Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	6BP9
BMRB ID	:	30374
Title	:	HSPB5 alpha-crystallin domain mutant R120G-ACD
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This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

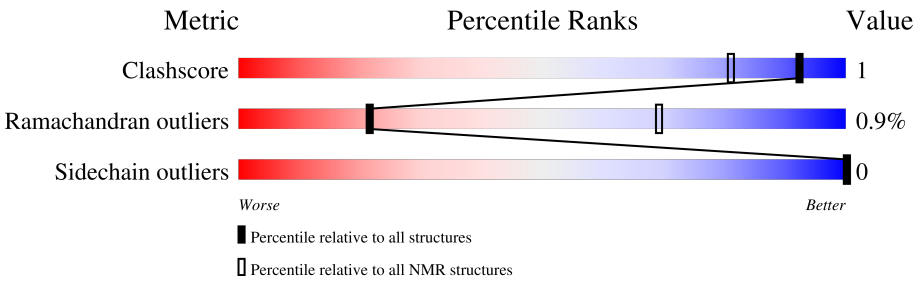
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 39%.

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	89	98%
1	B	89	100%

2 Ensemble composition and analysis (i)

This entry contains 8 models. Model 1 is the overall representative, medoid model (most similar to other models).

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

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:66-A:152, B:64-B:152 (176)	2.30	1

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

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

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

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2846 atoms, of which 1424 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Alpha-crystallin B chain.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	89	1423	444	712	128	138	1	0
1	B	89	1423	444	712	128	138	1	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	120	GLY	ARG	engineered mutation	UNP P02511
B	120	GLY	ARG	engineered mutation	UNP P02511

4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

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

• Molecule 1: Alpha-crystallin B chain

Chain A: 98%

• Molecule 1: Alpha-crystallin B chain

Chain B: 100%

There are no outlier residues in this chain.

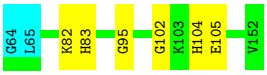
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

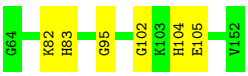
• Molecule 1: Alpha-crystallin B chain

Chain A: 91% 7%



• Molecule 1: Alpha-crystallin B chain

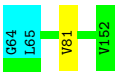
Chain B: 93% 7%



4.2.2 Score per residue for model 2

- Molecule 1: Alpha-crystallin B chain

Chain A: 97%



- Molecule 1: Alpha-crystallin B chain

Chain B: 99%

4.2.3 Score per residue for model 3

- Molecule 1: Alpha-crystallin B chain

Chain A: 98%

- Molecule 1: Alpha-crystallin B chain

Chain B: 98%

4.2.4 Score per residue for model 4

- Molecule 1: Alpha-crystallin B chain

Chain A: 96%

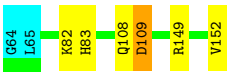
- Molecule 1: Alpha-crystallin B chain

Chain B: 98%

4.2.5 Score per residue for model 5

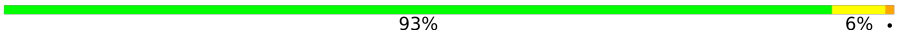
• Molecule 1: Alpha-crystallin B chain

Chain A:



• Molecule 1: Alpha-crystallin B chain

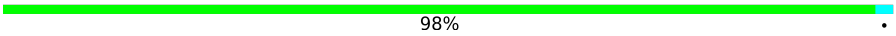
Chain B:



4.2.6 Score per residue for model 6

• Molecule 1: Alpha-crystallin B chain

Chain A:



• Molecule 1: Alpha-crystallin B chain

Chain B:

There are no outlier residues in this chain.

4.2.7 Score per residue for model 7

• Molecule 1: Alpha-crystallin B chain

Chain A:

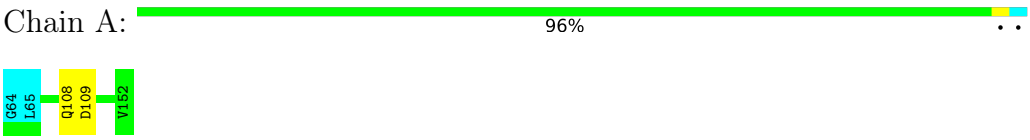
• Molecule 1: Alpha-crystallin B chain

Chain B:

4.2.8 Score per residue for model 8

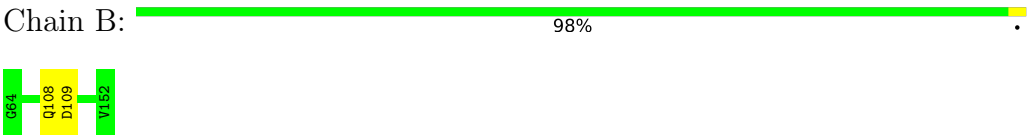
- Molecule 1: Alpha-crystallin B chain

Chain A:



- Molecule 1: Alpha-crystallin B chain

Chain B:



