6	1.49
(3,2546)	1:102:B:ILE:HD13	1:128:B:LEU:HG	3	1.49
(3,2545)	1:102:A:ILE:HD13	1:128:A:LEU:HG	3	1.49
(3,1522)	1:45:B:ILE:HG23	1:129:B:LYS:HB2	3	1.49
(3,1521)	1:45:A:ILE:HG23	1:129:A:LYS:HB2	3	1.49
(3,880)	1:69:B:LYS:HB2	1:140:B:LYS:HE3	2	1.49
(3,879)	1:69:A:LYS:HB2	1:140:A:LYS:HE3	2	1.49
(3,655)	1:45:A:ILE:HD13	1:125:A:ALA:H	7	1.49
(3,352)	1:98:B:LYS:HG2	1:90:B:LEU:H	2	1.49
(3,351)	1:98:A:LYS:HG2	1:90:A:LEU:H	2	1.49
(3,346)	1:106:B:ALA:HB1	1:114:B:THR:H	9	1.49
(3,345)	1:106:A:ALA:HB1	1:114:A:THR:H	9	1.49
(1,5809)	1:134:A:GLY:HA3	1:116:B:MET:HE1	3	1.49
(1,5404)	1:110:B:VAL:HG21	1:115:B:LEU:HB3	3	1.49
(1,5403)	1:110:A:VAL:HG21	1:115:A:LEU:HB3	3	1.49
(1,5403)	1:110:A:VAL:HG23	1:115:A:LEU:HB3	5	1.49
(1,4856)	1:98:B:LYS:HD3	1:126:B:GLY:HA2	10	1.49
(1,4855)	1:98:A:LYS:HD3	1:126:A:GLY:HA2	10	1.49
(1,4854)	1:98:B:LYS:HD3	1:51:A:ALA:HA	6	1.49
(1,4322)	1:127:B:TYR:HA	1:49:A:LEU:HB3	4	1.49
(1,2820)	1:54:B:ALA:HB1	1:44:A:ASP:HB2	7	1.49
(1,934)	1:82:B:ASN:HD22	1:84:B:ASP:H	4	1.49
(3,2925)	1:126:A:GLY:HA3	1:50:B:PRO:HG3	6	1.48
(3,2534)	1:102:B:ILE:HG21	1:133:B:VAL:HB	1	1.48
(3,2533)	1:102:A:ILE:HG21	1:133:A:VAL:HB	1	1.48
(3,1823)	1:129:A:LYS:HD2	1:45:A:ILE:HG23	3	1.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,1121)	1:54:A:ALA:HB2	1:57:A:GLN:HG2	5	1.48
(3,912)	1:45:B:ILE:HD11	1:46:B:ARG:HD3	1	1.48
(3,911)	1:45:A:ILE:HD11	1:46:A:ARG:HD3	1	1.48
(3,816)	1:88:B:SER:HB3	1:79:B:GLN:HE22	7	1.48
(3,656)	1:45:B:ILE:HD13	1:125:B:ALA:H	7	1.48
(3,304)	1:124:B:LYS:HG2	1:86:B:LEU:H	7	1.48
(3,303)	1:124:A:LYS:HG2	1:86:A:LEU:H	7	1.48
(1,5626)	1:87:B:THR:HG21	1:126:B:GLY:HA3	2	1.48
(1,5625)	1:87:A:THR:HG21	1:126:A:GLY:HA3	2	1.48
(1,4321)	1:127:A:TYR:HA	1:49:B:LEU:HB3	4	1.48
(1,3580)	1:115:B:LEU:HD12	1:75:B:TYR:HA	7	1.48
(1,3579)	1:115:A:LEU:HD12	1:75:A:TYR:HA	7	1.48
(1,2819)	1:54:A:ALA:HB1	1:44:B:ASP:HB2	7	1.48
(3,3072)	1:104:B:PHE:HE2	1:129:B:LYS:HG3	7	1.47
(3,3071)	1:104:A:PHE:HE2	1:129:A:LYS:HG3	7	1.47
(3,1824)	1:129:B:LYS:HD2	1:45:B:ILE:HG23	3	1.47
(3,1441)	1:61:A:GLU:HG2	1:62:A:LYS:HB3	1	1.47
(3,1122)	1:54:B:ALA:HB1	1:57:B:GLN:HG2	1	1.47
(3,1122)	1:54:B:ALA:HB2	1:57:B:GLN:HG2	5	1.47
(3,1080)	1:56:B:PRO:HG3	1:50:B:PRO:HD2	10	1.47
(3,1079)	1:56:A:PRO:HG3	1:50:A:PRO:HD2	10	1.47
(3,552)	1:90:B:LEU:HB3	1:103:B:PHE:H	8	1.47
(3,551)	1:90:A:LEU:HB3	1:103:A:PHE:H	8	1.47
(1,5810)	1:134:B:GLY:HA3	1:116:A:MET:HE1	3	1.47
(1,5312)	1:106:B:ALA:HB2	1:114:B:THR:HG23	5	1.47
(1,4711)	1:92:A:GLN:HG2	1:79:A:GLN:HB3	2	1.47
(3,2846)	1:51:B:ALA:HB1	1:127:A:TYR:HD2	6	1.46
(3,2534)	1:102:B:ILE:HG23	1:133:B:VAL:HB	4	1.46
(3,2533)	1:102:A:ILE:HG23	1:133:A:VAL:HB	4	1.46
(3,2458)	1:100:B:THR:HG21	1:66:B:LEU:HB3	5	1.46
(3,2457)	1:100:A:THR:HG21	1:66:A:LEU:HB3	5	1.46
(3,1442)	1:61:B:GLU:HG2	1:62:B:LYS:HB3	1	1.46
(3,1190)	1:108:B:LYS:HG3	1:114:B:THR:HG22	3	1.46
(3,1121)	1:54:A:ALA:HB1	1:57:A:GLN:HG2	1	1.46
(3,854)	1:88:B:SER:HA	1:124:B:LYS:HE3	5	1.46
(3,853)	1:88:A:SER:HA	1:124:A:LYS:HE3	5	1.46
(3,694)	1:45:B:ILE:HG23	1:128:B:LEU:H	5	1.46
(3,693)	1:45:A:ILE:HG23	1:128:A:LEU:H	5	1.46
(3,692)	1:45:B:ILE:HG23	1:128:B:LEU:H	1	1.46
(3,691)	1:45:A:ILE:HG23	1:128:A:LEU:H	1	1.46
(3,160)	1:129:B:LYS:HB3	1:62:B:LYS:H	8	1.46
(3,159)	1:129:A:LYS:HB3	1:62:A:LYS:H	8	1.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5558)	1:116:B:MET:HE2	1:119:B:MET:HE1	2	1.46
(1,5557)	1:116:A:MET:HE2	1:119:A:MET:HE1	2	1.46
(1,5504)	1:114:B:THR:HG21	1:104:B:PHE:HZ	6	1.46
(1,5504)	1:114:B:THR:HG21	1:104:B:PHE:HZ	7	1.46
(1,5503)	1:114:A:THR:HG21	1:104:A:PHE:HZ	6	1.46
(1,5503)	1:114:A:THR:HG21	1:104:A:PHE:HZ	7	1.46
(1,5311)	1:106:A:ALA:HB2	1:114:A:THR:HG21	1	1.46
(1,5311)	1:106:A:ALA:HB2	1:114:A:THR:HG23	5	1.46
(1,4712)	1:92:B:GLN:HG2	1:79:B:GLN:HB3	2	1.46
(1,3590)	1:115:B:LEU:HD11	1:112:B:TYR:HB3	8	1.46
(1,3589)	1:115:A:LEU:HD11	1:112:A:TYR:HB3	8	1.46
(3,2938)	1:127:B:TYR:HB2	1:45:B:ILE:HD13	5	1.45
(3,2937)	1:127:A:TYR:HB2	1:45:A:ILE:HD13	5	1.45
(3,2836)	1:116:B:MET:HE2	1:120:B:ASP:HA	1	1.45
(3,2835)	1:116:A:MET:HE2	1:120:A:ASP:HA	1	1.45
(3,2006)	1:81:B:VAL:HB	1:66:B:LEU:HG	4	1.45
(3,2006)	1:81:B:VAL:HB	1:93:B:ARG:HG3	10	1.45
(3,2005)	1:81:A:VAL:HB	1:93:A:ARG:HG3	10	1.45
(3,1668)	1:67:B:SER:HA	1:115:B:LEU:HD13	7	1.45
(3,1667)	1:67:A:SER:HA	1:115:A:LEU:HD13	7	1.45
(3,1189)	1:108:A:LYS:HG3	1:114:A:THR:HG22	3	1.45
(3,848)	1:44:B:ASP:HA	1:123:B:ARG:HG3	6	1.45
(3,847)	1:44:A:ASP:HA	1:123:A:ARG:HG3	6	1.45
(3,352)	1:98:B:LYS:HG2	1:90:B:LEU:H	1	1.45
(1,5386)	1:104:B:PHE:HZ	1:110:B:VAL:HG22	8	1.45
(1,5385)	1:104:A:PHE:HZ	1:110:A:VAL:HG22	8	1.45
(1,5312)	1:106:B:ALA:HB2	1:114:B:THR:HG21	1	1.45
(1,4444)	1:79:B:GLN:HB2	1:65:B:PHE:HB3	3	1.45
(1,4443)	1:79:A:GLN:HB2	1:65:A:PHE:HB3	3	1.45
(1,4321)	1:127:A:TYR:HA	1:49:B:LEU:HB3	8	1.45
(1,4321)	1:127:A:TYR:HA	1:49:B:LEU:HB3	10	1.45
(1,4122)	1:74:B:LEU:HB2	1:110:B:VAL:HG11	9	1.45
(1,4122)	1:74:B:LEU:HB2	1:110:B:VAL:HG12	10	1.45
(1,2871)	1:129:A:LYS:HB3	1:49:B:LEU:HB3	5	1.45
(1,2819)	1:54:A:ALA:HB1	1:44:B:ASP:HB2	5	1.45
(3,2845)	1:51:A:ALA:HB2	1:127:B:TYR:HD1	10	1.44
(3,2642)	1:115:B:LEU:HD13	1:116:B:MET:HG2	10	1.44
(3,2641)	1:115:A:LEU:HD13	1:116:A:MET:HG2	10	1.44
(3,2534)	1:102:B:ILE:HG21	1:133:B:VAL:HB	10	1.44
(3,2533)	1:102:A:ILE:HG21	1:133:A:VAL:HB	10	1.44
(3,2005)	1:81:A:VAL:HB	1:66:A:LEU:HG	4	1.44
(3,1830)	1:58:B:PRO:HG2	1:55:B:LYS:HE3	6	1.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,1829)	1:58:A:PRO:HG2	1:55:A:LYS:HE3	6	1.44
(3,1442)	1:61:B:GLU:HG2	1:62:B:LYS:HB3	8	1.44
(3,551)	1:90:A:LEU:HB3	1:103:A:PHE:H	9	1.44
(3,351)	1:98:A:LYS:HG2	1:90:A:LEU:H	1	1.44
(3,304)	1:124:B:LYS:HG2	1:86:B:LEU:H	8	1.44
(3,303)	1:124:A:LYS:HG2	1:86:A:LEU:H	8	1.44
(1,5798)	1:134:B:GLY:HA2	1:137:B:GLY:HA3	6	1.44
(1,5797)	1:134:A:GLY:HA2	1:137:A:GLY:HA3	6	1.44
(1,5797)	1:134:A:GLY:HA2	1:137:A:GLY:HA3	7	1.44
(1,5625)	1:87:A:THR:HG21	1:126:A:GLY:HA3	7	1.44
(1,4854)	1:98:B:LYS:HD3	1:51:A:ALA:HA	7	1.44
(1,4853)	1:98:A:LYS:HD3	1:51:B:ALA:HA	10	1.44
(1,4121)	1:74:A:LEU:HB2	1:110:A:VAL:HG11	9	1.44
(1,4121)	1:74:A:LEU:HB2	1:110:A:VAL:HG12	10	1.44
(1,4114)	1:74:B:LEU:HA	1:115:B:LEU:HD12	8	1.44
(1,4113)	1:74:A:LEU:HA	1:115:A:LEU:HD12	8	1.44
(1,3948)	1:91:B:ASP:HB2	1:96:B:ALA:HB3	8	1.44
(1,3947)	1:91:A:ASP:HB2	1:96:A:ALA:HB3	8	1.44
(1,3239)	1:99:A:GLU:HG2	1:49:B:LEU:HB3	6	1.44
(1,2872)	1:129:B:LYS:HB3	1:49:A:LEU:HB3	3	1.44
(1,2872)	1:129:B:LYS:HB3	1:49:A:LEU:HB3	4	1.44
(1,2871)	1:129:A:LYS:HB3	1:49:B:LEU:HB3	2	1.44
(1,2871)	1:129:A:LYS:HB3	1:49:B:LEU:HB3	8	1.44
(1,2820)	1:54:B:ALA:HB1	1:44:A:ASP:HB2	1	1.44
(1,2819)	1:54:A:ALA:HB1	1:44:B:ASP:HB2	1	1.44
(3,2334)	1:98:B:LYS:HG2	1:101:B:THR:HA	4	1.43
(3,1955)	1:79:A:GLN:HG2	1:91:A:ASP:HB3	9	1.43
(3,1286)	1:57:B:GLN:HG3	1:129:B:LYS:HD2	2	1.43
(3,1285)	1:57:A:GLN:HG3	1:129:A:LYS:HD2	2	1.43
(3,692)	1:45:B:ILE:HG23	1:128:B:LEU:H	3	1.43
(3,691)	1:45:A:ILE:HG23	1:128:A:LEU:H	3	1.43
(3,582)	1:72:B:LYS:HD3	1:116:B:MET:H	6	1.43
(3,552)	1:90:B:LEU:HB3	1:103:B:PHE:H	1	1.43
(3,552)	1:90:B:LEU:HB3	1:103:B:PHE:H	9	1.43
(3,552)	1:90:B:LEU:HB3	1:103:B:PHE:H	10	1.43
(3,551)	1:90:A:LEU:HB3	1:103:A:PHE:H	1	1.43
(3,551)	1:90:A:LEU:HB3	1:103:A:PHE:H	10	1.43
(1,5798)	1:134:B:GLY:HA2	1:137:B:GLY:HA3	7	1.43
(1,5626)	1:87:B:THR:HG23	1:126:B:GLY:HA3	3	1.43
(1,5626)	1:87:B:THR:HG21	1:126:B:GLY:HA3	7	1.43
(1,5558)	1:116:B:MET:HE3	1:119:B:MET:HE1	7	1.43
(1,5557)	1:116:A:MET:HE3	1:119:A:MET:HE1	7	1.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5404)	1:110:B:VAL:HG23	1:115:B:LEU:HB3	8	1.43
(1,5403)	1:110:A:VAL:HG23	1:115:A:LEU:HB3	8	1.43
(1,5313)	1:106:A:ALA:HB3	1:115:A:LEU:HD22	1	1.43
(1,4122)	1:74:B:LEU:HB2	1:110:B:VAL:HG11	8	1.43
(1,4121)	1:74:A:LEU:HB2	1:110:A:VAL:HG11	8	1.43
(1,4114)	1:74:B:LEU:HA	1:115:B:LEU:HD13	6	1.43
(1,4114)	1:74:B:LEU:HA	1:115:B:LEU:HD13	10	1.43
(1,4113)	1:74:A:LEU:HA	1:115:A:LEU:HD13	6	1.43
(1,4113)	1:74:A:LEU:HA	1:115:A:LEU:HD13	10	1.43
(1,2872)	1:129:B:LYS:HB3	1:49:A:LEU:HB3	5	1.43
(1,2871)	1:129:A:LYS:HB3	1:49:B:LEU:HB3	3	1.43
(1,2871)	1:129:A:LYS:HB3	1:49:B:LEU:HB3	4	1.43
(3,2873)	1:87:A:THR:HG21	1:124:A:LYS:HB2	10	1.42
(3,2333)	1:98:A:LYS:HG2	1:101:A:THR:HA	4	1.42
(3,2006)	1:81:B:VAL:HB	1:66:B:LEU:HG	6	1.42
(3,2005)	1:81:A:VAL:HB	1:66:A:LEU:HG	6	1.42
(3,1956)	1:79:B:GLN:HG2	1:91:B:ASP:HB3	9	1.42
(3,1850)	1:85:B:GLN:HB2	1:124:B:LYS:HE2	7	1.42
(3,1850)	1:85:B:GLN:HB2	1:124:B:LYS:HE2	9	1.42
(3,1849)	1:85:A:GLN:HB2	1:124:A:LYS:HE2	7	1.42
(3,1849)	1:85:A:GLN:HB2	1:124:A:LYS:HE2	9	1.42
(3,1823)	1:129:A:LYS:HD2	1:45:A:ILE:HG22	8	1.42
(3,1668)	1:67:B:SER:HA	1:115:B:LEU:HD11	1	1.42
(3,1667)	1:67:A:SER:HA	1:115:A:LEU:HD11	1	1.42
(3,1441)	1:61:A:GLU:HG2	1:62:A:LYS:HB3	8	1.42
(3,581)	1:49:A:LEU:HG	1:116:B:MET:H	6	1.42
(3,552)	1:90:B:LEU:HB3	1:103:B:PHE:H	4	1.42
(3,551)	1:90:A:LEU:HB3	1:103:A:PHE:H	4	1.42
(3,352)	1:98:B:LYS:HG2	1:90:B:LEU:H	7	1.42
(3,351)	1:98:A:LYS:HG2	1:90:A:LEU:H	7	1.42
(1,5625)	1:87:A:THR:HG23	1:126:A:GLY:HA3	3	1.42
(1,5314)	1:106:B:ALA:HB3	1:115:B:LEU:HD22	1	1.42
(1,4322)	1:127:B:TYR:HA	1:49:A:LEU:HB3	10	1.42
(1,4122)	1:74:B:LEU:HB2	1:110:B:VAL:HG13	7	1.42
(1,4121)	1:74:A:LEU:HB2	1:110:A:VAL:HG13	7	1.42
(1,2872)	1:129:B:LYS:HB3	1:49:A:LEU:HB3	7	1.42
(1,2872)	1:129:B:LYS:HB3	1:49:A:LEU:HB3	8	1.42
(1,2028)	1:98:B:LYS:HD3	1:125:B:ALA:H	1	1.42
(1,2028)	1:98:B:LYS:HD3	1:125:B:ALA:H	7	1.42
(1,2027)	1:98:A:LYS:HD3	1:125:A:ALA:H	1	1.42
(1,2027)	1:98:A:LYS:HD3	1:125:A:ALA:H	7	1.42
(1,1120)	1:93:B:ARG:HG3	1:90:B:LEU:H	8	1.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1119)	1:93:A:ARG:HG3	1:90:A:LEU:H	8	1.42
(3,3072)	1:104:B:PHE:HE1	1:129:B:LYS:HG3	4	1.41
(3,3071)	1:104:A:PHE:HE1	1:129:A:LYS:HG3	4	1.41
(3,2874)	1:87:B:THR:HG21	1:124:B:LYS:HB2	10	1.41
(3,2546)	1:102:B:ILE:HD11	1:128:B:LEU:HG	9	1.41
(3,2545)	1:102:A:ILE:HD11	1:128:A:LEU:HG	9	1.41
(3,2534)	1:102:B:ILE:HG21	1:119:B:MET:HB2	3	1.41
(3,2533)	1:102:A:ILE:HG21	1:119:A:MET:HB2	3	1.41
(3,2220)	1:93:B:ARG:HD3	1:66:B:LEU:HB3	9	1.41
(3,1824)	1:129:B:LYS:HD2	1:45:B:ILE:HG22	8	1.41
(3,1608)	1:65:B:PHE:HB2	1:60:B:PRO:HG2	6	1.41
(3,1607)	1:65:A:PHE:HB2	1:60:A:PRO:HG2	6	1.41
(3,1278)	1:57:B:GLN:HG3	1:50:B:PRO:HD2	9	1.41
(3,848)	1:44:B:ASP:HA	1:46:B:ARG:HG2	1	1.41
(3,847)	1:44:A:ASP:HA	1:46:A:ARG:HG2	1	1.41
(3,182)	1:115:B:LEU:HD12	1:66:B:LEU:H	9	1.41
(3,181)	1:115:A:LEU:HD12	1:66:A:LEU:H	9	1.41
(1,5626)	1:87:B:THR:HG23	1:126:B:GLY:HA3	10	1.41
(1,5625)	1:87:A:THR:HG23	1:126:A:GLY:HA3	10	1.41
(1,5552)	1:116:B:MET:HE2	1:113:B:GLU:HA	8	1.41
(1,5551)	1:116:A:MET:HE2	1:113:A:GLU:HA	8	1.41
(1,5386)	1:104:B:PHE:HZ	1:110:B:VAL:HG22	10	1.41
(1,5385)	1:104:A:PHE:HZ	1:110:A:VAL:HG22	10	1.41
(1,4853)	1:98:A:LYS:HD3	1:51:B:ALA:HA	6	1.41
(1,4853)	1:98:A:LYS:HD3	1:51:B:ALA:HA	7	1.41
(1,4322)	1:127:B:TYR:HA	1:49:A:LEU:HB3	3	1.41
(1,4322)	1:127:B:TYR:HA	1:49:A:LEU:HB3	8	1.41
(1,4122)	1:74:B:LEU:HB2	1:110:B:VAL:HG12	1	1.41
(1,4121)	1:74:A:LEU:HB2	1:110:A:VAL:HG12	1	1.41
(1,2872)	1:129:B:LYS:HB3	1:49:A:LEU:HB3	2	1.41
(1,2871)	1:129:A:LYS:HB3	1:49:B:LEU:HB3	7	1.41
(1,2820)	1:54:B:ALA:HB1	1:44:A:ASP:HB2	5	1.41
(1,934)	1:82:B:ASN:HD22	1:84:B:ASP:H	5	1.41
(3,2219)	1:93:A:ARG:HD3	1:66:A:LEU:HB3	9	1.4
(3,1668)	1:67:B:SER:HA	1:115:B:LEU:HD11	3	1.4
(3,1668)	1:115:B:LEU:HD11	1:104:B:PHE:HA	6	1.4
(3,1667)	1:67:A:SER:HA	1:115:A:LEU:HD11	3	1.4
(3,1667)	1:115:A:LEU:HD11	1:104:A:PHE:HA	6	1.4
(3,1667)	1:67:A:SER:HA	1:115:A:LEU:HD12	9	1.4
(3,1607)	1:65:A:PHE:HB2	1:60:A:PRO:HG2	7	1.4
(3,1441)	1:61:A:GLU:HG2	1:62:A:LYS:HB3	3	1.4
(3,1277)	1:57:A:GLN:HG3	1:50:A:PRO:HD2	9	1.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,692)	1:45:B:ILE:HG22	1:128:B:LEU:H	8	1.4
(3,691)	1:45:A:ILE:HG22	1:128:A:LEU:H	8	1.4
(1,5314)	1:106:B:ALA:HB1	1:115:B:LEU:HD21	3	1.4
(1,5313)	1:106:A:ALA:HB1	1:115:A:LEU:HD21	3	1.4
(1,3352)	1:124:B:LYS:HG2	1:84:B:ASP:HB3	10	1.4
(1,3351)	1:124:A:LYS:HG2	1:84:A:ASP:HB3	10	1.4
(1,933)	1:82:A:ASN:HD22	1:84:A:ASP:H	5	1.4
(3,2904)	1:87:B:THR:HG21	1:124:B:LYS:HB2	3	1.39
(3,2904)	1:87:B:THR:HG22	1:124:B:LYS:HB2	7	1.39
(3,2903)	1:87:A:THR:HG21	1:124:A:LYS:HB2	3	1.39
(3,2903)	1:87:A:THR:HG22	1:124:A:LYS:HB2	7	1.39
(3,2874)	1:87:B:THR:HG21	1:124:B:LYS:HB2	3	1.39
(3,2874)	1:87:B:THR:HG22	1:124:B:LYS:HB2	7	1.39
(3,2873)	1:87:A:THR:HG21	1:124:A:LYS:HB2	3	1.39
(3,2873)	1:87:A:THR:HG22	1:124:A:LYS:HB2	7	1.39
(3,2869)	1:87:A:THR:HG21	1:98:A:LYS:HE2	9	1.39
(3,1668)	1:67:B:SER:HA	1:115:B:LEU:HD12	9	1.39
(3,1608)	1:65:B:PHE:HB2	1:60:B:PRO:HG2	7	1.39
(3,1522)	1:45:B:ILE:HG22	1:129:B:LYS:HB2	10	1.39
(3,1521)	1:45:A:ILE:HG22	1:129:A:LYS:HB2	10	1.39
(3,1442)	1:61:B:GLU:HG2	1:62:B:LYS:HB3	3	1.39
(3,346)	1:106:B:ALA:HB1	1:114:B:THR:H	2	1.39
(3,345)	1:106:A:ALA:HB1	1:114:A:THR:H	2	1.39
(3,304)	1:124:B:LYS:HG2	1:86:B:LEU:H	3	1.39
(3,304)	1:124:B:LYS:HG2	1:86:B:LEU:H	4	1.39
(3,303)	1:124:A:LYS:HG2	1:86:A:LEU:H	3	1.39
(3,303)	1:124:A:LYS:HG2	1:86:A:LEU:H	4	1.39
(1,5926)	1:112:B:TYR:HE1	1:113:B:GLU:HB3	9	1.39
(1,5925)	1:112:A:TYR:HE1	1:113:A:GLU:HB3	9	1.39
(1,5311)	1:106:A:ALA:HB1	1:114:A:THR:HG23	4	1.39
(1,4711)	1:92:A:GLN:HG2	1:79:A:GLN:HB3	6	1.39
(1,4321)	1:127:A:TYR:HA	1:49:B:LEU:HB3	3	1.39
(1,4321)	1:127:A:TYR:HA	1:49:B:LEU:HB3	5	1.39
(1,3947)	1:91:A:ASP:HB2	1:96:A:ALA:HB2	3	1.39
(1,3580)	1:115:B:LEU:HD13	1:75:B:TYR:HA	10	1.39
(1,934)	1:82:B:ASN:HD22	1:84:B:ASP:H	10	1.39
(1,933)	1:82:A:ASN:HD22	1:84:A:ASP:H	10	1.39
(3,2870)	1:87:B:THR:HG21	1:98:B:LYS:HE2	9	1.38
(3,2682)	1:108:B:LYS:HB2	1:112:B:TYR:HB3	2	1.38
(3,2681)	1:108:A:LYS:HB2	1:112:A:TYR:HB3	2	1.38
(3,2334)	1:98:B:LYS:HG2	1:101:B:THR:HA	1	1.38
(3,2333)	1:98:A:LYS:HG2	1:101:A:THR:HA	1	1.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,2239)	1:94:A:THR:HG23	1:129:A:LYS:HE2	6	1.38
(3,1291)	1:119:A:MET:HB2	1:121:A:THR:HA	8	1.38
(1,5800)	1:134:B:GLY:HA2	1:137:B:GLY:HA2	9	1.38
(1,5799)	1:134:A:GLY:HA2	1:137:A:GLY:HA2	9	1.38
(1,5625)	1:87:A:THR:HG21	1:126:A:GLY:HA3	8	1.38
(1,5312)	1:106:B:ALA:HB3	1:114:B:THR:HG21	7	1.38
(1,5311)	1:106:A:ALA:HB3	1:114:A:THR:HG21	7	1.38
(1,4712)	1:92:B:GLN:HG2	1:79:B:GLN:HB3	6	1.38
(1,4122)	1:74:B:LEU:HB2	1:110:B:VAL:HG13	2	1.38
(1,4121)	1:74:A:LEU:HB2	1:110:A:VAL:HG13	2	1.38
(1,3948)	1:91:B:ASP:HB2	1:96:B:ALA:HB2	3	1.38
(1,3594)	1:115:B:LEU:HD13	1:75:B:TYR:HB3	3	1.38
(1,3593)	1:115:A:LEU:HD13	1:75:A:TYR:HB3	3	1.38
(1,3590)	1:115:B:LEU:HD12	1:112:B:TYR:HB3	3	1.38
(1,3589)	1:115:A:LEU:HD12	1:112:A:TYR:HB3	3	1.38
(1,3580)	1:115:B:LEU:HD12	1:75:B:TYR:HA	8	1.38
(1,3579)	1:115:A:LEU:HD12	1:75:A:TYR:HA	8	1.38
(1,3579)	1:115:A:LEU:HD13	1:75:A:TYR:HA	10	1.38
(3,2874)	1:87:B:THR:HG21	1:124:B:LYS:HB2	4	1.37
(3,2873)	1:87:A:THR:HG21	1:124:A:LYS:HB2	4	1.37
(3,2845)	1:51:A:ALA:HB3	1:127:B:TYR:HD1	7	1.37
(3,2240)	1:94:B:THR:HG23	1:129:B:LYS:HE2	6	1.37
(3,1850)	1:85:B:GLN:HB2	1:124:B:LYS:HE2	3	1.37
(3,1849)	1:85:A:GLN:HB2	1:124:A:LYS:HE2	3	1.37
(3,1829)	1:58:A:PRO:HG2	1:55:A:LYS:HE2	7	1.37
(3,1403)	1:122:A:LEU:HA	1:49:B:LEU:HB3	5	1.37
(3,1292)	1:119:B:MET:HB2	1:121:B:THR:HA	8	1.37
(3,1122)	1:54:B:ALA:HB2	1:57:B:GLN:HG2	10	1.37
(3,848)	1:44:B:ASP:HA	1:123:B:ARG:HG3	7	1.37
(3,847)	1:44:A:ASP:HA	1:123:A:ARG:HG3	7	1.37
(3,692)	1:45:B:ILE:HG22	1:128:B:LEU:H	6	1.37
(3,691)	1:45:A:ILE:HG21	1:128:A:LEU:H	2	1.37
(3,691)	1:45:A:ILE:HG22	1:128:A:LEU:H	6	1.37
(3,581)	1:72:A:LYS:HD3	1:116:A:MET:H	7	1.37
(3,575)	1:115:A:LEU:HD22	1:115:A:LEU:H	7	1.37
(1,5626)	1:87:B:THR:HG23	1:126:B:GLY:HA3	4	1.37
(1,5626)	1:87:B:THR:HG21	1:126:B:GLY:HA3	5	1.37
(1,5626)	1:87:B:THR:HG21	1:126:B:GLY:HA3	8	1.37
(1,5626)	1:87:B:THR:HG21	1:126:B:GLY:HA3	9	1.37
(1,5625)	1:87:A:THR:HG23	1:126:A:GLY:HA3	4	1.37
(1,5625)	1:87:A:THR:HG21	1:126:A:GLY:HA3	5	1.37
(1,5625)	1:87:A:THR:HG21	1:126:A:GLY:HA3	9	1.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5312)	1:106:B:ALA:HB1	1:114:B:THR:HG23	4	1.37
(1,4854)	1:98:B:LYS:HD3	1:51:A:ALA:HA	10	1.37
(1,4322)	1:127:B:TYR:HA	1:49:A:LEU:HB3	5	1.37
(1,4000)	1:72:B:LYS:HG2	1:114:B:THR:HG23	2	1.37
(1,3999)	1:72:A:LYS:HG2	1:114:A:THR:HG23	2	1.37
(1,3580)	1:115:B:LEU:HD13	1:75:B:TYR:HA	1	1.37
(1,3579)	1:115:A:LEU:HD13	1:75:A:TYR:HA	1	1.37
(1,3239)	1:99:A:GLU:HG2	1:49:B:LEU:HB3	9	1.37
(1,2266)	1:105:B:GLN:HA	1:138:B:ALA:H	2	1.37
(1,2265)	1:105:A:GLN:HA	1:138:A:ALA:H	2	1.37
(1,1860)	1:110:B:VAL:HG22	1:118:B:VAL:H	1	1.37
(1,1859)	1:110:A:VAL:HG22	1:118:A:VAL:H	1	1.37
(3,3100)	1:127:B:TYR:HE1	1:93:B:ARG:HG3	9	1.36
(3,3099)	1:127:A:TYR:HE1	1:93:A:ARG:HG3	9	1.36
(3,2925)	1:126:A:GLY:HA3	1:50:B:PRO:HG3	8	1.36
(3,2334)	1:98:B:LYS:HG2	1:101:B:THR:HA	5	1.36
(3,2333)	1:98:A:LYS:HG2	1:101:A:THR:HA	5	1.36
(3,2240)	1:94:B:THR:HG21	1:129:B:LYS:HE3	3	1.36
(3,2239)	1:94:A:THR:HG21	1:129:A:LYS:HE3	3	1.36
(3,1830)	1:58:B:PRO:HG2	1:55:B:LYS:HE2	7	1.36
(3,1668)	1:115:B:LEU:HD13	1:104:B:PHE:HA	8	1.36
(3,1667)	1:115:A:LEU:HD13	1:104:A:PHE:HA	8	1.36
(3,1522)	1:45:B:ILE:HG21	1:129:B:LYS:HB2	2	1.36
(3,1521)	1:45:A:ILE:HG21	1:129:A:LYS:HB2	2	1.36
(3,1121)	1:54:A:ALA:HB2	1:57:A:GLN:HG2	10	1.36
(3,692)	1:45:B:ILE:HG21	1:128:B:LEU:H	2	1.36
(3,582)	1:72:B:LYS:HD3	1:116:B:MET:H	7	1.36
(3,576)	1:115:B:LEU:HD22	1:115:B:LEU:H	7	1.36
(3,552)	1:90:B:LEU:HB3	1:103:B:PHE:H	3	1.36
(3,551)	1:90:A:LEU:HB3	1:103:A:PHE:H	3	1.36
(3,352)	1:98:B:LYS:HG2	1:90:B:LEU:H	6	1.36
(3,351)	1:98:A:LYS:HG2	1:90:A:LEU:H	6	1.36
(3,171)	1:46:A:ARG:HB2	1:64:B:VAL:H	5	1.36
(1,5552)	1:116:B:MET:HE1	1:113:B:GLU:HA	6	1.36
(1,5551)	1:116:A:MET:HE1	1:113:A:GLU:HA	6	1.36
(1,5528)	1:115:B:LEU:HD23	1:68:B:VAL:HA	4	1.36
(1,5528)	1:115:B:LEU:HD22	1:68:B:VAL:HA	7	1.36
(1,5527)	1:115:A:LEU:HD23	1:68:A:VAL:HA	4	1.36
(1,5527)	1:115:A:LEU:HD22	1:68:A:VAL:HA	7	1.36
(1,2819)	1:54:A:ALA:HB1	1:44:B:ASP:HB2	2	1.36
(1,2320)	1:57:B:GLN:HG2	1:57:B:GLN:HE22	5	1.36
(1,2319)	1:57:A:GLN:HG2	1:57:A:GLN:HE22	5	1.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,3092)	1:127:B:TYR:HE1	1:104:B:PHE:HB3	1	1.35
(3,3091)	1:127:A:TYR:HE1	1:104:A:PHE:HB3	1	1.35
(3,1830)	1:58:B:PRO:HG2	1:55:B:LYS:HE2	1	1.35
(3,1829)	1:58:A:PRO:HG2	1:55:A:LYS:HE2	1	1.35
(3,692)	1:45:B:ILE:HG21	1:128:B:LEU:H	9	1.35
(3,691)	1:45:A:ILE:HG21	1:128:A:LEU:H	9	1.35
(3,576)	1:115:B:LEU:HD23	1:115:B:LEU:H	2	1.35
(3,576)	1:115:B:LEU:HD21	1:115:B:LEU:H	10	1.35
(3,575)	1:115:A:LEU:HD23	1:115:A:LEU:H	2	1.35
(3,575)	1:115:A:LEU:HD23	1:115:A:LEU:H	9	1.35
(3,575)	1:115:A:LEU:HD21	1:115:A:LEU:H	10	1.35
(3,304)	1:124:B:LYS:HG2	1:86:B:LEU:H	9	1.35
(3,303)	1:124:A:LYS:HG2	1:86:A:LEU:H	9	1.35
(3,172)	1:46:B:ARG:HB2	1:64:A:VAL:H	5	1.35
(1,3590)	1:115:B:LEU:HD12	1:112:B:TYR:HB3	6	1.35
(1,3589)	1:115:A:LEU:HD12	1:112:A:TYR:HB3	6	1.35
(1,3240)	1:99:B:GLU:HG2	1:49:A:LEU:HB3	9	1.35
(1,2781)	1:51:A:ALA:HB1	1:126:B:GLY:HA3	4	1.35
(1,2320)	1:57:B:GLN:HG2	1:57:B:GLN:HE22	2	1.35
(1,2320)	1:57:B:GLN:HG2	1:57:B:GLN:HE22	3	1.35
(1,2320)	1:57:B:GLN:HG2	1:57:B:GLN:HE22	8	1.35
(1,2319)	1:57:A:GLN:HG2	1:57:A:GLN:HE22	2	1.35
(1,2319)	1:57:A:GLN:HG2	1:57:A:GLN:HE22	3	1.35
(1,2319)	1:57:A:GLN:HG2	1:57:A:GLN:HE22	8	1.35
(1,2028)	1:98:B:LYS:HD3	1:125:B:ALA:H	6	1.35
(1,2027)	1:98:A:LYS:HD3	1:125:A:ALA:H	6	1.35
(1,1120)	1:93:B:ARG:HG3	1:90:B:LEU:H	7	1.35
(1,1119)	1:93:A:ARG:HG3	1:90:A:LEU:H	7	1.35
(1,934)	1:82:B:ASN:HD22	1:84:B:ASP:H	8	1.35
(1,933)	1:82:A:ASN:HD22	1:84:A:ASP:H	8	1.35
(3,3092)	1:127:B:TYR:HE2	1:104:B:PHE:HB3	5	1.34
(3,3091)	1:127:A:TYR:HE2	1:104:A:PHE:HB3	5	1.34
(3,2642)	1:115:B:LEU:HD12	1:116:B:MET:HG2	7	1.34
(3,1830)	1:58:B:PRO:HG2	1:55:B:LYS:HE3	3	1.34
(3,1829)	1:58:A:PRO:HG2	1:55:A:LYS:HE3	3	1.34
(3,1608)	1:65:B:PHE:HB2	1:60:B:PRO:HG2	9	1.34
(3,1607)	1:65:A:PHE:HB2	1:60:A:PRO:HG2	9	1.34
(3,1404)	1:122:B:LEU:HA	1:49:A:LEU:HB3	5	1.34
(3,1292)	1:119:B:MET:HB2	1:121:B:THR:HA	9	1.34
(3,1291)	1:119:A:MET:HB2	1:121:A:THR:HA	9	1.34
(3,692)	1:45:B:ILE:HG22	1:128:B:LEU:H	10	1.34
(3,691)	1:45:A:ILE:HG22	1:128:A:LEU:H	10	1.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,576)	1:115:B:LEU:HD22	1:115:B:LEU:H	1	1.34
(3,576)	1:115:B:LEU:HD23	1:115:B:LEU:H	9	1.34
(3,575)	1:115:A:LEU:HD22	1:115:A:LEU:H	1	1.34
(3,182)	1:115:B:LEU:HD11	1:66:B:LEU:H	6	1.34
(3,181)	1:115:A:LEU:HD11	1:66:A:LEU:H	6	1.34
(1,5676)	1:125:B:ALA:HB1	1:102:B:ILE:HD12	1	1.34
(1,5675)	1:125:A:ALA:HB1	1:102:A:ILE:HD12	1	1.34
(1,5504)	1:114:B:THR:HG21	1:104:B:PHE:HZ	8	1.34
(1,5503)	1:114:A:THR:HG21	1:104:A:PHE:HZ	8	1.34
(1,4810)	1:96:B:ALA:HB1	1:100:B:THR:HB	4	1.34
(1,4809)	1:96:A:ALA:HB1	1:100:A:THR:HB	4	1.34
(1,4114)	1:74:B:LEU:HA	1:115:B:LEU:HD13	1	1.34
(1,4113)	1:74:A:LEU:HA	1:115:A:LEU:HD13	1	1.34
(1,3594)	1:115:B:LEU:HD12	1:75:B:TYR:HB3	8	1.34
(1,3594)	1:115:B:LEU:HD13	1:75:B:TYR:HB3	10	1.34
(1,3593)	1:115:A:LEU:HD12	1:75:A:TYR:HB3	8	1.34
(1,3593)	1:115:A:LEU:HD13	1:75:A:TYR:HB3	10	1.34
(1,2320)	1:57:B:GLN:HG2	1:57:B:GLN:HE22	1	1.34
(1,2320)	1:57:B:GLN:HG2	1:57:B:GLN:HE22	4	1.34
(1,2320)	1:57:B:GLN:HG2	1:57:B:GLN:HE22	6	1.34
(1,2320)	1:57:B:GLN:HG2	1:57:B:GLN:HE22	7	1.34
(1,2319)	1:57:A:GLN:HG2	1:57:A:GLN:HE22	1	1.34
(1,2319)	1:57:A:GLN:HG2	1:57:A:GLN:HE22	4	1.34
(1,2319)	1:57:A:GLN:HG2	1:57:A:GLN:HE22	6	1.34
(1,2319)	1:57:A:GLN:HG2	1:57:A:GLN:HE22	7	1.34
(1,933)	1:82:A:ASN:HD22	1:84:A:ASP:H	6	1.34
(3,3091)	1:127:A:TYR:HE1	1:104:A:PHE:HB3	3	1.33
(3,2846)	1:51:B:ALA:HB3	1:127:A:TYR:HD1	7	1.33
(3,2641)	1:115:A:LEU:HD12	1:116:A:MET:HG2	7	1.33
(3,352)	1:98:B:LYS:HG2	1:90:B:LEU:H	4	1.33
(3,351)	1:98:A:LYS:HG2	1:90:A:LEU:H	4	1.33
(1,5312)	1:106:B:ALA:HB2	1:114:B:THR:HG21	8	1.33
(1,5311)	1:106:A:ALA:HB2	1:114:A:THR:HG21	8	1.33
(1,4957)	1:100:A:THR:HG22	1:129:A:LYS:HD2	1	1.33
(1,4808)	1:96:B:ALA:HB1	1:127:B:TYR:HA	1	1.33
(1,4807)	1:96:A:ALA:HB1	1:127:A:TYR:HA	1	1.33
(1,4722)	1:93:B:ARG:HA	1:77:B:GLY:HA2	2	1.33
(1,4721)	1:93:A:ARG:HA	1:77:A:GLY:HA2	2	1.33
(1,4472)	1:86:B:LEU:HA	1:89:B:VAL:HB	1	1.33
(1,4471)	1:86:A:LEU:HA	1:89:A:VAL:HB	1	1.33
(1,4000)	1:72:B:LYS:HG2	1:114:B:THR:HG21	4	1.33
(1,3506)	1:120:B:ASP:HB3	1:116:B:MET:HB2	5	1.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3505)	1:120:A:ASP:HB3	1:116:A:MET:HB2	5	1.33
(1,3432)	1:64:B:VAL:HA	1:93:B:ARG:HG2	8	1.33
(1,3431)	1:64:A:VAL:HA	1:93:A:ARG:HG2	8	1.33
(1,3272)	1:140:B:LYS:HG3	1:67:B:SER:HB3	2	1.33
(1,3235)	1:61:A:GLU:HB3	1:62:A:LYS:HG2	3	1.33
(1,2819)	1:54:A:ALA:HB2	1:44:B:ASP:HB2	8	1.33
(1,2782)	1:51:B:ALA:HB1	1:126:A:GLY:HA3	4	1.33
(1,2495)	1:45:A:ILE:HA	1:54:B:ALA:HB2	1	1.33
(3,3092)	1:127:B:TYR:HE1	1:104:B:PHE:HB3	3	1.32
(3,3092)	1:127:B:TYR:HE1	1:104:B:PHE:HB3	8	1.32
(3,2926)	1:126:B:GLY:HA3	1:50:A:PRO:HG3	8	1.32
(3,2874)	1:121:B:THR:HG21	1:124:B:LYS:HB3	5	1.32
(3,2873)	1:121:A:THR:HG21	1:124:A:LYS:HB3	5	1.32
(3,2682)	1:108:B:LYS:HB2	1:112:B:TYR:HB3	9	1.32
(3,2681)	1:108:A:LYS:HB2	1:112:A:TYR:HB3	9	1.32
(3,2334)	1:98:B:LYS:HG2	1:101:B:THR:HA	6	1.32
(3,2333)	1:98:A:LYS:HG2	1:101:A:THR:HA	6	1.32
(3,1829)	1:58:A:PRO:HG2	1:55:A:LYS:HE2	4	1.32
(3,1668)	1:67:B:SER:HA	1:115:B:LEU:HD11	10	1.32
(3,1667)	1:67:A:SER:HA	1:115:A:LEU:HD11	10	1.32
(3,1608)	1:65:B:PHE:HB2	1:60:B:PRO:HG2	4	1.32
(3,1607)	1:65:A:PHE:HB2	1:60:A:PRO:HG2	4	1.32
(3,994)	1:47:B:VAL:HB	1:99:A:GLU:HG2	7	1.32
(3,952)	1:123:B:ARG:HB2	1:127:B:TYR:HB2	10	1.32
(3,951)	1:123:A:ARG:HB2	1:127:A:TYR:HB2	10	1.32
(3,576)	1:115:B:LEU:HD21	1:115:B:LEU:H	3	1.32
(3,576)	1:115:B:LEU:HD23	1:115:B:LEU:H	4	1.32
(3,576)	1:115:B:LEU:HD21	1:115:B:LEU:H	6	1.32
(3,575)	1:115:A:LEU:HD21	1:115:A:LEU:H	3	1.32
(3,575)	1:115:A:LEU:HD23	1:115:A:LEU:H	4	1.32
(3,575)	1:115:A:LEU:HD21	1:115:A:LEU:H	6	1.32
(1,5622)	1:119:B:MET:HE3	1:121:B:THR:HB	8	1.32
(1,5621)	1:119:A:MET:HE3	1:121:A:THR:HB	8	1.32
(1,5528)	1:115:B:LEU:HD21	1:68:B:VAL:HA	2	1.32
(1,5527)	1:115:A:LEU:HD21	1:68:A:VAL:HA	2	1.32
(1,5386)	1:104:B:PHE:HZ	1:110:B:VAL:HG23	3	1.32
(1,5385)	1:104:A:PHE:HZ	1:110:A:VAL:HG23	3	1.32
(1,4958)	1:100:B:THR:HG22	1:129:B:LYS:HD2	1	1.32
(1,4122)	1:74:B:LEU:HB2	1:110:B:VAL:HG11	3	1.32
(1,3999)	1:72:A:LYS:HG2	1:114:A:THR:HG21	4	1.32
(1,3352)	1:124:B:LYS:HG2	1:84:B:ASP:HB3	1	1.32
(1,3351)	1:124:A:LYS:HG2	1:84:A:ASP:HB3	1	1.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3271)	1:140:A:LYS:HG3	1:67:A:SER:HB3	2	1.32
(1,3236)	1:61:B:GLU:HB3	1:62:B:LYS:HG2	3	1.32
(1,2496)	1:45:B:ILE:HA	1:54:A:ALA:HB2	1	1.32
(1,1120)	1:93:B:ARG:HG3	1:90:B:LEU:H	10	1.32
(1,934)	1:82:B:ASN:HD22	1:84:B:ASP:H	6	1.32
(3,3091)	1:127:A:TYR:HE1	1:104:A:PHE:HB3	8	1.31
(3,1874)	1:105:B:GLN:HG3	1:119:B:MET:HE1	10	1.31
(3,1873)	1:105:A:GLN:HG3	1:119:A:MET:HE1	10	1.31
(3,1830)	1:58:B:PRO:HG2	1:55:B:LYS:HE2	4	1.31
(3,1441)	1:113:A:GLU:HG3	1:116:A:MET:HB3	9	1.31
(3,1080)	1:56:B:PRO:HG2	1:50:B:PRO:HD2	1	1.31
(3,1079)	1:56:A:PRO:HG2	1:50:A:PRO:HD2	1	1.31
(1,5800)	1:134:B:GLY:HA2	1:137:B:GLY:HA2	10	1.31
(1,5626)	1:87:B:THR:HG22	1:126:B:GLY:HA3	1	1.31
(1,5625)	1:87:A:THR:HG22	1:126:A:GLY:HA3	1	1.31
(1,5552)	1:116:B:MET:HE1	1:113:B:GLU:HA	5	1.31
(1,5551)	1:116:A:MET:HE1	1:113:A:GLU:HA	5	1.31
(1,5504)	1:114:B:THR:HG22	1:104:B:PHE:HZ	2	1.31
(1,5503)	1:114:A:THR:HG22	1:104:A:PHE:HZ	2	1.31
(1,4712)	1:92:B:GLN:HG2	1:79:B:GLN:HB3	5	1.31
(1,4711)	1:92:A:GLN:HG2	1:79:A:GLN:HB3	5	1.31
(1,4321)	1:127:A:TYR:HA	1:49:B:LEU:HB3	2	1.31
(1,4121)	1:74:A:LEU:HB2	1:110:A:VAL:HG11	3	1.31
(1,2820)	1:54:B:ALA:HB1	1:44:A:ASP:HB2	2	1.31
(1,1860)	1:110:B:VAL:HG22	1:118:B:VAL:H	5	1.31
(1,1859)	1:110:A:VAL:HG22	1:118:A:VAL:H	5	1.31
(1,1210)	1:89:B:VAL:HG21	1:93:B:ARG:H	4	1.31
(1,1209)	1:89:A:VAL:HG21	1:93:A:ARG:H	4	1.31
(1,1119)	1:93:A:ARG:HG3	1:90:A:LEU:H	10	1.31
(3,3072)	1:104:B:PHE:HE1	1:139:B:ALA:HB1	8	1.3
(3,3071)	1:104:A:PHE:HE1	1:139:A:ALA:HB1	8	1.3
(3,2926)	1:126:B:GLY:HA3	1:50:A:PRO:HG3	7	1.3
(3,2874)	1:121:B:THR:HG23	1:124:B:LYS:HB3	6	1.3
(3,2874)	1:121:B:THR:HG23	1:124:B:LYS:HB3	9	1.3
(3,2873)	1:121:A:THR:HG23	1:124:A:LYS:HB3	9	1.3
(3,2534)	1:102:B:ILE:HG23	1:119:B:MET:HB2	7	1.3
(3,2334)	1:98:B:LYS:HG2	1:101:B:THR:HA	7	1.3
(3,1522)	1:45:B:ILE:HG21	1:129:B:LYS:HB2	7	1.3
(3,1521)	1:45:A:ILE:HG21	1:129:A:LYS:HB2	7	1.3
(3,1122)	1:54:B:ALA:HB2	1:57:B:GLN:HG2	3	1.3
(3,1122)	1:54:B:ALA:HB1	1:57:B:GLN:HG2	4	1.3
(3,1121)	1:54:A:ALA:HB2	1:57:A:GLN:HG2	3	1.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,1121)	1:54:A:ALA:HB1	1:57:A:GLN:HG2	4	1.3
(3,993)	1:47:A:VAL:HB	1:99:B:GLU:HG2	7	1.3
(3,978)	1:104:B:PHE:HB2	1:131:B:GLY:HA3	7	1.3
(3,977)	1:104:A:PHE:HB2	1:131:A:GLY:HA3	7	1.3
(3,853)	1:88:A:SER:HA	1:124:A:LYS:HE3	7	1.3
(1,5799)	1:134:A:GLY:HA2	1:137:A:GLY:HA2	10	1.3
(1,5626)	1:87:B:THR:HG22	1:126:B:GLY:HA3	6	1.3
(1,5625)	1:87:A:THR:HG22	1:126:A:GLY:HA3	6	1.3
(1,2820)	1:54:B:ALA:HB2	1:44:A:ASP:HB2	8	1.3
(1,2354)	1:85:B:GLN:HE22	1:82:B:ASN:HD22	5	1.3
(3,3092)	1:127:B:TYR:HE1	1:104:B:PHE:HB3	4	1.29
(3,3091)	1:127:A:TYR:HE1	1:104:A:PHE:HB3	4	1.29
(3,2873)	1:121:A:THR:HG23	1:124:A:LYS:HB3	6	1.29
(3,2533)	1:102:A:ILE:HG23	1:119:A:MET:HB2	7	1.29
(3,2488)	1:101:B:THR:HB	1:98:B:LYS:HB2	4	1.29
(3,2333)	1:98:A:LYS:HG2	1:101:A:THR:HA	7	1.29
(3,2006)	1:81:B:VAL:HB	1:66:B:LEU:HG	2	1.29
(3,2005)	1:81:A:VAL:HB	1:66:A:LEU:HG	2	1.29
(3,1442)	1:113:B:GLU:HG3	1:116:B:MET:HB3	9	1.29
(3,978)	1:104:B:PHE:HB2	1:131:B:GLY:HA3	3	1.29
(3,977)	1:104:A:PHE:HB2	1:131:A:GLY:HA3	3	1.29
(3,920)	1:45:B:ILE:HD13	1:46:B:ARG:HG3	4	1.29
(3,919)	1:45:A:ILE:HD13	1:46:A:ARG:HG3	4	1.29
(3,854)	1:88:B:SER:HA	1:124:B:LYS:HE3	7	1.29
(3,694)	1:45:B:ILE:HG22	1:128:B:LEU:H	4	1.29
(3,693)	1:45:A:ILE:HG22	1:128:A:LEU:H	4	1.29
(1,5314)	1:106:B:ALA:HB2	1:115:B:LEU:HD23	9	1.29
(1,5313)	1:106:A:ALA:HB2	1:115:A:LEU:HD23	9	1.29
(1,4122)	1:74:B:LEU:HB2	1:110:B:VAL:HG11	5	1.29
(1,4121)	1:74:A:LEU:HB2	1:110:A:VAL:HG11	5	1.29
(1,2028)	1:98:B:LYS:HD3	1:125:B:ALA:H	2	1.29
(1,2027)	1:98:A:LYS:HD3	1:125:A:ALA:H	2	1.29
(1,796)	1:115:B:LEU:HD12	1:75:B:TYR:H	4	1.29
(1,795)	1:115:A:LEU:HD12	1:75:A:TYR:H	4	1.29
(3,2854)	1:119:B:MET:HE3	1:121:B:THR:HB	6	1.28
(3,2853)	1:119:A:MET:HE3	1:121:A:THR:HB	6	1.28
(3,2642)	1:115:B:LEU:HD11	1:116:B:MET:HG2	2	1.28
(3,2642)	1:115:B:LEU:HD11	1:116:B:MET:HG2	9	1.28
(3,2641)	1:115:A:LEU:HD11	1:116:A:MET:HG2	2	1.28
(3,2641)	1:115:A:LEU:HD11	1:116:A:MET:HG2	9	1.28
(3,2487)	1:101:A:THR:HB	1:98:A:LYS:HB2	4	1.28
(3,2334)	1:98:B:LYS:HG2	1:101:B:THR:HA	2	1.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,1522)	1:45:B:ILE:HG22	1:129:B:LYS:HB2	8	1.28
(3,1521)	1:45:A:ILE:HG22	1:129:A:LYS:HB2	8	1.28
(3,978)	1:104:B:PHE:HB2	1:131:B:GLY:HA3	6	1.28
(3,977)	1:104:A:PHE:HB2	1:131:A:GLY:HA3	6	1.28
(3,576)	1:115:B:LEU:HD23	1:115:B:LEU:H	5	1.28
(3,472)	1:90:B:LEU:HB3	1:102:B:ILE:H	9	1.28
(3,471)	1:90:A:LEU:HB3	1:102:A:ILE:H	9	1.28
(1,5422)	1:110:B:VAL:HG11	1:115:B:LEU:HD13	9	1.28
(1,5421)	1:110:A:VAL:HG11	1:115:A:LEU:HD13	9	1.28
(1,5404)	1:110:B:VAL:HG21	1:115:B:LEU:HB3	6	1.28
(1,5403)	1:110:A:VAL:HG21	1:115:A:LEU:HB3	6	1.28
(1,4809)	1:96:A:ALA:HB1	1:100:A:THR:HB	8	1.28
(1,4122)	1:74:B:LEU:HB2	1:110:B:VAL:HG13	6	1.28
(1,4121)	1:74:A:LEU:HB2	1:110:A:VAL:HG13	6	1.28
(1,3589)	1:115:A:LEU:HD12	1:112:A:TYR:HB3	5	1.28
(1,3432)	1:64:B:VAL:HA	1:93:B:ARG:HG2	3	1.28
(1,3431)	1:64:A:VAL:HA	1:93:A:ARG:HG2	3	1.28
(1,3236)	1:61:B:GLU:HB3	1:62:B:LYS:HG2	1	1.28
(1,2353)	1:85:A:GLN:HE22	1:82:A:ASN:HD22	5	1.28
(1,933)	1:82:A:ASN:HD22	1:84:A:ASP:H	1	1.28
(3,3077)	1:104:A:PHE:HD1	1:139:A:ALA:HB1	8	1.27
(3,2925)	1:126:A:GLY:HA3	1:50:B:PRO:HG3	7	1.27
(3,2903)	1:105:A:GLN:HB2	1:69:A:LYS:HD3	2	1.27
(3,2873)	1:87:A:THR:HG22	1:124:A:LYS:HB2	2	1.27
(3,2854)	1:119:B:MET:HE2	1:121:B:THR:HB	1	1.27
(3,2853)	1:119:A:MET:HE2	1:121:A:THR:HB	1	1.27
(3,2836)	1:116:B:MET:HE1	1:120:B:ASP:HA	6	1.27
(3,2835)	1:116:A:MET:HE1	1:120:A:ASP:HA	6	1.27
(3,2692)	1:108:B:LYS:HE2	1:109:B:SER:HB3	1	1.27
(3,2691)	1:108:A:LYS:HE2	1:109:A:SER:HB3	1	1.27
(3,2642)	1:115:B:LEU:HD13	1:116:B:MET:HG2	1	1.27
(3,2641)	1:115:A:LEU:HD13	1:116:A:MET:HG2	1	1.27
(3,2641)	1:115:A:LEU:HD12	1:116:A:MET:HG2	4	1.27
(3,2534)	1:102:B:ILE:HG23	1:133:B:VAL:HB	9	1.27
(3,2533)	1:102:A:ILE:HG23	1:133:A:VAL:HB	9	1.27
(3,2333)	1:98:A:LYS:HG2	1:101:A:THR:HA	2	1.27
(3,2220)	1:93:B:ARG:HD3	1:66:B:LEU:HB3	6	1.27
(3,2219)	1:93:A:ARG:HD3	1:66:A:LEU:HB3	6	1.27
(3,1521)	1:45:A:ILE:HG22	1:129:A:LYS:HB2	4	1.27
(3,1080)	1:56:B:PRO:HG3	1:50:B:PRO:HD2	7	1.27
(3,1079)	1:56:A:PRO:HG3	1:50:A:PRO:HD2	7	1.27
(3,952)	1:123:B:ARG:HB2	1:127:B:TYR:HB2	2	1.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,951)	1:123:A:ARG:HB2	1:127:A:TYR:HB2	2	1.27
(3,816)	1:88:B:SER:HB2	1:79:B:GLN:HE22	10	1.27
(3,582)	1:49:B:LEU:HG	1:116:A:MET:H	5	1.27
(3,576)	1:115:B:LEU:HD23	1:115:B:LEU:H	8	1.27
(3,575)	1:115:A:LEU:HD23	1:115:A:LEU:H	5	1.27
(1,4810)	1:96:B:ALA:HB1	1:100:B:THR:HB	8	1.27
(1,4660)	1:90:B:LEU:HG	1:89:B:VAL:HB	1	1.27
(1,4659)	1:90:A:LEU:HG	1:89:A:VAL:HB	1	1.27
(1,4322)	1:127:B:TYR:HA	1:49:A:LEU:HB3	2	1.27
(1,3778)	1:68:B:VAL:HB	1:114:B:THR:HG21	6	1.27
(1,3777)	1:68:A:VAL:HB	1:114:A:THR:HG21	6	1.27
(1,3590)	1:115:B:LEU:HD12	1:112:B:TYR:HB3	5	1.27
(1,3580)	1:115:B:LEU:HD13	1:75:B:TYR:HA	5	1.27
(1,3579)	1:115:A:LEU:HD13	1:75:A:TYR:HA	5	1.27
(1,3235)	1:61:A:GLU:HB3	1:62:A:LYS:HG2	1	1.27
(1,3235)	1:61:A:GLU:HB3	1:62:A:LYS:HG2	8	1.27
(3,3078)	1:104:B:PHE:HD1	1:139:B:ALA:HB1	8	1.26
(3,2904)	1:87:B:THR:HG22	1:124:B:LYS:HB2	2	1.26
(3,2874)	1:87:B:THR:HG22	1:124:B:LYS:HB2	2	1.26
(3,2642)	1:115:B:LEU:HD12	1:116:B:MET:HG2	4	1.26
(3,2006)	1:81:B:VAL:HB	1:66:B:LEU:HG	8	1.26
(3,1805)	1:98:A:LYS:HE2	1:124:A:LYS:HD2	10	1.26
(3,1522)	1:45:B:ILE:HG22	1:129:B:LYS:HB2	4	1.26
(3,815)	1:88:A:SER:HB2	1:79:A:GLN:HE22	10	1.26
(3,575)	1:115:A:LEU:HD23	1:115:A:LEU:H	8	1.26
(1,5798)	1:134:B:GLY:HA2	1:137:B:GLY:HA3	4	1.26
(1,5797)	1:134:A:GLY:HA2	1:137:A:GLY:HA3	4	1.26
(1,5528)	1:115:B:LEU:HD23	1:68:B:VAL:HA	9	1.26
(1,5314)	1:106:B:ALA:HB2	1:115:B:LEU:HD21	2	1.26
(1,5313)	1:106:A:ALA:HB2	1:115:A:LEU:HD21	2	1.26
(1,4154)	1:123:B:ARG:HG2	1:49:A:LEU:HB3	3	1.26
(1,4153)	1:123:A:ARG:HG2	1:49:B:LEU:HB3	3	1.26
(1,4078)	1:105:B:GLN:HG3	1:137:B:GLY:HA3	1	1.26
(1,4077)	1:105:A:GLN:HG3	1:137:A:GLY:HA3	1	1.26
(1,3594)	1:115:B:LEU:HD13	1:75:B:TYR:HB3	5	1.26
(1,3593)	1:115:A:LEU:HD13	1:75:A:TYR:HB3	5	1.26
(1,3236)	1:61:B:GLU:HB3	1:62:B:LYS:HG2	8	1.26
(1,2343)	1:89:A:VAL:HB	1:79:A:GLN:HE22	10	1.26
(1,2086)	1:98:B:LYS:HD3	1:127:B:TYR:H	2	1.26
(1,2085)	1:98:A:LYS:HD3	1:127:A:TYR:H	2	1.26
(1,934)	1:82:B:ASN:HD22	1:84:B:ASP:H	1	1.26
(3,2240)	1:94:B:THR:HG22	1:129:B:LYS:HE3	8	1.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,2006)	1:81:B:VAL:HB	1:66:B:LEU:HG	5	1.25
(3,2005)	1:81:A:VAL:HB	1:66:A:LEU:HG	5	1.25
(3,2005)	1:81:A:VAL:HB	1:66:A:LEU:HG	8	1.25
(3,1806)	1:98:B:LYS:HE2	1:124:B:LYS:HD2	10	1.25
(3,1122)	1:54:B:ALA:HB1	1:57:B:GLN:HG2	7	1.25
(3,1122)	1:54:B:ALA:HB3	1:57:B:GLN:HG2	8	1.25
(3,1121)	1:54:A:ALA:HB1	1:57:A:GLN:HG2	7	1.25
(3,1121)	1:54:A:ALA:HB3	1:57:A:GLN:HG2	8	1.25
(3,920)	1:45:B:ILE:HD11	1:46:B:ARG:HG3	3	1.25
(3,919)	1:45:A:ILE:HD11	1:46:A:ARG:HG3	3	1.25
(3,692)	1:45:B:ILE:HG22	1:128:B:LEU:H	7	1.25
(3,691)	1:45:A:ILE:HG22	1:128:A:LEU:H	7	1.25
(3,581)	1:49:A:LEU:HG	1:116:B:MET:H	5	1.25
(1,5527)	1:115:A:LEU:HD23	1:68:A:VAL:HA	9	1.25
(1,4322)	1:127:B:TYR:HA	1:49:A:LEU:HB3	7	1.25
(1,3506)	1:120:B:ASP:HB3	1:116:B:MET:HB2	3	1.25
(1,3505)	1:120:A:ASP:HB3	1:116:A:MET:HB2	3	1.25
(1,3368)	1:123:B:ARG:HG2	1:50:A:PRO:HD3	3	1.25
(1,2344)	1:89:B:VAL:HB	1:79:B:GLN:HE22	10	1.25
(3,2239)	1:94:A:THR:HG22	1:129:A:LYS:HE3	8	1.24
(3,1292)	1:119:B:MET:HB2	1:123:B:ARG:HA	5	1.24
(3,1291)	1:119:A:MET:HB2	1:123:A:ARG:HA	5	1.24
(3,1080)	1:56:B:PRO:HG3	1:50:B:PRO:HD2	9	1.24
(3,1079)	1:56:A:PRO:HG3	1:50:A:PRO:HD2	9	1.24
(3,552)	1:90:B:LEU:HB3	1:103:B:PHE:H	2	1.24
(3,551)	1:90:A:LEU:HB3	1:103:A:PHE:H	2	1.24
(3,304)	1:124:B:LYS:HG2	1:86:B:LEU:H	5	1.24
(3,303)	1:124:A:LYS:HG2	1:86:A:LEU:H	5	1.24
(1,5528)	1:115:B:LEU:HD21	1:68:B:VAL:HA	3	1.24
(1,5527)	1:115:A:LEU:HD21	1:68:A:VAL:HA	3	1.24
(1,4807)	1:96:A:ALA:HB1	1:127:A:TYR:HA	4	1.24
(1,4321)	1:127:A:TYR:HA	1:49:B:LEU:HB3	7	1.24
(1,4114)	1:74:B:LEU:HA	1:115:B:LEU:HD13	5	1.24
(1,4113)	1:74:A:LEU:HA	1:115:A:LEU:HD13	5	1.24
(1,3596)	1:115:B:LEU:HD11	1:119:B:MET:HG3	10	1.24
(1,3595)	1:115:A:LEU:HD11	1:119:A:MET:HG3	10	1.24
(3,3006)	1:106:B:ALA:HB2	1:135:B:MET:HG2	2	1.23
(3,3005)	1:106:A:ALA:HB2	1:135:A:MET:HG2	2	1.23
(3,2854)	1:119:B:MET:HE2	1:121:B:THR:HB	5	1.23
(3,2853)	1:119:A:MET:HE2	1:121:A:THR:HB	5	1.23
(3,2846)	1:51:B:ALA:HB1	1:127:A:TYR:HD1	2	1.23
(3,2220)	1:93:B:ARG:HD2	1:66:B:LEU:HB3	3	1.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,2112)	1:87:B:THR:HG23	1:124:B:LYS:HB2	1	1.23
(3,2111)	1:87:A:THR:HG23	1:124:A:LYS:HB2	1	1.23
(3,1292)	1:119:B:MET:HB2	1:123:B:ARG:HA	4	1.23
(3,1291)	1:119:A:MET:HB2	1:123:A:ARG:HA	4	1.23
(3,994)	1:47:B:VAL:HB	1:99:A:GLU:HG2	2	1.23
(3,993)	1:47:A:VAL:HB	1:99:B:GLU:HG2	2	1.23
(3,920)	1:45:B:ILE:HD11	1:46:B:ARG:HG3	9	1.23
(3,919)	1:45:A:ILE:HD11	1:46:A:ARG:HG3	9	1.23
(3,472)	1:90:B:LEU:HB3	1:102:B:ILE:H	4	1.23
(3,471)	1:90:A:LEU:HB3	1:102:A:ILE:H	4	1.23
(1,5582)	1:118:B:VAL:HB	1:83:B:ALA:HB2	10	1.23
(1,5581)	1:118:A:VAL:HB	1:83:A:ALA:HB2	10	1.23
(1,4958)	1:100:B:THR:HG21	1:129:B:LYS:HD2	5	1.23
(1,4957)	1:100:A:THR:HG21	1:129:A:LYS:HD2	5	1.23
(1,4808)	1:96:B:ALA:HB1	1:127:B:TYR:HA	4	1.23
(1,3596)	1:115:B:LEU:HD11	1:119:B:MET:HG3	1	1.23
(1,3595)	1:115:A:LEU:HD11	1:119:A:MET:HG3	1	1.23
(3,2534)	1:102:B:ILE:HG22	1:119:B:MET:HB2	6	1.22
(3,2533)	1:102:A:ILE:HG22	1:119:A:MET:HB2	6	1.22
(3,2220)	1:93:B:ARG:HD2	1:66:B:LEU:HB3	2	1.22
(3,2219)	1:93:A:ARG:HD2	1:66:A:LEU:HB3	2	1.22
(3,2219)	1:93:A:ARG:HD2	1:66:A:LEU:HB3	3	1.22
(3,1668)	1:67:B:SER:HA	1:115:B:LEU:HD11	5	1.22
(3,1667)	1:67:A:SER:HA	1:115:A:LEU:HD11	5	1.22
(3,1080)	1:56:B:PRO:HG2	1:50:B:PRO:HD2	4	1.22
(3,1079)	1:56:A:PRO:HG2	1:50:A:PRO:HD2	4	1.22
(3,552)	1:90:B:LEU:HB3	1:103:B:PHE:H	6	1.22
(3,472)	1:90:B:LEU:HB3	1:102:B:ILE:H	10	1.22
(3,471)	1:90:A:LEU:HB3	1:102:A:ILE:H	10	1.22
(3,150)	1:58:B:PRO:HB2	1:61:B:GLU:H	8	1.22
(3,149)	1:58:A:PRO:HB2	1:61:A:GLU:H	8	1.22
(1,5676)	1:125:B:ALA:HB1	1:102:B:ILE:HD13	8	1.22
(1,5675)	1:125:A:ALA:HB1	1:102:A:ILE:HD13	8	1.22
(1,5504)	1:114:B:THR:HG23	1:104:B:PHE:HZ	5	1.22
(1,5312)	1:106:B:ALA:HB1	1:114:B:THR:HG23	9	1.22
(1,4712)	1:92:B:GLN:HG2	1:79:B:GLN:HB3	9	1.22
(1,4012)	1:72:B:LYS:HD3	1:110:B:VAL:HG13	3	1.22
(1,3948)	1:91:B:ASP:HB2	1:96:B:ALA:HB3	9	1.22
(1,3947)	1:91:A:ASP:HB2	1:96:A:ALA:HB3	9	1.22
(1,3367)	1:123:A:ARG:HG2	1:50:B:PRO:HD3	3	1.22
(1,2086)	1:98:B:LYS:HD3	1:127:B:TYR:H	7	1.22
(1,2085)	1:98:A:LYS:HD3	1:127:A:TYR:H	7	1.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2028)	1:98:B:LYS:HD3	1:125:B:ALA:H	4	1.22
(1,2027)	1:98:A:LYS:HD3	1:125:A:ALA:H	4	1.22
(1,1996)	1:49:B:LEU:HB2	1:123:A:ARG:H	10	1.22
(1,1995)	1:49:A:LEU:HB2	1:123:B:ARG:H	10	1.22
(1,1860)	1:110:B:VAL:HG23	1:118:B:VAL:H	6	1.22
(1,1859)	1:110:A:VAL:HG23	1:118:A:VAL:H	6	1.22
(3,2874)	1:121:B:THR:HG23	1:124:B:LYS:HB3	8	1.21
(3,2873)	1:121:A:THR:HG23	1:124:A:LYS:HB3	8	1.21
(3,1522)	1:45:B:ILE:HG22	1:129:B:LYS:HB2	6	1.21
(3,1521)	1:45:A:ILE:HG22	1:129:A:LYS:HB2	6	1.21
(3,1292)	1:119:B:MET:HB2	1:123:B:ARG:HA	7	1.21
(3,1291)	1:119:A:MET:HB2	1:123:A:ARG:HA	7	1.21
(3,920)	1:45:B:ILE:HD11	1:46:B:ARG:HG3	7	1.21
(3,919)	1:45:A:ILE:HD11	1:46:A:ARG:HG3	7	1.21
(3,693)	1:45:A:ILE:HG23	1:128:A:LEU:H	1	1.21
(3,551)	1:90:A:LEU:HB3	1:103:A:PHE:H	6	1.21
(1,5503)	1:114:A:THR:HG23	1:104:A:PHE:HZ	5	1.21
(1,5311)	1:106:A:ALA:HB1	1:114:A:THR:HG22	2	1.21
(1,5311)	1:106:A:ALA:HB1	1:114:A:THR:HG21	9	1.21
(1,4711)	1:92:A:GLN:HG2	1:79:A:GLN:HB3	9	1.21
(1,4011)	1:72:A:LYS:HD3	1:110:A:VAL:HG13	3	1.21
(1,3594)	1:115:B:LEU:HD13	1:75:B:TYR:HB3	1	1.21
(1,3593)	1:115:A:LEU:HD13	1:75:A:TYR:HB3	1	1.21
(1,2816)	1:54:B:ALA:HB2	1:50:B:PRO:HD2	4	1.21
(1,2816)	1:54:B:ALA:HB2	1:50:B:PRO:HD2	5	1.21
(1,2815)	1:54:A:ALA:HB2	1:50:A:PRO:HD2	5	1.21
(1,1860)	1:110:B:VAL:HG21	1:118:B:VAL:H	7	1.21
(1,1859)	1:110:A:VAL:HG21	1:118:A:VAL:H	7	1.21
(1,1210)	1:89:B:VAL:HG21	1:93:B:ARG:H	5	1.21
(1,1209)	1:89:A:VAL:HG21	1:93:A:ARG:H	5	1.21
(1,524)	1:65:B:PHE:HB2	1:140:B:LYS:H	7	1.21
(1,523)	1:65:A:PHE:HB2	1:140:A:LYS:H	7	1.21
(3,2836)	1:116:B:MET:HE2	1:120:B:ASP:HA	2	1.2
(3,2835)	1:116:A:MET:HE2	1:120:A:ASP:HA	2	1.2
(3,2488)	1:101:B:THR:HB	1:98:B:LYS:HB2	1	1.2
(3,2487)	1:101:A:THR:HB	1:98:A:LYS:HB2	1	1.2
(3,1522)	1:45:B:ILE:HG21	1:129:B:LYS:HB2	9	1.2
(3,1521)	1:45:A:ILE:HG21	1:129:A:LYS:HB2	9	1.2
(3,1442)	1:61:B:GLU:HG2	1:62:B:LYS:HB3	7	1.2
(3,1441)	1:61:A:GLU:HG2	1:62:A:LYS:HB3	7	1.2
(3,1404)	1:122:B:LEU:HA	1:49:A:LEU:HB3	3	1.2
(3,694)	1:45:B:ILE:HG23	1:128:B:LEU:H	1	1.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,552)	1:90:B:LEU:HB3	1:103:B:PHE:H	5	1.2
(3,551)	1:90:A:LEU:HB3	1:103:A:PHE:H	5	1.2
(1,5798)	1:134:B:GLY:HA2	1:137:B:GLY:HA3	9	1.2
(1,5504)	1:114:B:THR:HG23	1:104:B:PHE:HZ	9	1.2
(1,5503)	1:114:A:THR:HG23	1:104:A:PHE:HZ	9	1.2
(1,5312)	1:106:B:ALA:HB1	1:114:B:THR:HG22	2	1.2
(1,4810)	1:96:B:ALA:HB1	1:100:B:THR:HB	6	1.2
(1,4809)	1:96:A:ALA:HB1	1:100:A:THR:HB	6	1.2
(1,3596)	1:115:B:LEU:HD11	1:119:B:MET:HG3	6	1.2
(1,3595)	1:115:A:LEU:HD11	1:119:A:MET:HG3	6	1.2
(1,3432)	1:64:B:VAL:HA	1:93:B:ARG:HG2	7	1.2
(1,3431)	1:64:A:VAL:HA	1:93:A:ARG:HG2	7	1.2
(1,2815)	1:54:A:ALA:HB2	1:50:A:PRO:HD2	4	1.2
(1,1860)	1:110:B:VAL:HG22	1:118:B:VAL:H	10	1.2
(1,1859)	1:110:A:VAL:HG22	1:118:A:VAL:H	10	1.2
(3,2914)	1:86:B:LEU:HB3	1:125:B:ALA:HA	5	1.19
(3,2913)	1:86:A:LEU:HB3	1:125:A:ALA:HA	5	1.19
(3,2845)	1:51:A:ALA:HB1	1:127:B:TYR:HD1	2	1.19
(3,2682)	1:108:B:LYS:HB2	1:112:B:TYR:HB3	8	1.19
(3,2681)	1:108:A:LYS:HB2	1:112:A:TYR:HB3	8	1.19
(3,2334)	1:98:B:LYS:HG2	1:101:B:THR:HA	9	1.19
(3,2333)	1:98:A:LYS:HG2	1:101:A:THR:HA	9	1.19
(3,1873)	1:105:A:GLN:HG3	1:119:A:MET:HE2	7	1.19
(3,845)	1:44:A:ASP:HA	1:105:B:GLN:HB3	2	1.19
(3,607)	1:134:A:GLY:HA3	1:119:B:MET:H	3	1.19
(3,551)	1:90:A:LEU:HB3	1:103:A:PHE:H	7	1.19
(3,352)	1:98:B:LYS:HG2	1:90:B:LEU:H	8	1.19
(3,351)	1:98:A:LYS:HG2	1:90:A:LEU:H	8	1.19
(3,172)	1:46:B:ARG:HB2	1:64:A:VAL:H	3	1.19
(3,171)	1:46:A:ARG:HB2	1:64:B:VAL:H	3	1.19
(1,5797)	1:134:A:GLY:HA2	1:137:A:GLY:HA3	9	1.19
(1,5557)	1:116:A:MET:HE2	1:119:A:MET:HE3	8	1.19
(1,5552)	1:116:B:MET:HE3	1:113:B:GLU:HA	3	1.19
(1,5551)	1:116:A:MET:HE3	1:113:A:GLU:HA	3	1.19
(1,5504)	1:114:B:THR:HG21	1:104:B:PHE:HZ	3	1.19
(1,5503)	1:114:A:THR:HG21	1:104:A:PHE:HZ	3	1.19
(1,5386)	1:104:B:PHE:HZ	1:110:B:VAL:HG22	1	1.19
(1,4974)	1:53:B:SER:HB2	1:45:A:ILE:HG12	4	1.19
(1,4973)	1:53:A:SER:HB2	1:45:B:ILE:HG12	4	1.19
(1,4810)	1:96:B:ALA:HB1	1:100:B:THR:HB	9	1.19
(1,4809)	1:96:A:ALA:HB2	1:100:A:THR:HB	1	1.19
(1,4809)	1:96:A:ALA:HB1	1:100:A:THR:HB	9	1.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4808)	1:96:B:ALA:HB3	1:127:B:TYR:HA	7	1.19
(1,4807)	1:96:A:ALA:HB3	1:127:A:TYR:HA	7	1.19
(1,4133)	1:74:A:LEU:HB3	1:110:A:VAL:HG11	9	1.19
(1,2086)	1:98:B:LYS:HD3	1:127:B:TYR:H	6	1.19
(1,1859)	1:110:A:VAL:HG23	1:118:A:VAL:H	9	1.19
(1,1210)	1:89:B:VAL:HG22	1:93:B:ARG:H	9	1.19
(1,1209)	1:89:A:VAL:HG22	1:93:A:ARG:H	9	1.19
(1,796)	1:115:B:LEU:HD13	1:75:B:TYR:H	6	1.19
(1,795)	1:115:A:LEU:HD13	1:75:A:TYR:H	6	1.19
(3,3092)	1:127:B:TYR:HE2	1:104:B:PHE:HB3	6	1.18
(3,3091)	1:127:A:TYR:HE2	1:104:A:PHE:HB3	6	1.18
(3,2904)	1:105:B:GLN:HB2	1:69:B:LYS:HD3	6	1.18
(3,2903)	1:105:A:GLN:HB2	1:69:A:LYS:HD3	6	1.18
(3,2836)	1:116:B:MET:HE3	1:120:B:ASP:HA	7	1.18
(3,2835)	1:116:A:MET:HE3	1:120:A:ASP:HA	7	1.18
(3,2005)	1:81:A:VAL:HB	1:66:A:LEU:HG	3	1.18
(3,1874)	1:105:B:GLN:HG3	1:119:B:MET:HE2	7	1.18
(3,1724)	1:135:B:MET:HG2	1:115:B:LEU:HD21	2	1.18
(3,1292)	1:119:B:MET:HB2	1:123:B:ARG:HA	1	1.18
(3,1291)	1:119:A:MET:HB2	1:123:A:ARG:HA	1	1.18
(3,1122)	1:54:B:ALA:HB1	1:57:B:GLN:HG2	2	1.18
(3,846)	1:44:B:ASP:HA	1:105:A:GLN:HB3	1	1.18
(3,845)	1:44:A:ASP:HA	1:105:B:GLN:HB3	1	1.18
(3,552)	1:90:B:LEU:HB3	1:103:B:PHE:H	7	1.18
(3,472)	1:90:B:LEU:HB3	1:102:B:ILE:H	8	1.18
(3,171)	1:46:A:ARG:HB2	1:64:B:VAL:H	9	1.18
(1,5676)	1:125:B:ALA:HB3	1:102:B:ILE:HD11	2	1.18
(1,5675)	1:125:A:ALA:HB3	1:102:A:ILE:HD11	2	1.18
(1,5558)	1:116:B:MET:HE2	1:119:B:MET:HE2	8	1.18
(1,5557)	1:116:A:MET:HE3	1:119:A:MET:HE3	3	1.18
(1,5386)	1:104:B:PHE:HZ	1:110:B:VAL:HG23	6	1.18
(1,5385)	1:104:A:PHE:HZ	1:110:A:VAL:HG22	1	1.18
(1,5385)	1:104:A:PHE:HZ	1:110:A:VAL:HG23	6	1.18
(1,4810)	1:96:B:ALA:HB2	1:100:B:THR:HB	1	1.18
(1,4444)	1:79:B:GLN:HB2	1:65:B:PHE:HB3	2	1.18
(1,4443)	1:79:A:GLN:HB2	1:65:A:PHE:HB3	2	1.18
(1,4134)	1:74:B:LEU:HB3	1:110:B:VAL:HG11	9	1.18
(1,2085)	1:98:A:LYS:HD3	1:127:A:TYR:H	6	1.18
(1,1860)	1:110:B:VAL:HG23	1:118:B:VAL:H	9	1.18
(1,796)	1:115:B:LEU:HD11	1:75:B:TYR:H	9	1.18
(1,795)	1:115:A:LEU:HD11	1:75:A:TYR:H	9	1.18
(3,2937)	1:127:A:TYR:HB2	1:45:A:ILE:HD11	1	1.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,2845)	1:51:A:ALA:HB2	1:127:B:TYR:HD1	9	1.17
(3,2175)	1:108:A:LYS:HA	1:139:A:ALA:HB2	6	1.17
(3,2006)	1:81:B:VAL:HB	1:66:B:LEU:HG	3	1.17
(3,1805)	1:98:A:LYS:HE2	1:124:A:LYS:HD2	1	1.17
(3,1723)	1:135:A:MET:HG2	1:115:A:LEU:HD21	2	1.17
(3,1403)	1:122:A:LEU:HA	1:49:B:LEU:HB3	3	1.17
(3,1121)	1:54:A:ALA:HB1	1:57:A:GLN:HG2	2	1.17
(3,978)	1:104:B:PHE:HB2	1:131:B:GLY:HA3	1	1.17
(3,977)	1:104:A:PHE:HB2	1:131:A:GLY:HA3	1	1.17
(3,879)	1:69:A:LYS:HB2	1:140:A:LYS:HE3	1	1.17
(3,846)	1:44:B:ASP:HA	1:105:A:GLN:HB3	2	1.17
(3,694)	1:45:B:ILE:HG23	1:128:B:LEU:H	3	1.17
(3,693)	1:45:A:ILE:HG23	1:128:A:LEU:H	3	1.17
(3,471)	1:90:A:LEU:HB3	1:102:A:ILE:H	8	1.17
(3,172)	1:46:B:ARG:HB2	1:64:A:VAL:H	9	1.17
(3,160)	1:58:B:PRO:HB2	1:62:B:LYS:H	1	1.17
(3,159)	1:58:A:PRO:HB2	1:62:A:LYS:H	1	1.17
(1,5582)	1:118:B:VAL:HB	1:83:B:ALA:HB2	5	1.17
(1,5581)	1:118:A:VAL:HB	1:83:A:ALA:HB2	5	1.17
(1,5558)	1:116:B:MET:HE3	1:119:B:MET:HE3	3	1.17
(1,5308)	1:106:B:ALA:HB3	1:116:B:MET:HE3	4	1.17
(1,5307)	1:106:A:ALA:HB3	1:116:A:MET:HE3	4	1.17
(1,4853)	1:98:A:LYS:HD3	1:51:B:ALA:HA	9	1.17
(1,4444)	1:79:B:GLN:HB2	1:65:B:PHE:HB3	7	1.17
(1,3590)	1:115:B:LEU:HD12	1:112:B:TYR:HB3	1	1.17
(1,3589)	1:115:A:LEU:HD12	1:112:A:TYR:HB3	1	1.17
(1,3140)	1:98:B:LYS:HE2	1:96:B:ALA:HB1	10	1.17
(1,2816)	1:54:B:ALA:HB3	1:50:B:PRO:HD2	8	1.17
(1,2815)	1:54:A:ALA:HB3	1:50:A:PRO:HD2	8	1.17
(1,2028)	1:98:B:LYS:HD3	1:125:B:ALA:H	8	1.17
(1,2027)	1:98:A:LYS:HD3	1:125:A:ALA:H	8	1.17
(3,3092)	1:127:B:TYR:HE1	1:104:B:PHE:HB3	7	1.16
(3,3092)	1:127:B:TYR:HE1	1:104:B:PHE:HB3	10	1.16
(3,3091)	1:127:A:TYR:HE1	1:104:A:PHE:HB3	7	1.16
(3,3091)	1:127:A:TYR:HE1	1:104:A:PHE:HB3	10	1.16
(3,2938)	1:127:B:TYR:HB2	1:45:B:ILE:HD11	1	1.16
(3,2904)	1:105:B:GLN:HB2	1:69:B:LYS:HD3	4	1.16
(3,2903)	1:105:A:GLN:HB2	1:69:A:LYS:HD3	4	1.16
(3,2846)	1:51:B:ALA:HB2	1:127:A:TYR:HD1	9	1.16
(3,2488)	1:101:B:THR:HB	1:50:B:PRO:HG2	10	1.16
(3,2487)	1:101:A:THR:HB	1:50:A:PRO:HG2	10	1.16
(3,2176)	1:108:B:LYS:HA	1:139:B:ALA:HB2	6	1.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,2176)	1:108:B:LYS:HA	1:139:B:ALA:HB2	7	1.16
(3,2175)	1:108:A:LYS:HA	1:139:A:ALA:HB2	7	1.16
(3,1806)	1:98:B:LYS:HE2	1:124:B:LYS:HD2	1	1.16
(3,1442)	1:61:B:GLU:HG2	1:62:B:LYS:HB3	4	1.16
(3,1441)	1:61:A:GLU:HG2	1:62:A:LYS:HB3	4	1.16
(3,952)	1:123:B:ARG:HB2	1:127:B:TYR:HB2	4	1.16
(3,951)	1:123:A:ARG:HB2	1:127:A:TYR:HB2	4	1.16
(3,920)	1:45:B:ILE:HD11	1:46:A:ARG:HG2	1	1.16
(3,919)	1:45:A:ILE:HD11	1:46:B:ARG:HG2	1	1.16
(3,880)	1:69:B:LYS:HB2	1:140:B:LYS:HE3	1	1.16
(3,854)	1:88:B:SER:HA	1:124:B:LYS:HE3	10	1.16
(3,853)	1:88:A:SER:HA	1:124:A:LYS:HE3	10	1.16
(3,286)	1:124:B:LYS:HG2	1:84:B:ASP:H	1	1.16
(3,160)	1:58:B:PRO:HB2	1:62:B:LYS:H	10	1.16
(3,159)	1:58:A:PRO:HB2	1:62:A:LYS:H	10	1.16
(1,5810)	1:134:B:GLY:HA3	1:116:A:MET:HE2	5	1.16
(1,4854)	1:98:B:LYS:HD3	1:51:A:ALA:HA	9	1.16
(1,4504)	1:86:B:LEU:HB2	1:121:B:THR:HG22	8	1.16
(1,4443)	1:79:A:GLN:HB2	1:65:A:PHE:HB3	7	1.16
(1,4134)	1:74:B:LEU:HB3	1:110:B:VAL:HG13	4	1.16
(1,4134)	1:74:B:LEU:HB3	1:110:B:VAL:HG12	10	1.16
(1,4133)	1:74:A:LEU:HB3	1:110:A:VAL:HG13	4	1.16
(1,4133)	1:74:A:LEU:HB3	1:110:A:VAL:HG12	10	1.16
(1,3139)	1:98:A:LYS:HE2	1:96:A:ALA:HB1	10	1.16
(1,1860)	1:110:B:VAL:HG22	1:118:B:VAL:H	8	1.16
(1,1859)	1:110:A:VAL:HG22	1:118:A:VAL:H	8	1.16
(3,2534)	1:102:B:ILE:HG23	1:133:B:VAL:HB	5	1.15
(3,2533)	1:102:A:ILE:HG23	1:133:A:VAL:HB	5	1.15
(3,1442)	1:61:B:GLU:HG2	1:62:B:LYS:HB3	2	1.15
(3,1442)	1:61:B:GLU:HG2	1:62:B:LYS:HB3	6	1.15
(3,1441)	1:61:A:GLU:HG2	1:62:A:LYS:HB3	5	1.15
(3,1441)	1:61:A:GLU:HG2	1:62:A:LYS:HB3	6	1.15
(3,1285)	1:57:A:GLN:HG3	1:129:A:LYS:HD2	10	1.15
(3,608)	1:134:B:GLY:HA3	1:119:A:MET:H	3	1.15
(3,285)	1:124:A:LYS:HG2	1:84:A:ASP:H	1	1.15
(3,160)	1:58:B:PRO:HB2	1:62:B:LYS:H	6	1.15
(3,159)	1:58:A:PRO:HB2	1:62:A:LYS:H	6	1.15
(1,5798)	1:134:B:GLY:HA2	1:137:B:GLY:HA3	10	1.15
(1,4503)	1:86:A:LEU:HB2	1:121:A:THR:HG22	8	1.15
(1,4134)	1:74:B:LEU:HB3	1:110:B:VAL:HG12	1	1.15
(1,4133)	1:74:A:LEU:HB3	1:110:A:VAL:HG12	1	1.15
(1,3505)	1:120:A:ASP:HB3	1:116:A:MET:HB2	8	1.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3432)	1:64:B:VAL:HA	1:93:B:ARG:HG2	1	1.15
(1,3432)	1:64:B:VAL:HA	1:93:B:ARG:HG2	6	1.15
(1,3431)	1:64:A:VAL:HA	1:93:A:ARG:HG2	6	1.15
(3,2682)	1:108:B:LYS:HB2	1:112:B:TYR:HB3	6	1.14
(3,2681)	1:108:A:LYS:HB2	1:112:A:TYR:HB3	6	1.14
(3,2334)	1:98:B:LYS:HG2	1:101:B:THR:HA	8	1.14
(3,2334)	1:98:B:LYS:HG2	1:101:B:THR:HA	10	1.14
(3,1670)	1:67:B:SER:HB2	1:80:B:PRO:HD3	9	1.14
(3,1669)	1:67:A:SER:HB2	1:80:A:PRO:HD3	9	1.14
(3,1442)	1:61:B:GLU:HG2	1:62:B:LYS:HB3	5	1.14
(3,1441)	1:61:A:GLU:HG2	1:62:A:LYS:HB3	2	1.14
(3,1292)	1:119:B:MET:HB2	1:123:B:ARG:HA	6	1.14
(3,1291)	1:119:A:MET:HB2	1:123:A:ARG:HA	6	1.14
(3,1286)	1:57:B:GLN:HG3	1:129:B:LYS:HD2	10	1.14
(3,952)	1:123:B:ARG:HB2	1:127:B:TYR:HB2	9	1.14
(3,951)	1:123:A:ARG:HB2	1:127:A:TYR:HB2	9	1.14
(3,920)	1:45:B:ILE:HD11	1:46:B:ARG:HG3	2	1.14
(3,920)	1:45:B:ILE:HD13	1:46:B:ARG:HG3	8	1.14
(3,919)	1:45:A:ILE:HD11	1:46:A:ARG:HG3	2	1.14
(3,919)	1:45:A:ILE:HD13	1:46:B:ARG:HG2	6	1.14
(3,919)	1:45:A:ILE:HD13	1:46:A:ARG:HG3	8	1.14
(3,694)	1:45:B:ILE:HG22	1:128:B:LEU:H	8	1.14
(3,693)	1:45:A:ILE:HG22	1:128:A:LEU:H	8	1.14
(3,171)	1:46:A:ARG:HB2	1:64:B:VAL:H	10	1.14
(1,5925)	1:112:A:TYR:HE2	1:113:A:GLU:HB3	8	1.14
(1,5809)	1:134:A:GLY:HA3	1:116:B:MET:HE2	5	1.14
(1,5797)	1:134:A:GLY:HA2	1:137:A:GLY:HA3	10	1.14
(1,5675)	1:125:A:ALA:HB2	1:102:A:ILE:HD13	3	1.14
(1,5483)	1:124:A:LYS:HA	1:123:A:ARG:HB2	2	1.14
(1,5312)	1:106:B:ALA:HB3	1:114:B:THR:HG21	3	1.14
(1,5311)	1:106:A:ALA:HB3	1:114:A:THR:HG21	3	1.14
(1,4721)	1:93:A:ARG:HA	1:77:A:GLY:HA2	10	1.14
(1,4012)	1:72:B:LYS:HD3	1:110:B:VAL:HG13	8	1.14
(1,4011)	1:72:A:LYS:HD3	1:110:A:VAL:HG13	8	1.14
(1,3506)	1:120:B:ASP:HB3	1:116:B:MET:HB2	8	1.14
(1,3505)	1:120:A:ASP:HB3	1:116:A:MET:HB2	6	1.14
(1,3431)	1:64:A:VAL:HA	1:93:A:ARG:HG2	1	1.14
(1,3431)	1:64:A:VAL:HA	1:93:A:ARG:HG2	5	1.14
(1,3240)	1:99:B:GLU:HG2	1:49:A:LEU:HB3	1	1.14
(1,3239)	1:99:A:GLU:HG2	1:49:B:LEU:HB3	1	1.14
(1,2824)	1:54:B:ALA:HB1	1:55:B:LYS:HB2	4	1.14
(1,2823)	1:54:A:ALA:HB1	1:55:A:LYS:HB2	4	1.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2782)	1:51:B:ALA:HB2	1:126:A:GLY:HA3	10	1.14
(1,2028)	1:98:B:LYS:HD3	1:125:B:ALA:H	5	1.14
(3,3060)	1:65:B:PHE:HE1	1:93:B:ARG:HB2	10	1.13
(3,3059)	1:65:A:PHE:HE1	1:93:A:ARG:HB2	10	1.13
(3,2963)	1:129:A:LYS:HG3	1:45:A:ILE:HG23	5	1.13
(3,2836)	1:116:B:MET:HE3	1:120:B:ASP:HA	3	1.13
(3,2488)	1:101:B:THR:HB	1:98:B:LYS:HB2	6	1.13
(3,2488)	1:101:B:THR:HB	1:98:B:LYS:HB2	8	1.13
(3,2487)	1:101:A:THR:HB	1:98:A:LYS:HB2	6	1.13
(3,2487)	1:101:A:THR:HB	1:98:A:LYS:HB2	7	1.13
(3,2487)	1:101:A:THR:HB	1:98:A:LYS:HB2	8	1.13
(3,2333)	1:98:A:LYS:HG2	1:101:A:THR:HA	8	1.13
(3,2333)	1:98:A:LYS:HG2	1:101:A:THR:HA	10	1.13
(3,2298)	1:90:B:LEU:HA	1:96:B:ALA:HB3	5	1.13
(3,2288)	1:95:B:GLN:HG2	1:63:B:PRO:HB2	8	1.13
(3,2287)	1:95:A:GLN:HG2	1:63:A:PRO:HB2	8	1.13
(3,2112)	1:87:B:THR:HG22	1:124:B:LYS:HB2	5	1.13
(3,2111)	1:87:A:THR:HG22	1:124:A:LYS:HB2	5	1.13
(3,952)	1:123:B:ARG:HB2	1:127:B:TYR:HB2	5	1.13
(3,951)	1:123:A:ARG:HB2	1:127:A:TYR:HB2	5	1.13
(3,920)	1:45:B:ILE:HD13	1:46:B:ARG:HG3	5	1.13
(3,286)	1:124:B:LYS:HG2	1:84:B:ASP:H	10	1.13
(3,285)	1:124:A:LYS:HG2	1:84:A:ASP:H	10	1.13
(1,5926)	1:112:B:TYR:HE2	1:113:B:GLU:HB3	8	1.13
(1,5676)	1:125:B:ALA:HB2	1:102:B:ILE:HD13	3	1.13
(1,5604)	1:119:B:MET:HE2	1:130:B:VAL:HA	7	1.13
(1,5603)	1:119:A:MET:HE2	1:130:A:VAL:HA	7	1.13
(1,5582)	1:118:B:VAL:HB	1:83:B:ALA:HB2	4	1.13
(1,5581)	1:118:A:VAL:HB	1:83:A:ALA:HB2	4	1.13
(1,5484)	1:124:B:LYS:HA	1:123:B:ARG:HB2	2	1.13
(1,5484)	1:124:B:LYS:HA	1:123:B:ARG:HB2	4	1.13
(1,5484)	1:124:B:LYS:HA	1:123:B:ARG:HB2	9	1.13
(1,5483)	1:124:A:LYS:HA	1:123:A:ARG:HB2	4	1.13
(1,5483)	1:124:A:LYS:HA	1:123:A:ARG:HB2	9	1.13
(1,4876)	1:99:B:GLU:HA	1:129:B:LYS:HD3	1	1.13
(1,4132)	1:74:B:LEU:HB3	1:119:B:MET:HE1	10	1.13
(1,4131)	1:74:A:LEU:HB3	1:119:A:MET:HE1	10	1.13
(1,4004)	1:72:B:LYS:HD3	1:110:B:VAL:HA	3	1.13
(1,3506)	1:120:B:ASP:HB3	1:116:B:MET:HB2	6	1.13
(1,3432)	1:64:B:VAL:HA	1:93:B:ARG:HG2	5	1.13
(1,2027)	1:98:A:LYS:HD3	1:125:A:ALA:H	5	1.13
(3,3072)	1:104:B:PHE:HE1	1:139:B:ALA:HB1	3	1.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,3071)	1:104:A:PHE:HE1	1:139:A:ALA:HB1	3	1.12
(3,2964)	1:129:B:LYS:HG3	1:45:B:ILE:HG23	5	1.12
(3,2914)	1:86:B:LEU:HB3	1:125:B:ALA:HA	6	1.12
(3,2913)	1:86:A:LEU:HB3	1:125:A:ALA:HA	6	1.12
(3,2904)	1:105:B:GLN:HB2	1:69:B:LYS:HD3	9	1.12
(3,2903)	1:105:A:GLN:HB2	1:69:A:LYS:HD3	9	1.12
(3,2854)	1:119:B:MET:HE3	1:121:B:THR:HB	3	1.12
(3,2853)	1:119:A:MET:HE3	1:121:A:THR:HB	3	1.12
(3,2835)	1:116:A:MET:HE3	1:120:A:ASP:HA	3	1.12
(3,2632)	1:105:B:GLN:HG3	1:110:B:VAL:HG22	2	1.12
(3,2631)	1:105:A:GLN:HG3	1:110:A:VAL:HG22	2	1.12
(3,2488)	1:101:B:THR:HB	1:98:B:LYS:HB2	2	1.12
(3,2488)	1:101:B:THR:HB	1:98:B:LYS:HB2	7	1.12
(3,2487)	1:101:A:THR:HB	1:98:A:LYS:HB2	2	1.12
(3,2297)	1:90:A:LEU:HA	1:96:A:ALA:HB3	5	1.12
(3,919)	1:45:A:ILE:HD13	1:46:A:ARG:HG3	5	1.12
(3,472)	1:90:B:LEU:HB3	1:102:B:ILE:H	3	1.12
(3,471)	1:90:A:LEU:HB3	1:102:A:ILE:H	3	1.12
(3,172)	1:46:B:ARG:HB2	1:64:A:VAL:H	10	1.12
(1,5582)	1:118:B:VAL:HB	1:83:B:ALA:HB3	2	1.12
(1,5581)	1:118:A:VAL:HB	1:83:A:ALA:HB3	2	1.12
(1,5558)	1:116:B:MET:HE2	1:119:B:MET:HE2	10	1.12
(1,5557)	1:116:A:MET:HE2	1:119:A:MET:HE2	10	1.12
(1,5238)	1:105:B:GLN:HB2	1:101:B:THR:HG23	8	1.12
(1,4875)	1:99:A:GLU:HA	1:129:A:LYS:HD3	1	1.12
(1,4808)	1:96:B:ALA:HB2	1:127:B:TYR:HA	2	1.12
(1,4807)	1:96:A:ALA:HB2	1:127:A:TYR:HA	2	1.12
(1,4722)	1:93:B:ARG:HA	1:77:B:GLY:HA2	10	1.12
(1,4134)	1:74:B:LEU:HB3	1:110:B:VAL:HG11	8	1.12
(1,4133)	1:74:A:LEU:HB3	1:110:A:VAL:HG11	8	1.12
(1,4003)	1:72:A:LYS:HD3	1:110:A:VAL:HA	3	1.12
(1,3590)	1:115:B:LEU:HD13	1:112:B:TYR:HB3	2	1.12
(1,3589)	1:115:A:LEU:HD13	1:112:A:TYR:HB3	2	1.12
(1,2816)	1:54:B:ALA:HB2	1:50:B:PRO:HD2	1	1.12
(1,2559)	1:45:A:ILE:HG23	1:54:B:ALA:HB2	1	1.12
(3,2845)	1:51:A:ALA:HB3	1:127:B:TYR:HD1	3	1.11
(3,2532)	1:102:B:ILE:HG22	1:133:B:VAL:HB	7	1.11
(3,2531)	1:102:A:ILE:HG22	1:133:A:VAL:HB	7	1.11
(3,2488)	1:101:B:THR:HB	1:98:B:LYS:HB2	3	1.11