5 Refinement protocol and experimental data overview (i)

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

Of the 100 calculated structures, 8 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
CSRosetta	structure calculation	

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	965
Number of shifts mapped to atoms	965
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	39%

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	699	696	691	2±2
1	B	711	712	704	2±2
All	All	11280	11264	11160	31

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:108:GLN:O	1:A:109:ASP:CB	0.72	2.38	5	2
1:B:108:GLN:O	1:B:109:ASP:CB	0.71	2.38	5	2
1:A:108:GLN:O	1:A:109:ASP:HB2	0.57	1.99	5	1
1:B:108:GLN:O	1:B:109:ASP:HB2	0.56	1.99	5	1
1:B:65:LEU:O	1:B:66:SER:C	0.51	2.48	4	1
1:B:126:ALA:O	1:B:127:ASP:C	0.50	2.50	7	1
1:A:126:ALA:O	1:A:127:ASP:C	0.49	2.50	7	1
1:A:104:HIS:O	1:A:105:GLU:C	0.48	2.52	1	2
1:A:152:VAL:HG13	1:A:152:VAL:OXT	0.47	2.09	5	1
1:B:152:VAL:HG13	1:B:152:VAL:OXT	0.47	2.09	5	1
1:A:82:LYS:O	1:A:83:HIS:HB2	0.47	2.10	1	3
1:B:82:LYS:O	1:B:83:HIS:HB2	0.47	2.10	5	3
1:B:81:VAL:O	1:B:81:VAL:HG23	0.47	2.10	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:104:HIS:O	1:B:105:GLU:C	0.46	2.52	1	2
1:A:81:VAL:HG23	1:A:81:VAL:O	0.46	2.10	7	2
1:B:129:ASP:O	1:B:132:THR:OG1	0.42	2.34	3	1
1:B:82:LYS:O	1:B:83:HIS:CB	0.41	2.69	1	2
1:A:82:LYS:O	1:A:83:HIS:CB	0.41	2.69	1	2
1:A:96:ASP:OD1	1:A:96:ASP:N	0.40	2.54	4	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

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	86/89 (97%)	77±2 (89±2%)	9±2 (10±2%)	1±1 (1±1%)	21	69
1	B	87/89 (98%)	78±2 (89±2%)	9±2 (10±2%)	1±1 (1±1%)	21	69
All	All	1384/1424 (97%)	1233 (89%)	139 (10%)	12 (1%)	21	69

All 12 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	95	GLY	1
1	A	102	GLY	1
1	B	95	GLY	1
1	B	102	GLY	1
1	A	66	SER	1
1	B	66	SER	1
1	A	109	ASP	1
1	A	149	ARG	1
1	B	109	ASP	1
1	B	149	ARG	1
1	A	105	GLU	1
1	B	105	GLU	1

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	80/81 (99%)	80±0 (100±0%)	0±0 (0±0%)	100	100
1	B	81/81 (100%)	81±0 (100±0%)	0±0 (0±0%)	100	100
All	All	1288/1296 (99%)	1288 (100%)	0 (0%)	100	100

There are no protein residues with a non-rotameric sidechain to report.

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 monosaccharides 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 (i)

The completeness of assignment taking into account all chemical shift lists is 39% for the well-defined parts and 39% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_0*

7.1.1 Bookkeeping (i)

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

Total number of shifts	965
Number of shifts mapped to atoms	965
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	89	0.17 ± 0.06	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	81	0.19 ± 0.19	None needed (< 0.5 ppm)
$^{13}C'$	80	0.44 ± 0.10	None needed (< 0.5 ppm)
^{15}N	84	-1.25 ± 0.36	Should be applied

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 39%, i.e. 946 atoms were assigned a chemical shift out of a possible 2446. 0 out of 35 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	418/877 (48%)	170/357 (48%)	165/352 (47%)	83/168 (49%)
Sidechain	461/1391 (33%)	279/895 (31%)	178/438 (41%)	4/58 (7%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	67/178 (38%)	32/88 (36%)	25/70 (36%)	10/20 (50%)
Overall	946/2446 (39%)	481/1340 (36%)	368/860 (43%)	97/246 (39%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 39%, i.e. 965 atoms were assigned a chemical shift out of a possible 2470. 0 out of 36 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	426/888 (48%)	173/362 (48%)	169/356 (47%)	84/170 (49%)
Sidechain	472/1404 (34%)	287/904 (32%)	181/442 (41%)	4/58 (7%)
Aromatic	67/178 (38%)	32/88 (36%)	25/70 (36%)	10/20 (50%)
Overall	965/2470 (39%)	492/1354 (36%)	375/868 (43%)	98/248 (40%)

7.1.4 Statistically unusual chemical shifts (i)

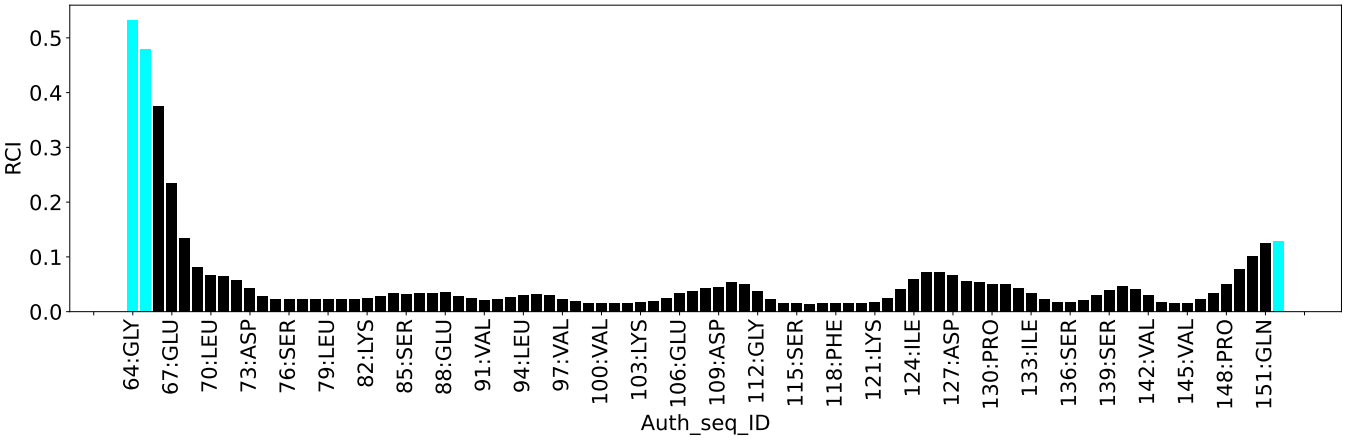
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	68	MET	CG	38.66	25.46 – 38.60	5.0

7.1.5 Random Coil Index (RCI) plots (i)

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

Random coil index (RCI) for chain A:


RCI
0.0
0.1
0.2
0.3
0.4
0.5
64:GLY
67:GLU
70:LEU
73:ASP
76:SER
79:LEU
82:LYS
85:SER
88:GLU
91:VAL
94:LEU
97:VAL
100:VAL
103:LYS
106:GLU
109:ASP
112:GLY
115:SER
118:PHE
121:LYS
124:ILE
127:ASP
130:PRO
133:ILE
136:SER
139:SER
142:VAL
145:VAL
148:PRO
151:GLN
Auth_seq_ID

8 NMR restraints analysis (i)

8.1 Conformationally restricting restraints (i)

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	1213
Intra-residue (|i-j|=0)	416
Sequential (|i-j|=1)	410
Medium range (|i-j|>1 and |i-j|<5)	72
Long range (|i-j|≥5)	315
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	6.8
Number of long range restraints per residue[1]	1.8

[1]Long 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 (i)

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 (i)

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)	1.9	0.2
0.2-0.5 (Medium)	6.6	0.49
>0.5 (Large)	65.4	30.9

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

Dihedral-angle violations less than 1° are not included in the calculation.There are no dihedral-angle violations

9 Distance violation analysis (i)

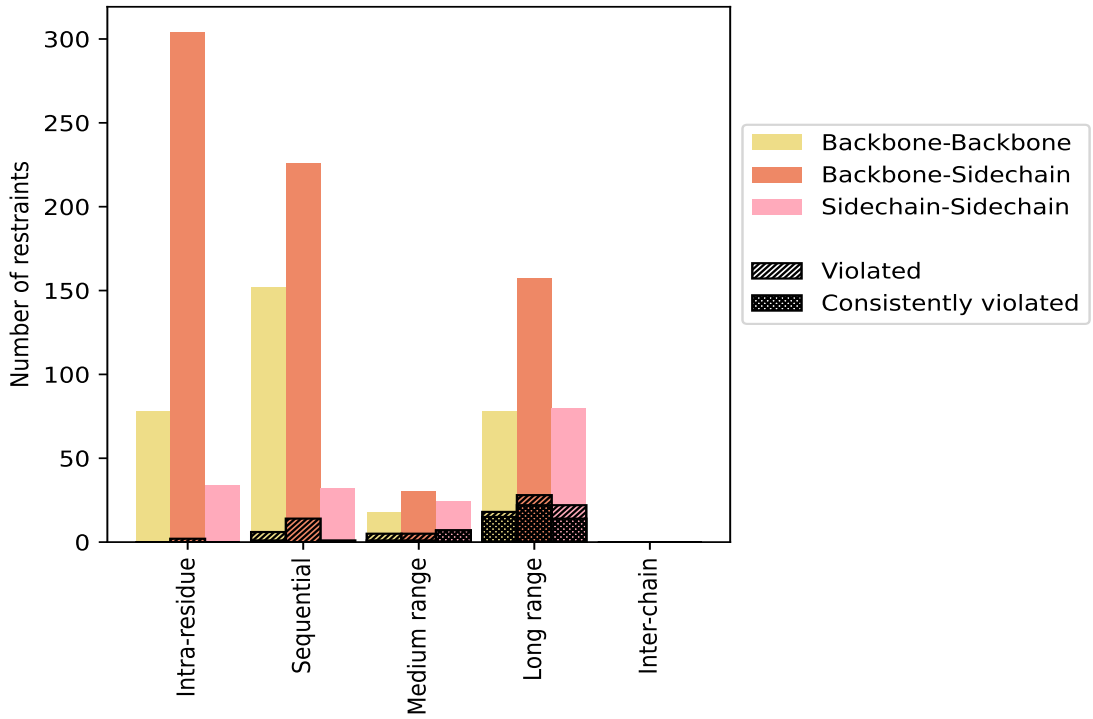
9.1 Summary of distance violations (i)