(3,2488)	1:101:B:THR:HB	1:98:B:LYS:HB2	5	1.11
(3,2487)	1:101:A:THR:HB	1:98:A:LYS:HB2	5	1.11
(3,2354)	1:98:B:LYS:HG2	1:96:B:ALA:HB2	2	1.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,2353)	1:98:A:LYS:HG2	1:96:A:ALA:HB2	2	1.11
(3,1830)	1:58:B:PRO:HG2	1:55:B:LYS:HE2	8	1.11
(3,1829)	1:58:A:PRO:HG2	1:55:A:LYS:HE2	8	1.11
(3,1286)	1:57:B:GLN:HG3	1:129:B:LYS:HD2	4	1.11
(3,1285)	1:57:A:GLN:HG3	1:129:A:LYS:HD2	4	1.11
(3,694)	1:45:B:ILE:HG22	1:128:B:LEU:H	6	1.11
(3,693)	1:45:A:ILE:HG21	1:128:A:LEU:H	2	1.11
(3,693)	1:45:A:ILE:HG22	1:128:A:LEU:H	6	1.11
(3,472)	1:90:B:LEU:HB3	1:102:B:ILE:H	1	1.11
(3,471)	1:90:A:LEU:HB3	1:102:A:ILE:H	1	1.11
(1,5810)	1:134:B:GLY:HA3	1:116:A:MET:HE3	8	1.11
(1,5607)	1:51:A:ALA:HB2	1:124:B:LYS:HA	2	1.11
(1,5558)	1:116:B:MET:HE2	1:119:B:MET:HE2	1	1.11
(1,5557)	1:116:A:MET:HE2	1:119:A:MET:HE2	1	1.11
(1,5422)	1:110:B:VAL:HG13	1:115:B:LEU:HD13	2	1.11
(1,5421)	1:110:A:VAL:HG13	1:115:A:LEU:HD13	2	1.11
(1,5237)	1:105:A:GLN:HB2	1:101:A:THR:HG23	8	1.11
(1,4808)	1:96:B:ALA:HB3	1:127:B:TYR:HA	6	1.11
(1,4807)	1:96:A:ALA:HB3	1:127:A:TYR:HA	6	1.11
(1,4722)	1:93:B:ARG:HA	1:77:B:GLY:HA2	5	1.11
(1,4721)	1:93:A:ARG:HA	1:77:A:GLY:HA2	5	1.11
(1,4717)	1:92:A:GLN:HG2	1:102:A:ILE:HG13	5	1.11
(1,4050)	1:85:B:GLN:HB2	1:88:B:SER:HB2	6	1.11
(1,4049)	1:85:A:GLN:HB2	1:88:A:SER:HB2	6	1.11
(1,2823)	1:54:A:ALA:HB1	1:55:A:LYS:HB2	9	1.11
(1,2815)	1:54:A:ALA:HB2	1:50:A:PRO:HD2	1	1.11
(1,2560)	1:45:B:ILE:HG23	1:54:A:ALA:HB2	1	1.11
(3,2844)	1:115:B:LEU:HD21	1:118:B:VAL:HA	4	1.1
(3,2843)	1:115:A:LEU:HD21	1:118:A:VAL:HA	4	1.1
(3,2487)	1:101:A:THR:HB	1:98:A:LYS:HB2	3	1.1
(3,978)	1:104:B:PHE:HB2	1:131:B:GLY:HA3	2	1.1
(3,977)	1:104:A:PHE:HB2	1:131:A:GLY:HA3	2	1.1
(3,920)	1:45:B:ILE:HD13	1:46:A:ARG:HG2	6	1.1
(3,845)	1:44:A:ASP:HA	1:105:B:GLN:HB3	9	1.1
(3,694)	1:45:B:ILE:HG21	1:128:B:LEU:H	2	1.1
(3,604)	1:87:B:THR:H	1:119:B:MET:H	2	1.1
(3,351)	1:98:A:LYS:HG2	1:90:A:LEU:H	3	1.1
(1,5809)	1:134:A:GLY:HA3	1:116:B:MET:HE3	8	1.1
(1,5676)	1:125:B:ALA:HB3	1:102:B:ILE:HD13	4	1.1
(1,5675)	1:125:A:ALA:HB3	1:102:A:ILE:HD13	4	1.1
(1,5528)	1:115:B:LEU:HD22	1:68:B:VAL:HA	1	1.1
(1,5527)	1:115:A:LEU:HD22	1:68:A:VAL:HA	1	1.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5484)	1:124:B:LYS:HA	1:123:B:ARG:HB2	10	1.1
(1,5483)	1:124:A:LYS:HA	1:123:A:ARG:HB2	7	1.1
(1,5483)	1:124:A:LYS:HA	1:123:A:ARG:HB2	10	1.1
(1,5406)	1:110:B:VAL:HG11	1:104:B:PHE:HZ	9	1.1
(1,5405)	1:110:A:VAL:HG11	1:104:A:PHE:HZ	9	1.1
(1,5386)	1:104:B:PHE:HZ	1:110:B:VAL:HG22	4	1.1
(1,4718)	1:92:B:GLN:HG2	1:102:B:ILE:HG13	5	1.1
(1,3967)	1:72:A:LYS:HB2	1:114:A:THR:HG22	8	1.1
(1,3604)	1:115:B:LEU:HD12	1:116:B:MET:HE3	4	1.1
(1,3603)	1:115:A:LEU:HD12	1:116:A:MET:HE3	4	1.1
(1,3590)	1:115:B:LEU:HD11	1:112:B:TYR:HB3	7	1.1
(1,3590)	1:115:B:LEU:HD13	1:112:B:TYR:HB3	9	1.1
(1,3589)	1:115:A:LEU:HD11	1:112:A:TYR:HB3	7	1.1
(1,3589)	1:115:A:LEU:HD13	1:112:A:TYR:HB3	9	1.1
(1,3352)	1:124:B:LYS:HG2	1:84:B:ASP:HB3	7	1.1
(1,3351)	1:124:A:LYS:HG2	1:84:A:ASP:HB3	7	1.1
(1,3271)	1:140:A:LYS:HG3	1:67:A:SER:HB3	1	1.1
(1,2824)	1:54:B:ALA:HB1	1:55:B:LYS:HB2	9	1.1
(3,2298)	1:90:B:LEU:HA	1:96:B:ALA:HB2	3	1.09
(3,2298)	1:90:B:LEU:HA	1:96:B:ALA:HB3	9	1.09
(3,1849)	1:85:A:GLN:HB2	1:124:A:LYS:HE3	8	1.09
(3,1824)	1:129:B:LYS:HD2	1:45:B:ILE:HG22	6	1.09
(3,1823)	1:129:A:LYS:HD2	1:45:A:ILE:HG22	6	1.09
(3,1442)	1:61:B:GLU:HG2	1:62:B:LYS:HB3	10	1.09
(3,1441)	1:113:A:GLU:HG3	1:116:A:MET:HB3	10	1.09
(3,952)	1:123:B:ARG:HB2	1:127:B:TYR:HB2	7	1.09
(3,951)	1:123:A:ARG:HB2	1:127:A:TYR:HB2	7	1.09
(3,694)	1:45:B:ILE:HG21	1:128:B:LEU:H	9	1.09
(3,694)	1:45:B:ILE:HG22	1:128:B:LEU:H	10	1.09
(3,693)	1:45:A:ILE:HG21	1:128:A:LEU:H	9	1.09
(3,693)	1:45:A:ILE:HG22	1:128:A:LEU:H	10	1.09
(3,603)	1:87:A:THR:H	1:119:A:MET:H	2	1.09
(3,460)	1:49:B:LEU:HB2	1:122:A:LEU:H	2	1.09
(3,352)	1:98:B:LYS:HG2	1:90:B:LEU:H	3	1.09
(1,5810)	1:134:B:GLY:HA3	1:116:A:MET:HE2	1	1.09
(1,5809)	1:134:A:GLY:HA3	1:116:B:MET:HE2	1	1.09
(1,5676)	1:125:B:ALA:HB1	1:102:B:ILE:HD13	10	1.09
(1,5608)	1:51:B:ALA:HB2	1:124:A:LYS:HA	2	1.09
(1,5558)	1:116:B:MET:HE1	1:119:B:MET:HE2	5	1.09
(1,5557)	1:116:A:MET:HE1	1:119:A:MET:HE2	5	1.09
(1,5528)	1:115:B:LEU:HD22	1:68:B:VAL:HA	10	1.09
(1,5527)	1:115:A:LEU:HD22	1:68:A:VAL:HA	10	1.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5503)	1:114:A:THR:HG23	1:104:A:PHE:HZ	4	1.09
(1,5484)	1:124:B:LYS:HA	1:123:B:ARG:HB2	7	1.09
(1,5385)	1:104:A:PHE:HZ	1:110:A:VAL:HG22	4	1.09
(1,5314)	1:106:B:ALA:HB2	1:115:B:LEU:HD22	10	1.09
(1,5066)	1:115:B:LEU:HD13	1:119:B:MET:HA	1	1.09
(1,5065)	1:115:A:LEU:HD13	1:119:A:MET:HA	1	1.09
(1,4134)	1:74:B:LEU:HB3	1:110:B:VAL:HG13	7	1.09
(1,4133)	1:74:A:LEU:HB3	1:110:A:VAL:HG13	7	1.09
(1,4012)	1:72:B:LYS:HD3	1:110:B:VAL:HG13	5	1.09
(1,4011)	1:72:A:LYS:HD3	1:110:A:VAL:HG13	5	1.09
(1,3968)	1:72:B:LYS:HB2	1:114:B:THR:HG22	8	1.09
(1,3432)	1:64:B:VAL:HA	1:93:B:ARG:HG2	2	1.09
(1,3431)	1:64:A:VAL:HA	1:93:A:ARG:HG2	2	1.09
(1,3272)	1:140:B:LYS:HG3	1:67:B:SER:HB3	1	1.09
(1,2824)	1:54:B:ALA:HB3	1:55:B:LYS:HB2	2	1.09
(1,2824)	1:54:B:ALA:HB1	1:55:B:LYS:HB2	10	1.09
(1,2823)	1:54:A:ALA:HB1	1:55:A:LYS:HB2	10	1.09
(3,3100)	1:127:B:TYR:HE1	1:93:B:ARG:HG3	1	1.08
(3,3099)	1:127:A:TYR:HE1	1:93:A:ARG:HG3	1	1.08
(3,3024)	1:129:B:LYS:HA	1:97:B:ASN:HB2	10	1.08
(3,3023)	1:129:A:LYS:HA	1:97:A:ASN:HB2	10	1.08
(3,2836)	1:116:B:MET:HE1	1:120:B:ASP:HA	5	1.08
(3,2835)	1:116:A:MET:HE1	1:120:A:ASP:HA	5	1.08
(3,2835)	1:116:A:MET:HE2	1:120:A:ASP:HA	8	1.08
(3,2632)	1:105:B:GLN:HG3	1:110:B:VAL:HG21	7	1.08
(3,2631)	1:105:A:GLN:HG3	1:110:A:VAL:HG21	7	1.08
(3,2474)	1:101:B:THR:HA	1:45:A:ILE:HG23	8	1.08
(3,2454)	1:94:B:THR:HG22	1:64:B:VAL:HB	6	1.08
(3,2453)	1:94:A:THR:HG22	1:64:A:VAL:HB	6	1.08
(3,2297)	1:90:A:LEU:HA	1:96:A:ALA:HB2	3	1.08
(3,2297)	1:90:A:LEU:HA	1:96:A:ALA:HB3	9	1.08
(3,1874)	1:105:B:GLN:HG3	1:119:B:MET:HE3	1	1.08
(3,1873)	1:105:A:GLN:HG3	1:119:A:MET:HE3	1	1.08
(3,1850)	1:85:B:GLN:HB2	1:124:B:LYS:HE3	8	1.08
(3,1646)	1:115:B:LEU:HD13	1:116:B:MET:HG2	3	1.08
(3,1645)	1:115:A:LEU:HD13	1:116:A:MET:HG2	3	1.08
(3,1292)	1:119:B:MET:HB2	1:123:B:ARG:HA	2	1.08
(3,1291)	1:119:A:MET:HB2	1:123:A:ARG:HA	2	1.08
(3,846)	1:44:B:ASP:HA	1:105:A:GLN:HB3	9	1.08
(3,459)	1:49:A:LEU:HB2	1:122:B:LEU:H	2	1.08
(3,160)	1:58:B:PRO:HB2	1:62:B:LYS:H	7	1.08
(3,159)	1:58:A:PRO:HB2	1:62:A:LYS:H	7	1.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5675)	1:125:A:ALA:HB1	1:102:A:ILE:HD13	10	1.08
(1,5581)	1:118:A:VAL:HB	1:83:A:ALA:HB1	7	1.08
(1,5504)	1:114:B:THR:HG23	1:104:B:PHE:HZ	4	1.08
(1,5484)	1:124:B:LYS:HA	1:123:B:ARG:HB2	3	1.08
(1,5484)	1:124:B:LYS:HA	1:123:B:ARG:HB2	5	1.08
(1,5483)	1:124:A:LYS:HA	1:123:A:ARG:HB2	3	1.08
(1,5313)	1:106:A:ALA:HB2	1:115:A:LEU:HD22	10	1.08
(1,5308)	1:106:B:ALA:HB3	1:116:B:MET:HE2	2	1.08
(1,5307)	1:106:A:ALA:HB3	1:116:A:MET:HE2	2	1.08
(1,4718)	1:92:B:GLN:HG2	1:102:B:ILE:HG13	6	1.08
(1,4717)	1:92:A:GLN:HG2	1:102:A:ILE:HG13	6	1.08
(1,4134)	1:74:B:LEU:HB3	1:110:B:VAL:HG11	5	1.08
(1,4133)	1:74:A:LEU:HB3	1:110:A:VAL:HG11	5	1.08
(1,3352)	1:124:B:LYS:HG2	1:84:B:ASP:HB3	5	1.08
(1,2824)	1:54:B:ALA:HB2	1:55:B:LYS:HB2	3	1.08
(1,2824)	1:54:B:ALA:HB1	1:55:B:LYS:HB2	6	1.08
(1,2823)	1:54:A:ALA:HB3	1:55:A:LYS:HB2	2	1.08
(1,2823)	1:54:A:ALA:HB2	1:55:A:LYS:HB2	3	1.08
(1,2823)	1:54:A:ALA:HB1	1:55:A:LYS:HB2	6	1.08
(1,2815)	1:54:A:ALA:HB3	1:50:A:PRO:HD2	3	1.08
(1,2343)	1:89:A:VAL:HB	1:79:A:GLN:HE22	7	1.08
(3,2854)	1:119:B:MET:HE1	1:121:B:THR:HB	7	1.07
(3,2853)	1:119:A:MET:HE1	1:121:A:THR:HB	7	1.07
(3,2836)	1:116:B:MET:HE2	1:120:B:ASP:HA	8	1.07
(3,2454)	1:94:B:THR:HG21	1:64:B:VAL:HB	4	1.07
(3,2453)	1:94:A:THR:HG21	1:64:A:VAL:HB	4	1.07
(3,2334)	1:98:B:LYS:HG2	1:101:B:THR:HA	3	1.07
(3,2006)	1:81:B:VAL:HB	1:66:B:LEU:HG	9	1.07
(3,2005)	1:81:A:VAL:HB	1:66:A:LEU:HG	9	1.07
(3,1522)	1:45:B:ILE:HG23	1:129:B:LYS:HB2	1	1.07
(3,1521)	1:45:A:ILE:HG23	1:129:A:LYS:HB2	1	1.07
(3,978)	1:104:B:PHE:HB2	1:131:B:GLY:HA3	4	1.07
(3,977)	1:104:A:PHE:HB2	1:131:A:GLY:HA3	4	1.07
(3,472)	1:90:B:LEU:HB3	1:102:B:ILE:H	6	1.07
(3,471)	1:90:A:LEU:HB3	1:102:A:ILE:H	6	1.07
(3,462)	1:102:B:ILE:HG22	1:101:B:THR:H	9	1.07
(3,461)	1:102:A:ILE:HG22	1:101:A:THR:H	9	1.07
(3,303)	1:124:A:LYS:HG2	1:86:A:LEU:H	2	1.07
(1,5582)	1:118:B:VAL:HB	1:83:B:ALA:HB1	7	1.07
(1,5504)	1:114:B:THR:HG21	1:104:B:PHE:HZ	1	1.07
(1,5503)	1:114:A:THR:HG21	1:104:A:PHE:HZ	1	1.07
(1,5484)	1:124:B:LYS:HA	1:123:B:ARG:HB2	1	1.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5483)	1:124:A:LYS:HA	1:123:A:ARG:HB2	1	1.07
(1,5483)	1:124:A:LYS:HA	1:123:A:ARG:HB2	5	1.07
(1,5314)	1:106:B:ALA:HB3	1:115:B:LEU:HD21	8	1.07
(1,5313)	1:106:A:ALA:HB3	1:115:A:LEU:HD21	8	1.07
(1,3604)	1:115:B:LEU:HD13	1:116:B:MET:HE2	10	1.07
(1,3603)	1:115:A:LEU:HD13	1:116:A:MET:HE2	10	1.07
(1,3596)	1:115:B:LEU:HD13	1:119:B:MET:HG3	8	1.07
(1,3595)	1:115:A:LEU:HD13	1:119:A:MET:HG3	8	1.07
(1,3351)	1:124:A:LYS:HG2	1:84:A:ASP:HB3	5	1.07
(1,2816)	1:54:B:ALA:HB3	1:50:B:PRO:HD2	3	1.07
(1,2782)	1:51:B:ALA:HB2	1:126:A:GLY:HA3	5	1.07
(1,2781)	1:51:A:ALA:HB2	1:126:B:GLY:HA3	10	1.07
(1,2495)	1:45:A:ILE:HA	1:54:B:ALA:HB2	4	1.07
(1,2344)	1:89:B:VAL:HB	1:79:B:GLN:HE22	7	1.07
(3,2846)	1:51:B:ALA:HB3	1:127:A:TYR:HD1	3	1.06
(3,2473)	1:101:A:THR:HA	1:45:B:ILE:HG23	8	1.06
(3,2394)	1:99:B:GLU:HG3	1:129:B:LYS:HD3	1	1.06
(3,2393)	1:99:A:GLU:HG3	1:129:A:LYS:HD3	1	1.06
(3,2354)	1:98:B:LYS:HG2	1:96:B:ALA:HB1	1	1.06
(3,2353)	1:98:A:LYS:HG2	1:96:A:ALA:HB1	1	1.06
(3,2353)	1:98:A:LYS:HG2	1:96:A:ALA:HB3	7	1.06
(3,2333)	1:98:A:LYS:HG2	1:101:A:THR:HA	3	1.06
(3,2112)	1:87:B:THR:HG23	1:124:B:LYS:HB2	6	1.06
(3,1292)	1:119:B:MET:HB2	1:123:B:ARG:HA	3	1.06
(3,1291)	1:119:A:MET:HB2	1:123:A:ARG:HA	3	1.06
(3,304)	1:124:B:LYS:HG2	1:86:B:LEU:H	2	1.06
(1,5926)	1:112:B:TYR:HE2	1:113:B:GLU:HB3	5	1.06
(1,5484)	1:124:B:LYS:HA	1:123:B:ARG:HB2	6	1.06
(1,5483)	1:124:A:LYS:HA	1:123:A:ARG:HB2	6	1.06
(1,5419)	1:110:A:VAL:HG12	1:114:A:THR:HG21	4	1.06
(1,2910)	1:55:B:LYS:HG3	1:58:B:PRO:HG2	10	1.06
(1,2824)	1:54:B:ALA:HB3	1:55:B:LYS:HB2	7	1.06
(1,2823)	1:54:A:ALA:HB3	1:55:A:LYS:HB2	7	1.06
(1,2496)	1:45:B:ILE:HA	1:54:A:ALA:HB2	4	1.06
(1,2320)	1:57:B:GLN:HG2	1:57:B:GLN:HE22	9	1.06
(1,1558)	1:115:B:LEU:HD13	1:105:B:GLN:H	4	1.06
(1,1557)	1:115:A:LEU:HD13	1:105:A:GLN:H	4	1.06
(3,3092)	1:127:B:TYR:HE1	1:104:B:PHE:HB3	9	1.05
(3,3091)	1:127:A:TYR:HE1	1:104:A:PHE:HB3	9	1.05
(3,2853)	1:119:A:MET:HE2	1:121:A:THR:HB	9	1.05
(3,2464)	1:100:B:THR:HG23	1:102:B:ILE:HG23	10	1.05
(3,2463)	1:100:A:THR:HG23	1:102:A:ILE:HG23	10	1.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,2354)	1:98:B:LYS:HG2	1:96:B:ALA:HB3	7	1.05
(3,2219)	1:93:A:ARG:HD2	1:66:A:LEU:HB3	4	1.05
(3,2111)	1:87:A:THR:HG23	1:124:A:LYS:HB2	6	1.05
(3,1806)	1:98:B:LYS:HE2	1:124:B:LYS:HD2	7	1.05
(3,472)	1:90:B:LEU:HB3	1:102:B:ILE:H	5	1.05
(3,471)	1:90:A:LEU:HB3	1:102:A:ILE:H	5	1.05
(3,462)	1:102:B:ILE:HG23	1:101:B:THR:H	10	1.05
(1,5925)	1:112:A:TYR:HE2	1:113:A:GLU:HB3	5	1.05
(1,5676)	1:125:B:ALA:HB1	1:102:B:ILE:HD12	5	1.05
(1,5676)	1:125:B:ALA:HB1	1:102:B:ILE:HD11	7	1.05
(1,5676)	1:125:B:ALA:HB3	1:102:B:ILE:HD11	9	1.05
(1,5675)	1:125:A:ALA:HB1	1:102:A:ILE:HD12	5	1.05
(1,5675)	1:125:A:ALA:HB1	1:102:A:ILE:HD11	7	1.05
(1,5675)	1:125:A:ALA:HB3	1:102:A:ILE:HD11	9	1.05
(1,5622)	1:119:B:MET:HE3	1:121:B:THR:HB	6	1.05
(1,5621)	1:119:A:MET:HE3	1:121:A:THR:HB	6	1.05
(1,5420)	1:110:B:VAL:HG12	1:114:B:THR:HG21	4	1.05
(1,5406)	1:110:B:VAL:HG13	1:104:B:PHE:HZ	7	1.05
(1,5405)	1:110:A:VAL:HG13	1:104:A:PHE:HZ	7	1.05
(1,5314)	1:106:B:ALA:HB2	1:115:B:LEU:HD21	5	1.05
(1,5313)	1:106:A:ALA:HB2	1:115:A:LEU:HD21	5	1.05
(1,4006)	1:72:B:LYS:HD3	1:107:B:ASP:HB3	8	1.05
(1,4005)	1:72:A:LYS:HD3	1:107:A:ASP:HB3	8	1.05
(1,3239)	1:99:A:GLU:HG2	1:49:B:LEU:HB3	10	1.05
(1,2909)	1:55:A:LYS:HG3	1:58:A:PRO:HG2	10	1.05
(1,2320)	1:57:B:GLN:HG2	1:57:B:GLN:HE22	10	1.05
(1,2319)	1:57:A:GLN:HG2	1:57:A:GLN:HE22	9	1.05
(1,2319)	1:57:A:GLN:HG2	1:57:A:GLN:HE22	10	1.05
(1,1995)	1:49:A:LEU:HB2	1:123:B:ARG:H	7	1.05
(1,796)	1:115:B:LEU:HD13	1:75:B:TYR:H	3	1.05
(1,795)	1:115:A:LEU:HD13	1:75:A:TYR:H	3	1.05
(3,2854)	1:119:B:MET:HE2	1:121:B:THR:HB	9	1.04
(3,2836)	1:116:B:MET:HE3	1:120:B:ASP:HA	4	1.04
(3,2835)	1:116:A:MET:HE3	1:120:A:ASP:HA	4	1.04
(3,2488)	1:101:B:THR:HB	1:50:B:PRO:HG2	9	1.04
(3,2454)	1:94:B:THR:HG23	1:64:B:VAL:HB	10	1.04
(3,2453)	1:94:A:THR:HG23	1:64:A:VAL:HB	10	1.04
(3,2220)	1:93:B:ARG:HD2	1:66:B:LEU:HB3	4	1.04
(3,1805)	1:98:A:LYS:HE2	1:124:A:LYS:HD2	7	1.04
(3,1760)	1:69:B:LYS:HE2	1:73:B:GLN:HG2	5	1.04
(3,1278)	1:57:B:GLN:HG2	1:50:B:PRO:HD2	10	1.04
(3,1277)	1:57:A:GLN:HG2	1:50:A:PRO:HD2	10	1.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,471)	1:90:A:LEU:HB3	1:102:A:ILE:H	2	1.04
(1,5810)	1:134:B:GLY:HA3	1:116:A:MET:HE3	10	1.04
(1,5622)	1:119:B:MET:HE2	1:121:B:THR:HB	1	1.04
(1,5621)	1:119:A:MET:HE2	1:121:A:THR:HB	1	1.04
(1,5582)	1:118:B:VAL:HB	1:83:B:ALA:HB3	3	1.04
(1,5581)	1:118:A:VAL:HB	1:83:A:ALA:HB3	3	1.04
(1,4752)	1:94:B:THR:HG21	1:96:B:ALA:HA	1	1.04
(1,4751)	1:94:A:THR:HG21	1:96:A:ALA:HA	1	1.04
(1,4718)	1:92:B:GLN:HG2	1:102:B:ILE:HG13	10	1.04
(1,4717)	1:92:A:GLN:HG2	1:102:A:ILE:HG13	10	1.04
(1,2824)	1:54:B:ALA:HB2	1:55:B:LYS:HB2	8	1.04
(1,2823)	1:54:A:ALA:HB2	1:55:A:LYS:HB2	8	1.04
(1,1996)	1:49:B:LEU:HB2	1:123:A:ARG:H	7	1.04
(1,1859)	1:110:A:VAL:HG22	1:118:A:VAL:H	4	1.04
(1,532)	1:102:B:ILE:HG23	1:65:B:PHE:H	10	1.04
(1,531)	1:102:A:ILE:HG23	1:65:A:PHE:H	10	1.04
(3,3100)	1:75:B:TYR:HE1	1:140:B:LYS:HD2	4	1.03
(3,3099)	1:75:A:TYR:HE1	1:140:A:LYS:HD2	4	1.03
(3,2944)	1:128:B:LEU:HA	1:125:B:ALA:HB3	2	1.03
(3,2943)	1:128:A:LEU:HA	1:125:A:ALA:HB3	2	1.03
(3,2514)	1:129:B:LYS:HD2	1:102:B:ILE:HG13	10	1.03
(3,2513)	1:129:A:LYS:HD2	1:102:A:ILE:HG13	10	1.03
(3,2487)	1:101:A:THR:HB	1:50:A:PRO:HG2	9	1.03
(3,1759)	1:69:A:LYS:HE2	1:73:A:GLN:HG2	5	1.03
(3,1724)	1:135:B:MET:HG2	1:115:B:LEU:HD21	5	1.03
(3,472)	1:90:B:LEU:HB3	1:102:B:ILE:H	2	1.03
(3,461)	1:102:A:ILE:HG23	1:101:A:THR:H	10	1.03
(3,172)	1:46:B:ARG:HB2	1:64:A:VAL:H	7	1.03
(1,5826)	1:135:B:MET:HE3	1:112:A:TYR:HD1	1	1.03
(1,5809)	1:134:A:GLY:HA3	1:116:B:MET:HE3	10	1.03
(1,5676)	1:125:B:ALA:HB3	1:102:B:ILE:HD11	6	1.03
(1,5675)	1:125:A:ALA:HB3	1:102:A:ILE:HD11	6	1.03
(1,4005)	1:72:A:LYS:HD3	1:107:A:ASP:HB3	9	1.03
(1,3604)	1:115:B:LEU:HD11	1:116:B:MET:HE3	9	1.03
(1,3603)	1:115:A:LEU:HD11	1:116:A:MET:HE3	9	1.03
(1,3596)	1:115:B:LEU:HD11	1:119:B:MET:HG3	3	1.03
(1,3595)	1:115:A:LEU:HD11	1:119:A:MET:HG3	3	1.03
(1,3432)	1:64:B:VAL:HA	1:93:B:ARG:HG2	9	1.03
(1,3431)	1:64:A:VAL:HA	1:93:A:ARG:HG2	9	1.03
(1,3021)	1:56:A:PRO:HD2	1:57:A:GLN:HG3	3	1.03
(1,2816)	1:54:B:ALA:HB1	1:50:B:PRO:HD2	2	1.03
(1,2815)	1:54:A:ALA:HB1	1:50:A:PRO:HD2	2	1.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2496)	1:45:B:ILE:HA	1:54:A:ALA:HB2	5	1.03
(1,1860)	1:110:B:VAL:HG22	1:118:B:VAL:H	4	1.03
(1,796)	1:115:B:LEU:HD12	1:75:B:TYR:H	7	1.03
(1,795)	1:115:A:LEU:HD12	1:75:A:TYR:H	7	1.03
(3,2642)	1:116:B:MET:HG2	1:45:B:ILE:HD11	6	1.02
(3,2641)	1:116:A:MET:HG2	1:45:A:ILE:HD11	6	1.02
(3,2632)	1:105:B:GLN:HG3	1:110:B:VAL:HG23	9	1.02
(3,2514)	1:129:B:LYS:HD2	1:102:B:ILE:HG13	7	1.02
(3,2513)	1:129:A:LYS:HD2	1:102:A:ILE:HG13	7	1.02
(3,2112)	1:87:B:THR:HG22	1:124:B:LYS:HB2	9	1.02
(3,2111)	1:87:A:THR:HG22	1:124:A:LYS:HB2	9	1.02
(3,1954)	1:79:B:GLN:HG2	1:88:B:SER:HB3	6	1.02
(3,1723)	1:135:A:MET:HG2	1:115:A:LEU:HD21	5	1.02
(3,978)	1:104:B:PHE:HB2	1:131:B:GLY:HA3	5	1.02
(3,977)	1:104:A:PHE:HB2	1:131:A:GLY:HA3	5	1.02
(3,854)	1:88:B:SER:HA	1:124:B:LYS:HE3	2	1.02
(3,171)	1:46:A:ARG:HB2	1:64:B:VAL:H	7	1.02
(3,160)	1:58:B:PRO:HB2	1:62:B:LYS:H	9	1.02
(3,159)	1:58:A:PRO:HB2	1:62:A:LYS:H	9	1.02
(1,5420)	1:110:B:VAL:HG13	1:114:B:THR:HG21	9	1.02
(1,5419)	1:110:A:VAL:HG13	1:114:A:THR:HG21	9	1.02
(1,4012)	1:72:B:LYS:HD3	1:110:B:VAL:HG12	6	1.02
(1,4011)	1:72:A:LYS:HD3	1:110:A:VAL:HG11	1	1.02
(1,4011)	1:72:A:LYS:HD3	1:110:A:VAL:HG12	6	1.02
(1,4006)	1:72:B:LYS:HD3	1:107:B:ASP:HB3	9	1.02
(1,3968)	1:72:B:LYS:HB2	1:114:B:THR:HG23	3	1.02
(1,3967)	1:72:A:LYS:HB2	1:114:A:THR:HG23	3	1.02
(1,3590)	1:115:B:LEU:HD11	1:112:B:TYR:HB3	4	1.02
(1,3589)	1:115:A:LEU:HD11	1:112:A:TYR:HB3	4	1.02
(1,3351)	1:124:A:LYS:HG2	1:84:A:ASP:HB3	6	1.02
(1,3240)	1:99:B:GLU:HG2	1:49:A:LEU:HB3	10	1.02
(1,3022)	1:56:B:PRO:HD2	1:57:B:GLN:HG3	3	1.02
(1,2824)	1:54:B:ALA:HB1	1:55:B:LYS:HB2	1	1.02
(1,2781)	1:51:A:ALA:HB2	1:126:B:GLY:HA3	5	1.02
(1,2495)	1:45:A:ILE:HA	1:54:B:ALA:HB2	5	1.02
(1,1860)	1:110:B:VAL:HG22	1:118:B:VAL:H	2	1.02
(1,1859)	1:110:A:VAL:HG22	1:118:A:VAL:H	2	1.02
(1,1210)	1:89:B:VAL:HG22	1:93:B:ARG:H	3	1.02
(1,1209)	1:89:A:VAL:HG22	1:93:A:ARG:H	3	1.02
(3,2821)	1:113:A:GLU:HG2	1:115:A:LEU:HD23	3	1.01
(3,2631)	1:105:A:GLN:HG3	1:110:A:VAL:HG23	9	1.01
(3,2394)	1:99:B:GLU:HG3	1:129:B:LYS:HD3	5	1.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,2393)	1:99:A:GLU:HG3	1:129:A:LYS:HD3	5	1.01
(3,1954)	1:79:B:GLN:HG2	1:88:B:SER:HB2	4	1.01
(3,1953)	1:79:A:GLN:HG2	1:88:A:SER:HB2	4	1.01
(3,1953)	1:79:A:GLN:HG2	1:88:A:SER:HB3	6	1.01
(3,1873)	1:105:A:GLN:HG3	1:119:A:MET:HE1	6	1.01
(3,1122)	1:54:B:ALA:HB2	1:57:B:GLN:HG2	6	1.01
(3,1121)	1:54:A:ALA:HB2	1:57:A:GLN:HG2	6	1.01
(3,1080)	1:56:B:PRO:HG3	1:50:B:PRO:HD2	8	1.01
(3,1079)	1:56:A:PRO:HG3	1:50:A:PRO:HD2	8	1.01
(3,853)	1:88:A:SER:HA	1:124:A:LYS:HE3	2	1.01
(3,461)	1:102:A:ILE:HG23	1:101:A:THR:H	6	1.01
(1,5825)	1:135:A:MET:HE3	1:112:B:TYR:HD1	1	1.01
(1,5308)	1:106:B:ALA:HB3	1:116:B:MET:HE3	9	1.01
(1,5307)	1:106:A:ALA:HB3	1:116:A:MET:HE3	9	1.01
(1,4682)	1:91:B:ASP:HA	1:96:B:ALA:HB3	5	1.01
(1,4682)	1:91:B:ASP:HA	1:96:B:ALA:HB3	9	1.01
(1,4681)	1:91:A:ASP:HA	1:96:A:ALA:HB3	9	1.01
(1,4012)	1:72:B:LYS:HD3	1:110:B:VAL:HG11	1	1.01
(1,4012)	1:72:B:LYS:HD3	1:110:B:VAL:HG13	9	1.01
(1,4011)	1:72:A:LYS:HD3	1:110:A:VAL:HG13	9	1.01
(1,3596)	1:115:B:LEU:HD11	1:119:B:MET:HG3	5	1.01
(1,3352)	1:124:B:LYS:HG2	1:84:B:ASP:HB3	6	1.01
(1,2823)	1:54:A:ALA:HB1	1:55:A:LYS:HB2	1	1.01
(1,2816)	1:54:B:ALA:HB1	1:50:B:PRO:HD2	7	1.01
(1,2815)	1:54:A:ALA:HB1	1:50:A:PRO:HD2	7	1.01
(3,2822)	1:113:B:GLU:HG2	1:115:B:LEU:HD23	3	1.0
(3,1874)	1:105:B:GLN:HG3	1:119:B:MET:HE1	6	1.0
(3,1806)	1:98:B:LYS:HE2	1:124:B:LYS:HD2	8	1.0
(3,1805)	1:98:A:LYS:HE2	1:124:A:LYS:HD2	8	1.0
(3,472)	1:90:B:LEU:HB3	1:102:B:ILE:H	7	1.0
(3,471)	1:90:A:LEU:HB3	1:102:A:ILE:H	7	1.0
(3,462)	1:102:B:ILE:HG23	1:101:B:THR:H	6	1.0
(1,5622)	1:119:B:MET:HE2	1:121:B:THR:HB	5	1.0
(1,5621)	1:119:A:MET:HE2	1:121:A:THR:HB	5	1.0
(1,5528)	1:115:B:LEU:HD21	1:68:B:VAL:HA	8	1.0
(1,5314)	1:106:B:ALA:HB1	1:115:B:LEU:HD22	6	1.0
(1,5313)	1:106:A:ALA:HB1	1:115:A:LEU:HD22	6	1.0
(1,5066)	1:115:B:LEU:HD13	1:119:B:MET:HA	6	1.0
(1,5065)	1:115:A:LEU:HD13	1:119:A:MET:HA	6	1.0
(1,4876)	1:99:B:GLU:HA	1:129:B:LYS:HD3	5	1.0
(1,4875)	1:99:A:GLU:HA	1:129:A:LYS:HD3	5	1.0
(1,4810)	1:96:B:ALA:HB3	1:100:B:THR:HB	3	1.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4772)	1:94:B:THR:HG23	1:102:B:ILE:HG22	4	1.0
(1,4771)	1:94:A:THR:HG23	1:102:A:ILE:HG22	4	1.0
(1,4681)	1:91:A:ASP:HA	1:96:A:ALA:HB3	5	1.0
(1,4006)	1:72:B:LYS:HD3	1:107:B:ASP:HB3	3	1.0
(1,3782)	1:115:B:LEU:HD13	1:68:B:VAL:HB	2	1.0
(1,3781)	1:115:A:LEU:HD13	1:68:A:VAL:HB	2	1.0
(1,3604)	1:115:B:LEU:HD12	1:116:B:MET:HE3	7	1.0
(1,3603)	1:115:A:LEU:HD12	1:116:A:MET:HE3	7	1.0
(1,3595)	1:115:A:LEU:HD11	1:119:A:MET:HG3	5	1.0
(1,3550)	1:66:B:LEU:HB3	1:122:B:LEU:HG	8	1.0
(1,3549)	1:66:A:LEU:HB3	1:122:A:LEU:HG	8	1.0
(1,2085)	1:98:A:LYS:HD3	1:127:A:TYR:H	1	1.0
(1,1862)	1:110:B:VAL:HG12	1:118:B:VAL:H	1	1.0
(1,1861)	1:110:A:VAL:HG12	1:118:A:VAL:H	1	1.0
(1,1210)	1:89:B:VAL:HG21	1:93:B:ARG:H	8	1.0
(1,46)	1:89:B:VAL:HG11	1:85:B:GLN:H	10	1.0
(1,45)	1:89:A:VAL:HG11	1:85:A:GLN:H	10	1.0
(3,2854)	1:119:B:MET:HE1	1:121:B:THR:HB	4	0.99
(3,2853)	1:119:A:MET:HE1	1:121:A:THR:HB	4	0.99
(3,2844)	1:102:B:ILE:HG21	1:118:B:VAL:HA	3	0.99
(3,2844)	1:115:B:LEU:HD21	1:118:B:VAL:HA	9	0.99
(3,2843)	1:102:A:ILE:HG21	1:118:A:VAL:HA	3	0.99
(3,2843)	1:115:A:LEU:HD21	1:118:A:VAL:HA	9	0.99
(3,2112)	1:87:B:THR:HG21	1:124:B:LYS:HB2	10	0.99
(3,2111)	1:87:A:THR:HG21	1:124:A:LYS:HB2	10	0.99
(3,2006)	1:81:B:VAL:HB	1:66:B:LEU:HG	7	0.99
(3,2005)	1:81:A:VAL:HB	1:66:A:LEU:HG	7	0.99
(3,1954)	1:79:B:GLN:HG2	1:88:B:SER:HB3	3	0.99
(3,1953)	1:79:A:GLN:HG2	1:88:A:SER:HB3	3	0.99
(3,1878)	1:105:B:GLN:HG3	1:110:B:VAL:HG11	8	0.99
(3,1877)	1:105:A:GLN:HG3	1:110:A:VAL:HG11	8	0.99
(3,1873)	1:73:A:GLN:HG2	1:69:A:LYS:HD2	4	0.99
(3,1805)	1:98:A:LYS:HE2	1:124:A:LYS:HD2	3	0.99
(3,694)	1:45:B:ILE:HG22	1:128:B:LEU:H	7	0.99
(3,693)	1:45:A:ILE:HG22	1:128:A:LEU:H	7	0.99
(1,5926)	1:112:B:TYR:HE2	1:113:B:GLU:HB3	10	0.99
(1,5925)	1:112:A:TYR:HE2	1:113:A:GLU:HB3	10	0.99
(1,5527)	1:115:A:LEU:HD21	1:68:A:VAL:HA	8	0.99
(1,5406)	1:110:B:VAL:HG13	1:104:B:PHE:HZ	2	0.99
(1,5405)	1:110:A:VAL:HG13	1:104:A:PHE:HZ	2	0.99
(1,4862)	1:98:B:LYS:HD3	1:127:B:TYR:HB2	6	0.99
(1,4861)	1:98:A:LYS:HD3	1:127:A:TYR:HB2	6	0.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4810)	1:96:B:ALA:HB1	1:100:B:THR:HB	7	0.99
(1,4809)	1:96:A:ALA:HB3	1:100:A:THR:HB	3	0.99
(1,4808)	1:96:B:ALA:HB1	1:127:B:TYR:HA	8	0.99
(1,4807)	1:96:A:ALA:HB1	1:127:A:TYR:HA	8	0.99
(1,4796)	1:96:B:ALA:HA	1:90:B:LEU:HB2	4	0.99
(1,4795)	1:96:A:ALA:HA	1:90:A:LEU:HB2	4	0.99
(1,4718)	1:92:B:GLN:HG2	1:102:B:ILE:HG13	3	0.99
(1,4718)	1:92:B:GLN:HG2	1:102:B:ILE:HG13	9	0.99
(1,4717)	1:92:A:GLN:HG2	1:102:A:ILE:HG13	3	0.99
(1,4717)	1:92:A:GLN:HG2	1:102:A:ILE:HG13	9	0.99
(1,4682)	1:91:B:ASP:HA	1:96:B:ALA:HB2	3	0.99
(1,4681)	1:91:A:ASP:HA	1:96:A:ALA:HB2	3	0.99
(1,4134)	1:74:B:LEU:HB3	1:110:B:VAL:HG13	6	0.99
(1,4133)	1:74:A:LEU:HB3	1:110:A:VAL:HG13	6	0.99
(1,4049)	1:85:A:GLN:HB2	1:88:A:SER:HB2	3	0.99
(1,4005)	1:72:A:LYS:HD3	1:107:A:ASP:HB3	3	0.99
(1,2823)	1:54:A:ALA:HB1	1:55:A:LYS:HB2	5	0.99
(1,2086)	1:98:B:LYS:HD3	1:127:B:TYR:H	1	0.99
(1,1209)	1:89:A:VAL:HG21	1:93:A:ARG:H	8	0.99
(1,45)	1:89:A:VAL:HG13	1:85:A:GLN:H	2	0.99
(3,2844)	1:115:B:LEU:HD22	1:118:B:VAL:HA	8	0.98
(3,2843)	1:115:A:LEU:HD22	1:118:A:VAL:HA	8	0.98
(3,2822)	1:113:B:GLU:HG2	1:115:B:LEU:HD23	8	0.98
(3,2514)	1:129:B:LYS:HD2	1:102:B:ILE:HG13	2	0.98
(3,2513)	1:129:A:LYS:HD2	1:102:A:ILE:HG13	2	0.98
(3,1878)	1:105:B:GLN:HG3	1:110:B:VAL:HG11	9	0.98
(3,1877)	1:105:A:GLN:HG3	1:110:A:VAL:HG11	9	0.98
(3,1874)	1:73:B:GLN:HG2	1:69:B:LYS:HD2	4	0.98
(3,1850)	1:73:B:GLN:HB3	1:140:B:LYS:HE2	4	0.98
(3,1806)	1:98:B:LYS:HE2	1:124:B:LYS:HD2	3	0.98
(1,5552)	1:116:B:MET:HE3	1:113:B:GLU:HA	4	0.98
(1,5551)	1:116:A:MET:HE3	1:113:A:GLU:HA	4	0.98
(1,5420)	1:110:B:VAL:HG12	1:114:B:THR:HG23	2	0.98
(1,5419)	1:110:A:VAL:HG12	1:114:A:THR:HG23	2	0.98
(1,5406)	1:110:B:VAL:HG11	1:104:B:PHE:HZ	5	0.98
(1,5405)	1:110:A:VAL:HG11	1:104:A:PHE:HZ	5	0.98
(1,4809)	1:96:A:ALA:HB1	1:100:A:THR:HB	7	0.98
(1,4278)	1:93:B:ARG:HG2	1:65:B:PHE:HB3	10	0.98
(1,4277)	1:93:A:ARG:HG2	1:65:A:PHE:HB3	10	0.98
(1,4134)	1:74:B:LEU:HB3	1:110:B:VAL:HG11	3	0.98
(1,4133)	1:74:A:LEU:HB3	1:110:A:VAL:HG11	3	0.98
(1,4050)	1:85:B:GLN:HB2	1:88:B:SER:HB2	3	0.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4004)	1:72:B:LYS:HD3	1:110:B:VAL:HA	8	0.98
(1,4003)	1:72:A:LYS:HD3	1:110:A:VAL:HA	8	0.98
(1,3966)	1:72:B:LYS:HA	1:110:B:VAL:HG13	3	0.98
(1,3965)	1:72:A:LYS:HA	1:110:A:VAL:HG13	3	0.98
(1,3604)	1:115:B:LEU:HD13	1:116:B:MET:HE2	1	0.98
(1,3604)	1:115:B:LEU:HD11	1:116:B:MET:HE2	2	0.98
(1,3603)	1:115:A:LEU:HD13	1:116:A:MET:HE2	1	0.98
(1,3603)	1:115:A:LEU:HD11	1:116:A:MET:HE2	2	0.98
(1,2824)	1:54:B:ALA:HB1	1:55:B:LYS:HB2	5	0.98
(1,2344)	1:89:B:VAL:HB	1:79:B:GLN:HE22	4	0.98
(1,2343)	1:89:A:VAL:HB	1:79:A:GLN:HE22	4	0.98
(1,46)	1:89:B:VAL:HG13	1:85:B:GLN:H	2	0.98
(3,3092)	1:127:B:TYR:HE1	1:104:B:PHE:HB3	2	0.97
(3,3091)	1:127:A:TYR:HE1	1:104:A:PHE:HB3	2	0.97
(3,2926)	1:126:B:GLY:HA3	1:50:A:PRO:HG3	3	0.97
(3,2632)	1:105:B:GLN:HG3	1:110:B:VAL:HG22	4	0.97
(3,2632)	1:105:B:GLN:HG3	1:110:B:VAL:HG22	10	0.97
(3,2631)	1:105:A:GLN:HG3	1:110:A:VAL:HG22	4	0.97
(3,2631)	1:105:A:GLN:HG3	1:110:A:VAL:HG22	10	0.97
(3,2220)	1:93:B:ARG:HD2	1:66:B:LEU:HB3	1	0.97
(3,2219)	1:93:A:ARG:HD2	1:66:A:LEU:HB3	1	0.97
(3,2111)	1:87:A:THR:HG21	1:124:A:LYS:HB2	3	0.97
(3,1849)	1:73:A:GLN:HB3	1:140:A:LYS:HE2	4	0.97
(3,1646)	1:115:B:LEU:HD12	1:116:B:MET:HG2	8	0.97
(3,1645)	1:115:A:LEU:HD12	1:116:A:MET:HG2	8	0.97
(3,1608)	1:65:B:PHE:HB2	1:136:B:GLU:HG3	5	0.97
(3,1607)	1:65:A:PHE:HB2	1:136:A:GLU:HG3	5	0.97
(3,604)	1:87:B:THR:H	1:119:B:MET:H	4	0.97
(3,603)	1:87:A:THR:H	1:119:A:MET:H	4	0.97
(3,582)	1:72:B:LYS:HD3	1:116:B:MET:H	10	0.97
(3,462)	1:102:B:ILE:HG21	1:101:B:THR:H	7	0.97
(1,5528)	1:115:B:LEU:HD21	1:68:B:VAL:HA	5	0.97
(1,5527)	1:115:A:LEU:HD21	1:68:A:VAL:HA	5	0.97
(1,5238)	1:105:B:GLN:HB2	1:101:B:THR:HG22	4	0.97
(1,5237)	1:105:A:GLN:HB2	1:101:A:THR:HG22	4	0.97
(1,4810)	1:96:B:ALA:HB1	1:100:B:THR:HB	10	0.97
(1,4809)	1:96:A:ALA:HB1	1:100:A:THR:HB	10	0.97
(1,4718)	1:92:B:GLN:HG2	1:102:B:ILE:HG13	4	0.97
(1,4717)	1:92:A:GLN:HG2	1:102:A:ILE:HG13	4	0.97
(1,4504)	1:86:B:LEU:HB2	1:121:B:THR:HG22	6	0.97
(1,4503)	1:86:A:LEU:HB2	1:121:A:THR:HG22	6	0.97
(1,4132)	1:74:B:LEU:HB3	1:119:B:MET:HE2	2	0.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4131)	1:74:A:LEU:HB3	1:119:A:MET:HE2	2	0.97
(1,3506)	1:120:B:ASP:HB3	1:116:B:MET:HB2	2	0.97
(1,1862)	1:110:B:VAL:HG11	1:118:B:VAL:H	5	0.97
(1,46)	1:89:B:VAL:HG11	1:85:B:GLN:H	9	0.97
(1,45)	1:89:A:VAL:HG12	1:85:A:GLN:H	8	0.97
(1,45)	1:89:A:VAL:HG11	1:85:A:GLN:H	9	0.97
(3,3078)	1:104:B:PHE:HD1	1:139:B:ALA:HB1	3	0.96
(3,3077)	1:104:A:PHE:HD1	1:139:A:ALA:HB1	3	0.96
(3,2938)	1:127:B:TYR:HB2	1:45:B:ILE:HD11	10	0.96
(3,2937)	1:127:A:TYR:HB2	1:45:A:ILE:HD11	10	0.96
(3,2836)	1:116:B:MET:HE3	1:120:B:ASP:HA	9	0.96
(3,2835)	1:116:A:MET:HE3	1:120:A:ASP:HA	9	0.96
(3,2821)	1:113:A:GLU:HG2	1:115:A:LEU:HD23	8	0.96
(3,2354)	1:98:B:LYS:HG2	1:96:B:ALA:HB1	5	0.96
(3,2353)	1:98:A:LYS:HG2	1:96:A:ALA:HB1	5	0.96
(3,2199)	1:92:A:GLN:HG2	1:87:A:THR:HG23	4	0.96
(3,2112)	1:87:B:THR:HG21	1:124:B:LYS:HB2	3	0.96
(3,2112)	1:87:B:THR:HG22	1:124:B:LYS:HB2	7	0.96
(3,2111)	1:87:A:THR:HG22	1:124:A:LYS:HB2	7	0.96
(3,2110)	1:87:B:THR:HG23	1:89:B:VAL:HB	2	0.96
(3,2110)	1:87:B:THR:HG23	1:89:B:VAL:HB	8	0.96
(3,2109)	1:87:A:THR:HG23	1:89:A:VAL:HB	2	0.96
(3,2109)	1:87:A:THR:HG23	1:89:A:VAL:HB	8	0.96
(3,1874)	1:105:B:GLN:HG3	1:119:B:MET:HE3	9	0.96
(3,1630)	1:66:B:LEU:HB3	1:140:B:LYS:HG3	2	0.96
(3,1629)	1:66:A:LEU:HB3	1:140:A:LYS:HG3	2	0.96
(3,1079)	1:56:A:PRO:HG3	1:50:A:PRO:HD2	6	0.96
(3,581)	1:72:A:LYS:HD3	1:116:A:MET:H	10	0.96
(3,264)	1:92:B:GLN:HG3	1:79:B:GLN:H	4	0.96
(3,263)	1:92:A:GLN:HG3	1:79:A:GLN:H	4	0.96
(1,5238)	1:105:B:GLN:HB2	1:101:B:THR:HG22	1	0.96
(1,5238)	1:105:B:GLN:HB2	1:101:B:THR:HG21	5	0.96
(1,5237)	1:105:A:GLN:HB2	1:101:A:THR:HG22	1	0.96
(1,5237)	1:105:A:GLN:HB2	1:101:A:THR:HG21	5	0.96
(1,4444)	1:79:B:GLN:HB2	1:65:B:PHE:HB3	1	0.96
(1,4444)	1:79:B:GLN:HB2	1:65:B:PHE:HB3	10	0.96
(1,4443)	1:79:A:GLN:HB2	1:65:A:PHE:HB3	10	0.96
(1,3855)	1:69:A:LYS:HD3	1:65:A:PHE:HB2	3	0.96
(1,3505)	1:120:A:ASP:HB3	1:116:A:MET:HB2	2	0.96
(1,3432)	1:64:B:VAL:HA	1:93:B:ARG:HG2	10	0.96
(1,3431)	1:64:A:VAL:HA	1:93:A:ARG:HG2	10	0.96
(1,2496)	1:45:B:ILE:HA	1:54:A:ALA:HB3	3	0.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2495)	1:45:A:ILE:HA	1:54:B:ALA:HB3	3	0.96
(1,2368)	1:84:B:ASP:HB2	1:85:B:GLN:HE22	4	0.96
(1,2086)	1:98:B:LYS:HD3	1:127:B:TYR:H	4	0.96
(1,2085)	1:98:A:LYS:HD3	1:127:A:TYR:H	4	0.96
(1,1995)	1:49:A:LEU:HB2	1:123:B:ARG:H	9	0.96
(1,1861)	1:110:A:VAL:HG11	1:118:A:VAL:H	5	0.96
(1,1860)	1:110:B:VAL:HG23	1:118:B:VAL:H	3	0.96
(1,1859)	1:110:A:VAL:HG23	1:118:A:VAL:H	3	0.96
(1,46)	1:89:B:VAL:HG12	1:85:B:GLN:H	8	0.96
(3,2914)	1:86:B:LEU:HB3	1:125:B:ALA:HA	4	0.95
(3,2913)	1:86:A:LEU:HB3	1:125:A:ALA:HA	4	0.95
(3,2474)	1:53:B:SER:HB2	1:45:A:ILE:HD13	3	0.95
(3,2473)	1:53:A:SER:HB2	1:45:B:ILE:HD13	3	0.95
(3,2200)	1:92:B:GLN:HG2	1:87:B:THR:HG23	4	0.95
(3,1873)	1:105:A:GLN:HG3	1:119:A:MET:HE3	9	0.95
(3,1080)	1:56:B:PRO:HG3	1:50:B:PRO:HD2	6	0.95
(3,978)	1:104:B:PHE:HB2	1:131:B:GLY:HA3	8	0.95
(3,977)	1:104:A:PHE:HB2	1:131:A:GLY:HA3	8	0.95
(3,846)	1:44:B:ASP:HA	1:105:A:GLN:HB3	5	0.95
(3,608)	1:134:B:GLY:HA3	1:119:A:MET:H	5	0.95
(3,582)	1:49:B:LEU:HG	1:116:A:MET:H	8	0.95
(3,581)	1:49:A:LEU:HG	1:116:B:MET:H	8	0.95
(3,461)	1:102:A:ILE:HG21	1:101:A:THR:H	7	0.95
(3,160)	1:58:B:PRO:HB2	1:62:B:LYS:H	4	0.95
(3,159)	1:58:A:PRO:HB2	1:62:A:LYS:H	4	0.95
(1,5528)	1:115:B:LEU:HD22	1:68:B:VAL:HA	6	0.95
(1,5527)	1:115:A:LEU:HD22	1:68:A:VAL:HA	6	0.95
(1,5308)	1:106:B:ALA:HB2	1:116:B:MET:HE3	7	0.95
(1,5307)	1:106:A:ALA:HB2	1:116:A:MET:HE3	7	0.95
(1,4810)	1:96:B:ALA:HB1	1:100:B:THR:HB	5	0.95
(1,4772)	1:94:B:THR:HG21	1:102:B:ILE:HG23	10	0.95
(1,4771)	1:94:A:THR:HG21	1:102:A:ILE:HG23	10	0.95
(1,4443)	1:79:A:GLN:HB2	1:65:A:PHE:HB3	1	0.95
(1,4012)	1:72:B:LYS:HD3	1:110:B:VAL:HG12	7	0.95
(1,4011)	1:72:A:LYS:HD3	1:110:A:VAL:HG12	7	0.95
(1,3856)	1:69:B:LYS:HD3	1:65:B:PHE:HB2	3	0.95
(1,3856)	1:69:B:LYS:HD3	1:65:B:PHE:HB2	8	0.95
(1,3855)	1:69:A:LYS:HD3	1:65:A:PHE:HB2	8	0.95
(1,3784)	1:68:B:VAL:HB	1:106:B:ALA:HB2	10	0.95
(1,3783)	1:68:A:VAL:HB	1:106:A:ALA:HB2	10	0.95
(1,3590)	1:115:B:LEU:HD12	1:112:B:TYR:HB3	10	0.95
(1,3589)	1:115:A:LEU:HD12	1:112:A:TYR:HB3	10	0.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2027)	1:98:A:LYS:HD3	1:125:A:ALA:H	3	0.95
(1,1996)	1:49:B:LEU:HB2	1:123:A:ARG:H	4	0.95
(1,1995)	1:49:A:LEU:HB2	1:123:B:ARG:H	4	0.95
(1,532)	1:102:B:ILE:HG22	1:65:B:PHE:H	2	0.95
(1,531)	1:102:A:ILE:HG22	1:65:A:PHE:H	2	0.95
(3,2844)	1:102:B:ILE:HG22	1:118:B:VAL:HA	1	0.94
(3,2843)	1:102:A:ILE:HG22	1:118:A:VAL:HA	1	0.94
(3,2632)	1:105:B:GLN:HG3	1:110:B:VAL:HG23	3	0.94
(3,2631)	1:105:A:GLN:HG3	1:110:A:VAL:HG23	3	0.94
(3,2464)	1:100:B:THR:HG23	1:102:B:ILE:HG23	6	0.94
(3,2463)	1:100:A:THR:HG23	1:102:A:ILE:HG23	6	0.94
(3,2353)	1:98:A:LYS:HG2	1:96:A:ALA:HB1	4	0.94
(3,2112)	1:87:B:THR:HG21	1:124:B:LYS:HB2	4	0.94
(3,2111)	1:87:A:THR:HG21	1:124:A:LYS:HB2	4	0.94
(3,1878)	1:105:B:GLN:HG3	1:110:B:VAL:HG13	7	0.94
(3,1877)	1:105:A:GLN:HG3	1:110:A:VAL:HG13	7	0.94
(3,1439)	1:136:A:GLU:HG3	1:105:A:GLN:HB3	1	0.94
(3,845)	1:44:A:ASP:HA	1:105:B:GLN:HB3	5	0.94
(3,816)	1:88:B:SER:HB3	1:79:B:GLN:HE22	1	0.94
(3,604)	1:87:B:THR:H	1:119:B:MET:H	1	0.94
(3,462)	1:102:B:ILE:HG22	1:101:B:THR:H	2	0.94
(3,461)	1:102:A:ILE:HG22	1:101:A:THR:H	2	0.94
(1,4862)	1:98:B:LYS:HD3	1:127:B:TYR:HB2	7	0.94
(1,4861)	1:98:A:LYS:HD3	1:127:A:TYR:HB2	7	0.94
(1,4809)	1:96:A:ALA:HB1	1:100:A:THR:HB	5	0.94
(1,4078)	1:105:B:GLN:HG3	1:137:B:GLY:HA3	8	0.94
(1,4050)	1:85:B:GLN:HB2	1:88:B:SER:HB2	7	0.94
(1,4049)	1:85:A:GLN:HB2	1:88:A:SER:HB2	7	0.94
(1,3351)	1:124:A:LYS:HG2	1:84:A:ASP:HB3	2	0.94
(1,2910)	1:55:B:LYS:HG3	1:58:B:PRO:HG2	2	0.94
(1,2367)	1:84:A:ASP:HB2	1:85:A:GLN:HE22	4	0.94
(1,2028)	1:98:B:LYS:HD3	1:125:B:ALA:H	3	0.94
(1,1996)	1:49:B:LEU:HB2	1:123:A:ARG:H	9	0.94
(3,2938)	1:127:B:TYR:HB2	1:45:B:ILE:HD13	8	0.93
(3,2937)	1:127:A:TYR:HB2	1:45:A:ILE:HD13	8	0.93
(3,2925)	1:126:A:GLY:HA3	1:50:B:PRO:HG3	3	0.93
(3,2904)	1:105:B:GLN:HB2	1:69:B:LYS:HD3	5	0.93
(3,2903)	1:105:A:GLN:HB2	1:69:A:LYS:HD3	5	0.93
(3,2534)	1:102:B:ILE:HG23	1:133:B:VAL:HB	2	0.93
(3,2533)	1:102:A:ILE:HG23	1:133:A:VAL:HB	2	0.93
(3,2474)	1:101:B:THR:HA	1:45:A:ILE:HG21	1	0.93
(3,2473)	1:101:A:THR:HA	1:45:B:ILE:HG21	1	0.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,2354)	1:98:B:LYS:HG2	1:96:B:ALA:HB1	4	0.93
(3,2288)	1:95:B:GLN:HG2	1:63:B:PRO:HB2	3	0.93
(3,2287)	1:95:A:GLN:HG2	1:63:A:PRO:HB2	3	0.93
(3,2200)	1:92:B:GLN:HG2	1:87:B:THR:HG22	6	0.93
(3,2199)	1:92:A:GLN:HG2	1:87:A:THR:HG22	6	0.93
(3,1440)	1:136:B:GLU:HG3	1:105:B:GLN:HB3	1	0.93
(3,815)	1:88:A:SER:HB3	1:79:A:GLN:HE22	1	0.93
(3,603)	1:87:A:THR:H	1:119:A:MET:H	1	0.93
(3,603)	1:87:A:THR:H	1:119:A:MET:H	10	0.93
(3,581)	1:49:A:LEU:HG	1:116:B:MET:H	3	0.93
(3,461)	1:102:A:ILE:HG22	1:101:A:THR:H	4	0.93
(3,150)	1:58:B:PRO:HB2	1:61:B:GLU:H	10	0.93
(1,5558)	1:116:B:MET:HE1	1:119:B:MET:HE3	6	0.93
(1,5557)	1:116:A:MET:HE1	1:119:A:MET:HE3	6	0.93
(1,5126)	1:102:B:ILE:HG23	1:66:B:LEU:HG	9	0.93
(1,5125)	1:102:A:ILE:HG23	1:66:A:LEU:HG	9	0.93
(1,4810)	1:96:B:ALA:HB3	1:100:B:THR:HB	2	0.93
(1,4809)	1:96:A:ALA:HB3	1:100:A:THR:HB	2	0.93
(1,4803)	1:96:A:ALA:HB1	1:127:A:TYR:HE1	1	0.93
(1,4772)	1:94:B:THR:HG23	1:102:B:ILE:HG23	8	0.93
(1,4771)	1:94:A:THR:HG23	1:102:A:ILE:HG23	8	0.93
(1,4751)	1:94:A:THR:HG23	1:96:A:ALA:HA	6	0.93
(1,4278)	1:93:B:ARG:HG2	1:65:B:PHE:HB3	6	0.93
(1,4077)	1:105:A:GLN:HG3	1:137:A:GLY:HA3	8	0.93
(1,4049)	1:85:A:GLN:HB2	1:88:A:SER:HB2	9	0.93
(1,3966)	1:72:B:LYS:HA	1:110:B:VAL:HG13	8	0.93
(1,3965)	1:72:A:LYS:HA	1:110:A:VAL:HG13	8	0.93
(1,3542)	1:66:B:LEU:HB2	1:106:B:ALA:HB1	5	0.93
(1,3352)	1:124:B:LYS:HG2	1:84:B:ASP:HB3	2	0.93
(1,2909)	1:55:A:LYS:HG3	1:58:A:PRO:HG2	2	0.93
(1,2841)	1:57:A:GLN:HA	1:60:A:PRO:HB3	5	0.93
(1,2816)	1:54:B:ALA:HB2	1:50:B:PRO:HD2	10	0.93
(1,2644)	1:125:B:ALA:HA	1:98:B:LYS:HD3	1	0.93
(1,796)	1:115:B:LEU:HD12	1:75:B:TYR:H	8	0.93
(1,796)	1:115:B:LEU:HD13	1:75:B:TYR:H	10	0.93
(3,3084)	1:112:B:TYR:HE1	1:116:B:MET:HE1	3	0.92
(3,3083)	1:112:A:TYR:HE1	1:116:A:MET:HE1	3	0.92
(3,3002)	1:135:B:MET:HA	1:116:A:MET:HE2	5	0.92
(3,3001)	1:135:A:MET:HA	1:116:B:MET:HE2	5	0.92
(3,2914)	1:86:B:LEU:HB3	1:125:B:ALA:HA	9	0.92
(3,2913)	1:86:A:LEU:HB3	1:125:A:ALA:HA	9	0.92
(3,2852)	1:49:B:LEU:HA	1:51:B:ALA:HB1	6	0.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,2851)	1:49:A:LEU:HA	1:51:A:ALA:HB1	6	0.92
(3,2844)	1:115:B:LEU:HD22	1:118:B:VAL:HA	2	0.92
(3,2843)	1:115:A:LEU:HD22	1:118:A:VAL:HA	2	0.92
(3,2834)	1:112:B:TYR:HE1	1:116:B:MET:HE1	3	0.92
(3,2833)	1:112:A:TYR:HE1	1:116:A:MET:HE1	3	0.92
(3,2640)	1:116:B:MET:HG2	1:110:A:VAL:HA	3	0.92
(3,2639)	1:116:A:MET:HG2	1:110:B:VAL:HA	3	0.92
(3,2632)	1:105:B:GLN:HG3	1:110:B:VAL:HG22	1	0.92
(3,2631)	1:105:A:GLN:HG3	1:110:A:VAL:HG22	1	0.92
(3,2220)	1:93:B:ARG:HD3	1:66:B:LEU:HB3	5	0.92
(3,2219)	1:93:A:ARG:HD3	1:66:A:LEU:HB3	5	0.92
(3,2109)	1:87:A:THR:HG21	1:89:A:VAL:HB	6	0.92
(3,1893)	1:123:A:ARG:HG2	1:124:A:LYS:HE2	8	0.92
(3,1646)	1:115:B:LEU:HD13	1:116:B:MET:HG2	6	0.92
(3,1645)	1:115:A:LEU:HD13	1:116:A:MET:HG2	6	0.92
(3,1292)	1:119:B:MET:HB2	1:123:B:ARG:HA	10	0.92
(3,1291)	1:119:A:MET:HB2	1:123:A:ARG:HA	10	0.92
(3,1102)	1:138:B:ALA:HA	1:136:B:GLU:HG3	2	0.92
(3,846)	1:44:B:ASP:HA	1:105:A:GLN:HB3	4	0.92
(3,604)	1:87:B:THR:H	1:119:B:MET:H	7	0.92
(3,604)	1:87:B:THR:H	1:119:B:MET:H	10	0.92
(3,603)	1:87:A:THR:H	1:119:A:MET:H	7	0.92
(3,462)	1:102:B:ILE:HG22	1:101:B:THR:H	4	0.92
(3,351)	1:98:A:LYS:HG2	1:90:A:LEU:H	10	0.92
(3,149)	1:58:A:PRO:HB2	1:61:A:GLU:H	10	0.92
(1,5406)	1:110:B:VAL:HG11	1:104:B:PHE:HZ	8	0.92
(1,5405)	1:110:A:VAL:HG11	1:104:A:PHE:HZ	8	0.92
(1,4804)	1:96:B:ALA:HB1	1:127:B:TYR:HE1	1	0.92
(1,4752)	1:94:B:THR:HG23	1:96:B:ALA:HA	6	0.92
(1,4496)	1:115:B:LEU:HB3	1:106:B:ALA:HB1	4	0.92
(1,4495)	1:115:A:LEU:HB3	1:106:A:ALA:HB1	4	0.92
(1,4277)	1:93:A:ARG:HG2	1:65:A:PHE:HB3	6	0.92
(1,4049)	1:85:A:GLN:HB2	1:88:A:SER:HB2	8	0.92
(1,3577)	1:66:A:LEU:HA	1:115:A:LEU:HD13	4	0.92
(1,3541)	1:66:A:LEU:HB2	1:106:A:ALA:HB1	5	0.92
(1,3022)	1:56:B:PRO:HD2	1:57:B:GLN:HG3	8	0.92
(1,3021)	1:56:A:PRO:HD2	1:57:A:GLN:HG3	8	0.92
(1,2974)	1:56:B:PRO:HD2	1:50:B:PRO:HD2	10	0.92
(1,2973)	1:56:A:PRO:HD2	1:50:A:PRO:HD2	10	0.92
(1,2842)	1:57:B:GLN:HA	1:60:B:PRO:HB3	5	0.92
(1,2815)	1:54:A:ALA:HB2	1:50:A:PRO:HD2	10	0.92
(1,2643)	1:125:A:ALA:HA	1:98:A:LYS:HD3	1	0.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2496)	1:45:B:ILE:HA	1:54:A:ALA:HB1	2	0.92
(1,2085)	1:98:A:LYS:HD3	1:127:A:TYR:H	5	0.92
(1,795)	1:115:A:LEU:HD12	1:75:A:TYR:H	8	0.92
(1,795)	1:115:A:LEU:HD13	1:75:A:TYR:H	10	0.92
(3,2904)	1:105:B:GLN:HB2	1:69:B:LYS:HD3	8	0.91
(3,2903)	1:105:A:GLN:HB2	1:69:A:LYS:HD3	8	0.91
(3,2296)	1:96:B:ALA:HA	1:100:B:THR:HG23	1	0.91
(3,2295)	1:96:A:ALA:HA	1:100:A:THR:HG23	1	0.91
(3,2110)	1:87:B:THR:HG21	1:89:B:VAL:HB	6	0.91
(3,1894)	1:123:B:ARG:HG2	1:124:B:LYS:HE2	8	0.91
(3,1824)	1:129:B:LYS:HD2	1:45:B:ILE:HG21	9	0.91
(3,1824)	1:129:B:LYS:HD2	1:45:B:ILE:HG22	10	0.91
(3,1823)	1:129:A:LYS:HD2	1:45:A:ILE:HG21	9	0.91
(3,1823)	1:129:A:LYS:HD2	1:45:A:ILE:HG22	10	0.91
(3,1806)	1:98:B:LYS:HE2	1:124:B:LYS:HD2	2	0.91
(3,1805)	1:98:A:LYS:HE2	1:124:A:LYS:HD2	2	0.91
(3,1646)	1:115:B:LEU:HD13	1:116:B:MET:HG2	5	0.91
(3,1645)	1:115:A:LEU:HD13	1:116:A:MET:HG2	5	0.91
(3,1101)	1:138:A:ALA:HA	1:136:A:GLU:HG3	2	0.91
(3,846)	1:44:B:ASP:HA	1:116:B:MET:HG3	10	0.91
(3,845)	1:44:A:ASP:HA	1:116:A:MET:HG3	10	0.91
(3,607)	1:134:A:GLY:HA3	1:119:B:MET:H	5	0.91
(3,582)	1:49:B:LEU:HG	1:116:A:MET:H	3	0.91
(3,461)	1:102:A:ILE:HG23	1:101:A:THR:H	8	0.91
(3,352)	1:98:B:LYS:HG2	1:90:B:LEU:H	10	0.91
(3,149)	1:58:A:PRO:HB2	1:61:A:GLU:H	3	0.91
(1,5066)	1:115:B:LEU:HD13	1:119:B:MET:HA	5	0.91
(1,4804)	1:96:B:ALA:HB2	1:127:B:TYR:HE2	2	0.91
(1,4752)	1:94:B:THR:HG23	1:96:B:ALA:HA	7	0.91
(1,4751)	1:94:A:THR:HG23	1:96:A:ALA:HA	7	0.91
(1,4718)	1:92:B:GLN:HG2	1:102:B:ILE:HG13	7	0.91
(1,4717)	1:92:A:GLN:HG2	1:102:A:ILE:HG13	7	0.91
(1,4050)	1:85:B:GLN:HB2	1:88:B:SER:HB2	5	0.91
(1,4050)	1:85:B:GLN:HB2	1:88:B:SER:HB2	8	0.91
(1,4050)	1:85:B:GLN:HB2	1:88:B:SER:HB2	9	0.91
(1,4049)	1:85:A:GLN:HB2	1:88:A:SER:HB2	5	0.91
(1,3784)	1:68:B:VAL:HB	1:106:B:ALA:HB2	5	0.91
(1,3578)	1:66:B:LEU:HA	1:115:B:LEU:HD13	4	0.91
(1,3432)	1:64:B:VAL:HA	1:93:B:ARG:HG2	4	0.91
(1,3431)	1:64:A:VAL:HA	1:93:A:ARG:HG2	4	0.91
(1,3352)	1:124:B:LYS:HG2	1:84:B:ASP:HB3	9	0.91
(1,3351)	1:124:A:LYS:HG2	1:84:A:ASP:HB3	9	0.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3022)	1:56:B:PRO:HD2	1:57:B:GLN:HG3	4	0.91
(1,2086)	1:98:B:LYS:HD3	1:127:B:TYR:H	5	0.91
(1,1558)	1:115:B:LEU:HD12	1:105:B:GLN:H	2	0.91
(1,1557)	1:115:A:LEU:HD12	1:105:A:GLN:H	2	0.91
(3,3100)	1:127:B:TYR:HE2	1:129:B:LYS:HD2	3	0.9
(3,3084)	1:112:B:TYR:HE1	1:116:B:MET:HE2	6	0.9
(3,3083)	1:112:A:TYR:HE1	1:116:A:MET:HE2	6	0.9
(3,2944)	1:128:B:LEU:HA	1:125:B:ALA:HB1	7	0.9
(3,2943)	1:128:A:LEU:HA	1:125:A:ALA:HB1	7	0.9
(3,2834)	1:112:B:TYR:HE1	1:116:B:MET:HE2	6	0.9
(3,2833)	1:112:A:TYR:HE1	1:116:A:MET:HE2	6	0.9
(3,2354)	1:98:B:LYS:HG2	1:96:B:ALA:HB3	6	0.9
(3,2353)	1:98:A:LYS:HG2	1:96:A:ALA:HB3	6	0.9
(3,2110)	1:87:B:THR:HG23	1:89:B:VAL:HB	7	0.9
(3,2109)	1:87:A:THR:HG23	1:89:A:VAL:HB	7	0.9
(3,978)	1:104:B:PHE:HB2	1:131:B:GLY:HA3	9	0.9
(3,977)	1:104:A:PHE:HB2	1:131:A:GLY:HA3	9	0.9
(3,845)	1:44:A:ASP:HA	1:105:B:GLN:HB3	4	0.9
(3,462)	1:102:B:ILE:HG23	1:101:B:THR:H	8	0.9
(3,351)	1:98:A:LYS:HG2	1:90:A:LEU:H	9	0.9
(3,150)	1:58:B:PRO:HB2	1:61:B:GLU:H	3	0.9
(1,5929)	1:112:A:TYR:HE2	1:110:B:VAL:HG12	8	0.9
(1,5809)	1:134:A:GLY:HA3	1:116:B:MET:HE2	6	0.9
(1,5608)	1:51:B:ALA:HB3	1:124:A:LYS:HA	5	0.9
(1,5065)	1:115:A:LEU:HD13	1:119:A:MET:HA	5	0.9
(1,4803)	1:96:A:ALA:HB2	1:127:A:TYR:HE2	2	0.9
(1,4718)	1:92:B:GLN:HG2	1:102:B:ILE:HG13	2	0.9
(1,4717)	1:92:A:GLN:HG2	1:102:A:ILE:HG13	2	0.9
(1,4496)	1:115:B:LEU:HB3	1:106:B:ALA:HB3	7	0.9
(1,4495)	1:115:A:LEU:HB3	1:106:A:ALA:HB3	7	0.9
(1,3783)	1:68:A:VAL:HB	1:106:A:ALA:HB2	5	0.9
(1,3604)	1:115:B:LEU:HD11	1:116:B:MET:HE2	3	0.9
(1,3603)	1:115:A:LEU:HD11	1:116:A:MET:HE2	3	0.9
(1,3021)	1:56:A:PRO:HD2	1:57:A:GLN:HG3	4	0.9
(1,2495)	1:45:A:ILE:HA	1:54:B:ALA:HB1	2	0.9
(1,2352)	1:85:B:GLN:HE22	1:82:B:ASN:HD21	3	0.9
(1,2351)	1:85:A:GLN:HE22	1:82:A:ASN:HD21	3	0.9
(1,2044)	1:98:B:LYS:HD3	1:126:B:GLY:H	2	0.9
(1,2043)	1:98:A:LYS:HD3	1:126:A:GLY:H	7	0.9
(1,1996)	1:49:B:LEU:HB2	1:123:A:ARG:H	8	0.9
(1,1995)	1:49:A:LEU:HB2	1:123:B:ARG:H	8	0.9
(1,1764)	1:118:B:VAL:HG12	1:115:B:LEU:H	4	0.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,796)	1:115:B:LEU:HD13	1:75:B:TYR:H	1	0.9
(1,795)	1:115:A:LEU:HD13	1:75:A:TYR:H	1	0.9
(3,3099)	1:127:A:TYR:HE2	1:129:A:LYS:HD2	3	0.89
(3,2913)	1:86:A:LEU:HB3	1:125:A:ALA:HA	3	0.89
(3,2514)	1:129:B:LYS:HD2	1:102:B:ILE:HG13	1	0.89
(3,2514)	1:129:B:LYS:HD2	1:102:B:ILE:HG13	9	0.89
(3,2513)	1:129:A:LYS:HD2	1:102:A:ILE:HG13	1	0.89
(3,1776)	1:71:B:ASP:HA	1:111:B:ASP:HB2	6	0.89
(3,1490)	1:129:B:LYS:HG2	1:46:A:ARG:HB3	8	0.89
(3,1403)	1:122:A:LEU:HA	1:49:B:LEU:HB3	8	0.89
(3,1079)	1:56:A:PRO:HG3	1:50:A:PRO:HD2	5	0.89
(3,880)	1:69:B:LYS:HB2	1:140:B:LYS:HE3	9	0.89
(3,879)	1:69:A:LYS:HB2	1:140:A:LYS:HE3	9	0.89
(3,462)	1:102:B:ILE:HG23	1:101:B:THR:H	1	0.89
(3,352)	1:98:B:LYS:HG2	1:90:B:LEU:H	9	0.89
(3,171)	1:46:A:ARG:HB2	1:64:B:VAL:H	2	0.89
(1,5929)	1:112:A:TYR:HE1	1:110:B:VAL:HG12	9	0.89
(1,5926)	1:112:B:TYR:HE2	1:113:B:GLU:HB3	3	0.89
(1,5925)	1:112:A:TYR:HE2	1:113:A:GLU:HB3	3	0.89
(1,5810)	1:134:B:GLY:HA3	1:116:A:MET:HE2	6	0.89
(1,5690)	1:126:B:GLY:HA3	1:98:B:LYS:HD3	2	0.89
(1,5689)	1:126:A:GLY:HA3	1:98:A:LYS:HD3	2	0.89
(1,5646)	1:124:B:LYS:HG3	1:124:B:LYS:HE3	1	0.89
(1,5645)	1:124:A:LYS:HG3	1:124:A:LYS:HE3	1	0.89
(1,5622)	1:119:B:MET:HE3	1:121:B:THR:HB	3	0.89
(1,5621)	1:119:A:MET:HE3	1:121:A:THR:HB	3	0.89
(1,5238)	1:105:B:GLN:HB2	1:101:B:THR:HG21	3	0.89
(1,5237)	1:105:A:GLN:HB2	1:101:A:THR:HG21	3	0.89
(1,4808)	1:96:B:ALA:HB1	1:127:B:TYR:HA	9	0.89
(1,4807)	1:96:A:ALA:HB1	1:127:A:TYR:HA	9	0.89
(1,4752)	1:94:B:THR:HG23	1:96:B:ALA:HA	2	0.89
(1,4751)	1:94:A:THR:HG23	1:96:A:ALA:HA	2	0.89
(1,4134)	1:74:B:LEU:HB3	1:110:B:VAL:HG13	2	0.89
(1,4006)	1:72:B:LYS:HD3	1:107:B:ASP:HB3	5	0.89
(1,4005)	1:72:A:LYS:HD3	1:107:A:ASP:HB3	5	0.89
(1,3239)	1:99:A:GLU:HG2	1:49:B:LEU:HB3	2	0.89
(1,2644)	1:125:B:ALA:HA	1:98:B:LYS:HD3	7	0.89
(1,2353)	1:85:A:GLN:HE22	1:82:A:ASN:HD22	7	0.89
(1,2044)	1:98:B:LYS:HD3	1:126:B:GLY:H	7	0.89
(1,2043)	1:98:A:LYS:HD3	1:126:A:GLY:H	2	0.89
(1,1861)	1:110:A:VAL:HG11	1:118:A:VAL:H	9	0.89
(1,1763)	1:118:A:VAL:HG12	1:115:A:LEU:H	4	0.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,46)	1:89:B:VAL:HG12	1:85:B:GLN:H	3	0.89
(1,45)	1:89:A:VAL:HG12	1:85:A:GLN:H	3	0.89
(3,2914)	1:86:B:LEU:HB3	1:125:B:ALA:HA	3	0.88
(3,2632)	1:105:B:GLN:HG3	1:110:B:VAL:HG23	6	0.88
(3,2631)	1:105:A:GLN:HG3	1:110:A:VAL:HG23	6	0.88
(3,2513)	1:129:A:LYS:HD2	1:102:A:ILE:HG13	9	0.88
(3,2454)	1:94:B:THR:HG21	1:64:B:VAL:HB	8	0.88
(3,2453)	1:94:A:THR:HG21	1:64:A:VAL:HB	8	0.88
(3,2200)	1:92:B:GLN:HG2	1:87:B:THR:HG21	7	0.88
(3,2199)	1:92:A:GLN:HG2	1:87:A:THR:HG21	7	0.88
(3,1775)	1:71:A:ASP:HA	1:111:A:ASP:HB2	6	0.88
(3,1080)	1:56:B:PRO:HG3	1:50:B:PRO:HD2	5	0.88
(3,854)	1:88:B:SER:HA	1:124:B:LYS:HE3	9	0.88
(3,853)	1:88:A:SER:HA	1:124:A:LYS:HE3	9	0.88
(3,489)	1:132:A:LEU:HG	1:105:A:GLN:H	4	0.88
(3,461)	1:102:A:ILE:HG23	1:101:A:THR:H	1	0.88
(3,286)	1:124:B:LYS:HG2	1:84:B:ASP:H	5	0.88
(3,285)	1:124:A:LYS:HG2	1:84:A:ASP:H	5	0.88
(1,5930)	1:112:B:TYR:HE2	1:110:A:VAL:HG12	8	0.88
(1,5646)	1:124:B:LYS:HG3	1:124:B:LYS:HE3	7	0.88
(1,5646)	1:124:B:LYS:HG3	1:124:B:LYS:HE3	8	0.88
(1,5646)	1:124:B:LYS:HG3	1:124:B:LYS:HE3	10	0.88
(1,5645)	1:124:A:LYS:HG3	1:124:A:LYS:HE3	7	0.88
(1,5645)	1:124:A:LYS:HG3	1:124:A:LYS:HE3	8	0.88
(1,5066)	1:115:B:LEU:HD12	1:119:B:MET:HA	8	0.88
(1,5065)	1:115:A:LEU:HD12	1:119:A:MET:HA	8	0.88
(1,4133)	1:74:A:LEU:HB3	1:110:A:VAL:HG13	2	0.88
(1,4010)	1:72:B:LYS:HD3	1:110:B:VAL:HG21	3	0.88
(1,4004)	1:72:B:LYS:HD3	1:110:B:VAL:HA	9	0.88
(1,4003)	1:72:A:LYS:HD3	1:110:A:VAL:HA	9	0.88
(1,3966)	1:72:B:LYS:HA	1:110:B:VAL:HG12	4	0.88
(1,3965)	1:72:A:LYS:HA	1:110:A:VAL:HG12	4	0.88
(1,2643)	1:125:A:ALA:HA	1:98:A:LYS:HD3	7	0.88
(1,2559)	1:45:A:ILE:HG22	1:54:B:ALA:HB2	4	0.88
(1,2559)	1:45:A:ILE:HG23	1:54:B:ALA:HB2	5	0.88
(1,2354)	1:85:B:GLN:HE22	1:82:B:ASN:HD22	7	0.88
(1,1862)	1:110:B:VAL:HG11	1:118:B:VAL:H	9	0.88
(1,1764)	1:118:B:VAL:HG11	1:115:B:LEU:H	3	0.88
(1,1764)	1:118:B:VAL:HG13	1:115:B:LEU:H	7	0.88
(1,1763)	1:118:A:VAL:HG11	1:115:A:LEU:H	3	0.88
(1,531)	1:102:A:ILE:HG22	1:65:A:PHE:H	5	0.88
(3,3006)	1:106:B:ALA:HB1	1:135:B:MET:HG2	3	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,3005)	1:106:A:ALA:HB1	1:135:A:MET:HG2	3	0.87
(3,2852)	1:49:B:LEU:HA	1:51:B:ALA:HB1	2	0.87
(3,2851)	1:49:A:LEU:HA	1:51:A:ALA:HB1	2	0.87
(3,2128)	1:87:B:THR:HG22	1:88:B:SER:HB2	4	0.87
(3,1878)	1:105:B:GLN:HG3	1:110:B:VAL:HG13	2	0.87
(3,1877)	1:105:A:GLN:HG3	1:110:A:VAL:HG13	2	0.87
(3,1806)	1:98:B:LYS:HE2	1:124:B:LYS:HD2	9	0.87
(3,1805)	1:98:A:LYS:HE2	1:124:A:LYS:HD2	9	0.87
(3,1759)	1:69:A:LYS:HE2	1:73:A:GLN:HG2	8	0.87
(3,1489)	1:129:A:LYS:HG2	1:46:B:ARG:HB3	8	0.87
(3,1404)	1:122:B:LEU:HA	1:49:A:LEU:HB3	8	0.87
(3,1286)	1:57:B:GLN:HG3	1:129:B:LYS:HD2	7	0.87
(3,1285)	1:57:A:GLN:HG3	1:129:A:LYS:HD2	7	0.87
(3,1080)	1:56:B:PRO:HG2	1:50:B:PRO:HD2	2	0.87
(3,1079)	1:56:A:PRO:HG2	1:50:A:PRO:HD2	2	0.87
(3,869)	1:43:A:VAL:HB	1:56:B:PRO:HD3	6	0.87
(3,862)	1:117:B:SER:HA	1:115:B:LEU:HG	6	0.87
(3,862)	1:117:B:SER:HA	1:115:B:LEU:HG	7	0.87
(3,861)	1:117:A:SER:HA	1:115:A:LEU:HG	6	0.87
(3,861)	1:117:A:SER:HA	1:115:A:LEU:HG	7	0.87
(3,490)	1:132:B:LEU:HG	1:105:B:GLN:H	4	0.87
(3,172)	1:46:B:ARG:HB2	1:64:A:VAL:H	2	0.87
(1,5930)	1:112:B:TYR:HE1	1:110:A:VAL:HG12	9	0.87
(1,5645)	1:124:A:LYS:HG3	1:124:A:LYS:HE3	10	0.87
(1,5582)	1:118:B:VAL:HB	1:83:B:ALA:HB1	8	0.87
(1,5581)	1:118:A:VAL:HB	1:83:A:ALA:HB1	8	0.87
(1,5530)	1:115:B:LEU:HD22	1:135:B:MET:HA	1	0.87
(1,5529)	1:115:A:LEU:HD22	1:135:A:MET:HA	1	0.87
(1,5406)	1:110:B:VAL:HG12	1:104:B:PHE:HZ	10	0.87
(1,5405)	1:110:A:VAL:HG12	1:104:A:PHE:HZ	10	0.87
(1,5066)	1:115:B:LEU:HD13	1:119:B:MET:HA	3	0.87
(1,4862)	1:98:B:LYS:HD3	1:127:B:TYR:HB2	2	0.87
(1,4861)	1:98:A:LYS:HD3	1:127:A:TYR:HB2	2	0.87
(1,4009)	1:72:A:LYS:HD3	1:110:A:VAL:HG21	3	0.87
(1,3968)	1:72:B:LYS:HB2	1:114:B:THR:HG23	2	0.87
(1,3506)	1:120:B:ASP:HB3	1:116:B:MET:HB2	1	0.87
(1,2910)	1:55:B:LYS:HG3	1:58:B:PRO:HG2	6	0.87
(1,2909)	1:55:A:LYS:HG3	1:58:A:PRO:HG2	6	0.87
(1,2560)	1:45:B:ILE:HG22	1:54:A:ALA:HB2	4	0.87
(1,2560)	1:45:B:ILE:HG23	1:54:A:ALA:HB2	5	0.87
(1,2496)	1:45:B:ILE:HA	1:54:A:ALA:HB3	8	0.87
(1,1763)	1:118:A:VAL:HG13	1:115:A:LEU:H	7	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,532)	1:102:B:ILE:HG22	1:65:B:PHE:H	5	0.87
(1,98)	1:106:B:ALA:HB2	1:107:B:ASP:H	10	0.87
(1,97)	1:106:A:ALA:HB2	1:107:A:ASP:H	10	0.87
(3,3001)	1:135:A:MET:HA	1:116:B:MET:HE1	6	0.86
(3,2944)	1:128:B:LEU:HA	1:125:B:ALA:HB3	6	0.86
(3,2944)	1:128:B:LEU:HA	1:125:B:ALA:HB1	10	0.86
(3,2943)	1:128:A:LEU:HA	1:125:A:ALA:HB3	6	0.86
(3,2943)	1:128:A:LEU:HA	1:125:A:ALA:HB1	10	0.86
(3,2914)	1:86:B:LEU:HB3	1:125:B:ALA:HA	8	0.86
(3,2913)	1:86:A:LEU:HB3	1:125:A:ALA:HA	8	0.86
(3,2821)	1:113:A:GLU:HG2	1:115:A:LEU:HD22	4	0.86
(3,2631)	1:105:A:GLN:HG3	1:110:A:VAL:HG22	5	0.86
(3,2463)	1:94:A:THR:HG21	1:102:A:ILE:HG22	9	0.86
(3,2128)	1:87:B:THR:HG22	1:88:B:SER:HB2	10	0.86
(3,2127)	1:87:A:THR:HG22	1:88:A:SER:HB2	4	0.86
(3,2127)	1:87:A:THR:HG22	1:88:A:SER:HB2	10	0.86
(3,1878)	1:105:B:GLN:HG3	1:110:B:VAL:HG11	3	0.86
(3,1877)	1:105:A:GLN:HG3	1:110:A:VAL:HG11	3	0.86
(3,1830)	1:58:B:PRO:HG2	1:55:B:LYS:HE3	9	0.86
(3,1829)	1:58:A:PRO:HG2	1:55:A:LYS:HE3	9	0.86
(3,1760)	1:69:B:LYS:HE2	1:73:B:GLN:HG2	8	0.86
(3,880)	1:69:B:LYS:HB2	1:140:B:LYS:HE3	7	0.86
(3,879)	1:69:A:LYS:HB2	1:140:A:LYS:HE3	7	0.86
(3,604)	1:87:B:THR:H	1:119:B:MET:H	9	0.86
(3,603)	1:87:A:THR:H	1:119:A:MET:H	9	0.86
(3,461)	1:102:A:ILE:HG22	1:101:A:THR:H	3	0.86
(3,460)	1:49:B:LEU:HB2	1:122:A:LEU:H	10	0.86
(3,459)	1:49:A:LEU:HB2	1:122:B:LEU:H	10	0.86
(1,5646)	1:124:B:LYS:HG3	1:124:B:LYS:HE3	2	0.86
(1,5646)	1:124:B:LYS:HG3	1:124:B:LYS:HE3	6	0.86
(1,5646)	1:124:B:LYS:HG3	1:124:B:LYS:HE3	9	0.86
(1,5645)	1:124:A:LYS:HG3	1:124:A:LYS:HE3	6	0.86
(1,5645)	1:124:A:LYS:HG3	1:124:A:LYS:HE3	9	0.86
(1,5607)	1:51:A:ALA:HB3	1:124:B:LYS:HA	5	0.86
(1,5406)	1:110:B:VAL:HG11	1:104:B:PHE:HZ	3	0.86
(1,5405)	1:110:A:VAL:HG11	1:104:A:PHE:HZ	3	0.86
(1,5238)	1:105:B:GLN:HB2	1:101:B:THR:HG21	10	0.86
(1,5237)	1:105:A:GLN:HB2	1:101:A:THR:HG21	10	0.86
(1,5065)	1:115:A:LEU:HD13	1:119:A:MET:HA	3	0.86
(1,3967)	1:72:A:LYS:HB2	1:114:A:THR:HG23	2	0.86
(1,3778)	1:68:B:VAL:HB	1:114:B:THR:HG22	10	0.86
(1,3777)	1:68:A:VAL:HB	1:114:A:THR:HG22	10	0.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3505)	1:120:A:ASP:HB3	1:116:A:MET:HB2	1	0.86
(1,3240)	1:99:B:GLU:HG2	1:49:A:LEU:HB3	2	0.86
(1,2587)	1:46:A:ARG:HG2	1:129:B:LYS:HG3	5	0.86
(1,2495)	1:45:A:ILE:HA	1:54:B:ALA:HB3	8	0.86
(1,1116)	1:89:B:VAL:HB	1:90:B:LEU:H	1	0.86
(1,1115)	1:89:A:VAL:HB	1:90:A:LEU:H	1	0.86
(1,46)	1:89:B:VAL:HG13	1:85:B:GLN:H	6	0.86
(1,45)	1:89:A:VAL:HG13	1:85:A:GLN:H	6	0.86
(3,3100)	1:75:B:TYR:HE2	1:140:B:LYS:HD2	2	0.85
(3,3099)	1:75:A:TYR:HE2	1:140:A:LYS:HD2	2	0.85
(3,2822)	1:113:B:GLU:HG2	1:115:B:LEU:HD22	4	0.85
(3,2821)	1:113:A:GLU:HG2	1:115:A:LEU:HD21	6	0.85
(3,2821)	1:113:A:GLU:HG2	1:115:A:LEU:HD21	7	0.85
(3,2730)	1:110:B:VAL:HG23	1:119:B:MET:HE1	9	0.85
(3,2729)	1:110:A:VAL:HG23	1:119:A:MET:HE1	9	0.85
(3,2632)	1:105:B:GLN:HG3	1:110:B:VAL:HG22	5	0.85
(3,2464)	1:94:B:THR:HG21	1:102:B:ILE:HG22	9	0.85
(3,1776)	1:71:B:ASP:HA	1:111:B:ASP:HB2	7	0.85
(3,1775)	1:71:A:ASP:HA	1:111:A:ASP:HB2	7	0.85
(3,912)	1:45:B:ILE:HD13	1:46:B:ARG:HD2	4	0.85
(3,911)	1:45:A:ILE:HD13	1:46:A:ARG:HD2	4	0.85
(3,616)	1:49:B:LEU:HA	1:120:A:ASP:H	2	0.85
(3,615)	1:49:A:LEU:HA	1:120:B:ASP:H	2	0.85
(3,604)	1:87:B:THR:H	1:119:B:MET:H	3	0.85
(3,603)	1:87:A:THR:H	1:119:A:MET:H	3	0.85
(3,462)	1:102:B:ILE:HG22	1:101:B:THR:H	3	0.85
(3,462)	1:102:B:ILE:HG22	1:101:B:THR:H	5	0.85
(3,461)	1:102:A:ILE:HG22	1:101:A:THR:H	5	0.85
(1,5645)	1:124:A:LYS:HG3	1:124:A:LYS:HE3	2	0.85
(1,5607)	1:51:A:ALA:HB1	1:124:B:LYS:HA	3	0.85
(1,4803)	1:96:A:ALA:HB1	1:127:A:TYR:HE2	8	0.85
(1,4772)	1:94:B:THR:HG21	1:102:B:ILE:HG23	6	0.85
(1,4771)	1:94:A:THR:HG21	1:102:A:ILE:HG23	6	0.85
(1,4518)	1:86:B:LEU:HG	1:90:B:LEU:HG	10	0.85
(1,4006)	1:72:B:LYS:HD3	1:107:B:ASP:HB3	6	0.85
(1,3968)	1:72:B:LYS:HB2	1:114:B:THR:HG21	9	0.85
(1,3578)	1:66:B:LEU:HA	1:115:B:LEU:HD12	2	0.85
(1,3577)	1:66:A:LEU:HA	1:115:A:LEU:HD12	2	0.85
(1,2588)	1:46:B:ARG:HG2	1:129:A:LYS:HG3	5	0.85
(1,2126)	1:129:B:LYS:HD3	1:129:B:LYS:H	1	0.85
(1,2125)	1:129:A:LYS:HD3	1:129:A:LYS:H	1	0.85
(1,1862)	1:110:B:VAL:HG13	1:118:B:VAL:H	7	0.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1861)	1:110:A:VAL:HG13	1:118:A:VAL:H	7	0.85
(1,1861)	1:110:A:VAL:HG12	1:118:A:VAL:H	10	0.85
(1,1210)	1:89:B:VAL:HG23	1:93:B:ARG:H	6	0.85
(1,1209)	1:89:A:VAL:HG23	1:93:A:ARG:H	6	0.85
(3,2943)	1:128:A:LEU:HA	1:125:A:ALA:HB1	5	0.84
(3,2914)	1:86:B:LEU:HB3	1:125:B:ALA:HA	1	0.84
(3,2914)	1:86:B:LEU:HB3	1:125:B:ALA:HA	2	0.84
(3,2913)	1:86:A:LEU:HB3	1:125:A:ALA:HA	1	0.84
(3,2913)	1:86:A:LEU:HB3	1:125:A:ALA:HA	2	0.84
(3,2852)	1:119:B:MET:HE3	1:114:B:THR:HB	3	0.84
(3,2822)	1:113:B:GLU:HG2	1:115:B:LEU:HD21	6	0.84
(3,2822)	1:113:B:GLU:HG2	1:115:B:LEU:HD21	7	0.84
(3,2682)	1:108:B:LYS:HB2	1:112:B:TYR:HB3	10	0.84
(3,2681)	1:108:A:LYS:HB2	1:112:A:TYR:HB3	10	0.84
(3,2238)	1:90:B:LEU:HA	1:94:B:THR:HG23	4	0.84
(3,2237)	1:90:A:LEU:HA	1:94:A:THR:HG23	4	0.84
(3,2220)	1:93:B:ARG:HD2	1:66:B:LEU:HB3	8	0.84
(3,2219)	1:93:A:ARG:HD2	1:66:A:LEU:HB3	8	0.84
(3,2111)	1:87:A:THR:HG22	1:124:A:LYS:HB2	2	0.84
(3,1956)	1:79:B:GLN:HG2	1:91:B:ASP:HB3	6	0.84
(3,1955)	1:79:A:GLN:HG2	1:91:A:ASP:HB3	6	0.84
(3,1760)	1:69:B:LYS:HE2	1:73:B:GLN:HG2	3	0.84
(3,1759)	1:69:A:LYS:HE2	1:73:A:GLN:HG2	3	0.84
(3,1526)	1:132:B:LEU:HG	1:106:B:ALA:HB2	2	0.84
(3,1525)	1:132:A:LEU:HG	1:106:A:ALA:HB2	2	0.84
(3,1279)	1:57:A:GLN:HG2	1:60:A:PRO:HG3	1	0.84
(3,1106)	1:51:B:ALA:HA	1:124:A:LYS:HB3	2	0.84
(3,1105)	1:51:A:ALA:HA	1:124:B:LYS:HB3	2	0.84
(3,1080)	1:56:B:PRO:HG2	1:50:B:PRO:HD2	3	0.84
(3,1079)	1:56:A:PRO:HG2	1:50:A:PRO:HD2	3	0.84
(3,870)	1:43:B:VAL:HB	1:56:A:PRO:HD3	6	0.84
(3,816)	1:88:B:SER:HB3	1:79:B:GLN:HE22	9	0.84
(3,815)	1:88:A:SER:HB3	1:79:A:GLN:HE22	9	0.84
(3,459)	1:49:A:LEU:HB2	1:122:B:LEU:H	7	0.84
(1,5929)	1:112:A:TYR:HE2	1:110:B:VAL:HG11	2	0.84
(1,5809)	1:134:A:GLY:HA3	1:116:B:MET:HE3	7	0.84
(1,5646)	1:124:B:LYS:HG3	1:124:B:LYS:HE3	3	0.84
(1,5645)	1:124:A:LYS:HG3	1:124:A:LYS:HE3	3	0.84
(1,5622)	1:119:B:MET:HE1	1:121:B:THR:HB	7	0.84
(1,5621)	1:119:A:MET:HE1	1:121:A:THR:HB	7	0.84
(1,5126)	1:102:B:ILE:HG23	1:66:B:LEU:HG	2	0.84
(1,5125)	1:102:A:ILE:HG23	1:66:A:LEU:HG	2	0.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4853)	1:98:A:LYS:HD3	1:51:B:ALA:HA	8	0.84
(1,4808)	1:96:B:ALA:HB1	1:127:B:TYR:HA	5	0.84
(1,4804)	1:96:B:ALA:HB1	1:127:B:TYR:HE2	8	0.84
(1,4517)	1:86:A:LEU:HG	1:90:A:LEU:HG	10	0.84
(1,4005)	1:72:A:LYS:HD3	1:107:A:ASP:HB3	6	0.84
(1,3967)	1:72:A:LYS:HB2	1:114:A:THR:HG21	9	0.84
(1,3780)	1:68:B:VAL:HB	1:110:B:VAL:HG23	6	0.84
(1,3779)	1:68:A:VAL:HB	1:110:A:VAL:HG23	6	0.84
(1,3609)	1:115:A:LEU:HD13	1:110:A:VAL:HG23	9	0.84
(1,2264)	1:135:B:MET:HA	1:138:B:ALA:H	2	0.84
(1,2263)	1:135:A:MET:HA	1:138:A:ALA:H	2	0.84
(1,1996)	1:49:B:LEU:HB2	1:123:A:ARG:H	6	0.84
(1,1862)	1:110:B:VAL:HG12	1:118:B:VAL:H	10	0.84
(1,1764)	1:118:B:VAL:HG13	1:115:B:LEU:H	5	0.84
(1,1763)	1:118:A:VAL:HG13	1:115:A:LEU:H	5	0.84
(1,1557)	1:115:A:LEU:HD11	1:105:A:GLN:H	1	0.84