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.

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	416	34.3	2	0.5	0.2	0	0.0	0.0
Backbone-Backbone	78	6.4	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	304	25.1	2	0.7	0.2	0	0.0	0.0
Sidechain-Sidechain	34	2.8	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	410	33.8	21	5.1	1.7	1	0.2	0.1
Backbone-Backbone	152	12.5	6	3.9	0.5	1	0.7	0.1
Backbone-Sidechain	226	18.6	14	6.2	1.2	0	0.0	0.0
Sidechain-Sidechain	32	2.6	1	3.1	0.1	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	72	5.9	17	23.6	1.4	9	12.5	0.7
Backbone-Backbone	18	1.5	5	27.8	0.4	1	5.6	0.1
Backbone-Sidechain	30	2.5	5	16.7	0.4	1	3.3	0.1
Sidechain-Sidechain	24	2.0	7	29.2	0.6	7	29.2	0.6
Long range (|i-j|≥5)	315	26.0	68	21.6	5.6	51	16.2	4.2
Backbone-Backbone	78	6.4	18	23.1	1.5	15	19.2	1.2
Backbone-Sidechain	157	12.9	28	17.8	2.3	22	14.0	1.8
Sidechain-Sidechain	80	6.6	22	27.5	1.8	14	17.5	1.2
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1213	100.0	108	8.9	8.9	61	5.0	5.0
Backbone-Backbone	326	26.9	29	8.9	2.4	17	5.2	1.4
Backbone-Sidechain	717	59.1	49	6.8	4.0	23	3.2	1.9
Sidechain-Sidechain	170	14.0	30	17.6	2.5	21	12.4	1.7

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

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



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

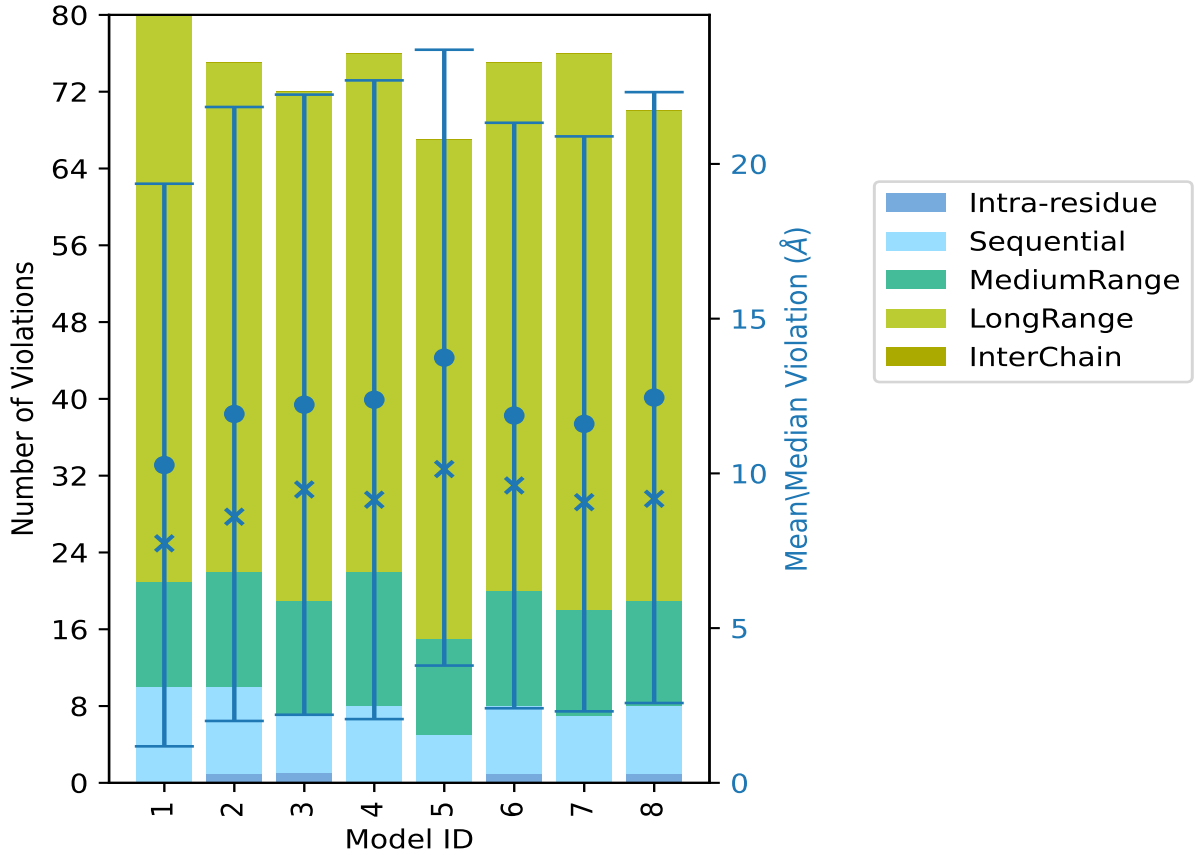
9.2 Distance violation statistics for each model (i)

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	0	10	11	59	0	80	10.27	27.32	9.09	7.74
2	1	9	12	53	0	75	11.92	29.35	9.92	8.6
3	1	6	12	53	0	72	12.22	30.02	10.02	9.48
4	0	8	14	54	0	76	12.38	30.9	10.32	9.15
5	0	5	10	52	0	67	13.74	29.84	9.95	10.14
6	1	7	12	55	0	75	11.87	27.87	9.46	9.61
7	0	7	11	58	0	76	11.6	27.36	9.29	9.07
8	1	7	11	51	0	70	12.45	28.62	9.87	9.18

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6]Standard 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, 1105(IR:414, SQ:389, MR:55, LR:247, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
0	9	3	9	0	21	1	12.5
2	6	1	6	0	15	2	25.0
0	0	2	2	0	4	3	37.5
0	1	1	0	0	2	4	50.0
0	0	0	0	0	0	5	62.5
0	2	1	0	0	3	6	75.0

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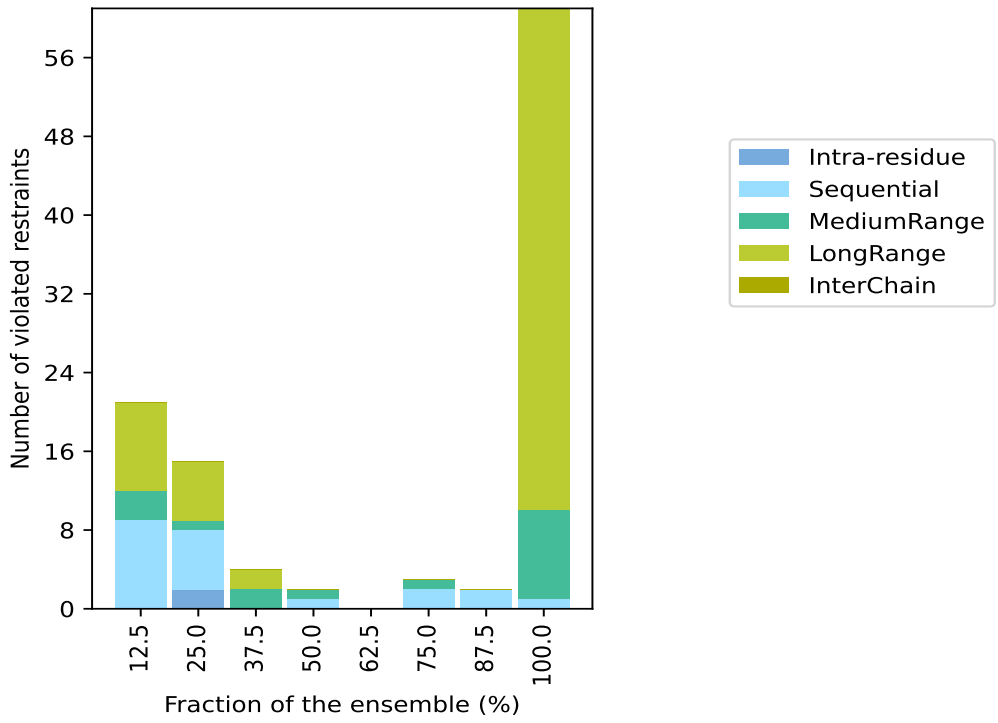
Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
0	2	0	0	0	2	7	87.5
0	1	9	51	0	61	8	100.0

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6] Number of models with violations