(1,1209)	1:89:A:VAL:HG23	1:93:A:ARG:H	2	0.84
(3,3059)	1:65:A:PHE:HE1	1:93:A:ARG:HB2	8	0.83
(3,2974)	1:130:B:VAL:HB	1:119:B:MET:HE3	7	0.83
(3,2973)	1:130:A:VAL:HB	1:119:A:MET:HE3	7	0.83
(3,2944)	1:128:B:LEU:HA	1:125:B:ALA:HB1	5	0.83
(3,2904)	1:105:B:GLN:HB2	1:69:B:LYS:HD3	1	0.83
(3,2903)	1:105:A:GLN:HB2	1:69:A:LYS:HD3	1	0.83
(3,2851)	1:119:A:MET:HE3	1:114:A:THR:HB	3	0.83
(3,2821)	1:113:A:GLU:HG2	1:115:A:LEU:HD23	5	0.83
(3,2464)	1:100:B:THR:HG21	1:102:B:ILE:HG21	7	0.83
(3,2463)	1:100:A:THR:HG21	1:102:A:ILE:HG21	7	0.83
(3,2200)	1:92:B:GLN:HG2	1:87:B:THR:HG23	3	0.83
(3,2199)	1:92:A:GLN:HG2	1:87:A:THR:HG23	3	0.83
(3,2112)	1:87:B:THR:HG22	1:124:B:LYS:HB2	2	0.83
(3,2112)	1:87:B:THR:HG22	1:124:B:LYS:HB2	8	0.83
(3,2111)	1:87:A:THR:HG22	1:124:A:LYS:HB2	8	0.83
(3,2110)	1:87:B:THR:HG23	1:89:B:VAL:HB	9	0.83
(3,2109)	1:87:A:THR:HG23	1:89:A:VAL:HB	9	0.83
(3,1873)	1:73:A:GLN:HG2	1:69:A:LYS:HD2	2	0.83
(3,1280)	1:57:B:GLN:HG2	1:60:B:PRO:HG3	1	0.83
(3,286)	1:124:B:LYS:HG2	1:84:B:ASP:H	6	0.83
(3,285)	1:124:A:LYS:HG2	1:84:A:ASP:H	7	0.83
(3,159)	1:58:A:PRO:HB2	1:62:A:LYS:H	2	0.83
(3,149)	1:58:A:PRO:HB2	1:61:A:GLU:H	6	0.83
(1,5930)	1:112:B:TYR:HE2	1:110:A:VAL:HG11	2	0.83
(1,5930)	1:112:B:TYR:HE2	1:110:A:VAL:HG12	3	0.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5929)	1:112:A:TYR:HE2	1:110:B:VAL:HG12	3	0.83
(1,5810)	1:134:B:GLY:HA3	1:116:A:MET:HE3	7	0.83
(1,5646)	1:124:B:LYS:HG3	1:124:B:LYS:HE3	4	0.83
(1,5645)	1:124:A:LYS:HG3	1:124:A:LYS:HE3	4	0.83
(1,5608)	1:51:B:ALA:HB1	1:124:A:LYS:HA	3	0.83
(1,5238)	1:105:B:GLN:HB2	1:101:B:THR:HG21	2	0.83
(1,5126)	1:102:B:ILE:HG23	1:66:B:LEU:HG	4	0.83
(1,5126)	1:102:B:ILE:HG21	1:66:B:LEU:HG	6	0.83
(1,5125)	1:102:A:ILE:HG23	1:66:A:LEU:HG	4	0.83
(1,5125)	1:102:A:ILE:HG21	1:66:A:LEU:HG	6	0.83
(1,4807)	1:96:A:ALA:HB1	1:127:A:TYR:HA	5	0.83
(1,4496)	1:115:B:LEU:HB3	1:106:B:ALA:HB2	1	0.83
(1,4495)	1:115:A:LEU:HB3	1:106:A:ALA:HB2	1	0.83
(1,3610)	1:115:B:LEU:HD13	1:110:B:VAL:HG23	9	0.83
(1,3542)	1:66:B:LEU:HB2	1:106:B:ALA:HB1	10	0.83
(1,3541)	1:66:A:LEU:HB2	1:106:A:ALA:HB1	10	0.83
(1,3506)	1:120:B:ASP:HB3	1:116:B:MET:HB2	10	0.83
(1,2027)	1:98:A:LYS:HD3	1:125:A:ALA:H	9	0.83
(1,1862)	1:110:B:VAL:HG13	1:118:B:VAL:H	6	0.83
(1,1861)	1:110:A:VAL:HG13	1:118:A:VAL:H	6	0.83
(1,1764)	1:118:B:VAL:HG13	1:115:B:LEU:H	1	0.83
(1,1764)	1:118:B:VAL:HG11	1:115:B:LEU:H	9	0.83
(1,1763)	1:118:A:VAL:HG13	1:115:A:LEU:H	1	0.83
(1,1763)	1:118:A:VAL:HG11	1:115:A:LEU:H	9	0.83
(1,1558)	1:115:B:LEU:HD11	1:105:B:GLN:H	1	0.83
(1,1557)	1:115:A:LEU:HD13	1:105:A:GLN:H	7	0.83
(1,1210)	1:89:B:VAL:HG23	1:93:B:ARG:H	2	0.83
(1,1210)	1:89:B:VAL:HG22	1:93:B:ARG:H	10	0.83
(1,1209)	1:89:A:VAL:HG22	1:93:A:ARG:H	10	0.83
(3,3060)	1:65:B:PHE:HE1	1:93:B:ARG:HB2	8	0.82
(3,3002)	1:135:B:MET:HA	1:116:A:MET:HE1	6	0.82
(3,2944)	1:128:B:LEU:HA	1:125:B:ALA:HB3	9	0.82
(3,2943)	1:128:A:LEU:HA	1:125:A:ALA:HB3	9	0.82
(3,2822)	1:113:B:GLU:HG2	1:115:B:LEU:HD23	5	0.82
(3,2730)	1:110:B:VAL:HG22	1:119:B:MET:HE1	2	0.82
(3,2730)	1:110:B:VAL:HG22	1:119:B:MET:HE2	10	0.82
(3,2729)	1:110:A:VAL:HG22	1:119:A:MET:HE1	2	0.82
(3,2729)	1:110:A:VAL:HG22	1:119:A:MET:HE2	10	0.82
(3,2555)	1:103:A:PHE:HA	1:45:B:ILE:HG23	6	0.82
(3,2474)	1:101:B:THR:HA	1:45:A:ILE:HG21	5	0.82
(3,2110)	1:87:B:THR:HG22	1:89:B:VAL:HB	3	0.82
(3,2109)	1:87:A:THR:HG22	1:89:A:VAL:HB	3	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,1874)	1:73:B:GLN:HG2	1:69:B:LYS:HD2	2	0.82
(3,1279)	1:57:A:GLN:HG2	1:60:A:PRO:HG3	6	0.82
(3,1102)	1:138:B:ALA:HA	1:136:B:GLU:HG3	1	0.82
(3,1101)	1:138:A:ALA:HA	1:136:A:GLU:HG3	1	0.82
(3,286)	1:124:B:LYS:HG2	1:84:B:ASP:H	7	0.82
(3,285)	1:124:A:LYS:HG2	1:84:A:ASP:H	6	0.82
(3,160)	1:58:B:PRO:HB2	1:62:B:LYS:H	2	0.82
(1,5622)	1:119:B:MET:HE2	1:121:B:THR:HB	9	0.82
(1,5621)	1:119:A:MET:HE2	1:121:A:THR:HB	9	0.82
(1,5552)	1:116:B:MET:HE2	1:113:B:GLU:HA	2	0.82
(1,5551)	1:116:A:MET:HE2	1:113:A:GLU:HA	2	0.82
(1,5308)	1:106:B:ALA:HB1	1:116:B:MET:HE2	1	0.82
(1,5307)	1:106:A:ALA:HB1	1:116:A:MET:HE2	1	0.82
(1,5237)	1:105:A:GLN:HB2	1:101:A:THR:HG21	2	0.82
(1,5066)	1:115:B:LEU:HD12	1:119:B:MET:HA	7	0.82
(1,5065)	1:115:A:LEU:HD12	1:119:A:MET:HA	7	0.82
(1,4862)	1:98:B:LYS:HD3	1:127:B:TYR:HB2	1	0.82
(1,4861)	1:98:A:LYS:HD3	1:127:A:TYR:HB2	1	0.82
(1,4804)	1:96:B:ALA:HB1	1:127:B:TYR:HE2	4	0.82
(1,4803)	1:96:A:ALA:HB1	1:127:A:TYR:HE2	4	0.82
(1,4796)	1:96:B:ALA:HA	1:90:B:LEU:HB2	8	0.82
(1,4795)	1:96:A:ALA:HA	1:90:A:LEU:HB2	8	0.82
(1,4772)	1:94:B:THR:HG22	1:102:B:ILE:HG23	1	0.82
(1,4771)	1:94:A:THR:HG22	1:102:A:ILE:HG23	1	0.82
(1,3968)	1:72:B:LYS:HB2	1:114:B:THR:HG21	4	0.82
(1,3782)	1:115:B:LEU:HD11	1:68:B:VAL:HB	4	0.82
(1,3782)	1:115:B:LEU:HD11	1:68:B:VAL:HB	7	0.82
(1,3781)	1:115:A:LEU:HD11	1:68:A:VAL:HB	4	0.82
(1,3781)	1:115:A:LEU:HD11	1:68:A:VAL:HB	7	0.82
(1,3506)	1:120:B:ASP:HB3	1:116:B:MET:HB2	4	0.82
(1,3505)	1:120:A:ASP:HB3	1:116:A:MET:HB2	10	0.82
(1,2028)	1:98:B:LYS:HD3	1:125:B:ALA:H	9	0.82
(1,1996)	1:49:B:LEU:HB2	1:123:A:ARG:H	5	0.82
(1,1558)	1:115:B:LEU:HD13	1:105:B:GLN:H	7	0.82
(1,796)	1:115:B:LEU:HD13	1:75:B:TYR:H	5	0.82
(1,795)	1:115:A:LEU:HD13	1:75:A:TYR:H	5	0.82
(1,98)	1:106:B:ALA:HB2	1:107:B:ASP:H	5	0.82
(1,45)	1:89:A:VAL:HG13	1:85:A:GLN:H	7	0.82
(3,3001)	1:135:A:MET:HA	1:116:B:MET:HE3	3	0.81
(3,2944)	1:128:B:LEU:HA	1:125:B:ALA:HB2	3	0.81
(3,2943)	1:128:A:LEU:HA	1:125:A:ALA:HB2	3	0.81
(3,2844)	1:102:B:ILE:HG21	1:118:B:VAL:HA	5	0.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,2843)	1:102:A:ILE:HG21	1:118:A:VAL:HA	5	0.81
(3,2464)	1:100:B:THR:HG23	1:102:B:ILE:HG22	4	0.81
(3,2463)	1:100:A:THR:HG23	1:102:A:ILE:HG22	4	0.81
(3,2200)	1:92:B:GLN:HG2	1:87:B:THR:HG21	9	0.81
(3,2199)	1:92:A:GLN:HG2	1:87:A:THR:HG21	9	0.81
(3,1805)	1:98:A:LYS:HE2	1:124:A:LYS:HD2	4	0.81
(3,1630)	1:66:B:LEU:HB3	1:140:B:LYS:HG2	5	0.81
(3,1280)	1:57:B:GLN:HG2	1:60:B:PRO:HG3	6	0.81
(3,903)	1:122:A:LEU:HB2	1:49:B:LEU:HB3	10	0.81
(3,846)	1:44:B:ASP:HA	1:116:B:MET:HG3	6	0.81
(3,845)	1:44:A:ASP:HA	1:116:A:MET:HG3	6	0.81
(3,460)	1:49:B:LEU:HB2	1:122:A:LEU:H	7	0.81
(3,150)	1:58:B:PRO:HB2	1:61:B:GLU:H	6	0.81
(3,149)	1:58:A:PRO:HB2	1:61:A:GLU:H	9	0.81
(1,5930)	1:112:B:TYR:HE2	1:110:A:VAL:HG12	5	0.81
(1,5929)	1:112:A:TYR:HE2	1:110:B:VAL:HG12	5	0.81
(1,5420)	1:110:B:VAL:HG13	1:114:B:THR:HG22	8	0.81
(1,5419)	1:110:A:VAL:HG13	1:114:A:THR:HG22	8	0.81
(1,5056)	1:119:B:MET:HA	1:122:B:LEU:HB3	4	0.81
(1,5055)	1:119:A:MET:HA	1:122:A:LEU:HB3	4	0.81
(1,4752)	1:94:B:THR:HG22	1:96:B:ALA:HA	4	0.81
(1,4751)	1:94:A:THR:HG22	1:96:A:ALA:HA	4	0.81
(1,4204)	1:107:B:ASP:HB2	1:110:B:VAL:HG13	1	0.81
(1,4203)	1:107:A:ASP:HB2	1:110:A:VAL:HG13	1	0.81
(1,3967)	1:72:A:LYS:HB2	1:114:A:THR:HG21	4	0.81
(1,2562)	1:45:B:ILE:HG23	1:49:A:LEU:HD11	2	0.81
(1,2240)	1:136:B:GLU:HB2	1:136:B:GLU:H	1	0.81
(1,2240)	1:136:B:GLU:HB2	1:136:B:GLU:H	2	0.81
(1,2239)	1:136:A:GLU:HB2	1:136:A:GLU:H	1	0.81
(1,2239)	1:136:A:GLU:HB2	1:136:A:GLU:H	2	0.81
(1,1995)	1:49:A:LEU:HB2	1:123:B:ARG:H	6	0.81
(1,97)	1:106:A:ALA:HB2	1:107:A:ASP:H	5	0.81
(1,46)	1:89:B:VAL:HG13	1:85:B:GLN:H	7	0.81
(3,3084)	1:112:B:TYR:HE1	1:116:B:MET:HE2	5	0.8
(3,3083)	1:112:A:TYR:HE1	1:116:A:MET:HE2	5	0.8
(3,3002)	1:135:B:MET:HA	1:116:A:MET:HE3	3	0.8
(3,2834)	1:112:B:TYR:HE1	1:116:B:MET:HE2	5	0.8
(3,2833)	1:112:A:TYR:HE1	1:116:A:MET:HE2	5	0.8
(3,2730)	1:110:B:VAL:HG22	1:119:B:MET:HE3	8	0.8
(3,2729)	1:110:A:VAL:HG22	1:119:A:MET:HE3	8	0.8
(3,2639)	1:116:A:MET:HG2	1:110:B:VAL:HA	8	0.8
(3,2473)	1:101:A:THR:HA	1:45:B:ILE:HG21	5	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,2464)	1:100:B:THR:HG21	1:102:B:ILE:HG23	8	0.8
(3,2463)	1:100:A:THR:HG21	1:102:A:ILE:HG23	8	0.8
(3,2456)	1:100:B:THR:HG23	1:129:B:LYS:HB3	6	0.8
(3,2454)	1:64:B:VAL:HB	1:100:B:THR:HG23	2	0.8
(3,2454)	1:94:B:THR:HG22	1:64:B:VAL:HB	9	0.8
(3,2453)	1:64:A:VAL:HB	1:100:A:THR:HG23	2	0.8
(3,2453)	1:94:A:THR:HG22	1:64:A:VAL:HB	9	0.8
(3,2296)	1:96:B:ALA:HA	1:100:B:THR:HG22	8	0.8
(3,2295)	1:96:A:ALA:HA	1:100:A:THR:HG22	8	0.8
(3,2199)	1:92:A:GLN:HG2	1:87:A:THR:HG23	10	0.8
(3,1806)	1:98:B:LYS:HE2	1:124:B:LYS:HD2	4	0.8
(3,1629)	1:66:A:LEU:HB3	1:140:A:LYS:HG2	5	0.8
(3,1280)	1:57:B:GLN:HG2	1:60:B:PRO:HG3	3	0.8
(3,1279)	1:57:A:GLN:HG2	1:60:A:PRO:HG3	3	0.8
(3,853)	1:88:A:SER:HA	1:124:A:LYS:HE3	4	0.8
(3,604)	1:87:B:THR:H	1:119:B:MET:H	5	0.8
(3,286)	1:124:B:LYS:HG2	1:84:B:ASP:H	4	0.8
(1,5552)	1:116:B:MET:HE3	1:113:B:GLU:HA	7	0.8
(1,5551)	1:116:A:MET:HE3	1:113:A:GLU:HA	7	0.8
(1,5066)	1:115:B:LEU:HD13	1:119:B:MET:HA	10	0.8
(1,4862)	1:98:B:LYS:HD3	1:127:B:TYR:HB2	5	0.8
(1,4861)	1:98:A:LYS:HD3	1:127:A:TYR:HB2	5	0.8
(1,4518)	1:86:B:LEU:HG	1:90:B:LEU:HG	9	0.8
(1,4203)	1:107:A:ASP:HB2	1:110:A:VAL:HG11	6	0.8
(1,3782)	1:115:B:LEU:HD13	1:68:B:VAL:HB	9	0.8
(1,3781)	1:115:A:LEU:HD13	1:68:A:VAL:HB	9	0.8
(1,3505)	1:120:A:ASP:HB3	1:116:A:MET:HB2	4	0.8
(1,2472)	1:43:B:VAL:HB	1:46:B:ARG:HA	6	0.8
(1,2471)	1:43:A:VAL:HB	1:46:A:ARG:HA	6	0.8
(1,1995)	1:49:A:LEU:HB2	1:123:B:ARG:H	5	0.8
(1,1126)	1:90:B:LEU:HG	1:90:B:LEU:H	4	0.8
(1,1125)	1:90:A:LEU:HG	1:90:A:LEU:H	4	0.8
(1,46)	1:89:B:VAL:HG13	1:85:B:GLN:H	5	0.8
(1,45)	1:89:A:VAL:HG13	1:85:A:GLN:H	5	0.8
(3,3059)	1:65:A:PHE:HE1	1:93:A:ARG:HB2	2	0.79
(3,2938)	1:127:B:TYR:HB2	1:45:B:ILE:HD11	3	0.79
(3,2937)	1:127:A:TYR:HB2	1:45:A:ILE:HD11	3	0.79
(3,2914)	1:86:B:LEU:HB3	1:125:B:ALA:HA	10	0.79
(3,2913)	1:86:A:LEU:HB3	1:125:A:ALA:HA	10	0.79
(3,2844)	1:102:B:ILE:HG22	1:118:B:VAL:HA	6	0.79
(3,2843)	1:102:A:ILE:HG22	1:118:A:VAL:HA	6	0.79
(3,2556)	1:103:B:PHE:HA	1:45:A:ILE:HG23	6	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,2464)	1:100:B:THR:HG22	1:102:B:ILE:HG23	1	0.79
(3,2455)	1:100:A:THR:HG23	1:129:A:LYS:HB3	6	0.79
(3,2238)	1:90:B:LEU:HA	1:94:B:THR:HG23	8	0.79
(3,2237)	1:90:A:LEU:HA	1:94:A:THR:HG23	8	0.79
(3,2220)	1:93:B:ARG:HD2	1:66:B:LEU:HB3	7	0.79
(3,2200)	1:92:B:GLN:HG2	1:87:B:THR:HG23	10	0.79
(3,2127)	1:87:A:THR:HG23	1:88:A:SER:HB2	5	0.79
(3,2110)	1:87:B:THR:HG22	1:89:B:VAL:HB	4	0.79
(3,2109)	1:87:A:THR:HG22	1:89:A:VAL:HB	4	0.79
(3,1878)	1:105:B:GLN:HG3	1:110:B:VAL:HG13	4	0.79
(3,1539)	1:46:A:ARG:HG2	1:128:B:LEU:HB3	10	0.79
(3,904)	1:122:B:LEU:HB2	1:49:A:LEU:HB3	10	0.79
(3,854)	1:88:B:SER:HA	1:124:B:LYS:HE3	4	0.79
(3,603)	1:87:A:THR:H	1:119:A:MET:H	5	0.79
(3,285)	1:124:A:LYS:HG2	1:84:A:ASP:H	2	0.79
(3,285)	1:124:A:LYS:HG2	1:84:A:ASP:H	4	0.79
(3,150)	1:58:B:PRO:HB2	1:61:B:GLU:H	9	0.79
(1,5929)	1:112:A:TYR:HE1	1:110:B:VAL:HG13	1	0.79
(1,5422)	1:110:B:VAL:HG13	1:115:B:LEU:HD11	4	0.79
(1,5422)	1:110:B:VAL:HG13	1:115:B:LEU:HD11	7	0.79
(1,5421)	1:110:A:VAL:HG13	1:115:A:LEU:HD11	4	0.79
(1,5421)	1:110:A:VAL:HG13	1:115:A:LEU:HD11	7	0.79
(1,5065)	1:115:A:LEU:HD13	1:119:A:MET:HA	10	0.79
(1,5056)	1:119:B:MET:HA	1:122:B:LEU:HB3	9	0.79
(1,5055)	1:119:A:MET:HA	1:122:A:LEU:HB3	9	0.79
(1,4718)	1:92:B:GLN:HG2	1:102:B:ILE:HG13	1	0.79
(1,4518)	1:86:B:LEU:HG	1:90:B:LEU:HG	4	0.79
(1,4517)	1:86:A:LEU:HG	1:90:A:LEU:HG	4	0.79
(1,4517)	1:86:A:LEU:HG	1:90:A:LEU:HG	9	0.79
(1,4278)	1:93:B:ARG:HG2	1:65:B:PHE:HB3	3	0.79
(1,4277)	1:93:A:ARG:HG2	1:65:A:PHE:HB3	3	0.79
(1,4204)	1:107:B:ASP:HB2	1:110:B:VAL:HG11	6	0.79
(1,4078)	1:105:B:GLN:HG3	1:137:B:GLY:HA3	4	0.79
(1,4077)	1:105:A:GLN:HG3	1:137:A:GLY:HA3	4	0.79
(1,4010)	1:72:B:LYS:HD3	1:110:B:VAL:HG23	8	0.79
(1,4009)	1:72:A:LYS:HD3	1:110:A:VAL:HG23	8	0.79
(1,3948)	1:91:B:ASP:HB2	1:96:B:ALA:HB3	10	0.79
(1,3947)	1:91:A:ASP:HB2	1:96:A:ALA:HB3	10	0.79
(1,3351)	1:124:A:LYS:HG2	1:84:A:ASP:HB3	4	0.79
(1,2734)	1:50:B:PRO:HG2	1:54:B:ALA:HB2	4	0.79
(1,2733)	1:50:A:PRO:HG2	1:54:A:ALA:HB2	4	0.79
(1,2561)	1:45:A:ILE:HG23	1:49:B:LEU:HD11	2	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2344)	1:89:B:VAL:HB	1:79:B:GLN:HE22	9	0.79
(1,1764)	1:118:B:VAL:HG11	1:115:B:LEU:H	2	0.79
(1,1763)	1:118:A:VAL:HG11	1:115:A:LEU:H	2	0.79
(1,532)	1:102:B:ILE:HG22	1:65:B:PHE:H	3	0.79
(1,98)	1:106:B:ALA:HB1	1:107:B:ASP:H	2	0.79
(1,98)	1:106:B:ALA:HB2	1:107:B:ASP:H	8	0.79
(1,97)	1:106:A:ALA:HB1	1:107:A:ASP:H	2	0.79
(3,3060)	1:65:B:PHE:HE1	1:93:B:ARG:HB2	2	0.78
(3,2914)	1:86:B:LEU:HB3	1:125:B:ALA:HA	7	0.78
(3,2913)	1:86:A:LEU:HB3	1:125:A:ALA:HA	7	0.78
(3,2822)	1:113:B:GLU:HG2	1:115:B:LEU:HD22	9	0.78
(3,2821)	1:113:A:GLU:HG2	1:115:A:LEU:HD22	9	0.78
(3,2640)	1:116:B:MET:HG2	1:110:A:VAL:HA	8	0.78
(3,2463)	1:100:A:THR:HG22	1:102:A:ILE:HG23	1	0.78
(3,2454)	1:94:B:THR:HG23	1:64:B:VAL:HB	3	0.78
(3,2453)	1:94:A:THR:HG23	1:64:A:VAL:HB	3	0.78
(3,2219)	1:93:A:ARG:HD2	1:66:A:LEU:HB3	7	0.78
(3,2200)	1:92:B:GLN:HG2	1:87:B:THR:HG22	1	0.78
(3,2128)	1:87:B:THR:HG23	1:88:B:SER:HB2	5	0.78
(3,1877)	1:105:A:GLN:HG3	1:110:A:VAL:HG13	4	0.78
(3,1724)	1:135:B:MET:HG2	1:115:B:LEU:HD21	3	0.78
(3,1723)	1:135:A:MET:HG2	1:115:A:LEU:HD21	3	0.78
(3,1526)	1:132:B:LEU:HG	1:106:B:ALA:HB2	9	0.78
(3,1525)	1:132:A:LEU:HG	1:106:A:ALA:HB2	9	0.78
(3,996)	1:47:B:VAL:HB	1:128:A:LEU:HG	1	0.78
(3,286)	1:124:B:LYS:HG2	1:84:B:ASP:H	2	0.78
(3,286)	1:124:B:LYS:HG2	1:84:B:ASP:H	3	0.78
(3,285)	1:124:A:LYS:HG2	1:84:A:ASP:H	3	0.78
(1,5930)	1:112:B:TYR:HE1	1:110:A:VAL:HG13	1	0.78
(1,5810)	1:134:B:GLY:HA3	1:116:A:MET:HE1	4	0.78
(1,5809)	1:134:A:GLY:HA3	1:116:B:MET:HE1	4	0.78
(1,5603)	1:119:A:MET:HE3	1:130:A:VAL:HA	9	0.78
(1,5238)	1:105:B:GLN:HB2	1:101:B:THR:HG22	6	0.78
(1,5237)	1:105:A:GLN:HB2	1:101:A:THR:HG22	6	0.78
(1,5056)	1:119:B:MET:HA	1:122:B:LEU:HB3	2	0.78
(1,4854)	1:98:B:LYS:HD3	1:51:A:ALA:HA	8	0.78
(1,4803)	1:96:A:ALA:HB3	1:127:A:TYR:HE1	6	0.78
(1,4772)	1:94:B:THR:HG21	1:102:B:ILE:HG22	2	0.78
(1,4771)	1:94:A:THR:HG21	1:102:A:ILE:HG22	2	0.78
(1,4752)	1:94:B:THR:HG23	1:96:B:ALA:HA	8	0.78
(1,4751)	1:94:A:THR:HG23	1:96:A:ALA:HA	8	0.78
(1,4717)	1:92:A:GLN:HG2	1:102:A:ILE:HG13	1	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4568)	1:87:B:THR:HG22	1:124:B:LYS:HD2	5	0.78
(1,4567)	1:87:A:THR:HG22	1:124:A:LYS:HD2	5	0.78
(1,4278)	1:93:B:ARG:HG2	1:65:B:PHE:HB3	8	0.78
(1,4277)	1:93:A:ARG:HG2	1:65:A:PHE:HB3	8	0.78
(1,3966)	1:72:B:LYS:HA	1:110:B:VAL:HG12	2	0.78
(1,3352)	1:124:B:LYS:HG2	1:84:B:ASP:HB3	4	0.78
(1,2819)	1:54:A:ALA:HB2	1:44:B:ASP:HB2	10	0.78
(1,2771)	1:60:A:PRO:HD3	1:63:A:PRO:HB2	2	0.78
(1,2560)	1:45:B:ILE:HG22	1:54:A:ALA:HB3	8	0.78
(1,2559)	1:45:A:ILE:HG22	1:54:B:ALA:HB3	8	0.78
(1,2367)	1:84:A:ASP:HB2	1:85:A:GLN:HE22	10	0.78
(1,2343)	1:89:A:VAL:HB	1:79:A:GLN:HE22	9	0.78
(1,1209)	1:89:A:VAL:HG22	1:93:A:ARG:H	7	0.78
(1,880)	1:73:B:GLN:HE21	1:81:B:VAL:H	6	0.78
(1,879)	1:73:A:GLN:HE21	1:81:A:VAL:H	6	0.78
(1,532)	1:102:B:ILE:HG23	1:65:B:PHE:H	6	0.78
(1,532)	1:102:B:ILE:HG21	1:65:B:PHE:H	7	0.78
(1,531)	1:102:A:ILE:HG22	1:65:A:PHE:H	3	0.78
(1,531)	1:102:A:ILE:HG23	1:65:A:PHE:H	6	0.78
(1,97)	1:106:A:ALA:HB2	1:107:A:ASP:H	8	0.78
(3,2714)	1:109:B:SER:HB3	1:72:B:LYS:HE2	2	0.77
(3,2500)	1:101:B:THR:HG23	1:50:B:PRO:HB3	6	0.77
(3,2499)	1:101:A:THR:HG23	1:50:A:PRO:HB3	6	0.77
(3,2464)	1:100:B:THR:HG22	1:102:B:ILE:HG22	3	0.77
(3,2463)	1:100:A:THR:HG22	1:102:A:ILE:HG22	3	0.77
(3,2296)	1:96:B:ALA:HA	1:100:B:THR:HG21	4	0.77
(3,2295)	1:96:A:ALA:HA	1:100:A:THR:HG21	4	0.77
(3,2295)	1:96:A:ALA:HA	1:100:A:THR:HG21	6	0.77
(3,2288)	1:95:B:GLN:HG2	1:63:B:PRO:HB2	10	0.77
(3,2287)	1:95:A:GLN:HG2	1:63:A:PRO:HB2	10	0.77
(3,2199)	1:92:A:GLN:HG2	1:87:A:THR:HG22	1	0.77
(3,2199)	1:92:A:GLN:HG2	1:87:A:THR:HG21	5	0.77
(3,2110)	1:87:B:THR:HG23	1:89:B:VAL:HB	5	0.77
(3,2110)	1:87:B:THR:HG22	1:89:B:VAL:HB	10	0.77
(3,2109)	1:87:A:THR:HG23	1:89:A:VAL:HB	5	0.77
(3,2109)	1:87:A:THR:HG22	1:89:A:VAL:HB	10	0.77
(3,1953)	1:79:A:GLN:HG2	1:88:A:SER:HB3	8	0.77
(3,1540)	1:46:B:ARG:HG2	1:128:A:LEU:HB3	10	0.77
(3,1279)	1:57:A:GLN:HG2	1:60:A:PRO:HG3	4	0.77
(3,1104)	1:51:B:ALA:HA	1:43:A:VAL:HB	4	0.77
(3,995)	1:47:A:VAL:HB	1:128:B:LEU:HG	1	0.77
(3,810)	1:89:B:VAL:HA	1:79:B:GLN:HE21	6	0.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,809)	1:89:A:VAL:HA	1:79:A:GLN:HE21	6	0.77
(3,490)	1:132:B:LEU:HG	1:105:B:GLN:H	1	0.77
(3,490)	1:122:B:LEU:HG	1:105:B:GLN:H	2	0.77
(3,489)	1:132:A:LEU:HG	1:105:A:GLN:H	1	0.77
(1,5604)	1:119:B:MET:HE3	1:130:B:VAL:HA	9	0.77
(1,5552)	1:116:B:MET:HE3	1:113:B:GLU:HA	9	0.77
(1,5551)	1:116:A:MET:HE3	1:113:A:GLU:HA	9	0.77
(1,5056)	1:119:B:MET:HA	1:122:B:LEU:HB3	7	0.77
(1,5055)	1:119:A:MET:HA	1:122:A:LEU:HB3	2	0.77
(1,5055)	1:119:A:MET:HA	1:122:A:LEU:HB3	7	0.77
(1,4804)	1:96:B:ALA:HB3	1:127:B:TYR:HE1	6	0.77
(1,4717)	1:92:A:GLN:HG2	1:102:A:ILE:HG13	8	0.77
(1,3965)	1:72:A:LYS:HA	1:110:A:VAL:HG12	2	0.77
(1,3578)	1:66:B:LEU:HA	1:115:B:LEU:HD11	3	0.77
(1,3577)	1:66:A:LEU:HA	1:115:A:LEU:HD13	1	0.77
(1,3542)	1:66:B:LEU:HB2	1:106:B:ALA:HB1	8	0.77
(1,3541)	1:66:A:LEU:HB2	1:106:A:ALA:HB1	8	0.77
(1,2772)	1:60:B:PRO:HD3	1:63:B:PRO:HB2	2	0.77
(1,2368)	1:84:B:ASP:HB2	1:85:B:GLN:HE22	10	0.77
(1,2351)	1:85:A:GLN:HE22	1:82:A:ASN:HD21	9	0.77
(1,2126)	1:129:B:LYS:HD3	1:129:B:LYS:H	5	0.77
(1,2125)	1:129:A:LYS:HD3	1:129:A:LYS:H	5	0.77
(1,2085)	1:98:A:LYS:HD3	1:127:A:TYR:H	8	0.77
(1,2028)	1:98:B:LYS:HD3	1:125:B:ALA:H	10	0.77
(1,2027)	1:98:A:LYS:HD3	1:125:A:ALA:H	10	0.77
(1,1210)	1:89:B:VAL:HG22	1:93:B:ARG:H	7	0.77
(1,1126)	1:90:B:LEU:HG	1:90:B:LEU:H	8	0.77
(1,1125)	1:90:A:LEU:HG	1:90:A:LEU:H	8	0.77
(1,531)	1:102:A:ILE:HG21	1:65:A:PHE:H	7	0.77
(1,194)	1:43:B:VAL:HB	1:44:B:ASP:H	7	0.77
(1,193)	1:43:A:VAL:HB	1:44:A:ASP:H	7	0.77
(3,2844)	1:102:B:ILE:HG23	1:118:B:VAL:HA	7	0.76
(3,2843)	1:102:A:ILE:HG23	1:118:A:VAL:HA	7	0.76
(3,2730)	1:110:B:VAL:HG22	1:119:B:MET:HE1	1	0.76
(3,2730)	1:110:B:VAL:HG22	1:119:B:MET:HE1	5	0.76
(3,2729)	1:110:A:VAL:HG22	1:119:A:MET:HE1	1	0.76
(3,2729)	1:110:A:VAL:HG22	1:119:A:MET:HE1	5	0.76
(3,2713)	1:109:A:SER:HB3	1:72:A:LYS:HE2	2	0.76
(3,2296)	1:96:B:ALA:HA	1:100:B:THR:HG21	6	0.76
(3,2200)	1:92:B:GLN:HG2	1:87:B:THR:HG21	5	0.76
(3,1954)	1:79:B:GLN:HG2	1:88:B:SER:HB3	8	0.76
(3,1776)	1:71:B:ASP:HA	1:111:B:ASP:HB2	1	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,1775)	1:71:A:ASP:HA	1:111:A:ASP:HB2	1	0.76
(3,1489)	1:129:A:LYS:HG2	1:46:B:ARG:HB3	3	0.76
(3,1280)	1:57:B:GLN:HG2	1:60:B:PRO:HG3	4	0.76
(3,995)	1:47:A:VAL:HB	1:128:B:LEU:HG	6	0.76
(3,489)	1:122:A:LEU:HG	1:105:A:GLN:H	2	0.76
(3,286)	1:124:B:LYS:HG2	1:84:B:ASP:H	9	0.76
(3,285)	1:124:A:LYS:HG2	1:84:A:ASP:H	9	0.76
(1,5622)	1:119:B:MET:HE1	1:121:B:THR:HB	4	0.76
(1,5621)	1:119:A:MET:HE1	1:121:A:THR:HB	4	0.76
(1,4771)	1:94:A:THR:HG22	1:102:A:ILE:HG22	3	0.76
(1,4496)	1:115:B:LEU:HB3	1:106:B:ALA:HB3	3	0.76
(1,4495)	1:115:A:LEU:HB3	1:106:A:ALA:HB3	3	0.76
(1,3780)	1:68:B:VAL:HB	1:110:B:VAL:HG22	8	0.76
(1,3779)	1:68:A:VAL:HB	1:110:A:VAL:HG22	8	0.76
(1,3777)	1:68:A:VAL:HB	1:114:A:THR:HG23	4	0.76
(1,3578)	1:66:B:LEU:HA	1:115:B:LEU:HD13	1	0.76
(1,3578)	1:66:B:LEU:HA	1:115:B:LEU:HD12	7	0.76
(1,3577)	1:66:A:LEU:HA	1:115:A:LEU:HD11	3	0.76
(1,3577)	1:66:A:LEU:HA	1:115:A:LEU:HD12	7	0.76
(1,3240)	1:99:B:GLU:HG2	1:49:A:LEU:HB3	4	0.76
(1,3239)	1:99:A:GLU:HG2	1:49:B:LEU:HB3	4	0.76
(1,2562)	1:45:B:ILE:HG22	1:49:A:LEU:HD12	3	0.76
(1,2561)	1:45:A:ILE:HG22	1:49:B:LEU:HD12	3	0.76
(1,2358)	1:82:B:ASN:HB2	1:82:B:ASN:HD22	3	0.76
(1,2357)	1:82:A:ASN:HB2	1:82:A:ASN:HD22	3	0.76
(1,2352)	1:85:B:GLN:HE22	1:82:B:ASN:HD21	9	0.76
(1,2086)	1:98:B:LYS:HD3	1:127:B:TYR:H	8	0.76
(3,3060)	1:65:B:PHE:HE2	1:93:B:ARG:HB2	7	0.75
(3,2846)	1:51:B:ALA:HB2	1:127:A:TYR:HD1	8	0.75
(3,2692)	1:108:B:LYS:HE3	1:109:B:SER:HB3	4	0.75
(3,2456)	1:100:B:THR:HG21	1:129:B:LYS:HB3	8	0.75
(3,2455)	1:100:A:THR:HG21	1:129:A:LYS:HB3	8	0.75
(3,1280)	1:57:B:GLN:HG2	1:60:B:PRO:HG3	9	0.75
(3,1103)	1:51:A:ALA:HA	1:43:B:VAL:HB	4	0.75
(3,996)	1:47:B:VAL:HB	1:128:A:LEU:HG	6	0.75
(3,904)	1:45:B:ILE:HB	1:49:A:LEU:HB3	2	0.75
(3,862)	1:43:B:VAL:HA	1:138:A:ALA:HB2	3	0.75
(3,848)	1:44:B:ASP:HA	1:46:B:ARG:HG2	10	0.75
(3,847)	1:44:A:ASP:HA	1:46:A:ARG:HG2	10	0.75
(3,264)	1:92:B:GLN:HG3	1:79:B:GLN:H	1	0.75
(1,5926)	1:112:B:TYR:HE2	1:113:B:GLU:HB3	6	0.75
(1,5925)	1:112:A:TYR:HE2	1:113:A:GLU:HB3	6	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5604)	1:119:B:MET:HE2	1:130:B:VAL:HA	4	0.75
(1,5603)	1:119:A:MET:HE2	1:130:A:VAL:HA	4	0.75
(1,4772)	1:94:B:THR:HG22	1:102:B:ILE:HG22	3	0.75
(1,4718)	1:92:B:GLN:HG2	1:102:B:ILE:HG13	8	0.75
(1,4518)	1:86:B:LEU:HG	1:90:B:LEU:HG	5	0.75
(1,4517)	1:86:A:LEU:HG	1:90:A:LEU:HG	5	0.75
(1,4050)	1:85:B:GLN:HB2	1:88:B:SER:HB2	2	0.75
(1,4049)	1:85:A:GLN:HB2	1:88:A:SER:HB2	2	0.75
(1,4006)	1:72:B:LYS:HD3	1:107:B:ASP:HB3	1	0.75
(1,4005)	1:72:A:LYS:HD3	1:107:A:ASP:HB3	1	0.75
(1,3778)	1:68:B:VAL:HB	1:114:B:THR:HG23	4	0.75
(1,3610)	1:115:B:LEU:HD13	1:110:B:VAL:HG22	2	0.75
(1,3609)	1:115:A:LEU:HD13	1:110:A:VAL:HG22	2	0.75
(1,3221)	1:122:A:LEU:HA	1:125:A:ALA:HB1	5	0.75
(1,3022)	1:56:B:PRO:HD2	1:57:B:GLN:HG3	7	0.75
(1,2816)	1:54:B:ALA:HB2	1:50:B:PRO:HD2	9	0.75
(1,2562)	1:45:B:ILE:HG23	1:49:A:LEU:HD11	9	0.75
(1,2561)	1:45:A:ILE:HG23	1:49:B:LEU:HD11	9	0.75
(1,2496)	1:45:B:ILE:HA	1:54:A:ALA:HB1	7	0.75
(1,2495)	1:45:A:ILE:HA	1:54:B:ALA:HB1	7	0.75
(1,2358)	1:82:B:ASN:HB2	1:82:B:ASN:HD22	9	0.75
(1,2357)	1:82:A:ASN:HB2	1:82:A:ASN:HD22	2	0.75
(1,2357)	1:82:A:ASN:HB2	1:82:A:ASN:HD22	9	0.75
(1,2044)	1:98:B:LYS:HD3	1:126:B:GLY:H	1	0.75
(1,2043)	1:98:A:LYS:HD3	1:126:A:GLY:H	1	0.75
(1,1764)	1:118:B:VAL:HG13	1:115:B:LEU:H	8	0.75
(1,1764)	1:118:B:VAL:HG11	1:115:B:LEU:H	10	0.75
(1,1763)	1:118:A:VAL:HG13	1:115:A:LEU:H	8	0.75
(1,1763)	1:118:A:VAL:HG11	1:115:A:LEU:H	10	0.75
(1,194)	1:43:B:VAL:HB	1:44:B:ASP:H	6	0.75
(1,193)	1:43:A:VAL:HB	1:44:A:ASP:H	6	0.75
(3,3059)	1:65:A:PHE:HE2	1:93:A:ARG:HB2	7	0.74
(3,2944)	1:128:B:LEU:HA	1:125:B:ALA:HB3	4	0.74
(3,2943)	1:128:A:LEU:HA	1:125:A:ALA:HB3	4	0.74
(3,2896)	1:123:B:ARG:HD3	1:51:A:ALA:HB1	2	0.74
(3,2691)	1:108:A:LYS:HE3	1:109:A:SER:HB3	4	0.74
(3,2532)	1:102:B:ILE:HG23	1:133:B:VAL:HB	3	0.74
(3,2531)	1:102:A:ILE:HG23	1:133:A:VAL:HB	3	0.74
(3,2199)	1:92:A:GLN:HG2	1:87:A:THR:HG21	2	0.74
(3,2114)	1:87:B:THR:HG22	1:124:B:LYS:HD3	5	0.74
(3,2113)	1:87:A:THR:HG22	1:124:A:LYS:HD3	5	0.74
(3,1535)	1:63:A:PRO:HG2	1:60:A:PRO:HD2	3	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,1490)	1:129:B:LYS:HG2	1:46:A:ARG:HB3	3	0.74
(3,1279)	1:57:A:GLN:HG2	1:60:A:PRO:HG3	9	0.74
(3,1010)	1:44:B:ASP:HB2	1:105:A:GLN:HG2	6	0.74
(3,996)	1:47:B:VAL:HB	1:128:A:LEU:HG	8	0.74
(3,995)	1:47:A:VAL:HB	1:128:B:LEU:HG	8	0.74
(3,854)	1:88:B:SER:HA	1:124:B:LYS:HE3	3	0.74
(3,853)	1:88:A:SER:HA	1:124:A:LYS:HE3	3	0.74
(3,263)	1:92:A:GLN:HG3	1:79:A:GLN:H	1	0.74
(1,5613)	1:121:A:THR:HA	1:124:A:LYS:HE3	8	0.74
(1,5604)	1:119:B:MET:HE1	1:130:B:VAL:HA	5	0.74
(1,5603)	1:119:A:MET:HE1	1:130:A:VAL:HA	5	0.74
(1,5308)	1:106:B:ALA:HB1	1:116:B:MET:HE2	10	0.74
(1,5307)	1:106:A:ALA:HB1	1:116:A:MET:HE2	10	0.74
(1,5126)	1:102:B:ILE:HG21	1:66:B:LEU:HG	1	0.74
(1,5126)	1:102:B:ILE:HG23	1:66:B:LEU:HG	3	0.74
(1,5126)	1:102:B:ILE:HG21	1:66:B:LEU:HG	8	0.74
(1,5125)	1:102:A:ILE:HG21	1:66:A:LEU:HG	1	0.74
(1,5125)	1:102:A:ILE:HG23	1:66:A:LEU:HG	3	0.74
(1,5125)	1:102:A:ILE:HG21	1:66:A:LEU:HG	8	0.74
(1,4722)	1:93:B:ARG:HA	1:77:B:GLY:HA2	3	0.74
(1,4721)	1:93:A:ARG:HA	1:77:A:GLY:HA2	3	0.74
(1,4204)	1:107:B:ASP:HB2	1:110:B:VAL:HG12	5	0.74
(1,4204)	1:107:B:ASP:HB2	1:110:B:VAL:HG13	10	0.74
(1,4203)	1:107:A:ASP:HB2	1:110:A:VAL:HG12	8	0.74
(1,4203)	1:107:A:ASP:HB2	1:110:A:VAL:HG12	9	0.74
(1,3603)	1:115:A:LEU:HD13	1:116:A:MET:HE1	8	0.74
(1,3542)	1:66:B:LEU:HB2	1:106:B:ALA:HB2	3	0.74
(1,3541)	1:66:A:LEU:HB2	1:106:A:ALA:HB2	3	0.74
(1,3506)	1:120:B:ASP:HB3	1:116:B:MET:HB2	7	0.74
(1,3222)	1:122:B:LEU:HA	1:125:B:ALA:HB1	5	0.74
(1,3021)	1:56:A:PRO:HD2	1:57:A:GLN:HG3	7	0.74
(1,2815)	1:54:A:ALA:HB2	1:50:A:PRO:HD2	9	0.74
(1,2733)	1:50:A:PRO:HG2	1:54:A:ALA:HB3	3	0.74
(1,2358)	1:82:B:ASN:HB2	1:82:B:ASN:HD22	2	0.74
(1,1995)	1:49:A:LEU:HB2	1:123:B:ARG:H	3	0.74
(1,1862)	1:110:B:VAL:HG11	1:118:B:VAL:H	8	0.74
(1,1861)	1:110:A:VAL:HG11	1:118:A:VAL:H	8	0.74
(1,1558)	1:115:B:LEU:HD12	1:105:B:GLN:H	9	0.74
(1,1557)	1:115:A:LEU:HD12	1:105:A:GLN:H	9	0.74
(3,3006)	1:106:B:ALA:HB3	1:135:B:MET:HG2	5	0.73
(3,3005)	1:106:A:ALA:HB3	1:135:A:MET:HG2	5	0.73
(3,2844)	1:102:B:ILE:HG22	1:118:B:VAL:HA	10	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,2843)	1:102:A:ILE:HG22	1:118:A:VAL:HA	10	0.73
(3,2200)	1:92:B:GLN:HG2	1:87:B:THR:HG21	2	0.73
(3,1536)	1:63:B:PRO:HG2	1:60:B:PRO:HD2	3	0.73
(3,1286)	1:57:B:GLN:HG3	1:129:B:LYS:HD2	3	0.73
(3,490)	1:132:B:LEU:HG	1:105:B:GLN:H	9	0.73
(3,489)	1:132:A:LEU:HG	1:105:A:GLN:H	9	0.73
(1,5930)	1:112:B:TYR:HE2	1:110:A:VAL:HG11	4	0.73
(1,5614)	1:121:B:THR:HA	1:124:B:LYS:HE3	8	0.73
(1,5607)	1:51:A:ALA:HB1	1:124:B:LYS:HA	7	0.73
(1,5126)	1:102:B:ILE:HG22	1:66:B:LEU:HG	7	0.73
(1,5125)	1:102:A:ILE:HG22	1:66:A:LEU:HG	7	0.73
(1,5056)	1:119:B:MET:HA	1:122:B:LEU:HB3	3	0.73
(1,5055)	1:119:A:MET:HA	1:122:A:LEU:HB3	3	0.73
(1,4808)	1:96:B:ALA:HB3	1:127:B:TYR:HA	3	0.73
(1,4278)	1:93:B:ARG:HG2	1:65:B:PHE:HB3	9	0.73
(1,4277)	1:93:A:ARG:HG2	1:65:A:PHE:HB3	9	0.73
(1,4204)	1:107:B:ASP:HB2	1:110:B:VAL:HG12	8	0.73
(1,4204)	1:107:B:ASP:HB2	1:110:B:VAL:HG12	9	0.73
(1,4203)	1:107:A:ASP:HB2	1:110:A:VAL:HG12	5	0.73
(1,4203)	1:107:A:ASP:HB2	1:110:A:VAL:HG13	10	0.73
(1,4131)	1:74:A:LEU:HB3	1:119:A:MET:HE3	1	0.73
(1,4050)	1:85:B:GLN:HB2	1:88:B:SER:HB2	1	0.73
(1,3777)	1:68:A:VAL:HB	1:114:A:THR:HG22	2	0.73
(1,3604)	1:115:B:LEU:HD13	1:116:B:MET:HE1	8	0.73
(1,3542)	1:66:B:LEU:HB2	1:106:B:ALA:HB3	6	0.73
(1,3541)	1:66:A:LEU:HB2	1:106:A:ALA:HB3	6	0.73
(1,3505)	1:120:A:ASP:HB3	1:116:A:MET:HB2	7	0.73
(1,2820)	1:54:B:ALA:HB2	1:44:A:ASP:HB2	10	0.73
(1,2734)	1:50:B:PRO:HG2	1:54:B:ALA:HB3	3	0.73
(1,2690)	1:93:B:ARG:HG3	1:92:B:GLN:HB3	8	0.73
(1,2689)	1:93:A:ARG:HG3	1:92:A:GLN:HB3	8	0.73
(1,2358)	1:82:B:ASN:HB2	1:82:B:ASN:HD22	6	0.73
(1,2357)	1:82:A:ASN:HB2	1:82:A:ASN:HD22	4	0.73
(1,2357)	1:82:A:ASN:HB2	1:82:A:ASN:HD22	6	0.73
(1,2044)	1:98:B:LYS:HD3	1:126:B:GLY:H	6	0.73
(1,2043)	1:98:A:LYS:HD3	1:126:A:GLY:H	6	0.73
(1,1996)	1:49:B:LEU:HB2	1:123:A:ARG:H	3	0.73
(1,1125)	1:90:A:LEU:HG	1:90:A:LEU:H	1	0.73
(1,1004)	1:89:B:VAL:HG13	1:86:B:LEU:H	2	0.73
(1,1003)	1:89:A:VAL:HG13	1:86:A:LEU:H	2	0.73
(1,532)	1:102:B:ILE:HG23	1:65:B:PHE:H	1	0.73
(1,531)	1:102:A:ILE:HG23	1:65:A:PHE:H	1	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,2938)	1:127:B:TYR:HB2	1:45:B:ILE:HD13	6	0.72
(3,2937)	1:127:A:TYR:HB2	1:45:A:ILE:HD13	6	0.72
(3,2822)	1:113:B:GLU:HG2	1:115:B:LEU:HD21	10	0.72
(3,2821)	1:113:A:GLU:HG2	1:115:A:LEU:HD21	10	0.72
(3,2640)	1:116:B:MET:HG2	1:110:A:VAL:HA	6	0.72
(3,2508)	1:86:B:LEU:HG	1:119:B:MET:HA	10	0.72
(3,2507)	1:86:A:LEU:HG	1:119:A:MET:HA	10	0.72
(3,2454)	1:94:B:THR:HG22	1:64:B:VAL:HB	7	0.72
(3,2453)	1:94:A:THR:HG22	1:64:A:VAL:HB	7	0.72
(3,2220)	1:93:B:ARG:HD2	1:66:B:LEU:HB3	10	0.72
(3,2219)	1:93:A:ARG:HD2	1:66:A:LEU:HB3	10	0.72
(3,1285)	1:57:A:GLN:HG3	1:129:A:LYS:HD2	3	0.72
(3,903)	1:45:A:ILE:HB	1:49:B:LEU:HB3	2	0.72
(3,861)	1:43:A:VAL:HA	1:138:B:ALA:HB2	3	0.72
(1,5929)	1:112:A:TYR:HE2	1:110:B:VAL:HG11	4	0.72
(1,4807)	1:96:A:ALA:HB3	1:127:A:TYR:HA	3	0.72
(1,4804)	1:96:B:ALA:HB3	1:127:B:TYR:HE2	7	0.72
(1,4803)	1:96:A:ALA:HB3	1:127:A:TYR:HE2	7	0.72
(1,4132)	1:74:B:LEU:HB3	1:119:B:MET:HE3	1	0.72
(1,4049)	1:85:A:GLN:HB2	1:88:A:SER:HB2	1	0.72
(1,3778)	1:68:B:VAL:HB	1:114:B:THR:HG22	2	0.72
(1,3506)	1:120:B:ASP:HB3	1:116:B:MET:HB2	9	0.72
(1,3505)	1:120:A:ASP:HB3	1:116:A:MET:HB2	9	0.72
(1,3022)	1:56:B:PRO:HD2	1:57:B:GLN:HG3	6	0.72
(1,2910)	1:55:B:LYS:HG3	1:58:B:PRO:HG2	7	0.72
(1,2909)	1:55:A:LYS:HG3	1:58:A:PRO:HG2	1	0.72
(1,2909)	1:55:A:LYS:HG3	1:58:A:PRO:HG2	7	0.72
(1,2781)	1:51:A:ALA:HB1	1:126:B:GLY:HA3	6	0.72
(1,2358)	1:82:B:ASN:HB2	1:82:B:ASN:HD22	4	0.72
(1,2357)	1:82:A:ASN:HB2	1:82:A:ASN:HD22	1	0.72
(1,1126)	1:90:B:LEU:HG	1:90:B:LEU:H	1	0.72
(1,1126)	1:90:B:LEU:HG	1:90:B:LEU:H	9	0.72
(1,1125)	1:90:A:LEU:HG	1:90:A:LEU:H	9	0.72
(1,46)	1:89:B:VAL:HG11	1:85:B:GLN:H	4	0.72
(1,45)	1:89:A:VAL:HG11	1:85:A:GLN:H	4	0.72
(3,3084)	1:112:B:TYR:HE1	1:116:B:MET:HE3	8	0.71
(3,3083)	1:112:A:TYR:HE1	1:116:A:MET:HE3	8	0.71
(3,2895)	1:123:A:ARG:HD3	1:51:B:ALA:HB1	2	0.71
(3,2845)	1:51:A:ALA:HB2	1:127:B:TYR:HD1	8	0.71
(3,2834)	1:112:B:TYR:HE1	1:116:B:MET:HE3	8	0.71
(3,2833)	1:112:A:TYR:HE1	1:116:A:MET:HE3	8	0.71
(3,2354)	1:98:B:LYS:HG2	1:96:B:ALA:HB1	10	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,2353)	1:98:A:LYS:HG2	1:96:A:ALA:HB1	10	0.71
(3,1768)	1:70:B:ALA:HA	1:74:B:LEU:HG	1	0.71
(3,1767)	1:70:A:ALA:HA	1:74:A:LEU:HG	1	0.71
(3,1490)	1:129:B:LYS:HG2	1:46:A:ARG:HB3	5	0.71
(3,904)	1:122:B:LEU:HB2	1:49:A:LEU:HB3	4	0.71
(3,604)	1:87:B:THR:H	1:119:B:MET:H	8	0.71
(3,603)	1:87:A:THR:H	1:119:A:MET:H	8	0.71
(3,460)	1:49:B:LEU:HB2	1:122:A:LEU:H	4	0.71
(3,459)	1:49:A:LEU:HB2	1:122:B:LEU:H	4	0.71
(3,150)	1:58:B:PRO:HB2	1:61:B:GLU:H	4	0.71
(3,150)	1:58:B:PRO:HB2	1:61:B:GLU:H	7	0.71
(3,149)	1:58:A:PRO:HB2	1:61:A:GLU:H	7	0.71
(1,5668)	1:87:B:THR:HA	1:125:B:ALA:HB2	5	0.71
(1,5667)	1:87:A:THR:HA	1:125:A:ALA:HB2	5	0.71
(1,5604)	1:119:B:MET:HE3	1:130:B:VAL:HA	1	0.71
(1,5603)	1:119:A:MET:HE3	1:130:A:VAL:HA	1	0.71
(1,5552)	1:116:B:MET:HE2	1:113:B:GLU:HA	1	0.71
(1,5551)	1:116:A:MET:HE2	1:113:A:GLU:HA	1	0.71
(1,5422)	1:110:B:VAL:HG11	1:115:B:LEU:HD12	3	0.71
(1,5421)	1:110:A:VAL:HG11	1:115:A:LEU:HD12	3	0.71
(1,5414)	1:68:B:VAL:HB	1:110:B:VAL:HG11	8	0.71
(1,5413)	1:68:A:VAL:HB	1:110:A:VAL:HG11	8	0.71
(1,5126)	1:102:B:ILE:HG21	1:66:B:LEU:HG	10	0.71
(1,5125)	1:102:A:ILE:HG21	1:66:A:LEU:HG	10	0.71
(1,5056)	1:119:B:MET:HA	1:122:B:LEU:HB3	10	0.71
(1,5055)	1:119:A:MET:HA	1:122:A:LEU:HB3	10	0.71
(1,4808)	1:96:B:ALA:HB1	1:127:B:TYR:HA	10	0.71
(1,4807)	1:96:A:ALA:HB1	1:127:A:TYR:HA	10	0.71
(1,4796)	1:96:B:ALA:HA	1:90:B:LEU:HB2	1	0.71
(1,4760)	1:94:B:THR:HG23	1:99:B:GLU:HG3	5	0.71
(1,4759)	1:94:A:THR:HG23	1:99:A:GLU:HG3	5	0.71
(1,4496)	1:115:B:LEU:HB3	1:106:B:ALA:HB1	2	0.71
(1,4495)	1:115:A:LEU:HB3	1:106:A:ALA:HB1	2	0.71
(1,4277)	1:93:A:ARG:HG2	1:65:A:PHE:HB3	7	0.71
(1,4204)	1:107:B:ASP:HB2	1:110:B:VAL:HG11	7	0.71
(1,4005)	1:72:A:LYS:HD3	1:107:A:ASP:HB3	7	0.71
(1,3783)	1:68:A:VAL:HB	1:106:A:ALA:HB3	6	0.71
(1,3022)	1:56:B:PRO:HD2	1:57:B:GLN:HG3	1	0.71
(1,3021)	1:56:A:PRO:HD2	1:57:A:GLN:HG3	1	0.71
(1,3021)	1:56:A:PRO:HD2	1:57:A:GLN:HG3	6	0.71
(1,2910)	1:55:B:LYS:HG3	1:58:B:PRO:HG2	1	0.71
(1,2644)	1:125:B:ALA:HA	1:98:B:LYS:HD3	4	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2643)	1:125:A:ALA:HA	1:98:A:LYS:HD3	4	0.71
(1,2358)	1:82:B:ASN:HB2	1:82:B:ASN:HD22	1	0.71
(1,2044)	1:98:B:LYS:HD3	1:126:B:GLY:H	4	0.71
(1,1764)	1:118:B:VAL:HG13	1:115:B:LEU:H	6	0.71
(1,1763)	1:118:A:VAL:HG13	1:115:A:LEU:H	6	0.71
(3,2508)	1:86:B:LEU:HG	1:119:B:MET:HA	2	0.7
(3,2507)	1:86:A:LEU:HG	1:119:A:MET:HA	2	0.7
(3,2456)	1:100:B:THR:HG22	1:129:B:LYS:HB3	3	0.7
(3,2455)	1:100:A:THR:HG22	1:129:A:LYS:HB3	3	0.7
(3,2454)	1:94:B:THR:HG22	1:64:B:VAL:HB	5	0.7
(3,2453)	1:94:A:THR:HG22	1:64:A:VAL:HB	5	0.7
(3,2387)	1:99:A:GLU:HG3	1:129:A:LYS:HE2	9	0.7
(3,2372)	1:98:B:LYS:HE2	1:126:B:GLY:HA2	10	0.7
(3,2371)	1:98:A:LYS:HE2	1:126:A:GLY:HA2	10	0.7
(3,2353)	1:98:A:LYS:HG2	1:96:A:ALA:HB1	9	0.7
(3,2199)	1:92:A:GLN:HG2	1:87:A:THR:HG21	8	0.7
(3,1874)	1:73:B:GLN:HG2	1:69:B:LYS:HD2	5	0.7
(3,1295)	1:58:A:PRO:HG2	1:55:A:LYS:HE3	2	0.7
(3,1279)	1:57:A:GLN:HG2	1:60:A:PRO:HG3	7	0.7
(3,903)	1:122:A:LEU:HB2	1:49:B:LEU:HB3	4	0.7
(3,149)	1:58:A:PRO:HB2	1:61:A:GLU:H	4	0.7
(1,5422)	1:110:B:VAL:HG11	1:115:B:LEU:HD11	8	0.7
(1,5421)	1:110:A:VAL:HG11	1:115:A:LEU:HD11	8	0.7
(1,4795)	1:96:A:ALA:HA	1:90:A:LEU:HB2	1	0.7
(1,4518)	1:86:B:LEU:HG	1:90:B:LEU:HG	3	0.7
(1,4495)	1:115:A:LEU:HB3	1:106:A:ALA:HB1	9	0.7
(1,4278)	1:93:B:ARG:HG2	1:65:B:PHE:HB3	7	0.7
(1,4203)	1:107:A:ASP:HB2	1:110:A:VAL:HG11	7	0.7
(1,4006)	1:72:B:LYS:HD3	1:107:B:ASP:HB3	7	0.7
(1,3784)	1:68:B:VAL:HB	1:106:B:ALA:HB3	6	0.7
(1,2819)	1:54:A:ALA:HB2	1:44:B:ASP:HB2	9	0.7
(1,2772)	1:60:B:PRO:HD3	1:63:B:PRO:HB2	4	0.7
(1,2771)	1:60:A:PRO:HD3	1:63:A:PRO:HB2	4	0.7
(1,2562)	1:45:B:ILE:HG22	1:49:A:LEU:HD13	1	0.7
(1,2561)	1:45:A:ILE:HG22	1:49:B:LEU:HD13	1	0.7
(1,2508)	1:122:B:LEU:HB2	1:130:B:VAL:HB	2	0.7
(1,2507)	1:122:A:LEU:HB2	1:130:A:VAL:HB	2	0.7
(1,2043)	1:98:A:LYS:HD3	1:126:A:GLY:H	4	0.7
(1,1125)	1:90:A:LEU:HG	1:90:A:LEU:H	2	0.7
(1,1067)	1:89:A:VAL:HG13	1:88:A:SER:H	10	0.7
(3,2852)	1:49:B:LEU:HA	1:51:B:ALA:HB3	7	0.69
(3,2851)	1:49:A:LEU:HA	1:51:A:ALA:HB3	7	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,2822)	1:113:B:GLU:HG2	1:115:B:LEU:HD23	2	0.69
(3,2821)	1:113:A:GLU:HG2	1:115:A:LEU:HD23	2	0.69
(3,2388)	1:99:B:GLU:HG3	1:129:B:LYS:HE2	9	0.69
(3,2354)	1:98:B:LYS:HG2	1:96:B:ALA:HB1	8	0.69
(3,2354)	1:98:B:LYS:HG2	1:96:B:ALA:HB1	9	0.69
(3,2353)	1:98:A:LYS:HG2	1:96:A:ALA:HB1	8	0.69
(3,2200)	1:92:B:GLN:HG2	1:87:B:THR:HG21	8	0.69
(3,2128)	1:87:B:THR:HG21	1:88:B:SER:HB2	6	0.69
(3,2127)	1:87:A:THR:HG21	1:88:A:SER:HB2	6	0.69
(3,1873)	1:73:A:GLN:HG2	1:69:A:LYS:HD2	5	0.69
(3,1776)	1:71:B:ASP:HA	1:111:B:ASP:HB2	5	0.69
(3,1775)	1:71:A:ASP:HA	1:111:A:ASP:HB2	5	0.69
(3,1735)	1:69:A:LYS:HD2	1:108:A:LYS:HE2	10	0.69
(3,1490)	1:129:B:LYS:HG2	1:46:A:ARG:HB3	10	0.69
(3,1296)	1:58:B:PRO:HG2	1:55:B:LYS:HE3	2	0.69
(3,1280)	1:57:B:GLN:HG2	1:60:B:PRO:HG3	7	0.69
(3,854)	1:88:B:SER:HA	1:124:B:LYS:HE3	6	0.69
(3,276)	1:73:B:GLN:HG2	1:79:B:GLN:H	2	0.69
(3,275)	1:73:A:GLN:HG2	1:79:A:GLN:H	2	0.69
(1,5582)	1:118:B:VAL:HB	1:83:B:ALA:HB3	9	0.69
(1,5581)	1:118:A:VAL:HB	1:83:A:ALA:HB3	9	0.69
(1,5422)	1:110:B:VAL:HG11	1:115:B:LEU:HD12	5	0.69
(1,5421)	1:110:A:VAL:HG11	1:115:A:LEU:HD12	5	0.69
(1,4772)	1:94:B:THR:HG21	1:102:B:ILE:HG22	5	0.69
(1,4772)	1:94:B:THR:HG21	1:102:B:ILE:HG21	7	0.69
(1,4771)	1:94:A:THR:HG21	1:102:A:ILE:HG22	5	0.69
(1,4771)	1:94:A:THR:HG21	1:102:A:ILE:HG21	7	0.69
(1,4518)	1:86:B:LEU:HG	1:90:B:LEU:HG	8	0.69
(1,4517)	1:86:A:LEU:HG	1:90:A:LEU:HG	3	0.69
(1,4517)	1:86:A:LEU:HG	1:90:A:LEU:HG	8	0.69
(1,4496)	1:115:B:LEU:HB3	1:106:B:ALA:HB1	9	0.69
(1,3784)	1:68:B:VAL:HB	1:106:B:ALA:HB1	8	0.69
(1,3596)	1:115:B:LEU:HD12	1:119:B:MET:HG3	2	0.69
(1,3542)	1:66:B:LEU:HB2	1:106:B:ALA:HB1	1	0.69
(1,3541)	1:66:A:LEU:HB2	1:106:A:ALA:HB1	1	0.69
(1,3022)	1:56:B:PRO:HD2	1:57:B:GLN:HG3	10	0.69
(1,2772)	1:60:B:PRO:HD3	1:63:B:PRO:HB2	10	0.69
(1,2771)	1:60:A:PRO:HD3	1:63:A:PRO:HB2	10	0.69
(1,1126)	1:90:B:LEU:HG	1:90:B:LEU:H	2	0.69
(1,1068)	1:89:B:VAL:HG13	1:88:B:SER:H	9	0.69
(1,1068)	1:89:B:VAL:HG13	1:88:B:SER:H	10	0.69
(1,1067)	1:89:A:VAL:HG13	1:88:A:SER:H	9	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,532)	1:102:B:ILE:HG22	1:65:B:PHE:H	4	0.69
(1,98)	1:106:B:ALA:HB1	1:107:B:ASP:H	4	0.69
(1,98)	1:106:B:ALA:HB1	1:107:B:ASP:H	6	0.69
(1,97)	1:106:A:ALA:HB1	1:107:A:ASP:H	4	0.69
(1,97)	1:106:A:ALA:HB1	1:107:A:ASP:H	6	0.69
(3,3100)	1:127:B:TYR:HE2	1:129:B:LYS:HD2	8	0.68
(3,2938)	1:127:B:TYR:HB2	1:45:B:ILE:HD11	9	0.68
(3,2937)	1:127:A:TYR:HB2	1:45:A:ILE:HD11	9	0.68
(3,2852)	1:49:B:LEU:HA	1:51:B:ALA:HB1	4	0.68
(3,2851)	1:49:A:LEU:HA	1:51:A:ALA:HB1	4	0.68
(3,2851)	1:49:A:LEU:HA	1:51:A:ALA:HB2	9	0.68
(3,2464)	1:100:B:THR:HG23	1:102:B:ILE:HG22	2	0.68
(3,1918)	1:75:B:TYR:HB2	1:140:B:LYS:HG2	2	0.68
(3,1917)	1:75:A:TYR:HB2	1:140:A:LYS:HG2	2	0.68
(3,1896)	1:123:B:ARG:HG2	1:50:A:PRO:HB3	3	0.68
(3,1768)	1:70:B:ALA:HA	1:105:B:GLN:HB3	5	0.68
(3,1767)	1:70:A:ALA:HA	1:105:A:GLN:HB3	5	0.68
(3,1736)	1:69:B:LYS:HD2	1:108:B:LYS:HE2	10	0.68
(3,1670)	1:67:B:SER:HB2	1:80:B:PRO:HD3	5	0.68
(3,1489)	1:129:A:LYS:HG2	1:46:B:ARG:HB3	5	0.68
(3,996)	1:47:B:VAL:HB	1:128:A:LEU:HG	4	0.68
(3,995)	1:47:A:VAL:HB	1:128:B:LEU:HG	4	0.68
(3,853)	1:88:A:SER:HA	1:124:A:LYS:HE3	6	0.68
(3,459)	1:49:A:LEU:HB2	1:122:B:LEU:H	9	0.68
(1,5608)	1:51:B:ALA:HB1	1:124:A:LYS:HA	7	0.68
(1,5422)	1:110:B:VAL:HG12	1:115:B:LEU:HD12	10	0.68
(1,5421)	1:110:A:VAL:HG12	1:115:A:LEU:HD12	10	0.68
(1,5056)	1:119:B:MET:HA	1:122:B:LEU:HB3	5	0.68
(1,5055)	1:119:A:MET:HA	1:122:A:LEU:HB3	5	0.68
(1,4518)	1:86:B:LEU:HG	1:90:B:LEU:HG	1	0.68
(1,4517)	1:86:A:LEU:HG	1:90:A:LEU:HG	1	0.68
(1,4204)	1:107:B:ASP:HB2	1:110:B:VAL:HG11	2	0.68
(1,4132)	1:74:B:LEU:HB3	1:119:B:MET:HE1	8	0.68
(1,4131)	1:74:A:LEU:HB3	1:119:A:MET:HE1	8	0.68
(1,3992)	1:72:B:LYS:HG3	1:72:B:LYS:HE2	2	0.68
(1,3992)	1:72:B:LYS:HG3	1:72:B:LYS:HE2	4	0.68
(1,3991)	1:72:A:LYS:HG3	1:72:A:LYS:HE2	2	0.68
(1,3991)	1:72:A:LYS:HG3	1:72:A:LYS:HE2	4	0.68
(1,3783)	1:68:A:VAL:HB	1:106:A:ALA:HB1	8	0.68
(1,3780)	1:68:B:VAL:HB	1:110:B:VAL:HG22	2	0.68
(1,3779)	1:68:A:VAL:HB	1:110:A:VAL:HG22	2	0.68
(1,3596)	1:115:B:LEU:HD13	1:119:B:MET:HG3	7	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3595)	1:115:A:LEU:HD12	1:119:A:MET:HG3	2	0.68
(1,3595)	1:115:A:LEU:HD13	1:119:A:MET:HG3	7	0.68
(1,3578)	1:66:B:LEU:HA	1:115:B:LEU:HD13	8	0.68
(1,3577)	1:66:A:LEU:HA	1:115:A:LEU:HD13	8	0.68
(1,3542)	1:66:B:LEU:HB2	1:106:B:ALA:HB2	7	0.68
(1,3541)	1:66:A:LEU:HB2	1:106:A:ALA:HB2	7	0.68
(1,2772)	1:60:B:PRO:HD3	1:63:B:PRO:HB2	9	0.68
(1,2771)	1:60:A:PRO:HD3	1:63:A:PRO:HB2	9	0.68
(1,2734)	1:50:B:PRO:HG2	1:54:B:ALA:HB3	8	0.68
(1,2664)	1:49:B:LEU:HB2	1:50:B:PRO:HD3	5	0.68
(1,2663)	1:49:A:LEU:HB2	1:50:A:PRO:HD3	5	0.68
(1,2644)	1:125:B:ALA:HA	1:98:B:LYS:HD3	6	0.68
(1,2643)	1:125:A:ALA:HA	1:98:A:LYS:HD3	6	0.68
(1,2624)	1:48:B:ASP:HB3	1:46:A:ARG:HB2	6	0.68
(1,1558)	1:115:B:LEU:HD11	1:105:B:GLN:H	5	0.68
(1,1557)	1:115:A:LEU:HD11	1:105:A:GLN:H	5	0.68
(1,531)	1:102:A:ILE:HG22	1:65:A:PHE:H	4	0.68
(3,3100)	1:75:B:TYR:HE1	1:140:B:LYS:HD3	5	0.67
(3,3099)	1:75:A:TYR:HE1	1:140:A:LYS:HD3	5	0.67
(3,3099)	1:127:A:TYR:HE2	1:129:A:LYS:HD2	8	0.67
(3,3024)	1:129:B:LYS:HA	1:97:B:ASN:HB2	2	0.67
(3,3023)	1:129:A:LYS:HA	1:97:A:ASN:HB2	2	0.67
(3,2944)	1:128:B:LEU:HA	1:125:B:ALA:HB1	1	0.67
(3,2943)	1:128:A:LEU:HA	1:125:A:ALA:HB1	1	0.67
(3,2852)	1:49:B:LEU:HA	1:51:B:ALA:HB2	9	0.67
(3,2730)	1:110:B:VAL:HG23	1:119:B:MET:HE3	6	0.67
(3,2729)	1:110:A:VAL:HG23	1:119:A:MET:HE3	6	0.67
(3,2642)	1:116:B:MET:HG2	1:45:B:ILE:HD11	5	0.67
(3,2639)	1:116:A:MET:HG2	1:110:B:VAL:HA	6	0.67
(3,2463)	1:100:A:THR:HG23	1:102:A:ILE:HG22	2	0.67
(3,2352)	1:98:B:LYS:HG3	1:125:B:ALA:HB3	1	0.67
(3,2351)	1:98:A:LYS:HG3	1:125:A:ALA:HB3	1	0.67
(3,2296)	1:96:B:ALA:HA	1:100:B:THR:HG21	2	0.67
(3,2296)	1:96:B:ALA:HA	1:100:B:THR:HG23	9	0.67
(3,2295)	1:96:A:ALA:HA	1:100:A:THR:HG21	2	0.67
(3,2295)	1:96:A:ALA:HA	1:100:A:THR:HG23	9	0.67
(3,2238)	1:90:B:LEU:HA	1:94:B:THR:HG21	1	0.67
(3,2237)	1:90:A:LEU:HA	1:94:A:THR:HG21	1	0.67
(3,1828)	1:108:B:LYS:HE3	1:113:A:GLU:HB2	1	0.67
(3,1768)	1:70:B:ALA:HA	1:74:B:LEU:HG	7	0.67
(3,1767)	1:70:A:ALA:HA	1:74:A:LEU:HG	7	0.67
(3,1669)	1:67:A:SER:HB2	1:80:A:PRO:HD3	5	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,1489)	1:129:A:LYS:HG2	1:46:B:ARG:HB3	10	0.67
(3,1286)	1:57:B:GLN:HG3	1:129:B:LYS:HD2	6	0.67
(3,1285)	1:57:A:GLN:HG3	1:129:A:LYS:HD2	6	0.67
(3,904)	1:45:B:ILE:HB	1:49:A:LEU:HB3	1	0.67
(3,232)	1:70:B:ALA:HB1	1:72:B:LYS:H	10	0.67
(1,5809)	1:134:A:GLY:HA3	1:116:B:MET:HE1	9	0.67
(1,5212)	1:104:B:PHE:HB2	1:115:B:LEU:HD13	4	0.67
(1,5211)	1:104:A:PHE:HB2	1:115:A:LEU:HD13	4	0.67
(1,5127)	1:100:A:THR:HG23	1:102:A:ILE:HG23	10	0.67
(1,5056)	1:119:B:MET:HA	1:122:B:LEU:HB3	8	0.67
(1,5055)	1:119:A:MET:HA	1:122:A:LEU:HB3	8	0.67
(1,4862)	1:98:B:LYS:HD3	1:127:B:TYR:HB2	4	0.67
(1,4861)	1:98:A:LYS:HD3	1:127:A:TYR:HB2	4	0.67
(1,4203)	1:107:A:ASP:HB2	1:110:A:VAL:HG11	2	0.67
(1,4078)	1:105:B:GLN:HG3	1:137:B:GLY:HA3	5	0.67
(1,4077)	1:105:A:GLN:HG3	1:137:A:GLY:HA3	5	0.67
(1,3856)	1:69:B:LYS:HD3	1:65:B:PHE:HB2	4	0.67
(1,3855)	1:69:A:LYS:HD3	1:65:A:PHE:HB2	4	0.67
(1,3780)	1:68:B:VAL:HB	1:110:B:VAL:HG22	10	0.67
(1,3779)	1:68:A:VAL:HB	1:110:A:VAL:HG22	10	0.67
(1,3022)	1:56:B:PRO:HD2	1:57:B:GLN:HG3	5	0.67
(1,3021)	1:56:A:PRO:HD2	1:57:A:GLN:HG3	5	0.67
(1,3021)	1:56:A:PRO:HD2	1:57:A:GLN:HG3	10	0.67
(1,2820)	1:54:B:ALA:HB2	1:44:A:ASP:HB2	9	0.67
(1,2772)	1:60:B:PRO:HD3	1:63:B:PRO:HB2	1	0.67
(1,2771)	1:60:A:PRO:HD3	1:63:A:PRO:HB2	1	0.67
(1,2733)	1:50:A:PRO:HG2	1:54:A:ALA:HB3	8	0.67
(1,2643)	1:125:A:ALA:HA	1:98:A:LYS:HD3	5	0.67
(1,2508)	1:122:B:LEU:HB2	1:130:B:VAL:HB	8	0.67
(1,2507)	1:122:A:LEU:HB2	1:130:A:VAL:HB	8	0.67
(1,1558)	1:115:B:LEU:HD11	1:105:B:GLN:H	3	0.67
(1,1557)	1:115:A:LEU:HD11	1:105:A:GLN:H	3	0.67
(1,1126)	1:90:B:LEU:HG	1:90:B:LEU:H	3	0.67
(1,1125)	1:90:A:LEU:HG	1:90:A:LEU:H	3	0.67
(1,532)	1:102:B:ILE:HG23	1:65:B:PHE:H	8	0.67
(1,531)	1:102:A:ILE:HG23	1:65:A:PHE:H	8	0.67
(1,382)	1:55:B:LYS:HB3	1:57:B:GLN:H	9	0.67
(3,3039)	1:112:A:TYR:HD2	1:109:B:SER:HB2	10	0.66
(3,2964)	1:129:B:LYS:HG3	1:45:B:ILE:HG22	10	0.66
(3,2963)	1:129:A:LYS:HG3	1:45:A:ILE:HG22	10	0.66
(3,2925)	1:126:A:GLY:HA3	1:50:B:PRO:HG3	2	0.66
(3,2641)	1:116:A:MET:HG2	1:45:A:ILE:HD11	5	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,2640)	1:116:B:MET:HG2	1:110:A:VAL:HA	5	0.66
(3,2237)	1:90:A:LEU:HA	1:94:A:THR:HG21	9	0.66
(3,1827)	1:108:A:LYS:HE3	1:113:B:GLU:HB2	1	0.66
(3,1824)	1:129:B:LYS:HD2	1:45:B:ILE:HG21	2	0.66
(3,1823)	1:129:A:LYS:HD2	1:45:A:ILE:HG21	2	0.66
(3,1806)	1:98:B:LYS:HE2	1:124:B:LYS:HD2	5	0.66
(3,1806)	1:98:B:LYS:HE2	1:124:B:LYS:HD2	6	0.66
(3,1068)	1:50:B:PRO:HA	1:54:B:ALA:HB2	6	0.66
(3,1067)	1:50:A:PRO:HA	1:54:A:ALA:HB2	6	0.66
(3,1009)	1:44:A:ASP:HB2	1:105:B:GLN:HG2	6	0.66
(3,904)	1:45:B:ILE:HB	1:49:A:LEU:HB3	7	0.66
(3,903)	1:45:A:ILE:HB	1:49:B:LEU:HB3	1	0.66
(3,903)	1:45:A:ILE:HB	1:49:B:LEU:HB3	7	0.66
(3,812)	1:89:B:VAL:HA	1:79:B:GLN:HE22	6	0.66
(3,460)	1:49:B:LEU:HB2	1:122:A:LEU:H	9	0.66
(3,231)	1:70:A:ALA:HB1	1:72:A:LYS:H	10	0.66
(1,5810)	1:134:B:GLY:HA3	1:116:A:MET:HE1	9	0.66
(1,5406)	1:110:B:VAL:HG12	1:104:B:PHE:HZ	1	0.66
(1,5405)	1:110:A:VAL:HG12	1:104:A:PHE:HZ	1	0.66
(1,5128)	1:100:B:THR:HG23	1:102:B:ILE:HG23	10	0.66
(1,5126)	1:102:B:ILE:HG23	1:66:B:LEU:HG	5	0.66
(1,5125)	1:102:A:ILE:HG23	1:66:A:LEU:HG	5	0.66
(1,4771)	1:94:A:THR:HG21	1:102:A:ILE:HG22	9	0.66
(1,4004)	1:72:B:LYS:HD3	1:110:B:VAL:HA	6	0.66
(1,3578)	1:66:B:LEU:HA	1:115:B:LEU:HD13	5	0.66
(1,3577)	1:66:A:LEU:HA	1:115:A:LEU:HD13	5	0.66
(1,3239)	1:99:A:GLU:HG2	1:49:B:LEU:HB3	7	0.66
(1,2782)	1:51:B:ALA:HB1	1:126:A:GLY:HA3	6	0.66
(1,2772)	1:60:B:PRO:HD3	1:63:B:PRO:HB2	5	0.66
(1,2733)	1:50:A:PRO:HG2	1:54:A:ALA:HB2	5	0.66
(1,2644)	1:125:B:ALA:HA	1:98:B:LYS:HD3	5	0.66
(1,2560)	1:45:B:ILE:HG21	1:54:A:ALA:HB1	2	0.66
(1,2559)	1:45:A:ILE:HG21	1:54:B:ALA:HB1	2	0.66
(1,1996)	1:49:B:LEU:HB2	1:123:A:ARG:H	1	0.66
(1,1995)	1:49:A:LEU:HB2	1:123:B:ARG:H	1	0.66
(1,381)	1:55:A:LYS:HB3	1:57:A:GLN:H	9	0.66
(3,2904)	1:105:B:GLN:HB2	1:69:B:LYS:HD3	10	0.65
(3,2903)	1:105:A:GLN:HB2	1:69:A:LYS:HD3	10	0.65
(3,2639)	1:116:A:MET:HG2	1:110:B:VAL:HA	5	0.65
(3,2288)	1:95:B:GLN:HG2	1:63:B:PRO:HB2	1	0.65
(3,2287)	1:95:A:GLN:HG2	1:63:A:PRO:HB2	1	0.65
(3,2238)	1:90:B:LEU:HA	1:94:B:THR:HG21	9	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,1805)	1:98:A:LYS:HE2	1:124:A:LYS:HD2	5	0.65
(3,1805)	1:98:A:LYS:HE2	1:124:A:LYS:HD2	6	0.65
(3,1489)	1:129:A:LYS:HG3	1:46:B:ARG:HB3	4	0.65
(3,811)	1:89:A:VAL:HA	1:79:A:GLN:HE22	6	0.65
(1,5406)	1:110:B:VAL:HG13	1:104:B:PHE:HZ	4	0.65
(1,5406)	1:110:B:VAL:HG13	1:104:B:PHE:HZ	6	0.65
(1,5405)	1:110:A:VAL:HG13	1:104:A:PHE:HZ	4	0.65
(1,5405)	1:110:A:VAL:HG13	1:104:A:PHE:HZ	6	0.65
(1,4912)	1:100:B:THR:HA	1:129:B:LYS:HD2	2	0.65
(1,4911)	1:100:A:THR:HA	1:129:A:LYS:HD2	2	0.65
(1,4772)	1:94:B:THR:HG21	1:102:B:ILE:HG22	9	0.65
(1,4444)	1:79:B:GLN:HB2	1:65:B:PHE:HB3	4	0.65
(1,4443)	1:79:A:GLN:HB2	1:65:A:PHE:HB3	4	0.65
(1,4278)	1:93:B:ARG:HG2	1:65:B:PHE:HB3	2	0.65
(1,4277)	1:93:A:ARG:HG2	1:65:A:PHE:HB3	2	0.65
(1,4204)	1:107:B:ASP:HB2	1:110:B:VAL:HG11	4	0.65
(1,4203)	1:107:A:ASP:HB2	1:110:A:VAL:HG11	4	0.65
(1,4004)	1:72:B:LYS:HD3	1:110:B:VAL:HA	5	0.65
(1,4003)	1:72:A:LYS:HD3	1:110:A:VAL:HA	5	0.65
(1,4003)	1:72:A:LYS:HD3	1:110:A:VAL:HA	6	0.65
(1,3781)	1:115:A:LEU:HD12	1:68:A:VAL:HB	3	0.65
(1,3604)	1:115:B:LEU:HD11	1:116:B:MET:HE3	5	0.65
(1,3603)	1:115:A:LEU:HD11	1:116:A:MET:HE3	5	0.65
(1,3240)	1:99:B:GLU:HG2	1:49:A:LEU:HB3	7	0.65
(1,2974)	1:56:B:PRO:HD2	1:50:B:PRO:HD2	6	0.65
(1,2973)	1:56:A:PRO:HD2	1:50:A:PRO:HD2	6	0.65
(1,2772)	1:60:B:PRO:HD3	1:63:B:PRO:HB2	7	0.65
(1,2771)	1:60:A:PRO:HD3	1:63:A:PRO:HB2	5	0.65
(1,2771)	1:60:A:PRO:HD3	1:63:A:PRO:HB2	7	0.65
(1,2734)	1:50:B:PRO:HG2	1:54:B:ALA:HB2	5	0.65
(1,1067)	1:89:A:VAL:HG11	1:88:A:SER:H	3	0.65
(1,1004)	1:89:B:VAL:HG11	1:86:B:LEU:H	9	0.65
(1,1003)	1:89:A:VAL:HG11	1:86:A:LEU:H	9	0.65
(1,532)	1:102:B:ILE:HG22	1:65:B:PHE:H	9	0.65
(1,531)	1:102:A:ILE:HG22	1:65:A:PHE:H	9	0.65
(1,194)	1:43:B:VAL:HB	1:44:B:ASP:H	10	0.65
(1,193)	1:43:A:VAL:HB	1:44:A:ASP:H	10	0.65
(3,3040)	1:112:B:TYR:HD2	1:109:A:SER:HB2	10	0.64
(3,2964)	1:129:B:LYS:HG3	1:45:B:ILE:HG23	3	0.64
(3,2963)	1:129:A:LYS:HG3	1:45:A:ILE:HG23	3	0.64
(3,2854)	1:119:B:MET:HE3	1:121:B:THR:HB	10	0.64
(3,2473)	1:101:A:THR:HA	1:45:B:ILE:HG23	4	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,2456)	1:100:B:THR:HG22	1:129:B:LYS:HB3	1	0.64
(3,2455)	1:100:A:THR:HG22	1:129:A:LYS:HB3	1	0.64
(3,2287)	1:95:A:GLN:HG2	1:63:A:PRO:HB2	6	0.64
(3,2176)	1:108:B:LYS:HA	1:139:B:ALA:HB3	2	0.64
(3,1895)	1:123:A:ARG:HG2	1:50:B:PRO:HB3	3	0.64
(3,1563)	1:110:A:VAL:HB	1:72:A:LYS:HG2	4	0.64
(3,1490)	1:129:B:LYS:HG3	1:46:A:ARG:HB3	4	0.64
(3,951)	1:46:A:ARG:HB2	1:48:B:ASP:HB2	6	0.64
(3,880)	1:69:B:LYS:HB2	1:140:B:LYS:HE2	6	0.64
(3,879)	1:69:A:LYS:HB2	1:140:A:LYS:HE2	6	0.64
(3,603)	1:87:A:THR:H	1:119:A:MET:H	6	0.64
(1,5930)	1:112:B:TYR:HE2	1:110:A:VAL:HG11	6	0.64
(1,4796)	1:96:B:ALA:HA	1:90:B:LEU:HB2	2	0.64
(1,4795)	1:96:A:ALA:HA	1:90:A:LEU:HB2	2	0.64
(1,3782)	1:115:B:LEU:HD12	1:68:B:VAL:HB	3	0.64
(1,3726)	1:67:B:SER:HB3	1:114:B:THR:HG23	9	0.64
(1,3725)	1:67:A:SER:HB3	1:114:A:THR:HG23	9	0.64
(1,3344)	1:129:B:LYS:HB2	1:101:B:THR:HG23	9	0.64
(1,3343)	1:129:A:LYS:HB2	1:101:A:THR:HG23	9	0.64
(1,3022)	1:56:B:PRO:HD2	1:57:B:GLN:HG3	2	0.64
(1,3021)	1:56:A:PRO:HD2	1:57:A:GLN:HG3	2	0.64
(1,2974)	1:56:B:PRO:HD2	1:50:B:PRO:HD2	7	0.64
(1,2973)	1:56:A:PRO:HD2	1:50:A:PRO:HD2	7	0.64
(1,2772)	1:60:B:PRO:HD3	1:63:B:PRO:HB2	6	0.64
(1,2623)	1:48:A:ASP:HB3	1:46:B:ARG:HB2	6	0.64
(1,2562)	1:45:B:ILE:HG21	1:49:A:LEU:HD13	8	0.64
(1,1558)	1:115:B:LEU:HD13	1:105:B:GLN:H	8	0.64
(1,1557)	1:115:A:LEU:HD13	1:105:A:GLN:H	8	0.64
(1,1126)	1:90:B:LEU:HG	1:90:B:LEU:H	5	0.64
(1,1126)	1:90:B:LEU:HG	1:90:B:LEU:H	6	0.64
(1,1125)	1:90:A:LEU:HG	1:90:A:LEU:H	5	0.64
(1,1125)	1:90:A:LEU:HG	1:90:A:LEU:H	6	0.64
(1,1068)	1:89:B:VAL:HG11	1:88:B:SER:H	3	0.64
(3,2877)	1:83:A:ALA:HB3	1:121:A:THR:HG23	5	0.63
(3,2853)	1:119:A:MET:HE3	1:121:A:THR:HB	10	0.63
(3,2556)	1:103:B:PHE:HA	1:45:A:ILE:HG23	10	0.63
(3,2474)	1:101:B:THR:HA	1:45:A:ILE:HG23	4	0.63
(3,2464)	1:100:B:THR:HG21	1:102:B:ILE:HG22	5	0.63
(3,2463)	1:100:A:THR:HG21	1:102:A:ILE:HG22	5	0.63
(3,2352)	1:98:B:LYS:HG3	1:125:B:ALA:HB3	8	0.63
(3,2351)	1:98:A:LYS:HG3	1:125:A:ALA:HB3	8	0.63
(3,2288)	1:95:B:GLN:HG2	1:63:B:PRO:HB2	6	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,2175)	1:108:A:LYS:HA	1:139:A:ALA:HB3	2	0.63
(3,1956)	1:79:B:GLN:HG2	1:91:B:ASP:HB3	8	0.63
(3,1955)	1:79:A:GLN:HG2	1:91:A:ASP:HB3	8	0.63
(3,1824)	1:129:B:LYS:HD2	1:45:B:ILE:HG22	7	0.63
(3,1823)	1:129:A:LYS:HD2	1:45:A:ILE:HG22	7	0.63
(3,1564)	1:110:B:VAL:HB	1:72:B:LYS:HG2	4	0.63
(3,1268)	1:48:B:ASP:HB3	1:57:B:GLN:HB3	6	0.63
(3,1267)	1:48:A:ASP:HB3	1:57:A:GLN:HB3	6	0.63
(3,604)	1:87:B:THR:H	1:119:B:MET:H	6	0.63
(3,263)	1:92:A:GLN:HG3	1:79:A:GLN:H	6	0.63
(1,5604)	1:119:B:MET:HE2	1:130:B:VAL:HA	6	0.63
(1,5603)	1:119:A:MET:HE2	1:130:A:VAL:HA	6	0.63
(1,5056)	1:119:B:MET:HA	1:122:B:LEU:HB3	1	0.63
(1,5055)	1:119:A:MET:HA	1:122:A:LEU:HB3	1	0.63
(1,4443)	1:79:A:GLN:HB2	1:65:A:PHE:HB3	5	0.63
(1,3948)	1:91:B:ASP:HB2	1:96:B:ALA:HB3	5	0.63
(1,3782)	1:115:B:LEU:HD12	1:68:B:VAL:HB	10	0.63
(1,3781)	1:115:A:LEU:HD12	1:68:A:VAL:HB	10	0.63
(1,3778)	1:68:B:VAL:HB	1:114:B:THR:HG21	1	0.63
(1,3777)	1:68:A:VAL:HB	1:114:A:THR:HG21	1	0.63
(1,3730)	1:67:B:SER:HB3	1:115:B:LEU:HD13	9	0.63
(1,3729)	1:67:A:SER:HB3	1:115:A:LEU:HD13	9	0.63
(1,3578)	1:66:B:LEU:HA	1:115:B:LEU:HD11	10	0.63
(1,3577)	1:66:A:LEU:HA	1:115:A:LEU:HD11	10	0.63
(1,3368)	1:123:B:ARG:HG2	1:50:A:PRO:HD3	9	0.63
(1,2910)	1:55:B:LYS:HG3	1:58:B:PRO:HG2	8	0.63
(1,2909)	1:55:A:LYS:HG3	1:58:A:PRO:HG2	8	0.63
(1,2772)	1:60:B:PRO:HD3	1:63:B:PRO:HB2	3	0.63
(1,2771)	1:60:A:PRO:HD3	1:63:A:PRO:HB2	3	0.63
(1,2771)	1:60:A:PRO:HD3	1:63:A:PRO:HB2	6	0.63
(1,2644)	1:125:B:ALA:HA	1:98:B:LYS:HD3	2	0.63
(1,2643)	1:125:A:ALA:HA	1:98:A:LYS:HD3	2	0.63
(3,2878)	1:83:B:ALA:HB3	1:121:B:THR:HG23	5	0.62
(3,2456)	1:100:B:THR:HG21	1:129:B:LYS:HB3	5	0.62
(3,1878)	1:105:B:GLN:HG3	1:110:B:VAL:HG13	6	0.62
(3,1877)	1:105:A:GLN:HG3	1:110:A:VAL:HG13	6	0.62
(3,1296)	1:58:B:PRO:HG2	1:55:B:LYS:HE3	10	0.62
(3,1280)	1:57:B:GLN:HG2	1:60:B:PRO:HG3	2	0.62
(3,1279)	1:57:A:GLN:HG2	1:60:A:PRO:HG3	2	0.62
(3,952)	1:46:B:ARG:HB2	1:48:A:ASP:HB2	6	0.62
(3,903)	1:45:A:ILE:HB	1:49:B:LEU:HB3	6	0.62
(3,862)	1:88:B:SER:HA	1:96:B:ALA:HB3	10	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,861)	1:88:A:SER:HA	1:96:A:ALA:HB3	10	0.62
(1,5690)	1:126:B:GLY:HA3	1:98:B:LYS:HD3	7	0.62
(1,5689)	1:126:A:GLY:HA3	1:98:A:LYS:HD3	7	0.62
(1,5422)	1:110:B:VAL:HG12	1:115:B:LEU:HD12	1	0.62
(1,5421)	1:110:A:VAL:HG12	1:115:A:LEU:HD12	1	0.62
(1,5420)	1:110:B:VAL:HG13	1:114:B:THR:HG22	3	0.62
(1,5419)	1:110:A:VAL:HG13	1:114:A:THR:HG22	3	0.62
(1,5238)	1:105:B:GLN:HB2	1:101:B:THR:HG21	9	0.62
(1,5237)	1:105:A:GLN:HB2	1:101:A:THR:HG21	9	0.62
(1,4795)	1:96:A:ALA:HA	1:90:A:LEU:HB2	7	0.62
(1,4518)	1:86:B:LEU:HG	1:90:B:LEU:HG	2	0.62
(1,4517)	1:86:A:LEU:HG	1:90:A:LEU:HG	2	0.62
(1,4444)	1:79:B:GLN:HB2	1:65:B:PHE:HB3	5	0.62
(1,3972)	1:72:B:LYS:HB3	1:72:B:LYS:HD2	10	0.62
(1,3971)	1:72:A:LYS:HB3	1:72:A:LYS:HD2	10	0.62
(1,3778)	1:68:B:VAL:HB	1:114:B:THR:HG21	8	0.62
(1,3777)	1:68:A:VAL:HB	1:114:A:THR:HG21	8	0.62
(1,3604)	1:115:B:LEU:HD11	1:116:B:MET:HE3	6	0.62
(1,3603)	1:115:A:LEU:HD11	1:116:A:MET:HE3	6	0.62
(1,3596)	1:115:B:LEU:HD13	1:119:B:MET:HG3	4	0.62
(1,3595)	1:115:A:LEU:HD13	1:119:A:MET:HG3	4	0.62
(1,3577)	1:66:A:LEU:HA	1:115:A:LEU:HD12	9	0.62
(1,3550)	1:66:B:LEU:HB3	1:122:B:LEU:HG	3	0.62
(1,3549)	1:66:A:LEU:HB3	1:122:A:LEU:HG	3	0.62
(1,3367)	1:123:A:ARG:HG2	1:50:B:PRO:HD3	9	0.62
(1,3138)	1:98:B:LYS:HE3	1:125:B:ALA:HB3	8	0.62
(1,3137)	1:98:A:LYS:HE3	1:125:A:ALA:HB3	8	0.62
(1,2842)	1:57:B:GLN:HA	1:60:B:PRO:HB3	10	0.62
(1,2841)	1:57:A:GLN:HA	1:60:A:PRO:HB3	10	0.62
(1,2816)	1:54:B:ALA:HB2	1:50:B:PRO:HD2	6	0.62
(1,2815)	1:54:A:ALA:HB2	1:50:A:PRO:HD2	6	0.62
(1,2689)	1:93:A:ARG:HG3	1:92:A:GLN:HB3	1	0.62
(1,2664)	1:49:B:LEU:HB2	1:50:B:PRO:HD3	3	0.62
(1,2663)	1:49:A:LEU:HB2	1:50:A:PRO:HD3	3	0.62
(1,2561)	1:45:A:ILE:HG21	1:49:B:LEU:HD13	8	0.62
(1,1861)	1:110:A:VAL:HG13	1:118:A:VAL:H	2	0.62
(1,1126)	1:90:B:LEU:HG	1:90:B:LEU:H	10	0.62
(1,1125)	1:90:A:LEU:HG	1:90:A:LEU:H	10	0.62
(1,1068)	1:89:B:VAL:HG11	1:88:B:SER:H	8	0.62
(1,1067)	1:89:A:VAL:HG11	1:88:A:SER:H	8	0.62
(3,2926)	1:126:B:GLY:HA3	1:50:A:PRO:HG3	2	0.61
(3,2851)	1:49:A:LEU:HA	1:51:A:ALA:HB2	8	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,2555)	1:103:A:PHE:HA	1:45:B:ILE:HG23	10	0.61
(3,2513)	1:129:A:LYS:HD2	1:102:A:ILE:HG13	6	0.61
(3,2455)	1:100:A:THR:HG21	1:129:A:LYS:HB3	5	0.61
(3,2114)	1:87:B:THR:HG23	1:124:B:LYS:HD3	6	0.61
(3,2113)	1:87:A:THR:HG23	1:124:A:LYS:HD3	6	0.61
(3,1878)	1:105:B:GLN:HG3	1:110:B:VAL:HG12	10	0.61
(3,1877)	1:105:A:GLN:HG3	1:110:A:VAL:HG12	10	0.61
(3,1824)	1:129:B:LYS:HD2	1:45:B:ILE:HG22	4	0.61
(3,1823)	1:129:A:LYS:HD2	1:45:A:ILE:HG22	4	0.61
(3,1295)	1:58:A:PRO:HG2	1:55:A:LYS:HE3	10	0.61
(3,414)	1:93:B:ARG:HA	1:97:B:ASN:H	7	0.61
(3,275)	1:73:A:GLN:HG2	1:79:A:GLN:H	7	0.61
(3,264)	1:92:B:GLN:HG3	1:79:B:GLN:H	6	0.61
(1,5810)	1:134:B:GLY:HA3	1:116:A:MET:HE3	2	0.61
(1,5608)	1:51:B:ALA:HB2	1:124:A:LYS:HA	6	0.61
(1,5414)	1:68:B:VAL:HB	1:110:B:VAL:HG11	9	0.61
(1,5413)	1:68:A:VAL:HB	1:110:A:VAL:HG11	9	0.61
(1,5258)	1:105:B:GLN:HG2	1:65:B:PHE:HB2	7	0.61
(1,5257)	1:105:A:GLN:HG2	1:65:A:PHE:HB2	7	0.61
(1,4796)	1:96:B:ALA:HA	1:90:B:LEU:HB2	7	0.61
(1,3960)	1:72:B:LYS:HA	1:72:B:LYS:HD3	1	0.61
(1,3960)	1:72:B:LYS:HA	1:72:B:LYS:HD3	5	0.61
(1,3959)	1:72:A:LYS:HA	1:72:A:LYS:HD3	1	0.61
(1,3784)	1:68:B:VAL:HB	1:106:B:ALA:HB2	1	0.61
(1,3783)	1:68:A:VAL:HB	1:106:A:ALA:HB2	1	0.61
(1,3578)	1:66:B:LEU:HA	1:115:B:LEU:HD12	9	0.61
(1,3222)	1:122:B:LEU:HA	1:125:B:ALA:HB3	4	0.61
(1,3221)	1:122:A:LEU:HA	1:125:A:ALA:HB3	4	0.61
(1,2910)	1:55:B:LYS:HG3	1:58:B:PRO:HG2	3	0.61
(1,2909)	1:55:A:LYS:HG3	1:58:A:PRO:HG2	3	0.61
(1,2690)	1:93:B:ARG:HG3	1:92:B:GLN:HB3	1	0.61
(1,2690)	1:93:B:ARG:HG3	1:92:B:GLN:HB3	7	0.61
(1,2689)	1:93:A:ARG:HG3	1:92:A:GLN:HB3	7	0.61
(1,1862)	1:110:B:VAL:HG13	1:118:B:VAL:H	2	0.61
(1,1558)	1:115:B:LEU:HD11	1:105:B:GLN:H	10	0.61
(1,1126)	1:90:B:LEU:HG	1:90:B:LEU:H	7	0.61
(1,1125)	1:90:A:LEU:HG	1:90:A:LEU:H	7	0.61
(1,952)	1:84:B:ASP:HB2	1:84:B:ASP:H	3	0.61
(1,951)	1:84:A:ASP:HB2	1:84:A:ASP:H	3	0.61
(1,98)	1:106:B:ALA:HB3	1:107:B:ASP:H	3	0.61