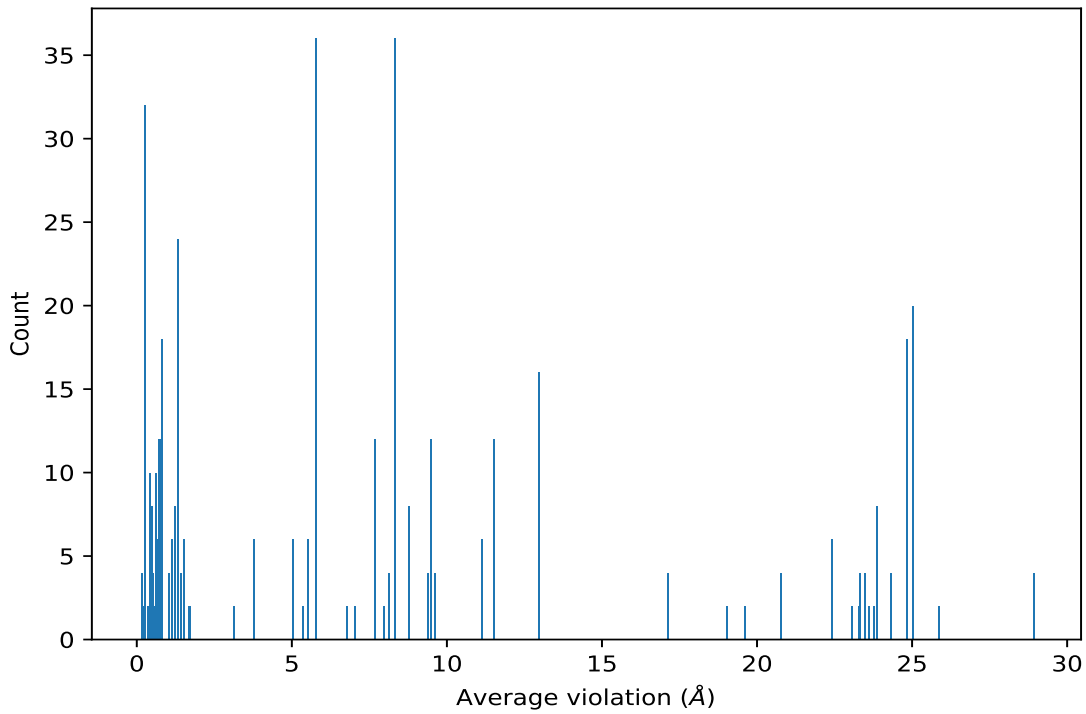
9.3.1 Bar graph : Distance violation statistics for the ensemble (i)



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)
(5,5)	1:B:110:GLU:H	1:B:123:ARG:HB2	8	28.91	1.24	28.98
(5,5)	1:B:110:GLU:H	1:B:123:ARG:HB3	8	28.91	1.24	28.98
(5,5)	1:A:110:GLU:H	1:A:123:ARG:HB2	8	28.91	1.24	28.98
(5,5)	1:A:110:GLU:H	1:A:123:ARG:HB3	8	28.91	1.24	28.98
(4,49)	1:A:113:PHE:H	1:A:123:ARG:HG3	8	25.86	1.08	25.65
(4,49)	1:B:113:PHE:H	1:B:123:ARG:HG3	8	25.86	1.08	25.65
(4,2)	1:A:111:HIS:HB2	1:A:123:ARG:HB2	8	25.04	2.05	26.27
(4,2)	1:A:111:HIS:HB2	1:A:123:ARG:HB3	8	25.04	2.05	26.27
(4,2)	1:B:111:HIS:HB2	1:B:123:ARG:HB2	8	25.04	2.05	26.27
(4,2)	1:B:111:HIS:HB2	1:B:123:ARG:HB3	8	25.04	2.05	26.27
(4,4)	1:A:111:HIS:HB2	1:A:123:ARG:HB2	8	25.04	2.05	26.27
(4,4)	1:A:111:HIS:HB2	1:A:123:ARG:HB3	8	25.04	2.05	26.27
(4,4)	1:B:111:HIS:HB2	1:B:123:ARG:HB2	8	25.04	2.05	26.27
(4,4)	1:B:111:HIS:HB2	1:B:123:ARG:HB3	8	25.04	2.05	26.27
(4,6)	1:A:111:HIS:HB2	1:A:123:ARG:HB2	8	25.04	2.05	26.27
(4,6)	1:A:111:HIS:HB2	1:A:123:ARG:HB3	8	25.04	2.05	26.27

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(4,6)	1:B:111:HIS:HB2	1:B:123:ARG:HB2	8	25.04	2.05	26.27
(4,6)	1:B:111:HIS:HB2	1:B:123:ARG:HB3	8	25.04	2.05	26.27
(4,7)	1:A:111:HIS:HB2	1:A:123:ARG:HB2	8	25.04	2.05	26.27
(4,7)	1:A:111:HIS:HB2	1:A:123:ARG:HB3	8	25.04	2.05	26.27
(4,7)	1:B:111:HIS:HB2	1:B:123:ARG:HB2	8	25.04	2.05	26.27
(4,7)	1:B:111:HIS:HB2	1:B:123:ARG:HB3	8	25.04	2.05	26.27
(4,9)	1:A:111:HIS:HB2	1:A:123:ARG:HB2	8	25.04	2.05	26.27
(4,9)	1:A:111:HIS:HB2	1:A:123:ARG:HB3	8	25.04	2.05	26.27
(4,9)	1:B:111:HIS:HB2	1:B:123:ARG:HB2	8	25.04	2.05	26.27
(4,9)	1:B:111:HIS:HB2	1:B:123:ARG:HB3	8	25.04	2.05	26.27
(5,8)	1:A:113:PHE:H	1:A:123:ARG:H	8	24.83	0.87	24.53
(5,8)	1:B:113:PHE:H	1:B:123:ARG:H	8	24.83	0.87	24.53
(4,3)	1:A:111:HIS:HB3	1:A:123:ARG:HB2	8	24.82	1.46	25.54
(4,3)	1:A:111:HIS:HB3	1:A:123:ARG:HB3	8	24.82	1.46	25.54
(4,3)	1:B:111:HIS:HB3	1:B:123:ARG:HB2	8	24.82	1.46	25.54
(4,3)	1:B:111:HIS:HB3	1:B:123:ARG:HB3	8	24.82	1.46	25.54
(4,5)	1:A:111:HIS:HB3	1:A:123:ARG:HB2	8	24.82	1.46	25.54
(4,5)	1:A:111:HIS:HB3	1:A:123:ARG:HB3	8	24.82	1.46	25.54
(4,5)	1:B:111:HIS:HB3	1:B:123:ARG:HB2	8	24.82	1.46	25.54
(4,5)	1:B:111:HIS:HB3	1:B:123:ARG:HB3	8	24.82	1.46	25.54
(4,8)	1:A:111:HIS:HB3	1:A:123:ARG:HB2	8	24.82	1.46	25.54
(4,8)	1:A:111:HIS:HB3	1:A:123:ARG:HB3	8	24.82	1.46	25.54
(4,8)	1:B:111:HIS:HB3	1:B:123:ARG:HB2	8	24.82	1.46	25.54
(4,8)	1:B:111:HIS:HB3	1:B:123:ARG:HB3	8	24.82	1.46	25.54
(4,10)	1:A:111:HIS:HB3	1:A:123:ARG:HB2	8	24.82	1.46	25.54
(4,10)	1:A:111:HIS:HB3	1:A:123:ARG:HB3	8	24.82	1.46	25.54
(4,10)	1:B:111:HIS:HB3	1:B:123:ARG:HB2	8	24.82	1.46	25.54
(4,10)	1:B:111:HIS:HB3	1:B:123:ARG:HB3	8	24.82	1.46	25.54
(5,9)	1:A:113:PHE:H	1:A:123:ARG:HG2	8	24.34	0.92	24.14
(5,9)	1:A:113:PHE:H	1:A:123:ARG:HG3	8	24.34	0.92	24.14
(5,9)	1:B:113:PHE:H	1:B:123:ARG:HG2	8	24.34	0.92	24.14
(5,9)	1:B:113:PHE:H	1:B:123:ARG:HG3	8	24.34	0.92	24.14
(4,56)	1:A:122:TYR:H	1:A:110:GLU:HB2	8	23.89	1.21	24.06
(4,56)	1:A:122:TYR:H	1:A:110:GLU:HB3	8	23.89	1.21	24.06
(4,56)	1:B:122:TYR:H	1:B:110:GLU:HB2	8	23.89	1.21	24.06
(4,56)	1:B:122:TYR:H	1:B:110:GLU:HB3	8	23.89	1.21	24.06
(4,57)	1:A:122:TYR:H	1:A:110:GLU:HB2	8	23.89	1.21	24.06
(4,57)	1:A:122:TYR:H	1:A:110:GLU:HB3	8	23.89	1.21	24.06
(4,57)	1:B:122:TYR:H	1:B:110:GLU:HB2	8	23.89	1.21	24.06
(4,57)	1:B:122:TYR:H	1:B:110:GLU:HB3	8	23.89	1.21	24.06
(5,7)	1:A:113:PHE:H	1:A:122:TYR:HA	8	23.77	0.7	23.38
(5,7)	1:B:113:PHE:H	1:B:122:TYR:HA	8	23.77	0.7	23.38