(1,97)	1:106:A:ALA:HB2	1:107:A:ASP:H	1	0.61
(1,97)	1:106:A:ALA:HB3	1:107:A:ASP:H	3	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,2944)	1:128:B:LEU:HA	1:125:B:ALA:HB1	8	0.6
(3,2943)	1:128:A:LEU:HA	1:125:A:ALA:HB1	8	0.6
(3,2852)	1:49:B:LEU:HA	1:51:B:ALA:HB2	8	0.6
(3,2532)	1:102:B:ILE:HG21	1:133:B:VAL:HB	6	0.6
(3,2531)	1:102:A:ILE:HG21	1:133:A:VAL:HB	6	0.6
(3,2514)	1:129:B:LYS:HD2	1:102:B:ILE:HG13	6	0.6
(3,2454)	1:94:B:THR:HG22	1:64:B:VAL:HB	1	0.6
(3,2453)	1:94:A:THR:HG22	1:64:A:VAL:HB	1	0.6
(3,2392)	1:136:B:GLU:HG3	1:140:B:LYS:HB3	4	0.6
(3,2391)	1:136:A:GLU:HG3	1:140:A:LYS:HB3	4	0.6
(3,2374)	1:98:B:LYS:HG2	1:98:B:LYS:HE2	8	0.6
(3,2354)	1:98:B:LYS:HG2	1:96:B:ALA:HB3	3	0.6
(3,1640)	1:115:B:LEU:HD11	1:131:B:GLY:HA3	1	0.6
(3,1639)	1:115:A:LEU:HD11	1:131:A:GLY:HA3	1	0.6
(3,1286)	1:57:B:GLN:HG3	1:129:B:LYS:HD2	8	0.6
(3,1278)	1:57:B:GLN:HG2	1:50:B:PRO:HD2	7	0.6
(3,1277)	1:57:A:GLN:HG2	1:50:A:PRO:HD2	6	0.6
(3,1277)	1:57:A:GLN:HG2	1:50:A:PRO:HD2	7	0.6
(3,845)	1:44:A:ASP:HA	1:105:B:GLN:HB3	7	0.6
(3,413)	1:93:A:ARG:HA	1:97:A:ASN:H	7	0.6
(3,276)	1:73:B:GLN:HG2	1:79:B:GLN:H	7	0.6
(1,5809)	1:134:A:GLY:HA3	1:116:B:MET:HE3	2	0.6
(1,5212)	1:104:B:PHE:HB2	1:115:B:LEU:HD13	7	0.6
(1,5211)	1:104:A:PHE:HB2	1:115:A:LEU:HD13	7	0.6
(1,5066)	1:115:B:LEU:HD12	1:119:B:MET:HA	4	0.6
(1,5065)	1:115:A:LEU:HD12	1:119:A:MET:HA	4	0.6
(1,4010)	1:72:B:LYS:HD3	1:110:B:VAL:HG21	9	0.6
(1,3960)	1:72:B:LYS:HA	1:72:B:LYS:HD3	9	0.6
(1,3959)	1:72:A:LYS:HA	1:72:A:LYS:HD3	5	0.6
(1,3959)	1:72:A:LYS:HA	1:72:A:LYS:HD3	9	0.6
(1,3947)	1:91:A:ASP:HB2	1:96:A:ALA:HB3	5	0.6
(1,3726)	1:67:B:SER:HB3	1:114:B:THR:HG21	6	0.6
(1,3725)	1:67:A:SER:HB3	1:114:A:THR:HG21	6	0.6
(1,3542)	1:66:B:LEU:HB2	1:106:B:ALA:HB3	2	0.6
(1,3541)	1:66:A:LEU:HB2	1:106:A:ALA:HB3	2	0.6
(1,2562)	1:45:B:ILE:HG21	1:49:A:LEU:HD11	7	0.6
(1,2561)	1:45:A:ILE:HG21	1:49:B:LEU:HD11	7	0.6
(1,1557)	1:115:A:LEU:HD11	1:105:A:GLN:H	10	0.6
(1,1004)	1:89:B:VAL:HG12	1:86:B:LEU:H	3	0.6
(1,98)	1:106:B:ALA:HB2	1:107:B:ASP:H	1	0.6
(3,3059)	1:65:A:PHE:HE1	1:93:A:ARG:HB2	1	0.59
(3,2852)	1:49:B:LEU:HA	1:51:B:ALA:HB1	1	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,2852)	1:49:B:LEU:HA	1:51:B:ALA:HB2	10	0.59
(3,2851)	1:49:A:LEU:HA	1:51:A:ALA:HB1	1	0.59
(3,2851)	1:49:A:LEU:HA	1:51:A:ALA:HB2	10	0.59
(3,2730)	1:110:B:VAL:HG23	1:119:B:MET:HE3	3	0.59
(3,2729)	1:110:A:VAL:HG23	1:119:A:MET:HE3	3	0.59
(3,2374)	1:98:B:LYS:HG2	1:98:B:LYS:HE2	9	0.59
(3,2373)	1:98:A:LYS:HG2	1:98:A:LYS:HE2	8	0.59
(3,2373)	1:98:A:LYS:HG2	1:98:A:LYS:HE2	9	0.59
(3,2353)	1:98:A:LYS:HG2	1:96:A:ALA:HB3	3	0.59
(3,2295)	1:96:A:ALA:HA	1:100:A:THR:HG22	7	0.59
(3,2127)	1:87:A:THR:HG23	1:88:A:SER:HB2	2	0.59
(3,1878)	1:105:B:GLN:HG3	1:110:B:VAL:HG12	1	0.59
(3,1877)	1:105:A:GLN:HG3	1:110:A:VAL:HG12	1	0.59
(3,1640)	1:115:B:LEU:HD13	1:131:B:GLY:HA2	7	0.59
(3,1639)	1:115:A:LEU:HD13	1:131:A:GLY:HA2	7	0.59
(3,1285)	1:57:A:GLN:HG3	1:129:A:LYS:HD2	8	0.59
(3,1285)	1:57:A:GLN:HG3	1:129:A:LYS:HD2	9	0.59
(3,1278)	1:57:B:GLN:HG2	1:50:B:PRO:HD2	6	0.59
(3,1278)	1:57:B:GLN:HG2	1:50:B:PRO:HD2	8	0.59
(3,1277)	1:57:A:GLN:HG2	1:50:A:PRO:HD2	8	0.59
(3,904)	1:45:B:ILE:HB	1:49:A:LEU:HB3	9	0.59
(3,880)	1:69:B:LYS:HB2	1:140:B:LYS:HE3	4	0.59
(3,879)	1:69:A:LYS:HB2	1:140:A:LYS:HE3	4	0.59
(3,846)	1:44:B:ASP:HA	1:105:A:GLN:HB3	7	0.59
(3,232)	1:72:B:LYS:HG2	1:72:B:LYS:H	9	0.59
(1,5929)	1:112:A:TYR:HE2	1:110:B:VAL:HG11	6	0.59
(1,4204)	1:107:B:ASP:HB2	1:110:B:VAL:HG12	3	0.59
(1,4203)	1:107:A:ASP:HB2	1:110:A:VAL:HG12	3	0.59
(1,4132)	1:74:B:LEU:HB3	1:119:B:MET:HE1	3	0.59
(1,4131)	1:74:A:LEU:HB3	1:119:A:MET:HE1	3	0.59
(1,4009)	1:72:A:LYS:HD3	1:110:A:VAL:HG21	9	0.59
(1,4004)	1:72:B:LYS:HD3	1:110:B:VAL:HA	1	0.59
(1,4003)	1:72:A:LYS:HD3	1:110:A:VAL:HA	1	0.59
(1,3784)	1:68:B:VAL:HB	1:106:B:ALA:HB3	3	0.59
(1,3783)	1:68:A:VAL:HB	1:106:A:ALA:HB3	3	0.59
(1,3778)	1:68:B:VAL:HB	1:114:B:THR:HG21	7	0.59
(1,3777)	1:68:A:VAL:HB	1:114:A:THR:HG21	7	0.59
(1,2902)	1:55:B:LYS:HB2	1:45:A:ILE:HG12	10	0.59
(1,2496)	1:45:B:ILE:HA	1:54:A:ALA:HB2	10	0.59
(1,1861)	1:110:A:VAL:HG13	1:118:A:VAL:H	4	0.59
(1,1003)	1:89:A:VAL:HG12	1:86:A:LEU:H	3	0.59
(1,944)	1:121:B:THR:HB	1:84:B:ASP:H	10	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,943)	1:121:A:THR:HB	1:84:A:ASP:H	10	0.59
(3,3060)	1:65:B:PHE:HE1	1:93:B:ARG:HB2	1	0.58
(3,3060)	1:65:B:PHE:HE2	1:93:B:ARG:HB2	5	0.58
(3,3060)	1:65:B:PHE:HE2	1:93:B:ARG:HB2	6	0.58
(3,3059)	1:65:A:PHE:HE2	1:93:A:ARG:HB2	5	0.58
(3,3059)	1:65:A:PHE:HE2	1:93:A:ARG:HB2	6	0.58
(3,2974)	1:130:B:VAL:HB	1:119:B:MET:HE1	9	0.58
(3,2973)	1:130:A:VAL:HB	1:119:A:MET:HE1	9	0.58
(3,2508)	1:86:B:LEU:HG	1:119:B:MET:HA	6	0.58
(3,2507)	1:86:A:LEU:HG	1:119:A:MET:HA	6	0.58
(3,2374)	1:98:B:LYS:HG2	1:98:B:LYS:HE2	3	0.58
(3,2373)	1:98:A:LYS:HG2	1:98:A:LYS:HE2	3	0.58
(3,2296)	1:96:B:ALA:HA	1:100:B:THR:HG22	7	0.58
(3,2128)	1:87:B:THR:HG23	1:88:B:SER:HB2	2	0.58
(3,2114)	1:87:B:THR:HG23	1:124:B:LYS:HD3	1	0.58
(3,1878)	1:105:B:GLN:HG3	1:110:B:VAL:HG11	5	0.58
(3,1877)	1:105:A:GLN:HG3	1:110:A:VAL:HG11	5	0.58
(3,1286)	1:57:B:GLN:HG3	1:129:B:LYS:HD2	9	0.58
(3,1106)	1:51:B:ALA:HA	1:124:A:LYS:HB3	5	0.58
(3,995)	1:47:A:VAL:HB	1:128:B:LEU:HG	5	0.58
(3,904)	1:45:B:ILE:HB	1:49:A:LEU:HB3	6	0.58
(3,903)	1:45:A:ILE:HB	1:49:B:LEU:HB3	9	0.58
(3,437)	1:87:A:THR:HG22	1:100:A:THR:H	1	0.58
(3,384)	1:98:B:LYS:H	1:93:B:ARG:H	7	0.58
(3,383)	1:98:A:LYS:H	1:93:A:ARG:H	7	0.58
(3,275)	1:73:A:GLN:HG2	1:79:A:GLN:H	9	0.58
(3,231)	1:72:A:LYS:HG2	1:72:A:LYS:H	9	0.58
(3,74)	1:46:B:ARG:HG2	1:46:B:ARG:H	10	0.58
(3,73)	1:46:A:ARG:HG2	1:46:A:ARG:H	10	0.58
(1,4912)	1:100:B:THR:HA	1:129:B:LYS:HD2	7	0.58
(1,4573)	1:87:A:THR:HG22	1:90:A:LEU:HG	1	0.58
(1,4496)	1:115:B:LEU:HB3	1:106:B:ALA:HB2	5	0.58
(1,4008)	1:72:B:LYS:HD3	1:114:B:THR:HG22	1	0.58
(1,4007)	1:72:A:LYS:HD3	1:114:A:THR:HG22	1	0.58
(1,3782)	1:115:B:LEU:HD12	1:68:B:VAL:HB	1	0.58
(1,3781)	1:115:A:LEU:HD12	1:68:A:VAL:HB	1	0.58
(1,2782)	1:51:B:ALA:HB2	1:126:A:GLY:HA3	9	0.58
(1,2781)	1:51:A:ALA:HB2	1:126:B:GLY:HA3	9	0.58
(1,2495)	1:45:A:ILE:HA	1:54:B:ALA:HB2	10	0.58
(1,2086)	1:98:B:LYS:HD3	1:127:B:TYR:H	3	0.58
(1,2085)	1:98:A:LYS:HD3	1:127:A:TYR:H	3	0.58
(1,1862)	1:110:B:VAL:HG13	1:118:B:VAL:H	4	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1004)	1:89:B:VAL:HG11	1:86:B:LEU:H	10	0.58
(1,1003)	1:89:A:VAL:HG11	1:86:A:LEU:H	10	0.58
(3,2906)	1:124:B:LYS:HD2	1:121:B:THR:HA	8	0.57
(3,2238)	1:90:B:LEU:HA	1:94:B:THR:HG21	6	0.57
(3,2237)	1:90:A:LEU:HA	1:94:A:THR:HG21	6	0.57
(3,2127)	1:87:A:THR:HG23	1:88:A:SER:HB2	9	0.57
(3,2113)	1:87:A:THR:HG23	1:124:A:LYS:HD3	1	0.57
(3,1630)	1:66:B:LEU:HB3	1:140:B:LYS:HG2	1	0.57
(3,1629)	1:66:A:LEU:HB3	1:140:A:LYS:HG2	1	0.57
(3,812)	1:89:B:VAL:HA	1:79:B:GLN:HE22	3	0.57
(3,811)	1:89:A:VAL:HA	1:79:A:GLN:HE22	3	0.57
(3,438)	1:87:B:THR:HG22	1:100:B:THR:H	1	0.57
(3,286)	1:124:B:LYS:HG2	1:84:B:ASP:H	8	0.57
(3,285)	1:124:A:LYS:HG2	1:84:A:ASP:H	8	0.57
(3,276)	1:73:B:GLN:HG2	1:79:B:GLN:H	9	0.57
(3,111)	1:98:A:LYS:HB3	1:51:B:ALA:H	1	0.57
(1,4911)	1:100:A:THR:HA	1:129:A:LYS:HD2	7	0.57
(1,4760)	1:94:B:THR:HG23	1:99:B:GLU:HG3	1	0.57
(1,4759)	1:94:A:THR:HG23	1:99:A:GLU:HG3	1	0.57
(1,4759)	1:94:A:THR:HG23	1:99:A:GLU:HG3	7	0.57
(1,4752)	1:94:B:THR:HG21	1:96:B:ALA:HA	3	0.57
(1,4751)	1:94:A:THR:HG21	1:96:A:ALA:HA	3	0.57
(1,4574)	1:87:B:THR:HG22	1:90:B:LEU:HG	1	0.57
(1,4504)	1:86:B:LEU:HB2	1:121:B:THR:HG22	9	0.57
(1,4503)	1:86:A:LEU:HB2	1:121:A:THR:HG22	9	0.57
(1,4496)	1:115:B:LEU:HB3	1:106:B:ALA:HB1	6	0.57
(1,4495)	1:115:A:LEU:HB3	1:106:A:ALA:HB2	5	0.57
(1,4495)	1:115:A:LEU:HB3	1:106:A:ALA:HB1	6	0.57
(1,4350)	1:82:B:ASN:HB2	1:82:B:ASN:HA	1	0.57
(1,4350)	1:82:B:ASN:HB2	1:82:B:ASN:HA	4	0.57
(1,4350)	1:82:B:ASN:HB2	1:82:B:ASN:HA	6	0.57
(1,4350)	1:82:B:ASN:HB2	1:82:B:ASN:HA	7	0.57
(1,4350)	1:82:B:ASN:HB2	1:82:B:ASN:HA	8	0.57
(1,4349)	1:82:A:ASN:HB2	1:82:A:ASN:HA	1	0.57
(1,4349)	1:82:A:ASN:HB2	1:82:A:ASN:HA	4	0.57
(1,4349)	1:82:A:ASN:HB2	1:82:A:ASN:HA	6	0.57
(1,4349)	1:82:A:ASN:HB2	1:82:A:ASN:HA	8	0.57
(1,4349)	1:82:A:ASN:HB2	1:82:A:ASN:HA	10	0.57
(1,4278)	1:93:B:ARG:HG2	1:65:B:PHE:HB3	1	0.57
(1,4277)	1:93:A:ARG:HG2	1:65:A:PHE:HB3	1	0.57
(1,3962)	1:72:B:LYS:HA	1:72:B:LYS:HG3	2	0.57
(1,3961)	1:72:A:LYS:HA	1:72:A:LYS:HG3	2	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3779)	1:68:A:VAL:HB	1:110:A:VAL:HG22	4	0.57
(1,3730)	1:67:B:SER:HB3	1:115:B:LEU:HD12	6	0.57
(1,3729)	1:67:A:SER:HB3	1:115:A:LEU:HD12	6	0.57
(1,3542)	1:66:B:LEU:HB2	1:106:B:ALA:HB3	9	0.57
(1,2901)	1:55:A:LYS:HB2	1:45:B:ILE:HG12	10	0.57
(1,2664)	1:49:B:LEU:HB2	1:50:B:PRO:HD3	4	0.57
(1,2663)	1:49:A:LEU:HB2	1:50:A:PRO:HD3	4	0.57
(1,2044)	1:98:B:LYS:HD3	1:126:B:GLY:H	5	0.57
(1,1004)	1:89:B:VAL:HG12	1:86:B:LEU:H	8	0.57
(1,1003)	1:89:A:VAL:HG12	1:86:A:LEU:H	8	0.57
(1,97)	1:106:A:ALA:HB1	1:107:A:ASP:H	9	0.57
(3,2963)	1:129:A:LYS:HG3	1:45:A:ILE:HG21	2	0.56
(3,2905)	1:124:A:LYS:HD2	1:121:A:THR:HA	8	0.56
(3,2852)	1:49:B:LEU:HA	1:51:B:ALA:HB2	5	0.56
(3,2851)	1:49:A:LEU:HA	1:51:A:ALA:HB2	5	0.56
(3,2824)	1:115:B:LEU:HD22	1:116:A:MET:HG2	10	0.56
(3,2323)	1:127:A:TYR:HE1	1:98:A:LYS:HG2	1	0.56
(3,2238)	1:90:B:LEU:HA	1:94:B:THR:HG22	10	0.56
(3,2237)	1:90:A:LEU:HA	1:94:A:THR:HG22	10	0.56
(3,1998)	1:81:B:VAL:HA	1:66:B:LEU:HB2	1	0.56
(3,1997)	1:81:A:VAL:HA	1:66:A:LEU:HB2	1	0.56
(3,1955)	1:79:A:GLN:HG3	1:91:A:ASP:HB3	5	0.56
(3,1564)	1:110:B:VAL:HB	1:72:B:LYS:HG2	2	0.56
(3,1563)	1:110:A:VAL:HB	1:72:A:LYS:HG2	2	0.56
(3,1104)	1:139:B:ALA:HA	1:136:B:GLU:HB2	3	0.56
(3,870)	1:43:B:VAL:HB	1:56:A:PRO:HD3	7	0.56
(3,276)	1:73:B:GLN:HG2	1:79:B:GLN:H	8	0.56
(3,232)	1:72:B:LYS:HG2	1:72:B:LYS:H	5	0.56
(3,232)	1:72:B:LYS:HG2	1:72:B:LYS:H	7	0.56
(3,231)	1:72:A:LYS:HG2	1:72:A:LYS:H	5	0.56
(1,5607)	1:51:A:ALA:HB2	1:124:B:LYS:HA	6	0.56
(1,5582)	1:118:B:VAL:HB	1:83:B:ALA:HB2	1	0.56
(1,5552)	1:116:B:MET:HE2	1:113:B:GLU:HA	10	0.56
(1,5212)	1:104:B:PHE:HB2	1:115:B:LEU:HD12	9	0.56
(1,5211)	1:104:A:PHE:HB2	1:115:A:LEU:HD12	9	0.56
(1,5127)	1:100:A:THR:HG23	1:102:A:ILE:HG23	6	0.56
(1,4760)	1:94:B:THR:HG23	1:99:B:GLU:HG3	7	0.56
(1,4364)	1:82:B:ASN:HB3	1:85:B:GLN:HG2	5	0.56
(1,4350)	1:82:B:ASN:HB2	1:82:B:ASN:HA	5	0.56
(1,4350)	1:82:B:ASN:HB2	1:82:B:ASN:HA	10	0.56
(1,4349)	1:82:A:ASN:HB2	1:82:A:ASN:HA	5	0.56
(1,4349)	1:82:A:ASN:HB2	1:82:A:ASN:HA	7	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4277)	1:93:A:ARG:HG2	1:65:A:PHE:HB3	5	0.56
(1,3966)	1:72:B:LYS:HA	1:110:B:VAL:HG13	9	0.56
(1,3780)	1:68:B:VAL:HB	1:110:B:VAL:HG22	4	0.56
(1,3779)	1:68:A:VAL:HB	1:110:A:VAL:HG23	3	0.56
(1,3541)	1:66:A:LEU:HB2	1:106:A:ALA:HB3	9	0.56
(1,3540)	1:66:B:LEU:HB2	1:102:B:ILE:HG22	6	0.56
(1,3440)	1:64:B:VAL:HA	1:102:B:ILE:HG22	5	0.56
(1,3439)	1:64:A:VAL:HA	1:102:A:ILE:HG22	5	0.56
(1,3344)	1:129:B:LYS:HB2	1:101:B:THR:HG23	10	0.56
(1,2601)	1:47:A:VAL:HB	1:119:B:MET:HB3	2	0.56
(1,2562)	1:45:B:ILE:HG21	1:49:A:LEU:HD12	10	0.56
(1,2561)	1:45:A:ILE:HG21	1:49:B:LEU:HD11	6	0.56
(1,2043)	1:98:A:LYS:HD3	1:126:A:GLY:H	5	0.56
(1,1122)	1:110:B:VAL:HG21	1:114:B:THR:H	6	0.56
(1,1121)	1:110:A:VAL:HG21	1:114:A:THR:H	6	0.56
(1,1068)	1:89:B:VAL:HG12	1:88:B:SER:H	2	0.56
(1,1067)	1:89:A:VAL:HG12	1:88:A:SER:H	2	0.56
(1,98)	1:106:B:ALA:HB1	1:107:B:ASP:H	9	0.56
(3,2964)	1:129:B:LYS:HG3	1:45:B:ILE:HG21	2	0.55
(3,2938)	1:127:B:TYR:HB2	1:45:B:ILE:HD11	2	0.55
(3,2937)	1:127:A:TYR:HB2	1:45:A:ILE:HD11	2	0.55
(3,2896)	1:123:B:ARG:HD2	1:54:A:ALA:HB3	3	0.55
(3,2823)	1:115:A:LEU:HD22	1:116:B:MET:HG2	10	0.55
(3,2556)	1:103:B:PHE:HA	1:115:B:LEU:HD13	8	0.55
(3,2555)	1:103:A:PHE:HA	1:115:A:LEU:HD13	8	0.55
(3,2392)	1:136:B:GLU:HG3	1:140:B:LYS:HB3	3	0.55
(3,2391)	1:136:A:GLU:HG3	1:140:A:LYS:HB3	3	0.55
(3,2352)	1:98:B:LYS:HG3	1:125:B:ALA:HB1	3	0.55
(3,2351)	1:98:A:LYS:HG3	1:125:A:ALA:HB1	3	0.55
(3,2324)	1:127:B:TYR:HE1	1:98:B:LYS:HG2	1	0.55
(3,2176)	1:108:B:LYS:HA	1:139:B:ALA:HB2	10	0.55
(3,2175)	1:108:A:LYS:HA	1:139:A:ALA:HB2	10	0.55
(3,2128)	1:87:B:THR:HG23	1:88:B:SER:HB2	9	0.55
(3,1956)	1:79:B:GLN:HG3	1:91:B:ASP:HB3	5	0.55
(3,1727)	1:69:A:LYS:HB3	1:66:A:LEU:HG	7	0.55
(3,1103)	1:139:A:ALA:HA	1:136:A:GLU:HB2	3	0.55
(3,996)	1:47:B:VAL:HB	1:128:A:LEU:HG	5	0.55
(3,974)	1:46:B:ARG:HD2	1:46:B:ARG:HA	4	0.55
(3,973)	1:46:A:ARG:HD2	1:46:A:ARG:HA	4	0.55
(3,460)	1:49:B:LEU:HB2	1:122:A:LEU:H	5	0.55
(3,437)	1:87:A:THR:HG21	1:100:A:THR:H	7	0.55
(3,414)	1:93:B:ARG:HA	1:97:B:ASN:H	6	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,413)	1:93:A:ARG:HA	1:97:A:ASN:H	6	0.55
(3,275)	1:73:A:GLN:HG2	1:79:A:GLN:H	8	0.55
(3,231)	1:72:A:LYS:HG2	1:72:A:LYS:H	7	0.55
(3,112)	1:98:B:LYS:HB3	1:51:A:ALA:H	1	0.55
(1,5805)	1:134:A:GLY:HA3	1:116:B:MET:HB2	3	0.55
(1,5581)	1:118:A:VAL:HB	1:83:A:ALA:HB2	1	0.55
(1,5551)	1:116:A:MET:HE2	1:113:A:GLU:HA	10	0.55
(1,5212)	1:104:B:PHE:HB2	1:115:B:LEU:HD11	1	0.55
(1,5211)	1:104:A:PHE:HB2	1:115:A:LEU:HD11	1	0.55
(1,5128)	1:100:B:THR:HG23	1:102:B:ILE:HG23	6	0.55
(1,5056)	1:119:B:MET:HA	1:122:B:LEU:HB3	6	0.55
(1,5055)	1:119:A:MET:HA	1:122:A:LEU:HB3	6	0.55
(1,4496)	1:115:B:LEU:HB3	1:106:B:ALA:HB2	10	0.55
(1,4495)	1:115:A:LEU:HB3	1:106:A:ALA:HB2	10	0.55
(1,4363)	1:82:A:ASN:HB3	1:85:A:GLN:HG2	5	0.55
(1,4278)	1:93:B:ARG:HG2	1:65:B:PHE:HB3	5	0.55
(1,4132)	1:74:B:LEU:HB3	1:119:B:MET:HE3	5	0.55
(1,4077)	1:105:A:GLN:HG3	1:137:A:GLY:HA3	3	0.55
(1,3965)	1:72:A:LYS:HA	1:110:A:VAL:HG13	9	0.55
(1,3962)	1:72:B:LYS:HA	1:72:B:LYS:HG3	4	0.55
(1,3961)	1:72:A:LYS:HA	1:72:A:LYS:HG3	4	0.55
(1,3856)	1:69:B:LYS:HD3	1:65:B:PHE:HB2	2	0.55
(1,3855)	1:69:A:LYS:HD3	1:65:A:PHE:HB2	2	0.55
(1,3780)	1:68:B:VAL:HB	1:110:B:VAL:HG22	1	0.55
(1,3780)	1:68:B:VAL:HB	1:110:B:VAL:HG23	3	0.55
(1,3779)	1:68:A:VAL:HB	1:110:A:VAL:HG22	1	0.55
(1,3542)	1:66:B:LEU:HB2	1:106:B:ALA:HB3	4	0.55
(1,3541)	1:66:A:LEU:HB2	1:106:A:ALA:HB3	4	0.55
(1,3539)	1:66:A:LEU:HB2	1:102:A:ILE:HG22	6	0.55
(1,3344)	1:129:B:LYS:HB2	1:101:B:THR:HG21	4	0.55
(1,3343)	1:129:A:LYS:HB2	1:101:A:THR:HG21	4	0.55
(1,3343)	1:129:A:LYS:HB2	1:101:A:THR:HG23	10	0.55
(1,2781)	1:51:A:ALA:HB3	1:126:B:GLY:HA3	7	0.55
(1,2664)	1:49:B:LEU:HB2	1:50:B:PRO:HD3	9	0.55
(1,2663)	1:49:A:LEU:HB2	1:50:A:PRO:HD3	9	0.55
(1,2602)	1:47:B:VAL:HB	1:119:A:MET:HB3	2	0.55
(1,2508)	1:122:B:LEU:HB2	1:130:B:VAL:HB	10	0.55
(1,2507)	1:122:A:LEU:HB2	1:130:A:VAL:HB	10	0.55
(1,1067)	1:89:A:VAL:HG12	1:88:A:SER:H	5	0.55
(3,2964)	1:129:B:LYS:HG3	1:45:B:ILE:HG22	7	0.54
(3,2556)	1:103:B:PHE:HA	1:45:A:ILE:HG23	7	0.54
(3,2555)	1:103:A:PHE:HA	1:45:B:ILE:HG23	7	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,2373)	1:98:A:LYS:HG2	1:98:A:LYS:HE2	10	0.54
(3,2114)	1:87:B:THR:HG22	1:124:B:LYS:HD3	9	0.54
(3,2108)	1:87:B:THR:HG21	1:124:B:LYS:HA	10	0.54
(3,2107)	1:87:A:THR:HG21	1:124:A:LYS:HA	10	0.54
(3,1736)	1:69:B:LYS:HD2	1:72:B:LYS:HE2	2	0.54
(3,1728)	1:69:B:LYS:HB3	1:66:B:LEU:HG	7	0.54
(3,997)	1:47:A:VAL:HB	1:129:B:LYS:HG3	5	0.54
(3,974)	1:46:B:ARG:HD3	1:46:B:ARG:HA	6	0.54
(3,974)	1:46:B:ARG:HD3	1:46:B:ARG:HA	9	0.54
(3,973)	1:46:A:ARG:HD3	1:46:A:ARG:HA	6	0.54
(3,869)	1:43:A:VAL:HB	1:56:B:PRO:HD3	7	0.54
(3,810)	1:86:B:LEU:HA	1:79:B:GLN:HE21	3	0.54
(3,438)	1:87:B:THR:HG21	1:100:B:THR:H	7	0.54
(3,438)	1:87:B:THR:HG21	1:100:B:THR:H	8	0.54
(3,437)	1:87:A:THR:HG21	1:100:A:THR:H	8	0.54
(3,437)	1:87:A:THR:HG23	1:100:A:THR:H	10	0.54
(3,264)	1:92:B:GLN:HG3	1:79:B:GLN:H	7	0.54
(3,232)	1:72:B:LYS:HG2	1:72:B:LYS:H	6	0.54
(3,231)	1:72:A:LYS:HG2	1:72:A:LYS:H	6	0.54
(1,5908)	1:65:B:PHE:HE1	1:100:B:THR:HG21	10	0.54
(1,5907)	1:65:A:PHE:HE1	1:100:A:THR:HG21	10	0.54
(1,4795)	1:96:A:ALA:HA	1:90:A:LEU:HB2	6	0.54
(1,4278)	1:93:B:ARG:HG2	1:65:B:PHE:HB3	4	0.54
(1,4277)	1:93:A:ARG:HG2	1:65:A:PHE:HB3	4	0.54
(1,4132)	1:74:B:LEU:HB3	1:119:B:MET:HE1	6	0.54
(1,4131)	1:74:A:LEU:HB3	1:119:A:MET:HE3	5	0.54
(1,4131)	1:74:A:LEU:HB3	1:119:A:MET:HE1	6	0.54
(1,4078)	1:105:B:GLN:HG3	1:137:B:GLY:HA3	3	0.54
(1,4010)	1:72:B:LYS:HD3	1:110:B:VAL:HG21	6	0.54
(1,4009)	1:72:A:LYS:HD3	1:110:A:VAL:HG21	6	0.54
(1,3960)	1:72:B:LYS:HA	1:72:B:LYS:HD3	6	0.54
(1,3959)	1:72:A:LYS:HA	1:72:A:LYS:HD3	6	0.54
(1,3855)	1:69:A:LYS:HD3	1:65:A:PHE:HB2	6	0.54
(1,3726)	1:67:B:SER:HB3	1:114:B:THR:HG23	5	0.54
(1,3354)	1:122:B:LEU:HG	1:119:B:MET:HB2	10	0.54
(1,3353)	1:122:A:LEU:HG	1:119:A:MET:HB2	10	0.54
(1,2561)	1:45:A:ILE:HG21	1:49:B:LEU:HD12	10	0.54
(1,1068)	1:89:B:VAL:HG12	1:88:B:SER:H	5	0.54
(1,406)	1:58:B:PRO:HB3	1:59:B:ARG:H	5	0.54
(1,405)	1:58:A:PRO:HB3	1:59:A:ARG:H	5	0.54
(3,2963)	1:129:A:LYS:HG3	1:45:A:ILE:HG22	7	0.53
(3,2374)	1:98:B:LYS:HG2	1:98:B:LYS:HE2	10	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,2352)	1:98:B:LYS:HG3	1:125:B:ALA:HB2	9	0.53
(3,2351)	1:98:A:LYS:HG3	1:125:A:ALA:HB2	9	0.53
(3,2250)	1:94:B:THR:HG21	1:64:B:VAL:HB	4	0.53
(3,2249)	1:94:A:THR:HG21	1:64:A:VAL:HB	4	0.53
(3,2113)	1:87:A:THR:HG22	1:124:A:LYS:HD3	9	0.53
(3,1954)	1:79:B:GLN:HG2	1:88:B:SER:HB3	7	0.53
(3,1953)	1:79:A:GLN:HG2	1:88:A:SER:HB3	7	0.53
(3,1892)	1:74:B:LEU:HB3	1:86:B:LEU:HB3	2	0.53
(3,1891)	1:74:A:LEU:HB3	1:86:A:LEU:HB3	2	0.53
(3,1888)	1:74:B:LEU:HB2	1:83:B:ALA:HB2	5	0.53
(3,1887)	1:74:A:LEU:HB2	1:83:A:ALA:HB2	5	0.53
(3,1735)	1:69:A:LYS:HD2	1:72:A:LYS:HE2	2	0.53
(3,1640)	1:115:B:LEU:HD11	1:131:B:GLY:HA2	6	0.53
(3,1639)	1:115:A:LEU:HD11	1:131:A:GLY:HA2	6	0.53
(3,1526)	1:132:B:LEU:HG	1:106:B:ALA:HB3	1	0.53
(3,1489)	1:129:A:LYS:HG2	1:46:B:ARG:HB3	6	0.53
(3,1105)	1:51:A:ALA:HA	1:124:B:LYS:HB3	5	0.53
(3,974)	1:46:B:ARG:HD3	1:46:B:ARG:HA	3	0.53
(3,973)	1:46:A:ARG:HD3	1:46:A:ARG:HA	3	0.53
(3,973)	1:46:A:ARG:HD3	1:46:A:ARG:HA	9	0.53
(3,809)	1:86:A:LEU:HA	1:79:A:GLN:HE21	3	0.53
(3,479)	1:115:A:LEU:HD11	1:104:A:PHE:H	6	0.53
(3,460)	1:49:B:LEU:HB2	1:122:A:LEU:H	6	0.53
(3,438)	1:87:B:THR:HG23	1:100:B:THR:H	10	0.53
(3,414)	1:93:B:ARG:HA	1:97:B:ASN:H	2	0.53
(3,413)	1:93:A:ARG:HA	1:97:A:ASN:H	2	0.53
(3,276)	1:73:B:GLN:HG2	1:79:B:GLN:H	10	0.53
(3,275)	1:73:A:GLN:HG2	1:79:A:GLN:H	3	0.53
(3,275)	1:73:A:GLN:HG2	1:79:A:GLN:H	10	0.53
(3,263)	1:92:A:GLN:HG3	1:79:A:GLN:H	7	0.53
(3,232)	1:72:B:LYS:HG2	1:72:B:LYS:H	8	0.53
(3,231)	1:72:A:LYS:HG2	1:72:A:LYS:H	8	0.53
(1,5929)	1:112:A:TYR:HE2	1:110:B:VAL:HG13	10	0.53
(1,5238)	1:105:B:GLN:HB2	1:101:B:THR:HG23	7	0.53
(1,5237)	1:105:A:GLN:HB2	1:101:A:THR:HG23	7	0.53
(1,5212)	1:104:B:PHE:HB2	1:115:B:LEU:HD12	2	0.53
(1,5211)	1:104:A:PHE:HB2	1:115:A:LEU:HD12	2	0.53
(1,5128)	1:100:B:THR:HG22	1:102:B:ILE:HG22	9	0.53
(1,5127)	1:100:A:THR:HG22	1:102:A:ILE:HG22	9	0.53
(1,4796)	1:96:B:ALA:HA	1:90:B:LEU:HB2	6	0.53
(1,4751)	1:94:A:THR:HG23	1:96:A:ALA:HA	9	0.53
(1,4008)	1:72:B:LYS:HD3	1:114:B:THR:HG21	5	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4007)	1:72:A:LYS:HD3	1:114:A:THR:HG21	5	0.53
(1,3960)	1:72:B:LYS:HA	1:72:B:LYS:HD3	7	0.53
(1,3959)	1:72:A:LYS:HA	1:72:A:LYS:HD3	7	0.53
(1,3856)	1:69:B:LYS:HD3	1:65:B:PHE:HB2	6	0.53
(1,3782)	1:115:B:LEU:HD12	1:68:B:VAL:HB	5	0.53
(1,3781)	1:115:A:LEU:HD12	1:68:A:VAL:HB	5	0.53
(1,3780)	1:68:B:VAL:HB	1:110:B:VAL:HG22	5	0.53
(1,3779)	1:68:A:VAL:HB	1:110:A:VAL:HG22	5	0.53
(1,3778)	1:68:B:VAL:HB	1:114:B:THR:HG23	9	0.53
(1,3777)	1:68:A:VAL:HB	1:114:A:THR:HG23	9	0.53
(1,3725)	1:67:A:SER:HB3	1:114:A:THR:HG23	5	0.53
(1,2974)	1:56:B:PRO:HD2	1:50:B:PRO:HD2	9	0.53
(1,2734)	1:50:B:PRO:HG2	1:54:B:ALA:HB1	7	0.53
(1,2733)	1:50:A:PRO:HG2	1:54:A:ALA:HB1	7	0.53
(1,2690)	1:93:B:ARG:HG3	1:92:B:GLN:HB3	4	0.53
(1,2689)	1:93:A:ARG:HG3	1:92:A:GLN:HB3	4	0.53
(1,2508)	1:122:B:LEU:HB2	1:130:B:VAL:HB	4	0.53
(1,2507)	1:122:A:LEU:HB2	1:130:A:VAL:HB	4	0.53
(1,1690)	1:140:B:LYS:HB2	1:140:B:LYS:H	3	0.53
(1,1689)	1:140:A:LYS:HB2	1:140:A:LYS:H	3	0.53
(1,1068)	1:89:B:VAL:HG12	1:88:B:SER:H	6	0.53
(1,1067)	1:89:A:VAL:HG12	1:88:A:SER:H	6	0.53
(1,1004)	1:89:B:VAL:HG13	1:86:B:LEU:H	5	0.53
(1,1003)	1:89:A:VAL:HG13	1:86:A:LEU:H	5	0.53
(1,98)	1:106:B:ALA:HB3	1:107:B:ASP:H	7	0.53
(3,3060)	1:65:B:PHE:HE1	1:93:B:ARG:HB2	3	0.52
(3,3059)	1:65:A:PHE:HE1	1:93:A:ARG:HB2	3	0.52
(3,2930)	1:126:B:GLY:HA2	1:91:B:ASP:HA	5	0.52
(3,2929)	1:126:A:GLY:HA2	1:91:A:ASP:HA	5	0.52
(3,2508)	1:86:B:LEU:HG	1:119:B:MET:HA	1	0.52
(3,2507)	1:86:A:LEU:HG	1:119:A:MET:HA	1	0.52
(3,2499)	1:101:A:THR:HG22	1:50:A:PRO:HB3	3	0.52
(3,2371)	1:98:A:LYS:HE2	1:126:A:GLY:HA2	8	0.52
(3,2288)	1:95:B:GLN:HG2	1:63:B:PRO:HB2	4	0.52
(3,2250)	1:94:B:THR:HG21	1:93:B:ARG:HB3	6	0.52
(3,2249)	1:94:A:THR:HG21	1:93:A:ARG:HB3	6	0.52
(3,1564)	1:110:B:VAL:HB	1:72:B:LYS:HG2	3	0.52
(3,1564)	1:110:B:VAL:HB	1:72:B:LYS:HG2	8	0.52
(3,1563)	1:110:A:VAL:HB	1:72:A:LYS:HG2	3	0.52
(3,1563)	1:110:A:VAL:HB	1:72:A:LYS:HG2	8	0.52
(3,1525)	1:132:A:LEU:HG	1:106:A:ALA:HB3	1	0.52
(3,1490)	1:129:B:LYS:HG2	1:46:A:ARG:HB3	6	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,974)	1:46:B:ARG:HD3	1:46:B:ARG:HA	7	0.52
(3,973)	1:46:A:ARG:HD3	1:46:A:ARG:HA	7	0.52
(3,580)	1:108:B:LYS:HG3	1:116:A:MET:H	3	0.52
(3,579)	1:108:A:LYS:HG3	1:116:B:MET:H	3	0.52
(3,480)	1:115:B:LEU:HD11	1:104:B:PHE:H	6	0.52
(3,459)	1:49:A:LEU:HB2	1:122:B:LEU:H	5	0.52
(3,276)	1:73:B:GLN:HG2	1:79:B:GLN:H	3	0.52
(3,232)	1:72:B:LYS:HG2	1:72:B:LYS:H	3	0.52
(3,149)	1:58:A:PRO:HB2	1:61:A:GLU:H	2	0.52
(3,112)	1:98:B:LYS:HB3	1:51:A:ALA:H	4	0.52
(1,5930)	1:112:B:TYR:HE2	1:110:A:VAL:HG11	7	0.52
(1,5929)	1:112:A:TYR:HE2	1:110:B:VAL:HG11	7	0.52
(1,5690)	1:126:B:GLY:HA3	1:98:B:LYS:HD3	6	0.52
(1,5689)	1:126:A:GLY:HA3	1:98:A:LYS:HD3	6	0.52
(1,5582)	1:118:B:VAL:HB	1:83:B:ALA:HB2	6	0.52
(1,5581)	1:118:A:VAL:HB	1:83:A:ALA:HB2	6	0.52
(1,4752)	1:94:B:THR:HG23	1:96:B:ALA:HA	9	0.52
(1,4150)	1:74:B:LEU:HB3	1:74:B:LEU:HG	2	0.52
(1,4149)	1:74:A:LEU:HB3	1:74:A:LEU:HG	2	0.52
(1,3784)	1:68:B:VAL:HB	1:106:B:ALA:HB1	2	0.52
(1,3783)	1:68:A:VAL:HB	1:106:A:ALA:HB1	2	0.52
(1,3783)	1:68:A:VAL:HB	1:106:A:ALA:HB1	4	0.52
(1,3606)	1:115:B:LEU:HD13	1:119:B:MET:HE2	1	0.52
(1,3605)	1:115:A:LEU:HD13	1:119:A:MET:HE2	1	0.52
(1,2973)	1:56:A:PRO:HD2	1:50:A:PRO:HD2	9	0.52
(1,2664)	1:49:B:LEU:HB2	1:50:B:PRO:HD3	8	0.52
(1,2663)	1:49:A:LEU:HB2	1:50:A:PRO:HD3	8	0.52
(1,2562)	1:45:B:ILE:HG21	1:49:A:LEU:HD11	6	0.52
(1,2508)	1:122:B:LEU:HB2	1:130:B:VAL:HB	5	0.52
(1,2507)	1:122:A:LEU:HB2	1:130:A:VAL:HB	5	0.52
(1,2344)	1:89:B:VAL:HB	1:79:B:GLN:HE22	2	0.52
(1,2086)	1:98:B:LYS:HD3	1:127:B:TYR:H	9	0.52
(1,2085)	1:98:A:LYS:HD3	1:127:A:TYR:H	9	0.52
(1,1689)	1:140:A:LYS:HB2	1:140:A:LYS:H	9	0.52
(1,1121)	1:110:A:VAL:HG22	1:114:A:THR:H	7	0.52
(1,1068)	1:89:B:VAL:HG13	1:88:B:SER:H	4	0.52
(1,1067)	1:89:A:VAL:HG13	1:88:A:SER:H	4	0.52
(1,97)	1:106:A:ALA:HB3	1:107:A:ASP:H	7	0.52
(3,2878)	1:83:B:ALA:HB2	1:121:B:THR:HG21	7	0.51
(3,2877)	1:83:A:ALA:HB2	1:121:A:THR:HG21	7	0.51
(3,2532)	1:102:B:ILE:HG21	1:133:B:VAL:HB	8	0.51
(3,2531)	1:102:A:ILE:HG21	1:133:A:VAL:HB	8	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,2500)	1:101:B:THR:HG22	1:50:B:PRO:HB3	3	0.51
(3,2372)	1:98:B:LYS:HE2	1:126:B:GLY:HA2	8	0.51
(3,2287)	1:95:A:GLN:HG2	1:63:A:PRO:HB2	4	0.51
(3,1888)	1:74:B:LEU:HB2	1:83:B:ALA:HB1	7	0.51
(3,1887)	1:74:A:LEU:HB2	1:83:A:ALA:HB1	7	0.51
(3,1850)	1:73:B:GLN:HB3	1:140:B:LYS:HE2	6	0.51
(3,1849)	1:73:A:GLN:HB3	1:140:A:LYS:HE2	6	0.51
(3,1640)	1:115:B:LEU:HD11	1:131:B:GLY:HA3	5	0.51
(3,1640)	1:115:B:LEU:HD11	1:131:B:GLY:HA2	10	0.51
(3,1639)	1:115:A:LEU:HD11	1:131:A:GLY:HA2	10	0.51
(3,1386)	1:60:B:PRO:HG2	1:129:B:LYS:HB3	9	0.51
(3,1385)	1:60:A:PRO:HG2	1:129:A:LYS:HB3	9	0.51
(3,998)	1:47:B:VAL:HB	1:129:A:LYS:HG3	1	0.51
(3,998)	1:47:B:VAL:HB	1:129:A:LYS:HG3	5	0.51
(3,997)	1:47:A:VAL:HB	1:129:B:LYS:HG3	1	0.51
(3,974)	1:46:B:ARG:HD3	1:46:B:ARG:HA	2	0.51
(3,480)	1:115:B:LEU:HD13	1:104:B:PHE:H	7	0.51
(3,479)	1:115:A:LEU:HD13	1:104:A:PHE:H	7	0.51
(3,459)	1:49:A:LEU:HB2	1:122:B:LEU:H	6	0.51
(3,264)	1:92:B:GLN:HG3	1:79:B:GLN:H	2	0.51
(3,263)	1:92:A:GLN:HG3	1:79:A:GLN:H	2	0.51
(3,231)	1:72:A:LYS:HG2	1:72:A:LYS:H	3	0.51
(3,150)	1:58:B:PRO:HB2	1:61:B:GLU:H	2	0.51
(1,5806)	1:134:B:GLY:HA3	1:116:A:MET:HB2	3	0.51
(1,5554)	1:116:B:MET:HE2	1:114:B:THR:HA	8	0.51
(1,5553)	1:116:A:MET:HE2	1:114:A:THR:HA	8	0.51
(1,4568)	1:87:B:THR:HG23	1:124:B:LYS:HD2	6	0.51
(1,4567)	1:87:A:THR:HG23	1:124:A:LYS:HD2	6	0.51
(1,4504)	1:86:B:LEU:HB2	1:121:B:THR:HG22	4	0.51
(1,4503)	1:86:A:LEU:HB2	1:121:A:THR:HG22	4	0.51
(1,3996)	1:72:B:LYS:HG3	1:114:B:THR:HG23	2	0.51
(1,3995)	1:72:A:LYS:HG3	1:114:A:THR:HG23	2	0.51
(1,3784)	1:68:B:VAL:HB	1:106:B:ALA:HB1	4	0.51
(1,3578)	1:66:B:LEU:HA	1:115:B:LEU:HD11	6	0.51
(1,3577)	1:66:A:LEU:HA	1:115:A:LEU:HD11	6	0.51
(1,3550)	1:66:B:LEU:HB3	1:122:B:LEU:HG	1	0.51
(1,3550)	1:66:B:LEU:HB3	1:122:B:LEU:HG	6	0.51
(1,3549)	1:66:A:LEU:HB3	1:122:A:LEU:HG	1	0.51
(1,3440)	1:64:B:VAL:HA	1:102:B:ILE:HG22	2	0.51
(1,3439)	1:64:A:VAL:HA	1:102:A:ILE:HG22	2	0.51
(1,2910)	1:55:B:LYS:HG3	1:58:B:PRO:HG2	4	0.51
(1,2909)	1:55:A:LYS:HG3	1:58:A:PRO:HG2	4	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2560)	1:45:B:ILE:HG23	1:54:A:ALA:HB3	3	0.51
(1,2560)	1:45:B:ILE:HG21	1:54:A:ALA:HB2	9	0.51
(1,2552)	1:45:B:ILE:HG22	1:56:A:PRO:HB3	10	0.51
(1,2551)	1:45:A:ILE:HG22	1:56:B:PRO:HB3	10	0.51
(1,2367)	1:84:A:ASP:HB2	1:85:A:GLN:HE22	2	0.51
(1,2343)	1:89:A:VAL:HB	1:79:A:GLN:HE22	2	0.51
(1,1690)	1:140:B:LYS:HB2	1:140:B:LYS:H	9	0.51
(1,1689)	1:140:A:LYS:HB2	1:140:A:LYS:H	10	0.51
(1,1122)	1:110:B:VAL:HG22	1:114:B:THR:H	7	0.51
(1,382)	1:55:B:LYS:HB3	1:57:B:GLN:H	5	0.51
(1,381)	1:55:A:LYS:HB3	1:57:A:GLN:H	5	0.51
(1,254)	1:45:B:ILE:HG23	1:47:B:VAL:H	10	0.51
(1,253)	1:45:A:ILE:HG23	1:47:A:VAL:H	10	0.51
(3,2895)	1:123:A:ARG:HD2	1:54:B:ALA:HB3	3	0.5
(3,2128)	1:87:B:THR:HG23	1:88:B:SER:HB2	8	0.5
(3,2127)	1:87:A:THR:HG23	1:88:A:SER:HB2	8	0.5
(3,2108)	1:87:B:THR:HG22	1:124:B:LYS:HA	5	0.5
(3,2107)	1:87:A:THR:HG22	1:124:A:LYS:HA	5	0.5
(3,1768)	1:70:B:ALA:HA	1:105:B:GLN:HB3	10	0.5
(3,1767)	1:70:A:ALA:HA	1:105:A:GLN:HB3	10	0.5
(3,1639)	1:115:A:LEU:HD11	1:131:A:GLY:HA3	5	0.5
(3,1488)	1:61:B:GLU:HB2	1:62:B:LYS:HG2	2	0.5
(3,1487)	1:61:A:GLU:HB2	1:62:A:LYS:HG2	2	0.5
(3,974)	1:46:B:ARG:HD3	1:46:B:ARG:HA	1	0.5
(3,973)	1:46:A:ARG:HD3	1:46:A:ARG:HA	1	0.5
(3,973)	1:46:A:ARG:HD3	1:46:A:ARG:HA	2	0.5
(3,460)	1:49:B:LEU:HB2	1:122:A:LEU:H	1	0.5
(3,459)	1:49:A:LEU:HB2	1:122:B:LEU:H	1	0.5
(3,438)	1:87:B:THR:HG23	1:100:B:THR:H	3	0.5
(3,437)	1:87:A:THR:HG23	1:100:A:THR:H	3	0.5
(3,414)	1:93:B:ARG:HA	1:97:B:ASN:H	1	0.5
(3,413)	1:93:A:ARG:HA	1:97:A:ASN:H	1	0.5
(3,263)	1:85:A:GLN:HG3	1:79:A:GLN:H	3	0.5
(3,232)	1:72:B:LYS:HG2	1:72:B:LYS:H	1	0.5
(3,231)	1:72:A:LYS:HG2	1:72:A:LYS:H	1	0.5
(3,111)	1:98:A:LYS:HB3	1:51:B:ALA:H	4	0.5
(1,5930)	1:112:B:TYR:HE2	1:110:A:VAL:HG13	10	0.5
(1,5604)	1:119:B:MET:HE2	1:130:B:VAL:HA	3	0.5
(1,5603)	1:119:A:MET:HE2	1:130:A:VAL:HA	3	0.5
(1,4912)	1:100:B:THR:HA	1:129:B:LYS:HD2	10	0.5
(1,4911)	1:100:A:THR:HA	1:129:A:LYS:HD2	10	0.5
(1,4132)	1:74:B:LEU:HB3	1:119:B:MET:HE2	4	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4131)	1:74:A:LEU:HB3	1:119:A:MET:HE2	4	0.5
(1,3782)	1:115:B:LEU:HD12	1:68:B:VAL:HB	6	0.5
(1,3781)	1:115:A:LEU:HD12	1:68:A:VAL:HB	6	0.5
(1,3675)	1:67:A:SER:HB2	1:105:A:GLN:HG2	7	0.5
(1,3549)	1:66:A:LEU:HB3	1:122:A:LEU:HG	6	0.5
(1,3222)	1:122:B:LEU:HA	1:125:B:ALA:HB3	6	0.5
(1,3221)	1:122:A:LEU:HA	1:125:A:ALA:HB3	6	0.5
(1,2782)	1:51:B:ALA:HB3	1:126:A:GLY:HA3	7	0.5
(1,2690)	1:93:B:ARG:HG3	1:92:B:GLN:HB3	10	0.5
(1,2664)	1:49:B:LEU:HB2	1:50:B:PRO:HD3	6	0.5
(1,2663)	1:49:A:LEU:HB2	1:50:A:PRO:HD3	6	0.5
(1,2559)	1:45:A:ILE:HG21	1:54:B:ALA:HB2	9	0.5
(1,2368)	1:84:B:ASP:HB2	1:85:B:GLN:HE22	2	0.5
(1,1690)	1:140:B:LYS:HB2	1:140:B:LYS:H	8	0.5
(1,1690)	1:140:B:LYS:HB2	1:140:B:LYS:H	10	0.5
(1,1689)	1:140:A:LYS:HB2	1:140:A:LYS:H	8	0.5
(1,1226)	1:93:B:ARG:HG3	1:93:B:ARG:H	9	0.5
(1,1225)	1:93:A:ARG:HG3	1:93:A:ARG:H	9	0.5
(1,1122)	1:110:B:VAL:HG23	1:114:B:THR:H	1	0.5
(1,1121)	1:110:A:VAL:HG23	1:114:A:THR:H	1	0.5
(1,1003)	1:89:A:VAL:HG13	1:86:A:LEU:H	6	0.5
(1,382)	1:55:B:LYS:HB3	1:57:B:GLN:H	3	0.5
(1,381)	1:55:A:LYS:HB3	1:57:A:GLN:H	3	0.5
(1,100)	1:110:B:VAL:HG12	1:107:B:ASP:H	8	0.5
(1,99)	1:110:A:VAL:HG12	1:107:A:ASP:H	8	0.5
(3,2974)	1:130:B:VAL:HB	1:119:B:MET:HE3	4	0.49
(3,2973)	1:130:A:VAL:HB	1:119:A:MET:HE3	4	0.49
(3,2729)	1:110:A:VAL:HG21	1:119:A:MET:HE3	7	0.49
(3,2691)	1:108:A:LYS:HE3	1:109:A:SER:HB3	9	0.49
(3,2238)	1:90:B:LEU:HA	1:94:B:THR:HG22	3	0.49
(3,2237)	1:90:A:LEU:HA	1:94:A:THR:HG22	3	0.49
(3,1526)	1:132:B:LEU:HG	1:106:B:ALA:HB2	4	0.49
(3,1525)	1:132:A:LEU:HG	1:106:A:ALA:HB2	4	0.49
(3,974)	1:46:B:ARG:HD3	1:46:B:ARG:HA	8	0.49
(3,810)	1:86:B:LEU:HA	1:79:B:GLN:HE21	8	0.49
(3,414)	1:93:B:ARG:HA	1:97:B:ASN:H	5	0.49
(3,413)	1:93:A:ARG:HA	1:97:A:ASN:H	5	0.49
(3,264)	1:85:B:GLN:HG3	1:79:B:GLN:H	3	0.49
(3,257)	1:81:A:VAL:HA	1:77:A:GLY:H	6	0.49
(3,150)	1:58:B:PRO:HB2	1:61:B:GLU:H	1	0.49
(3,149)	1:58:A:PRO:HB2	1:61:A:GLU:H	1	0.49
(3,78)	1:46:B:ARG:HD2	1:47:B:VAL:H	8	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,77)	1:46:A:ARG:HD2	1:47:A:VAL:H	8	0.49
(1,5414)	1:68:B:VAL:HB	1:110:B:VAL:HG13	6	0.49
(1,5413)	1:68:A:VAL:HB	1:110:A:VAL:HG13	6	0.49
(1,5066)	1:115:B:LEU:HD11	1:119:B:MET:HA	9	0.49
(1,4504)	1:86:B:LEU:HB2	1:121:B:THR:HG23	1	0.49
(1,4503)	1:86:A:LEU:HB2	1:121:A:THR:HG23	1	0.49
(1,4010)	1:72:B:LYS:HD3	1:110:B:VAL:HG23	1	0.49
(1,4009)	1:72:A:LYS:HD3	1:110:A:VAL:HG23	1	0.49
(1,4004)	1:72:B:LYS:HD3	1:110:B:VAL:HA	7	0.49
(1,4003)	1:72:A:LYS:HD3	1:110:A:VAL:HA	7	0.49
(1,3992)	1:72:B:LYS:HG3	1:72:B:LYS:HE2	10	0.49
(1,3991)	1:72:A:LYS:HG3	1:72:A:LYS:HE2	10	0.49
(1,3960)	1:72:B:LYS:HA	1:72:B:LYS:HD3	3	0.49
(1,3959)	1:72:A:LYS:HA	1:72:A:LYS:HD3	3	0.49
(1,3780)	1:68:B:VAL:HB	1:110:B:VAL:HG21	7	0.49
(1,3779)	1:68:A:VAL:HB	1:110:A:VAL:HG21	7	0.49
(1,3778)	1:68:B:VAL:HB	1:114:B:THR:HG23	5	0.49
(1,3676)	1:67:B:SER:HB2	1:105:B:GLN:HG2	7	0.49
(1,2814)	1:54:B:ALA:HB3	1:53:B:SER:HB2	10	0.49
(1,2813)	1:54:A:ALA:HB3	1:53:A:SER:HB2	10	0.49
(1,2734)	1:50:B:PRO:HG2	1:54:B:ALA:HB2	1	0.49
(1,2734)	1:50:B:PRO:HG2	1:54:B:ALA:HB1	2	0.49
(1,2733)	1:50:A:PRO:HG2	1:54:A:ALA:HB1	2	0.49
(1,2689)	1:93:A:ARG:HG3	1:92:A:GLN:HB3	10	0.49
(1,2559)	1:45:A:ILE:HG23	1:54:B:ALA:HB3	3	0.49
(1,2496)	1:45:B:ILE:HA	1:54:A:ALA:HB2	9	0.49
(1,2268)	1:138:B:ALA:HB3	1:138:B:ALA:H	2	0.49
(1,2267)	1:138:A:ALA:HB3	1:138:A:ALA:H	2	0.49
(1,1862)	1:110:B:VAL:HG11	1:118:B:VAL:H	3	0.49
(1,1861)	1:110:A:VAL:HG11	1:118:A:VAL:H	3	0.49
(1,1226)	1:93:B:ARG:HG3	1:93:B:ARG:H	5	0.49
(1,1225)	1:93:A:ARG:HG3	1:93:A:ARG:H	5	0.49
(1,1004)	1:89:B:VAL:HG13	1:86:B:LEU:H	6	0.49
(1,100)	1:110:B:VAL:HG11	1:107:B:ASP:H	9	0.49
(1,99)	1:110:A:VAL:HG11	1:107:A:ASP:H	9	0.49
(3,2730)	1:110:B:VAL:HG21	1:119:B:MET:HE3	7	0.48
(3,2692)	1:108:B:LYS:HE3	1:109:B:SER:HB3	9	0.48
(3,2542)	1:102:B:ILE:HD12	1:61:B:GLU:HG3	2	0.48
(3,2541)	1:102:A:ILE:HD12	1:61:A:GLU:HG3	2	0.48
(3,2324)	1:127:B:TYR:HE2	1:98:B:LYS:HG2	2	0.48
(3,2323)	1:127:A:TYR:HE2	1:98:A:LYS:HG2	2	0.48
(3,2238)	1:90:B:LEU:HA	1:94:B:THR:HG21	7	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,2237)	1:90:A:LEU:HA	1:94:A:THR:HG21	7	0.48
(3,1752)	1:69:B:LYS:HE2	1:77:B:GLY:HA3	6	0.48
(3,1751)	1:69:A:LYS:HE2	1:77:A:GLY:HA3	6	0.48
(3,1642)	1:115:B:LEU:HD11	1:131:B:GLY:HA3	1	0.48
(3,1641)	1:115:A:LEU:HD11	1:131:A:GLY:HA3	1	0.48
(3,973)	1:46:A:ARG:HD3	1:46:A:ARG:HA	8	0.48
(3,816)	1:88:B:SER:HB3	1:79:B:GLN:HE22	2	0.48
(3,815)	1:88:A:SER:HB3	1:79:A:GLN:HE22	2	0.48
(3,809)	1:86:A:LEU:HA	1:79:A:GLN:HE21	8	0.48
(3,802)	1:79:B:GLN:HG3	1:79:B:GLN:HE22	10	0.48
(3,801)	1:79:A:GLN:HG3	1:79:A:GLN:HE22	10	0.48
(3,258)	1:81:B:VAL:HA	1:77:B:GLY:H	6	0.48
(1,5402)	1:110:B:VAL:HG23	1:116:B:MET:HE1	2	0.48
(1,5401)	1:110:A:VAL:HG23	1:116:A:MET:HE1	2	0.48
(1,5065)	1:115:A:LEU:HD11	1:119:A:MET:HA	9	0.48
(1,4496)	1:115:B:LEU:HB3	1:106:B:ALA:HB2	8	0.48
(1,4495)	1:115:A:LEU:HB3	1:106:A:ALA:HB2	8	0.48
(1,3974)	1:72:B:LYS:HB3	1:72:B:LYS:HD3	3	0.48
(1,3973)	1:72:A:LYS:HB3	1:72:A:LYS:HD3	3	0.48
(1,3777)	1:68:A:VAL:HB	1:114:A:THR:HG23	5	0.48
(1,3730)	1:67:B:SER:HB3	1:115:B:LEU:HD11	5	0.48
(1,3729)	1:67:A:SER:HB3	1:115:A:LEU:HD11	5	0.48
(1,3606)	1:115:B:LEU:HD13	1:119:B:MET:HE2	5	0.48
(1,3367)	1:123:A:ARG:HG2	1:50:B:PRO:HD3	5	0.48
(1,3352)	1:124:B:LYS:HG2	1:84:B:ASP:HB3	8	0.48
(1,3351)	1:124:A:LYS:HG2	1:84:A:ASP:HB3	8	0.48
(1,3343)	1:129:A:LYS:HB2	1:101:A:THR:HG23	2	0.48
(1,3236)	1:61:B:GLU:HB3	1:62:B:LYS:HG2	10	0.48
(1,3235)	1:61:A:GLU:HB3	1:62:A:LYS:HG2	10	0.48
(1,2733)	1:50:A:PRO:HG2	1:54:A:ALA:HB2	1	0.48
(1,2560)	1:45:B:ILE:HG22	1:54:A:ALA:HB1	7	0.48
(1,1690)	1:140:B:LYS:HB2	1:140:B:LYS:H	1	0.48
(1,1689)	1:140:A:LYS:HB2	1:140:A:LYS:H	1	0.48
(1,1226)	1:93:B:ARG:HG3	1:93:B:ARG:H	4	0.48
(1,1225)	1:93:A:ARG:HG3	1:93:A:ARG:H	4	0.48
(3,2964)	1:129:B:LYS:HG3	1:45:B:ILE:HG23	1	0.47
(3,2963)	1:129:A:LYS:HG3	1:45:A:ILE:HG23	1	0.47
(3,2714)	1:109:B:SER:HB3	1:72:B:LYS:HE3	3	0.47
(3,2713)	1:109:A:SER:HB3	1:72:A:LYS:HE3	3	0.47
(3,2642)	1:116:B:MET:HG2	1:45:B:ILE:HD11	8	0.47
(3,2641)	1:116:A:MET:HG2	1:45:A:ILE:HD11	8	0.47
(3,2296)	1:96:B:ALA:HA	1:100:B:THR:HG21	10	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,2295)	1:96:A:ALA:HA	1:100:A:THR:HG21	10	0.47
(3,2118)	1:88:B:SER:HB2	1:96:B:ALA:HA	8	0.47
(3,2117)	1:88:A:SER:HB2	1:96:A:ALA:HA	8	0.47
(3,1892)	1:74:B:LEU:HB3	1:86:B:LEU:HB3	5	0.47
(3,1891)	1:74:A:LEU:HB3	1:86:A:LEU:HB3	5	0.47
(3,1642)	1:115:B:LEU:HD13	1:131:B:GLY:HA2	7	0.47
(3,1641)	1:115:A:LEU:HD13	1:131:A:GLY:HA2	7	0.47
(3,1489)	1:129:A:LYS:HG3	1:46:B:ARG:HB2	7	0.47
(3,869)	1:43:A:VAL:HB	1:56:B:PRO:HD3	10	0.47
(3,802)	1:79:B:GLN:HG2	1:79:B:GLN:HE22	2	0.47
(3,802)	1:79:B:GLN:HG3	1:79:B:GLN:HE22	3	0.47
(3,802)	1:79:B:GLN:HG3	1:79:B:GLN:HE22	4	0.47
(3,802)	1:79:B:GLN:HG3	1:79:B:GLN:HE22	5	0.47
(3,802)	1:79:B:GLN:HG3	1:79:B:GLN:HE22	7	0.47
(3,802)	1:79:B:GLN:HG2	1:79:B:GLN:HE22	9	0.47
(3,801)	1:79:A:GLN:HG2	1:79:A:GLN:HE22	1	0.47
(3,801)	1:79:A:GLN:HG3	1:79:A:GLN:HE22	3	0.47
(3,801)	1:79:A:GLN:HG3	1:79:A:GLN:HE22	4	0.47
(3,801)	1:79:A:GLN:HG3	1:79:A:GLN:HE22	5	0.47
(3,608)	1:134:B:GLY:HA3	1:119:A:MET:H	8	0.47
(3,438)	1:87:B:THR:HG21	1:100:B:THR:H	2	0.47
(3,437)	1:87:A:THR:HG21	1:100:A:THR:H	2	0.47
(1,5553)	1:116:A:MET:HE1	1:114:A:THR:HA	5	0.47
(1,5356)	1:107:B:ASP:HB2	1:109:B:SER:HB3	9	0.47
(1,5355)	1:107:A:ASP:HB2	1:109:A:SER:HB3	9	0.47
(1,4760)	1:94:B:THR:HG23	1:99:B:GLU:HG3	2	0.47
(1,4759)	1:94:A:THR:HG23	1:99:A:GLU:HG3	2	0.47
(1,4721)	1:93:A:ARG:HA	1:77:A:GLY:HA2	7	0.47
(1,4000)	1:72:B:LYS:HG2	1:114:B:THR:HG23	8	0.47
(1,3999)	1:72:A:LYS:HG2	1:114:A:THR:HG23	8	0.47
(1,3974)	1:72:B:LYS:HB3	1:72:B:LYS:HD3	8	0.47
(1,3973)	1:72:A:LYS:HB3	1:72:A:LYS:HD3	8	0.47
(1,3606)	1:115:B:LEU:HD13	1:119:B:MET:HE3	7	0.47
(1,3606)	1:115:B:LEU:HD11	1:119:B:MET:HE2	10	0.47
(1,3605)	1:115:A:LEU:HD13	1:119:A:MET:HE2	5	0.47
(1,3605)	1:115:A:LEU:HD13	1:119:A:MET:HE3	7	0.47
(1,3605)	1:115:A:LEU:HD11	1:119:A:MET:HE2	10	0.47
(1,3344)	1:129:B:LYS:HB2	1:101:B:THR:HG23	2	0.47
(1,3222)	1:122:B:LEU:HA	1:125:B:ALA:HB3	9	0.47
(1,3221)	1:122:A:LEU:HA	1:125:A:ALA:HB3	9	0.47
(1,2974)	1:56:B:PRO:HD2	1:50:B:PRO:HD2	8	0.47
(1,2973)	1:56:A:PRO:HD2	1:50:A:PRO:HD2	8	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2664)	1:49:B:LEU:HB2	1:50:B:PRO:HD3	1	0.47
(1,2663)	1:49:A:LEU:HB2	1:50:A:PRO:HD3	1	0.47
(1,2559)	1:45:A:ILE:HG22	1:54:B:ALA:HB1	7	0.47
(1,2508)	1:122:B:LEU:HB2	1:130:B:VAL:HB	6	0.47
(1,2507)	1:122:A:LEU:HB2	1:130:A:VAL:HB	6	0.47
(1,2495)	1:45:A:ILE:HA	1:54:B:ALA:HB2	9	0.47
(1,2272)	1:139:B:ALA:HB1	1:139:B:ALA:H	4	0.47
(1,2105)	1:129:A:LYS:HD3	1:128:A:LEU:H	1	0.47
(1,1690)	1:140:B:LYS:HB2	1:140:B:LYS:H	5	0.47
(1,1689)	1:140:A:LYS:HB2	1:140:A:LYS:H	5	0.47
(1,1226)	1:93:B:ARG:HG3	1:93:B:ARG:H	1	0.47
(1,1225)	1:93:A:ARG:HG3	1:93:A:ARG:H	1	0.47
(1,1004)	1:89:B:VAL:HG13	1:86:B:LEU:H	7	0.47
(1,1003)	1:89:A:VAL:HG13	1:86:A:LEU:H	7	0.47
(1,405)	1:58:A:PRO:HB3	1:59:A:ARG:H	1	0.47
(3,3074)	1:104:B:PHE:HD2	1:65:B:PHE:HB2	7	0.46
(3,3073)	1:104:A:PHE:HD2	1:65:A:PHE:HB2	7	0.46
(3,2556)	1:103:B:PHE:HA	1:115:B:LEU:HD11	3	0.46
(3,2455)	1:100:A:THR:HG23	1:129:A:LYS:HB3	10	0.46
(3,2324)	1:127:B:TYR:HE1	1:98:B:LYS:HG2	6	0.46
(3,2323)	1:127:A:TYR:HE1	1:98:A:LYS:HG2	6	0.46
(3,2288)	1:95:B:GLN:HG2	1:63:B:PRO:HB2	5	0.46
(3,2108)	1:87:B:THR:HG22	1:124:B:LYS:HA	9	0.46
(3,2107)	1:87:A:THR:HG22	1:124:A:LYS:HA	9	0.46
(3,1753)	1:69:A:LYS:HE3	1:71:A:ASP:HB2	10	0.46
(3,1490)	1:129:B:LYS:HG3	1:46:A:ARG:HB2	2	0.46
(3,1044)	1:49:B:LEU:HB2	1:56:B:PRO:HG3	9	0.46
(3,1043)	1:49:A:LEU:HB2	1:56:A:PRO:HG3	9	0.46
(3,870)	1:43:B:VAL:HB	1:56:A:PRO:HD3	10	0.46
(3,812)	1:89:B:VAL:HA	1:79:B:GLN:HE22	8	0.46
(3,802)	1:79:B:GLN:HG2	1:79:B:GLN:HE22	1	0.46
(3,802)	1:79:B:GLN:HG3	1:79:B:GLN:HE22	6	0.46
(3,802)	1:79:B:GLN:HG3	1:79:B:GLN:HE22	8	0.46
(3,801)	1:79:A:GLN:HG2	1:79:A:GLN:HE22	2	0.46
(3,801)	1:79:A:GLN:HG3	1:79:A:GLN:HE22	6	0.46
(3,801)	1:79:A:GLN:HG3	1:79:A:GLN:HE22	7	0.46
(3,801)	1:79:A:GLN:HG3	1:79:A:GLN:HE22	8	0.46
(3,801)	1:79:A:GLN:HG2	1:79:A:GLN:HE22	9	0.46
(3,414)	1:93:B:ARG:HA	1:97:B:ASN:H	3	0.46
(3,73)	1:46:A:ARG:HG2	1:46:A:ARG:H	1	0.46
(1,5613)	1:121:A:THR:HA	1:124:A:LYS:HE3	9	0.46
(1,5554)	1:116:B:MET:HE1	1:114:B:THR:HA	5	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5402)	1:110:B:VAL:HG21	1:116:B:MET:HE2	9	0.46
(1,5401)	1:110:A:VAL:HG21	1:116:A:MET:HE2	9	0.46
(1,4722)	1:93:B:ARG:HA	1:77:B:GLY:HA2	7	0.46
(1,4010)	1:72:B:LYS:HD3	1:110:B:VAL:HG23	5	0.46
(1,4009)	1:72:A:LYS:HD3	1:110:A:VAL:HG23	5	0.46
(1,3960)	1:72:B:LYS:HA	1:72:B:LYS:HD3	8	0.46
(1,3959)	1:72:A:LYS:HA	1:72:A:LYS:HD3	8	0.46
(1,3784)	1:68:B:VAL:HB	1:106:B:ALA:HB3	7	0.46
(1,3784)	1:68:B:VAL:HB	1:106:B:ALA:HB1	9	0.46
(1,3783)	1:68:A:VAL:HB	1:106:A:ALA:HB3	7	0.46
(1,3783)	1:68:A:VAL:HB	1:106:A:ALA:HB1	9	0.46
(1,3610)	1:115:B:LEU:HD11	1:110:B:VAL:HG22	8	0.46
(1,3609)	1:115:A:LEU:HD11	1:110:A:VAL:HG22	8	0.46
(1,3606)	1:115:B:LEU:HD13	1:119:B:MET:HE3	6	0.46
(1,3605)	1:115:A:LEU:HD13	1:119:A:MET:HE3	6	0.46
(1,2842)	1:57:B:GLN:HA	1:60:B:PRO:HB3	8	0.46
(1,2841)	1:57:A:GLN:HA	1:60:A:PRO:HB3	8	0.46
(1,2734)	1:50:B:PRO:HG2	1:54:B:ALA:HB2	10	0.46
(1,2508)	1:122:B:LEU:HB2	1:130:B:VAL:HB	1	0.46
(1,2508)	1:122:B:LEU:HB2	1:130:B:VAL:HB	9	0.46
(1,2507)	1:122:A:LEU:HB2	1:130:A:VAL:HB	1	0.46
(1,2507)	1:122:A:LEU:HB2	1:130:A:VAL:HB	9	0.46
(1,2358)	1:82:B:ASN:HB2	1:82:B:ASN:HD22	5	0.46
(1,2358)	1:82:B:ASN:HB2	1:82:B:ASN:HD22	7	0.46
(1,2358)	1:82:B:ASN:HB2	1:82:B:ASN:HD22	8	0.46
(1,2358)	1:82:B:ASN:HB2	1:82:B:ASN:HD22	10	0.46
(1,2357)	1:82:A:ASN:HB2	1:82:A:ASN:HD22	7	0.46
(1,2357)	1:82:A:ASN:HB2	1:82:A:ASN:HD22	8	0.46
(1,2357)	1:82:A:ASN:HB2	1:82:A:ASN:HD22	10	0.46
(1,2352)	1:85:B:GLN:HE22	1:82:B:ASN:HD21	5	0.46
(1,2271)	1:139:A:ALA:HB1	1:139:A:ALA:H	4	0.46
(1,2271)	1:139:A:ALA:HB2	1:139:A:ALA:H	9	0.46
(1,2106)	1:129:B:LYS:HD3	1:128:B:LEU:H	1	0.46
(1,1744)	1:139:B:ALA:HB3	1:140:B:LYS:H	4	0.46
(1,1743)	1:139:A:ALA:HB3	1:140:A:LYS:H	4	0.46
(1,1526)	1:66:B:LEU:HB2	1:104:B:PHE:H	6	0.46
(1,1525)	1:66:A:LEU:HB2	1:104:A:PHE:H	6	0.46
(1,944)	1:121:B:THR:HB	1:84:B:ASP:H	2	0.46
(1,943)	1:121:A:THR:HB	1:84:A:ASP:H	2	0.46
(1,406)	1:58:B:PRO:HB3	1:59:B:ARG:H	1	0.46
(1,406)	1:58:B:PRO:HB3	1:59:B:ARG:H	2	0.46
(1,405)	1:58:A:PRO:HB3	1:59:A:ARG:H	2	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,99)	1:110:A:VAL:HG11	1:107:A:ASP:H	2	0.46
(3,3100)	1:75:B:TYR:HE2	1:140:B:LYS:HD3	7	0.45
(3,2924)	1:126:B:GLY:HA3	1:120:B:ASP:HA	8	0.45
(3,2923)	1:126:A:GLY:HA3	1:120:A:ASP:HA	8	0.45
(3,2555)	1:103:A:PHE:HA	1:115:A:LEU:HD11	3	0.45
(3,2456)	1:100:B:THR:HG23	1:129:B:LYS:HB3	2	0.45
(3,2456)	1:100:B:THR:HG23	1:129:B:LYS:HB3	10	0.45
(3,2287)	1:95:A:GLN:HG2	1:63:A:PRO:HB2	5	0.45
(3,2238)	1:90:B:LEU:HA	1:94:B:THR:HG21	2	0.45
(3,2237)	1:90:A:LEU:HA	1:94:A:THR:HG21	2	0.45
(3,2128)	1:87:B:THR:HG21	1:88:B:SER:HB2	1	0.45
(3,2127)	1:87:A:THR:HG21	1:88:A:SER:HB2	1	0.45
(3,2108)	1:87:B:THR:HG21	1:88:B:SER:HB2	1	0.45
(3,2107)	1:87:A:THR:HG21	1:88:A:SER:HB2	1	0.45
(3,1954)	1:79:B:GLN:HG2	1:88:B:SER:HB2	10	0.45
(3,1953)	1:79:A:GLN:HG2	1:88:A:SER:HB2	10	0.45
(3,1768)	1:70:B:ALA:HA	1:74:B:LEU:HG	9	0.45
(3,1767)	1:70:A:ALA:HA	1:74:A:LEU:HG	9	0.45
(3,1754)	1:69:B:LYS:HE3	1:71:B:ASP:HB2	10	0.45
(3,1728)	1:69:B:LYS:HB3	1:66:B:LEU:HG	5	0.45
(3,1727)	1:69:A:LYS:HB3	1:66:A:LEU:HG	5	0.45
(3,1490)	1:129:B:LYS:HG3	1:46:A:ARG:HB2	7	0.45
(3,1278)	1:57:B:GLN:HG2	1:50:B:PRO:HD2	4	0.45
(3,1277)	1:57:A:GLN:HG2	1:50:A:PRO:HD2	4	0.45
(3,1068)	1:50:B:PRO:HA	1:54:B:ALA:HB2	9	0.45
(3,1067)	1:50:A:PRO:HA	1:54:A:ALA:HB2	9	0.45
(3,811)	1:89:A:VAL:HA	1:79:A:GLN:HE22	8	0.45
(3,413)	1:93:A:ARG:HA	1:97:A:ASN:H	3	0.45
(3,390)	1:49:B:LEU:HB2	1:121:A:THR:H	2	0.45
(3,389)	1:49:A:LEU:HB2	1:121:B:THR:H	2	0.45
(3,383)	1:98:A:LYS:H	1:93:A:ARG:H	10	0.45
(3,264)	1:92:B:GLN:HG3	1:79:B:GLN:H	10	0.45
(3,263)	1:92:A:GLN:HG3	1:79:A:GLN:H	10	0.45
(3,74)	1:46:B:ARG:HG2	1:46:B:ARG:H	1	0.45
(1,5614)	1:121:B:THR:HA	1:124:B:LYS:HE3	9	0.45
(1,5417)	1:72:A:LYS:HG3	1:110:A:VAL:HG13	3	0.45
(1,5128)	1:100:B:THR:HG21	1:102:B:ILE:HG21	7	0.45
(1,4912)	1:100:B:THR:HA	1:129:B:LYS:HD2	4	0.45
(1,4911)	1:100:A:THR:HA	1:129:A:LYS:HD2	4	0.45
(1,4853)	1:98:A:LYS:HD3	1:51:B:ALA:HA	2	0.45
(1,4804)	1:96:B:ALA:HB1	1:127:B:TYR:HE2	9	0.45
(1,4803)	1:96:A:ALA:HB1	1:127:A:TYR:HE2	9	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4568)	1:87:B:THR:HG22	1:124:B:LYS:HD2	9	0.45
(1,4567)	1:87:A:THR:HG22	1:124:A:LYS:HD2	9	0.45
(1,4132)	1:74:B:LEU:HB3	1:119:B:MET:HE3	9	0.45
(1,4131)	1:74:A:LEU:HB3	1:119:A:MET:HE3	9	0.45
(1,3780)	1:68:B:VAL:HB	1:110:B:VAL:HG23	9	0.45
(1,3779)	1:68:A:VAL:HB	1:110:A:VAL:HG23	9	0.45
(1,3777)	1:68:A:VAL:HB	1:114:A:THR:HG21	3	0.45
(1,3606)	1:115:B:LEU:HD13	1:119:B:MET:HE3	3	0.45
(1,3605)	1:115:A:LEU:HD13	1:119:A:MET:HE3	3	0.45
(1,3368)	1:123:B:ARG:HG2	1:50:A:PRO:HD3	5	0.45
(1,3367)	1:123:A:ARG:HG2	1:50:B:PRO:HD3	10	0.45
(1,3344)	1:129:B:LYS:HB2	1:101:B:THR:HG22	7	0.45
(1,3343)	1:129:A:LYS:HB2	1:101:A:THR:HG22	7	0.45
(1,2733)	1:50:A:PRO:HG2	1:54:A:ALA:HB2	10	0.45
(1,2588)	1:46:B:ARG:HG2	1:129:A:LYS:HG3	1	0.45
(1,2587)	1:46:A:ARG:HG2	1:129:B:LYS:HG3	1	0.45
(1,2508)	1:122:B:LEU:HB2	1:130:B:VAL:HB	3	0.45
(1,2507)	1:122:A:LEU:HB2	1:130:A:VAL:HB	3	0.45
(1,2357)	1:82:A:ASN:HB2	1:82:A:ASN:HD22	5	0.45
(1,2272)	1:139:B:ALA:HB2	1:139:B:ALA:H	9	0.45
(1,1690)	1:140:B:LYS:HB2	1:140:B:LYS:H	4	0.45
(1,1689)	1:140:A:LYS:HB2	1:140:A:LYS:H	4	0.45
(1,1068)	1:89:B:VAL:HG12	1:88:B:SER:H	7	0.45
(1,1067)	1:89:A:VAL:HG12	1:88:A:SER:H	7	0.45
(1,406)	1:58:B:PRO:HB3	1:59:B:ARG:H	10	0.45
(1,405)	1:58:A:PRO:HB3	1:59:A:ARG:H	10	0.45
(1,254)	1:45:B:ILE:HG21	1:47:B:VAL:H	3	0.45
(1,254)	1:45:B:ILE:HG23	1:47:B:VAL:H	7	0.45
(1,253)	1:45:A:ILE:HG21	1:47:A:VAL:H	3	0.45
(1,253)	1:45:A:ILE:HG23	1:47:A:VAL:H	7	0.45
(1,100)	1:110:B:VAL:HG11	1:107:B:ASP:H	2	0.45
(3,3099)	1:75:A:TYR:HE2	1:140:A:LYS:HD3	7	0.44
(3,2692)	1:108:B:LYS:HE2	1:109:B:SER:HB3	7	0.44
(3,2508)	1:86:B:LEU:HG	1:119:B:MET:HA	7	0.44
(3,2507)	1:86:A:LEU:HG	1:119:A:MET:HA	7	0.44
(3,2474)	1:53:B:SER:HB2	1:45:A:ILE:HD13	2	0.44
(3,2473)	1:53:A:SER:HB2	1:45:B:ILE:HD13	2	0.44
(3,2456)	1:100:B:THR:HG21	1:129:B:LYS:HB3	7	0.44
(3,2455)	1:100:A:THR:HG23	1:129:A:LYS:HB3	2	0.44
(3,2372)	1:98:B:LYS:HE2	1:126:B:GLY:HA2	3	0.44
(3,2371)	1:98:A:LYS:HE2	1:126:A:GLY:HA2	3	0.44
(3,2318)	1:123:B:ARG:HB2	1:124:B:LYS:HG3	3	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,2296)	1:96:B:ALA:HA	1:100:B:THR:HG23	3	0.44
(3,1998)	1:81:B:VAL:HA	1:66:B:LEU:HB2	2	0.44
(3,1997)	1:81:A:VAL:HA	1:66:A:LEU:HB2	2	0.44
(3,1896)	1:123:B:ARG:HG2	1:50:A:PRO:HB3	9	0.44
(3,1728)	1:69:B:LYS:HB3	1:66:B:LEU:HG	10	0.44
(3,1727)	1:69:A:LYS:HB3	1:66:A:LEU:HG	10	0.44
(3,1554)	1:64:B:VAL:HA	1:61:B:GLU:HG2	9	0.44
(3,1553)	1:64:A:VAL:HA	1:61:A:GLU:HG2	9	0.44
(3,1490)	1:129:B:LYS:HG2	1:46:A:ARG:HB3	1	0.44
(3,1489)	1:129:A:LYS:HG2	1:46:B:ARG:HB3	1	0.44
(3,1489)	1:129:A:LYS:HG3	1:46:B:ARG:HB2	2	0.44
(3,1055)	1:49:A:LEU:HG	1:45:B:ILE:HA	5	0.44
(3,580)	1:108:B:LYS:HG3	1:116:A:MET:H	9	0.44
(3,384)	1:98:B:LYS:H	1:93:B:ARG:H	10	0.44
(3,108)	1:49:B:LEU:HG	1:51:B:ALA:H	1	0.44
(1,5418)	1:72:B:LYS:HG3	1:110:B:VAL:HG13	3	0.44
(1,5418)	1:72:B:LYS:HG3	1:110:B:VAL:HG13	8	0.44
(1,5414)	1:68:B:VAL:HB	1:110:B:VAL:HG11	3	0.44
(1,5413)	1:68:A:VAL:HB	1:110:A:VAL:HG11	3	0.44
(1,5212)	1:104:B:PHE:HB2	1:115:B:LEU:HD11	5	0.44
(1,5212)	1:104:B:PHE:HB2	1:115:B:LEU:HD11	6	0.44
(1,5211)	1:104:A:PHE:HB2	1:115:A:LEU:HD11	5	0.44
(1,5211)	1:104:A:PHE:HB2	1:115:A:LEU:HD11	6	0.44
(1,5127)	1:100:A:THR:HG21	1:102:A:ILE:HG21	7	0.44
(1,5106)	1:102:B:ILE:HG22	1:127:B:TYR:HE2	4	0.44
(1,5105)	1:102:A:ILE:HG22	1:127:A:TYR:HE2	4	0.44
(1,5066)	1:115:B:LEU:HD11	1:119:B:MET:HA	2	0.44
(1,5065)	1:115:A:LEU:HD11	1:119:A:MET:HA	2	0.44
(1,4752)	1:94:B:THR:HG23	1:96:B:ALA:HA	5	0.44
(1,4751)	1:94:A:THR:HG23	1:96:A:ALA:HA	5	0.44
(1,4574)	1:87:B:THR:HG21	1:90:B:LEU:HG	7	0.44
(1,4573)	1:87:A:THR:HG21	1:90:A:LEU:HG	7	0.44
(1,4568)	1:87:B:THR:HG23	1:124:B:LYS:HD2	1	0.44
(1,4567)	1:87:A:THR:HG23	1:124:A:LYS:HD2	1	0.44
(1,4154)	1:123:B:ARG:HG2	1:49:A:LEU:HB3	2	0.44
(1,4153)	1:123:A:ARG:HG2	1:49:B:LEU:HB3	2	0.44
(1,3778)	1:68:B:VAL:HB	1:114:B:THR:HG21	3	0.44
(1,3750)	1:68:B:VAL:HA	1:110:B:VAL:HG11	8	0.44
(1,3749)	1:68:A:VAL:HA	1:110:A:VAL:HG11	8	0.44
(1,3368)	1:123:B:ARG:HG2	1:50:A:PRO:HD3	6	0.44
(1,3236)	1:61:B:GLU:HB3	1:62:B:LYS:HG2	5	0.44
(1,3235)	1:61:A:GLU:HB3	1:62:A:LYS:HG2	5	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2552)	1:45:B:ILE:HG21	1:56:A:PRO:HB3	9	0.44
(1,1197)	1:92:A:GLN:HG2	1:92:A:GLN:H	10	0.44
(1,764)	1:73:B:GLN:HG2	1:74:B:LEU:H	8	0.44
(1,763)	1:73:A:GLN:HG2	1:74:A:LEU:H	8	0.44
(1,406)	1:58:B:PRO:HB3	1:59:B:ARG:H	3	0.44
(1,406)	1:58:B:PRO:HB3	1:59:B:ARG:H	7	0.44
(1,406)	1:58:B:PRO:HB3	1:59:B:ARG:H	8	0.44
(1,405)	1:58:A:PRO:HB3	1:59:A:ARG:H	3	0.44
(1,405)	1:58:A:PRO:HB3	1:59:A:ARG:H	7	0.44
(1,405)	1:58:A:PRO:HB3	1:59:A:ARG:H	8	0.44
(3,2878)	1:83:B:ALA:HB3	1:121:B:THR:HG23	1	0.43
(3,2878)	1:83:B:ALA:HB3	1:121:B:THR:HG22	4	0.43
(3,2730)	1:110:B:VAL:HG22	1:119:B:MET:HE3	4	0.43
(3,2455)	1:100:A:THR:HG21	1:129:A:LYS:HB3	7	0.43
(3,2442)	1:100:B:THR:HB	1:100:B:THR:HG22	3	0.43
(3,2442)	1:100:B:THR:HB	1:100:B:THR:HG21	5	0.43
(3,2441)	1:100:A:THR:HB	1:100:A:THR:HG22	3	0.43
(3,2441)	1:100:A:THR:HB	1:100:A:THR:HG21	5	0.43
(3,2388)	1:99:B:GLU:HG3	1:129:B:LYS:HE2	7	0.43
(3,2387)	1:99:A:GLU:HG3	1:129:A:LYS:HE2	10	0.43
(3,2352)	1:98:B:LYS:HG3	1:125:B:ALA:HB2	4	0.43
(3,2351)	1:98:A:LYS:HG3	1:125:A:ALA:HB2	4	0.43
(3,2324)	1:127:B:TYR:HE1	1:98:B:LYS:HG2	5	0.43
(3,2317)	1:123:A:ARG:HB2	1:124:A:LYS:HG3	3	0.43
(3,2295)	1:96:A:ALA:HA	1:100:A:THR:HG23	3	0.43
(3,2108)	1:87:B:THR:HG23	1:124:B:LYS:HA	6	0.43
(3,2107)	1:87:A:THR:HG23	1:124:A:LYS:HA	6	0.43
(3,1954)	1:79:B:GLN:HG2	1:88:B:SER:HB3	1	0.43
(3,1895)	1:123:A:ARG:HG2	1:50:B:PRO:HB3	9	0.43
(3,1105)	1:51:A:ALA:HA	1:124:B:LYS:HB3	3	0.43
(3,1044)	1:49:B:LEU:HB2	1:56:B:PRO:HG3	10	0.43
(3,1043)	1:49:A:LEU:HB2	1:56:A:PRO:HG3	10	0.43
(3,974)	1:46:B:ARG:HD3	1:46:B:ARG:HA	5	0.43
(3,973)	1:46:A:ARG:HD3	1:46:A:ARG:HA	5	0.43
(3,607)	1:134:A:GLY:HA3	1:119:B:MET:H	4	0.43
(3,607)	1:134:A:GLY:HA3	1:119:B:MET:H	8	0.43
(3,107)	1:49:A:LEU:HG	1:51:A:ALA:H	1	0.43
(3,78)	1:46:B:ARG:HD2	1:47:B:VAL:H	5	0.43
(3,77)	1:46:A:ARG:HD2	1:47:A:VAL:H	5	0.43
(3,74)	1:46:B:ARG:HG2	1:46:B:ARG:H	4	0.43
(3,74)	1:46:B:ARG:HG2	1:46:B:ARG:H	6	0.43
(3,73)	1:46:A:ARG:HG2	1:46:A:ARG:H	4	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,73)	1:46:A:ARG:HG2	1:46:A:ARG:H	6	0.43
(1,5417)	1:72:A:LYS:HG3	1:110:A:VAL:HG13	8	0.43
(1,5306)	1:106:B:ALA:HB2	1:110:B:VAL:HB	5	0.43
(1,5305)	1:106:A:ALA:HB2	1:110:A:VAL:HB	5	0.43
(1,5128)	1:100:B:THR:HG23	1:102:B:ILE:HG22	4	0.43
(1,5106)	1:102:B:ILE:HG22	1:127:B:TYR:HE1	5	0.43
(1,5105)	1:102:A:ILE:HG22	1:127:A:TYR:HE1	5	0.43
(1,4815)	1:92:A:GLN:HG3	1:96:A:ALA:HB3	1	0.43
(1,4804)	1:96:B:ALA:HB3	1:127:B:TYR:HE2	3	0.43
(1,4008)	1:72:B:LYS:HD3	1:114:B:THR:HG21	9	0.43
(1,4007)	1:72:A:LYS:HD3	1:114:A:THR:HG21	9	0.43
(1,3730)	1:67:B:SER:HB3	1:115:B:LEU:HD13	2	0.43
(1,3729)	1:67:A:SER:HB3	1:115:A:LEU:HD13	2	0.43
(1,3676)	1:67:B:SER:HB2	1:105:B:GLN:HG2	2	0.43
(1,3675)	1:67:A:SER:HB2	1:105:A:GLN:HG2	2	0.43
(1,3550)	1:66:B:LEU:HB3	1:122:B:LEU:HG	2	0.43
(1,3549)	1:66:A:LEU:HB3	1:122:A:LEU:HG	2	0.43
(1,3549)	1:66:A:LEU:HB3	1:122:A:LEU:HG	5	0.43
(1,3440)	1:64:B:VAL:HA	1:102:B:ILE:HG23	1	0.43
(1,3440)	1:64:B:VAL:HA	1:102:B:ILE:HG21	7	0.43
(1,3439)	1:64:A:VAL:HA	1:102:A:ILE:HG23	1	0.43
(1,3354)	1:122:B:LEU:HG	1:119:B:MET:HB2	2	0.43
(1,3354)	1:122:B:LEU:HG	1:119:B:MET:HB2	4	0.43
(1,3353)	1:122:A:LEU:HG	1:119:A:MET:HB2	2	0.43
(1,3353)	1:122:A:LEU:HG	1:119:A:MET:HB2	4	0.43
(1,3235)	1:61:A:GLU:HB3	1:62:A:LYS:HG2	4	0.43
(1,2820)	1:54:B:ALA:HB2	1:44:A:ASP:HB2	6	0.43
(1,2682)	1:93:B:ARG:HG3	1:91:B:ASP:HB3	10	0.43
(1,2664)	1:49:B:LEU:HB2	1:50:B:PRO:HD3	2	0.43
(1,2663)	1:49:A:LEU:HB2	1:50:A:PRO:HD3	2	0.43
(1,2643)	1:125:A:ALA:HA	1:98:A:LYS:HD3	9	0.43
(1,2351)	1:85:A:GLN:HE22	1:82:A:ASN:HD21	5	0.43
(1,2044)	1:98:B:LYS:HD3	1:126:B:GLY:H	8	0.43
(1,2043)	1:98:A:LYS:HD3	1:126:A:GLY:H	8	0.43
(1,1198)	1:92:B:GLN:HG2	1:92:B:GLN:H	10	0.43
(1,1122)	1:110:B:VAL:HG23	1:114:B:THR:H	5	0.43
(1,930)	1:83:B:ALA:HB1	1:83:B:ALA:H	8	0.43
(1,929)	1:83:A:ALA:HB1	1:83:A:ALA:H	8	0.43
(1,764)	1:73:B:GLN:HG2	1:74:B:LEU:H	3	0.43
(1,763)	1:73:A:GLN:HG2	1:74:A:LEU:H	3	0.43
(1,100)	1:110:B:VAL:HG12	1:107:B:ASP:H	5	0.43
(1,99)	1:110:A:VAL:HG12	1:107:A:ASP:H	5	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,2877)	1:83:A:ALA:HB3	1:121:A:THR:HG22	4	0.42
(3,2850)	1:119:B:MET:HE3	1:103:B:PHE:HA	7	0.42
(3,2849)	1:119:A:MET:HE3	1:103:A:PHE:HA	7	0.42
(3,2729)	1:110:A:VAL:HG22	1:119:A:MET:HE3	4	0.42
(3,2691)	1:108:A:LYS:HE2	1:109:A:SER:HB3	7	0.42
(3,2508)	1:86:B:LEU:HG	1:119:B:MET:HA	3	0.42
(3,2507)	1:86:A:LEU:HG	1:119:A:MET:HA	3	0.42
(3,2388)	1:99:B:GLU:HG3	1:129:B:LYS:HE2	10	0.42
(3,2387)	1:99:A:GLU:HG3	1:129:A:LYS:HE2	7	0.42
(3,2323)	1:127:A:TYR:HE1	1:98:A:LYS:HG2	5	0.42
(3,2318)	1:123:B:ARG:HB2	1:124:B:LYS:HG3	9	0.42
(3,2317)	1:123:A:ARG:HB2	1:124:A:LYS:HG3	9	0.42
(3,1953)	1:79:A:GLN:HG2	1:88:A:SER:HB3	1	0.42
(3,1834)	1:72:B:LYS:HE2	1:110:B:VAL:HG23	8	0.42
(3,1833)	1:72:A:LYS:HE2	1:110:A:VAL:HG23	8	0.42
(3,1728)	1:69:B:LYS:HB3	1:66:B:LEU:HG	1	0.42
(3,1727)	1:69:A:LYS:HB3	1:66:A:LEU:HG	1	0.42
(3,1110)	1:139:B:ALA:HA	1:140:B:LYS:HD2	6	0.42
(3,1109)	1:139:A:ALA:HA	1:140:A:LYS:HD2	6	0.42
(3,1106)	1:51:B:ALA:HA	1:124:A:LYS:HB3	6	0.42
(3,1056)	1:49:B:LEU:HG	1:45:A:ILE:HA	5	0.42
(3,996)	1:47:B:VAL:HB	1:128:A:LEU:HG	9	0.42
(3,903)	1:122:A:LEU:HB2	1:49:B:LEU:HB3	5	0.42
(3,608)	1:134:B:GLY:HA3	1:119:A:MET:H	10	0.42
(3,579)	1:108:A:LYS:HG3	1:116:B:MET:H	9	0.42
(3,480)	1:115:B:LEU:HD11	1:104:B:PHE:H	10	0.42
(3,479)	1:115:A:LEU:HD11	1:104:A:PHE:H	10	0.42
(1,5908)	1:65:B:PHE:HE2	1:100:B:THR:HG22	5	0.42
(1,5907)	1:65:A:PHE:HE2	1:100:A:THR:HG22	5	0.42
(1,5590)	1:119:B:MET:HG3	1:119:B:MET:HE1	2	0.42
(1,5589)	1:119:A:MET:HG3	1:119:A:MET:HE1	2	0.42
(1,5212)	1:104:B:PHE:HB2	1:115:B:LEU:HD11	10	0.42
(1,5128)	1:100:B:THR:HG21	1:102:B:ILE:HG23	8	0.42
(1,5127)	1:100:A:THR:HG23	1:102:A:ILE:HG22	4	0.42
(1,5127)	1:100:A:THR:HG21	1:102:A:ILE:HG23	8	0.42
(1,4816)	1:92:B:GLN:HG3	1:96:B:ALA:HB3	1	0.42
(1,4803)	1:96:A:ALA:HB3	1:127:A:TYR:HE2	3	0.42
(1,4574)	1:87:B:THR:HG23	1:90:B:LEU:HG	4	0.42
(1,4364)	1:82:B:ASN:HB3	1:85:B:GLN:HG2	7	0.42
(1,4182)	1:98:B:LYS:HE2	1:96:B:ALA:HA	5	0.42
(1,4181)	1:98:A:LYS:HE2	1:96:A:ALA:HA	5	0.42
(1,4132)	1:74:B:LEU:HB3	1:119:B:MET:HE2	7	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4008)	1:72:B:LYS:HD3	1:114:B:THR:HG22	7	0.42
(1,4007)	1:72:A:LYS:HD3	1:114:A:THR:HG22	7	0.42
(1,3968)	1:72:B:LYS:HB2	1:114:B:THR:HG21	5	0.42
(1,3967)	1:72:A:LYS:HB2	1:114:A:THR:HG21	5	0.42
(1,3782)	1:115:B:LEU:HD11	1:68:B:VAL:HB	8	0.42
(1,3781)	1:115:A:LEU:HD11	1:68:A:VAL:HB	8	0.42
(1,3610)	1:115:B:LEU:HD12	1:110:B:VAL:HG22	10	0.42
(1,3609)	1:115:A:LEU:HD12	1:110:A:VAL:HG22	10	0.42
(1,3606)	1:115:B:LEU:HD13	1:119:B:MET:HE3	4	0.42
(1,3605)	1:115:A:LEU:HD13	1:119:A:MET:HE3	4	0.42
(1,3598)	1:115:B:LEU:HD13	1:119:B:MET:HG2	1	0.42
(1,3597)	1:115:A:LEU:HD13	1:119:A:MET:HG2	1	0.42
(1,3550)	1:66:B:LEU:HB3	1:122:B:LEU:HG	5	0.42
(1,3439)	1:64:A:VAL:HA	1:102:A:ILE:HG21	7	0.42
(1,3368)	1:123:B:ARG:HG2	1:50:A:PRO:HD3	10	0.42
(1,3367)	1:123:A:ARG:HG2	1:50:B:PRO:HD3	6	0.42
(1,3236)	1:61:B:GLU:HB3	1:62:B:LYS:HG2	4	0.42
(1,3222)	1:122:B:LEU:HA	1:125:B:ALA:HB1	7	0.42
(1,2814)	1:54:B:ALA:HB2	1:53:B:SER:HB2	7	0.42
(1,2813)	1:54:A:ALA:HB2	1:53:A:SER:HB2	7	0.42
(1,2681)	1:93:A:ARG:HG3	1:91:A:ASP:HB3	10	0.42
(1,2644)	1:125:B:ALA:HA	1:98:B:LYS:HD3	9	0.42
(1,2643)	1:125:A:ALA:HA	1:98:A:LYS:HD3	3	0.42
(1,2559)	1:45:A:ILE:HG22	1:54:B:ALA:HB2	10	0.42
(1,2551)	1:45:A:ILE:HG21	1:56:B:PRO:HB3	9	0.42
(1,1121)	1:110:A:VAL:HG23	1:114:A:THR:H	5	0.42
(1,930)	1:83:B:ALA:HB2	1:83:B:ALA:H	1	0.42
(1,930)	1:83:B:ALA:HB2	1:83:B:ALA:H	6	0.42
(1,929)	1:83:A:ALA:HB2	1:83:A:ALA:H	1	0.42
(1,929)	1:83:A:ALA:HB2	1:83:A:ALA:H	6	0.42
(1,254)	1:45:B:ILE:HG23	1:47:B:VAL:H	6	0.42
(1,253)	1:45:A:ILE:HG23	1:47:A:VAL:H	6	0.42
(3,3074)	1:104:B:PHE:HD1	1:65:B:PHE:HB2	4	0.41
(3,3073)	1:104:A:PHE:HD1	1:65:A:PHE:HB2	4	0.41
(3,3023)	1:129:A:LYS:HA	1:97:A:ASN:HB2	8	0.41
(3,2963)	1:129:A:LYS:HG3	1:45:A:ILE:HG22	8	0.41
(3,2877)	1:83:A:ALA:HB3	1:121:A:THR:HG23	1	0.41
(3,2824)	1:115:B:LEU:HD21	1:116:A:MET:HG2	2	0.41
(3,2508)	1:86:B:LEU:HG	1:119:B:MET:HA	8	0.41
(3,2508)	1:86:B:LEU:HG	1:119:B:MET:HA	9	0.41
(3,2507)	1:86:A:LEU:HG	1:119:A:MET:HA	8	0.41
(3,2507)	1:86:A:LEU:HG	1:119:A:MET:HA	9	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,2442)	1:100:B:THR:HB	1:100:B:THR:HG23	2	0.41
(3,2442)	1:100:B:THR:HB	1:100:B:THR:HG21	7	0.41
(3,2442)	1:100:B:THR:HB	1:100:B:THR:HG22	9	0.41
(3,2441)	1:100:A:THR:HB	1:100:A:THR:HG23	2	0.41
(3,2441)	1:100:A:THR:HB	1:100:A:THR:HG21	7	0.41
(3,2441)	1:100:A:THR:HB	1:100:A:THR:HG22	9	0.41
(3,1997)	1:81:A:VAL:HA	1:66:A:LEU:HB2	9	0.41
(3,1728)	1:69:B:LYS:HB3	1:66:B:LEU:HG	6	0.41
(3,1727)	1:69:A:LYS:HB3	1:66:A:LEU:HG	6	0.41
(3,1642)	1:115:B:LEU:HD11	1:131:B:GLY:HA2	6	0.41
(3,1641)	1:115:A:LEU:HD11	1:131:A:GLY:HA2	6	0.41
(3,1546)	1:63:B:PRO:HD2	1:93:B:ARG:HD3	8	0.41
(3,1545)	1:63:A:PRO:HD2	1:93:A:ARG:HD3	8	0.41
(3,1540)	1:46:B:ARG:HG2	1:128:A:LEU:HB3	7	0.41
(3,1106)	1:51:B:ALA:HA	1:124:A:LYS:HB3	3	0.41
(3,1009)	1:48:A:ASP:HB3	1:57:A:GLN:HB3	1	0.41
(3,995)	1:47:A:VAL:HB	1:128:B:LEU:HG	9	0.41
(3,744)	1:116:B:MET:HE1	1:135:A:MET:H	3	0.41
(3,608)	1:134:B:GLY:HA3	1:119:A:MET:H	4	0.41
(1,5830)	1:135:B:MET:HE2	1:108:B:LYS:HA	3	0.41
(1,5829)	1:135:A:MET:HE2	1:108:A:LYS:HA	3	0.41
(1,5622)	1:119:B:MET:HE3	1:121:B:THR:HB	10	0.41
(1,5621)	1:119:A:MET:HE3	1:121:A:THR:HB	10	0.41
(1,5306)	1:106:B:ALA:HB2	1:110:B:VAL:HB	8	0.41
(1,5305)	1:106:A:ALA:HB2	1:110:A:VAL:HB	8	0.41
(1,5211)	1:104:A:PHE:HB2	1:115:A:LEU:HD11	10	0.41
(1,5128)	1:100:B:THR:HG22	1:102:B:ILE:HG23	1	0.41
(1,4861)	1:98:A:LYS:HD3	1:127:A:TYR:HB2	8	0.41
(1,4812)	1:96:B:ALA:HA	1:96:B:ALA:HB1	5	0.41
(1,4812)	1:96:B:ALA:HA	1:96:B:ALA:HB1	8	0.41
(1,4812)	1:96:B:ALA:HA	1:96:B:ALA:HB1	10	0.41
(1,4811)	1:96:A:ALA:HA	1:96:A:ALA:HB1	5	0.41
(1,4573)	1:87:A:THR:HG23	1:90:A:LEU:HG	4	0.41
(1,4396)	1:83:B:ALA:HA	1:83:B:ALA:HB3	6	0.41
(1,4396)	1:83:B:ALA:HA	1:83:B:ALA:HB2	8	0.41
(1,4395)	1:83:A:ALA:HA	1:83:A:ALA:HB2	8	0.41
(1,4363)	1:82:A:ASN:HB3	1:85:A:GLN:HG2	7	0.41
(1,4131)	1:74:A:LEU:HB3	1:119:A:MET:HE2	7	0.41
(1,3996)	1:72:B:LYS:HG3	1:114:B:THR:HG21	4	0.41
(1,3974)	1:72:B:LYS:HB3	1:72:B:LYS:HD3	1	0.41
(1,3974)	1:72:B:LYS:HB3	1:72:B:LYS:HD3	9	0.41
(1,3973)	1:72:A:LYS:HB3	1:72:A:LYS:HD3	1	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3973)	1:72:A:LYS:HB3	1:72:A:LYS:HD3	9	0.41
(1,3730)	1:67:B:SER:HB3	1:115:B:LEU:HD11	4	0.41
(1,3606)	1:115:B:LEU:HD12	1:119:B:MET:HE3	8	0.41
(1,3605)	1:115:A:LEU:HD12	1:119:A:MET:HE3	8	0.41
(1,3440)	1:64:B:VAL:HA	1:102:B:ILE:HG22	3	0.41
(1,3236)	1:61:B:GLU:HB3	1:62:B:LYS:HG2	9	0.41
(1,3235)	1:61:A:GLU:HB3	1:62:A:LYS:HG2	9	0.41
(1,3222)	1:122:B:LEU:HA	1:125:B:ALA:HB1	1	0.41
(1,3221)	1:122:A:LEU:HA	1:125:A:ALA:HB1	1	0.41
(1,3221)	1:122:A:LEU:HA	1:125:A:ALA:HB1	7	0.41
(1,3138)	1:98:B:LYS:HE3	1:125:B:ALA:HB3	10	0.41
(1,3137)	1:98:A:LYS:HE3	1:125:A:ALA:HB3	10	0.41
(1,2664)	1:49:B:LEU:HB2	1:50:B:PRO:HD3	10	0.41
(1,2663)	1:49:A:LEU:HB2	1:50:A:PRO:HD3	10	0.41
(1,2560)	1:45:B:ILE:HG22	1:54:A:ALA:HB2	10	0.41
(1,1070)	1:90:B:LEU:HB3	1:88:B:SER:H	10	0.41
(1,1069)	1:90:A:LEU:HB3	1:88:A:SER:H	10	0.41
(1,930)	1:83:B:ALA:HB2	1:83:B:ALA:H	4	0.41
(1,930)	1:83:B:ALA:HB2	1:83:B:ALA:H	5	0.41
(1,929)	1:83:A:ALA:HB2	1:83:A:ALA:H	4	0.41
(1,929)	1:83:A:ALA:HB2	1:83:A:ALA:H	5	0.41
(1,100)	1:110:B:VAL:HG13	1:107:B:ASP:H	10	0.41
(1,24)	1:92:B:GLN:HG2	1:92:B:GLN:HE22	1	0.41
(1,24)	1:92:B:GLN:HG2	1:92:B:GLN:HE22	2	0.41
(1,24)	1:92:B:GLN:HG2	1:92:B:GLN:HE22	3	0.41
(1,24)	1:92:B:GLN:HG2	1:92:B:GLN:HE22	5	0.41
(1,24)	1:92:B:GLN:HG2	1:92:B:GLN:HE22	7	0.41
(1,24)	1:92:B:GLN:HG2	1:92:B:GLN:HE22	8	0.41
(1,24)	1:92:B:GLN:HG2	1:92:B:GLN:HE22	9	0.41
(1,24)	1:92:B:GLN:HG2	1:92:B:GLN:HE22	10	0.41
(1,23)	1:92:A:GLN:HG2	1:92:A:GLN:HE22	1	0.41
(1,23)	1:92:A:GLN:HG2	1:92:A:GLN:HE22	2	0.41
(1,23)	1:92:A:GLN:HG2	1:92:A:GLN:HE22	3	0.41
(1,23)	1:92:A:GLN:HG2	1:92:A:GLN:HE22	4	0.41
(1,23)	1:92:A:GLN:HG2	1:92:A:GLN:HE22	5	0.41
(1,23)	1:92:A:GLN:HG2	1:92:A:GLN:HE22	8	0.41
(1,23)	1:92:A:GLN:HG2	1:92:A:GLN:HE22	9	0.41
(1,23)	1:92:A:GLN:HG2	1:92:A:GLN:HE22	10	0.41
(3,3074)	1:104:B:PHE:HD2	1:65:B:PHE:HB2	3	0.4
(3,3073)	1:104:A:PHE:HD2	1:65:A:PHE:HB2	3	0.4
(3,3024)	1:129:B:LYS:HA	1:97:B:ASN:HB2	8	0.4
(3,3005)	1:106:A:ALA:HB2	1:135:A:MET:HG2	4	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,2964)	1:129:B:LYS:HG3	1:45:B:ILE:HG22	8	0.4
(3,2823)	1:115:A:LEU:HD21	1:116:B:MET:HG2	2	0.4
(3,2351)	1:98:A:LYS:HG3	1:125:A:ALA:HB3	7	0.4
(3,2108)	1:87:B:THR:HG21	1:124:B:LYS:HA	4	0.4
(3,2107)	1:87:A:THR:HG21	1:124:A:LYS:HA	4	0.4
(3,1998)	1:81:B:VAL:HA	1:66:B:LEU:HB2	9	0.4
(3,1895)	1:123:A:ARG:HG2	1:50:B:PRO:HB3	10	0.4
(3,1894)	1:123:B:ARG:HG2	1:124:B:LYS:HE2	2	0.4
(3,1892)	1:74:B:LEU:HB3	1:86:B:LEU:HB3	7	0.4
(3,1891)	1:74:A:LEU:HB3	1:86:A:LEU:HB3	7	0.4
(3,1834)	1:72:B:LYS:HE2	1:110:B:VAL:HG21	3	0.4
(3,1539)	1:46:A:ARG:HG2	1:128:B:LEU:HB3	7	0.4
(3,1105)	1:51:A:ALA:HA	1:124:B:LYS:HB3	6	0.4
(3,1056)	1:49:B:LEU:HG	1:45:A:ILE:HA	4	0.4
(3,1010)	1:48:B:ASP:HB3	1:57:B:GLN:HB3	1	0.4
(3,743)	1:116:A:MET:HE1	1:135:B:MET:H	3	0.4
(3,384)	1:98:B:LYS:H	1:93:B:ARG:H	2	0.4
(1,5908)	1:65:B:PHE:HE1	1:100:B:THR:HG21	2	0.4
(1,5907)	1:65:A:PHE:HE1	1:100:A:THR:HG21	2	0.4
(1,5752)	1:86:B:LEU:HG	1:102:B:ILE:HD13	9	0.4
(1,5751)	1:86:A:LEU:HG	1:102:A:ILE:HD13	9	0.4
(1,5607)	1:51:A:ALA:HB2	1:124:B:LYS:HA	4	0.4
(1,5520)	1:115:B:LEU:HG	1:116:B:MET:HE3	4	0.4
(1,5519)	1:115:A:LEU:HG	1:116:A:MET:HE3	4	0.4
(1,5416)	1:110:B:VAL:HG13	1:70:B:ALA:HB2	10	0.4
(1,5415)	1:110:A:VAL:HG13	1:70:A:ALA:HB2	10	0.4
(1,5414)	1:68:B:VAL:HB	1:110:B:VAL:HG13	4	0.4
(1,5413)	1:68:A:VAL:HB	1:110:A:VAL:HG13	4	0.4
(1,5212)	1:104:B:PHE:HB2	1:115:B:LEU:HD11	3	0.4
(1,5211)	1:104:A:PHE:HB2	1:115:A:LEU:HD11	3	0.4
(1,5127)	1:100:A:THR:HG22	1:102:A:ILE:HG23	1	0.4
(1,4862)	1:98:B:LYS:HD3	1:127:B:TYR:HB2	8	0.4
(1,4812)	1:96:B:ALA:HA	1:96:B:ALA:HB1	4	0.4
(1,4812)	1:96:B:ALA:HA	1:96:B:ALA:HB3	7	0.4
(1,4812)	1:96:B:ALA:HA	1:96:B:ALA:HB1	9	0.4
(1,4811)	1:96:A:ALA:HA	1:96:A:ALA:HB1	1	0.4
(1,4811)	1:96:A:ALA:HA	1:96:A:ALA:HB1	4	0.4
(1,4811)	1:96:A:ALA:HA	1:96:A:ALA:HB3	7	0.4
(1,4811)	1:96:A:ALA:HA	1:96:A:ALA:HB1	8	0.4
(1,4811)	1:96:A:ALA:HA	1:96:A:ALA:HB1	9	0.4
(1,4811)	1:96:A:ALA:HA	1:96:A:ALA:HB1	10	0.4
(1,4518)	1:86:B:LEU:HG	1:90:B:LEU:HG	6	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4515)	1:128:A:LEU:HG	1:49:B:LEU:HB3	9	0.4
(1,4396)	1:83:B:ALA:HA	1:83:B:ALA:HB3	1	0.4
(1,4396)	1:83:B:ALA:HA	1:83:B:ALA:HB1	3	0.4
(1,4396)	1:83:B:ALA:HA	1:83:B:ALA:HB3	4	0.4
(1,4396)	1:83:B:ALA:HA	1:83:B:ALA:HB3	5	0.4
(1,4396)	1:83:B:ALA:HA	1:83:B:ALA:HB2	7	0.4
(1,4396)	1:83:B:ALA:HA	1:83:B:ALA:HB1	9	0.4
(1,4395)	1:83:A:ALA:HA	1:83:A:ALA:HB3	1	0.4
(1,4395)	1:83:A:ALA:HA	1:83:A:ALA:HB1	3	0.4
(1,4395)	1:83:A:ALA:HA	1:83:A:ALA:HB3	6	0.4
(1,4395)	1:83:A:ALA:HA	1:83:A:ALA:HB2	7	0.4
(1,3995)	1:72:A:LYS:HG3	1:114:A:THR:HG21	4	0.4
(1,3974)	1:72:B:LYS:HB3	1:72:B:LYS:HD3	6	0.4
(1,3973)	1:72:A:LYS:HB3	1:72:A:LYS:HD3	6	0.4
(1,3729)	1:67:A:SER:HB3	1:115:A:LEU:HD11	4	0.4
(1,3439)	1:64:A:VAL:HA	1:102:A:ILE:HG22	3	0.4
(1,3368)	1:123:B:ARG:HG2	1:50:A:PRO:HD3	4	0.4
(1,3367)	1:123:A:ARG:HG2	1:50:B:PRO:HD3	4	0.4
(1,3344)	1:129:B:LYS:HB2	1:101:B:THR:HG21	1	0.4
(1,3343)	1:129:A:LYS:HB2	1:101:A:THR:HG21	1	0.4
(1,3236)	1:61:B:GLU:HB3	1:62:B:LYS:HG2	7	0.4
(1,3235)	1:61:A:GLU:HB3	1:62:A:LYS:HG2	7	0.4
(1,2974)	1:56:B:PRO:HD2	1:50:B:PRO:HD2	5	0.4
(1,2973)	1:56:A:PRO:HD2	1:50:A:PRO:HD2	5	0.4
(1,2920)	1:56:B:PRO:HA	1:45:A:ILE:HA	10	0.4
(1,2919)	1:56:A:PRO:HA	1:45:B:ILE:HA	10	0.4
(1,2901)	1:55:A:LYS:HB2	1:45:B:ILE:HG12	9	0.4
(1,2690)	1:93:B:ARG:HG3	1:92:B:GLN:HB3	9	0.4
(1,2689)	1:93:A:ARG:HG3	1:92:A:GLN:HB3	2	0.4
(1,2644)	1:125:B:ALA:HA	1:98:B:LYS:HD3	3	0.4
(1,2272)	1:139:B:ALA:HB3	1:139:B:ALA:H	3	0.4
(1,1226)	1:93:B:ARG:HG3	1:93:B:ARG:H	8	0.4
(1,1225)	1:93:A:ARG:HG3	1:93:A:ARG:H	8	0.4
(1,1198)	1:92:B:GLN:HG2	1:92:B:GLN:H	6	0.4
(1,1197)	1:92:A:GLN:HG2	1:92:A:GLN:H	6	0.4
(1,930)	1:83:B:ALA:HB1	1:83:B:ALA:H	7	0.4
(1,930)	1:83:B:ALA:HB2	1:83:B:ALA:H	10	0.4
(1,929)	1:83:A:ALA:HB1	1:83:A:ALA:H	7	0.4
(1,929)	1:83:A:ALA:HB2	1:83:A:ALA:H	10	0.4
(1,100)	1:110:B:VAL:HG11	1:107:B:ASP:H	4	0.4
(1,99)	1:110:A:VAL:HG11	1:107:A:ASP:H	4	0.4
(1,99)	1:110:A:VAL:HG13	1:107:A:ASP:H	10	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,24)	1:92:B:GLN:HG2	1:92:B:GLN:HE22	4	0.4
(1,24)	1:92:B:GLN:HG2	1:92:B:GLN:HE22	6	0.4
(1,23)	1:92:A:GLN:HG2	1:92:A:GLN:HE22	6	0.4
(1,23)	1:92:A:GLN:HG2	1:92:A:GLN:HE22	7	0.4
(3,3074)	1:104:B:PHE:HD2	1:65:B:PHE:HB2	8	0.39
(3,3073)	1:104:A:PHE:HD2	1:65:A:PHE:HB2	8	0.39
(3,3006)	1:106:B:ALA:HB2	1:135:B:MET:HG2	4	0.39
(3,2964)	1:129:B:LYS:HG3	1:45:B:ILE:HG22	4	0.39
(3,2963)	1:129:A:LYS:HG3	1:45:A:ILE:HG22	4	0.39
(3,2878)	1:83:B:ALA:HB1	1:121:B:THR:HG22	9	0.39
(3,2877)	1:83:A:ALA:HB1	1:121:A:THR:HG22	9	0.39
(3,2850)	1:119:B:MET:HE1	1:103:B:PHE:HA	9	0.39
(3,2849)	1:119:A:MET:HE1	1:103:A:PHE:HA	9	0.39
(3,2738)	1:108:B:LYS:HD2	1:110:B:VAL:HG11	6	0.39
(3,2737)	1:108:A:LYS:HD2	1:110:A:VAL:HG11	6	0.39
(3,2372)	1:98:B:LYS:HE2	1:126:B:GLY:HA2	9	0.39
(3,2352)	1:98:B:LYS:HG3	1:125:B:ALA:HB3	7	0.39
(3,2128)	1:87:B:THR:HG23	1:88:B:SER:HB2	7	0.39
(3,2127)	1:87:A:THR:HG23	1:88:A:SER:HB2	7	0.39
(3,2114)	1:87:B:THR:HG21	1:124:B:LYS:HD3	3	0.39
(3,2113)	1:87:A:THR:HG21	1:124:A:LYS:HD3	3	0.39
(3,2108)	1:87:B:THR:HG23	1:88:B:SER:HB2	7	0.39
(3,2107)	1:87:A:THR:HG23	1:88:A:SER:HB2	7	0.39
(3,2060)	1:119:B:MET:HG2	1:49:A:LEU:HG	9	0.39
(3,1893)	1:123:A:ARG:HG2	1:124:A:LYS:HE2	2	0.39
(3,1833)	1:72:A:LYS:HE2	1:110:A:VAL:HG21	3	0.39
(3,1728)	1:69:B:LYS:HB3	1:66:B:LEU:HG	9	0.39
(3,1727)	1:69:A:LYS:HB3	1:66:A:LEU:HG	9	0.39
(3,1642)	1:115:B:LEU:HD11	1:131:B:GLY:HA3	5	0.39
(3,1640)	1:115:B:LEU:HD13	1:131:B:GLY:HA3	8	0.39
(3,1488)	1:61:B:GLU:HB2	1:62:B:LYS:HG2	6	0.39
(3,1240)	1:56:B:PRO:HD2	1:57:B:GLN:HG3	9	0.39
(3,1239)	1:56:A:PRO:HD2	1:57:A:GLN:HG3	9	0.39
(3,1100)	1:139:B:ALA:HA	1:139:B:ALA:HB2	4	0.39
(3,1100)	1:138:B:ALA:HA	1:138:B:ALA:HB1	5	0.39
(3,1100)	1:139:B:ALA:HA	1:139:B:ALA:HB2	7	0.39
(3,1099)	1:139:A:ALA:HA	1:139:A:ALA:HB2	3	0.39
(3,1099)	1:139:A:ALA:HA	1:139:A:ALA:HB3	4	0.39
(3,1099)	1:139:A:ALA:HA	1:139:A:ALA:HB2	7	0.39
(3,1099)	1:139:A:ALA:HA	1:139:A:ALA:HB3	9	0.39
(3,1055)	1:49:A:LEU:HG	1:45:B:ILE:HA	4	0.39
(3,607)	1:134:A:GLY:HA3	1:119:B:MET:H	10	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,580)	1:108:B:LYS:HG3	1:116:A:MET:H	8	0.39
(3,490)	1:132:B:LEU:HG	1:105:B:GLN:H	7	0.39
(3,489)	1:132:A:LEU:HG	1:105:A:GLN:H	7	0.39
(3,383)	1:98:A:LYS:H	1:93:A:ARG:H	2	0.39
(3,257)	1:81:A:VAL:HA	1:77:A:GLY:H	1	0.39
(1,5608)	1:51:B:ALA:HB2	1:124:A:LYS:HA	4	0.39
(1,5604)	1:119:B:MET:HE2	1:130:B:VAL:HA	8	0.39
(1,5603)	1:119:A:MET:HE2	1:130:A:VAL:HA	8	0.39
(1,5530)	1:115:B:LEU:HD21	1:135:B:MET:HA	3	0.39
(1,5529)	1:115:A:LEU:HD21	1:135:A:MET:HA	3	0.39
(1,5306)	1:106:B:ALA:HB1	1:110:B:VAL:HB	9	0.39
(1,5305)	1:106:A:ALA:HB1	1:110:A:VAL:HB	9	0.39
(1,5127)	1:100:A:THR:HG22	1:102:A:ILE:HG22	3	0.39
(1,4854)	1:98:B:LYS:HD3	1:51:A:ALA:HA	2	0.39
(1,4812)	1:96:B:ALA:HA	1:96:B:ALA:HB1	1	0.39
(1,4812)	1:96:B:ALA:HA	1:96:B:ALA:HB2	2	0.39
(1,4812)	1:96:B:ALA:HA	1:96:B:ALA:HB3	3	0.39
(1,4811)	1:96:A:ALA:HA	1:96:A:ALA:HB2	2	0.39
(1,4811)	1:96:A:ALA:HA	1:96:A:ALA:HB3	3	0.39
(1,4760)	1:94:B:THR:HG21	1:99:B:GLU:HG3	10	0.39
(1,4759)	1:94:A:THR:HG21	1:99:A:GLU:HG3	10	0.39
(1,4518)	1:86:B:LEU:HG	1:90:B:LEU:HG	7	0.39
(1,4517)	1:86:A:LEU:HG	1:90:A:LEU:HG	6	0.39
(1,4517)	1:86:A:LEU:HG	1:90:A:LEU:HG	7	0.39
(1,4446)	1:119:B:MET:HG2	1:112:A:TYR:HB3	1	0.39
(1,4445)	1:119:A:MET:HG2	1:112:B:TYR:HB3	1	0.39
(1,4396)	1:83:B:ALA:HA	1:83:B:ALA:HB1	2	0.39
(1,4396)	1:83:B:ALA:HA	1:83:B:ALA:HB3	10	0.39
(1,4395)	1:83:A:ALA:HA	1:83:A:ALA:HB3	4	0.39
(1,4395)	1:83:A:ALA:HA	1:83:A:ALA:HB3	5	0.39
(1,4395)	1:83:A:ALA:HA	1:83:A:ALA:HB1	9	0.39
(1,4395)	1:83:A:ALA:HA	1:83:A:ALA:HB3	10	0.39
(1,4007)	1:72:A:LYS:HD3	1:114:A:THR:HG22	6	0.39
(1,3965)	1:72:A:LYS:HA	1:110:A:VAL:HG12	6	0.39
(1,3550)	1:66:B:LEU:HB3	1:122:B:LEU:HG	4	0.39
(1,3550)	1:66:B:LEU:HB3	1:122:B:LEU:HG	10	0.39
(1,3549)	1:66:A:LEU:HB3	1:122:A:LEU:HG	4	0.39
(1,3549)	1:66:A:LEU:HB3	1:122:A:LEU:HG	10	0.39
(1,3022)	1:56:B:PRO:HD2	1:57:B:GLN:HG3	9	0.39
(1,3021)	1:56:A:PRO:HD2	1:57:A:GLN:HG3	9	0.39
(1,2902)	1:55:B:LYS:HB2	1:45:A:ILE:HG12	9	0.39
(1,2782)	1:51:B:ALA:HB3	1:126:A:GLY:HA3	8	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2690)	1:93:B:ARG:HG3	1:92:B:GLN:HB3	2	0.39
(1,2689)	1:93:A:ARG:HG3	1:92:A:GLN:HB3	9	0.39
(1,2230)	1:107:B:ASP:HA	1:136:B:GLU:H	3	0.39
(1,2229)	1:107:A:ASP:HA	1:136:A:GLU:H	3	0.39
(1,2085)	1:98:A:LYS:HD3	1:127:A:TYR:H	10	0.39
(1,1557)	1:115:A:LEU:HD11	1:105:A:GLN:H	6	0.39
(1,405)	1:58:A:PRO:HB3	1:59:A:ARG:H	6	0.39
(3,2974)	1:130:B:VAL:HB	1:119:B:MET:HE1	5	0.38
(3,2877)	1:83:A:ALA:HB1	1:121:A:THR:HG22	3	0.38
(3,2514)	1:129:B:LYS:HD2	1:102:B:ILE:HG13	3	0.38
(3,2508)	1:86:B:LEU:HG	1:119:B:MET:HA	4	0.38
(3,2507)	1:86:A:LEU:HG	1:119:A:MET:HA	4	0.38
(3,2371)	1:98:A:LYS:HE2	1:126:A:GLY:HA2	9	0.38
(3,2242)	1:98:B:LYS:HE3	1:94:B:THR:HG23	1	0.38
(3,2241)	1:98:A:LYS:HE3	1:94:A:THR:HG23	1	0.38
(3,2059)	1:119:A:MET:HG2	1:49:B:LEU:HG	9	0.38
(3,1998)	1:81:B:VAL:HA	1:66:B:LEU:HB2	8	0.38
(3,1814)	1:72:B:LYS:HB3	1:72:B:LYS:HD3	7	0.38
(3,1813)	1:72:A:LYS:HB3	1:72:A:LYS:HD3	7	0.38
(3,1641)	1:115:A:LEU:HD11	1:131:A:GLY:HA3	5	0.38
(3,1639)	1:115:A:LEU:HD13	1:131:A:GLY:HA3	8	0.38
(3,1487)	1:61:A:GLU:HB2	1:62:A:LYS:HG2	6	0.38
(3,1100)	1:139:B:ALA:HA	1:139:B:ALA:HB1	1	0.38
(3,1100)	1:139:B:ALA:HA	1:139:B:ALA:HB2	3	0.38
(3,1100)	1:139:B:ALA:HA	1:139:B:ALA:HB2	6	0.38
(3,1100)	1:139:B:ALA:HA	1:139:B:ALA:HB2	8	0.38
(3,1100)	1:139:B:ALA:HA	1:139:B:ALA:HB3	9	0.38
(3,1100)	1:139:B:ALA:HA	1:139:B:ALA:HB3	10	0.38
(3,1099)	1:138:A:ALA:HA	1:138:A:ALA:HB3	1	0.38
(3,1099)	1:138:A:ALA:HA	1:138:A:ALA:HB1	5	0.38
(3,1099)	1:139:A:ALA:HA	1:139:A:ALA:HB2	6	0.38
(3,1099)	1:139:A:ALA:HA	1:139:A:ALA:HB2	8	0.38
(3,1099)	1:139:A:ALA:HA	1:139:A:ALA:HB3	10	0.38
(3,904)	1:122:B:LEU:HB2	1:49:A:LEU:HB3	5	0.38
(3,615)	1:49:A:LEU:HA	1:120:B:ASP:H	9	0.38
(3,437)	1:87:A:THR:HG21	1:100:A:THR:H	9	0.38
(3,413)	1:93:A:ARG:HA	1:97:A:ASN:H	10	0.38
(3,258)	1:81:B:VAL:HA	1:77:B:GLY:H	1	0.38
(3,257)	1:81:A:VAL:HA	1:77:A:GLY:H	9	0.38
(1,5690)	1:126:B:GLY:HA3	1:98:B:LYS:HD3	4	0.38
(1,5689)	1:126:A:GLY:HA3	1:98:A:LYS:HD3	4	0.38
(1,5614)	1:121:B:THR:HA	1:124:B:LYS:HE3	6	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5613)	1:121:A:THR:HA	1:124:A:LYS:HE3	6	0.38
(1,5422)	1:110:B:VAL:HG13	1:115:B:LEU:HD12	6	0.38
(1,5421)	1:110:A:VAL:HG13	1:115:A:LEU:HD12	6	0.38
(1,5414)	1:68:B:VAL:HB	1:110:B:VAL:HG13	2	0.38
(1,5413)	1:68:A:VAL:HB	1:110:A:VAL:HG13	2	0.38
(1,5356)	1:107:B:ASP:HB2	1:109:B:SER:HB3	8	0.38
(1,5355)	1:107:A:ASP:HB2	1:109:A:SER:HB3	8	0.38
(1,5342)	1:109:B:SER:HA	1:111:A:ASP:HB2	10	0.38
(1,5258)	1:105:B:GLN:HG2	1:65:B:PHE:HB2	2	0.38
(1,5257)	1:105:A:GLN:HG2	1:65:A:PHE:HB2	2	0.38
(1,5128)	1:100:B:THR:HG22	1:102:B:ILE:HG22	3	0.38
(1,4816)	1:92:B:GLN:HG3	1:96:B:ALA:HB3	5	0.38
(1,4812)	1:96:B:ALA:HA	1:96:B:ALA:HB3	6	0.38
(1,4811)	1:96:A:ALA:HA	1:96:A:ALA:HB3	6	0.38
(1,4516)	1:128:B:LEU:HG	1:49:A:LEU:HB3	9	0.38
(1,4395)	1:83:A:ALA:HA	1:83:A:ALA:HB1	2	0.38
(1,4008)	1:72:B:LYS:HD3	1:114:B:THR:HG22	6	0.38
(1,3974)	1:72:B:LYS:HB3	1:72:B:LYS:HD3	7	0.38
(1,3973)	1:72:A:LYS:HB3	1:72:A:LYS:HD3	7	0.38
(1,3966)	1:72:B:LYS:HA	1:110:B:VAL:HG12	6	0.38
(1,3610)	1:115:B:LEU:HD12	1:110:B:VAL:HG22	5	0.38
(1,3609)	1:115:A:LEU:HD12	1:110:A:VAL:HG22	5	0.38
(1,3440)	1:64:B:VAL:HA	1:102:B:ILE:HG23	6	0.38
(1,3439)	1:64:A:VAL:HA	1:102:A:ILE:HG23	6	0.38
(1,3367)	1:123:A:ARG:HG2	1:50:B:PRO:HD3	1	0.38
(1,3222)	1:122:B:LEU:HA	1:125:B:ALA:HB3	2	0.38
(1,3221)	1:122:A:LEU:HA	1:125:A:ALA:HB3	2	0.38
(1,2644)	1:125:B:ALA:HA	1:98:B:LYS:HD3	8	0.38
(1,2643)	1:125:A:ALA:HA	1:98:A:LYS:HD3	8	0.38
(1,2271)	1:139:A:ALA:HB3	1:139:A:ALA:H	3	0.38
(1,2212)	1:45:B:ILE:H	1:135:A:MET:H	2	0.38
(1,2211)	1:45:A:ILE:H	1:135:B:MET:H	2	0.38
(1,2086)	1:98:B:LYS:HD3	1:127:B:TYR:H	10	0.38
(1,1558)	1:115:B:LEU:HD11	1:105:B:GLN:H	6	0.38
(1,1226)	1:93:B:ARG:HG3	1:93:B:ARG:H	3	0.38
(1,1198)	1:92:B:GLN:HG2	1:92:B:GLN:H	4	0.38
(1,1198)	1:92:B:GLN:HG2	1:92:B:GLN:H	9	0.38
(1,1197)	1:92:A:GLN:HG2	1:92:A:GLN:H	2	0.38
(1,1197)	1:92:A:GLN:HG2	1:92:A:GLN:H	4	0.38
(1,1197)	1:92:A:GLN:HG2	1:92:A:GLN:H	9	0.38
(1,406)	1:58:B:PRO:HB3	1:59:B:ARG:H	4	0.38
(1,406)	1:58:B:PRO:HB3	1:59:B:ARG:H	6	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,405)	1:58:A:PRO:HB3	1:59:A:ARG:H	4	0.38
(1,382)	1:55:B:LYS:HB3	1:57:B:GLN:H	2	0.38
(3,2973)	1:130:A:VAL:HB	1:119:A:MET:HE1	5	0.37
(3,2513)	1:129:A:LYS:HD2	1:102:A:ILE:HG13	3	0.37
(3,2442)	1:94:B:THR:HG23	1:100:B:THR:HB	6	0.37
(3,2441)	1:94:A:THR:HG23	1:100:A:THR:HB	6	0.37
(3,2324)	1:127:B:TYR:HE2	1:98:B:LYS:HG2	10	0.37
(3,2323)	1:127:A:TYR:HE2	1:98:A:LYS:HG2	10	0.37
(3,2127)	1:87:A:THR:HG22	1:88:A:SER:HB2	3	0.37
(3,2107)	1:87:A:THR:HG22	1:88:A:SER:HB2	3	0.37
(3,1997)	1:81:A:VAL:HA	1:66:A:LEU:HB2	8	0.37
(3,1896)	1:123:B:ARG:HG2	1:50:A:PRO:HB3	10	0.37
(3,1873)	1:73:A:GLN:HG2	1:69:A:LYS:HD2	8	0.37
(3,1728)	1:69:B:LYS:HB3	1:66:B:LEU:HG	2	0.37
(3,1575)	1:120:A:ASP:HB2	1:50:B:PRO:HD3	2	0.37
(3,1278)	1:57:B:GLN:HG2	1:50:B:PRO:HD2	3	0.37
(3,1277)	1:57:A:GLN:HG2	1:50:A:PRO:HD2	3	0.37
(3,1100)	1:139:B:ALA:HA	1:139:B:ALA:HB1	2	0.37
(3,1099)	1:139:A:ALA:HA	1:139:A:ALA:HB1	2	0.37
(3,996)	1:47:B:VAL:HB	1:128:A:LEU:HG	3	0.37
(3,580)	1:108:B:LYS:HG3	1:116:A:MET:H	2	0.37
(3,580)	1:108:B:LYS:HG3	1:116:A:MET:H	7	0.37
(3,579)	1:108:A:LYS:HG3	1:116:B:MET:H	6	0.37
(3,579)	1:108:A:LYS:HG3	1:116:B:MET:H	8	0.37
(3,438)	1:87:B:THR:HG21	1:100:B:THR:H	9	0.37
(3,414)	1:93:B:ARG:HA	1:97:B:ASN:H	10	0.37
(3,276)	1:73:B:GLN:HG2	1:79:B:GLN:H	5	0.37
(3,275)	1:73:A:GLN:HG2	1:79:A:GLN:H	5	0.37
(3,258)	1:81:B:VAL:HA	1:77:B:GLY:H	9	0.37
(3,160)	1:58:B:PRO:HB2	1:62:B:LYS:H	5	0.37
(3,78)	1:46:B:ARG:HD2	1:47:B:VAL:H	2	0.37
(1,5614)	1:121:B:THR:HA	1:124:B:LYS:HE3	4	0.37
(1,5613)	1:121:A:THR:HA	1:124:A:LYS:HE3	4	0.37
(1,5414)	1:68:B:VAL:HB	1:110:B:VAL:HG11	5	0.37
(1,5413)	1:68:A:VAL:HB	1:110:A:VAL:HG11	5	0.37
(1,5356)	1:107:B:ASP:HB2	1:109:B:SER:HB3	5	0.37
(1,5355)	1:107:A:ASP:HB2	1:109:A:SER:HB3	5	0.37
(1,4752)	1:94:B:THR:HG22	1:96:B:ALA:HA	10	0.37
(1,4673)	1:91:A:ASP:HA	1:96:A:ALA:HA	4	0.37
(1,4515)	1:128:A:LEU:HG	1:49:B:LEU:HB3	1	0.37
(1,3974)	1:72:B:LYS:HB3	1:72:B:LYS:HD3	5	0.37
(1,3973)	1:72:A:LYS:HB3	1:72:A:LYS:HD3	5	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3968)	1:72:B:LYS:HB2	1:114:B:THR:HG22	1	0.37
(1,3967)	1:72:A:LYS:HB2	1:114:A:THR:HG22	1	0.37
(1,3856)	1:69:B:LYS:HD3	1:65:B:PHE:HB2	7	0.37
(1,3440)	1:64:B:VAL:HA	1:102:B:ILE:HG22	4	0.37
(1,3439)	1:64:A:VAL:HA	1:102:A:ILE:HG22	4	0.37
(1,3368)	1:123:B:ARG:HG2	1:50:A:PRO:HD3	1	0.37
(1,3138)	1:98:B:LYS:HE3	1:125:B:ALA:HB1	3	0.37
(1,3137)	1:98:A:LYS:HE3	1:125:A:ALA:HB1	3	0.37
(1,2924)	1:56:B:PRO:HA	1:50:B:PRO:HD2	10	0.37
(1,2923)	1:56:A:PRO:HA	1:50:A:PRO:HD2	10	0.37
(1,2682)	1:93:B:ARG:HG3	1:91:B:ASP:HB3	3	0.37
(1,2681)	1:93:A:ARG:HG3	1:91:A:ASP:HB3	3	0.37
(1,2570)	1:136:B:GLU:HB3	1:107:B:ASP:HB2	3	0.37
(1,2569)	1:136:A:GLU:HB3	1:107:A:ASP:HB2	3	0.37
(1,1743)	1:139:A:ALA:HB3	1:140:A:LYS:H	7	0.37
(1,1225)	1:93:A:ARG:HG3	1:93:A:ARG:H	3	0.37
(1,1198)	1:92:B:GLN:HG2	1:92:B:GLN:H	2	0.37
(1,930)	1:83:B:ALA:HB3	1:83:B:ALA:H	3	0.37
(1,929)	1:83:A:ALA:HB3	1:83:A:ALA:H	3	0.37
(1,381)	1:55:A:LYS:HB3	1:57:A:GLN:H	2	0.37
(1,100)	1:110:B:VAL:HG12	1:107:B:ASP:H	3	0.37
(1,100)	1:110:B:VAL:HG11	1:107:B:ASP:H	6	0.37
(1,99)	1:110:A:VAL:HG12	1:107:A:ASP:H	3	0.37
(1,99)	1:110:A:VAL:HG11	1:107:A:ASP:H	6	0.37
(3,2938)	1:127:B:TYR:HB2	1:45:B:ILE:HD11	7	0.36
(3,2937)	1:127:A:TYR:HB2	1:45:A:ILE:HD11	7	0.36
(3,2878)	1:83:B:ALA:HB1	1:121:B:THR:HG22	3	0.36
(3,2352)	1:98:B:LYS:HG3	1:125:B:ALA:HB3	5	0.36
(3,2351)	1:98:A:LYS:HG3	1:125:A:ALA:HB3	5	0.36
(3,2288)	1:95:B:GLN:HG2	1:63:B:PRO:HB2	7	0.36
(3,2287)	1:95:A:GLN:HG2	1:63:A:PRO:HB2	7	0.36
(3,2128)	1:87:B:THR:HG22	1:88:B:SER:HB2	3	0.36
(3,2108)	1:87:B:THR:HG22	1:124:B:LYS:HA	2	0.36
(3,2108)	1:87:B:THR:HG22	1:88:B:SER:HB2	3	0.36
(3,1874)	1:73:B:GLN:HG2	1:69:B:LYS:HD2	8	0.36
(3,1814)	1:62:B:LYS:HD2	1:95:B:GLN:HB2	5	0.36
(3,1813)	1:62:A:LYS:HD2	1:95:A:GLN:HB2	5	0.36
(3,1727)	1:69:A:LYS:HB3	1:66:A:LEU:HG	2	0.36
(3,1576)	1:120:B:ASP:HB2	1:50:A:PRO:HD3	2	0.36
(3,1539)	1:46:A:ARG:HG2	1:128:B:LEU:HB3	2	0.36
(3,1418)	1:61:B:GLU:HG2	1:103:B:PHE:HD1	4	0.36
(3,1417)	1:61:A:GLU:HG2	1:103:A:PHE:HD1	4	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,996)	1:47:B:VAL:HB	1:128:A:LEU:HG	7	0.36
(3,972)	1:46:B:ARG:HD3	1:103:A:PHE:HE2	4	0.36
(3,971)	1:46:A:ARG:HD3	1:103:B:PHE:HE2	4	0.36
(3,616)	1:49:B:LEU:HA	1:120:A:ASP:H	9	0.36
(3,579)	1:108:A:LYS:HG3	1:116:B:MET:H	2	0.36
(3,579)	1:108:A:LYS:HG3	1:116:B:MET:H	7	0.36
(3,479)	1:115:A:LEU:HD13	1:104:A:PHE:H	4	0.36
(3,263)	1:92:A:GLN:HG3	1:79:A:GLN:H	8	0.36
(3,258)	1:81:B:VAL:HA	1:77:B:GLY:H	7	0.36
(3,257)	1:81:A:VAL:HA	1:77:A:GLY:H	3	0.36
(3,257)	1:81:A:VAL:HA	1:77:A:GLY:H	7	0.36
(3,159)	1:58:A:PRO:HB2	1:62:A:LYS:H	5	0.36
(3,77)	1:46:A:ARG:HD2	1:47:A:VAL:H	2	0.36
(1,5908)	1:65:B:PHE:HE1	1:100:B:THR:HG23	1	0.36
(1,5907)	1:65:A:PHE:HE1	1:100:A:THR:HG23	1	0.36
(1,5394)	1:110:B:VAL:HG21	1:112:B:TYR:HB3	3	0.36
(1,5393)	1:110:A:VAL:HG21	1:112:A:TYR:HB3	3	0.36
(1,5306)	1:106:B:ALA:HB2	1:110:B:VAL:HB	10	0.36
(1,5305)	1:106:A:ALA:HB2	1:110:A:VAL:HB	10	0.36
(1,5150)	1:100:B:THR:HG23	1:102:B:ILE:HD11	10	0.36
(1,5149)	1:100:A:THR:HG23	1:102:A:ILE:HD11	10	0.36
(1,4816)	1:92:B:GLN:HG3	1:96:B:ALA:HB1	2	0.36
(1,4815)	1:92:A:GLN:HG3	1:96:A:ALA:HB1	2	0.36
(1,4751)	1:94:A:THR:HG22	1:96:A:ALA:HA	10	0.36
(1,4722)	1:93:B:ARG:HA	1:77:B:GLY:HA2	8	0.36
(1,4722)	1:93:B:ARG:HA	1:77:B:GLY:HA2	9	0.36
(1,4721)	1:93:A:ARG:HA	1:77:A:GLY:HA2	9	0.36
(1,4674)	1:91:B:ASP:HA	1:96:B:ALA:HA	4	0.36
(1,4568)	1:87:B:THR:HG21	1:124:B:LYS:HD2	3	0.36
(1,4567)	1:87:A:THR:HG21	1:124:A:LYS:HD2	3	0.36
(1,4516)	1:128:B:LEU:HG	1:49:A:LEU:HB3	1	0.36
(1,4516)	1:128:B:LEU:HG	1:49:A:LEU:HB3	6	0.36
(1,4010)	1:72:B:LYS:HD3	1:110:B:VAL:HG22	7	0.36
(1,4009)	1:72:A:LYS:HD3	1:110:A:VAL:HG22	7	0.36
(1,3855)	1:69:A:LYS:HD3	1:65:A:PHE:HB2	7	0.36
(1,3838)	1:69:B:LYS:HG3	1:115:B:LEU:HD13	2	0.36
(1,3837)	1:69:A:LYS:HG3	1:115:A:LEU:HD13	2	0.36
(1,3596)	1:115:B:LEU:HD12	1:119:B:MET:HG3	9	0.36
(1,3595)	1:115:A:LEU:HD12	1:119:A:MET:HG3	9	0.36
(1,3222)	1:122:B:LEU:HA	1:125:B:ALA:HB1	8	0.36
(1,3221)	1:122:A:LEU:HA	1:125:A:ALA:HB1	8	0.36
(1,2812)	1:54:B:ALA:HA	1:54:B:ALA:HB2	3	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2812)	1:54:B:ALA:HA	1:54:B:ALA:HB1	4	0.36
(1,2811)	1:54:A:ALA:HA	1:54:A:ALA:HB2	3	0.36
(1,2811)	1:54:A:ALA:HA	1:54:A:ALA:HB1	4	0.36
(1,2780)	1:51:B:ALA:HB2	1:51:B:ALA:HA	6	0.36
(1,2779)	1:51:A:ALA:HB3	1:51:A:ALA:HA	9	0.36
(1,2689)	1:93:A:ARG:HG3	1:92:A:GLN:HB3	5	0.36
(1,2495)	1:45:A:ILE:HA	1:54:B:ALA:HB2	6	0.36
(1,2106)	1:129:B:LYS:HD3	1:128:B:LEU:H	5	0.36
(1,2105)	1:129:A:LYS:HD3	1:128:A:LEU:H	5	0.36
(1,1744)	1:139:B:ALA:HB3	1:140:B:LYS:H	7	0.36
(1,1744)	1:139:B:ALA:HB1	1:140:B:LYS:H	9	0.36
(1,1004)	1:89:B:VAL:HG11	1:86:B:LEU:H	4	0.36
(1,1003)	1:89:A:VAL:HG11	1:86:A:LEU:H	4	0.36
(1,944)	1:121:B:THR:HB	1:84:B:ASP:H	3	0.36
(1,943)	1:121:A:THR:HB	1:84:A:ASP:H	7	0.36
(1,930)	1:83:B:ALA:HB3	1:83:B:ALA:H	9	0.36
(1,929)	1:83:A:ALA:HB3	1:83:A:ALA:H	9	0.36
(1,764)	1:73:B:GLN:HG2	1:74:B:LEU:H	5	0.36
(1,763)	1:73:A:GLN:HG2	1:74:A:LEU:H	5	0.36
(1,381)	1:55:A:LYS:HB3	1:57:A:GLN:H	8	0.36
(1,100)	1:110:B:VAL:HG11	1:107:B:ASP:H	7	0.36
(1,99)	1:110:A:VAL:HG11	1:107:A:ASP:H	7	0.36
(3,2924)	1:126:B:GLY:HA3	1:120:B:ASP:HA	1	0.35
(3,2923)	1:126:A:GLY:HA3	1:120:A:ASP:HA	1	0.35
(3,2906)	1:124:B:LYS:HD2	1:121:B:THR:HA	5	0.35
(3,2850)	1:119:B:MET:HE2	1:103:B:PHE:HA	4	0.35
(3,2849)	1:119:A:MET:HE2	1:103:A:PHE:HA	4	0.35
(3,2532)	1:102:B:ILE:HG21	1:133:B:VAL:HB	1	0.35
(3,2531)	1:102:A:ILE:HG21	1:133:A:VAL:HB	1	0.35
(3,2508)	1:86:B:LEU:HG	1:119:B:MET:HA	5	0.35
(3,2507)	1:86:A:LEU:HG	1:119:A:MET:HA	5	0.35
(3,2238)	1:90:B:LEU:HA	1:94:B:THR:HG21	5	0.35
(3,2237)	1:90:A:LEU:HA	1:94:A:THR:HG21	5	0.35
(3,2114)	1:87:B:THR:HG21	1:124:B:LYS:HD3	4	0.35
(3,2113)	1:87:A:THR:HG21	1:124:A:LYS:HD3	4	0.35
(3,2107)	1:87:A:THR:HG22	1:124:A:LYS:HA	2	0.35
(3,1888)	1:74:B:LEU:HB2	1:86:B:LEU:HB3	3	0.35
(3,1887)	1:74:A:LEU:HB2	1:86:A:LEU:HB3	3	0.35
(3,1639)	1:115:A:LEU:HD13	1:131:A:GLY:HA3	4	0.35
(3,995)	1:47:A:VAL:HB	1:128:B:LEU:HG	3	0.35
(3,995)	1:47:A:VAL:HB	1:128:B:LEU:HG	7	0.35
(3,480)	1:115:B:LEU:HD11	1:104:B:PHE:H	1	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,480)	1:115:B:LEU:HD13	1:104:B:PHE:H	4	0.35
(3,480)	1:115:B:LEU:HD11	1:104:B:PHE:H	5	0.35
(3,479)	1:115:A:LEU:HD11	1:104:A:PHE:H	1	0.35
(3,479)	1:115:A:LEU:HD11	1:104:A:PHE:H	5	0.35
(3,264)	1:92:B:GLN:HG3	1:79:B:GLN:H	8	0.35
(3,258)	1:81:B:VAL:HA	1:77:B:GLY:H	3	0.35
(3,258)	1:81:B:VAL:HA	1:77:B:GLY:H	8	0.35
(3,108)	1:49:B:LEU:HG	1:51:B:ALA:H	5	0.35
(1,5806)	1:134:B:GLY:HA3	1:116:A:MET:HB2	5	0.35
(1,5752)	1:86:B:LEU:HG	1:102:B:ILE:HD11	1	0.35
(1,5752)	1:86:B:LEU:HG	1:102:B:ILE:HD12	4	0.35
(1,5751)	1:86:A:LEU:HG	1:102:A:ILE:HD11	1	0.35
(1,5751)	1:86:A:LEU:HG	1:102:A:ILE:HD12	4	0.35
(1,5732)	1:128:B:LEU:HA	1:49:A:LEU:HB3	6	0.35
(1,5554)	1:116:B:MET:HE1	1:114:B:THR:HA	6	0.35
(1,5553)	1:116:A:MET:HE1	1:114:A:THR:HA	6	0.35
(1,5520)	1:115:B:LEU:HG	1:116:B:MET:HE2	10	0.35
(1,5519)	1:115:A:LEU:HG	1:116:A:MET:HE2	10	0.35
(1,5370)	1:110:B:VAL:HA	1:110:B:VAL:HG23	8	0.35
(1,5106)	1:102:B:ILE:HG21	1:127:B:TYR:HE2	7	0.35
(1,5105)	1:102:A:ILE:HG21	1:127:A:TYR:HE2	7	0.35
(1,4815)	1:92:A:GLN:HG3	1:96:A:ALA:HB3	5	0.35
(1,4754)	1:94:B:THR:HG23	1:97:B:ASN:HB3	5	0.35
(1,4753)	1:94:A:THR:HG23	1:97:A:ASN:HB3	5	0.35
(1,4152)	1:123:B:ARG:HG2	1:51:A:ALA:HB1	3	0.35
(1,3966)	1:72:B:LYS:HA	1:110:B:VAL:HG13	5	0.35
(1,3966)	1:72:B:LYS:HA	1:110:B:VAL:HG12	7	0.35
(1,3965)	1:72:A:LYS:HA	1:110:A:VAL:HG13	5	0.35
(1,3965)	1:72:A:LYS:HA	1:110:A:VAL:HG12	7	0.35
(1,3750)	1:68:B:VAL:HA	1:110:B:VAL:HG13	6	0.35
(1,3750)	1:68:B:VAL:HA	1:110:B:VAL:HG11	9	0.35
(1,3749)	1:68:A:VAL:HA	1:110:A:VAL:HG13	6	0.35
(1,3749)	1:68:A:VAL:HA	1:110:A:VAL:HG11	9	0.35
(1,3606)	1:115:B:LEU:HD12	1:119:B:MET:HE1	9	0.35
(1,3605)	1:115:A:LEU:HD12	1:119:A:MET:HE1	9	0.35
(1,3598)	1:115:B:LEU:HD13	1:119:B:MET:HG2	6	0.35
(1,3597)	1:115:A:LEU:HD13	1:119:A:MET:HG2	6	0.35
(1,3550)	1:66:B:LEU:HB3	1:122:B:LEU:HG	7	0.35
(1,3549)	1:66:A:LEU:HB3	1:122:A:LEU:HG	7	0.35
(1,3440)	1:64:B:VAL:HA	1:102:B:ILE:HG22	9	0.35
(1,3439)	1:64:A:VAL:HA	1:102:A:ILE:HG22	9	0.35
(1,3354)	1:122:B:LEU:HG	1:119:B:MET:HB2	1	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3353)	1:122:A:LEU:HG	1:119:A:MET:HB2	1	0.35
(1,2819)	1:54:A:ALA:HB2	1:44:B:ASP:HB2	6	0.35
(1,2812)	1:54:B:ALA:HA	1:54:B:ALA:HB2	8	0.35
(1,2811)	1:54:A:ALA:HA	1:54:A:ALA:HB2	8	0.35
(1,2780)	1:51:B:ALA:HB1	1:51:B:ALA:HA	1	0.35
(1,2780)	1:51:B:ALA:HB1	1:51:B:ALA:HA	2	0.35
(1,2780)	1:51:B:ALA:HB3	1:51:B:ALA:HA	3	0.35
(1,2780)	1:51:B:ALA:HB2	1:51:B:ALA:HA	4	0.35
(1,2780)	1:51:B:ALA:HB2	1:51:B:ALA:HA	5	0.35
(1,2780)	1:51:B:ALA:HB3	1:51:B:ALA:HA	7	0.35
(1,2780)	1:51:B:ALA:HB3	1:51:B:ALA:HA	8	0.35
(1,2780)	1:51:B:ALA:HB3	1:51:B:ALA:HA	9	0.35
(1,2780)	1:51:B:ALA:HB3	1:51:B:ALA:HA	10	0.35
(1,2779)	1:51:A:ALA:HB1	1:51:A:ALA:HA	1	0.35
(1,2779)	1:51:A:ALA:HB1	1:51:A:ALA:HA	2	0.35
(1,2779)	1:51:A:ALA:HB3	1:51:A:ALA:HA	3	0.35
(1,2779)	1:51:A:ALA:HB2	1:51:A:ALA:HA	4	0.35
(1,2779)	1:51:A:ALA:HB2	1:51:A:ALA:HA	5	0.35
(1,2779)	1:51:A:ALA:HB2	1:51:A:ALA:HA	6	0.35
(1,2779)	1:51:A:ALA:HB3	1:51:A:ALA:HA	7	0.35
(1,2779)	1:51:A:ALA:HB3	1:51:A:ALA:HA	8	0.35
(1,2779)	1:51:A:ALA:HB3	1:51:A:ALA:HA	10	0.35
(1,2690)	1:93:B:ARG:HG3	1:92:B:GLN:HB3	3	0.35
(1,2690)	1:93:B:ARG:HG3	1:92:B:GLN:HB3	5	0.35
(1,2689)	1:93:A:ARG:HG3	1:92:A:GLN:HB3	3	0.35
(1,2508)	1:122:B:LEU:HB2	1:130:B:VAL:HB	7	0.35
(1,2507)	1:122:A:LEU:HB2	1:130:A:VAL:HB	7	0.35
(1,2353)	1:85:A:GLN:HE22	1:82:A:ASN:HD22	2	0.35
(1,2241)	1:136:A:GLU:HB3	1:136:A:GLU:H	10	0.35
(1,944)	1:121:B:THR:HB	1:84:B:ASP:H	7	0.35
(1,943)	1:121:A:THR:HB	1:84:A:ASP:H	3	0.35
(1,930)	1:83:B:ALA:HB3	1:83:B:ALA:H	2	0.35
(1,382)	1:55:B:LYS:HB3	1:57:B:GLN:H	8	0.35
(3,3060)	1:65:B:PHE:HE1	1:93:B:ARG:HB2	4	0.34
(3,3059)	1:65:A:PHE:HE1	1:93:A:ARG:HB2	4	0.34
(3,2905)	1:124:A:LYS:HD2	1:121:A:THR:HA	5	0.34
(3,2876)	1:87:B:THR:HG21	1:124:B:LYS:HD3	10	0.34
(3,2875)	1:87:A:THR:HG21	1:124:A:LYS:HD3	10	0.34
(3,2854)	1:119:B:MET:HE2	1:121:B:THR:HB	2	0.34
(3,2853)	1:119:A:MET:HE2	1:121:A:THR:HB	2	0.34
(3,2823)	1:115:A:LEU:HD23	1:116:B:MET:HG2	4	0.34
(3,2532)	1:102:B:ILE:HG23	1:133:B:VAL:HB	4	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,2466)	1:94:B:THR:HG23	1:102:B:ILE:HD11	6	0.34
(3,2465)	1:94:A:THR:HG23	1:102:A:ILE:HD11	6	0.34
(3,2456)	1:100:B:THR:HG22	1:129:B:LYS:HB3	9	0.34
(3,2455)	1:100:A:THR:HG22	1:129:A:LYS:HB3	9	0.34
(3,2388)	1:99:B:GLU:HG3	1:129:B:LYS:HE2	4	0.34
(3,2387)	1:99:A:GLU:HG3	1:129:A:LYS:HE2	4	0.34
(3,2324)	1:127:B:TYR:HE2	1:98:B:LYS:HG2	7	0.34
(3,2323)	1:127:A:TYR:HE2	1:98:A:LYS:HG2	7	0.34
(3,2318)	1:123:B:ARG:HB2	1:124:B:LYS:HG3	4	0.34
(3,2317)	1:123:A:ARG:HB2	1:124:A:LYS:HG3	4	0.34
(3,2114)	1:87:B:THR:HG22	1:124:B:LYS:HD3	7	0.34
(3,2113)	1:87:A:THR:HG22	1:124:A:LYS:HD3	7	0.34
(3,1814)	1:72:B:LYS:HB3	1:72:B:LYS:HD3	10	0.34
(3,1813)	1:72:A:LYS:HB3	1:72:A:LYS:HD3	10	0.34
(3,1724)	1:135:B:MET:HG2	1:115:B:LEU:HD22	6	0.34
(3,1723)	1:135:A:MET:HG2	1:115:A:LEU:HD22	6	0.34
(3,1640)	1:115:B:LEU:HD13	1:131:B:GLY:HA3	4	0.34
(3,1540)	1:46:B:ARG:HG2	1:128:A:LEU:HB3	2	0.34
(3,737)	1:117:A:SER:HA	1:135:B:MET:H	10	0.34
(3,619)	1:124:A:LYS:HE2	1:120:A:ASP:H	8	0.34
(3,480)	1:115:B:LEU:HD12	1:104:B:PHE:H	9	0.34
(3,479)	1:115:A:LEU:HD12	1:104:A:PHE:H	9	0.34
(3,414)	1:93:B:ARG:HA	1:97:B:ASN:H	4	0.34
(3,414)	1:93:B:ARG:HA	1:97:B:ASN:H	8	0.34
(3,413)	1:93:A:ARG:HA	1:97:A:ASN:H	4	0.34
(3,413)	1:93:A:ARG:HA	1:97:A:ASN:H	8	0.34
(3,384)	1:98:B:LYS:H	1:93:B:ARG:H	6	0.34
(3,383)	1:98:A:LYS:H	1:93:A:ARG:H	6	0.34
(3,257)	1:81:A:VAL:HA	1:77:A:GLY:H	8	0.34
(3,107)	1:49:A:LEU:HG	1:51:A:ALA:H	5	0.34
(3,107)	1:49:A:LEU:HG	1:51:A:ALA:H	9	0.34
(1,5731)	1:128:A:LEU:HA	1:49:B:LEU:HB3	9	0.34
(1,5690)	1:126:B:GLY:HA3	1:98:B:LYS:HD3	5	0.34
(1,5668)	1:87:B:THR:HA	1:125:B:ALA:HB3	3	0.34
(1,5667)	1:87:A:THR:HA	1:125:A:ALA:HB3	3	0.34
(1,5414)	1:68:B:VAL:HB	1:110:B:VAL:HG12	1	0.34
(1,5414)	1:68:B:VAL:HB	1:110:B:VAL:HG12	10	0.34
(1,5413)	1:68:A:VAL:HB	1:110:A:VAL:HG12	1	0.34
(1,5413)	1:68:A:VAL:HB	1:110:A:VAL:HG12	10	0.34
(1,5370)	1:110:B:VAL:HA	1:110:B:VAL:HG21	3	0.34
(1,5370)	1:110:B:VAL:HA	1:110:B:VAL:HG21	9	0.34
(1,5369)	1:110:A:VAL:HA	1:110:A:VAL:HG21	3	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5369)	1:110:A:VAL:HA	1:110:A:VAL:HG23	8	0.34
(1,5369)	1:110:A:VAL:HA	1:110:A:VAL:HG21	9	0.34
(1,5356)	1:107:B:ASP:HB2	1:109:B:SER:HB3	4	0.34
(1,5341)	1:109:A:SER:HA	1:111:B:ASP:HB2	10	0.34
(1,5308)	1:106:B:ALA:HB2	1:116:B:MET:HE2	3	0.34
(1,5307)	1:106:A:ALA:HB2	1:116:A:MET:HE2	3	0.34
(1,5212)	1:104:B:PHE:HB2	1:115:B:LEU:HD13	8	0.34
(1,5211)	1:104:A:PHE:HB2	1:115:A:LEU:HD13	8	0.34
(1,4754)	1:94:B:THR:HG23	1:97:B:ASN:HB3	7	0.34
(1,4753)	1:94:A:THR:HG23	1:97:A:ASN:HB3	7	0.34
(1,4721)	1:93:A:ARG:HA	1:77:A:GLY:HA2	8	0.34
(1,4151)	1:123:A:ARG:HG2	1:51:B:ALA:HB1	3	0.34
(1,3974)	1:72:B:LYS:HB3	1:72:B:LYS:HD3	10	0.34
(1,3973)	1:72:A:LYS:HB3	1:72:A:LYS:HD3	10	0.34
(1,3968)	1:72:B:LYS:HB2	1:114:B:THR:HG22	6	0.34
(1,3967)	1:72:A:LYS:HB2	1:114:A:THR:HG22	6	0.34
(1,3856)	1:69:B:LYS:HD3	1:65:B:PHE:HB2	9	0.34
(1,3855)	1:69:A:LYS:HD3	1:65:A:PHE:HB2	9	0.34
(1,3608)	1:115:B:LEU:HD13	1:115:B:LEU:HG	1	0.34
(1,3608)	1:115:B:LEU:HD11	1:115:B:LEU:HG	2	0.34
(1,3608)	1:115:B:LEU:HD12	1:115:B:LEU:HG	4	0.34
(1,3608)	1:115:B:LEU:HD13	1:115:B:LEU:HG	5	0.34
(1,3608)	1:115:B:LEU:HD13	1:115:B:LEU:HG	6	0.34
(1,3608)	1:115:B:LEU:HD12	1:115:B:LEU:HG	7	0.34
(1,3607)	1:115:A:LEU:HD13	1:115:A:LEU:HG	1	0.34
(1,3607)	1:115:A:LEU:HD11	1:115:A:LEU:HG	2	0.34
(1,3607)	1:115:A:LEU:HD12	1:115:A:LEU:HG	4	0.34
(1,3607)	1:115:A:LEU:HD13	1:115:A:LEU:HG	5	0.34
(1,3607)	1:115:A:LEU:HD13	1:115:A:LEU:HG	6	0.34
(1,3607)	1:115:A:LEU:HD12	1:115:A:LEU:HG	7	0.34
(1,3032)	1:119:B:MET:HG2	1:119:B:MET:HE2	2	0.34
(1,3031)	1:119:A:MET:HG2	1:119:A:MET:HE2	2	0.34
(1,2781)	1:51:A:ALA:HB3	1:126:B:GLY:HA3	8	0.34
(1,2664)	1:49:B:LEU:HB2	1:50:B:PRO:HD3	7	0.34
(1,2663)	1:49:A:LEU:HB2	1:50:A:PRO:HD3	7	0.34
(1,2354)	1:85:B:GLN:HE22	1:82:B:ASN:HD22	2	0.34
(1,2272)	1:139:B:ALA:HB1	1:139:B:ALA:H	6	0.34
(1,2271)	1:139:A:ALA:HB1	1:139:A:ALA:H	6	0.34
(1,2268)	1:138:B:ALA:HB1	1:138:B:ALA:H	4	0.34
(1,2267)	1:138:A:ALA:HB1	1:138:A:ALA:H	4	0.34
(1,2242)	1:136:B:GLU:HB3	1:136:B:GLU:H	10	0.34
(1,2241)	1:136:A:GLU:HB3	1:136:A:GLU:H	4	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1743)	1:139:A:ALA:HB1	1:140:A:LYS:H	9	0.34
(1,1688)	1:139:B:ALA:HA	1:140:B:LYS:H	8	0.34
(1,1687)	1:139:A:ALA:HA	1:140:A:LYS:H	8	0.34
(1,1226)	1:93:B:ARG:HG3	1:93:B:ARG:H	6	0.34
(1,1225)	1:93:A:ARG:HG3	1:93:A:ARG:H	6	0.34
(1,929)	1:83:A:ALA:HB3	1:83:A:ALA:H	2	0.34
(1,764)	1:73:B:GLN:HG2	1:74:B:LEU:H	1	0.34
(1,763)	1:73:A:GLN:HG2	1:74:A:LEU:H	1	0.34
(1,254)	1:45:B:ILE:HG21	1:47:B:VAL:H	1	0.34
(1,253)	1:45:A:ILE:HG21	1:47:A:VAL:H	1	0.34
(3,3074)	1:104:B:PHE:HD1	1:65:B:PHE:HB2	5	0.33
(3,3074)	1:104:B:PHE:HD2	1:65:B:PHE:HB2	10	0.33
(3,3073)	1:104:A:PHE:HD1	1:65:A:PHE:HB2	5	0.33
(3,3073)	1:104:A:PHE:HD2	1:65:A:PHE:HB2	10	0.33
(3,2824)	1:115:B:LEU:HD23	1:116:A:MET:HG2	4	0.33
(3,2714)	1:109:B:SER:HB3	1:72:B:LYS:HE2	4	0.33
(3,2556)	1:103:B:PHE:HA	1:45:A:ILE:HG22	9	0.33
(3,2531)	1:102:A:ILE:HG23	1:133:A:VAL:HB	4	0.33
(3,2250)	1:94:B:THR:HG21	1:64:B:VAL:HB	8	0.33
(3,2249)	1:94:A:THR:HG21	1:64:A:VAL:HB	8	0.33
(3,2158)	1:127:B:TYR:HA	1:90:B:LEU:HG	7	0.33
(3,2060)	1:119:B:MET:HG2	1:49:A:LEU:HG	7	0.33
(3,1998)	1:81:B:VAL:HA	1:66:B:LEU:HB2	3	0.33
(3,1997)	1:81:A:VAL:HA	1:66:A:LEU:HB2	3	0.33
(3,1540)	1:46:B:ARG:HG2	1:128:A:LEU:HB3	4	0.33
(3,1539)	1:46:A:ARG:HG2	1:128:B:LEU:HB3	4	0.33
(3,1539)	1:46:A:ARG:HG2	1:128:B:LEU:HB3	8	0.33
(3,1386)	1:60:B:PRO:HG2	1:129:B:LYS:HB3	1	0.33
(3,1385)	1:60:A:PRO:HG2	1:129:A:LYS:HB3	1	0.33
(3,1104)	1:139:B:ALA:HA	1:136:B:GLU:HB2	9	0.33
(3,1103)	1:139:A:ALA:HA	1:136:A:GLU:HB2	9	0.33
(3,696)	1:129:B:LYS:HB3	1:128:B:LEU:H	3	0.33
(3,695)	1:129:A:LYS:HB3	1:128:A:LEU:H	3	0.33
(3,620)	1:124:B:LYS:HE2	1:120:B:ASP:H	8	0.33
(3,414)	1:93:B:ARG:HA	1:97:B:ASN:H	9	0.33
(3,413)	1:93:A:ARG:HA	1:97:A:ASN:H	9	0.33
(3,384)	1:98:B:LYS:H	1:93:B:ARG:H	5	0.33
(3,383)	1:98:A:LYS:H	1:93:A:ARG:H	5	0.33
(3,108)	1:49:B:LEU:HG	1:51:B:ALA:H	6	0.33
(3,108)	1:49:B:LEU:HG	1:51:B:ALA:H	9	0.33
(3,107)	1:49:A:LEU:HG	1:51:A:ALA:H	6	0.33
(1,5805)	1:134:A:GLY:HA3	1:116:B:MET:HB2	5	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5752)	1:86:B:LEU:HG	1:102:B:ILE:HD12	8	0.33
(1,5751)	1:86:A:LEU:HG	1:102:A:ILE:HD12	8	0.33
(1,5731)	1:128:A:LEU:HA	1:49:B:LEU:HB3	3	0.33
(1,5689)	1:126:A:GLY:HA3	1:98:A:LYS:HD3	5	0.33
(1,5604)	1:119:B:MET:HE1	1:130:B:VAL:HA	10	0.33
(1,5603)	1:119:A:MET:HE1	1:130:A:VAL:HA	10	0.33
(1,5394)	1:110:B:VAL:HG22	1:112:B:TYR:HB3	7	0.33
(1,5393)	1:110:A:VAL:HG22	1:112:A:TYR:HB3	7	0.33
(1,5370)	1:110:B:VAL:HA	1:110:B:VAL:HG23	1	0.33
(1,5370)	1:110:B:VAL:HA	1:110:B:VAL:HG23	4	0.33
(1,5370)	1:110:B:VAL:HA	1:110:B:VAL:HG23	10	0.33
(1,5369)	1:110:A:VAL:HA	1:110:A:VAL:HG23	1	0.33
(1,5369)	1:110:A:VAL:HA	1:110:A:VAL:HG23	4	0.33
(1,5369)	1:110:A:VAL:HA	1:110:A:VAL:HG23	10	0.33
(1,5355)	1:107:A:ASP:HB2	1:109:A:SER:HB3	1	0.33
(1,5355)	1:107:A:ASP:HB2	1:109:A:SER:HB3	4	0.33
(1,5306)	1:106:B:ALA:HB1	1:110:B:VAL:HB	6	0.33
(1,5305)	1:106:A:ALA:HB3	1:110:A:VAL:HB	3	0.33
(1,5305)	1:106:A:ALA:HB1	1:110:A:VAL:HB	6	0.33
(1,5150)	1:100:B:THR:HG22	1:102:B:ILE:HD12	9	0.33
(1,5149)	1:100:A:THR:HG22	1:102:A:ILE:HD12	9	0.33
(1,4816)	1:92:B:GLN:HG3	1:96:B:ALA:HB3	4	0.33
(1,4504)	1:86:B:LEU:HB2	1:121:B:THR:HG22	3	0.33
(1,4503)	1:86:A:LEU:HB2	1:121:A:THR:HG22	3	0.33
(1,4326)	1:127:B:TYR:HA	1:90:B:LEU:HG	7	0.33
(1,4112)	1:74:B:LEU:HA	1:110:B:VAL:HG13	4	0.33
(1,4111)	1:74:A:LEU:HA	1:110:A:VAL:HG13	4	0.33
(1,3750)	1:68:B:VAL:HA	1:110:B:VAL:HG13	4	0.33
(1,3749)	1:68:A:VAL:HA	1:110:A:VAL:HG13	4	0.33
(1,3608)	1:115:B:LEU:HD11	1:115:B:LEU:HG	9	0.33
(1,3608)	1:115:B:LEU:HD13	1:115:B:LEU:HG	10	0.33
(1,3607)	1:115:A:LEU:HD11	1:115:A:LEU:HG	9	0.33
(1,3607)	1:115:A:LEU:HD13	1:115:A:LEU:HG	10	0.33
(1,3440)	1:64:B:VAL:HA	1:102:B:ILE:HG23	8	0.33
(1,3440)	1:64:B:VAL:HA	1:102:B:ILE:HG23	10	0.33
(1,3439)	1:64:A:VAL:HA	1:102:A:ILE:HG23	8	0.33
(1,3439)	1:64:A:VAL:HA	1:102:A:ILE:HG23	10	0.33
(1,2812)	1:54:B:ALA:HA	1:54:B:ALA:HB3	1	0.33
(1,2812)	1:54:B:ALA:HA	1:54:B:ALA:HB1	5	0.33
(1,2811)	1:54:A:ALA:HA	1:54:A:ALA:HB3	1	0.33
(1,2811)	1:54:A:ALA:HA	1:54:A:ALA:HB1	5	0.33
(1,2682)	1:93:B:ARG:HG3	1:91:B:ASP:HB3	9	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2681)	1:93:A:ARG:HG3	1:91:A:ASP:HB3	9	0.33
(1,2496)	1:45:B:ILE:HA	1:54:A:ALA:HB2	6	0.33
(1,2472)	1:43:B:VAL:HB	1:46:B:ARG:HA	7	0.33
(1,2471)	1:43:A:VAL:HB	1:46:A:ARG:HA	7	0.33
(1,2267)	1:138:A:ALA:HB1	1:138:A:ALA:H	1	0.33
(1,2242)	1:136:B:GLU:HB3	1:136:B:GLU:H	4	0.33
(1,2242)	1:136:B:GLU:HB3	1:136:B:GLU:H	9	0.33
(1,1198)	1:92:B:GLN:HG2	1:92:B:GLN:H	3	0.33
(1,1198)	1:92:B:GLN:HG2	1:92:B:GLN:H	5	0.33
(1,1198)	1:92:B:GLN:HG2	1:92:B:GLN:H	7	0.33
(1,1197)	1:92:A:GLN:HG2	1:92:A:GLN:H	3	0.33
(1,1197)	1:92:A:GLN:HG2	1:92:A:GLN:H	5	0.33
(1,1197)	1:92:A:GLN:HG2	1:92:A:GLN:H	7	0.33
(3,3074)	1:104:B:PHE:HD1	1:65:B:PHE:HB2	1	0.32
(3,3073)	1:104:A:PHE:HD1	1:65:A:PHE:HB2	1	0.32
(3,3060)	1:65:B:PHE:HE2	1:93:B:ARG:HB2	9	0.32
(3,3059)	1:65:A:PHE:HE2	1:93:A:ARG:HB2	9	0.32
(3,2877)	1:86:A:LEU:HB3	1:121:A:THR:HG22	2	0.32
(3,2824)	1:115:B:LEU:HD23	1:116:A:MET:HG2	1	0.32
(3,2823)	1:115:A:LEU:HD23	1:116:B:MET:HG2	1	0.32
(3,2738)	1:108:B:LYS:HD3	1:110:B:VAL:HG12	8	0.32
(3,2737)	1:108:A:LYS:HD3	1:110:A:VAL:HG12	8	0.32
(3,2713)	1:109:A:SER:HB3	1:72:A:LYS:HE2	4	0.32
(3,2555)	1:103:A:PHE:HA	1:45:B:ILE:HG22	9	0.32
(3,2466)	1:94:B:THR:HG21	1:102:B:ILE:HD13	10	0.32
(3,2465)	1:94:A:THR:HG21	1:102:A:ILE:HD13	10	0.32
(3,2318)	1:123:B:ARG:HB2	1:124:B:LYS:HG3	5	0.32
(3,2317)	1:123:A:ARG:HB2	1:124:A:LYS:HG3	5	0.32
(3,2157)	1:127:A:TYR:HA	1:90:A:LEU:HG	7	0.32
(3,1997)	1:81:A:VAL:HA	1:66:A:LEU:HB2	4	0.32
(3,1874)	1:73:B:GLN:HG2	1:69:B:LYS:HD2	3	0.32
(3,1768)	1:70:B:ALA:HA	1:74:B:LEU:HG	4	0.32
(3,1767)	1:70:A:ALA:HA	1:74:A:LEU:HG	4	0.32
(3,1386)	1:60:B:PRO:HG2	1:129:B:LYS:HB3	6	0.32
(3,1385)	1:60:A:PRO:HG2	1:129:A:LYS:HB3	6	0.32
(3,1043)	1:49:A:LEU:HB2	1:56:A:PRO:HG3	6	0.32
(3,996)	1:47:B:VAL:HB	1:128:A:LEU:HG	10	0.32
(3,995)	1:47:A:VAL:HB	1:128:B:LEU:HG	10	0.32
(3,738)	1:117:B:SER:HA	1:135:A:MET:H	10	0.32
(3,580)	1:108:B:LYS:HG3	1:116:A:MET:H	5	0.32
(3,579)	1:108:A:LYS:HG3	1:116:B:MET:H	5	0.32
(3,108)	1:49:B:LEU:HG	1:51:B:ALA:H	3	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,107)	1:49:A:LEU:HG	1:51:A:ALA:H	3	0.32
(3,74)	1:46:B:ARG:HG2	1:46:B:ARG:H	9	0.32
(3,73)	1:46:A:ARG:HG2	1:46:A:ARG:H	9	0.32
(1,5732)	1:128:B:LEU:HA	1:49:A:LEU:HB3	3	0.32
(1,5732)	1:128:B:LEU:HA	1:49:A:LEU:HB3	9	0.32
(1,5731)	1:128:A:LEU:HA	1:49:B:LEU:HB3	8	0.32
(1,5668)	1:87:B:THR:HA	1:125:B:ALA:HB1	9	0.32
(1,5667)	1:87:A:THR:HA	1:125:A:ALA:HB1	9	0.32
(1,5614)	1:121:B:THR:HA	1:124:B:LYS:HE3	3	0.32
(1,5613)	1:121:A:THR:HA	1:124:A:LYS:HE3	3	0.32
(1,5590)	1:119:B:MET:HG3	1:119:B:MET:HE2	10	0.32
(1,5589)	1:119:A:MET:HG3	1:119:A:MET:HE2	10	0.32
(1,5507)	1:114:A:THR:HB	1:114:A:THR:HG21	5	0.32
(1,5370)	1:110:B:VAL:HA	1:110:B:VAL:HG23	5	0.32
(1,5370)	1:110:B:VAL:HA	1:110:B:VAL:HG21	6	0.32
(1,5369)	1:110:A:VAL:HA	1:110:A:VAL:HG23	5	0.32
(1,5369)	1:110:A:VAL:HA	1:110:A:VAL:HG21	6	0.32
(1,5356)	1:107:B:ASP:HB2	1:109:B:SER:HB3	1	0.32
(1,5356)	1:107:B:ASP:HB2	1:109:B:SER:HB3	7	0.32
(1,5355)	1:107:A:ASP:HB2	1:109:A:SER:HB3	7	0.32
(1,5306)	1:106:B:ALA:HB2	1:110:B:VAL:HB	1	0.32
(1,5306)	1:106:B:ALA:HB3	1:110:B:VAL:HB	3	0.32
(1,5305)	1:106:A:ALA:HB2	1:110:A:VAL:HB	1	0.32
(1,4815)	1:92:A:GLN:HG3	1:96:A:ALA:HB3	4	0.32
(1,4574)	1:87:B:THR:HG21	1:90:B:LEU:HG	2	0.32
(1,4573)	1:87:A:THR:HG21	1:90:A:LEU:HG	2	0.32
(1,4535)	1:87:A:THR:HA	1:90:A:LEU:HG	1	0.32
(1,4325)	1:127:A:TYR:HA	1:90:A:LEU:HG	7	0.32
(1,3855)	1:69:A:LYS:HD3	1:65:A:PHE:HB2	5	0.32
(1,3750)	1:68:B:VAL:HA	1:110:B:VAL:HG12	10	0.32
(1,3749)	1:68:A:VAL:HA	1:110:A:VAL:HG11	3	0.32
(1,3749)	1:68:A:VAL:HA	1:110:A:VAL:HG12	10	0.32
(1,3608)	1:115:B:LEU:HD13	1:115:B:LEU:HG	3	0.32
(1,3608)	1:115:B:LEU:HD12	1:115:B:LEU:HG	8	0.32
(1,3607)	1:115:A:LEU:HD13	1:115:A:LEU:HG	3	0.32
(1,3607)	1:115:A:LEU:HD12	1:115:A:LEU:HG	8	0.32
(1,3458)	1:110:B:VAL:HB	1:114:B:THR:HG22	6	0.32
(1,2812)	1:54:B:ALA:HA	1:54:B:ALA:HB1	6	0.32
(1,2812)	1:54:B:ALA:HA	1:54:B:ALA:HB3	7	0.32
(1,2812)	1:54:B:ALA:HA	1:54:B:ALA:HB1	10	0.32
(1,2811)	1:54:A:ALA:HA	1:54:A:ALA:HB1	6	0.32
(1,2811)	1:54:A:ALA:HA	1:54:A:ALA:HB3	7	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2811)	1:54:A:ALA:HA	1:54:A:ALA:HB1	10	0.32
(1,2644)	1:125:B:ALA:HA	1:98:B:LYS:HD3	10	0.32
(1,2643)	1:125:A:ALA:HA	1:98:A:LYS:HD3	10	0.32
(1,2367)	1:84:A:ASP:HB2	1:85:A:GLN:HE22	8	0.32
(1,2268)	1:138:B:ALA:HB1	1:138:B:ALA:H	1	0.32
(1,2242)	1:136:B:GLU:HB3	1:136:B:GLU:H	5	0.32
(1,2241)	1:136:A:GLU:HB3	1:136:A:GLU:H	5	0.32
(1,2241)	1:136:A:GLU:HB3	1:136:A:GLU:H	9	0.32
(1,1225)	1:93:A:ARG:HG3	1:93:A:ARG:H	2	0.32
(1,62)	1:85:B:GLN:HB3	1:82:B:ASN:H	2	0.32
(1,61)	1:85:A:GLN:HB3	1:82:A:ASN:H	2	0.32
(3,3074)	1:104:B:PHE:HD1	1:65:B:PHE:HB2	2	0.31
(3,3073)	1:104:A:PHE:HD1	1:65:A:PHE:HB2	2	0.31
(3,2954)	1:128:B:LEU:HB3	1:122:B:LEU:HB2	2	0.31
(3,2953)	1:128:A:LEU:HB3	1:122:A:LEU:HB2	2	0.31
(3,2878)	1:86:B:LEU:HB3	1:121:B:THR:HG22	2	0.31
(3,2738)	1:108:B:LYS:HD3	1:110:B:VAL:HG13	10	0.31
(3,2737)	1:108:A:LYS:HD3	1:110:A:VAL:HG13	10	0.31
(3,2532)	1:102:B:ILE:HG21	1:133:B:VAL:HB	10	0.31
(3,2531)	1:102:A:ILE:HG21	1:133:A:VAL:HB	10	0.31
(3,2514)	1:129:B:LYS:HD2	1:102:B:ILE:HG13	8	0.31
(3,2513)	1:129:A:LYS:HD2	1:102:A:ILE:HG13	8	0.31
(3,2500)	1:101:B:THR:HG21	1:50:B:PRO:HB3	8	0.31
(3,2499)	1:101:A:THR:HG21	1:50:A:PRO:HB3	8	0.31
(3,2450)	1:100:B:THR:HG22	1:129:B:LYS:HE3	1	0.31
(3,2449)	1:100:A:THR:HG21	1:129:A:LYS:HE3	1	0.31
(3,2442)	1:94:B:THR:HG22	1:100:B:THR:HB	4	0.31
(3,2441)	1:94:A:THR:HG22	1:100:A:THR:HB	4	0.31
(3,2118)	1:88:B:SER:HB2	1:96:B:ALA:HA	3	0.31
(3,2117)	1:88:A:SER:HB2	1:96:A:ALA:HA	3	0.31
(3,2114)	1:87:B:THR:HG22	1:124:B:LYS:HD3	8	0.31
(3,2113)	1:87:A:THR:HG22	1:124:A:LYS:HD3	8	0.31
(3,1998)	1:81:B:VAL:HA	1:66:B:LEU:HB2	4	0.31
(3,1956)	1:79:B:GLN:HG2	1:91:B:ASP:HB3	4	0.31
(3,1892)	1:74:B:LEU:HB3	1:86:B:LEU:HB3	9	0.31
(3,1873)	1:73:A:GLN:HG2	1:69:A:LYS:HD2	3	0.31
(3,1642)	1:115:B:LEU:HD13	1:120:B:ASP:HB3	10	0.31
(3,1641)	1:115:A:LEU:HD13	1:120:A:ASP:HB3	10	0.31
(3,1639)	1:115:A:LEU:HD12	1:131:A:GLY:HA3	2	0.31
(3,1540)	1:46:B:ARG:HG2	1:128:A:LEU:HB3	8	0.31
(3,1539)	1:46:A:ARG:HG2	1:128:B:LEU:HB3	5	0.31
(3,1278)	1:57:B:GLN:HG2	1:50:B:PRO:HD2	1	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,1277)	1:57:A:GLN:HG2	1:50:A:PRO:HD2	1	0.31
(3,1105)	1:51:A:ALA:HA	1:124:B:LYS:HB3	7	0.31
(3,1044)	1:49:B:LEU:HB2	1:56:B:PRO:HG3	6	0.31
(3,580)	1:108:B:LYS:HG3	1:116:A:MET:H	6	0.31
(3,362)	1:102:B:ILE:HA	1:91:B:ASP:H	10	0.31
(3,361)	1:102:A:ILE:HA	1:91:A:ASP:H	10	0.31
(3,74)	1:46:B:ARG:HG2	1:46:B:ARG:H	5	0.31
(3,73)	1:46:A:ARG:HG2	1:46:A:ARG:H	5	0.31
(1,5508)	1:114:B:THR:HB	1:114:B:THR:HG21	5	0.31
(1,5508)	1:114:B:THR:HB	1:114:B:THR:HG23	10	0.31
(1,5507)	1:114:A:THR:HB	1:114:A:THR:HG23	10	0.31
(1,5394)	1:110:B:VAL:HG23	1:112:B:TYR:HB3	1	0.31
(1,5393)	1:110:A:VAL:HG23	1:112:A:TYR:HB3	1	0.31
(1,5370)	1:110:B:VAL:HA	1:110:B:VAL:HG22	7	0.31
(1,5369)	1:110:A:VAL:HA	1:110:A:VAL:HG22	7	0.31
(1,5356)	1:107:B:ASP:HB2	1:109:B:SER:HB3	3	0.31
(1,5355)	1:107:A:ASP:HB2	1:109:A:SER:HB3	3	0.31
(1,4573)	1:87:A:THR:HG21	1:90:A:LEU:HG	8	0.31
(1,4536)	1:87:B:THR:HA	1:90:B:LEU:HG	1	0.31
(1,4364)	1:82:B:ASN:HB3	1:85:B:GLN:HG2	2	0.31
(1,4363)	1:82:A:ASN:HB3	1:85:A:GLN:HG2	2	0.31
(1,4182)	1:98:B:LYS:HE2	1:96:B:ALA:HA	2	0.31
(1,4181)	1:98:A:LYS:HE2	1:96:A:ALA:HA	2	0.31
(1,4112)	1:74:B:LEU:HA	1:110:B:VAL:HG11	9	0.31
(1,4111)	1:74:A:LEU:HA	1:110:A:VAL:HG11	9	0.31
(1,3965)	1:72:A:LYS:HA	1:110:A:VAL:HG11	1	0.31
(1,3856)	1:69:B:LYS:HD3	1:65:B:PHE:HB2	1	0.31
(1,3856)	1:69:B:LYS:HD3	1:65:B:PHE:HB2	5	0.31
(1,3855)	1:69:A:LYS:HD3	1:65:A:PHE:HB2	1	0.31
(1,3750)	1:68:B:VAL:HA	1:110:B:VAL:HG13	2	0.31
(1,3750)	1:68:B:VAL:HA	1:110:B:VAL:HG11	3	0.31
(1,3749)	1:68:A:VAL:HA	1:110:A:VAL:HG13	2	0.31
(1,3610)	1:115:B:LEU:HD11	1:110:B:VAL:HG21	7	0.31
(1,3609)	1:115:A:LEU:HD11	1:110:A:VAL:HG21	7	0.31
(1,3540)	1:66:B:LEU:HB2	1:102:B:ILE:HG23	4	0.31
(1,3539)	1:66:A:LEU:HB2	1:102:A:ILE:HG23	4	0.31
(1,3457)	1:110:A:VAL:HB	1:114:A:THR:HG22	6	0.31
(1,3367)	1:123:A:ARG:HG2	1:50:B:PRO:HD3	2	0.31
(1,3032)	1:119:B:MET:HG2	1:119:B:MET:HE3	8	0.31
(1,3031)	1:119:A:MET:HG2	1:119:A:MET:HE3	8	0.31
(1,2368)	1:84:B:ASP:HB2	1:85:B:GLN:HE22	6	0.31
(1,2242)	1:136:B:GLU:HB3	1:136:B:GLU:H	6	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2241)	1:136:A:GLU:HB3	1:136:A:GLU:H	6	0.31
(1,1964)	1:121:B:THR:HG21	1:121:B:THR:H	4	0.31
(1,1963)	1:121:A:THR:HG21	1:121:A:THR:H	4	0.31
(1,1744)	1:139:B:ALA:HB1	1:140:B:LYS:H	2	0.31
(1,1226)	1:93:B:ARG:HG3	1:93:B:ARG:H	2	0.31
(1,1226)	1:93:B:ARG:HG3	1:93:B:ARG:H	7	0.31
(1,1226)	1:93:B:ARG:HG3	1:93:B:ARG:H	10	0.31
(1,1225)	1:93:A:ARG:HG3	1:93:A:ARG:H	7	0.31
(1,1121)	1:110:A:VAL:HG23	1:114:A:THR:H	10	0.31
(1,1066)	1:87:B:THR:HG23	1:88:B:SER:H	5	0.31
(1,1066)	1:87:B:THR:HG21	1:88:B:SER:H	6	0.31
(1,1065)	1:87:A:THR:HG23	1:88:A:SER:H	5	0.31
(1,944)	1:121:B:THR:HB	1:84:B:ASP:H	4	0.31
(1,943)	1:121:A:THR:HB	1:84:A:ASP:H	5	0.31
(1,100)	1:110:B:VAL:HG13	1:107:B:ASP:H	1	0.31
(1,99)	1:110:A:VAL:HG13	1:107:A:ASP:H	1	0.31
(3,3056)	1:103:B:PHE:HD2	1:138:B:ALA:HB2	2	0.3
(3,3055)	1:103:A:PHE:HD2	1:138:A:ALA:HB2	2	0.3
(3,3024)	1:129:B:LYS:HA	1:97:B:ASN:HB2	6	0.3
(3,3023)	1:129:A:LYS:HA	1:97:A:ASN:HB2	6	0.3
(3,2878)	1:83:B:ALA:HB3	1:121:B:THR:HG22	6	0.3
(3,2877)	1:83:A:ALA:HB3	1:121:A:THR:HG22	6	0.3
(3,2877)	1:83:A:ALA:HB2	1:121:A:THR:HG22	8	0.3
(3,2466)	1:94:B:THR:HG23	1:102:B:ILE:HD11	9	0.3
(3,2442)	1:94:B:THR:HG22	1:100:B:THR:HB	8	0.3
(3,2441)	1:94:A:THR:HG22	1:100:A:THR:HB	8	0.3
(3,2114)	1:87:B:THR:HG21	1:124:B:LYS:HD3	10	0.3
(3,2113)	1:87:A:THR:HG21	1:124:A:LYS:HD3	10	0.3
(3,2059)	1:119:A:MET:HG2	1:49:B:LEU:HG	7	0.3
(3,1956)	1:79:B:GLN:HG2	1:91:B:ASP:HB3	1	0.3
(3,1955)	1:79:A:GLN:HG2	1:91:A:ASP:HB3	1	0.3
(3,1955)	1:79:A:GLN:HG2	1:91:A:ASP:HB3	4	0.3
(3,1894)	1:123:B:ARG:HG2	1:124:B:LYS:HE2	6	0.3
(3,1893)	1:123:A:ARG:HG2	1:124:A:LYS:HE2	6	0.3
(3,1891)	1:74:A:LEU:HB3	1:86:A:LEU:HB3	9	0.3
(3,1888)	1:74:B:LEU:HB2	1:83:B:ALA:HB3	9	0.3
(3,1887)	1:74:A:LEU:HB2	1:83:A:ALA:HB3	9	0.3
(3,1728)	1:69:B:LYS:HB3	1:66:B:LEU:HG	4	0.3
(3,1640)	1:115:B:LEU:HD12	1:131:B:GLY:HA3	2	0.3
(3,1540)	1:46:B:ARG:HG2	1:128:A:LEU:HB3	5	0.3
(3,1526)	1:132:B:LEU:HG	1:106:B:ALA:HB1	7	0.3
(3,1525)	1:132:A:LEU:HG	1:106:A:ALA:HB1	7	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,995)	1:47:A:VAL:HB	1:128:B:LEU:HG	2	0.3
(3,861)	1:43:A:VAL:HA	1:138:B:ALA:HB2	2	0.3
(3,743)	1:116:A:MET:HE2	1:135:B:MET:H	5	0.3
(3,615)	1:49:A:LEU:HA	1:120:B:ASP:H	7	0.3
(3,489)	1:116:A:MET:HE3	1:105:A:GLN:H	6	0.3
(3,263)	1:92:A:GLN:HG3	1:79:A:GLN:H	5	0.3
(3,108)	1:49:B:LEU:HG	1:51:B:ALA:H	7	0.3
(3,107)	1:49:A:LEU:HG	1:51:A:ALA:H	7	0.3
(1,5752)	1:86:B:LEU:HG	1:102:B:ILE:HD12	10	0.3
(1,5751)	1:86:A:LEU:HG	1:102:A:ILE:HD12	10	0.3
(1,5732)	1:128:B:LEU:HA	1:49:A:LEU:HB3	8	0.3
(1,5668)	1:87:B:THR:HA	1:125:B:ALA:HB1	2	0.3
(1,5667)	1:87:A:THR:HA	1:125:A:ALA:HB1	2	0.3
(1,5520)	1:115:B:LEU:HG	1:116:B:MET:HE2	2	0.3
(1,5520)	1:115:B:LEU:HG	1:116:B:MET:HE3	9	0.3
(1,5519)	1:115:A:LEU:HG	1:116:A:MET:HE2	2	0.3
(1,5519)	1:115:A:LEU:HG	1:116:A:MET:HE3	9	0.3
(1,5508)	1:114:B:THR:HB	1:114:B:THR:HG22	1	0.3
(1,5508)	1:114:B:THR:HB	1:114:B:THR:HG22	6	0.3
(1,5508)	1:114:B:THR:HB	1:114:B:THR:HG22	7	0.3
(1,5507)	1:114:A:THR:HB	1:114:A:THR:HG22	1	0.3
(1,5507)	1:114:A:THR:HB	1:114:A:THR:HG22	6	0.3
(1,5507)	1:114:A:THR:HB	1:114:A:THR:HG22	7	0.3
(1,5128)	1:100:B:THR:HG23	1:102:B:ILE:HG22	2	0.3
(1,5106)	1:102:B:ILE:HG22	1:127:B:TYR:HE2	3	0.3
(1,5106)	1:102:B:ILE:HG23	1:127:B:TYR:HE1	6	0.3
(1,5105)	1:102:A:ILE:HG22	1:127:A:TYR:HE2	3	0.3
(1,5105)	1:102:A:ILE:HG23	1:127:A:TYR:HE1	6	0.3
(1,4862)	1:98:B:LYS:HD3	1:127:B:TYR:HB2	3	0.3
(1,4861)	1:98:A:LYS:HD3	1:127:A:TYR:HB2	3	0.3
(1,4816)	1:92:B:GLN:HG3	1:96:B:ALA:HB2	6	0.3
(1,4815)	1:92:A:GLN:HG3	1:96:A:ALA:HB2	6	0.3
(1,4804)	1:96:B:ALA:HB1	1:127:B:TYR:HE1	10	0.3
(1,4759)	1:94:A:THR:HG22	1:99:A:GLU:HG3	4	0.3
(1,4574)	1:87:B:THR:HG21	1:90:B:LEU:HG	8	0.3
(1,4515)	1:128:A:LEU:HG	1:49:B:LEU:HB3	6	0.3
(1,4515)	1:128:A:LEU:HG	1:49:B:LEU:HB3	8	0.3
(1,4504)	1:86:B:LEU:HB2	1:121:B:THR:HG23	5	0.3
(1,4503)	1:86:A:LEU:HB2	1:121:A:THR:HG23	5	0.3
(1,4364)	1:82:B:ASN:HB3	1:85:B:GLN:HG2	8	0.3
(1,4363)	1:82:A:ASN:HB3	1:85:A:GLN:HG2	8	0.3
(1,4112)	1:74:B:LEU:HA	1:110:B:VAL:HG13	2	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4111)	1:74:A:LEU:HA	1:110:A:VAL:HG13	2	0.3
(1,4007)	1:72:A:LYS:HD3	1:114:A:THR:HG22	8	0.3
(1,4000)	1:72:B:LYS:HG2	1:114:B:THR:HG23	3	0.3
(1,3999)	1:72:A:LYS:HG2	1:114:A:THR:HG23	3	0.3
(1,3968)	1:72:B:LYS:HB2	1:114:B:THR:HG22	7	0.3
(1,3967)	1:72:A:LYS:HB2	1:114:A:THR:HG22	7	0.3
(1,3966)	1:72:B:LYS:HA	1:110:B:VAL:HG11	1	0.3
(1,3606)	1:115:B:LEU:HD12	1:119:B:MET:HE1	2	0.3
(1,3605)	1:115:A:LEU:HD12	1:119:A:MET:HE1	2	0.3
(1,3539)	1:66:A:LEU:HB2	1:102:A:ILE:HG21	10	0.3
(1,3507)	1:65:A:PHE:HB2	1:140:A:LYS:HB2	7	0.3
(1,3032)	1:119:B:MET:HG2	1:119:B:MET:HE1	4	0.3
(1,3032)	1:119:B:MET:HG2	1:119:B:MET:HE3	10	0.3
(1,3031)	1:119:A:MET:HG2	1:119:A:MET:HE1	4	0.3
(1,3031)	1:119:A:MET:HG2	1:119:A:MET:HE3	6	0.3
(1,3031)	1:119:A:MET:HG2	1:119:A:MET:HE3	10	0.3
(1,2812)	1:54:B:ALA:HA	1:54:B:ALA:HB3	2	0.3
(1,2812)	1:54:B:ALA:HA	1:54:B:ALA:HB1	9	0.3
(1,2811)	1:54:A:ALA:HA	1:54:A:ALA:HB3	2	0.3
(1,2811)	1:54:A:ALA:HA	1:54:A:ALA:HB1	9	0.3
(1,2690)	1:93:B:ARG:HG3	1:92:B:GLN:HB3	6	0.3
(1,2689)	1:93:A:ARG:HG3	1:92:A:GLN:HB3	6	0.3
(1,2368)	1:84:B:ASP:HB2	1:85:B:GLN:HE22	8	0.3
(1,2242)	1:136:B:GLU:HB3	1:136:B:GLU:H	8	0.3
(1,1964)	1:121:B:THR:HG22	1:121:B:THR:H	5	0.3
(1,1964)	1:121:B:THR:HG23	1:121:B:THR:H	8	0.3
(1,1963)	1:121:A:THR:HG22	1:121:A:THR:H	5	0.3
(1,1963)	1:121:A:THR:HG23	1:121:A:THR:H	8	0.3
(1,1743)	1:139:A:ALA:HB1	1:140:A:LYS:H	2	0.3
(1,1688)	1:139:B:ALA:HA	1:140:B:LYS:H	1	0.3
(1,1688)	1:139:B:ALA:HA	1:140:B:LYS:H	5	0.3
(1,1687)	1:139:A:ALA:HA	1:140:A:LYS:H	1	0.3
(1,1225)	1:93:A:ARG:HG3	1:93:A:ARG:H	10	0.3
(1,1122)	1:110:B:VAL:HG23	1:114:B:THR:H	10	0.3
(1,1065)	1:87:A:THR:HG21	1:88:A:SER:H	6	0.3
(1,944)	1:121:B:THR:HB	1:84:B:ASP:H	5	0.3
(1,943)	1:121:A:THR:HB	1:84:A:ASP:H	4	0.3
(1,762)	1:110:B:VAL:HG13	1:74:B:LEU:H	4	0.3
(1,761)	1:110:A:VAL:HG13	1:74:A:LEU:H	4	0.3
(1,62)	1:85:B:GLN:HB3	1:82:B:ASN:H	1	0.3
(3,2964)	1:129:B:LYS:HG3	1:45:B:ILE:HG21	9	0.29
(3,2963)	1:129:A:LYS:HG3	1:45:A:ILE:HG21	9	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,2906)	1:124:B:LYS:HD2	1:121:B:THR:HA	9	0.29
(3,2905)	1:124:A:LYS:HD2	1:121:A:THR:HA	9	0.29
(3,2878)	1:83:B:ALA:HB2	1:121:B:THR:HG22	8	0.29
(3,2850)	1:119:B:MET:HE2	1:103:B:PHE:HA	6	0.29
(3,2849)	1:119:A:MET:HE2	1:103:A:PHE:HA	6	0.29
(3,2789)	1:136:A:GLU:HG3	1:136:A:GLU:HA	2	0.29
(3,2466)	1:100:B:THR:HG21	1:102:B:ILE:HD11	8	0.29
(3,2465)	1:100:A:THR:HG21	1:102:A:ILE:HD11	8	0.29
(3,2465)	1:94:A:THR:HG23	1:102:A:ILE:HD11	9	0.29
(3,2324)	1:127:B:TYR:HE2	1:98:B:LYS:HG2	4	0.29
(3,2323)	1:127:A:TYR:HE2	1:98:A:LYS:HG2	4	0.29
(3,2298)	1:90:B:LEU:HA	1:96:B:ALA:HB3	10	0.29
(3,2297)	1:90:A:LEU:HA	1:96:A:ALA:HB3	10	0.29
(3,1998)	1:81:B:VAL:HA	1:66:B:LEU:HB2	10	0.29
(3,1997)	1:81:A:VAL:HA	1:66:A:LEU:HB2	10	0.29
(3,1888)	1:74:B:LEU:HB2	1:86:B:LEU:HB3	8	0.29
(3,1887)	1:74:A:LEU:HB2	1:86:A:LEU:HB3	8	0.29
(3,1727)	1:69:A:LYS:HB3	1:66:A:LEU:HG	4	0.29
(3,1630)	1:66:B:LEU:HB3	1:140:B:LYS:HG3	6	0.29
(3,1629)	1:66:A:LEU:HB3	1:140:A:LYS:HG3	6	0.29
(3,1326)	1:59:B:ARG:HG2	1:103:B:PHE:HE1	10	0.29
(3,1296)	1:58:B:PRO:HG2	1:55:B:LYS:HE3	6	0.29
(3,1295)	1:58:A:PRO:HG2	1:55:A:LYS:HE3	6	0.29
(3,1032)	1:46:B:ARG:HG3	1:48:B:ASP:HB2	1	0.29
(3,1032)	1:46:B:ARG:HG3	1:48:B:ASP:HB2	6	0.29
(3,1031)	1:46:A:ARG:HG3	1:48:A:ASP:HB2	1	0.29
(3,1031)	1:46:A:ARG:HG3	1:48:A:ASP:HB2	6	0.29
(3,996)	1:47:B:VAL:HB	1:128:A:LEU:HG	2	0.29
(3,750)	1:135:B:MET:HB2	1:136:B:GLU:H	2	0.29
(3,749)	1:135:A:MET:HB2	1:136:A:GLU:H	2	0.29
(3,744)	1:116:B:MET:HE2	1:135:A:MET:H	5	0.29
(3,696)	1:129:B:LYS:HB3	1:128:B:LEU:H	6	0.29
(3,695)	1:129:A:LYS:HB3	1:128:A:LEU:H	6	0.29
(3,490)	1:116:B:MET:HE3	1:105:B:GLN:H	6	0.29
(3,438)	1:87:B:THR:HG23	1:100:B:THR:H	4	0.29
(3,437)	1:87:A:THR:HG23	1:100:A:THR:H	4	0.29
(3,264)	1:92:B:GLN:HG3	1:79:B:GLN:H	5	0.29
(3,78)	1:46:B:ARG:HD2	1:47:B:VAL:H	9	0.29
(3,77)	1:46:A:ARG:HD2	1:47:A:VAL:H	9	0.29
(1,5908)	1:65:B:PHE:HE2	1:100:B:THR:HG22	7	0.29
(1,5907)	1:65:A:PHE:HE2	1:100:A:THR:HG22	7	0.29
(1,5762)	1:129:B:LYS:HG2	1:129:B:LYS:HA	2	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5762)	1:129:B:LYS:HG2	1:129:B:LYS:HA	4	0.29
(1,5761)	1:129:A:LYS:HG2	1:129:A:LYS:HA	2	0.29
(1,5731)	1:128:A:LEU:HA	1:49:B:LEU:HB3	6	0.29
(1,5540)	1:115:B:LEU:HG	1:115:B:LEU:HD22	4	0.29
(1,5539)	1:115:A:LEU:HG	1:115:A:LEU:HD22	4	0.29
(1,5520)	1:115:B:LEU:HG	1:116:B:MET:HE3	3	0.29
(1,5519)	1:115:A:LEU:HG	1:116:A:MET:HE3	3	0.29
(1,5472)	1:112:B:TYR:HB3	1:115:B:LEU:HD23	3	0.29
(1,5471)	1:112:A:TYR:HB3	1:115:A:LEU:HD23	3	0.29
(1,5416)	1:110:B:VAL:HG13	1:70:B:ALA:HB3	1	0.29
(1,5416)	1:110:B:VAL:HG12	1:70:B:ALA:HB1	5	0.29
(1,5415)	1:110:A:VAL:HG12	1:70:A:ALA:HB1	5	0.29
(1,5370)	1:110:B:VAL:HA	1:110:B:VAL:HG23	2	0.29
(1,5369)	1:110:A:VAL:HA	1:110:A:VAL:HG23	2	0.29
(1,5150)	1:100:B:THR:HG23	1:102:B:ILE:HD12	6	0.29
(1,5149)	1:100:A:THR:HG23	1:102:A:ILE:HD12	6	0.29
(1,5127)	1:100:A:THR:HG23	1:102:A:ILE:HG22	2	0.29
(1,5106)	1:102:B:ILE:HG22	1:127:B:TYR:HE2	9	0.29
(1,5105)	1:102:A:ILE:HG22	1:127:A:TYR:HE2	9	0.29
(1,4815)	1:92:A:GLN:HG3	1:96:A:ALA:HB2	3	0.29
(1,4803)	1:96:A:ALA:HB1	1:127:A:TYR:HE1	10	0.29
(1,4770)	1:94:B:THR:HG22	1:102:B:ILE:HG13	4	0.29
(1,4769)	1:94:A:THR:HG22	1:102:A:ILE:HG13	4	0.29
(1,4760)	1:94:B:THR:HG22	1:99:B:GLU:HG3	4	0.29
(1,4482)	1:86:B:LEU:HA	1:90:B:LEU:HG	9	0.29
(1,4481)	1:86:A:LEU:HA	1:90:A:LEU:HG	9	0.29
(1,4008)	1:72:B:LYS:HD3	1:114:B:THR:HG22	8	0.29
(1,3750)	1:68:B:VAL:HA	1:110:B:VAL:HG11	5	0.29
(1,3749)	1:68:A:VAL:HA	1:110:A:VAL:HG11	5	0.29
(1,3612)	1:115:B:LEU:HD11	1:106:B:ALA:HB3	4	0.29
(1,3611)	1:115:A:LEU:HD11	1:106:A:ALA:HB3	4	0.29
(1,3540)	1:66:B:LEU:HB2	1:102:B:ILE:HG21	10	0.29
(1,3508)	1:65:B:PHE:HB2	1:140:B:LYS:HB2	7	0.29
(1,3032)	1:119:B:MET:HG2	1:119:B:MET:HE3	3	0.29
(1,3032)	1:119:B:MET:HG2	1:119:B:MET:HE3	6	0.29
(1,3032)	1:119:B:MET:HG2	1:119:B:MET:HE2	9	0.29
(1,3031)	1:119:A:MET:HG2	1:119:A:MET:HE3	3	0.29
(1,3031)	1:119:A:MET:HG2	1:119:A:MET:HE2	9	0.29
(1,2514)	1:45:B:ILE:HD11	1:49:A:LEU:HA	10	0.29
(1,2353)	1:85:A:GLN:HE22	1:82:A:ASN:HD22	8	0.29
(1,2241)	1:136:A:GLU:HB3	1:136:A:GLU:H	8	0.29
(1,1964)	1:121:B:THR:HG21	1:121:B:THR:H	6	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1964)	1:121:B:THR:HG21	1:121:B:THR:H	9	0.29
(1,1963)	1:121:A:THR:HG21	1:121:A:THR:H	6	0.29
(1,1963)	1:121:A:THR:HG21	1:121:A:THR:H	9	0.29
(1,1198)	1:92:B:GLN:HG2	1:92:B:GLN:H	1	0.29
(1,1197)	1:92:A:GLN:HG2	1:92:A:GLN:H	1	0.29
(1,916)	1:82:B:ASN:HB3	1:82:B:ASN:H	5	0.29
(1,916)	1:82:B:ASN:HB3	1:82:B:ASN:H	7	0.29
(1,915)	1:82:A:ASN:HB3	1:82:A:ASN:H	5	0.29
(1,915)	1:82:A:ASN:HB3	1:82:A:ASN:H	7	0.29
(1,824)	1:79:B:GLN:HB2	1:76:B:VAL:H	9	0.29
(1,823)	1:79:A:GLN:HB2	1:76:A:VAL:H	9	0.29
(1,350)	1:54:B:ALA:HA	1:55:B:LYS:H	2	0.29
(1,349)	1:54:A:ALA:HA	1:55:A:LYS:H	2	0.29
(1,61)	1:85:A:GLN:HB3	1:82:A:ASN:H	1	0.29
(3,3002)	1:135:B:MET:HA	1:116:A:MET:HE3	8	0.28
(3,2906)	1:124:B:LYS:HD2	1:121:B:THR:HA	3	0.28
(3,2905)	1:124:A:LYS:HD2	1:121:A:THR:HA	3	0.28
(3,2878)	1:86:B:LEU:HB3	1:121:B:THR:HG22	10	0.28
(3,2877)	1:86:A:LEU:HB3	1:121:A:THR:HG22	10	0.28
(3,2790)	1:136:B:GLU:HG3	1:136:B:GLU:HA	2	0.28
(3,2318)	1:123:B:ARG:HB2	1:124:B:LYS:HG3	7	0.28
(3,2317)	1:123:A:ARG:HB2	1:124:A:LYS:HG3	7	0.28
(3,2118)	1:88:B:SER:HB2	1:96:B:ALA:HA	9	0.28
(3,2117)	1:88:A:SER:HB2	1:96:A:ALA:HA	9	0.28
(3,2114)	1:87:B:THR:HG22	1:124:B:LYS:HD3	2	0.28
(3,2113)	1:87:A:THR:HG22	1:124:A:LYS:HD3	2	0.28
(3,1892)	1:74:B:LEU:HB3	1:86:B:LEU:HB3	3	0.28
(3,1891)	1:74:A:LEU:HB3	1:86:A:LEU:HB3	3	0.28
(3,1359)	1:79:A:GLN:HG3	1:86:A:LEU:HB3	6	0.28
(3,1325)	1:59:A:ARG:HG2	1:103:A:PHE:HE1	10	0.28
(3,1106)	1:51:B:ALA:HA	1:124:A:LYS:HB3	7	0.28
(3,1105)	1:51:A:ALA:HA	1:124:B:LYS:HB3	9	0.28
(3,846)	1:44:B:ASP:HA	1:116:B:MET:HG3	3	0.28
(3,845)	1:44:A:ASP:HA	1:116:A:MET:HG3	3	0.28
(3,733)	1:120:A:ASP:HA	1:134:B:GLY:H	10	0.28
(3,696)	1:129:B:LYS:HB3	1:128:B:LEU:H	8	0.28
(3,695)	1:129:A:LYS:HB3	1:128:A:LEU:H	8	0.28
(3,616)	1:49:B:LEU:HA	1:120:A:ASP:H	7	0.28
(3,480)	1:115:B:LEU:HD13	1:104:B:PHE:H	8	0.28
(3,479)	1:115:A:LEU:HD13	1:104:A:PHE:H	8	0.28
(3,111)	1:98:A:LYS:HB3	1:51:B:ALA:H	5	0.28
(3,108)	1:49:B:LEU:HG	1:51:B:ALA:H	2	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,107)	1:49:A:LEU:HG	1:51:A:ALA:H	8	0.28
(3,78)	1:46:B:ARG:HD2	1:47:B:VAL:H	3	0.28
(3,77)	1:46:A:ARG:HD2	1:47:A:VAL:H	3	0.28
(1,5761)	1:129:A:LYS:HG2	1:129:A:LYS:HA	4	0.28
(1,5731)	1:128:A:LEU:HA	1:49:B:LEU:HB3	1	0.28
(1,5668)	1:87:B:THR:HA	1:125:B:ALA:HB2	1	0.28
(1,5668)	1:87:B:THR:HA	1:125:B:ALA:HB1	6	0.28
(1,5667)	1:87:A:THR:HA	1:125:A:ALA:HB2	1	0.28
(1,5667)	1:87:A:THR:HA	1:125:A:ALA:HB1	6	0.28
(1,5540)	1:115:B:LEU:HG	1:115:B:LEU:HD23	1	0.28
(1,5540)	1:115:B:LEU:HG	1:115:B:LEU:HD22	2	0.28
(1,5540)	1:115:B:LEU:HG	1:115:B:LEU:HD21	7	0.28
(1,5540)	1:115:B:LEU:HG	1:115:B:LEU:HD22	9	0.28
(1,5539)	1:115:A:LEU:HG	1:115:A:LEU:HD23	1	0.28
(1,5539)	1:115:A:LEU:HG	1:115:A:LEU:HD22	2	0.28
(1,5539)	1:115:A:LEU:HG	1:115:A:LEU:HD21	7	0.28
(1,5539)	1:115:A:LEU:HG	1:115:A:LEU:HD22	9	0.28
(1,5415)	1:110:A:VAL:HG13	1:70:A:ALA:HB3	1	0.28
(1,5394)	1:110:B:VAL:HG23	1:112:B:TYR:HB3	5	0.28
(1,5356)	1:107:B:ASP:HB2	1:109:B:SER:HB3	6	0.28
(1,5306)	1:106:B:ALA:HB1	1:110:B:VAL:HB	4	0.28
(1,5305)	1:106:A:ALA:HB1	1:110:A:VAL:HB	4	0.28
(1,4816)	1:92:B:GLN:HG3	1:96:B:ALA:HB2	3	0.28
(1,4815)	1:92:A:GLN:HG3	1:96:A:ALA:HB2	7	0.28
(1,4760)	1:94:B:THR:HG21	1:99:B:GLU:HG3	3	0.28
(1,4568)	1:87:B:THR:HG21	1:124:B:LYS:HD2	4	0.28
(1,4567)	1:87:A:THR:HG21	1:124:A:LYS:HD2	4	0.28
(1,4536)	1:87:B:THR:HA	1:90:B:LEU:HG	7	0.28
(1,4516)	1:128:B:LEU:HG	1:49:A:LEU:HB3	8	0.28
(1,4112)	1:74:B:LEU:HA	1:110:B:VAL:HG12	10	0.28
(1,4111)	1:74:A:LEU:HA	1:110:A:VAL:HG12	10	0.28
(1,3610)	1:115:B:LEU:HD12	1:110:B:VAL:HG23	3	0.28
(1,3610)	1:115:B:LEU:HD11	1:110:B:VAL:HG22	4	0.28
(1,3609)	1:115:A:LEU:HD12	1:110:A:VAL:HG23	3	0.28
(1,3609)	1:115:A:LEU:HD11	1:110:A:VAL:HG22	4	0.28
(1,3598)	1:115:B:LEU:HD13	1:119:B:MET:HG2	10	0.28
(1,3597)	1:115:A:LEU:HD13	1:119:A:MET:HG2	10	0.28
(1,3420)	1:64:B:VAL:HA	1:67:B:SER:HB2	5	0.28
(1,3419)	1:64:A:VAL:HA	1:67:A:SER:HB2	5	0.28
(1,3368)	1:123:B:ARG:HG2	1:50:A:PRO:HD3	2	0.28
(1,3032)	1:119:B:MET:HG2	1:119:B:MET:HE2	1	0.28
(1,3032)	1:119:B:MET:HG2	1:119:B:MET:HE2	5	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3031)	1:119:A:MET:HG2	1:119:A:MET:HE2	1	0.28
(1,3031)	1:119:A:MET:HG2	1:119:A:MET:HE2	5	0.28
(1,2973)	1:56:A:PRO:HD2	1:50:A:PRO:HD2	4	0.28
(1,2513)	1:45:A:ILE:HD11	1:49:B:LEU:HA	10	0.28
(1,2367)	1:84:A:ASP:HB2	1:85:A:GLN:HE22	6	0.28
(1,2354)	1:85:B:GLN:HE22	1:82:B:ASN:HD22	8	0.28
(1,2242)	1:136:B:GLU:HB3	1:136:B:GLU:H	3	0.28
(1,2242)	1:136:B:GLU:HB3	1:136:B:GLU:H	7	0.28
(1,2241)	1:136:A:GLU:HB3	1:136:A:GLU:H	3	0.28
(1,2241)	1:136:A:GLU:HB3	1:136:A:GLU:H	7	0.28
(1,1842)	1:118:B:VAL:HG12	1:117:B:SER:H	7	0.28
(1,1841)	1:118:A:VAL:HG12	1:117:A:SER:H	7	0.28
(1,1688)	1:139:B:ALA:HA	1:140:B:LYS:H	6	0.28
(1,1687)	1:139:A:ALA:HA	1:140:A:LYS:H	5	0.28
(1,1687)	1:139:A:ALA:HA	1:140:A:LYS:H	6	0.28
(1,761)	1:110:A:VAL:HG13	1:74:A:LEU:H	2	0.28
(1,382)	1:55:B:LYS:HB3	1:57:B:GLN:H	6	0.28
(1,382)	1:55:B:LYS:HB3	1:57:B:GLN:H	7	0.28
(1,381)	1:55:A:LYS:HB3	1:57:A:GLN:H	6	0.28
(1,381)	1:55:A:LYS:HB3	1:57:A:GLN:H	7	0.28
(3,3001)	1:135:A:MET:HA	1:116:B:MET:HE2	8	0.27
(3,2738)	1:108:B:LYS:HD3	1:110:B:VAL:HG12	3	0.27
(3,2471)	1:53:A:SER:HB2	1:123:B:ARG:HG2	4	0.27
(3,2296)	1:96:B:ALA:HA	1:100:B:THR:HG22	5	0.27
(3,2250)	1:94:B:THR:HG22	1:64:B:VAL:HB	2	0.27
(3,2249)	1:94:A:THR:HG22	1:64:A:VAL:HB	2	0.27
(3,2108)	1:87:B:THR:HG22	1:124:B:LYS:HA	8	0.27
(3,2107)	1:87:A:THR:HG22	1:124:A:LYS:HA	8	0.27
(3,1954)	1:79:B:GLN:HG2	1:88:B:SER:HB3	2	0.27
(3,1953)	1:79:A:GLN:HG2	1:88:A:SER:HB3	2	0.27
(3,1895)	1:123:A:ARG:HG2	1:50:B:PRO:HB3	1	0.27
(3,1894)	1:123:B:ARG:HG2	1:124:B:LYS:HE2	1	0.27
(3,1894)	1:123:B:ARG:HG2	1:124:B:LYS:HE2	4	0.27
(3,1893)	1:123:A:ARG:HG2	1:124:A:LYS:HE2	4	0.27
(3,1642)	1:115:B:LEU:HD13	1:131:B:GLY:HA3	8	0.27
(3,1386)	1:60:B:PRO:HG2	1:129:B:LYS:HB3	4	0.27
(3,1385)	1:60:A:PRO:HG2	1:129:A:LYS:HB3	4	0.27
(3,1360)	1:79:B:GLN:HG3	1:86:B:LEU:HB3	6	0.27
(3,1106)	1:51:B:ALA:HA	1:124:A:LYS:HB3	9	0.27
(3,276)	1:73:B:GLN:HG2	1:79:B:GLN:H	4	0.27
(3,275)	1:73:A:GLN:HG2	1:79:A:GLN:H	4	0.27
(3,108)	1:49:B:LEU:HG	1:51:B:ALA:H	8	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,107)	1:49:A:LEU:HG	1:51:A:ALA:H	2	0.27
(3,74)	1:46:B:ARG:HG2	1:46:B:ARG:H	7	0.27
(3,73)	1:46:A:ARG:HG2	1:46:A:ARG:H	7	0.27
(1,5762)	1:129:B:LYS:HG2	1:129:B:LYS:HA	7	0.27
(1,5761)	1:129:A:LYS:HG2	1:129:A:LYS:HA	7	0.27
(1,5732)	1:128:B:LEU:HA	1:49:A:LEU:HB3	1	0.27
(1,5604)	1:119:B:MET:HE3	1:130:B:VAL:HA	2	0.27
(1,5603)	1:119:A:MET:HE3	1:130:A:VAL:HA	2	0.27
(1,5590)	1:119:B:MET:HG3	1:119:B:MET:HE3	4	0.27
(1,5589)	1:119:A:MET:HG3	1:119:A:MET:HE3	4	0.27
(1,5554)	1:116:B:MET:HE3	1:114:B:THR:HA	3	0.27
(1,5554)	1:116:B:MET:HE3	1:114:B:THR:HA	4	0.27
(1,5553)	1:116:A:MET:HE3	1:114:A:THR:HA	3	0.27
(1,5540)	1:115:B:LEU:HG	1:115:B:LEU:HD22	3	0.27
(1,5540)	1:115:B:LEU:HG	1:115:B:LEU:HD23	10	0.27
(1,5539)	1:115:A:LEU:HG	1:115:A:LEU:HD22	3	0.27
(1,5539)	1:115:A:LEU:HG	1:115:A:LEU:HD23	10	0.27
(1,5520)	1:115:B:LEU:HG	1:116:B:MET:HE1	8	0.27
(1,5519)	1:115:A:LEU:HG	1:116:A:MET:HE2	1	0.27
(1,5519)	1:115:A:LEU:HG	1:116:A:MET:HE1	8	0.27
(1,5508)	1:114:B:THR:HB	1:114:B:THR:HG23	2	0.27
(1,5508)	1:114:B:THR:HB	1:114:B:THR:HG22	3	0.27
(1,5508)	1:114:B:THR:HB	1:114:B:THR:HG22	8	0.27
(1,5507)	1:114:A:THR:HB	1:114:A:THR:HG23	2	0.27
(1,5507)	1:114:A:THR:HB	1:114:A:THR:HG22	3	0.27
(1,5507)	1:114:A:THR:HB	1:114:A:THR:HG22	8	0.27
(1,5393)	1:110:A:VAL:HG23	1:112:A:TYR:HB3	5	0.27
(1,5355)	1:107:A:ASP:HB2	1:109:A:SER:HB3	6	0.27
(1,5306)	1:106:B:ALA:HB3	1:110:B:VAL:HB	7	0.27
(1,5305)	1:106:A:ALA:HB3	1:110:A:VAL:HB	7	0.27
(1,5260)	1:116:B:MET:HG2	1:116:B:MET:HE1	3	0.27
(1,5259)	1:116:A:MET:HG2	1:116:A:MET:HE1	3	0.27
(1,4816)	1:92:B:GLN:HG3	1:96:B:ALA:HB2	7	0.27
(1,4759)	1:94:A:THR:HG21	1:99:A:GLU:HG3	3	0.27
(1,4610)	1:90:B:LEU:HB3	1:99:B:GLU:HA	8	0.27
(1,4609)	1:90:A:LEU:HB3	1:99:A:GLU:HA	8	0.27
(1,4535)	1:87:A:THR:HA	1:90:A:LEU:HG	7	0.27
(1,4516)	1:128:B:LEU:HG	1:49:A:LEU:HB3	3	0.27
(1,4515)	1:128:A:LEU:HG	1:49:B:LEU:HB3	3	0.27
(1,4112)	1:74:B:LEU:HA	1:110:B:VAL:HG11	8	0.27
(1,4111)	1:74:A:LEU:HA	1:110:A:VAL:HG11	8	0.27
(1,3750)	1:68:B:VAL:HA	1:110:B:VAL:HG12	1	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3610)	1:115:B:LEU:HD12	1:110:B:VAL:HG22	1	0.27
(1,3609)	1:115:A:LEU:HD12	1:110:A:VAL:HG22	1	0.27
(1,3550)	1:66:B:LEU:HB3	1:122:B:LEU:HG	9	0.27
(1,3549)	1:66:A:LEU:HB3	1:122:A:LEU:HG	9	0.27
(1,3210)	1:122:B:LEU:HA	1:87:B:THR:HB	10	0.27
(1,3209)	1:122:A:LEU:HA	1:87:A:THR:HB	10	0.27
(1,2974)	1:56:B:PRO:HD2	1:50:B:PRO:HD2	4	0.27
(1,2814)	1:54:B:ALA:HB3	1:53:B:SER:HB2	6	0.27
(1,2813)	1:54:A:ALA:HB3	1:53:A:SER:HB2	6	0.27
(1,2044)	1:98:B:LYS:HD3	1:126:B:GLY:H	3	0.27
(1,2043)	1:98:A:LYS:HD3	1:126:A:GLY:H	3	0.27
(1,1964)	1:121:B:THR:HG21	1:121:B:THR:H	2	0.27
(1,1964)	1:121:B:THR:HG21	1:121:B:THR:H	3	0.27
(1,1964)	1:121:B:THR:HG21	1:121:B:THR:H	10	0.27
(1,1963)	1:121:A:THR:HG21	1:121:A:THR:H	2	0.27
(1,1963)	1:121:A:THR:HG21	1:121:A:THR:H	10	0.27
(1,1842)	1:118:B:VAL:HG13	1:117:B:SER:H	9	0.27
(1,1841)	1:118:A:VAL:HG13	1:117:A:SER:H	9	0.27
(1,1743)	1:139:A:ALA:HB3	1:140:A:LYS:H	10	0.27
(1,1526)	1:66:B:LEU:HB2	1:104:B:PHE:H	8	0.27
(1,1525)	1:66:A:LEU:HB2	1:104:A:PHE:H	8	0.27
(1,916)	1:82:B:ASN:HB3	1:82:B:ASN:H	8	0.27
(1,916)	1:82:B:ASN:HB3	1:82:B:ASN:H	10	0.27
(1,915)	1:82:A:ASN:HB3	1:82:A:ASN:H	8	0.27
(1,915)	1:82:A:ASN:HB3	1:82:A:ASN:H	10	0.27
(1,824)	1:79:B:GLN:HB2	1:76:B:VAL:H	3	0.27
(1,823)	1:79:A:GLN:HB2	1:76:A:VAL:H	3	0.27
(1,762)	1:110:B:VAL:HG13	1:74:B:LEU:H	2	0.27
(1,406)	1:58:B:PRO:HB3	1:59:B:ARG:H	9	0.27
(1,405)	1:58:A:PRO:HB3	1:59:A:ARG:H	9	0.27
(1,254)	1:45:B:ILE:HG23	1:47:B:VAL:H	4	0.27
(1,253)	1:45:A:ILE:HG23	1:47:A:VAL:H	4	0.27
(3,2824)	1:115:B:LEU:HD23	1:116:A:MET:HG2	9	0.26
(3,2823)	1:115:A:LEU:HD23	1:116:B:MET:HG2	9	0.26
(3,2738)	1:108:B:LYS:HD3	1:110:B:VAL:HG12	5	0.26
(3,2737)	1:108:A:LYS:HD3	1:110:A:VAL:HG12	3	0.26
(3,2737)	1:108:A:LYS:HD3	1:110:A:VAL:HG12	5	0.26
(3,2472)	1:53:B:SER:HB2	1:123:A:ARG:HG2	4	0.26
(3,2450)	1:100:B:THR:HG22	1:129:B:LYS:HE2	2	0.26
(3,2449)	1:100:A:THR:HG22	1:129:A:LYS:HE2	2	0.26
(3,2295)	1:96:A:ALA:HA	1:100:A:THR:HG22	5	0.26
(3,1953)	1:79:A:GLN:HG2	1:88:A:SER:HB3	9	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,1896)	1:123:B:ARG:HG2	1:50:A:PRO:HB3	4	0.26
(3,1894)	1:123:B:ARG:HG2	1:124:B:LYS:HE2	10	0.26
(3,1893)	1:123:A:ARG:HG2	1:124:A:LYS:HE2	1	0.26
(3,1768)	1:70:B:ALA:HA	1:74:B:LEU:HG	2	0.26
(3,1641)	1:115:A:LEU:HD13	1:131:A:GLY:HA3	8	0.26
(3,918)	1:45:B:ILE:HB	1:45:B:ILE:HD11	5	0.26
(3,917)	1:45:A:ILE:HB	1:45:A:ILE:HD11	5	0.26
(3,459)	1:49:A:LEU:HB2	1:122:B:LEU:H	3	0.26
(3,74)	1:46:B:ARG:HG2	1:46:B:ARG:H	2	0.26
(3,73)	1:46:A:ARG:HG2	1:46:A:ARG:H	2	0.26
(1,5762)	1:129:B:LYS:HG2	1:129:B:LYS:HA	3	0.26
(1,5762)	1:129:B:LYS:HG2	1:129:B:LYS:HA	10	0.26
(1,5761)	1:129:A:LYS:HG2	1:129:A:LYS:HA	3	0.26
(1,5761)	1:129:A:LYS:HG2	1:129:A:LYS:HA	10	0.26
(1,5752)	1:86:B:LEU:HG	1:102:B:ILE:HD13	2	0.26
(1,5752)	1:86:B:LEU:HG	1:102:B:ILE:HD12	3	0.26
(1,5751)	1:86:A:LEU:HG	1:102:A:ILE:HD13	2	0.26
(1,5751)	1:86:A:LEU:HG	1:102:A:ILE:HD12	3	0.26
(1,5590)	1:119:B:MET:HG3	1:119:B:MET:HE1	9	0.26
(1,5589)	1:119:A:MET:HG3	1:119:A:MET:HE1	9	0.26
(1,5553)	1:116:A:MET:HE3	1:114:A:THR:HA	4	0.26
(1,5540)	1:115:B:LEU:HG	1:115:B:LEU:HD23	6	0.26
(1,5539)	1:115:A:LEU:HG	1:115:A:LEU:HD23	6	0.26
(1,5520)	1:115:B:LEU:HG	1:116:B:MET:HE2	1	0.26
(1,5508)	1:114:B:THR:HB	1:114:B:THR:HG21	4	0.26
(1,5507)	1:114:A:THR:HB	1:114:A:THR:HG21	4	0.26
(1,5507)	1:114:A:THR:HB	1:114:A:THR:HG21	9	0.26
(1,5378)	1:110:B:VAL:HB	1:110:B:VAL:HG22	1	0.26
(1,5378)	1:110:B:VAL:HB	1:110:B:VAL:HG22	5	0.26
(1,5378)	1:110:B:VAL:HB	1:110:B:VAL:HG23	9	0.26
(1,5377)	1:110:A:VAL:HB	1:110:A:VAL:HG22	1	0.26
(1,5377)	1:110:A:VAL:HB	1:110:A:VAL:HG22	5	0.26
(1,5377)	1:110:A:VAL:HB	1:110:A:VAL:HG23	9	0.26
(1,5106)	1:102:B:ILE:HG23	1:127:B:TYR:HE2	8	0.26
(1,4796)	1:96:B:ALA:HA	1:90:B:LEU:HB2	9	0.26
(1,4609)	1:90:A:LEU:HB3	1:99:A:GLU:HA	3	0.26
(1,4565)	1:87:A:THR:HG23	1:125:A:ALA:HB1	6	0.26
(1,4552)	1:87:B:THR:HB	1:87:B:THR:HG21	8	0.26
(1,4535)	1:87:A:THR:HA	1:90:A:LEU:HG	4	0.26
(1,4482)	1:86:B:LEU:HA	1:90:B:LEU:HG	10	0.26
(1,4481)	1:86:A:LEU:HA	1:90:A:LEU:HG	10	0.26
(1,4428)	1:84:B:ASP:HB2	1:85:B:GLN:HG2	10	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4427)	1:84:A:ASP:HB2	1:85:A:GLN:HG2	10	0.26
(1,3750)	1:68:B:VAL:HA	1:110:B:VAL:HG13	7	0.26
(1,3749)	1:68:A:VAL:HA	1:110:A:VAL:HG12	1	0.26
(1,3420)	1:64:B:VAL:HA	1:67:B:SER:HB2	9	0.26
(1,3419)	1:64:A:VAL:HA	1:67:A:SER:HB2	9	0.26
(1,3032)	1:119:B:MET:HG2	1:119:B:MET:HE1	7	0.26
(1,3031)	1:119:A:MET:HG2	1:119:A:MET:HE1	7	0.26
(1,2974)	1:56:B:PRO:HD2	1:50:B:PRO:HD2	3	0.26
(1,2973)	1:56:A:PRO:HD2	1:50:A:PRO:HD2	3	0.26
(1,2814)	1:54:B:ALA:HB1	1:53:B:SER:HB2	3	0.26
(1,2813)	1:54:A:ALA:HB1	1:53:A:SER:HB2	3	0.26
(1,2552)	1:45:B:ILE:HG23	1:56:A:PRO:HB3	1	0.26
(1,2551)	1:45:A:ILE:HG23	1:56:B:PRO:HB3	1	0.26
(1,2466)	1:88:B:SER:HA	1:87:B:THR:HG21	5	0.26
(1,2465)	1:88:A:SER:HA	1:87:A:THR:HG21	5	0.26
(1,2271)	1:139:A:ALA:HB3	1:139:A:ALA:H	2	0.26
(1,1963)	1:121:A:THR:HG21	1:121:A:THR:H	3	0.26
(1,1526)	1:66:B:LEU:HB2	1:104:B:PHE:H	4	0.26
(1,1525)	1:66:A:LEU:HB2	1:104:A:PHE:H	4	0.26
(1,824)	1:79:B:GLN:HB2	1:76:B:VAL:H	6	0.26
(3,3024)	1:129:B:LYS:HA	1:97:B:ASN:HB2	3	0.25
(3,3023)	1:129:A:LYS:HA	1:97:A:ASN:HB2	3	0.25
(3,2974)	1:130:B:VAL:HB	1:119:B:MET:HE1	1	0.25
(3,2973)	1:130:A:VAL:HB	1:119:A:MET:HE1	1	0.25
(3,2964)	1:129:B:LYS:HG3	1:45:B:ILE:HG22	6	0.25
(3,2963)	1:129:A:LYS:HG3	1:45:A:ILE:HG22	6	0.25
(3,2868)	1:121:B:THR:HA	1:121:B:THR:HG22	7	0.25
(3,2738)	1:108:B:LYS:HD3	1:110:B:VAL:HG11	2	0.25
(3,2737)	1:108:A:LYS:HD3	1:110:A:VAL:HG11	2	0.25
(3,2466)	1:100:B:THR:HG22	1:102:B:ILE:HD13	1	0.25
(3,2465)	1:100:A:THR:HG22	1:102:A:ILE:HD13	1	0.25
(3,2388)	1:99:B:GLU:HG3	1:129:B:LYS:HE2	2	0.25
(3,2387)	1:99:A:GLU:HG3	1:129:A:LYS:HE2	2	0.25
(3,2250)	1:94:B:THR:HG22	1:64:B:VAL:HB	9	0.25
(3,2249)	1:94:A:THR:HG22	1:64:A:VAL:HB	9	0.25
(3,1954)	1:79:B:GLN:HG2	1:88:B:SER:HB3	9	0.25
(3,1896)	1:123:B:ARG:HG2	1:50:A:PRO:HB3	1	0.25
(3,1895)	1:123:A:ARG:HG2	1:50:B:PRO:HB3	4	0.25
(3,1893)	1:123:A:ARG:HG2	1:124:A:LYS:HE2	10	0.25
(3,1767)	1:70:A:ALA:HA	1:74:A:LEU:HG	2	0.25
(3,1640)	1:115:B:LEU:HD12	1:131:B:GLY:HA3	9	0.25
(3,1639)	1:115:A:LEU:HD12	1:131:A:GLY:HA3	9	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,1540)	1:46:B:ARG:HG2	1:128:A:LEU:HB3	1	0.25
(3,1540)	1:46:B:ARG:HG2	1:128:A:LEU:HB3	3	0.25
(3,1539)	1:46:A:ARG:HG2	1:128:B:LEU:HB3	1	0.25
(3,1106)	1:51:B:ALA:HA	1:124:A:LYS:HB3	4	0.25
(3,1105)	1:51:A:ALA:HA	1:124:B:LYS:HB3	4	0.25
(3,918)	1:45:B:ILE:HB	1:45:B:ILE:HD12	3	0.25
(3,696)	1:129:B:LYS:HB3	1:128:B:LEU:H	2	0.25
(3,696)	1:129:B:LYS:HB3	1:128:B:LEU:H	9	0.25
(3,695)	1:129:A:LYS:HB3	1:128:A:LEU:H	2	0.25
(3,695)	1:129:A:LYS:HB3	1:128:A:LEU:H	9	0.25
(3,580)	1:108:B:LYS:HG3	1:116:A:MET:H	1	0.25
(3,579)	1:108:A:LYS:HG2	1:116:B:MET:H	1	0.25
(1,5762)	1:129:B:LYS:HG2	1:129:B:LYS:HA	6	0.25
(1,5761)	1:129:A:LYS:HG2	1:129:A:LYS:HA	6	0.25
(1,5668)	1:87:B:THR:HA	1:125:B:ALA:HB2	10	0.25
(1,5667)	1:87:A:THR:HA	1:125:A:ALA:HB2	10	0.25
(1,5590)	1:119:B:MET:HG3	1:119:B:MET:HE3	7	0.25
(1,5589)	1:119:A:MET:HG3	1:119:A:MET:HE3	7	0.25
(1,5576)	1:118:B:VAL:HA	1:121:B:THR:HG22	8	0.25
(1,5575)	1:118:A:VAL:HA	1:121:A:THR:HG22	8	0.25
(1,5520)	1:115:B:LEU:HG	1:116:B:MET:HE3	7	0.25
(1,5519)	1:115:A:LEU:HG	1:116:A:MET:HE3	7	0.25
(1,5508)	1:114:B:THR:HB	1:114:B:THR:HG21	9	0.25
(1,5414)	1:68:B:VAL:HB	1:110:B:VAL:HG13	7	0.25
(1,5413)	1:68:A:VAL:HB	1:110:A:VAL:HG13	7	0.25
(1,5402)	1:110:B:VAL:HG23	1:116:B:MET:HE2	4	0.25
(1,5394)	1:110:B:VAL:HG23	1:112:B:TYR:HB3	4	0.25
(1,5393)	1:110:A:VAL:HG23	1:112:A:TYR:HB3	4	0.25
(1,5378)	1:110:B:VAL:HB	1:110:B:VAL:HG23	3	0.25
(1,5378)	1:110:B:VAL:HB	1:110:B:VAL:HG22	4	0.25
(1,5378)	1:110:B:VAL:HB	1:110:B:VAL:HG23	6	0.25
(1,5378)	1:110:B:VAL:HB	1:110:B:VAL:HG21	7	0.25
(1,5378)	1:110:B:VAL:HB	1:110:B:VAL:HG22	8	0.25
(1,5378)	1:110:B:VAL:HB	1:110:B:VAL:HG22	10	0.25
(1,5377)	1:110:A:VAL:HB	1:110:A:VAL:HG23	3	0.25
(1,5377)	1:110:A:VAL:HB	1:110:A:VAL:HG22	4	0.25
(1,5377)	1:110:A:VAL:HB	1:110:A:VAL:HG23	6	0.25
(1,5377)	1:110:A:VAL:HB	1:110:A:VAL:HG21	7	0.25
(1,5377)	1:110:A:VAL:HB	1:110:A:VAL:HG22	8	0.25
(1,5306)	1:106:B:ALA:HB1	1:110:B:VAL:HB	2	0.25
(1,5305)	1:106:A:ALA:HB1	1:110:A:VAL:HB	2	0.25
(1,5128)	1:100:B:THR:HG21	1:102:B:ILE:HG22	5	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5127)	1:100:A:THR:HG21	1:102:A:ILE:HG22	5	0.25
(1,5105)	1:102:A:ILE:HG23	1:127:A:TYR:HE2	8	0.25
(1,4795)	1:96:A:ALA:HA	1:90:A:LEU:HB2	9	0.25
(1,4610)	1:90:B:LEU:HB3	1:99:B:GLU:HA	3	0.25
(1,4566)	1:87:B:THR:HG23	1:125:B:ALA:HB1	6	0.25
(1,4552)	1:87:B:THR:HB	1:87:B:THR:HG22	1	0.25
(1,4552)	1:87:B:THR:HB	1:87:B:THR:HG21	2	0.25
(1,4552)	1:87:B:THR:HB	1:87:B:THR:HG22	7	0.25
(1,4552)	1:87:B:THR:HB	1:87:B:THR:HG21	10	0.25
(1,4551)	1:87:A:THR:HB	1:87:A:THR:HG22	1	0.25
(1,4551)	1:87:A:THR:HB	1:87:A:THR:HG21	2	0.25
(1,4551)	1:87:A:THR:HB	1:87:A:THR:HG22	7	0.25
(1,4551)	1:87:A:THR:HB	1:87:A:THR:HG21	8	0.25
(1,4551)	1:87:A:THR:HB	1:87:A:THR:HG21	10	0.25
(1,4536)	1:87:B:THR:HA	1:90:B:LEU:HG	4	0.25
(1,4398)	1:83:B:ALA:HA	1:121:B:THR:HG22	8	0.25
(1,4397)	1:83:A:ALA:HA	1:121:A:THR:HG22	8	0.25
(1,4358)	1:82:B:ASN:HB2	1:83:B:ALA:HB2	2	0.25
(1,4357)	1:82:A:ASN:HB2	1:83:A:ALA:HB2	2	0.25
(1,4182)	1:98:B:LYS:HE2	1:96:B:ALA:HA	1	0.25
(1,3968)	1:72:B:LYS:HB2	1:114:B:THR:HG23	10	0.25
(1,3967)	1:72:A:LYS:HB2	1:114:A:THR:HG23	10	0.25
(1,3749)	1:68:A:VAL:HA	1:110:A:VAL:HG13	7	0.25
(1,3354)	1:122:B:LEU:HG	1:119:B:MET:HB2	7	0.25
(1,3353)	1:122:A:LEU:HG	1:119:A:MET:HB2	7	0.25
(1,2919)	1:56:A:PRO:HA	1:45:B:ILE:HA	9	0.25
(1,2784)	1:70:B:ALA:HB2	1:70:B:ALA:HA	3	0.25
(1,2784)	1:70:B:ALA:HB3	1:70:B:ALA:HA	4	0.25
(1,2784)	1:70:B:ALA:HB1	1:70:B:ALA:HA	5	0.25
(1,2784)	1:70:B:ALA:HB2	1:70:B:ALA:HA	6	0.25
(1,2783)	1:70:A:ALA:HB2	1:70:A:ALA:HA	3	0.25
(1,2783)	1:70:A:ALA:HB3	1:70:A:ALA:HA	4	0.25
(1,2783)	1:70:A:ALA:HB2	1:70:A:ALA:HA	5	0.25
(1,2783)	1:70:A:ALA:HB1	1:70:A:ALA:HA	6	0.25
(1,2571)	1:46:A:ARG:HB2	1:48:B:ASP:HB3	6	0.25
(1,2272)	1:139:B:ALA:HB2	1:139:B:ALA:H	1	0.25
(1,2272)	1:139:B:ALA:HB3	1:139:B:ALA:H	2	0.25
(1,2272)	1:139:B:ALA:HB3	1:139:B:ALA:H	8	0.25
(1,2272)	1:139:B:ALA:HB1	1:139:B:ALA:H	10	0.25
(1,1964)	1:121:B:THR:HG22	1:121:B:THR:H	1	0.25
(1,1963)	1:121:A:THR:HG22	1:121:A:THR:H	1	0.25
(1,1744)	1:139:B:ALA:HB2	1:140:B:LYS:H	3	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1744)	1:139:B:ALA:HB3	1:140:B:LYS:H	10	0.25
(1,1122)	1:110:B:VAL:HG23	1:114:B:THR:H	4	0.25
(1,916)	1:82:B:ASN:HB3	1:82:B:ASN:H	6	0.25
(1,915)	1:82:A:ASN:HB3	1:82:A:ASN:H	4	0.25
(1,915)	1:82:A:ASN:HB3	1:82:A:ASN:H	6	0.25
(1,823)	1:79:A:GLN:HB2	1:76:A:VAL:H	6	0.25
(1,349)	1:54:A:ALA:HA	1:55:A:LYS:H	5	0.25
(3,2905)	1:124:A:LYS:HD2	1:121:A:THR:HA	6	0.24
(3,2867)	1:121:A:THR:HA	1:121:A:THR:HG22	7	0.24
(3,2850)	1:119:B:MET:HE1	1:103:B:PHE:HA	5	0.24
(3,2849)	1:119:A:MET:HE1	1:103:A:PHE:HA	5	0.24
(3,2832)	1:112:B:TYR:HD1	1:116:B:MET:HE3	5	0.24
(3,2831)	1:112:A:TYR:HD1	1:116:A:MET:HE3	5	0.24
(3,2823)	1:115:A:LEU:HD23	1:116:A:MET:HG3	3	0.24
(3,2790)	1:136:B:GLU:HG3	1:136:B:GLU:HA	1	0.24
(3,2789)	1:136:A:GLU:HG3	1:136:A:GLU:HA	1	0.24
(3,2450)	1:100:B:THR:HG23	1:129:B:LYS:HE2	7	0.24
(3,2449)	1:100:A:THR:HG23	1:129:A:LYS:HE2	7	0.24
(3,2250)	1:94:B:THR:HG23	1:64:B:VAL:HB	3	0.24
(3,2249)	1:94:A:THR:HG23	1:64:A:VAL:HB	3	0.24
(3,1896)	1:123:B:ARG:HG2	1:50:A:PRO:HB3	6	0.24
(3,1106)	1:51:B:ALA:HA	1:124:A:LYS:HB3	10	0.24
(3,1054)	1:93:B:ARG:HG3	1:94:B:THR:HA	4	0.24
(3,1053)	1:93:A:ARG:HG3	1:94:A:THR:HA	4	0.24
(3,918)	1:45:B:ILE:HB	1:45:B:ILE:HD11	6	0.24
(3,918)	1:45:B:ILE:HB	1:45:B:ILE:HD12	7	0.24
(3,917)	1:45:A:ILE:HB	1:45:A:ILE:HD12	3	0.24
(3,917)	1:45:A:ILE:HB	1:45:A:ILE:HD11	6	0.24
(3,917)	1:45:A:ILE:HB	1:45:A:ILE:HD12	7	0.24
(3,750)	1:135:B:MET:HB3	1:136:B:GLU:H	7	0.24
(3,749)	1:135:A:MET:HB3	1:136:A:GLU:H	7	0.24
(3,749)	1:135:A:MET:HB3	1:136:A:GLU:H	9	0.24
(3,734)	1:120:B:ASP:HA	1:134:A:GLY:H	10	0.24
(3,616)	1:49:B:LEU:HA	1:120:A:ASP:H	10	0.24
(3,615)	1:49:A:LEU:HA	1:120:B:ASP:H	10	0.24
(3,258)	1:81:B:VAL:HA	1:77:B:GLY:H	4	0.24
(3,74)	1:46:B:ARG:HG2	1:46:B:ARG:H	3	0.24
(3,74)	1:46:B:ARG:HG2	1:46:B:ARG:H	8	0.24
(3,73)	1:46:A:ARG:HG2	1:46:A:ARG:H	3	0.24
(3,73)	1:46:A:ARG:HG2	1:46:A:ARG:H	8	0.24
(1,5752)	1:86:B:LEU:HG	1:102:B:ILE:HD11	5	0.24
(1,5751)	1:86:A:LEU:HG	1:102:A:ILE:HD11	5	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5690)	1:126:B:GLY:HA3	1:98:B:LYS:HD3	8	0.24
(1,5689)	1:126:A:GLY:HA3	1:98:A:LYS:HD3	8	0.24
(1,5668)	1:87:B:THR:HA	1:125:B:ALA:HB1	4	0.24
(1,5667)	1:87:A:THR:HA	1:125:A:ALA:HB1	4	0.24
(1,5628)	1:121:B:THR:HG22	1:84:B:ASP:HB3	10	0.24
(1,5627)	1:121:A:THR:HG22	1:84:A:ASP:HB3	10	0.24
(1,5590)	1:119:B:MET:HG3	1:119:B:MET:HE1	5	0.24
(1,5589)	1:119:A:MET:HG3	1:119:A:MET:HE1	5	0.24
(1,5553)	1:116:A:MET:HE3	1:114:A:THR:HA	9	0.24
(1,5540)	1:115:B:LEU:HG	1:115:B:LEU:HD22	5	0.24
(1,5540)	1:115:B:LEU:HG	1:115:B:LEU:HD22	8	0.24
(1,5539)	1:115:A:LEU:HG	1:115:A:LEU:HD22	5	0.24
(1,5539)	1:115:A:LEU:HG	1:115:A:LEU:HD22	8	0.24
(1,5401)	1:110:A:VAL:HG23	1:116:A:MET:HE2	4	0.24
(1,5377)	1:110:A:VAL:HB	1:110:A:VAL:HG22	10	0.24
(1,5260)	1:116:B:MET:HG2	1:116:B:MET:HE2	5	0.24
(1,5260)	1:116:B:MET:HG2	1:116:B:MET:HE2	6	0.24
(1,5259)	1:116:A:MET:HG2	1:116:A:MET:HE2	5	0.24
(1,5259)	1:116:A:MET:HG2	1:116:A:MET:HE2	6	0.24
(1,4816)	1:92:B:GLN:HG3	1:96:B:ALA:HB3	8	0.24
(1,4815)	1:92:A:GLN:HG3	1:96:A:ALA:HB3	8	0.24
(1,4636)	1:90:B:LEU:HB2	1:64:B:VAL:HB	7	0.24
(1,4635)	1:90:A:LEU:HB2	1:64:A:VAL:HB	7	0.24
(1,4574)	1:87:B:THR:HG23	1:90:B:LEU:HG	3	0.24
(1,4573)	1:87:A:THR:HG23	1:90:A:LEU:HG	3	0.24
(1,4552)	1:87:B:THR:HB	1:87:B:THR:HG23	3	0.24
(1,4552)	1:87:B:THR:HB	1:87:B:THR:HG23	4	0.24
(1,4551)	1:87:A:THR:HB	1:87:A:THR:HG23	3	0.24
(1,4551)	1:87:A:THR:HB	1:87:A:THR:HG23	4	0.24
(1,4536)	1:87:B:THR:HA	1:90:B:LEU:HG	2	0.24
(1,4535)	1:87:A:THR:HA	1:90:A:LEU:HG	2	0.24
(1,4182)	1:98:B:LYS:HE2	1:96:B:ALA:HA	7	0.24
(1,4181)	1:98:A:LYS:HE2	1:96:A:ALA:HA	1	0.24
(1,4181)	1:98:A:LYS:HE2	1:96:A:ALA:HA	7	0.24
(1,3676)	1:67:B:SER:HB2	1:105:B:GLN:HG2	6	0.24
(1,3675)	1:67:A:SER:HB2	1:105:A:GLN:HG2	6	0.24
(1,3540)	1:66:B:LEU:HB2	1:102:B:ILE:HG21	1	0.24
(1,3540)	1:66:B:LEU:HB2	1:102:B:ILE:HG23	5	0.24
(1,3539)	1:66:A:LEU:HB2	1:102:A:ILE:HG21	1	0.24
(1,3539)	1:66:A:LEU:HB2	1:102:A:ILE:HG23	5	0.24
(1,3354)	1:122:B:LEU:HG	1:119:B:MET:HB2	5	0.24
(1,2814)	1:54:B:ALA:HB3	1:53:B:SER:HB2	9	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2813)	1:54:A:ALA:HB3	1:53:A:SER:HB2	9	0.24
(1,2784)	1:70:B:ALA:HB1	1:70:B:ALA:HA	1	0.24
(1,2784)	1:70:B:ALA:HB3	1:70:B:ALA:HA	2	0.24
(1,2784)	1:70:B:ALA:HB2	1:70:B:ALA:HA	7	0.24
(1,2784)	1:70:B:ALA:HB2	1:70:B:ALA:HA	8	0.24
(1,2784)	1:70:B:ALA:HB3	1:70:B:ALA:HA	9	0.24
(1,2784)	1:70:B:ALA:HB3	1:70:B:ALA:HA	10	0.24
(1,2783)	1:70:A:ALA:HB1	1:70:A:ALA:HA	1	0.24
(1,2783)	1:70:A:ALA:HB3	1:70:A:ALA:HA	2	0.24
(1,2783)	1:70:A:ALA:HB2	1:70:A:ALA:HA	7	0.24
(1,2783)	1:70:A:ALA:HB2	1:70:A:ALA:HA	8	0.24
(1,2783)	1:70:A:ALA:HB3	1:70:A:ALA:HA	10	0.24
(1,2559)	1:45:A:ILE:HG22	1:54:B:ALA:HB2	6	0.24
(1,2271)	1:139:A:ALA:HB2	1:139:A:ALA:H	1	0.24
(1,2271)	1:139:A:ALA:HB3	1:139:A:ALA:H	8	0.24
(1,2271)	1:139:A:ALA:HB1	1:139:A:ALA:H	10	0.24
(1,2212)	1:45:B:ILE:H	1:135:A:MET:H	1	0.24
(1,1526)	1:66:B:LEU:HB2	1:104:B:PHE:H	10	0.24
(1,1525)	1:66:A:LEU:HB2	1:104:A:PHE:H	10	0.24
(1,1121)	1:110:A:VAL:HG23	1:114:A:THR:H	4	0.24
(1,916)	1:82:B:ASN:HB3	1:82:B:ASN:H	4	0.24
(1,915)	1:82:A:ASN:HB3	1:82:A:ASN:H	1	0.24
(1,382)	1:55:B:LYS:HB3	1:57:B:GLN:H	1	0.24
(1,381)	1:55:A:LYS:HB3	1:57:A:GLN:H	1	0.24
(1,350)	1:54:B:ALA:HA	1:55:B:LYS:H	5	0.24
(3,3039)	1:112:A:TYR:HD2	1:109:B:SER:HB2	2	0.23
(3,2906)	1:124:B:LYS:HD2	1:121:B:THR:HA	4	0.23
(3,2906)	1:124:B:LYS:HD2	1:121:B:THR:HA	6	0.23
(3,2905)	1:124:A:LYS:HD2	1:121:A:THR:HA	4	0.23
(3,2824)	1:115:B:LEU:HD23	1:116:B:MET:HG3	3	0.23
(3,2542)	1:102:B:ILE:HD11	1:61:B:GLU:HG3	4	0.23
(3,2541)	1:102:A:ILE:HD11	1:61:A:GLU:HG3	4	0.23
(3,2500)	1:101:B:THR:HG22	1:50:B:PRO:HB3	2	0.23
(3,2499)	1:101:A:THR:HG22	1:50:A:PRO:HB3	2	0.23
(3,2466)	1:100:B:THR:HG22	1:102:B:ILE:HD11	3	0.23
(3,2465)	1:100:A:THR:HG22	1:102:A:ILE:HD11	3	0.23
(3,2450)	1:100:B:THR:HG21	1:129:B:LYS:HE3	5	0.23
(3,2449)	1:100:A:THR:HG21	1:129:A:LYS:HE3	5	0.23
(3,2158)	1:127:B:TYR:HA	1:90:B:LEU:HG	6	0.23
(3,2157)	1:127:A:TYR:HA	1:90:A:LEU:HG	6	0.23
(3,1895)	1:123:A:ARG:HG2	1:50:B:PRO:HB3	5	0.23
(3,1895)	1:123:A:ARG:HG2	1:50:B:PRO:HB3	6	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,1641)	1:115:A:LEU:HD13	1:131:A:GLY:HA3	4	0.23
(3,1539)	1:46:A:ARG:HG2	1:128:B:LEU:HB3	3	0.23
(3,1360)	1:79:B:GLN:HG3	1:86:B:LEU:HB3	3	0.23
(3,1295)	1:58:A:PRO:HG2	1:55:A:LYS:HE2	7	0.23
(3,1280)	1:57:B:GLN:HG2	1:60:B:PRO:HG3	8	0.23
(3,1279)	1:57:A:GLN:HG2	1:60:A:PRO:HG3	8	0.23
(3,1278)	1:57:B:GLN:HG2	1:50:B:PRO:HD2	5	0.23
(3,1277)	1:57:A:GLN:HG2	1:50:A:PRO:HD2	5	0.23
(3,1105)	1:51:A:ALA:HA	1:124:B:LYS:HB3	10	0.23
(3,918)	1:45:B:ILE:HB	1:45:B:ILE:HD11	8	0.23
(3,917)	1:45:A:ILE:HB	1:45:A:ILE:HD11	8	0.23
(3,904)	1:122:B:LEU:HB2	1:49:A:LEU:HB3	3	0.23
(3,862)	1:43:B:VAL:HA	1:138:A:ALA:HB2	2	0.23
(3,750)	1:135:B:MET:HB3	1:136:B:GLU:H	9	0.23
(3,750)	1:135:B:MET:HB3	1:136:B:GLU:H	10	0.23
(3,696)	1:129:B:LYS:HB3	1:128:B:LEU:H	7	0.23
(3,607)	1:134:A:GLY:HA3	1:119:B:MET:H	6	0.23
(3,460)	1:49:B:LEU:HB2	1:122:A:LEU:H	3	0.23
(3,257)	1:81:A:VAL:HA	1:77:A:GLY:H	4	0.23
(3,126)	1:56:B:PRO:HG2	1:57:B:GLN:H	4	0.23
(3,125)	1:56:A:PRO:HG2	1:57:A:GLN:H	4	0.23
(3,112)	1:98:B:LYS:HB3	1:51:A:ALA:H	5	0.23
(1,5762)	1:129:B:LYS:HG2	1:129:B:LYS:HA	8	0.23
(1,5762)	1:129:B:LYS:HG2	1:129:B:LYS:HA	9	0.23
(1,5761)	1:129:A:LYS:HG2	1:129:A:LYS:HA	8	0.23
(1,5761)	1:129:A:LYS:HG2	1:129:A:LYS:HA	9	0.23
(1,5607)	1:51:A:ALA:HB3	1:124:B:LYS:HA	9	0.23
(1,5589)	1:119:A:MET:HG3	1:119:A:MET:HE1	1	0.23
(1,5554)	1:116:B:MET:HE3	1:114:B:THR:HA	9	0.23
(1,5530)	1:115:B:LEU:HD21	1:135:B:MET:HA	2	0.23
(1,5529)	1:115:A:LEU:HD21	1:135:A:MET:HA	2	0.23
(1,5378)	1:110:B:VAL:HB	1:110:B:VAL:HG22	2	0.23
(1,5377)	1:110:A:VAL:HB	1:110:A:VAL:HG22	2	0.23
(1,5260)	1:116:B:MET:HG2	1:116:B:MET:HE3	8	0.23
(1,5259)	1:116:A:MET:HG2	1:116:A:MET:HE3	8	0.23
(1,5106)	1:102:B:ILE:HG23	1:127:B:TYR:HE1	1	0.23
(1,5105)	1:102:A:ILE:HG23	1:127:A:TYR:HE1	1	0.23
(1,4871)	1:99:A:GLU:HA	1:60:A:PRO:HB3	2	0.23
(1,4861)	1:98:A:LYS:HD3	1:127:A:TYR:HB2	9	0.23
(1,4770)	1:94:B:THR:HG22	1:102:B:ILE:HG13	8	0.23
(1,4769)	1:94:A:THR:HG22	1:102:A:ILE:HG13	8	0.23
(1,4760)	1:94:B:THR:HG23	1:99:B:GLU:HG3	6	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4759)	1:94:A:THR:HG23	1:99:A:GLU:HG3	6	0.23
(1,4704)	1:108:B:LYS:HA	1:115:B:LEU:HD13	2	0.23
(1,4552)	1:87:B:THR:HB	1:87:B:THR:HG21	5	0.23
(1,4552)	1:87:B:THR:HB	1:87:B:THR:HG22	6	0.23
(1,4552)	1:87:B:THR:HB	1:87:B:THR:HG21	9	0.23
(1,4551)	1:87:A:THR:HB	1:87:A:THR:HG21	5	0.23
(1,4551)	1:87:A:THR:HB	1:87:A:THR:HG22	6	0.23
(1,4551)	1:87:A:THR:HB	1:87:A:THR:HG21	9	0.23
(1,4326)	1:127:B:TYR:HA	1:90:B:LEU:HG	6	0.23
(1,4325)	1:127:A:TYR:HA	1:90:A:LEU:HG	6	0.23
(1,4078)	1:105:B:GLN:HG3	1:137:B:GLY:HA3	9	0.23
(1,4077)	1:105:A:GLN:HG3	1:137:A:GLY:HA3	9	0.23
(1,4000)	1:72:B:LYS:HG2	1:114:B:THR:HG21	9	0.23
(1,3508)	1:65:B:PHE:HB2	1:140:B:LYS:HB2	3	0.23
(1,3507)	1:65:A:PHE:HB2	1:140:A:LYS:HB2	3	0.23
(1,3462)	1:64:B:VAL:HB	1:102:B:ILE:HD11	5	0.23
(1,3461)	1:64:A:VAL:HB	1:102:A:ILE:HD11	5	0.23
(1,3354)	1:122:B:LEU:HG	1:119:B:MET:HB2	9	0.23
(1,3353)	1:122:A:LEU:HG	1:119:A:MET:HB2	5	0.23
(1,3353)	1:122:A:LEU:HG	1:119:A:MET:HB2	9	0.23
(1,3344)	1:129:B:LYS:HB2	1:101:B:THR:HG23	5	0.23
(1,3343)	1:129:A:LYS:HB2	1:101:A:THR:HG23	5	0.23
(1,3138)	1:98:B:LYS:HE3	1:125:B:ALA:HB2	9	0.23
(1,3137)	1:98:A:LYS:HE3	1:125:A:ALA:HB2	9	0.23
(1,2974)	1:56:B:PRO:HD2	1:50:B:PRO:HD2	2	0.23
(1,2973)	1:56:A:PRO:HD2	1:50:A:PRO:HD2	2	0.23
(1,2783)	1:70:A:ALA:HB3	1:70:A:ALA:HA	9	0.23
(1,2560)	1:45:B:ILE:HG22	1:54:A:ALA:HB2	6	0.23
(1,2352)	1:85:B:GLN:HE22	1:82:B:ASN:HD21	7	0.23
(1,2351)	1:85:A:GLN:HE22	1:82:A:ASN:HD21	7	0.23
(1,2272)	1:139:B:ALA:HB2	1:139:B:ALA:H	5	0.23
(1,2271)	1:139:A:ALA:HB2	1:139:A:ALA:H	5	0.23
(1,2271)	1:139:A:ALA:HB1	1:139:A:ALA:H	7	0.23
(1,2211)	1:45:A:ILE:H	1:135:B:MET:H	1	0.23
(1,2044)	1:98:B:LYS:HD3	1:126:B:GLY:H	9	0.23
(1,1964)	1:121:B:THR:HG23	1:121:B:THR:H	7	0.23
(1,1743)	1:139:A:ALA:HB2	1:140:A:LYS:H	3	0.23
(1,1526)	1:66:B:LEU:HB2	1:104:B:PHE:H	1	0.23
(1,1525)	1:66:A:LEU:HB2	1:104:A:PHE:H	1	0.23
(1,1525)	1:66:A:LEU:HB2	1:104:A:PHE:H	3	0.23
(1,1197)	1:92:A:GLN:HG2	1:92:A:GLN:H	8	0.23
(1,1070)	1:90:B:LEU:HB3	1:88:B:SER:H	3	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1069)	1:90:A:LEU:HB3	1:88:A:SER:H	3	0.23
(1,916)	1:82:B:ASN:HB3	1:82:B:ASN:H	1	0.23
(1,350)	1:54:B:ALA:HA	1:55:B:LYS:H	1	0.23
(1,349)	1:54:A:ALA:HA	1:55:A:LYS:H	1	0.23
(1,2)	1:57:B:GLN:HG3	1:57:B:GLN:H	4	0.23
(1,1)	1:57:A:GLN:HG3	1:57:A:GLN:H	4	0.23
(3,3023)	1:129:A:LYS:HA	1:97:A:ASN:HB2	1	0.22
(3,2974)	1:130:B:VAL:HB	1:119:B:MET:HE2	6	0.22
(3,2973)	1:130:A:VAL:HB	1:119:A:MET:HE2	6	0.22
(3,2867)	1:121:A:THR:HA	1:121:A:THR:HG21	1	0.22
(3,2556)	1:103:B:PHE:HA	1:45:A:ILE:HG21	1	0.22
(3,2555)	1:103:A:PHE:HA	1:45:B:ILE:HG21	1	0.22
(3,2555)	1:103:A:PHE:HA	1:45:B:ILE:HG23	4	0.22
(3,2499)	1:101:A:THR:HG22	1:50:A:PRO:HB3	10	0.22
(3,2442)	1:94:B:THR:HG23	1:100:B:THR:HB	1	0.22
(3,2352)	1:98:B:LYS:HG3	1:125:B:ALA:HB2	6	0.22
(3,2352)	1:98:B:LYS:HG3	1:125:B:ALA:HB3	10	0.22
(3,2351)	1:98:A:LYS:HG3	1:125:A:ALA:HB2	6	0.22
(3,2351)	1:98:A:LYS:HG3	1:125:A:ALA:HB3	10	0.22
(3,2318)	1:123:B:ARG:HB2	1:124:B:LYS:HG3	2	0.22
(3,2317)	1:123:A:ARG:HB2	1:124:A:LYS:HG3	2	0.22
(3,2244)	1:60:B:PRO:HB3	1:94:B:THR:HG22	2	0.22
(3,2243)	1:60:A:PRO:HB3	1:94:A:THR:HG22	2	0.22
(3,1892)	1:74:B:LEU:HB3	1:86:B:LEU:HB3	1	0.22
(3,1891)	1:74:A:LEU:HB3	1:86:A:LEU:HB3	1	0.22
(3,1888)	1:74:B:LEU:HB2	1:83:B:ALA:HB2	4	0.22
(3,1887)	1:74:A:LEU:HB2	1:83:A:ALA:HB2	4	0.22
(3,1850)	1:136:B:GLU:HB2	1:140:B:LYS:HE3	2	0.22
(3,1849)	1:136:A:GLU:HB2	1:140:A:LYS:HE3	2	0.22
(3,1768)	1:70:B:ALA:HA	1:74:B:LEU:HG	6	0.22
(3,1767)	1:70:A:ALA:HA	1:74:A:LEU:HG	6	0.22
(3,1743)	1:69:A:LYS:HE2	1:74:A:LEU:HA	1	0.22
(3,1642)	1:115:B:LEU:HD13	1:131:B:GLY:HA3	4	0.22
(3,1552)	1:64:B:VAL:HA	1:79:B:GLN:HG2	8	0.22
(3,1551)	1:64:A:VAL:HA	1:79:A:GLN:HG2	8	0.22
(3,1490)	1:129:B:LYS:HG2	1:46:A:ARG:HB3	9	0.22
(3,1489)	1:129:A:LYS:HG2	1:46:B:ARG:HB3	9	0.22
(3,1359)	1:79:A:GLN:HG3	1:86:A:LEU:HB3	3	0.22
(3,1296)	1:58:B:PRO:HG2	1:55:B:LYS:HE2	7	0.22
(3,952)	1:46:B:ARG:HB2	1:48:A:ASP:HB2	1	0.22
(3,750)	1:135:B:MET:HB3	1:136:B:GLU:H	4	0.22
(3,749)	1:135:A:MET:HB3	1:136:A:GLU:H	4	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,749)	1:135:A:MET:HB3	1:136:A:GLU:H	10	0.22
(3,736)	1:132:B:LEU:HG	1:134:B:GLY:H	8	0.22
(3,735)	1:132:A:LEU:HG	1:134:A:GLY:H	8	0.22
(3,695)	1:129:A:LYS:HB3	1:128:A:LEU:H	7	0.22
(3,620)	1:124:B:LYS:HE2	1:120:B:ASP:H	9	0.22
(3,619)	1:124:A:LYS:HE3	1:120:A:ASP:H	5	0.22
(3,619)	1:124:A:LYS:HE2	1:120:A:ASP:H	9	0.22
(3,318)	1:96:B:ALA:HA	1:88:B:SER:H	8	0.22
(3,317)	1:96:A:ALA:HA	1:88:A:SER:H	8	0.22
(3,111)	1:98:A:LYS:HB3	1:51:B:ALA:H	10	0.22
(1,5920)	1:104:B:PHE:HD1	1:115:B:LEU:HD12	9	0.22
(1,5919)	1:104:A:PHE:HD1	1:115:A:LEU:HD12	9	0.22
(1,5590)	1:119:B:MET:HG3	1:119:B:MET:HE1	1	0.22
(1,5590)	1:119:B:MET:HG3	1:119:B:MET:HE2	3	0.22
(1,5538)	1:115:B:LEU:HD23	1:116:B:MET:HE1	2	0.22
(1,5537)	1:115:A:LEU:HD23	1:116:A:MET:HE1	2	0.22
(1,5520)	1:115:B:LEU:HG	1:116:B:MET:HE3	5	0.22
(1,5519)	1:115:A:LEU:HG	1:116:A:MET:HE3	5	0.22
(1,5416)	1:110:B:VAL:HG11	1:70:B:ALA:HB1	7	0.22
(1,5415)	1:110:A:VAL:HG11	1:70:A:ALA:HB1	7	0.22
(1,5376)	1:110:B:VAL:HB	1:112:B:TYR:HB3	7	0.22
(1,5375)	1:110:A:VAL:HB	1:112:A:TYR:HB3	7	0.22
(1,5152)	1:102:B:ILE:HG22	1:102:B:ILE:HD12	4	0.22
(1,5152)	1:102:B:ILE:HG23	1:102:B:ILE:HD12	8	0.22
(1,5151)	1:102:A:ILE:HG22	1:102:A:ILE:HD12	4	0.22
(1,5151)	1:102:A:ILE:HG23	1:102:A:ILE:HD12	8	0.22
(1,5149)	1:100:A:THR:HG21	1:102:A:ILE:HD11	8	0.22
(1,4872)	1:99:B:GLU:HA	1:60:B:PRO:HB3	2	0.22
(1,4862)	1:98:B:LYS:HD3	1:127:B:TYR:HB2	9	0.22
(1,4703)	1:108:A:LYS:HA	1:115:A:LEU:HD13	2	0.22
(1,4568)	1:87:B:THR:HG22	1:124:B:LYS:HD2	7	0.22
(1,4567)	1:87:A:THR:HG22	1:124:A:LYS:HD2	7	0.22
(1,4536)	1:87:B:THR:HA	1:90:B:LEU:HG	8	0.22
(1,4535)	1:87:A:THR:HA	1:90:A:LEU:HG	8	0.22
(1,4534)	1:87:B:THR:HA	1:87:B:THR:HG22	1	0.22
(1,4533)	1:87:A:THR:HA	1:87:A:THR:HG22	1	0.22
(1,4182)	1:98:B:LYS:HE2	1:96:B:ALA:HA	4	0.22
(1,4181)	1:98:A:LYS:HE2	1:96:A:ALA:HA	4	0.22
(1,4112)	1:74:B:LEU:HA	1:110:B:VAL:HG13	6	0.22
(1,4111)	1:74:A:LEU:HA	1:110:A:VAL:HG13	6	0.22
(1,4052)	1:93:B:ARG:HB3	1:64:B:VAL:HA	8	0.22
(1,4051)	1:93:A:ARG:HB3	1:64:A:VAL:HA	8	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4008)	1:72:B:LYS:HD3	1:114:B:THR:HG22	3	0.22
(1,3999)	1:72:A:LYS:HG2	1:114:A:THR:HG21	9	0.22
(1,3722)	1:67:B:SER:HB3	1:69:B:LYS:HD2	5	0.22
(1,3721)	1:67:A:SER:HB3	1:69:A:LYS:HD2	5	0.22
(1,3612)	1:115:B:LEU:HD12	1:106:B:ALA:HB1	1	0.22
(1,3611)	1:115:A:LEU:HD12	1:106:A:ALA:HB1	1	0.22
(1,3540)	1:66:B:LEU:HB2	1:102:B:ILE:HG23	9	0.22
(1,3539)	1:66:A:LEU:HB2	1:102:A:ILE:HG23	9	0.22
(1,3273)	1:61:A:GLU:HG2	1:62:A:LYS:HG2	7	0.22
(1,3222)	1:122:B:LEU:HA	1:125:B:ALA:HB2	3	0.22
(1,3221)	1:122:A:LEU:HA	1:125:A:ALA:HB2	3	0.22
(1,2920)	1:56:B:PRO:HA	1:45:A:ILE:HA	9	0.22
(1,2272)	1:139:B:ALA:HB1	1:139:B:ALA:H	7	0.22
(1,2043)	1:98:A:LYS:HD3	1:126:A:GLY:H	9	0.22
(1,1963)	1:121:A:THR:HG23	1:121:A:THR:H	7	0.22
(1,1526)	1:66:B:LEU:HB2	1:104:B:PHE:H	3	0.22
(1,1526)	1:66:B:LEU:HB2	1:104:B:PHE:H	5	0.22
(1,1525)	1:66:A:LEU:HB2	1:104:A:PHE:H	5	0.22
(1,1198)	1:92:B:GLN:HG2	1:92:B:GLN:H	8	0.22
(1,964)	1:83:B:ALA:HB1	1:84:B:ASP:H	1	0.22
(1,460)	1:61:B:GLU:HG3	1:62:B:LYS:H	8	0.22
(1,459)	1:61:A:GLU:HG3	1:62:A:LYS:H	8	0.22
(1,254)	1:45:B:ILE:HG22	1:47:B:VAL:H	2	0.22
(1,253)	1:45:A:ILE:HG22	1:47:A:VAL:H	2	0.22
(3,3074)	1:104:B:PHE:HD1	1:65:B:PHE:HB2	6	0.21
(3,3073)	1:104:A:PHE:HD1	1:65:A:PHE:HB2	6	0.21
(3,3040)	1:112:B:TYR:HD2	1:109:A:SER:HB2	2	0.21
(3,3024)	1:129:B:LYS:HA	1:97:B:ASN:HB2	1	0.21
(3,2868)	1:121:B:THR:HA	1:121:B:THR:HG21	1	0.21
(3,2692)	1:108:B:LYS:HE3	1:109:B:SER:HB3	8	0.21
(3,2556)	1:103:B:PHE:HA	1:45:A:ILE:HG23	4	0.21
(3,2500)	1:101:B:THR:HG22	1:50:B:PRO:HB3	10	0.21
(3,2441)	1:94:A:THR:HG23	1:100:A:THR:HB	1	0.21
(3,2318)	1:123:B:ARG:HB2	1:124:B:LYS:HG3	6	0.21
(3,2317)	1:123:A:ARG:HB2	1:124:A:LYS:HG3	6	0.21
(3,2175)	1:108:A:LYS:HA	1:139:A:ALA:HB1	8	0.21
(3,1744)	1:69:B:LYS:HE2	1:74:B:LEU:HA	1	0.21
(3,1554)	1:64:B:VAL:HA	1:61:B:GLU:HG2	4	0.21
(3,1553)	1:64:A:VAL:HA	1:61:A:GLU:HG2	4	0.21
(3,1068)	1:50:B:PRO:HA	1:54:B:ALA:HB2	1	0.21
(3,1067)	1:50:A:PRO:HA	1:54:A:ALA:HB2	1	0.21
(3,951)	1:46:A:ARG:HB2	1:48:B:ASP:HB2	1	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,908)	1:45:B:ILE:HD12	1:104:A:PHE:HD2	3	0.21
(3,620)	1:124:B:LYS:HE3	1:120:B:ASP:H	5	0.21
(3,608)	1:134:B:GLY:HA3	1:119:A:MET:H	2	0.21
(3,480)	1:115:B:LEU:HD11	1:104:B:PHE:H	3	0.21
(3,479)	1:115:A:LEU:HD11	1:104:A:PHE:H	3	0.21
(3,383)	1:98:A:LYS:H	1:93:A:ARG:H	3	0.21
(3,78)	1:46:B:ARG:HD2	1:47:B:VAL:H	6	0.21
(3,77)	1:46:A:ARG:HD2	1:47:A:VAL:H	6	0.21
(3,77)	1:46:A:ARG:HD2	1:47:A:VAL:H	7	0.21
(1,5830)	1:135:B:MET:HE2	1:108:B:LYS:HA	2	0.21
(1,5829)	1:135:A:MET:HE2	1:108:A:LYS:HA	2	0.21
(1,5690)	1:126:B:GLY:HA3	1:98:B:LYS:HD3	3	0.21
(1,5689)	1:126:A:GLY:HA3	1:98:A:LYS:HD3	3	0.21
(1,5662)	1:125:B:ALA:HA	1:125:B:ALA:HB1	4	0.21
(1,5662)	1:125:B:ALA:HA	1:125:B:ALA:HB2	5	0.21
(1,5662)	1:125:B:ALA:HA	1:125:B:ALA:HB1	6	0.21
(1,5661)	1:125:A:ALA:HA	1:125:A:ALA:HB1	4	0.21
(1,5661)	1:125:A:ALA:HA	1:125:A:ALA:HB1	6	0.21
(1,5644)	1:120:B:ASP:HA	1:123:B:ARG:HD3	5	0.21
(1,5643)	1:120:A:ASP:HA	1:123:A:ARG:HD3	5	0.21
(1,5608)	1:51:B:ALA:HB3	1:124:A:LYS:HA	9	0.21
(1,5589)	1:119:A:MET:HG3	1:119:A:MET:HE2	3	0.21
(1,5472)	1:112:B:TYR:HB3	1:115:B:LEU:HD23	8	0.21
(1,5471)	1:112:A:TYR:HB3	1:115:A:LEU:HD23	8	0.21
(1,5394)	1:110:B:VAL:HG23	1:112:B:TYR:HB3	8	0.21
(1,5393)	1:110:A:VAL:HG23	1:112:A:TYR:HB3	8	0.21
(1,5380)	1:110:B:VAL:HB	1:110:B:VAL:HG12	4	0.21
(1,5380)	1:110:B:VAL:HB	1:110:B:VAL:HG11	10	0.21
(1,5379)	1:110:A:VAL:HB	1:110:A:VAL:HG13	3	0.21
(1,5379)	1:110:A:VAL:HB	1:110:A:VAL:HG12	4	0.21
(1,5379)	1:110:A:VAL:HB	1:110:A:VAL:HG11	10	0.21
(1,5152)	1:102:B:ILE:HG22	1:102:B:ILE:HD12	3	0.21
(1,5152)	1:102:B:ILE:HG23	1:102:B:ILE:HD13	6	0.21
(1,5152)	1:102:B:ILE:HG23	1:102:B:ILE:HD12	10	0.21
(1,5151)	1:102:A:ILE:HG22	1:102:A:ILE:HD12	3	0.21
(1,5151)	1:102:A:ILE:HG23	1:102:A:ILE:HD13	6	0.21
(1,5151)	1:102:A:ILE:HG23	1:102:A:ILE:HD12	10	0.21
(1,5150)	1:100:B:THR:HG21	1:102:B:ILE:HD12	7	0.21
(1,5150)	1:100:B:THR:HG21	1:102:B:ILE:HD11	8	0.21
(1,5149)	1:100:A:THR:HG21	1:102:A:ILE:HD12	7	0.21
(1,4912)	1:100:B:THR:HA	1:129:B:LYS:HD2	9	0.21
(1,4911)	1:100:A:THR:HA	1:129:A:LYS:HD2	9	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4682)	1:91:B:ASP:HA	1:96:B:ALA:HB3	10	0.21
(1,4681)	1:91:A:ASP:HA	1:96:A:ALA:HB3	10	0.21
(1,4636)	1:90:B:LEU:HB2	1:64:B:VAL:HB	10	0.21
(1,4635)	1:90:A:LEU:HB2	1:64:A:VAL:HB	10	0.21
(1,4573)	1:87:A:THR:HG23	1:90:A:LEU:HG	10	0.21
(1,4428)	1:84:B:ASP:HB2	1:85:B:GLN:HG2	4	0.21
(1,4358)	1:82:B:ASN:HB2	1:83:B:ALA:HB2	9	0.21
(1,4007)	1:72:A:LYS:HD3	1:114:A:THR:HG22	3	0.21
(1,3966)	1:72:B:LYS:HA	1:110:B:VAL:HG11	10	0.21
(1,3856)	1:69:B:LYS:HD3	1:65:B:PHE:HB2	10	0.21
(1,3838)	1:69:B:LYS:HG3	1:115:B:LEU:HD11	7	0.21
(1,3837)	1:69:A:LYS:HG3	1:115:A:LEU:HD11	7	0.21
(1,3598)	1:115:B:LEU:HD13	1:119:B:MET:HG2	5	0.21
(1,3598)	1:115:B:LEU:HD12	1:119:B:MET:HG2	8	0.21
(1,3597)	1:115:A:LEU:HD12	1:119:A:MET:HG2	8	0.21
(1,3540)	1:66:B:LEU:HB2	1:102:B:ILE:HG23	3	0.21
(1,3539)	1:66:A:LEU:HB2	1:102:A:ILE:HG23	3	0.21
(1,3460)	1:64:B:VAL:HB	1:102:B:ILE:HG22	2	0.21
(1,3459)	1:64:A:VAL:HB	1:102:A:ILE:HG22	2	0.21
(1,3274)	1:61:B:GLU:HG2	1:62:B:LYS:HG2	7	0.21
(1,3248)	1:99:B:GLU:HG2	1:99:B:GLU:HB2	3	0.21
(1,3248)	1:99:B:GLU:HG2	1:99:B:GLU:HB2	6	0.21
(1,3248)	1:99:B:GLU:HG2	1:99:B:GLU:HB2	8	0.21
(1,3248)	1:99:B:GLU:HG2	1:99:B:GLU:HB2	9	0.21
(1,3247)	1:99:A:GLU:HG2	1:99:A:GLU:HB2	3	0.21
(1,3247)	1:99:A:GLU:HG2	1:99:A:GLU:HB2	6	0.21
(1,3247)	1:99:A:GLU:HG2	1:99:A:GLU:HB2	8	0.21
(1,2572)	1:46:B:ARG:HB2	1:48:A:ASP:HB3	6	0.21
(1,1842)	1:118:B:VAL:HG12	1:117:B:SER:H	1	0.21
(1,1842)	1:118:B:VAL:HG13	1:117:B:SER:H	2	0.21
(1,1842)	1:118:B:VAL:HG11	1:117:B:SER:H	4	0.21
(1,1841)	1:118:A:VAL:HG12	1:117:A:SER:H	1	0.21
(1,1841)	1:118:A:VAL:HG13	1:117:A:SER:H	2	0.21
(1,1841)	1:118:A:VAL:HG11	1:117:A:SER:H	4	0.21
(1,1474)	1:122:B:LEU:HD13	1:122:B:LEU:H	8	0.21
(1,1474)	1:122:B:LEU:HD13	1:122:B:LEU:H	9	0.21
(1,1473)	1:122:A:LEU:HD13	1:122:A:LEU:H	8	0.21
(1,1473)	1:122:A:LEU:HD13	1:122:A:LEU:H	9	0.21
(1,963)	1:83:A:ALA:HB1	1:84:A:ASP:H	1	0.21
(1,802)	1:74:B:LEU:HB2	1:75:B:TYR:H	6	0.21
(1,350)	1:54:B:ALA:HA	1:55:B:LYS:H	6	0.21
(1,349)	1:54:A:ALA:HA	1:55:A:LYS:H	6	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,254)	1:45:B:ILE:HG22	1:47:B:VAL:H	9	0.21
(1,253)	1:45:A:ILE:HG22	1:47:A:VAL:H	9	0.21
(1,61)	1:85:A:GLN:HB3	1:82:A:ASN:H	9	0.21
(3,2832)	1:112:B:TYR:HD1	1:116:B:MET:HE1	8	0.2
(3,2831)	1:112:A:TYR:HD1	1:116:A:MET:HE1	8	0.2
(3,2691)	1:108:A:LYS:HE3	1:109:A:SER:HB3	8	0.2
(3,2642)	1:116:B:MET:HG2	1:45:B:ILE:HD12	3	0.2
(3,2641)	1:116:A:MET:HG2	1:45:A:ILE:HD12	3	0.2
(3,2466)	1:100:B:THR:HG23	1:102:B:ILE:HD11	4	0.2
(3,2465)	1:100:A:THR:HG23	1:102:A:ILE:HD11	4	0.2
(3,2442)	1:94:B:THR:HG21	1:100:B:THR:HB	10	0.2
(3,2176)	1:108:B:LYS:HA	1:139:B:ALA:HB1	8	0.2
(3,2160)	1:90:B:LEU:HG	1:98:B:LYS:HE3	5	0.2
(3,2159)	1:90:A:LEU:HG	1:98:A:LYS:HE3	5	0.2
(3,2059)	1:119:A:MET:HG2	1:49:B:LEU:HG	2	0.2
(3,2008)	1:82:B:ASN:HB2	1:85:B:GLN:HG2	9	0.2
(3,2007)	1:82:A:ASN:HB2	1:85:A:GLN:HG2	9	0.2
(3,1998)	1:81:B:VAL:HA	1:66:B:LEU:HB2	5	0.2
(3,1997)	1:81:A:VAL:HA	1:66:A:LEU:HB2	5	0.2
(3,1894)	1:123:B:ARG:HG2	1:124:B:LYS:HE2	9	0.2
(3,1888)	1:74:B:LEU:HB2	1:86:B:LEU:HB3	6	0.2
(3,1887)	1:74:A:LEU:HB2	1:86:A:LEU:HB3	6	0.2
(3,1672)	1:67:B:SER:HB2	1:69:B:LYS:HE3	1	0.2
(3,1553)	1:64:A:VAL:HA	1:61:A:GLU:HG2	5	0.2
(3,1386)	1:60:B:PRO:HG2	1:129:B:LYS:HB3	2	0.2
(3,1386)	1:60:B:PRO:HG2	1:129:B:LYS:HB3	3	0.2
(3,1385)	1:60:A:PRO:HG2	1:129:A:LYS:HB3	2	0.2
(3,1385)	1:60:A:PRO:HG2	1:129:A:LYS:HB3	3	0.2
(3,1360)	1:79:B:GLN:HG3	1:86:B:LEU:HB3	1	0.2
(3,1296)	1:58:B:PRO:HG2	1:55:B:LYS:HE2	1	0.2
(3,1295)	1:58:A:PRO:HG2	1:55:A:LYS:HE2	1	0.2
(3,1295)	1:58:A:PRO:HG2	1:55:A:LYS:HE3	3	0.2
(3,903)	1:122:A:LEU:HB2	1:49:B:LEU:HB3	3	0.2
(3,734)	1:120:B:ASP:HA	1:134:A:GLY:H	3	0.2
(3,696)	1:129:B:LYS:HB3	1:128:B:LEU:H	4	0.2
(3,695)	1:129:A:LYS:HB3	1:128:A:LEU:H	4	0.2
(3,384)	1:98:B:LYS:H	1:93:B:ARG:H	1	0.2
(3,384)	1:98:B:LYS:H	1:93:B:ARG:H	3	0.2
(3,383)	1:98:A:LYS:H	1:93:A:ARG:H	1	0.2
(3,257)	1:81:A:VAL:HA	1:77:A:GLY:H	10	0.2
(3,78)	1:46:B:ARG:HD2	1:47:B:VAL:H	7	0.2
(1,5752)	1:86:B:LEU:HG	1:102:B:ILE:HD13	7	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5751)	1:86:A:LEU:HG	1:102:A:ILE:HD13	7	0.2
(1,5662)	1:125:B:ALA:HA	1:125:B:ALA:HB2	8	0.2
(1,5662)	1:125:B:ALA:HA	1:125:B:ALA:HB1	9	0.2
(1,5661)	1:125:A:ALA:HA	1:125:A:ALA:HB2	5	0.2
(1,5661)	1:125:A:ALA:HA	1:125:A:ALA:HB2	8	0.2
(1,5661)	1:125:A:ALA:HA	1:125:A:ALA:HB1	9	0.2
(1,5590)	1:119:B:MET:HG3	1:119:B:MET:HE2	6	0.2
(1,5589)	1:119:A:MET:HG3	1:119:A:MET:HE2	6	0.2
(1,5520)	1:115:B:LEU:HG	1:116:B:MET:HE3	6	0.2
(1,5519)	1:115:A:LEU:HG	1:116:A:MET:HE3	6	0.2
(1,5380)	1:110:B:VAL:HB	1:110:B:VAL:HG11	1	0.2
(1,5380)	1:110:B:VAL:HB	1:110:B:VAL:HG12	2	0.2
(1,5380)	1:110:B:VAL:HB	1:110:B:VAL:HG13	3	0.2
(1,5380)	1:110:B:VAL:HB	1:110:B:VAL:HG13	5	0.2
(1,5380)	1:110:B:VAL:HB	1:110:B:VAL:HG12	6	0.2
(1,5380)	1:110:B:VAL:HB	1:110:B:VAL:HG12	7	0.2
(1,5379)	1:110:A:VAL:HB	1:110:A:VAL:HG11	1	0.2
(1,5379)	1:110:A:VAL:HB	1:110:A:VAL:HG12	2	0.2
(1,5379)	1:110:A:VAL:HB	1:110:A:VAL:HG13	5	0.2
(1,5379)	1:110:A:VAL:HB	1:110:A:VAL:HG12	6	0.2
(1,5379)	1:110:A:VAL:HB	1:110:A:VAL:HG12	7	0.2
(1,5152)	1:102:B:ILE:HG21	1:102:B:ILE:HD13	7	0.2
(1,5152)	1:102:B:ILE:HG22	1:102:B:ILE:HD13	9	0.2
(1,5151)	1:102:A:ILE:HG23	1:102:A:ILE:HD11	1	0.2
(1,5151)	1:102:A:ILE:HG21	1:102:A:ILE:HD13	7	0.2
(1,5151)	1:102:A:ILE:HG22	1:102:A:ILE:HD13	9	0.2
(1,4704)	1:108:B:LYS:HA	1:115:B:LEU:HD13	9	0.2
(1,4703)	1:108:A:LYS:HA	1:115:A:LEU:HD13	9	0.2
(1,4574)	1:87:B:THR:HG23	1:90:B:LEU:HG	10	0.2
(1,4566)	1:87:B:THR:HG21	1:125:B:ALA:HB2	8	0.2
(1,4565)	1:87:A:THR:HG21	1:125:A:ALA:HB2	8	0.2
(1,4534)	1:87:B:THR:HA	1:87:B:THR:HG23	3	0.2
(1,4427)	1:84:A:ASP:HB2	1:85:A:GLN:HG2	4	0.2
(1,4357)	1:82:A:ASN:HB2	1:83:A:ALA:HB2	9	0.2
(1,4112)	1:74:B:LEU:HA	1:110:B:VAL:HG12	1	0.2
(1,4112)	1:74:B:LEU:HA	1:110:B:VAL:HG13	7	0.2
(1,4111)	1:74:A:LEU:HA	1:110:A:VAL:HG12	1	0.2
(1,4111)	1:74:A:LEU:HA	1:110:A:VAL:HG13	7	0.2
(1,3972)	1:72:B:LYS:HB3	1:72:B:LYS:HD2	5	0.2
(1,3971)	1:72:A:LYS:HB3	1:72:A:LYS:HD2	5	0.2
(1,3965)	1:72:A:LYS:HA	1:110:A:VAL:HG11	10	0.2
(1,3855)	1:69:A:LYS:HD3	1:65:A:PHE:HB2	10	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3676)	1:67:B:SER:HB2	1:105:B:GLN:HG2	4	0.2
(1,3675)	1:67:A:SER:HB2	1:105:A:GLN:HG2	4	0.2
(1,3610)	1:115:B:LEU:HD12	1:110:B:VAL:HG23	6	0.2
(1,3609)	1:115:A:LEU:HD12	1:110:A:VAL:HG23	6	0.2
(1,3597)	1:115:A:LEU:HD13	1:119:A:MET:HG2	5	0.2
(1,3540)	1:66:B:LEU:HB2	1:102:B:ILE:HG23	2	0.2
(1,3539)	1:66:A:LEU:HB2	1:102:A:ILE:HG23	2	0.2
(1,3460)	1:64:B:VAL:HB	1:102:B:ILE:HG22	5	0.2
(1,3459)	1:64:A:VAL:HB	1:102:A:ILE:HG22	5	0.2
(1,3354)	1:122:B:LEU:HG	1:119:B:MET:HB2	3	0.2
(1,3353)	1:122:A:LEU:HG	1:119:A:MET:HB2	3	0.2
(1,3248)	1:99:B:GLU:HG2	1:99:B:GLU:HB2	2	0.2
(1,3248)	1:99:B:GLU:HG2	1:99:B:GLU:HB2	4	0.2
(1,3248)	1:99:B:GLU:HG2	1:99:B:GLU:HB2	5	0.2
(1,3248)	1:99:B:GLU:HG2	1:99:B:GLU:HB2	7	0.2
(1,3248)	1:99:B:GLU:HG2	1:99:B:GLU:HB2	10	0.2
(1,3247)	1:99:A:GLU:HG2	1:99:A:GLU:HB2	2	0.2
(1,3247)	1:99:A:GLU:HG2	1:99:A:GLU:HB2	4	0.2
(1,3247)	1:99:A:GLU:HG2	1:99:A:GLU:HB2	5	0.2
(1,3247)	1:99:A:GLU:HG2	1:99:A:GLU:HB2	7	0.2
(1,3247)	1:99:A:GLU:HG2	1:99:A:GLU:HB2	9	0.2
(1,3247)	1:99:A:GLU:HG2	1:99:A:GLU:HB2	10	0.2
(1,2466)	1:88:B:SER:HA	1:87:B:THR:HG23	2	0.2
(1,2466)	1:88:B:SER:HA	1:87:B:THR:HG22	6	0.2
(1,2466)	1:88:B:SER:HA	1:87:B:THR:HG23	9	0.2
(1,2465)	1:88:A:SER:HA	1:87:A:THR:HG22	6	0.2
(1,2465)	1:88:A:SER:HA	1:87:A:THR:HG23	9	0.2
(1,1842)	1:118:B:VAL:HG12	1:117:B:SER:H	5	0.2
(1,1841)	1:118:A:VAL:HG12	1:117:A:SER:H	5	0.2
(1,1650)	1:110:B:VAL:HG23	1:115:B:LEU:H	1	0.2
(1,1649)	1:110:A:VAL:HG23	1:115:A:LEU:H	1	0.2
(1,1404)	1:99:B:GLU:HG2	1:99:B:GLU:H	10	0.2
(1,1403)	1:99:A:GLU:HG2	1:99:A:GLU:H	10	0.2
(1,824)	1:79:B:GLN:HB2	1:76:B:VAL:H	8	0.2
(1,823)	1:79:A:GLN:HB2	1:76:A:VAL:H	8	0.2
(1,801)	1:74:A:LEU:HB2	1:75:A:TYR:H	6	0.2
(1,350)	1:54:B:ALA:HA	1:55:B:LYS:H	7	0.2
(1,349)	1:54:A:ALA:HA	1:55:A:LYS:H	7	0.2
(1,62)	1:85:B:GLN:HB3	1:82:B:ASN:H	9	0.2
(1,2)	1:57:B:GLN:HG3	1:57:B:GLN:H	10	0.2
(3,3006)	1:106:B:ALA:HB1	1:135:B:MET:HG2	7	0.19
(3,3005)	1:106:A:ALA:HB1	1:135:A:MET:HG2	7	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,2974)	1:130:B:VAL:HB	1:119:B:MET:HE3	2	0.19
(3,2973)	1:130:A:VAL:HB	1:119:A:MET:HE3	2	0.19
(3,2867)	1:121:A:THR:HA	1:121:A:THR:HG23	3	0.19
(3,2832)	1:116:B:MET:HE3	1:112:A:TYR:HD1	6	0.19
(3,2824)	1:115:B:LEU:HD21	1:116:B:MET:HG3	6	0.19
(3,2823)	1:115:A:LEU:HD21	1:116:A:MET:HG3	6	0.19
(3,2822)	1:113:B:GLU:HG2	1:115:B:LEU:HD21	1	0.19
(3,2821)	1:113:A:GLU:HG2	1:115:A:LEU:HD21	1	0.19
(3,2738)	1:108:B:LYS:HD3	1:110:B:VAL:HG11	4	0.19
(3,2737)	1:108:A:LYS:HD3	1:110:A:VAL:HG11	4	0.19
(3,2441)	1:94:A:THR:HG21	1:100:A:THR:HB	10	0.19
(3,2324)	1:127:B:TYR:HE2	1:98:B:LYS:HG2	8	0.19
(3,2323)	1:127:A:TYR:HE2	1:98:A:LYS:HG2	8	0.19
(3,2060)	1:119:B:MET:HG2	1:49:A:LEU:HG	2	0.19
(3,1893)	1:123:A:ARG:HG2	1:124:A:LYS:HE2	9	0.19
(3,1892)	1:74:B:LEU:HB3	1:86:B:LEU:HB3	10	0.19
(3,1891)	1:74:A:LEU:HB3	1:86:A:LEU:HB3	10	0.19
(3,1888)	1:74:B:LEU:HB2	1:83:B:ALA:HB2	10	0.19
(3,1887)	1:74:A:LEU:HB2	1:83:A:ALA:HB2	10	0.19
(3,1671)	1:67:A:SER:HB2	1:69:A:LYS:HE3	1	0.19
(3,1554)	1:64:B:VAL:HA	1:61:B:GLU:HG2	2	0.19
(3,1554)	1:64:B:VAL:HA	1:61:B:GLU:HG2	5	0.19
(3,1536)	1:123:B:ARG:HG2	1:50:A:PRO:HD2	9	0.19
(3,1535)	1:123:A:ARG:HG2	1:50:B:PRO:HD2	9	0.19
(3,1359)	1:79:A:GLN:HG3	1:86:A:LEU:HB3	1	0.19
(3,1296)	1:58:B:PRO:HG2	1:55:B:LYS:HE3	3	0.19
(3,1054)	1:93:B:ARG:HG3	1:94:B:THR:HA	5	0.19
(3,1053)	1:93:A:ARG:HG3	1:94:A:THR:HA	5	0.19
(3,907)	1:45:A:ILE:HD12	1:104:B:PHE:HD2	3	0.19
(3,750)	1:135:B:MET:HB3	1:136:B:GLU:H	3	0.19
(3,750)	1:135:B:MET:HB3	1:136:B:GLU:H	6	0.19
(3,750)	1:135:B:MET:HB3	1:136:B:GLU:H	8	0.19
(3,749)	1:135:A:MET:HB3	1:136:A:GLU:H	3	0.19
(3,749)	1:135:A:MET:HB3	1:136:A:GLU:H	6	0.19
(3,749)	1:135:A:MET:HB3	1:136:A:GLU:H	8	0.19
(3,696)	1:129:B:LYS:HB3	1:128:B:LEU:H	10	0.19
(3,695)	1:129:A:LYS:HB3	1:128:A:LEU:H	10	0.19
(3,480)	1:115:B:LEU:HD12	1:104:B:PHE:H	2	0.19
(3,479)	1:115:A:LEU:HD12	1:104:A:PHE:H	2	0.19
(3,258)	1:81:B:VAL:HA	1:77:B:GLY:H	10	0.19
(3,188)	1:110:B:VAL:HG13	1:67:B:SER:H	6	0.19
(3,187)	1:110:A:VAL:HG13	1:67:A:SER:H	6	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,108)	1:49:B:LEU:HG	1:51:B:ALA:H	10	0.19
(3,107)	1:49:A:LEU:HG	1:51:A:ALA:H	4	0.19
(3,107)	1:49:A:LEU:HG	1:51:A:ALA:H	10	0.19
(1,5889)	1:65:A:PHE:HD2	1:101:A:THR:HB	4	0.19
(1,5825)	1:135:A:MET:HE2	1:112:B:TYR:HD2	2	0.19
(1,5668)	1:87:B:THR:HA	1:125:B:ALA:HB2	7	0.19
(1,5667)	1:87:A:THR:HA	1:125:A:ALA:HB2	7	0.19
(1,5624)	1:121:B:THR:HB	1:121:B:THR:HG22	4	0.19
(1,5624)	1:121:B:THR:HB	1:121:B:THR:HG21	8	0.19
(1,5623)	1:121:A:THR:HB	1:121:A:THR:HG22	4	0.19
(1,5623)	1:121:A:THR:HB	1:121:A:THR:HG21	8	0.19
(1,5553)	1:116:A:MET:HE2	1:114:A:THR:HA	1	0.19
(1,5380)	1:110:B:VAL:HB	1:110:B:VAL:HG13	8	0.19
(1,5379)	1:110:A:VAL:HB	1:110:A:VAL:HG13	8	0.19
(1,5379)	1:110:A:VAL:HB	1:110:A:VAL:HG13	9	0.19
(1,5258)	1:105:B:GLN:HG2	1:65:B:PHE:HB2	3	0.19
(1,5257)	1:105:A:GLN:HG2	1:65:A:PHE:HB2	3	0.19
(1,5152)	1:102:B:ILE:HG23	1:102:B:ILE:HD11	1	0.19
(1,5106)	1:102:B:ILE:HG22	1:127:B:TYR:HE2	2	0.19
(1,5105)	1:102:A:ILE:HG22	1:127:A:TYR:HE2	2	0.19
(1,4796)	1:96:B:ALA:HA	1:90:B:LEU:HB2	3	0.19
(1,4795)	1:96:A:ALA:HA	1:90:A:LEU:HB2	3	0.19
(1,4770)	1:94:B:THR:HG21	1:102:B:ILE:HG13	10	0.19
(1,4769)	1:94:A:THR:HG21	1:102:A:ILE:HG13	10	0.19
(1,4534)	1:87:B:THR:HA	1:87:B:THR:HG21	9	0.19
(1,4533)	1:87:A:THR:HA	1:87:A:THR:HG23	3	0.19
(1,4533)	1:87:A:THR:HA	1:87:A:THR:HG21	9	0.19
(1,4152)	1:123:B:ARG:HG2	1:51:A:ALA:HB2	8	0.19
(1,3972)	1:72:B:LYS:HB3	1:72:B:LYS:HD2	7	0.19
(1,3971)	1:72:A:LYS:HB3	1:72:A:LYS:HD2	7	0.19
(1,3612)	1:115:B:LEU:HD11	1:106:B:ALA:HB2	7	0.19
(1,3611)	1:115:A:LEU:HD11	1:106:A:ALA:HB2	7	0.19
(1,3248)	1:99:B:GLU:HG2	1:99:B:GLU:HB2	1	0.19
(1,3247)	1:99:A:GLU:HG2	1:99:A:GLU:HB2	1	0.19
(1,3222)	1:122:B:LEU:HA	1:125:B:ALA:HB1	10	0.19
(1,3221)	1:122:A:LEU:HA	1:125:A:ALA:HB1	10	0.19
(1,3210)	1:122:B:LEU:HA	1:87:B:THR:HB	2	0.19
(1,2551)	1:45:A:ILE:HG23	1:56:B:PRO:HB3	5	0.19
(1,2466)	1:88:B:SER:HA	1:87:B:THR:HG22	4	0.19
(1,2466)	1:88:B:SER:HA	1:87:B:THR:HG23	8	0.19
(1,2465)	1:88:A:SER:HA	1:87:A:THR:HG23	2	0.19
(1,2465)	1:88:A:SER:HA	1:87:A:THR:HG22	4	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2465)	1:88:A:SER:HA	1:87:A:THR:HG23	8	0.19
(1,1842)	1:118:B:VAL:HG13	1:117:B:SER:H	3	0.19
(1,1480)	1:122:B:LEU:HB3	1:122:B:LEU:H	2	0.19
(1,1479)	1:122:A:LEU:HB3	1:122:A:LEU:H	2	0.19
(1,1479)	1:122:A:LEU:HB3	1:122:A:LEU:H	9	0.19
(1,1474)	1:122:B:LEU:HD11	1:122:B:LEU:H	5	0.19
(1,1474)	1:122:B:LEU:HD12	1:122:B:LEU:H	6	0.19
(1,1473)	1:122:A:LEU:HD11	1:122:A:LEU:H	5	0.19
(1,1473)	1:122:A:LEU:HD12	1:122:A:LEU:H	6	0.19
(1,1070)	1:90:B:LEU:HB3	1:88:B:SER:H	5	0.19
(1,1069)	1:90:A:LEU:HB3	1:88:A:SER:H	5	0.19
(1,964)	1:83:B:ALA:HB2	1:84:B:ASP:H	3	0.19
(1,963)	1:83:A:ALA:HB2	1:84:A:ASP:H	3	0.19
(1,1)	1:57:A:GLN:HG3	1:57:A:GLN:H	10	0.19
(3,2868)	1:121:B:THR:HA	1:121:B:THR:HG23	3	0.18
(3,2868)	1:121:B:THR:HA	1:121:B:THR:HG23	6	0.18
(3,2868)	1:121:B:THR:HA	1:121:B:THR:HG23	9	0.18
(3,2868)	1:121:B:THR:HA	1:121:B:THR:HG23	10	0.18
(3,2850)	1:119:B:MET:HE1	1:103:B:PHE:HA	1	0.18
(3,2849)	1:119:A:MET:HE1	1:103:A:PHE:HA	1	0.18
(3,2824)	1:115:B:LEU:HD23	1:116:B:MET:HG3	5	0.18
(3,2823)	1:115:A:LEU:HD23	1:116:A:MET:HG3	5	0.18
(3,2466)	1:94:B:THR:HG23	1:102:B:ILE:HD11	7	0.18
(3,2465)	1:94:A:THR:HG23	1:102:A:ILE:HD11	7	0.18
(3,2317)	1:123:A:ARG:HB2	1:124:A:LYS:HG3	1	0.18
(3,2250)	1:94:B:THR:HG22	1:64:B:VAL:HB	7	0.18
(3,2250)	1:94:B:THR:HG22	1:93:B:ARG:HB3	10	0.18
(3,2249)	1:94:A:THR:HG22	1:64:A:VAL:HB	7	0.18
(3,2249)	1:94:A:THR:HG22	1:93:A:ARG:HB3	10	0.18
(3,2008)	1:82:B:ASN:HB2	1:85:B:GLN:HG2	3	0.18
(3,2007)	1:82:A:ASN:HB2	1:85:A:GLN:HG2	3	0.18
(3,1896)	1:123:B:ARG:HG2	1:50:A:PRO:HB3	5	0.18
(3,1894)	1:123:B:ARG:HG2	1:124:B:LYS:HE2	7	0.18
(3,1386)	1:60:B:PRO:HG2	1:129:B:LYS:HB3	7	0.18
(3,1385)	1:60:A:PRO:HG2	1:129:A:LYS:HB3	7	0.18
(3,1218)	1:54:B:ALA:HB2	1:56:B:PRO:HG3	1	0.18
(3,1217)	1:54:A:ALA:HB2	1:56:A:PRO:HG3	1	0.18
(3,1067)	1:50:A:PRO:HA	1:54:A:ALA:HB3	8	0.18
(3,912)	1:45:B:ILE:HD11	1:46:B:ARG:HD2	10	0.18
(3,911)	1:45:A:ILE:HD11	1:46:A:ARG:HD2	10	0.18
(3,750)	1:135:B:MET:HB2	1:136:B:GLU:H	5	0.18
(3,749)	1:135:A:MET:HB2	1:136:A:GLU:H	5	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,608)	1:134:B:GLY:HA3	1:119:A:MET:H	6	0.18
(3,580)	1:108:B:LYS:HG3	1:116:A:MET:H	10	0.18
(3,125)	1:56:A:PRO:HG2	1:57:A:GLN:H	10	0.18
(3,108)	1:49:B:LEU:HG	1:51:B:ALA:H	4	0.18
(3,78)	1:46:B:ARG:HD2	1:47:B:VAL:H	1	0.18
(3,77)	1:46:A:ARG:HD2	1:47:A:VAL:H	1	0.18
(1,5890)	1:65:B:PHE:HD2	1:101:B:THR:HB	4	0.18
(1,5830)	1:135:B:MET:HE1	1:108:B:LYS:HA	5	0.18
(1,5829)	1:135:A:MET:HE1	1:108:A:LYS:HA	5	0.18
(1,5662)	1:125:B:ALA:HA	1:125:B:ALA:HB3	3	0.18
(1,5662)	1:125:B:ALA:HA	1:125:B:ALA:HB2	7	0.18
(1,5661)	1:125:A:ALA:HA	1:125:A:ALA:HB3	3	0.18
(1,5661)	1:125:A:ALA:HA	1:125:A:ALA:HB2	7	0.18
(1,5624)	1:121:B:THR:HB	1:121:B:THR:HG22	3	0.18
(1,5624)	1:121:B:THR:HB	1:121:B:THR:HG23	5	0.18
(1,5624)	1:121:B:THR:HB	1:121:B:THR:HG22	6	0.18
(1,5624)	1:121:B:THR:HB	1:121:B:THR:HG21	7	0.18
(1,5624)	1:121:B:THR:HB	1:121:B:THR:HG21	10	0.18
(1,5623)	1:121:A:THR:HB	1:121:A:THR:HG22	3	0.18
(1,5623)	1:121:A:THR:HB	1:121:A:THR:HG23	5	0.18
(1,5623)	1:121:A:THR:HB	1:121:A:THR:HG22	6	0.18
(1,5623)	1:121:A:THR:HB	1:121:A:THR:HG23	7	0.18
(1,5623)	1:121:A:THR:HB	1:121:A:THR:HG21	10	0.18
(1,5590)	1:119:B:MET:HG3	1:119:B:MET:HE2	8	0.18
(1,5589)	1:119:A:MET:HG3	1:119:A:MET:HE2	8	0.18
(1,5554)	1:116:B:MET:HE2	1:114:B:THR:HA	1	0.18
(1,5380)	1:110:B:VAL:HB	1:110:B:VAL:HG13	9	0.18
(1,5376)	1:110:B:VAL:HB	1:112:B:TYR:HB3	1	0.18
(1,5375)	1:110:A:VAL:HB	1:112:A:TYR:HB3	1	0.18
(1,5152)	1:102:B:ILE:HG22	1:102:B:ILE:HD13	2	0.18
(1,5130)	1:102:B:ILE:HG21	1:102:B:ILE:HG13	2	0.18
(1,5130)	1:102:B:ILE:HG21	1:102:B:ILE:HG13	5	0.18
(1,5129)	1:102:A:ILE:HG21	1:102:A:ILE:HG13	2	0.18
(1,5129)	1:102:A:ILE:HG21	1:102:A:ILE:HG13	5	0.18
(1,5106)	1:102:B:ILE:HG23	1:127:B:TYR:HE2	10	0.18
(1,5105)	1:102:A:ILE:HG23	1:127:A:TYR:HE2	10	0.18
(1,4674)	1:91:B:ASP:HA	1:96:B:ALA:HA	8	0.18
(1,4673)	1:91:A:ASP:HA	1:96:A:ALA:HA	8	0.18
(1,4636)	1:90:B:LEU:HB2	1:64:B:VAL:HB	1	0.18
(1,4635)	1:90:A:LEU:HB2	1:64:A:VAL:HB	1	0.18
(1,4610)	1:90:B:LEU:HB3	1:99:B:GLU:HA	5	0.18
(1,4568)	1:87:B:THR:HG22	1:124:B:LYS:HD2	2	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4567)	1:87:A:THR:HG22	1:124:A:LYS:HD2	2	0.18
(1,4534)	1:87:B:THR:HA	1:87:B:THR:HG23	4	0.18
(1,4534)	1:87:B:THR:HA	1:87:B:THR:HG23	10	0.18
(1,4533)	1:87:A:THR:HA	1:87:A:THR:HG23	4	0.18
(1,4533)	1:87:A:THR:HA	1:87:A:THR:HG21	7	0.18
(1,4533)	1:87:A:THR:HA	1:87:A:THR:HG23	10	0.18
(1,4482)	1:86:B:LEU:HA	1:90:B:LEU:HG	4	0.18
(1,4481)	1:86:A:LEU:HA	1:90:A:LEU:HG	4	0.18
(1,4154)	1:123:B:ARG:HG2	1:49:A:LEU:HB3	9	0.18
(1,4153)	1:123:A:ARG:HG2	1:49:B:LEU:HB3	9	0.18
(1,4151)	1:123:A:ARG:HG2	1:51:B:ALA:HB2	8	0.18
(1,4052)	1:93:B:ARG:HB3	1:64:B:VAL:HA	6	0.18
(1,4051)	1:93:A:ARG:HB3	1:64:A:VAL:HA	6	0.18
(1,3972)	1:72:B:LYS:HB3	1:72:B:LYS:HD2	6	0.18
(1,3971)	1:72:A:LYS:HB3	1:72:A:LYS:HD2	6	0.18
(1,3690)	1:67:B:SER:HB2	1:115:B:LEU:HD11	4	0.18
(1,3689)	1:67:A:SER:HB2	1:115:A:LEU:HD11	4	0.18
(1,3676)	1:67:B:SER:HB2	1:105:B:GLN:HG2	3	0.18
(1,3540)	1:66:B:LEU:HB2	1:102:B:ILE:HG22	7	0.18
(1,3540)	1:66:B:LEU:HB2	1:102:B:ILE:HG21	8	0.18
(1,3539)	1:66:A:LEU:HB2	1:102:A:ILE:HG22	7	0.18
(1,3460)	1:64:B:VAL:HB	1:102:B:ILE:HG23	1	0.18
(1,3459)	1:64:A:VAL:HB	1:102:A:ILE:HG23	1	0.18
(1,3458)	1:110:B:VAL:HB	1:114:B:THR:HG23	10	0.18
(1,3457)	1:110:A:VAL:HB	1:114:A:THR:HG23	10	0.18
(1,3209)	1:122:A:LEU:HA	1:87:A:THR:HB	2	0.18
(1,3016)	1:57:B:GLN:HB3	1:60:B:PRO:HB3	5	0.18
(1,3015)	1:57:A:GLN:HB3	1:60:A:PRO:HB3	5	0.18
(1,2822)	1:54:B:ALA:HB2	1:56:B:PRO:HG3	1	0.18
(1,2821)	1:54:A:ALA:HB2	1:56:A:PRO:HG3	1	0.18
(1,2680)	1:93:B:ARG:HG3	1:90:B:LEU:HA	9	0.18
(1,2679)	1:93:A:ARG:HG3	1:90:A:LEU:HA	9	0.18
(1,2576)	1:98:B:LYS:HB2	1:98:B:LYS:HD3	1	0.18
(1,2576)	1:98:B:LYS:HB2	1:98:B:LYS:HD3	4	0.18
(1,2576)	1:98:B:LYS:HB2	1:98:B:LYS:HD3	6	0.18
(1,2575)	1:98:A:LYS:HB2	1:98:A:LYS:HD3	1	0.18
(1,2575)	1:98:A:LYS:HB2	1:98:A:LYS:HD3	4	0.18
(1,2575)	1:98:A:LYS:HB2	1:98:A:LYS:HD3	6	0.18
(1,1841)	1:118:A:VAL:HG13	1:117:A:SER:H	3	0.18
(1,1480)	1:122:B:LEU:HB3	1:122:B:LEU:H	1	0.18
(1,1480)	1:122:B:LEU:HB3	1:122:B:LEU:H	3	0.18
(1,1480)	1:122:B:LEU:HB3	1:122:B:LEU:H	4	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1480)	1:122:B:LEU:HB3	1:122:B:LEU:H	5	0.18
(1,1480)	1:122:B:LEU:HB3	1:122:B:LEU:H	6	0.18
(1,1480)	1:122:B:LEU:HB3	1:122:B:LEU:H	7	0.18
(1,1480)	1:122:B:LEU:HB3	1:122:B:LEU:H	9	0.18
(1,1480)	1:122:B:LEU:HB3	1:122:B:LEU:H	10	0.18
(1,1479)	1:122:A:LEU:HB3	1:122:A:LEU:H	1	0.18
(1,1479)	1:122:A:LEU:HB3	1:122:A:LEU:H	3	0.18
(1,1479)	1:122:A:LEU:HB3	1:122:A:LEU:H	4	0.18
(1,1479)	1:122:A:LEU:HB3	1:122:A:LEU:H	5	0.18
(1,1479)	1:122:A:LEU:HB3	1:122:A:LEU:H	6	0.18
(1,1479)	1:122:A:LEU:HB3	1:122:A:LEU:H	7	0.18
(1,1479)	1:122:A:LEU:HB3	1:122:A:LEU:H	10	0.18
(1,1474)	1:122:B:LEU:HD13	1:122:B:LEU:H	2	0.18
(1,1474)	1:122:B:LEU:HD13	1:122:B:LEU:H	3	0.18
(1,1473)	1:122:A:LEU:HD13	1:122:A:LEU:H	2	0.18
(1,1473)	1:122:A:LEU:HD13	1:122:A:LEU:H	3	0.18
(1,1274)	1:94:B:THR:HG21	1:94:B:THR:H	2	0.18
(1,1066)	1:87:B:THR:HG23	1:88:B:SER:H	2	0.18
(1,964)	1:83:B:ALA:HB1	1:84:B:ASP:H	6	0.18
(1,964)	1:83:B:ALA:HB2	1:84:B:ASP:H	9	0.18
(1,964)	1:83:B:ALA:HB1	1:84:B:ASP:H	10	0.18
(1,963)	1:83:A:ALA:HB1	1:84:A:ASP:H	6	0.18
(1,963)	1:83:A:ALA:HB2	1:84:A:ASP:H	9	0.18
(1,963)	1:83:A:ALA:HB1	1:84:A:ASP:H	10	0.18
(1,350)	1:54:B:ALA:HA	1:55:B:LYS:H	10	0.18
(1,254)	1:45:B:ILE:HG23	1:47:B:VAL:H	8	0.18
(1,253)	1:45:A:ILE:HG23	1:47:A:VAL:H	8	0.18
(3,2867)	1:121:A:THR:HA	1:121:A:THR:HG23	9	0.17
(3,2867)	1:121:A:THR:HA	1:121:A:THR:HG23	10	0.17
(3,2831)	1:116:A:MET:HE3	1:112:B:TYR:HD1	6	0.17
(3,2692)	1:108:B:LYS:HE3	1:109:B:SER:HB3	5	0.17
(3,2318)	1:123:B:ARG:HB2	1:124:B:LYS:HG3	1	0.17
(3,1956)	1:79:B:GLN:HG2	1:91:B:ASP:HB3	7	0.17
(3,1955)	1:79:A:GLN:HG2	1:91:A:ASP:HB3	7	0.17
(3,1893)	1:123:A:ARG:HG2	1:124:A:LYS:HE2	7	0.17
(3,1834)	1:72:B:LYS:HE2	1:110:B:VAL:HG21	6	0.17
(3,1723)	1:135:A:MET:HG2	1:115:A:LEU:HD23	4	0.17
(3,1620)	1:120:B:ASP:HB3	1:115:B:LEU:HD23	3	0.17
(3,1619)	1:120:A:ASP:HB3	1:115:A:LEU:HD23	3	0.17
(3,1553)	1:64:A:VAL:HA	1:61:A:GLU:HG2	2	0.17
(3,1376)	1:60:B:PRO:HG3	1:97:B:ASN:HB2	10	0.17
(3,1359)	1:79:A:GLN:HG3	1:86:A:LEU:HB3	2	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,1296)	1:58:B:PRO:HG2	1:55:B:LYS:HE2	4	0.17
(3,1295)	1:58:A:PRO:HG2	1:55:A:LYS:HE2	4	0.17
(3,1068)	1:50:B:PRO:HA	1:54:B:ALA:HB3	8	0.17
(3,607)	1:134:A:GLY:HA3	1:119:B:MET:H	9	0.17
(3,361)	1:102:A:ILE:HA	1:91:A:ASP:H	3	0.17
(3,258)	1:81:B:VAL:HA	1:77:B:GLY:H	2	0.17
(3,258)	1:81:B:VAL:HA	1:77:B:GLY:H	5	0.17
(3,257)	1:81:A:VAL:HA	1:77:A:GLY:H	2	0.17
(3,257)	1:81:A:VAL:HA	1:77:A:GLY:H	5	0.17
(3,126)	1:56:B:PRO:HG2	1:57:B:GLN:H	10	0.17
(1,5920)	1:104:B:PHE:HD2	1:115:B:LEU:HD13	4	0.17
(1,5919)	1:104:A:PHE:HD2	1:115:A:LEU:HD13	4	0.17
(1,5826)	1:135:B:MET:HE2	1:112:A:TYR:HD2	2	0.17
(1,5690)	1:126:B:GLY:HA3	1:98:B:LYS:HD3	1	0.17
(1,5690)	1:126:B:GLY:HA3	1:98:B:LYS:HD3	9	0.17
(1,5689)	1:126:A:GLY:HA3	1:98:A:LYS:HD3	1	0.17
(1,5689)	1:126:A:GLY:HA3	1:98:A:LYS:HD3	9	0.17
(1,5662)	1:125:B:ALA:HA	1:125:B:ALA:HB2	1	0.17
(1,5661)	1:125:A:ALA:HA	1:125:A:ALA:HB2	1	0.17
(1,5661)	1:125:A:ALA:HA	1:125:A:ALA:HB1	2	0.17
(1,5624)	1:121:B:THR:HB	1:121:B:THR:HG23	1	0.17
(1,5624)	1:121:B:THR:HB	1:121:B:THR:HG21	2	0.17
(1,5624)	1:121:B:THR:HB	1:121:B:THR:HG22	9	0.17
(1,5623)	1:121:A:THR:HB	1:121:A:THR:HG23	1	0.17
(1,5623)	1:121:A:THR:HB	1:121:A:THR:HG21	2	0.17
(1,5623)	1:121:A:THR:HB	1:121:A:THR:HG22	9	0.17
(1,5608)	1:51:B:ALA:HB3	1:124:A:LYS:HA	10	0.17
(1,5376)	1:110:B:VAL:HB	1:112:B:TYR:HB3	5	0.17
(1,5375)	1:110:A:VAL:HB	1:112:A:TYR:HB3	5	0.17
(1,5152)	1:102:B:ILE:HG22	1:102:B:ILE:HD11	5	0.17
(1,5151)	1:102:A:ILE:HG22	1:102:A:ILE:HD13	2	0.17
(1,5151)	1:102:A:ILE:HG22	1:102:A:ILE:HD11	5	0.17
(1,5150)	1:100:B:THR:HG22	1:102:B:ILE:HD13	1	0.17
(1,5149)	1:100:A:THR:HG22	1:102:A:ILE:HD13	1	0.17
(1,5130)	1:102:B:ILE:HG22	1:102:B:ILE:HG13	1	0.17
(1,5130)	1:102:B:ILE:HG22	1:102:B:ILE:HG13	6	0.17
(1,5130)	1:102:B:ILE:HG22	1:102:B:ILE:HG13	8	0.17
(1,5130)	1:102:B:ILE:HG21	1:102:B:ILE:HG13	9	0.17
(1,5129)	1:102:A:ILE:HG22	1:102:A:ILE:HG13	1	0.17
(1,5129)	1:102:A:ILE:HG22	1:102:A:ILE:HG13	6	0.17
(1,5129)	1:102:A:ILE:HG22	1:102:A:ILE:HG13	8	0.17
(1,5129)	1:102:A:ILE:HG21	1:102:A:ILE:HG13	9	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4609)	1:90:A:LEU:HB3	1:99:A:GLU:HA	5	0.17
(1,4566)	1:87:B:THR:HG21	1:125:B:ALA:HB1	4	0.17
(1,4565)	1:87:A:THR:HG21	1:125:A:ALA:HB1	4	0.17
(1,4534)	1:87:B:THR:HA	1:87:B:THR:HG21	2	0.17
(1,4534)	1:87:B:THR:HA	1:87:B:THR:HG21	7	0.17
(1,4533)	1:87:A:THR:HA	1:87:A:THR:HG21	2	0.17
(1,4504)	1:86:B:LEU:HB2	1:121:B:THR:HG21	7	0.17
(1,4503)	1:86:A:LEU:HB2	1:121:A:THR:HG21	7	0.17
(1,4482)	1:86:B:LEU:HA	1:90:B:LEU:HG	5	0.17
(1,4481)	1:86:A:LEU:HA	1:90:A:LEU:HG	5	0.17
(1,4000)	1:72:B:LYS:HG2	1:114:B:THR:HG22	1	0.17
(1,3999)	1:72:A:LYS:HG2	1:114:A:THR:HG22	1	0.17
(1,3972)	1:72:B:LYS:HB3	1:72:B:LYS:HD2	9	0.17
(1,3539)	1:66:A:LEU:HB2	1:102:A:ILE:HG21	8	0.17
(1,3210)	1:122:B:LEU:HA	1:87:B:THR:HB	1	0.17
(1,2576)	1:98:B:LYS:HB2	1:98:B:LYS:HD3	2	0.17
(1,2576)	1:98:B:LYS:HB2	1:98:B:LYS:HD3	5	0.17
(1,2576)	1:98:B:LYS:HB2	1:98:B:LYS:HD3	7	0.17
(1,2575)	1:98:A:LYS:HB2	1:98:A:LYS:HD3	2	0.17
(1,2575)	1:98:A:LYS:HB2	1:98:A:LYS:HD3	7	0.17
(1,2552)	1:45:B:ILE:HG23	1:56:A:PRO:HB3	5	0.17
(1,2466)	1:88:B:SER:HA	1:87:B:THR:HG23	7	0.17
(1,2465)	1:88:A:SER:HA	1:87:A:THR:HG23	7	0.17
(1,1842)	1:118:B:VAL:HG13	1:117:B:SER:H	10	0.17
(1,1841)	1:118:A:VAL:HG13	1:117:A:SER:H	10	0.17
(1,1687)	1:139:A:ALA:HA	1:140:A:LYS:H	3	0.17
(1,1480)	1:122:B:LEU:HB3	1:122:B:LEU:H	8	0.17
(1,1479)	1:122:A:LEU:HB3	1:122:A:LEU:H	8	0.17
(1,1403)	1:99:A:GLU:HG2	1:99:A:GLU:H	5	0.17
(1,1274)	1:94:B:THR:HG21	1:94:B:THR:H	9	0.17
(1,1273)	1:94:A:THR:HG21	1:94:A:THR:H	2	0.17
(1,1273)	1:94:A:THR:HG21	1:94:A:THR:H	9	0.17
(1,1065)	1:87:A:THR:HG23	1:88:A:SER:H	2	0.17
(1,964)	1:83:B:ALA:HB1	1:84:B:ASP:H	5	0.17
(1,963)	1:83:A:ALA:HB1	1:84:A:ASP:H	5	0.17
(1,963)	1:83:A:ALA:HB3	1:84:A:ASP:H	7	0.17
(1,349)	1:54:A:ALA:HA	1:55:A:LYS:H	10	0.17
(3,2930)	1:126:B:GLY:HA2	1:91:B:ASP:HA	2	0.16
(3,2929)	1:126:A:GLY:HA2	1:91:A:ASP:HA	2	0.16
(3,2868)	1:121:B:THR:HA	1:121:B:THR:HG23	2	0.16
(3,2867)	1:121:A:THR:HA	1:121:A:THR:HG23	6	0.16
(3,2691)	1:108:A:LYS:HE3	1:109:A:SER:HB3	5	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,2564)	1:60:B:PRO:HA	1:103:B:PHE:HB2	2	0.16
(3,2563)	1:60:A:PRO:HA	1:103:A:PHE:HB2	2	0.16
(3,2542)	1:102:B:ILE:HD12	1:95:B:GLN:HG2	5	0.16
(3,2541)	1:102:A:ILE:HD12	1:95:A:GLN:HG2	5	0.16
(3,2352)	1:98:B:LYS:HG3	1:125:B:ALA:HB2	2	0.16
(3,2351)	1:98:A:LYS:HG3	1:125:A:ALA:HB2	2	0.16
(3,2250)	1:94:B:THR:HG22	1:64:B:VAL:HB	5	0.16
(3,2249)	1:94:A:THR:HG22	1:64:A:VAL:HB	5	0.16
(3,1888)	1:74:B:LEU:HB2	1:83:B:ALA:HB3	2	0.16
(3,1887)	1:74:A:LEU:HB2	1:83:A:ALA:HB3	2	0.16
(3,1833)	1:72:A:LYS:HE2	1:110:A:VAL:HG23	4	0.16
(3,1833)	1:72:A:LYS:HE2	1:110:A:VAL:HG23	5	0.16
(3,1833)	1:72:A:LYS:HE2	1:110:A:VAL:HG21	6	0.16
(3,1724)	1:135:B:MET:HG2	1:115:B:LEU:HD23	4	0.16
(3,1640)	1:115:B:LEU:HD11	1:131:B:GLY:HA2	3	0.16
(3,1639)	1:115:A:LEU:HD11	1:131:A:GLY:HA2	3	0.16
(3,1546)	1:63:B:PRO:HD2	1:93:B:ARG:HD3	3	0.16
(3,1545)	1:63:A:PRO:HD2	1:93:A:ARG:HD3	3	0.16
(3,1540)	1:46:B:ARG:HG2	1:128:A:LEU:HB3	9	0.16
(3,1539)	1:46:A:ARG:HG2	1:128:B:LEU:HB3	9	0.16
(3,1375)	1:60:A:PRO:HG3	1:97:A:ASN:HB2	10	0.16
(3,1360)	1:79:B:GLN:HG3	1:86:B:LEU:HB3	2	0.16
(3,853)	1:88:A:SER:HA	1:124:A:LYS:HE3	8	0.16
(3,608)	1:134:B:GLY:HA3	1:119:A:MET:H	9	0.16
(3,607)	1:134:A:GLY:HA3	1:119:B:MET:H	2	0.16
(3,362)	1:102:B:ILE:HA	1:91:B:ASP:H	3	0.16
(3,318)	1:96:B:ALA:HA	1:88:B:SER:H	4	0.16
(3,317)	1:96:A:ALA:HA	1:88:A:SER:H	4	0.16
(3,276)	1:73:B:GLN:HG2	1:79:B:GLN:H	1	0.16
(1,5898)	1:103:B:PHE:HD2	1:102:B:ILE:HG13	8	0.16
(1,5897)	1:103:A:PHE:HD2	1:102:A:ILE:HG13	8	0.16
(1,5886)	1:65:B:PHE:HD1	1:93:B:ARG:H	10	0.16
(1,5885)	1:65:A:PHE:HD1	1:93:A:ARG:H	10	0.16
(1,5731)	1:128:A:LEU:HA	1:49:B:LEU:HB3	2	0.16
(1,5662)	1:125:B:ALA:HA	1:125:B:ALA:HB1	2	0.16
(1,5662)	1:125:B:ALA:HA	1:125:B:ALA:HB2	10	0.16
(1,5650)	1:124:B:LYS:HA	1:124:B:LYS:HD3	5	0.16
(1,5608)	1:51:B:ALA:HB3	1:124:A:LYS:HA	8	0.16
(1,5607)	1:51:A:ALA:HB3	1:124:B:LYS:HA	8	0.16
(1,5554)	1:116:B:MET:HE2	1:114:B:THR:HA	2	0.16
(1,5553)	1:116:A:MET:HE2	1:114:A:THR:HA	2	0.16
(1,5538)	1:115:B:LEU:HD22	1:116:B:MET:HE2	4	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5537)	1:115:A:LEU:HD22	1:116:A:MET:HE2	4	0.16
(1,5514)	1:115:B:LEU:HB2	1:115:B:LEU:HG	1	0.16
(1,5514)	1:115:B:LEU:HB2	1:115:B:LEU:HG	2	0.16
(1,5514)	1:115:B:LEU:HB2	1:115:B:LEU:HG	3	0.16
(1,5514)	1:115:B:LEU:HB2	1:115:B:LEU:HG	4	0.16
(1,5514)	1:115:B:LEU:HB2	1:115:B:LEU:HG	6	0.16
(1,5514)	1:115:B:LEU:HB2	1:115:B:LEU:HG	7	0.16
(1,5514)	1:115:B:LEU:HB2	1:115:B:LEU:HG	10	0.16
(1,5513)	1:115:A:LEU:HB2	1:115:A:LEU:HG	1	0.16
(1,5513)	1:115:A:LEU:HB2	1:115:A:LEU:HG	2	0.16
(1,5513)	1:115:A:LEU:HB2	1:115:A:LEU:HG	4	0.16
(1,5513)	1:115:A:LEU:HB2	1:115:A:LEU:HG	6	0.16
(1,5513)	1:115:A:LEU:HB2	1:115:A:LEU:HG	9	0.16
(1,5513)	1:115:A:LEU:HB2	1:115:A:LEU:HG	10	0.16
(1,5394)	1:110:B:VAL:HG23	1:112:B:TYR:HB3	2	0.16
(1,5394)	1:110:B:VAL:HG21	1:112:B:TYR:HB3	6	0.16
(1,5393)	1:110:A:VAL:HG23	1:112:A:TYR:HB3	2	0.16
(1,5393)	1:110:A:VAL:HG21	1:112:A:TYR:HB3	6	0.16
(1,5258)	1:105:B:GLN:HG2	1:65:B:PHE:HB2	4	0.16
(1,5130)	1:102:B:ILE:HG21	1:102:B:ILE:HG13	3	0.16
(1,5130)	1:102:B:ILE:HG21	1:102:B:ILE:HG13	4	0.16
(1,5130)	1:102:B:ILE:HG23	1:102:B:ILE:HG13	7	0.16
(1,5129)	1:102:A:ILE:HG21	1:102:A:ILE:HG13	3	0.16
(1,5129)	1:102:A:ILE:HG21	1:102:A:ILE:HG13	4	0.16
(1,5129)	1:102:A:ILE:HG23	1:102:A:ILE:HG13	7	0.16
(1,5100)	1:102:B:ILE:HG13	1:102:B:ILE:HD11	2	0.16
(1,5100)	1:102:B:ILE:HG13	1:102:B:ILE:HD13	3	0.16
(1,5100)	1:102:B:ILE:HG13	1:102:B:ILE:HD13	8	0.16
(1,5099)	1:102:A:ILE:HG13	1:102:A:ILE:HD12	1	0.16
(1,5099)	1:102:A:ILE:HG13	1:102:A:ILE:HD11	2	0.16
(1,5099)	1:102:A:ILE:HG13	1:102:A:ILE:HD13	3	0.16
(1,5099)	1:102:A:ILE:HG13	1:102:A:ILE:HD13	8	0.16
(1,5022)	1:101:B:THR:HG23	1:130:B:VAL:HA	2	0.16
(1,5021)	1:101:A:THR:HG23	1:130:A:VAL:HA	2	0.16
(1,4938)	1:100:B:THR:HB	1:100:B:THR:HG21	5	0.16
(1,4937)	1:100:A:THR:HB	1:100:A:THR:HG21	5	0.16
(1,4568)	1:87:B:THR:HG21	1:124:B:LYS:HD2	10	0.16
(1,4567)	1:87:A:THR:HG21	1:124:A:LYS:HD2	10	0.16
(1,4566)	1:87:B:THR:HG22	1:125:B:ALA:HB2	7	0.16
(1,4565)	1:87:A:THR:HG22	1:125:A:ALA:HB2	7	0.16
(1,4534)	1:87:B:THR:HA	1:87:B:THR:HG21	8	0.16
(1,4533)	1:87:A:THR:HA	1:87:A:THR:HG21	8	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3971)	1:72:A:LYS:HB3	1:72:A:LYS:HD2	9	0.16
(1,3838)	1:69:B:LYS:HG3	1:115:B:LEU:HD11	4	0.16
(1,3837)	1:69:A:LYS:HG3	1:115:A:LEU:HD11	4	0.16
(1,3721)	1:67:A:SER:HB3	1:69:A:LYS:HD2	9	0.16
(1,3690)	1:67:B:SER:HB2	1:115:B:LEU:HD13	2	0.16
(1,3689)	1:67:A:SER:HB2	1:115:A:LEU:HD13	2	0.16
(1,3675)	1:67:A:SER:HB2	1:105:A:GLN:HG2	3	0.16
(1,3612)	1:115:B:LEU:HD12	1:106:B:ALA:HB3	6	0.16
(1,3611)	1:115:A:LEU:HD12	1:106:A:ALA:HB3	6	0.16
(1,3598)	1:115:B:LEU:HD13	1:119:B:MET:HG2	3	0.16
(1,3597)	1:115:A:LEU:HD13	1:119:A:MET:HG2	3	0.16
(1,3209)	1:122:A:LEU:HA	1:87:A:THR:HB	1	0.16
(1,2924)	1:56:B:PRO:HA	1:50:B:PRO:HD2	4	0.16
(1,2898)	1:55:B:LYS:HB2	1:55:B:LYS:HG2	1	0.16
(1,2898)	1:55:B:LYS:HB2	1:55:B:LYS:HG2	2	0.16
(1,2898)	1:55:B:LYS:HB2	1:55:B:LYS:HG2	3	0.16
(1,2898)	1:55:B:LYS:HB2	1:55:B:LYS:HG2	4	0.16
(1,2898)	1:55:B:LYS:HB2	1:55:B:LYS:HG2	5	0.16
(1,2898)	1:55:B:LYS:HB2	1:55:B:LYS:HG2	6	0.16
(1,2898)	1:55:B:LYS:HB2	1:55:B:LYS:HG2	7	0.16
(1,2898)	1:55:B:LYS:HB2	1:55:B:LYS:HG2	8	0.16
(1,2898)	1:55:B:LYS:HB2	1:55:B:LYS:HG2	9	0.16
(1,2898)	1:55:B:LYS:HB2	1:55:B:LYS:HG2	10	0.16
(1,2897)	1:55:A:LYS:HB2	1:55:A:LYS:HG2	1	0.16
(1,2897)	1:55:A:LYS:HB2	1:55:A:LYS:HG2	2	0.16
(1,2897)	1:55:A:LYS:HB2	1:55:A:LYS:HG2	3	0.16
(1,2897)	1:55:A:LYS:HB2	1:55:A:LYS:HG2	4	0.16
(1,2897)	1:55:A:LYS:HB2	1:55:A:LYS:HG2	5	0.16
(1,2897)	1:55:A:LYS:HB2	1:55:A:LYS:HG2	6	0.16
(1,2897)	1:55:A:LYS:HB2	1:55:A:LYS:HG2	7	0.16
(1,2897)	1:55:A:LYS:HB2	1:55:A:LYS:HG2	8	0.16
(1,2897)	1:55:A:LYS:HB2	1:55:A:LYS:HG2	9	0.16
(1,2897)	1:55:A:LYS:HB2	1:55:A:LYS:HG2	10	0.16
(1,2852)	1:55:B:LYS:HA	1:55:B:LYS:HG3	9	0.16
(1,2851)	1:55:A:LYS:HA	1:55:A:LYS:HG3	9	0.16
(1,2576)	1:98:B:LYS:HB2	1:98:B:LYS:HD3	8	0.16
(1,2576)	1:98:B:LYS:HB2	1:98:B:LYS:HD3	9	0.16
(1,2575)	1:98:A:LYS:HB2	1:98:A:LYS:HD3	5	0.16
(1,2575)	1:98:A:LYS:HB2	1:98:A:LYS:HD3	8	0.16
(1,2575)	1:98:A:LYS:HB2	1:98:A:LYS:HD3	9	0.16
(1,2268)	1:138:B:ALA:HB2	1:138:B:ALA:H	3	0.16
(1,2267)	1:138:A:ALA:HB2	1:138:A:ALA:H	3	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1842)	1:118:B:VAL:HG12	1:117:B:SER:H	6	0.16
(1,1841)	1:118:A:VAL:HG12	1:117:A:SER:H	6	0.16
(1,1688)	1:139:B:ALA:HA	1:140:B:LYS:H	3	0.16
(1,1649)	1:110:A:VAL:HG23	1:115:A:LEU:H	5	0.16
(1,1474)	1:122:B:LEU:HD11	1:122:B:LEU:H	4	0.16
(1,1473)	1:122:A:LEU:HD11	1:122:A:LEU:H	4	0.16
(1,1404)	1:99:B:GLU:HG2	1:99:B:GLU:H	5	0.16
(1,1274)	1:94:B:THR:HG22	1:94:B:THR:H	3	0.16
(1,1273)	1:94:A:THR:HG21	1:94:A:THR:H	6	0.16
(1,1066)	1:87:B:THR:HG23	1:88:B:SER:H	7	0.16
(1,1036)	1:89:B:VAL:HG12	1:87:B:THR:H	2	0.16
(1,1036)	1:89:B:VAL:HG11	1:87:B:THR:H	8	0.16
(1,1035)	1:89:A:VAL:HG12	1:87:A:THR:H	2	0.16
(1,1035)	1:89:A:VAL:HG11	1:87:A:THR:H	8	0.16
(1,981)	1:85:A:GLN:HG2	1:85:A:GLN:H	10	0.16
(1,974)	1:85:B:GLN:HB3	1:85:B:GLN:H	1	0.16
(1,974)	1:85:B:GLN:HB3	1:85:B:GLN:H	3	0.16
(1,973)	1:85:A:GLN:HB3	1:85:A:GLN:H	1	0.16
(1,964)	1:83:B:ALA:HB3	1:84:B:ASP:H	7	0.16
(1,762)	1:110:B:VAL:HG12	1:74:B:LEU:H	10	0.16
(1,761)	1:110:A:VAL:HG12	1:74:A:LEU:H	10	0.16
(1,614)	1:115:B:LEU:HD13	1:68:B:VAL:H	2	0.16
(1,613)	1:115:A:LEU:HD13	1:68:A:VAL:H	2	0.16
(1,349)	1:54:A:ALA:HA	1:55:A:LYS:H	9	0.16
(3,2868)	1:121:B:THR:HA	1:121:B:THR:HG21	5	0.15
(3,2867)	1:121:A:THR:HA	1:121:A:THR:HG23	2	0.15
(3,2867)	1:121:A:THR:HA	1:121:A:THR:HG21	5	0.15
(3,2856)	1:119:B:MET:HE2	1:104:B:PHE:HB3	7	0.15
(3,2855)	1:119:A:MET:HE2	1:104:A:PHE:HB3	7	0.15
(3,2692)	1:108:B:LYS:HE3	1:109:B:SER:HB3	3	0.15
(3,2691)	1:108:A:LYS:HE3	1:109:A:SER:HB3	3	0.15
(3,2532)	1:102:B:ILE:HG23	1:133:B:VAL:HB	9	0.15
(3,2500)	1:101:B:THR:HG21	1:50:B:PRO:HB3	7	0.15
(3,2499)	1:101:A:THR:HG21	1:50:A:PRO:HB3	7	0.15
(3,2118)	1:88:B:SER:HB2	1:96:B:ALA:HA	1	0.15
(3,2117)	1:88:A:SER:HB2	1:96:A:ALA:HA	1	0.15
(3,2080)	1:115:B:LEU:HA	1:115:B:LEU:HB3	1	0.15
(3,2080)	1:115:B:LEU:HA	1:115:B:LEU:HB3	2	0.15
(3,2080)	1:115:B:LEU:HA	1:115:B:LEU:HB3	3	0.15
(3,2080)	1:115:B:LEU:HA	1:115:B:LEU:HB3	4	0.15
(3,2080)	1:115:B:LEU:HA	1:115:B:LEU:HB3	5	0.15
(3,2080)	1:115:B:LEU:HA	1:115:B:LEU:HB3	6	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,2080)	1:115:B:LEU:HA	1:115:B:LEU:HB3	7	0.15
(3,2080)	1:115:B:LEU:HA	1:115:B:LEU:HB3	8	0.15
(3,2080)	1:115:B:LEU:HA	1:115:B:LEU:HB3	9	0.15
(3,2080)	1:115:B:LEU:HA	1:115:B:LEU:HB3	10	0.15
(3,2079)	1:115:A:LEU:HA	1:115:A:LEU:HB3	1	0.15
(3,2079)	1:115:A:LEU:HA	1:115:A:LEU:HB3	2	0.15
(3,2079)	1:115:A:LEU:HA	1:115:A:LEU:HB3	3	0.15
(3,2079)	1:115:A:LEU:HA	1:115:A:LEU:HB3	4	0.15
(3,2079)	1:115:A:LEU:HA	1:115:A:LEU:HB3	5	0.15
(3,2079)	1:115:A:LEU:HA	1:115:A:LEU:HB3	6	0.15
(3,2079)	1:115:A:LEU:HA	1:115:A:LEU:HB3	7	0.15
(3,2079)	1:115:A:LEU:HA	1:115:A:LEU:HB3	8	0.15
(3,2079)	1:115:A:LEU:HA	1:115:A:LEU:HB3	9	0.15
(3,2079)	1:115:A:LEU:HA	1:115:A:LEU:HB3	10	0.15
(3,1998)	1:81:B:VAL:HA	1:66:B:LEU:HB2	7	0.15
(3,1997)	1:81:A:VAL:HA	1:66:A:LEU:HB2	7	0.15
(3,1834)	1:72:B:LYS:HE2	1:110:B:VAL:HG23	4	0.15
(3,1834)	1:72:B:LYS:HE2	1:110:B:VAL:HG23	5	0.15
(3,1278)	1:57:B:GLN:HG2	1:50:B:PRO:HD2	2	0.15
(3,1277)	1:57:A:GLN:HG2	1:50:A:PRO:HD2	2	0.15
(3,1067)	1:50:A:PRO:HA	1:54:A:ALA:HB1	2	0.15
(3,1010)	1:48:B:ASP:HB3	1:57:B:GLN:HB3	10	0.15
(3,929)	1:45:A:ILE:HG23	1:57:B:GLN:HG2	10	0.15
(3,854)	1:88:B:SER:HA	1:124:B:LYS:HE3	8	0.15
(3,735)	1:132:A:LEU:HG	1:134:A:GLY:H	2	0.15
(3,733)	1:120:A:ASP:HA	1:134:B:GLY:H	3	0.15
(3,695)	1:129:A:LYS:HB3	1:128:A:LEU:H	1	0.15
(3,579)	1:108:A:LYS:HG3	1:116:B:MET:H	10	0.15
(3,275)	1:73:A:GLN:HG2	1:79:A:GLN:H	1	0.15
(3,112)	1:98:B:LYS:HB3	1:51:A:ALA:H	10	0.15
(1,5661)	1:125:A:ALA:HA	1:125:A:ALA:HB2	10	0.15
(1,5649)	1:124:A:LYS:HA	1:124:A:LYS:HD3	5	0.15
(1,5607)	1:51:A:ALA:HB3	1:124:B:LYS:HA	10	0.15
(1,5538)	1:115:B:LEU:HD21	1:116:B:MET:HE1	10	0.15
(1,5537)	1:115:A:LEU:HD21	1:116:A:MET:HE1	10	0.15
(1,5530)	1:115:B:LEU:HD21	1:135:B:MET:HA	5	0.15
(1,5529)	1:115:A:LEU:HD21	1:135:A:MET:HA	5	0.15
(1,5514)	1:115:B:LEU:HB2	1:115:B:LEU:HG	5	0.15
(1,5514)	1:115:B:LEU:HB2	1:115:B:LEU:HG	8	0.15
(1,5514)	1:115:B:LEU:HB2	1:115:B:LEU:HG	9	0.15
(1,5513)	1:115:A:LEU:HB2	1:115:A:LEU:HG	3	0.15
(1,5513)	1:115:A:LEU:HB2	1:115:A:LEU:HG	5	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5513)	1:115:A:LEU:HB2	1:115:A:LEU:HG	7	0.15
(1,5513)	1:115:A:LEU:HB2	1:115:A:LEU:HG	8	0.15
(1,5290)	1:106:B:ALA:HA	1:106:B:ALA:HB1	1	0.15
(1,5290)	1:106:B:ALA:HA	1:106:B:ALA:HB3	2	0.15
(1,5290)	1:106:B:ALA:HA	1:106:B:ALA:HB2	3	0.15
(1,5290)	1:106:B:ALA:HA	1:106:B:ALA:HB3	4	0.15
(1,5290)	1:106:B:ALA:HA	1:106:B:ALA:HB1	5	0.15
(1,5290)	1:106:B:ALA:HA	1:106:B:ALA:HB3	6	0.15
(1,5290)	1:106:B:ALA:HA	1:106:B:ALA:HB3	7	0.15
(1,5290)	1:106:B:ALA:HA	1:106:B:ALA:HB1	8	0.15
(1,5290)	1:106:B:ALA:HA	1:106:B:ALA:HB3	9	0.15
(1,5289)	1:106:A:ALA:HA	1:106:A:ALA:HB1	1	0.15
(1,5289)	1:106:A:ALA:HA	1:106:A:ALA:HB3	2	0.15
(1,5289)	1:106:A:ALA:HA	1:106:A:ALA:HB2	3	0.15
(1,5289)	1:106:A:ALA:HA	1:106:A:ALA:HB3	4	0.15
(1,5289)	1:106:A:ALA:HA	1:106:A:ALA:HB1	5	0.15
(1,5289)	1:106:A:ALA:HA	1:106:A:ALA:HB3	6	0.15
(1,5289)	1:106:A:ALA:HA	1:106:A:ALA:HB3	7	0.15
(1,5289)	1:106:A:ALA:HA	1:106:A:ALA:HB1	8	0.15
(1,5289)	1:106:A:ALA:HA	1:106:A:ALA:HB3	9	0.15
(1,5257)	1:105:A:GLN:HG2	1:65:A:PHE:HB2	4	0.15
(1,5150)	1:100:B:THR:HG22	1:102:B:ILE:HD11	3	0.15
(1,5149)	1:100:A:THR:HG22	1:102:A:ILE:HD11	3	0.15
(1,5130)	1:102:B:ILE:HG22	1:102:B:ILE:HG13	10	0.15
(1,5129)	1:102:A:ILE:HG22	1:102:A:ILE:HG13	10	0.15
(1,5100)	1:102:B:ILE:HG13	1:102:B:ILE:HD12	1	0.15
(1,5100)	1:102:B:ILE:HG13	1:102:B:ILE:HD13	4	0.15
(1,5100)	1:102:B:ILE:HG13	1:102:B:ILE:HD12	5	0.15
(1,5100)	1:102:B:ILE:HG13	1:102:B:ILE:HD11	6	0.15
(1,5100)	1:102:B:ILE:HG13	1:102:B:ILE:HD11	7	0.15
(1,5100)	1:102:B:ILE:HG13	1:102:B:ILE:HD11	9	0.15
(1,5100)	1:102:B:ILE:HG13	1:102:B:ILE:HD13	10	0.15
(1,5099)	1:102:A:ILE:HG13	1:102:A:ILE:HD13	4	0.15
(1,5099)	1:102:A:ILE:HG13	1:102:A:ILE:HD12	5	0.15
(1,5099)	1:102:A:ILE:HG13	1:102:A:ILE:HD11	6	0.15
(1,5099)	1:102:A:ILE:HG13	1:102:A:ILE:HD11	7	0.15
(1,5099)	1:102:A:ILE:HG13	1:102:A:ILE:HD11	9	0.15
(1,5099)	1:102:A:ILE:HG13	1:102:A:ILE:HD13	10	0.15
(1,4942)	1:100:B:THR:HB	1:102:B:ILE:HD13	10	0.15
(1,4938)	1:100:B:THR:HB	1:100:B:THR:HG22	1	0.15
(1,4938)	1:100:B:THR:HB	1:100:B:THR:HG22	3	0.15
(1,4938)	1:100:B:THR:HB	1:100:B:THR:HG23	4	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4938)	1:100:B:THR:HB	1:100:B:THR:HG21	8	0.15
(1,4938)	1:100:B:THR:HB	1:100:B:THR:HG23	10	0.15
(1,4937)	1:100:A:THR:HB	1:100:A:THR:HG22	1	0.15
(1,4937)	1:100:A:THR:HB	1:100:A:THR:HG22	3	0.15
(1,4937)	1:100:A:THR:HB	1:100:A:THR:HG23	4	0.15
(1,4937)	1:100:A:THR:HB	1:100:A:THR:HG21	8	0.15
(1,4636)	1:90:B:LEU:HB2	1:64:B:VAL:HB	2	0.15
(1,4636)	1:90:B:LEU:HB2	1:64:B:VAL:HB	5	0.15
(1,4635)	1:90:A:LEU:HB2	1:64:A:VAL:HB	2	0.15
(1,4566)	1:87:B:THR:HG22	1:125:B:ALA:HB1	2	0.15
(1,4566)	1:87:B:THR:HG21	1:125:B:ALA:HB3	3	0.15
(1,4566)	1:87:B:THR:HG22	1:125:B:ALA:HB1	9	0.15
(1,4565)	1:87:A:THR:HG21	1:125:A:ALA:HB3	3	0.15
(1,4565)	1:87:A:THR:HG22	1:125:A:ALA:HB1	9	0.15
(1,4516)	1:128:B:LEU:HG	1:49:A:LEU:HB3	5	0.15
(1,4515)	1:128:A:LEU:HG	1:49:B:LEU:HB3	5	0.15
(1,4482)	1:86:B:LEU:HA	1:90:B:LEU:HG	1	0.15
(1,4481)	1:86:A:LEU:HA	1:90:A:LEU:HG	1	0.15
(1,4472)	1:86:B:LEU:HA	1:89:B:VAL:HB	2	0.15
(1,4471)	1:86:A:LEU:HA	1:89:A:VAL:HB	2	0.15
(1,4363)	1:82:A:ASN:HB3	1:85:A:GLN:HG2	1	0.15
(1,4358)	1:82:B:ASN:HB2	1:83:B:ALA:HB2	3	0.15
(1,4152)	1:123:B:ARG:HG2	1:51:A:ALA:HB2	2	0.15
(1,3972)	1:72:B:LYS:HB3	1:72:B:LYS:HD2	1	0.15
(1,3971)	1:72:A:LYS:HB3	1:72:A:LYS:HD2	1	0.15
(1,3722)	1:67:B:SER:HB3	1:69:B:LYS:HD2	9	0.15
(1,3690)	1:67:B:SER:HB2	1:115:B:LEU:HD12	6	0.15
(1,3689)	1:67:A:SER:HB2	1:115:A:LEU:HD12	6	0.15
(1,2974)	1:56:B:PRO:HD2	1:50:B:PRO:HD2	1	0.15
(1,2973)	1:56:A:PRO:HD2	1:50:A:PRO:HD2	1	0.15
(1,2923)	1:56:A:PRO:HA	1:50:A:PRO:HD2	4	0.15
(1,2734)	1:50:B:PRO:HG2	1:54:B:ALA:HB2	9	0.15
(1,2732)	1:50:B:PRO:HG2	1:44:A:ASP:HB3	3	0.15
(1,2680)	1:93:B:ARG:HG3	1:90:B:LEU:HA	2	0.15
(1,2623)	1:48:A:ASP:HB3	1:46:B:ARG:HB2	1	0.15
(1,2576)	1:98:B:LYS:HB2	1:98:B:LYS:HD3	3	0.15
(1,2575)	1:98:A:LYS:HB2	1:98:A:LYS:HD3	3	0.15
(1,2466)	1:88:B:SER:HA	1:87:B:THR:HG21	1	0.15
(1,2356)	1:82:B:ASN:HB3	1:82:B:ASN:HD22	8	0.15
(1,2355)	1:82:A:ASN:HB3	1:82:A:ASN:HD22	8	0.15
(1,2355)	1:82:A:ASN:HB3	1:82:A:ASN:HD22	10	0.15
(1,1650)	1:110:B:VAL:HG23	1:115:B:LEU:H	5	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1650)	1:110:B:VAL:HG21	1:115:B:LEU:H	6	0.15
(1,1649)	1:110:A:VAL:HG21	1:115:A:LEU:H	6	0.15
(1,1474)	1:122:B:LEU:HD13	1:122:B:LEU:H	10	0.15
(1,1473)	1:122:A:LEU:HD13	1:122:A:LEU:H	10	0.15
(1,1468)	1:100:B:THR:HG23	1:101:B:THR:H	5	0.15
(1,1467)	1:100:A:THR:HG23	1:101:A:THR:H	5	0.15
(1,1274)	1:94:B:THR:HG21	1:94:B:THR:H	6	0.15
(1,1273)	1:94:A:THR:HG22	1:94:A:THR:H	3	0.15
(1,1122)	1:110:B:VAL:HG23	1:114:B:THR:H	2	0.15
(1,1121)	1:110:A:VAL:HG23	1:114:A:THR:H	2	0.15
(1,1078)	1:88:B:SER:HB2	1:89:B:VAL:H	5	0.15
(1,1077)	1:88:A:SER:HB2	1:89:A:VAL:H	5	0.15
(1,1066)	1:87:B:THR:HG23	1:88:B:SER:H	8	0.15
(1,1065)	1:87:A:THR:HG23	1:88:A:SER:H	7	0.15
(1,1065)	1:87:A:THR:HG23	1:88:A:SER:H	8	0.15
(1,1036)	1:89:B:VAL:HG13	1:87:B:THR:H	9	0.15
(1,982)	1:85:B:GLN:HG2	1:85:B:GLN:H	10	0.15
(1,974)	1:85:B:GLN:HB3	1:85:B:GLN:H	2	0.15
(1,974)	1:85:B:GLN:HB3	1:85:B:GLN:H	5	0.15
(1,974)	1:85:B:GLN:HB3	1:85:B:GLN:H	7	0.15
(1,973)	1:85:A:GLN:HB3	1:85:A:GLN:H	2	0.15
(1,973)	1:85:A:GLN:HB3	1:85:A:GLN:H	3	0.15
(1,973)	1:85:A:GLN:HB3	1:85:A:GLN:H	5	0.15
(1,973)	1:85:A:GLN:HB3	1:85:A:GLN:H	7	0.15
(1,964)	1:83:B:ALA:HB1	1:84:B:ASP:H	4	0.15
(1,963)	1:83:A:ALA:HB2	1:84:A:ASP:H	2	0.15
(1,350)	1:54:B:ALA:HA	1:55:B:LYS:H	9	0.15
(1,270)	1:45:B:ILE:HG22	1:48:A:ASP:H	2	0.15
(1,2)	1:57:B:GLN:HG3	1:57:B:GLN:H	3	0.15
(1,2)	1:57:B:GLN:HG3	1:57:B:GLN:H	6	0.15
(1,2)	1:57:B:GLN:HG3	1:57:B:GLN:H	8	0.15
(1,1)	1:57:A:GLN:HG3	1:57:A:GLN:H	3	0.15
(1,1)	1:57:A:GLN:HG3	1:57:A:GLN:H	8	0.15
(3,2868)	1:121:B:THR:HA	1:121:B:THR:HG23	4	0.14
(3,2867)	1:121:A:THR:HA	1:121:A:THR:HG23	4	0.14
(3,2531)	1:102:A:ILE:HG23	1:133:A:VAL:HB	9	0.14
(3,2500)	1:101:B:THR:HG22	1:50:B:PRO:HB3	9	0.14
(3,2499)	1:101:A:THR:HG22	1:50:A:PRO:HB3	9	0.14
(3,2473)	1:53:A:SER:HB2	1:45:B:ILE:HD13	9	0.14
(3,2446)	1:100:B:THR:HG23	1:97:B:ASN:HB3	5	0.14
(3,2445)	1:100:A:THR:HG23	1:97:A:ASN:HB3	5	0.14
(3,2050)	1:119:B:MET:HG2	1:72:B:LYS:HA	10	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,2049)	1:119:A:MET:HG2	1:72:A:LYS:HA	10	0.14
(3,1896)	1:123:B:ARG:HG2	1:50:A:PRO:HB3	7	0.14
(3,1834)	1:72:B:LYS:HE2	1:110:B:VAL:HG21	9	0.14
(3,1833)	1:72:A:LYS:HE2	1:110:A:VAL:HG21	9	0.14
(3,1796)	1:72:B:LYS:HG2	1:72:B:LYS:HE2	3	0.14
(3,1795)	1:72:A:LYS:HG2	1:72:A:LYS:HE2	3	0.14
(3,1754)	1:69:B:LYS:HE3	1:71:B:ASP:HB2	9	0.14
(3,1753)	1:69:A:LYS:HE3	1:71:A:ASP:HB2	9	0.14
(3,1736)	1:69:B:LYS:HD2	1:108:B:LYS:HE2	8	0.14
(3,1735)	1:69:A:LYS:HD2	1:108:A:LYS:HE2	8	0.14
(3,1068)	1:50:B:PRO:HA	1:54:B:ALA:HB1	2	0.14
(3,1009)	1:48:A:ASP:HB3	1:57:A:GLN:HB3	10	0.14
(3,930)	1:45:B:ILE:HG23	1:57:A:GLN:HG2	10	0.14
(3,736)	1:132:B:LEU:HG	1:134:B:GLY:H	2	0.14
(3,696)	1:129:B:LYS:HB3	1:128:B:LEU:H	1	0.14
(3,696)	1:129:B:LYS:HB3	1:128:B:LEU:H	5	0.14
(3,695)	1:129:A:LYS:HB3	1:128:A:LEU:H	5	0.14
(3,580)	1:108:B:LYS:HG3	1:116:A:MET:H	4	0.14
(3,579)	1:108:A:LYS:HG3	1:116:B:MET:H	4	0.14
(1,5890)	1:65:B:PHE:HD2	1:101:B:THR:HB	3	0.14
(1,5828)	1:135:B:MET:HE3	1:135:B:MET:HA	1	0.14
(1,5732)	1:128:B:LEU:HA	1:49:A:LEU:HB3	2	0.14
(1,5402)	1:110:B:VAL:HG22	1:116:B:MET:HE2	7	0.14
(1,5401)	1:110:A:VAL:HG22	1:116:A:MET:HE2	7	0.14
(1,5290)	1:106:B:ALA:HA	1:106:B:ALA:HB1	10	0.14
(1,5289)	1:106:A:ALA:HA	1:106:A:ALA:HB1	10	0.14
(1,4941)	1:100:A:THR:HB	1:102:A:ILE:HD13	10	0.14
(1,4938)	1:100:B:THR:HB	1:100:B:THR:HG23	2	0.14
(1,4938)	1:100:B:THR:HB	1:100:B:THR:HG23	6	0.14
(1,4938)	1:100:B:THR:HB	1:100:B:THR:HG21	7	0.14
(1,4938)	1:100:B:THR:HB	1:100:B:THR:HG22	9	0.14
(1,4937)	1:100:A:THR:HB	1:100:A:THR:HG23	2	0.14
(1,4937)	1:100:A:THR:HB	1:100:A:THR:HG23	6	0.14
(1,4937)	1:100:A:THR:HB	1:100:A:THR:HG21	7	0.14
(1,4937)	1:100:A:THR:HB	1:100:A:THR:HG22	9	0.14
(1,4937)	1:100:A:THR:HB	1:100:A:THR:HG23	10	0.14
(1,4674)	1:91:B:ASP:HA	1:96:B:ALA:HA	1	0.14
(1,4635)	1:90:A:LEU:HB2	1:64:A:VAL:HB	5	0.14
(1,4574)	1:87:B:THR:HG22	1:90:B:LEU:HG	6	0.14
(1,4573)	1:87:A:THR:HG22	1:90:A:LEU:HG	6	0.14
(1,4566)	1:87:B:THR:HG23	1:125:B:ALA:HB2	1	0.14
(1,4565)	1:87:A:THR:HG23	1:125:A:ALA:HB2	1	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4565)	1:87:A:THR:HG22	1:125:A:ALA:HB1	2	0.14
(1,4534)	1:87:B:THR:HA	1:87:B:THR:HG21	5	0.14
(1,4534)	1:87:B:THR:HA	1:87:B:THR:HG22	6	0.14
(1,4533)	1:87:A:THR:HA	1:87:A:THR:HG21	5	0.14
(1,4533)	1:87:A:THR:HA	1:87:A:THR:HG22	6	0.14
(1,4482)	1:86:B:LEU:HA	1:90:B:LEU:HG	3	0.14
(1,4481)	1:86:A:LEU:HA	1:90:A:LEU:HG	3	0.14
(1,4398)	1:83:B:ALA:HA	1:121:B:THR:HG22	6	0.14
(1,4397)	1:83:A:ALA:HA	1:121:A:THR:HG22	6	0.14
(1,4364)	1:82:B:ASN:HB3	1:85:B:GLN:HG2	1	0.14
(1,4357)	1:82:A:ASN:HB2	1:83:A:ALA:HB2	3	0.14
(1,4112)	1:74:B:LEU:HA	1:110:B:VAL:HG11	3	0.14
(1,4111)	1:74:A:LEU:HA	1:110:A:VAL:HG11	3	0.14
(1,4051)	1:93:A:ARG:HB3	1:64:A:VAL:HA	3	0.14
(1,3462)	1:64:B:VAL:HB	1:102:B:ILE:HD13	2	0.14
(1,3461)	1:64:A:VAL:HB	1:102:A:ILE:HD13	2	0.14
(1,3460)	1:64:B:VAL:HB	1:102:B:ILE:HG21	7	0.14
(1,3459)	1:64:A:VAL:HB	1:102:A:ILE:HG21	7	0.14
(1,3210)	1:122:B:LEU:HA	1:87:B:THR:HB	7	0.14
(1,3209)	1:122:A:LEU:HA	1:87:A:THR:HB	7	0.14
(1,3164)	1:60:B:PRO:HG2	1:57:B:GLN:HA	9	0.14
(1,3163)	1:60:A:PRO:HG2	1:57:A:GLN:HA	9	0.14
(1,2852)	1:55:B:LYS:HA	1:55:B:LYS:HG3	2	0.14
(1,2851)	1:55:A:LYS:HA	1:55:A:LYS:HG3	2	0.14
(1,2733)	1:50:A:PRO:HG2	1:54:A:ALA:HB2	9	0.14
(1,2679)	1:93:A:ARG:HG3	1:90:A:LEU:HA	2	0.14
(1,2624)	1:48:B:ASP:HB3	1:46:A:ARG:HB2	1	0.14
(1,2513)	1:45:A:ILE:HD13	1:49:B:LEU:HA	5	0.14
(1,2466)	1:88:B:SER:HA	1:87:B:THR:HG22	10	0.14
(1,2465)	1:88:A:SER:HA	1:87:A:THR:HG21	1	0.14
(1,2456)	1:88:B:SER:HA	1:91:B:ASP:HB3	9	0.14
(1,2455)	1:88:A:SER:HA	1:91:A:ASP:HB3	9	0.14
(1,2356)	1:82:B:ASN:HB3	1:82:B:ASN:HD22	5	0.14
(1,2356)	1:82:B:ASN:HB3	1:82:B:ASN:HD22	7	0.14
(1,2356)	1:82:B:ASN:HB3	1:82:B:ASN:HD22	10	0.14
(1,2355)	1:82:A:ASN:HB3	1:82:A:ASN:HD22	7	0.14
(1,1474)	1:122:B:LEU:HD12	1:122:B:LEU:H	1	0.14
(1,1404)	1:99:B:GLU:HG2	1:99:B:GLU:H	4	0.14
(1,1274)	1:94:B:THR:HG21	1:94:B:THR:H	7	0.14
(1,1273)	1:94:A:THR:HG21	1:94:A:THR:H	7	0.14
(1,1070)	1:90:B:LEU:HB3	1:88:B:SER:H	9	0.14
(1,1069)	1:90:A:LEU:HB3	1:88:A:SER:H	9	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1066)	1:87:B:THR:HG23	1:88:B:SER:H	9	0.14
(1,1065)	1:87:A:THR:HG22	1:88:A:SER:H	4	0.14
(1,1065)	1:87:A:THR:HG23	1:88:A:SER:H	9	0.14
(1,1035)	1:89:A:VAL:HG13	1:87:A:THR:H	9	0.14
(1,964)	1:83:B:ALA:HB2	1:84:B:ASP:H	2	0.14
(1,964)	1:83:B:ALA:HB3	1:84:B:ASP:H	8	0.14
(1,963)	1:83:A:ALA:HB1	1:84:A:ASP:H	4	0.14
(1,349)	1:54:A:ALA:HA	1:55:A:LYS:H	8	0.14
(1,269)	1:45:A:ILE:HG22	1:48:B:ASP:H	2	0.14
(1,62)	1:85:B:GLN:HB3	1:82:B:ASN:H	7	0.14
(1,61)	1:85:A:GLN:HB3	1:82:A:ASN:H	7	0.14
(1,1)	1:57:A:GLN:HG3	1:57:A:GLN:H	6	0.14
(3,3044)	1:112:B:TYR:HD1	1:116:B:MET:HE3	5	0.13
(3,3043)	1:112:A:TYR:HD1	1:116:A:MET:HE3	5	0.13
(3,3006)	1:106:B:ALA:HB2	1:135:B:MET:HG2	6	0.13
(3,3005)	1:106:A:ALA:HB2	1:135:A:MET:HG2	6	0.13
(3,2974)	1:130:B:VAL:HB	1:119:B:MET:HE1	10	0.13
(3,2954)	1:128:B:LEU:HB3	1:122:B:LEU:HB2	7	0.13
(3,2953)	1:128:A:LEU:HB3	1:122:A:LEU:HB2	7	0.13
(3,2474)	1:53:B:SER:HB2	1:45:A:ILE:HD13	9	0.13
(3,2450)	1:100:B:THR:HG21	1:129:B:LYS:HE3	8	0.13
(3,2449)	1:100:A:THR:HG21	1:129:A:LYS:HE3	8	0.13
(3,2324)	1:127:B:TYR:HE2	1:98:B:LYS:HG2	3	0.13
(3,2323)	1:127:A:TYR:HE2	1:98:A:LYS:HG2	3	0.13
(3,2242)	1:98:B:LYS:HE3	1:94:B:THR:HG23	5	0.13
(3,2241)	1:98:A:LYS:HE3	1:94:A:THR:HG22	4	0.13
(3,2241)	1:98:A:LYS:HE3	1:94:A:THR:HG23	5	0.13
(3,2158)	1:127:B:TYR:HA	1:90:B:LEU:HG	2	0.13
(3,2157)	1:127:A:TYR:HA	1:90:A:LEU:HG	2	0.13
(3,2050)	1:119:B:MET:HG2	1:72:B:LYS:HA	1	0.13
(3,2050)	1:119:B:MET:HG2	1:72:B:LYS:HA	2	0.13
(3,2049)	1:119:A:MET:HG2	1:72:A:LYS:HA	1	0.13
(3,2049)	1:119:A:MET:HG2	1:72:A:LYS:HA	2	0.13
(3,2049)	1:119:A:MET:HG2	1:72:A:LYS:HA	8	0.13
(3,1990)	1:127:B:TYR:HA	1:87:B:THR:HB	10	0.13
(3,1989)	1:127:A:TYR:HA	1:87:A:THR:HB	10	0.13
(3,1956)	1:79:B:GLN:HG2	1:91:B:ASP:HB3	2	0.13
(3,1894)	1:123:B:ARG:HG2	1:124:B:LYS:HE3	5	0.13
(3,1893)	1:123:A:ARG:HG2	1:124:A:LYS:HE3	5	0.13
(3,1834)	1:72:B:LYS:HE2	1:110:B:VAL:HG23	2	0.13
(3,1833)	1:72:A:LYS:HE2	1:110:A:VAL:HG23	2	0.13
(3,1642)	1:115:B:LEU:HD12	1:131:B:GLY:HA3	9	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,1641)	1:115:A:LEU:HD12	1:131:A:GLY:HA3	9	0.13
(3,1535)	1:123:A:ARG:HG2	1:50:B:PRO:HD2	5	0.13
(3,126)	1:56:B:PRO:HG2	1:57:B:GLN:H	8	0.13
(3,125)	1:56:A:PRO:HG2	1:57:A:GLN:H	8	0.13
(1,5919)	1:104:A:PHE:HD2	1:115:A:LEU:HD12	2	0.13
(1,5889)	1:65:A:PHE:HD2	1:101:A:THR:HB	3	0.13
(1,5827)	1:135:A:MET:HE3	1:135:A:MET:HA	1	0.13
(1,5608)	1:51:B:ALA:HB2	1:124:A:LYS:HA	1	0.13
(1,5607)	1:51:A:ALA:HB2	1:124:B:LYS:HA	1	0.13
(1,5258)	1:105:B:GLN:HG2	1:65:B:PHE:HB2	10	0.13
(1,5257)	1:105:A:GLN:HG2	1:65:A:PHE:HB2	10	0.13
(1,4804)	1:96:B:ALA:HB1	1:127:B:TYR:HE1	5	0.13
(1,4803)	1:96:A:ALA:HB1	1:127:A:TYR:HE1	5	0.13
(1,4770)	1:94:B:THR:HG23	1:102:B:ILE:HG13	6	0.13
(1,4769)	1:94:A:THR:HG23	1:102:A:ILE:HG13	6	0.13
(1,4673)	1:91:A:ASP:HA	1:96:A:ALA:HA	1	0.13
(1,4636)	1:90:B:LEU:HB2	1:64:B:VAL:HB	9	0.13
(1,4635)	1:90:A:LEU:HB2	1:64:A:VAL:HB	9	0.13
(1,4568)	1:87:B:THR:HG22	1:124:B:LYS:HD2	8	0.13
(1,4567)	1:87:A:THR:HG22	1:124:A:LYS:HD2	8	0.13
(1,4514)	1:86:B:LEU:HG	1:86:B:LEU:HB2	2	0.13
(1,4514)	1:86:B:LEU:HG	1:86:B:LEU:HB2	3	0.13
(1,4514)	1:86:B:LEU:HG	1:86:B:LEU:HB2	4	0.13
(1,4514)	1:86:B:LEU:HG	1:86:B:LEU:HB2	7	0.13
(1,4514)	1:86:B:LEU:HG	1:86:B:LEU:HB2	10	0.13
(1,4513)	1:86:A:LEU:HG	1:86:A:LEU:HB2	2	0.13
(1,4513)	1:86:A:LEU:HG	1:86:A:LEU:HB2	3	0.13
(1,4513)	1:86:A:LEU:HG	1:86:A:LEU:HB2	4	0.13
(1,4513)	1:86:A:LEU:HG	1:86:A:LEU:HB2	7	0.13
(1,4513)	1:86:A:LEU:HG	1:86:A:LEU:HB2	9	0.13
(1,4513)	1:86:A:LEU:HG	1:86:A:LEU:HB2	10	0.13
(1,4326)	1:127:B:TYR:HA	1:90:B:LEU:HG	2	0.13
(1,4325)	1:127:A:TYR:HA	1:90:A:LEU:HG	2	0.13
(1,4182)	1:98:B:LYS:HE2	1:96:B:ALA:HA	6	0.13
(1,4181)	1:98:A:LYS:HE2	1:96:A:ALA:HA	6	0.13
(1,4052)	1:93:B:ARG:HB3	1:64:B:VAL:HA	3	0.13
(1,3838)	1:69:B:LYS:HG3	1:115:B:LEU:HD13	9	0.13
(1,3837)	1:69:A:LYS:HG3	1:115:A:LEU:HD13	9	0.13
(1,3354)	1:122:B:LEU:HG	1:119:B:MET:HB2	6	0.13
(1,3353)	1:122:A:LEU:HG	1:119:A:MET:HB2	6	0.13
(1,2852)	1:55:B:LYS:HA	1:55:B:LYS:HG3	3	0.13
(1,2851)	1:55:A:LYS:HA	1:55:A:LYS:HG3	3	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2680)	1:93:B:ARG:HG3	1:90:B:LEU:HA	3	0.13
(1,2679)	1:93:A:ARG:HG3	1:90:A:LEU:HA	3	0.13
(1,2514)	1:45:B:ILE:HD13	1:49:A:LEU:HA	5	0.13
(1,2466)	1:88:B:SER:HA	1:87:B:THR:HG22	3	0.13
(1,2465)	1:88:A:SER:HA	1:87:A:THR:HG22	3	0.13
(1,2465)	1:88:A:SER:HA	1:87:A:THR:HG22	10	0.13
(1,2355)	1:82:A:ASN:HB3	1:82:A:ASN:HD22	5	0.13
(1,2268)	1:138:B:ALA:HB2	1:138:B:ALA:H	10	0.13
(1,2267)	1:138:A:ALA:HB2	1:138:A:ALA:H	10	0.13
(1,1688)	1:139:B:ALA:HA	1:140:B:LYS:H	9	0.13
(1,1688)	1:139:B:ALA:HA	1:140:B:LYS:H	10	0.13
(1,1687)	1:139:A:ALA:HA	1:140:A:LYS:H	9	0.13
(1,1687)	1:139:A:ALA:HA	1:140:A:LYS:H	10	0.13
(1,1526)	1:66:B:LEU:HB2	1:104:B:PHE:H	9	0.13
(1,1525)	1:66:A:LEU:HB2	1:104:A:PHE:H	9	0.13
(1,1474)	1:122:B:LEU:HD13	1:122:B:LEU:H	7	0.13
(1,1473)	1:122:A:LEU:HD12	1:122:A:LEU:H	1	0.13
(1,1473)	1:122:A:LEU:HD13	1:122:A:LEU:H	7	0.13
(1,1468)	1:100:B:THR:HG21	1:101:B:THR:H	9	0.13
(1,1404)	1:99:B:GLU:HG2	1:99:B:GLU:H	1	0.13
(1,1403)	1:99:A:GLU:HG2	1:99:A:GLU:H	1	0.13
(1,1403)	1:99:A:GLU:HG2	1:99:A:GLU:H	4	0.13
(1,1077)	1:88:A:SER:HB2	1:89:A:VAL:H	8	0.13
(1,1066)	1:87:B:THR:HG22	1:88:B:SER:H	4	0.13
(1,974)	1:85:B:GLN:HB3	1:85:B:GLN:H	4	0.13
(1,974)	1:85:B:GLN:HB3	1:85:B:GLN:H	9	0.13
(1,973)	1:85:A:GLN:HB3	1:85:A:GLN:H	4	0.13
(1,973)	1:85:A:GLN:HB3	1:85:A:GLN:H	9	0.13
(1,963)	1:83:A:ALA:HB3	1:84:A:ASP:H	8	0.13
(1,944)	1:121:B:THR:HB	1:84:B:ASP:H	9	0.13
(1,943)	1:121:A:THR:HB	1:84:A:ASP:H	9	0.13
(1,761)	1:110:A:VAL:HG11	1:74:A:LEU:H	9	0.13
(1,434)	1:61:B:GLU:HB2	1:61:B:GLU:H	3	0.13
(1,433)	1:61:A:GLU:HB2	1:61:A:GLU:H	3	0.13
(1,382)	1:55:B:LYS:HB3	1:57:B:GLN:H	10	0.13
(1,381)	1:55:A:LYS:HB3	1:57:A:GLN:H	10	0.13
(1,350)	1:54:B:ALA:HA	1:55:B:LYS:H	8	0.13
(1,254)	1:45:B:ILE:HG21	1:47:B:VAL:H	5	0.13
(1,253)	1:45:A:ILE:HG21	1:47:A:VAL:H	5	0.13
(3,3039)	1:112:A:TYR:HD1	1:109:B:SER:HB2	9	0.12
(3,2973)	1:130:A:VAL:HB	1:119:A:MET:HE1	10	0.12
(3,2924)	1:126:B:GLY:HA3	1:120:B:ASP:HA	5	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,2923)	1:126:A:GLY:HA3	1:120:A:ASP:HA	5	0.12
(3,2875)	1:121:A:THR:HG21	1:124:A:LYS:HG2	1	0.12
(3,2868)	1:121:B:THR:HA	1:121:B:THR:HG23	8	0.12
(3,2867)	1:121:A:THR:HA	1:121:A:THR:HG23	8	0.12
(3,2856)	1:119:B:MET:HE3	1:104:B:PHE:HB3	9	0.12
(3,2855)	1:119:A:MET:HE3	1:104:A:PHE:HB3	9	0.12
(3,2850)	1:119:B:MET:HE2	1:103:B:PHE:HA	8	0.12
(3,2849)	1:119:A:MET:HE2	1:103:A:PHE:HA	8	0.12
(3,2556)	1:103:B:PHE:HA	1:45:A:ILE:HG21	5	0.12
(3,2555)	1:103:A:PHE:HA	1:45:B:ILE:HG21	5	0.12
(3,2466)	1:100:B:THR:HG23	1:102:B:ILE:HD12	2	0.12
(3,2314)	1:94:B:THR:HG23	1:97:B:ASN:HB3	6	0.12
(3,2313)	1:94:A:THR:HG23	1:97:A:ASN:HB3	6	0.12
(3,2158)	1:127:B:TYR:HA	1:90:B:LEU:HG	5	0.12
(3,2157)	1:127:A:TYR:HA	1:90:A:LEU:HG	5	0.12
(3,2050)	1:119:B:MET:HG2	1:72:B:LYS:HA	8	0.12
(3,1955)	1:79:A:GLN:HG2	1:91:A:ASP:HB3	2	0.12
(3,1745)	1:69:A:LYS:HE2	1:105:A:GLN:HA	6	0.12
(3,1279)	1:57:A:GLN:HG2	1:60:A:PRO:HG3	10	0.12
(3,1109)	1:139:A:ALA:HA	1:140:A:LYS:HD3	2	0.12
(3,1104)	1:139:B:ALA:HA	1:136:B:GLU:HB2	8	0.12
(3,1103)	1:139:A:ALA:HA	1:136:A:GLU:HB2	8	0.12
(3,994)	1:47:B:VAL:HB	1:116:A:MET:HG3	5	0.12
(3,750)	1:135:B:MET:HB2	1:136:B:GLU:H	1	0.12
(3,749)	1:135:A:MET:HB2	1:136:A:GLU:H	1	0.12
(3,735)	1:132:A:LEU:HG	1:134:A:GLY:H	3	0.12
(3,362)	1:102:B:ILE:HA	1:91:B:ASP:H	9	0.12
(3,361)	1:102:A:ILE:HA	1:91:A:ASP:H	9	0.12
(1,5920)	1:104:B:PHE:HD2	1:115:B:LEU:HD12	2	0.12
(1,5908)	1:65:B:PHE:HE1	1:100:B:THR:HG21	4	0.12
(1,5907)	1:65:A:PHE:HE1	1:100:A:THR:HG21	4	0.12
(1,5376)	1:110:B:VAL:HB	1:112:B:TYR:HB3	4	0.12
(1,5375)	1:110:A:VAL:HB	1:112:A:TYR:HB3	4	0.12
(1,5250)	1:105:B:GLN:HG3	1:102:B:ILE:HD12	8	0.12
(1,5249)	1:105:A:GLN:HG3	1:102:A:ILE:HD12	8	0.12
(1,5150)	1:100:B:THR:HG23	1:102:B:ILE:HD11	4	0.12
(1,5149)	1:100:A:THR:HG23	1:102:A:ILE:HD11	4	0.12
(1,5022)	1:101:B:THR:HG23	1:130:B:VAL:HA	5	0.12
(1,5021)	1:101:A:THR:HG23	1:130:A:VAL:HA	5	0.12
(1,4754)	1:94:B:THR:HG23	1:97:B:ASN:HB3	6	0.12
(1,4753)	1:94:A:THR:HG23	1:97:A:ASN:HB3	6	0.12
(1,4566)	1:87:B:THR:HG23	1:125:B:ALA:HB2	10	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4565)	1:87:A:THR:HG23	1:125:A:ALA:HB2	10	0.12
(1,4514)	1:86:B:LEU:HG	1:86:B:LEU:HB2	1	0.12
(1,4514)	1:86:B:LEU:HG	1:86:B:LEU:HB2	5	0.12
(1,4514)	1:86:B:LEU:HG	1:86:B:LEU:HB2	6	0.12
(1,4514)	1:86:B:LEU:HG	1:86:B:LEU:HB2	8	0.12
(1,4514)	1:86:B:LEU:HG	1:86:B:LEU:HB2	9	0.12
(1,4513)	1:86:A:LEU:HG	1:86:A:LEU:HB2	1	0.12
(1,4513)	1:86:A:LEU:HG	1:86:A:LEU:HB2	5	0.12
(1,4513)	1:86:A:LEU:HG	1:86:A:LEU:HB2	6	0.12
(1,4513)	1:86:A:LEU:HG	1:86:A:LEU:HB2	8	0.12
(1,4481)	1:86:A:LEU:HA	1:90:A:LEU:HG	8	0.12
(1,4472)	1:86:B:LEU:HA	1:89:B:VAL:HB	8	0.12
(1,4472)	1:86:B:LEU:HA	1:89:B:VAL:HB	9	0.12
(1,4326)	1:127:B:TYR:HA	1:90:B:LEU:HG	5	0.12
(1,4325)	1:127:A:TYR:HA	1:90:A:LEU:HG	5	0.12
(1,4151)	1:123:A:ARG:HG2	1:51:B:ALA:HB2	2	0.12
(1,4112)	1:74:B:LEU:HA	1:110:B:VAL:HG11	5	0.12
(1,4111)	1:74:A:LEU:HA	1:110:A:VAL:HG11	5	0.12
(1,3972)	1:72:B:LYS:HB3	1:72:B:LYS:HD2	8	0.12
(1,3971)	1:72:A:LYS:HB3	1:72:A:LYS:HD2	8	0.12
(1,3462)	1:64:B:VAL:HB	1:102:B:ILE:HD13	7	0.12
(1,3461)	1:64:A:VAL:HB	1:102:A:ILE:HD13	7	0.12
(1,2852)	1:55:B:LYS:HA	1:55:B:LYS:HG3	1	0.12
(1,2851)	1:55:A:LYS:HA	1:55:A:LYS:HG3	1	0.12
(1,2514)	1:45:B:ILE:HD11	1:49:A:LEU:HA	3	0.12
(1,2267)	1:138:A:ALA:HB1	1:138:A:ALA:H	9	0.12
(1,2212)	1:45:B:ILE:H	1:135:A:MET:H	6	0.12
(1,1526)	1:66:B:LEU:HB2	1:104:B:PHE:H	7	0.12
(1,1525)	1:66:A:LEU:HB2	1:104:A:PHE:H	7	0.12
(1,1467)	1:100:A:THR:HG21	1:101:A:THR:H	9	0.12
(1,1406)	1:99:B:GLU:HB3	1:99:B:GLU:H	4	0.12
(1,1406)	1:99:B:GLU:HB3	1:99:B:GLU:H	9	0.12
(1,1405)	1:99:A:GLU:HB3	1:99:A:GLU:H	4	0.12
(1,1405)	1:99:A:GLU:HB3	1:99:A:GLU:H	9	0.12
(1,1078)	1:88:B:SER:HB2	1:89:B:VAL:H	8	0.12
(1,974)	1:85:B:GLN:HB3	1:85:B:GLN:H	6	0.12
(1,974)	1:85:B:GLN:HB3	1:85:B:GLN:H	10	0.12
(1,973)	1:85:A:GLN:HB3	1:85:A:GLN:H	10	0.12
(1,928)	1:82:B:ASN:HB2	1:83:B:ALA:H	2	0.12
(1,927)	1:82:A:ASN:HB2	1:83:A:ALA:H	2	0.12
(1,824)	1:79:B:GLN:HB2	1:76:B:VAL:H	7	0.12
(1,762)	1:110:B:VAL:HG11	1:74:B:LEU:H	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,434)	1:61:B:GLU:HB2	1:61:B:GLU:H	1	0.12
(1,434)	1:61:B:GLU:HB2	1:61:B:GLU:H	8	0.12
(1,434)	1:61:B:GLU:HB2	1:61:B:GLU:H	10	0.12
(1,433)	1:61:A:GLU:HB2	1:61:A:GLU:H	1	0.12
(1,433)	1:61:A:GLU:HB2	1:61:A:GLU:H	8	0.12
(1,433)	1:61:A:GLU:HB2	1:61:A:GLU:H	9	0.12
(1,62)	1:85:B:GLN:HB3	1:82:B:ASN:H	3	0.12
(1,61)	1:85:A:GLN:HB3	1:82:A:ASN:H	3	0.12
(1,20)	1:105:B:GLN:HG2	1:105:B:GLN:HE22	10	0.12
(3,2930)	1:126:B:GLY:HA2	1:91:B:ASP:HA	9	0.11
(3,2929)	1:126:A:GLY:HA2	1:91:A:ASP:HA	9	0.11
(3,2876)	1:121:B:THR:HG21	1:124:B:LYS:HG2	1	0.11
(3,2850)	1:119:B:MET:HE2	1:103:B:PHE:HA	3	0.11
(3,2849)	1:119:A:MET:HE2	1:103:A:PHE:HA	3	0.11
(3,2556)	1:103:B:PHE:HA	1:45:A:ILE:HG22	2	0.11
(3,2542)	1:102:B:ILE:HD11	1:95:B:GLN:HG2	7	0.11
(3,2542)	1:102:B:ILE:HD11	1:61:B:GLU:HG3	10	0.11
(3,2541)	1:102:A:ILE:HD11	1:95:A:GLN:HG2	7	0.11
(3,2465)	1:100:A:THR:HG23	1:102:A:ILE:HD12	2	0.11
(3,2456)	1:100:B:THR:HG23	1:129:B:LYS:HB3	4	0.11
(3,2242)	1:98:B:LYS:HE3	1:94:B:THR:HG22	4	0.11
(3,2242)	1:98:B:LYS:HE3	1:94:B:THR:HG23	6	0.11
(3,2241)	1:98:A:LYS:HE3	1:94:A:THR:HG23	6	0.11
(3,1895)	1:123:A:ARG:HG2	1:50:B:PRO:HB3	7	0.11
(3,1892)	1:74:B:LEU:HB3	1:86:B:LEU:HB3	6	0.11
(3,1892)	1:74:B:LEU:HB3	1:86:B:LEU:HB3	8	0.11
(3,1891)	1:74:A:LEU:HB3	1:86:A:LEU:HB3	6	0.11
(3,1891)	1:74:A:LEU:HB3	1:86:A:LEU:HB3	8	0.11
(3,1746)	1:69:B:LYS:HE2	1:105:B:GLN:HA	6	0.11
(3,1710)	1:68:B:VAL:HB	1:71:B:ASP:HB2	6	0.11
(3,1709)	1:68:A:VAL:HB	1:71:A:ASP:HB2	6	0.11
(3,1280)	1:57:B:GLN:HG2	1:60:B:PRO:HG3	10	0.11
(3,1279)	1:57:A:GLN:HG2	1:60:A:PRO:HG3	5	0.11
(3,1192)	1:108:B:LYS:HE3	1:108:B:LYS:HD2	3	0.11
(3,1192)	1:108:B:LYS:HE2	1:108:B:LYS:HD3	5	0.11
(3,1192)	1:108:B:LYS:HE3	1:108:B:LYS:HD2	8	0.11
(3,1191)	1:108:A:LYS:HE3	1:108:A:LYS:HD2	3	0.11
(3,1191)	1:108:A:LYS:HE2	1:108:A:LYS:HD3	5	0.11
(3,1191)	1:108:A:LYS:HE3	1:108:A:LYS:HD2	8	0.11
(3,1110)	1:139:B:ALA:HA	1:140:B:LYS:HD3	2	0.11
(3,993)	1:47:A:VAL:HB	1:116:B:MET:HG3	5	0.11
(3,736)	1:132:B:LEU:HG	1:134:B:GLY:H	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,620)	1:124:B:LYS:HE2	1:120:B:ASP:H	4	0.11
(3,619)	1:124:A:LYS:HE2	1:120:A:ASP:H	4	0.11
(3,430)	1:95:B:GLN:HB3	1:99:B:GLU:H	2	0.11
(3,429)	1:95:A:GLN:HB3	1:99:A:GLU:H	2	0.11
(1,5908)	1:65:B:PHE:HE2	1:100:B:THR:HG21	6	0.11
(1,5907)	1:65:A:PHE:HE2	1:100:A:THR:HG21	6	0.11
(1,5622)	1:119:B:MET:HE2	1:121:B:THR:HB	2	0.11
(1,5621)	1:119:A:MET:HE2	1:121:A:THR:HB	2	0.11
(1,5614)	1:121:B:THR:HA	1:124:B:LYS:HE3	2	0.11
(1,5613)	1:121:A:THR:HA	1:124:A:LYS:HE3	2	0.11
(1,5554)	1:116:B:MET:HE3	1:114:B:THR:HA	7	0.11
(1,5553)	1:116:A:MET:HE3	1:114:A:THR:HA	7	0.11
(1,5402)	1:110:B:VAL:HG23	1:116:B:MET:HE1	10	0.11
(1,5401)	1:110:A:VAL:HG23	1:116:A:MET:HE1	10	0.11
(1,5376)	1:110:B:VAL:HB	1:112:B:TYR:HB3	3	0.11
(1,5375)	1:110:A:VAL:HB	1:112:A:TYR:HB3	3	0.11
(1,5084)	1:102:B:ILE:HB	1:102:B:ILE:HG21	2	0.11
(1,5084)	1:102:B:ILE:HB	1:102:B:ILE:HG23	5	0.11
(1,5084)	1:102:B:ILE:HB	1:102:B:ILE:HG21	6	0.11
(1,5083)	1:102:A:ILE:HB	1:102:A:ILE:HG21	2	0.11
(1,5083)	1:102:A:ILE:HB	1:102:A:ILE:HG23	5	0.11
(1,5083)	1:102:A:ILE:HB	1:102:A:ILE:HG21	6	0.11
(1,4636)	1:90:B:LEU:HB2	1:64:B:VAL:HB	3	0.11
(1,4635)	1:90:A:LEU:HB2	1:64:A:VAL:HB	3	0.11
(1,4569)	1:86:A:LEU:HB3	1:87:A:THR:HG23	5	0.11
(1,4569)	1:86:A:LEU:HB3	1:87:A:THR:HG22	10	0.11
(1,4482)	1:86:B:LEU:HA	1:90:B:LEU:HG	8	0.11
(1,4472)	1:86:B:LEU:HA	1:89:B:VAL:HB	3	0.11
(1,4471)	1:86:A:LEU:HA	1:89:A:VAL:HB	3	0.11
(1,4471)	1:86:A:LEU:HA	1:89:A:VAL:HB	8	0.11
(1,4471)	1:86:A:LEU:HA	1:89:A:VAL:HB	9	0.11
(1,4154)	1:123:B:ARG:HG2	1:49:A:LEU:HB3	10	0.11
(1,3972)	1:72:B:LYS:HB3	1:72:B:LYS:HD2	3	0.11
(1,3971)	1:72:A:LYS:HB3	1:72:A:LYS:HD2	3	0.11
(1,3730)	1:67:B:SER:HB3	1:115:B:LEU:HD12	1	0.11
(1,3729)	1:67:A:SER:HB3	1:115:A:LEU:HD12	1	0.11
(1,3612)	1:115:B:LEU:HD12	1:106:B:ALA:HB1	10	0.11
(1,3611)	1:115:A:LEU:HD12	1:106:A:ALA:HB1	10	0.11
(1,3274)	1:61:B:GLU:HG2	1:62:B:LYS:HG2	10	0.11
(1,3273)	1:61:A:GLU:HG2	1:62:A:LYS:HG2	10	0.11
(1,2920)	1:56:B:PRO:HA	1:45:A:ILE:HA	1	0.11
(1,2919)	1:56:A:PRO:HA	1:45:B:ILE:HA	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2852)	1:55:B:LYS:HA	1:55:B:LYS:HG3	4	0.11
(1,2852)	1:55:B:LYS:HA	1:55:B:LYS:HG3	5	0.11
(1,2852)	1:55:B:LYS:HA	1:55:B:LYS:HG3	6	0.11
(1,2852)	1:55:B:LYS:HA	1:55:B:LYS:HG3	10	0.11
(1,2851)	1:55:A:LYS:HA	1:55:A:LYS:HG3	4	0.11
(1,2851)	1:55:A:LYS:HA	1:55:A:LYS:HG3	5	0.11
(1,2851)	1:55:A:LYS:HA	1:55:A:LYS:HG3	6	0.11
(1,2851)	1:55:A:LYS:HA	1:55:A:LYS:HG3	10	0.11
(1,2731)	1:50:A:PRO:HG2	1:44:B:ASP:HB3	3	0.11
(1,2680)	1:93:B:ARG:HG3	1:90:B:LEU:HA	5	0.11
(1,2679)	1:93:A:ARG:HG3	1:90:A:LEU:HA	5	0.11
(1,2268)	1:138:B:ALA:HB1	1:138:B:ALA:H	6	0.11
(1,2268)	1:138:B:ALA:HB1	1:138:B:ALA:H	9	0.11
(1,2267)	1:138:A:ALA:HB1	1:138:A:ALA:H	6	0.11
(1,1688)	1:139:B:ALA:HA	1:140:B:LYS:H	7	0.11
(1,1649)	1:110:A:VAL:HG23	1:115:A:LEU:H	10	0.11
(1,1512)	1:101:B:THR:HG21	1:102:B:ILE:H	2	0.11
(1,1511)	1:101:A:THR:HG21	1:102:A:ILE:H	2	0.11
(1,1406)	1:99:B:GLU:HB3	1:99:B:GLU:H	6	0.11
(1,1406)	1:99:B:GLU:HB3	1:99:B:GLU:H	8	0.11
(1,1406)	1:99:B:GLU:HB3	1:99:B:GLU:H	10	0.11
(1,1405)	1:99:A:GLU:HB3	1:99:A:GLU:H	6	0.11
(1,1405)	1:99:A:GLU:HB3	1:99:A:GLU:H	8	0.11
(1,1405)	1:99:A:GLU:HB3	1:99:A:GLU:H	10	0.11
(1,1404)	1:99:B:GLU:HG2	1:99:B:GLU:H	7	0.11
(1,1403)	1:99:A:GLU:HG2	1:99:A:GLU:H	7	0.11
(1,1124)	1:89:B:VAL:HG23	1:90:B:LEU:H	4	0.11
(1,1123)	1:89:A:VAL:HG23	1:90:A:LEU:H	4	0.11
(1,1122)	1:110:B:VAL:HG21	1:114:B:THR:H	9	0.11
(1,1078)	1:88:B:SER:HB2	1:89:B:VAL:H	9	0.11
(1,1077)	1:88:A:SER:HB2	1:89:A:VAL:H	9	0.11
(1,1066)	1:87:B:THR:HG21	1:88:B:SER:H	1	0.11
(1,974)	1:85:B:GLN:HB3	1:85:B:GLN:H	8	0.11
(1,973)	1:85:A:GLN:HB3	1:85:A:GLN:H	6	0.11
(1,973)	1:85:A:GLN:HB3	1:85:A:GLN:H	8	0.11
(1,928)	1:82:B:ASN:HB2	1:83:B:ALA:H	9	0.11
(1,927)	1:82:A:ASN:HB2	1:83:A:ALA:H	9	0.11
(1,823)	1:79:A:GLN:HB2	1:76:A:VAL:H	7	0.11
(1,434)	1:61:B:GLU:HB2	1:61:B:GLU:H	5	0.11
(1,434)	1:61:B:GLU:HB2	1:61:B:GLU:H	9	0.11
(1,433)	1:61:A:GLU:HB2	1:61:A:GLU:H	5	0.11
(1,433)	1:61:A:GLU:HB2	1:61:A:GLU:H	6	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,433)	1:61:A:GLU:HB2	1:61:A:GLU:H	10	0.11
(1,62)	1:85:B:GLN:HB3	1:82:B:ASN:H	5	0.11
(1,61)	1:85:A:GLN:HB3	1:82:A:ASN:H	5	0.11
(1,19)	1:105:A:GLN:HG2	1:105:A:GLN:HE22	10	0.11
(3,3040)	1:112:B:TYR:HD1	1:109:A:SER:HB2	9	0.1
(3,2930)	1:126:B:GLY:HA2	1:91:B:ASP:HA	3	0.1
(3,2905)	1:124:A:LYS:HD2	1:121:A:THR:HA	2	0.1
(3,2824)	1:115:B:LEU:HD23	1:116:B:MET:HG3	8	0.1
(3,2823)	1:115:A:LEU:HD23	1:116:A:MET:HG3	8	0.1
(3,2780)	1:124:B:LYS:HG2	1:124:B:LYS:HA	4	0.1
(3,2779)	1:124:A:LYS:HG2	1:124:A:LYS:HA	4	0.1
(3,2713)	1:109:A:SER:HB3	1:72:A:LYS:HE3	8	0.1
(3,2493)	1:101:A:THR:HG22	1:129:A:LYS:HE2	8	0.1
(3,2465)	1:100:A:THR:HG21	1:102:A:ILE:HD13	5	0.1
(3,2455)	1:100:A:THR:HG23	1:129:A:LYS:HB3	4	0.1
(3,1892)	1:74:B:LEU:HB3	1:86:B:LEU:HB3	4	0.1
(3,1891)	1:74:A:LEU:HB3	1:86:A:LEU:HB3	4	0.1
(3,1553)	1:64:A:VAL:HA	1:61:A:GLU:HG2	1	0.1
(3,1280)	1:57:B:GLN:HG2	1:60:B:PRO:HG3	5	0.1
(3,1192)	1:108:B:LYS:HE2	1:108:B:LYS:HD3	4	0.1
(3,1192)	1:108:B:LYS:HE3	1:108:B:LYS:HD3	7	0.1
(3,1191)	1:108:A:LYS:HE2	1:108:A:LYS:HD3	4	0.1
(3,1191)	1:108:A:LYS:HE2	1:108:A:LYS:HD3	6	0.1
(3,1191)	1:108:A:LYS:HE3	1:108:A:LYS:HD3	7	0.1
(3,1068)	1:50:B:PRO:HA	1:54:B:ALA:HB1	7	0.1
(3,1067)	1:50:A:PRO:HA	1:54:A:ALA:HB1	7	0.1
(3,845)	1:44:A:ASP:HA	1:116:A:MET:HG3	8	0.1
(3,736)	1:132:B:LEU:HG	1:134:B:GLY:H	5	0.1
(1,5614)	1:121:B:THR:HA	1:124:B:LYS:HE3	7	0.1
(1,5613)	1:121:A:THR:HA	1:124:A:LYS:HE3	7	0.1
(1,5084)	1:102:B:ILE:HB	1:102:B:ILE:HG21	1	0.1
(1,5084)	1:102:B:ILE:HB	1:102:B:ILE:HG21	8	0.1
(1,5084)	1:102:B:ILE:HB	1:102:B:ILE:HG23	9	0.1
(1,5084)	1:102:B:ILE:HB	1:102:B:ILE:HG21	10	0.1
(1,5083)	1:102:A:ILE:HB	1:102:A:ILE:HG21	1	0.1
(1,5083)	1:102:A:ILE:HB	1:102:A:ILE:HG21	8	0.1
(1,5083)	1:102:A:ILE:HB	1:102:A:ILE:HG23	9	0.1
(1,4862)	1:98:B:LYS:HD3	1:127:B:TYR:HB2	10	0.1
(1,4861)	1:98:A:LYS:HD3	1:127:A:TYR:HB2	10	0.1
(1,4570)	1:86:B:LEU:HB3	1:87:B:THR:HG23	5	0.1
(1,4570)	1:86:B:LEU:HB3	1:87:B:THR:HG22	10	0.1
(1,4398)	1:83:B:ALA:HA	1:121:B:THR:HG23	1	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4397)	1:83:A:ALA:HA	1:121:A:THR:HG23	1	0.1
(1,4153)	1:123:A:ARG:HG2	1:49:B:LEU:HB3	10	0.1
(1,3729)	1:67:A:SER:HB3	1:115:A:LEU:HD11	7	0.1
(1,3612)	1:115:B:LEU:HD12	1:106:B:ALA:HB2	3	0.1
(1,3611)	1:115:A:LEU:HD12	1:106:A:ALA:HB2	3	0.1
(1,2919)	1:56:A:PRO:HA	1:45:B:ILE:HA	3	0.1
(1,2919)	1:56:A:PRO:HA	1:45:B:ILE:HA	7	0.1
(1,2852)	1:55:B:LYS:HA	1:55:B:LYS:HG3	7	0.1
(1,2852)	1:55:B:LYS:HA	1:55:B:LYS:HG3	8	0.1
(1,2851)	1:55:A:LYS:HA	1:55:A:LYS:HG3	7	0.1
(1,2851)	1:55:A:LYS:HA	1:55:A:LYS:HG3	8	0.1
(1,2678)	1:124:B:LYS:HG2	1:124:B:LYS:HA	4	0.1
(1,2677)	1:124:A:LYS:HG2	1:124:A:LYS:HA	4	0.1
(1,2513)	1:45:A:ILE:HD11	1:49:B:LEU:HA	3	0.1
(1,2044)	1:98:B:LYS:HD3	1:126:B:GLY:H	10	0.1
(1,2043)	1:98:A:LYS:HD3	1:126:A:GLY:H	10	0.1
(1,1687)	1:139:A:ALA:HA	1:140:A:LYS:H	7	0.1
(1,1650)	1:110:B:VAL:HG22	1:115:B:LEU:H	7	0.1
(1,1650)	1:110:B:VAL:HG23	1:115:B:LEU:H	10	0.1
(1,1649)	1:110:A:VAL:HG22	1:115:A:LEU:H	7	0.1
(1,1468)	1:100:B:THR:HG22	1:101:B:THR:H	6	0.1
(1,1467)	1:100:A:THR:HG22	1:101:A:THR:H	6	0.1
(1,1467)	1:100:A:THR:HG23	1:101:A:THR:H	8	0.1
(1,1405)	1:99:A:GLU:HB3	1:99:A:GLU:H	3	0.1
(1,1121)	1:110:A:VAL:HG21	1:114:A:THR:H	9	0.1
(1,1078)	1:88:B:SER:HB2	1:89:B:VAL:H	3	0.1
(1,1077)	1:88:A:SER:HB2	1:89:A:VAL:H	3	0.1
(1,762)	1:110:B:VAL:HG13	1:74:B:LEU:H	6	0.1
(1,761)	1:110:A:VAL:HG13	1:74:A:LEU:H	6	0.1
(1,434)	1:61:B:GLU:HB2	1:61:B:GLU:H	4	0.1
(1,434)	1:61:B:GLU:HB2	1:61:B:GLU:H	6	0.1
(1,434)	1:61:B:GLU:HB2	1:61:B:GLU:H	7	0.1
(1,433)	1:61:A:GLU:HB2	1:61:A:GLU:H	4	0.1
(1,20)	1:105:B:GLN:HG2	1:105:B:GLN:HE22	8	0.1
(1,19)	1:105:A:GLN:HG2	1:105:A:GLN:HE22	8	0.1

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

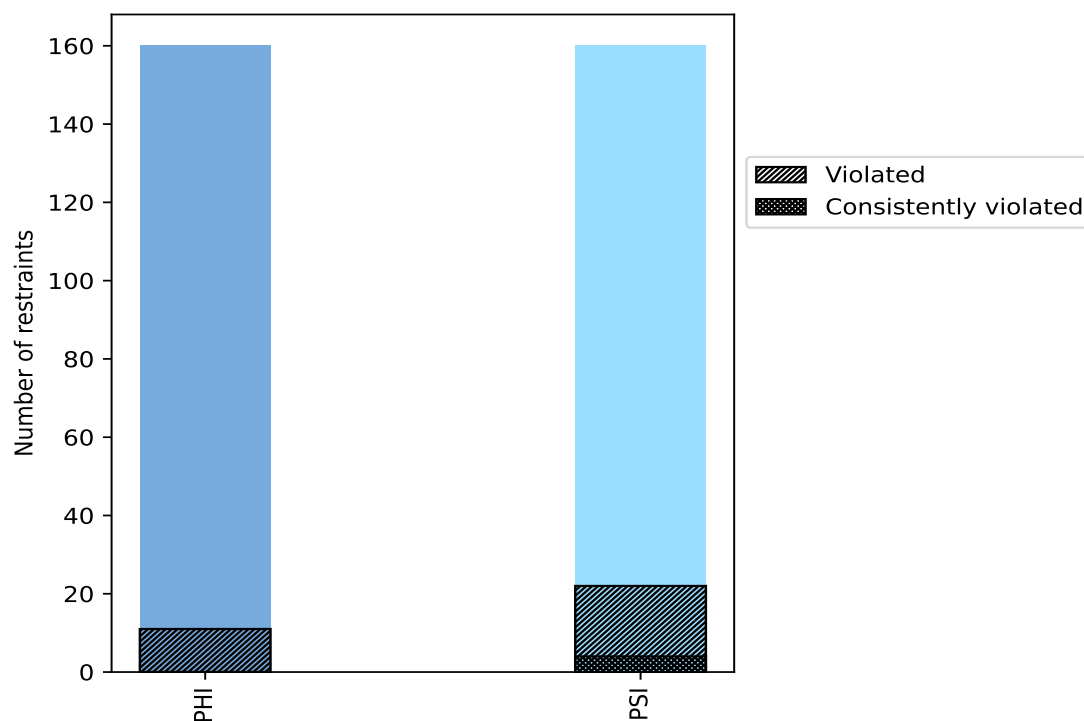
10.1 Summary of dihedral-angle violations [i](#)

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	160	50.0	11	6.9	3.4	0	0.0	0.0
PSI	160	50.0	22	13.8	6.9	4	2.5	1.2
Total	320	100.0	33	10.3	10.3	4	1.2	1.2

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

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



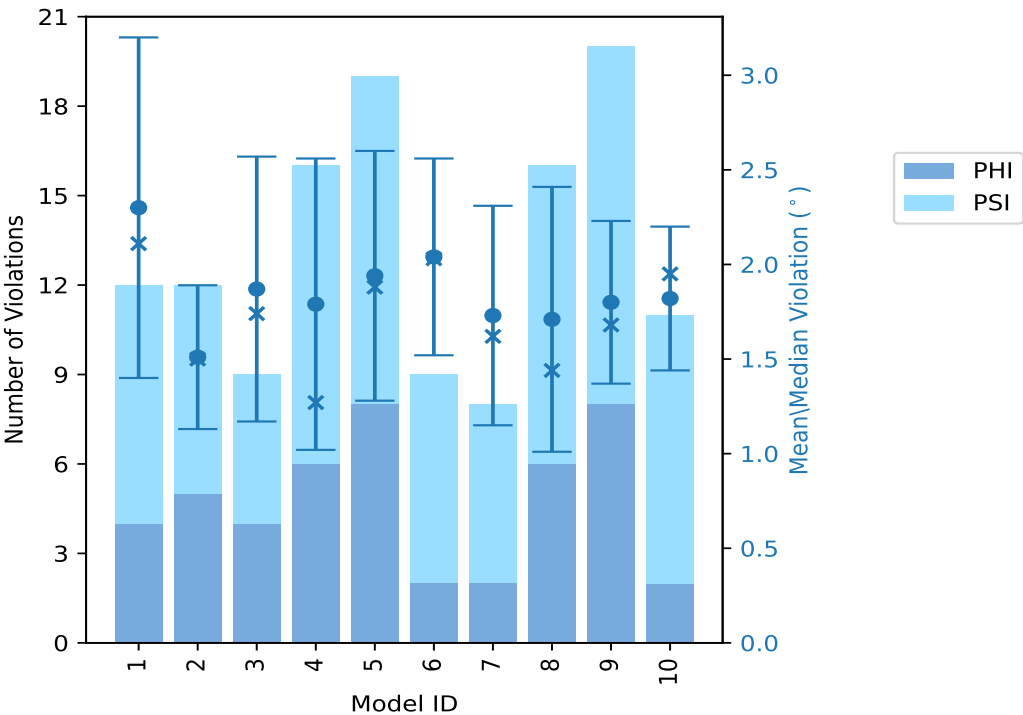
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model ⓘ

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	4	8	12	2.3	3.54	0.9	2.11
2	5	7	12	1.51	2.22	0.38	1.5
3	4	5	9	1.87	3.02	0.7	1.74
4	6	10	16	1.79	2.95	0.77	1.27
5	8	11	19	1.94	3.48	0.66	1.88
6	2	7	9	2.04	2.63	0.52	2.03
7	2	6	8	1.73	2.72	0.58	1.62
8	6	10	16	1.71	3.13	0.7	1.44
9	8	12	20	1.8	2.56	0.43	1.68
10	2	9	11	1.82	2.26	0.38	1.95

10.2.1 Bar graph : Dihedral violation statistics for each model ⓘ



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

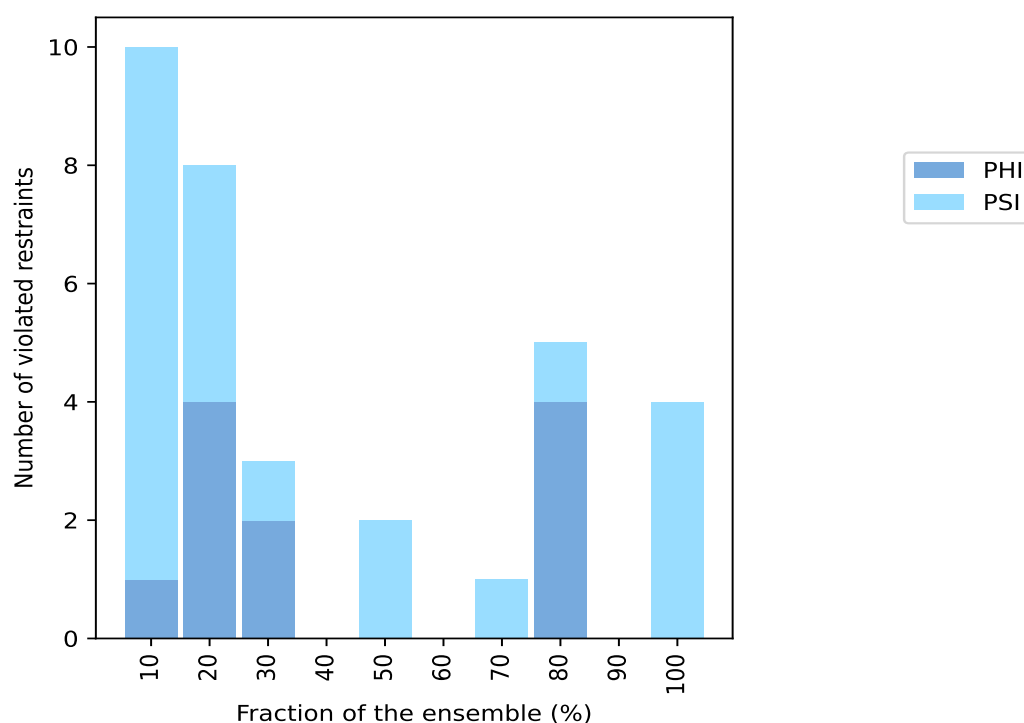
10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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

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

¹ Number of models with violations

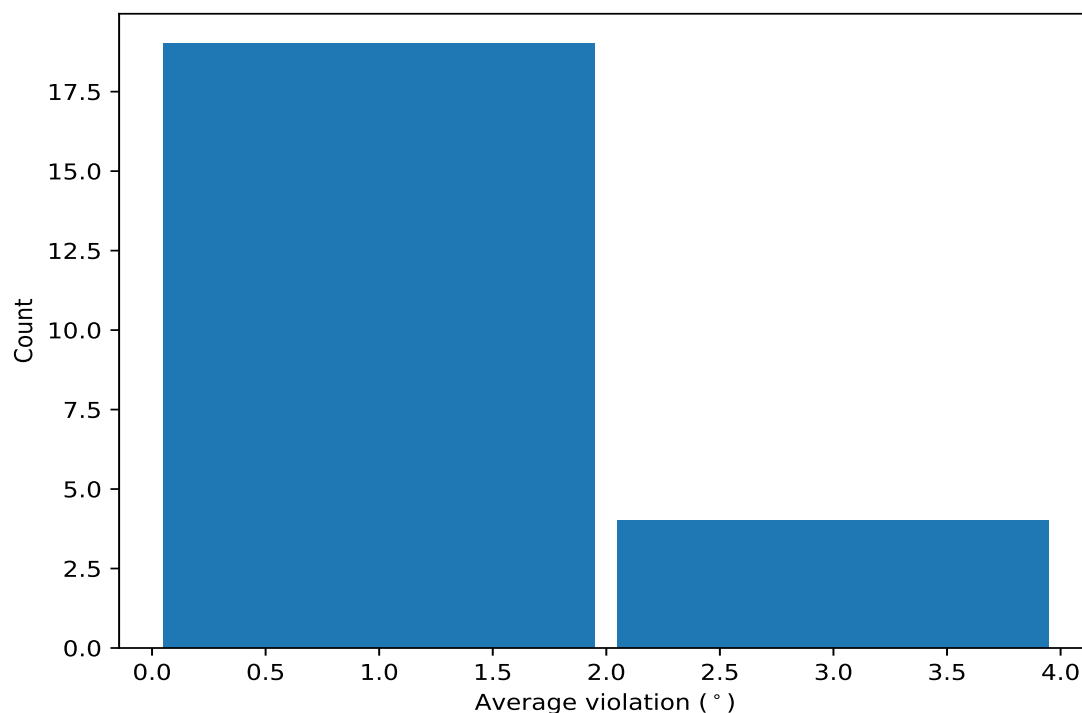
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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
(1,102)	1:105:B:GLN:N	1:105:B:GLN:CA	1:105:B:GLN:C	1:106:B:ALA:N	10	2.63	0.59	2.65
(2,102)	1:105:A:GLN:N	1:105:A:GLN:CA	1:105:A:GLN:C	1:106:A:ALA:N	10	2.62	0.56	2.59
(2,14)	1:50:A:PRO:N	1:50:A:PRO:CA	1:50:A:PRO:C	1:51:A:ALA:N	10	2.17	0.55	2.01
(1,14)	1:50:B:PRO:N	1:50:B:PRO:CA	1:50:B:PRO:C	1:51:B:ALA:N	10	2.14	0.52	2.04
(2,145)	1:128:A:LEU:C	1:129:A:LYS:N	1:129:A:LYS:CA	1:129:A:LYS:C	8	1.91	0.73	1.78
(1,145)	1:128:B:LEU:C	1:129:B:LYS:N	1:129:B:LYS:CA	1:129:B:LYS:C	8	1.85	0.72	1.74
(1,24)	1:63:B:PRO:N	1:63:B:PRO:CA	1:63:B:PRO:C	1:64:B:VAL:N	8	1.69	0.6	1.4
(1,29)	1:65:B:PHE:C	1:66:B:LEU:N	1:66:B:LEU:CA	1:66:B:LEU:C	8	1.57	0.37	1.42
(2,29)	1:65:A:PHE:C	1:66:A:LEU:N	1:66:A:LEU:CA	1:66:A:LEU:C	8	1.57	0.42	1.41
(2,24)	1:63:A:PRO:N	1:63:A:PRO:CA	1:63:A:PRO:C	1:64:A:VAL:N	7	1.79	0.57	1.65
(2,96)	1:102:A:ILE:N	1:102:A:ILE:CA	1:102:A:ILE:C	1:103:A:PHE:N	5	1.65	0.22	1.74
(1,96)	1:102:B:ILE:N	1:102:B:ILE:CA	1:102:B:ILE:C	1:103:B:PHE:N	5	1.6	0.21	1.59
(1,25)	1:63:B:PRO:C	1:64:B:VAL:N	1:64:B:VAL:CA	1:64:B:VAL:C	3	1.72	0.45	1.69

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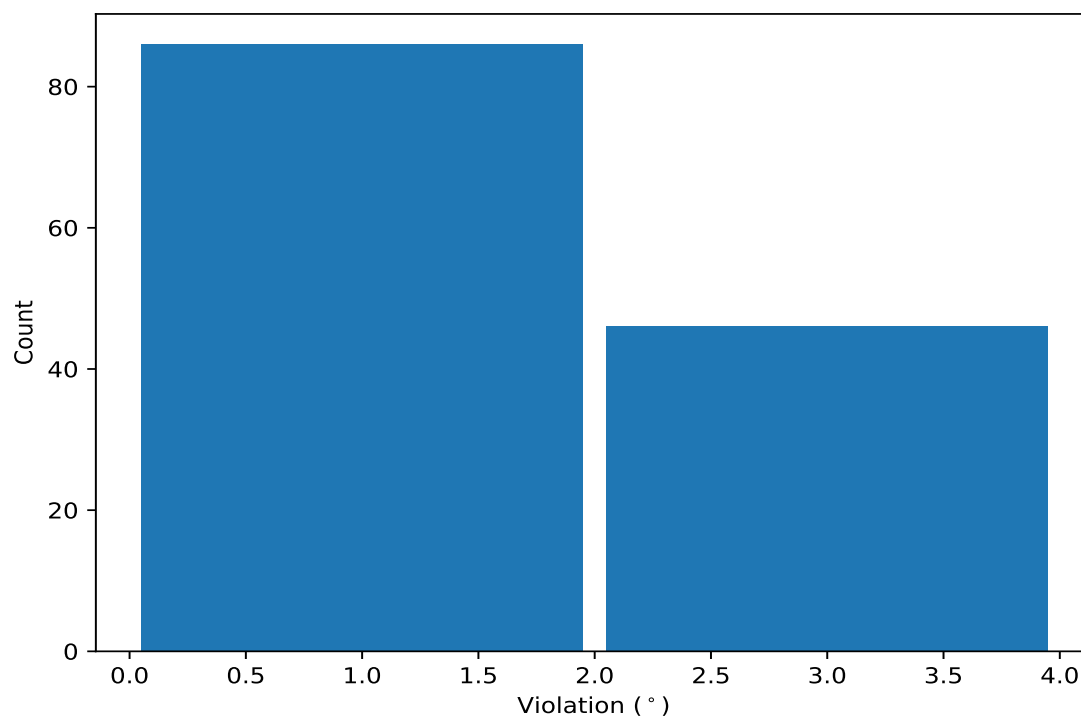
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(2,25)	1:63:A:PRO:C	1:64:A:VAL:N	1:64:A:VAL:CA	1:64:A:VAL:C	3	1.69	0.42	1.74
(2,22)	1:62:A:LYS:N	1:62:A:LYS:CA	1:62:A:LYS:C	1:63:A:PRO:N	3	1.38	0.42	1.12
(1,154)	1:133:B:VAL:N	1:133:B:VAL:CA	1:133:B:VAL:C	1:134:B:GLY:N	2	1.74	0.15	1.74
(2,154)	1:133:A:VAL:N	1:133:A:VAL:CA	1:133:A:VAL:C	1:134:A:GLY:N	2	1.72	0.12	1.72
(1,22)	1:62:B:LYS:N	1:62:B:LYS:CA	1:62:B:LYS:C	1:63:B:PRO:N	2	1.68	0.53	1.68
(1,95)	1:101:B:THR:C	1:102:B:ILE:N	1:102:B:ILE:CA	1:102:B:ILE:C	2	1.63	0.02	1.63
(1,48)	1:75:B:TYR:N	1:75:B:TYR:CA	1:75:B:TYR:C	1:76:B:VAL:N	2	1.54	0.49	1.54
(2,95)	1:101:A:THR:C	1:102:A:ILE:N	1:102:A:ILE:CA	1:102:A:ILE:C	2	1.5	0.03	1.5
(1,1)	1:43:B:VAL:C	1:44:B:ASP:N	1:44:B:ASP:CA	1:44:B:ASP:C	2	1.08	0.01	1.08
(2,1)	1:43:A:VAL:C	1:44:A:ASP:N	1:44:A:ASP:CA	1:44:A:ASP:C	2	1.06	0.02	1.06

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

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

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

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



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(2,102)	1:105:A:GLN:N	1:105:A:GLN:CA	1:105:A:GLN:C	1:106:A:ALA:N	1	3.54
(1,102)	1:105:B:GLN:N	1:105:B:GLN:CA	1:105:B:GLN:C	1:106:B:ALA:N	1	3.51
(2,14)	1:50:A:PRO:N	1:50:A:PRO:CA	1:50:A:PRO:C	1:51:A:ALA:N	5	3.48
(2,145)	1:128:A:LEU:C	1:129:A:LYS:N	1:129:A:LYS:CA	1:129:A:LYS:C	1	3.43
(1,145)	1:128:B:LEU:C	1:129:B:LYS:N	1:129:B:LYS:CA	1:129:B:LYS:C	1	3.41
(1,14)	1:50:B:PRO:N	1:50:B:PRO:CA	1:50:B:PRO:C	1:51:B:ALA:N	5	3.24
(2,102)	1:105:A:GLN:N	1:105:A:GLN:CA	1:105:A:GLN:C	1:106:A:ALA:N	8	3.13
(1,102)	1:105:B:GLN:N	1:105:B:GLN:CA	1:105:B:GLN:C	1:106:B:ALA:N	8	3.1
(2,102)	1:105:A:GLN:N	1:105:A:GLN:CA	1:105:A:GLN:C	1:106:A:ALA:N	3	3.02
(1,102)	1:105:B:GLN:N	1:105:B:GLN:CA	1:105:B:GLN:C	1:106:B:ALA:N	3	2.95
(1,102)	1:105:B:GLN:N	1:105:B:GLN:CA	1:105:B:GLN:C	1:106:B:ALA:N	4	2.95
(2,102)	1:105:A:GLN:N	1:105:A:GLN:CA	1:105:A:GLN:C	1:106:A:ALA:N	4	2.91
(2,24)	1:63:A:PRO:N	1:63:A:PRO:CA	1:63:A:PRO:C	1:64:A:VAL:N	4	2.78
(1,24)	1:63:B:PRO:N	1:63:B:PRO:CA	1:63:B:PRO:C	1:64:B:VAL:N	4	2.74
(1,102)	1:105:B:GLN:N	1:105:B:GLN:CA	1:105:B:GLN:C	1:106:B:ALA:N	7	2.72
(2,14)	1:50:A:PRO:N	1:50:A:PRO:CA	1:50:A:PRO:C	1:51:A:ALA:N	4	2.66
(2,102)	1:105:A:GLN:N	1:105:A:GLN:CA	1:105:A:GLN:C	1:106:A:ALA:N	6	2.63
(1,14)	1:50:B:PRO:N	1:50:B:PRO:CA	1:50:B:PRO:C	1:51:B:ALA:N	4	2.62
(2,145)	1:128:A:LEU:C	1:129:A:LYS:N	1:129:A:LYS:CA	1:129:A:LYS:C	6	2.58
(1,102)	1:105:B:GLN:N	1:105:B:GLN:CA	1:105:B:GLN:C	1:106:B:ALA:N	5	2.58
(1,102)	1:105:B:GLN:N	1:105:B:GLN:CA	1:105:B:GLN:C	1:106:B:ALA:N	9	2.56
(2,102)	1:105:A:GLN:N	1:105:A:GLN:CA	1:105:A:GLN:C	1:106:A:ALA:N	5	2.55
(1,14)	1:50:B:PRO:N	1:50:B:PRO:CA	1:50:B:PRO:C	1:51:B:ALA:N	8	2.55
(1,102)	1:105:B:GLN:N	1:105:B:GLN:CA	1:105:B:GLN:C	1:106:B:ALA:N	6	2.52
(2,102)	1:105:A:GLN:N	1:105:A:GLN:CA	1:105:A:GLN:C	1:106:A:ALA:N	9	2.51
(2,14)	1:50:A:PRO:N	1:50:A:PRO:CA	1:50:A:PRO:C	1:51:A:ALA:N	8	2.48
(2,102)	1:105:A:GLN:N	1:105:A:GLN:CA	1:105:A:GLN:C	1:106:A:ALA:N	7	2.45
(1,145)	1:128:B:LEU:C	1:129:B:LYS:N	1:129:B:LYS:CA	1:129:B:LYS:C	6	2.45
(1,24)	1:63:B:PRO:N	1:63:B:PRO:CA	1:63:B:PRO:C	1:64:B:VAL:N	5	2.36
(2,29)	1:65:A:PHE:C	1:66:A:LEU:N	1:66:A:LEU:CA	1:66:A:LEU:C	1	2.3
(1,25)	1:63:B:PRO:C	1:64:B:VAL:N	1:64:B:VAL:CA	1:64:B:VAL:C	9	2.29
(2,29)	1:65:A:PHE:C	1:66:A:LEU:N	1:66:A:LEU:CA	1:66:A:LEU:C	10	2.26
(1,29)	1:65:B:PHE:C	1:66:B:LEU:N	1:66:B:LEU:CA	1:66:B:LEU:C	1	2.26
(2,24)	1:63:A:PRO:N	1:63:A:PRO:CA	1:63:A:PRO:C	1:64:A:VAL:N	5	2.25
(1,102)	1:105:B:GLN:N	1:105:B:GLN:CA	1:105:B:GLN:C	1:106:B:ALA:N	2	2.22
(1,22)	1:62:B:LYS:N	1:62:B:LYS:CA	1:62:B:LYS:C	1:63:B:PRO:N	9	2.21
(1,14)	1:50:B:PRO:N	1:50:B:PRO:CA	1:50:B:PRO:C	1:51:B:ALA:N	9	2.19
(2,25)	1:63:A:PRO:C	1:64:A:VAL:N	1:64:A:VAL:CA	1:64:A:VAL:C	9	2.18
(1,24)	1:63:B:PRO:N	1:63:B:PRO:CA	1:63:B:PRO:C	1:64:B:VAL:N	10	2.16
(2,102)	1:105:A:GLN:N	1:105:A:GLN:CA	1:105:A:GLN:C	1:106:A:ALA:N	2	2.13
(2,14)	1:50:A:PRO:N	1:50:A:PRO:CA	1:50:A:PRO:C	1:51:A:ALA:N	9	2.13
(2,24)	1:63:A:PRO:N	1:63:A:PRO:CA	1:63:A:PRO:C	1:64:A:VAL:N	10	2.11
(1,14)	1:50:B:PRO:N	1:50:B:PRO:CA	1:50:B:PRO:C	1:51:B:ALA:N	3	2.1
(1,29)	1:65:B:PHE:C	1:66:B:LEU:N	1:66:B:LEU:CA	1:66:B:LEU:C	10	2.09
(2,14)	1:50:A:PRO:N	1:50:A:PRO:CA	1:50:A:PRO:C	1:51:A:ALA:N	3	2.06
(1,48)	1:75:B:TYR:N	1:75:B:TYR:CA	1:75:B:TYR:C	1:76:B:VAL:N	6	2.03
(2,145)	1:128:A:LEU:C	1:129:A:LYS:N	1:129:A:LYS:CA	1:129:A:LYS:C	5	1.99
(1,14)	1:50:B:PRO:N	1:50:B:PRO:CA	1:50:B:PRO:C	1:51:B:ALA:N	10	1.98
(2,22)	1:62:A:LYS:N	1:62:A:LYS:CA	1:62:A:LYS:C	1:63:A:PRO:N	9	1.97
(2,14)	1:50:A:PRO:N	1:50:A:PRO:CA	1:50:A:PRO:C	1:51:A:ALA:N	1	1.96
(2,48)	1:75:A:TYR:N	1:75:A:TYR:CA	1:75:A:TYR:C	1:76:A:VAL:N	6	1.95
(2,14)	1:50:A:PRO:N	1:50:A:PRO:CA	1:50:A:PRO:C	1:51:A:ALA:N	10	1.95

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,14)	1:50:B:PRO:N	1:50:B:PRO:CA	1:50:B:PRO:C	1:51:B:ALA:N	1	1.95
(1,14)	1:50:B:PRO:N	1:50:B:PRO:CA	1:50:B:PRO:C	1:51:B:ALA:N	7	1.94
(1,145)	1:128:B:LEU:C	1:129:B:LYS:N	1:129:B:LYS:CA	1:129:B:LYS:C	5	1.92
(1,96)	1:102:B:ILE:N	1:102:B:ILE:CA	1:102:B:ILE:C	1:103:B:PHE:N	5	1.9
(2,14)	1:50:A:PRO:N	1:50:A:PRO:CA	1:50:A:PRO:C	1:51:A:ALA:N	7	1.89
(1,154)	1:133:B:VAL:N	1:133:B:VAL:CA	1:133:B:VAL:C	1:134:B:GLY:N	10	1.89
(2,96)	1:102:A:ILE:N	1:102:A:ILE:CA	1:102:A:ILE:C	1:103:A:PHE:N	5	1.88
(2,154)	1:133:A:VAL:N	1:133:A:VAL:CA	1:133:A:VAL:C	1:134:A:GLY:N	10	1.84
(2,145)	1:128:A:LEU:C	1:129:A:LYS:N	1:129:A:LYS:CA	1:129:A:LYS:C	8	1.81
(2,96)	1:102:A:ILE:N	1:102:A:ILE:CA	1:102:A:ILE:C	1:103:A:PHE:N	2	1.81
(1,145)	1:128:B:LEU:C	1:129:B:LYS:N	1:129:B:LYS:CA	1:129:B:LYS:C	8	1.81
(2,145)	1:128:A:LEU:C	1:129:A:LYS:N	1:129:A:LYS:CA	1:129:A:LYS:C	3	1.74
(2,96)	1:102:A:ILE:N	1:102:A:ILE:CA	1:102:A:ILE:C	1:103:A:PHE:N	9	1.74
(2,25)	1:63:A:PRO:C	1:64:A:VAL:N	1:64:A:VAL:CA	1:64:A:VAL:C	5	1.74
(1,96)	1:102:B:ILE:N	1:102:B:ILE:CA	1:102:B:ILE:C	1:103:B:PHE:N	9	1.72
(1,25)	1:63:B:PRO:C	1:64:B:VAL:N	1:64:B:VAL:CA	1:64:B:VAL:C	5	1.69
(1,145)	1:128:B:LEU:C	1:129:B:LYS:N	1:129:B:LYS:CA	1:129:B:LYS:C	3	1.66
(2,24)	1:63:A:PRO:N	1:63:A:PRO:CA	1:63:A:PRO:C	1:64:A:VAL:N	9	1.65
(1,95)	1:101:B:THR:C	1:102:B:ILE:N	1:102:B:ILE:CA	1:102:B:ILE:C	9	1.65
(2,154)	1:133:A:VAL:N	1:133:A:VAL:CA	1:133:A:VAL:C	1:134:A:GLY:N	9	1.61
(1,95)	1:101:B:THR:C	1:102:B:ILE:N	1:102:B:ILE:CA	1:102:B:ILE:C	5	1.61
(1,29)	1:65:B:PHE:C	1:66:B:LEU:N	1:66:B:LEU:CA	1:66:B:LEU:C	2	1.6
(1,154)	1:133:B:VAL:N	1:133:B:VAL:CA	1:133:B:VAL:C	1:134:B:GLY:N	9	1.59
(1,96)	1:102:B:ILE:N	1:102:B:ILE:CA	1:102:B:ILE:C	1:103:B:PHE:N	2	1.59
(2,96)	1:102:A:ILE:N	1:102:A:ILE:CA	1:102:A:ILE:C	1:103:A:PHE:N	8	1.58
(2,14)	1:50:A:PRO:N	1:50:A:PRO:CA	1:50:A:PRO:C	1:51:A:ALA:N	6	1.56
(1,96)	1:102:B:ILE:N	1:102:B:ILE:CA	1:102:B:ILE:C	1:103:B:PHE:N	8	1.54
(2,95)	1:101:A:THR:C	1:102:A:ILE:N	1:102:A:ILE:CA	1:102:A:ILE:C	9	1.52
(2,14)	1:50:A:PRO:N	1:50:A:PRO:CA	1:50:A:PRO:C	1:51:A:ALA:N	2	1.52
(1,24)	1:63:B:PRO:N	1:63:B:PRO:CA	1:63:B:PRO:C	1:64:B:VAL:N	9	1.5
(2,29)	1:65:A:PHE:C	1:66:A:LEU:N	1:66:A:LEU:CA	1:66:A:LEU:C	9	1.48
(2,95)	1:101:A:THR:C	1:102:A:ILE:N	1:102:A:ILE:CA	1:102:A:ILE:C	5	1.47
(2,29)	1:65:A:PHE:C	1:66:A:LEU:N	1:66:A:LEU:CA	1:66:A:LEU:C	2	1.47
(1,14)	1:50:B:PRO:N	1:50:B:PRO:CA	1:50:B:PRO:C	1:51:B:ALA:N	6	1.46
(1,29)	1:65:B:PHE:C	1:66:B:LEU:N	1:66:B:LEU:CA	1:66:B:LEU:C	5	1.45
(2,24)	1:63:A:PRO:N	1:63:A:PRO:CA	1:63:A:PRO:C	1:64:A:VAL:N	1	1.4
(1,29)	1:65:B:PHE:C	1:66:B:LEU:N	1:66:B:LEU:CA	1:66:B:LEU:C	4	1.4
(1,14)	1:50:B:PRO:N	1:50:B:PRO:CA	1:50:B:PRO:C	1:51:B:ALA:N	2	1.39
(2,102)	1:105:A:GLN:N	1:105:A:GLN:CA	1:105:A:GLN:C	1:106:A:ALA:N	10	1.38
(2,29)	1:65:A:PHE:C	1:66:A:LEU:N	1:66:A:LEU:CA	1:66:A:LEU:C	8	1.35
(2,145)	1:128:A:LEU:C	1:129:A:LYS:N	1:129:A:LYS:CA	1:129:A:LYS:C	7	1.34
(1,29)	1:65:B:PHE:C	1:66:B:LEU:N	1:66:B:LEU:CA	1:66:B:LEU:C	8	1.32
(1,24)	1:63:B:PRO:N	1:63:B:PRO:CA	1:63:B:PRO:C	1:64:B:VAL:N	1	1.31
(1,24)	1:63:B:PRO:N	1:63:B:PRO:CA	1:63:B:PRO:C	1:64:B:VAL:N	8	1.29
(2,29)	1:65:A:PHE:C	1:66:A:LEU:N	1:66:A:LEU:CA	1:66:A:LEU:C	4	1.28
(1,145)	1:128:B:LEU:C	1:129:B:LYS:N	1:129:B:LYS:CA	1:129:B:LYS:C	7	1.28
(1,29)	1:65:B:PHE:C	1:66:B:LEU:N	1:66:B:LEU:CA	1:66:B:LEU:C	9	1.28
(2,29)	1:65:A:PHE:C	1:66:A:LEU:N	1:66:A:LEU:CA	1:66:A:LEU:C	5	1.27
(1,110)	1:109:B:SER:N	1:109:B:SER:CA	1:109:B:SER:C	1:110:B:VAL:N	4	1.26
(2,96)	1:102:A:ILE:N	1:102:A:ILE:CA	1:102:A:ILE:C	1:103:A:PHE:N	1	1.25
(1,96)	1:102:B:ILE:N	1:102:B:ILE:CA	1:102:B:ILE:C	1:103:B:PHE:N	1	1.25

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(2,50)	1:77:A:GLY:N	1:77:A:GLY:CA	1:77:A:GLY:C	1:78:A:ASP:N	5	1.24
(2,145)	1:128:A:LEU:C	1:129:A:LYS:N	1:129:A:LYS:CA	1:129:A:LYS:C	4	1.21
(1,102)	1:105:B:GLN:N	1:105:B:GLN:CA	1:105:B:GLN:C	1:106:B:ALA:N	10	1.2
(1,25)	1:63:B:PRO:C	1:64:B:VAL:N	1:64:B:VAL:CA	1:64:B:VAL:C	4	1.19
(2,110)	1:109:A:SER:N	1:109:A:SER:CA	1:109:A:SER:C	1:110:A:VAL:N	4	1.18
(2,24)	1:63:A:PRO:N	1:63:A:PRO:CA	1:63:A:PRO:C	1:64:A:VAL:N	7	1.16
(2,24)	1:63:A:PRO:N	1:63:A:PRO:CA	1:63:A:PRO:C	1:64:A:VAL:N	8	1.16
(1,145)	1:128:B:LEU:C	1:129:B:LYS:N	1:129:B:LYS:CA	1:129:B:LYS:C	4	1.16
(1,29)	1:65:B:PHE:C	1:66:B:LEU:N	1:66:B:LEU:CA	1:66:B:LEU:C	3	1.16
(2,28)	1:65:A:PHE:N	1:65:A:PHE:CA	1:65:A:PHE:C	1:66:A:LEU:N	6	1.15
(2,25)	1:63:A:PRO:C	1:64:A:VAL:N	1:64:A:VAL:CA	1:64:A:VAL:C	4	1.15
(1,22)	1:62:B:LYS:N	1:62:B:LYS:CA	1:62:B:LYS:C	1:63:B:PRO:N	4	1.15
(2,145)	1:128:A:LEU:C	1:129:A:LYS:N	1:129:A:LYS:CA	1:129:A:LYS:C	2	1.14
(2,54)	1:80:A:PRO:N	1:80:A:PRO:CA	1:80:A:PRO:C	1:81:A:VAL:N	10	1.14
(2,29)	1:65:A:PHE:C	1:66:A:LEU:N	1:66:A:LEU:CA	1:66:A:LEU:C	3	1.14
(1,145)	1:128:B:LEU:C	1:129:B:LYS:N	1:129:B:LYS:CA	1:129:B:LYS:C	2	1.14
(2,22)	1:62:A:LYS:N	1:62:A:LYS:CA	1:62:A:LYS:C	1:63:A:PRO:N	5	1.12
(1,24)	1:63:B:PRO:N	1:63:B:PRO:CA	1:63:B:PRO:C	1:64:B:VAL:N	2	1.09
(1,24)	1:63:B:PRO:N	1:63:B:PRO:CA	1:63:B:PRO:C	1:64:B:VAL:N	7	1.09
(1,1)	1:43:B:VAL:C	1:44:B:ASP:N	1:44:B:ASP:CA	1:44:B:ASP:C	9	1.09
(2,1)	1:43:A:VAL:C	1:44:A:ASP:N	1:44:A:ASP:CA	1:44:A:ASP:C	9	1.08
(1,50)	1:77:B:GLY:N	1:77:B:GLY:CA	1:77:B:GLY:C	1:78:B:ASP:N	5	1.07
(1,1)	1:43:B:VAL:C	1:44:B:ASP:N	1:44:B:ASP:CA	1:44:B:ASP:C	8	1.07
(2,22)	1:62:A:LYS:N	1:62:A:LYS:CA	1:62:A:LYS:C	1:63:A:PRO:N	4	1.06
(2,1)	1:43:A:VAL:C	1:44:A:ASP:N	1:44:A:ASP:CA	1:44:A:ASP:C	8	1.05
(1,48)	1:75:B:TYR:N	1:75:B:TYR:CA	1:75:B:TYR:C	1:76:B:VAL:N	3	1.04
(1,30)	1:66:B:LEU:N	1:66:B:LEU:CA	1:66:B:LEU:C	1:67:B:SER:N	8	1.04
(2,30)	1:66:A:LEU:N	1:66:A:LEU:CA	1:66:A:LEU:C	1:67:A:SER:N	8	1.03
(1,23)	1:62:B:LYS:C	1:63:B:PRO:N	1:63:B:PRO:CA	1:63:B:PRO:C	2	1.0