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(4,13)	1:A:112:GLY:HA2	1:A:122:TYR:HB3	8	23.64	0.77	23.54
(4,13)	1:B:112:GLY:HA2	1:B:122:TYR:HB3	8	23.64	0.77	23.54
(4,11)	1:A:112:GLY:HA2	1:A:122:TYR:HA	8	23.47	0.8	23.0
(4,11)	1:B:112:GLY:HA2	1:B:122:TYR:HA	8	23.47	0.8	23.0
(4,47)	1:A:122:TYR:HA	1:A:112:GLY:HA2	8	23.47	0.8	23.0
(4,47)	1:B:122:TYR:HA	1:B:112:GLY:HA2	8	23.47	0.8	23.0
(4,12)	1:A:112:GLY:HA3	1:A:122:TYR:HA	8	23.34	0.81	23.4
(4,12)	1:B:112:GLY:HA3	1:B:122:TYR:HA	8	23.34	0.81	23.4
(4,48)	1:A:122:TYR:HA	1:A:112:GLY:HA3	8	23.34	0.81	23.4
(4,48)	1:B:122:TYR:HA	1:B:112:GLY:HA3	8	23.34	0.81	23.4
(4,15)	1:A:112:GLY:HA2	1:A:122:TYR:HB2	8	23.27	0.74	23.22
(4,15)	1:B:112:GLY:HA2	1:B:122:TYR:HB2	8	23.27	0.74	23.22
(4,14)	1:A:112:GLY:HA3	1:A:122:TYR:HB2	8	23.09	1.17	23.48
(4,14)	1:B:112:GLY:HA3	1:B:122:TYR:HB2	8	23.09	1.17	23.48
(4,17)	1:A:112:GLY:HA2	1:A:124:ILE:HD11	8	22.43	0.88	22.56
(4,17)	1:A:112:GLY:HA2	1:A:124:ILE:HD12	8	22.43	0.88	22.56
(4,17)	1:A:112:GLY:HA2	1:A:124:ILE:HD13	8	22.43	0.88	22.56
(4,17)	1:B:112:GLY:HA2	1:B:124:ILE:HD11	8	22.43	0.88	22.56
(4,17)	1:B:112:GLY:HA2	1:B:124:ILE:HD12	8	22.43	0.88	22.56
(4,17)	1:B:112:GLY:HA2	1:B:124:ILE:HD13	8	22.43	0.88	22.56
(4,16)	1:A:112:GLY:HA2	1:A:122:TYR:HD1	8	20.77	1.35	21.04
(4,16)	1:A:112:GLY:HA2	1:A:122:TYR:HD2	8	20.77	1.35	21.04
(4,16)	1:B:112:GLY:HA2	1:B:122:TYR:HD1	8	20.77	1.35	21.04
(4,16)	1:B:112:GLY:HA2	1:B:122:TYR:HD2	8	20.77	1.35	21.04
(5,6)	1:A:113:PHE:H	1:A:121:LYS:H	8	19.63	0.71	19.24
(5,6)	1:B:113:PHE:H	1:B:121:LYS:H	8	19.63	0.71	19.24
(5,12)	1:A:121:LYS:H	1:A:113:PHE:H	8	19.03	0.71	18.64
(5,12)	1:B:121:LYS:H	1:B:113:PHE:H	8	19.03	0.71	18.64
(4,28)	1:A:116:ARG:HA	1:A:71:GLU:HG2	8	17.15	1.09	17.49
(4,28)	1:A:116:ARG:HA	1:A:71:GLU:HG3	8	17.15	1.09	17.49
(4,28)	1:B:116:ARG:HA	1:B:71:GLU:HG2	8	17.15	1.09	17.49
(4,28)	1:B:116:ARG:HA	1:B:71:GLU:HG3	8	17.15	1.09	17.49
(4,45)	1:A:121:LYS:HD2	1:A:113:PHE:HD1	8	12.96	0.67	13.04
(4,45)	1:A:121:LYS:HD2	1:A:113:PHE:HD2	8	12.96	0.67	13.04
(4,45)	1:A:121:LYS:HD3	1:A:113:PHE:HD1	8	12.96	0.67	13.04
(4,45)	1:A:121:LYS:HD3	1:A:113:PHE:HD2	8	12.96	0.67	13.04
(4,45)	1:B:121:LYS:HD2	1:B:113:PHE:HD1	8	12.96	0.67	13.04
(4,45)	1:B:121:LYS:HD2	1:B:113:PHE:HD2	8	12.96	0.67	13.04
(4,45)	1:B:121:LYS:HD3	1:B:113:PHE:HD1	8	12.96	0.67	13.04
(4,45)	1:B:121:LYS:HD3	1:B:113:PHE:HD2	8	12.96	0.67	13.04
(4,46)	1:A:121:LYS:HD2	1:A:113:PHE:HD1	8	12.96	0.67	13.04
(4,46)	1:A:121:LYS:HD2	1:A:113:PHE:HD2	8	12.96	0.67	13.04

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(4,46)	1:A:121:LYS:HD3	1:A:113:PHE:HD1	8	12.96	0.67	13.04
(4,46)	1:A:121:LYS:HD3	1:A:113:PHE:HD2	8	12.96	0.67	13.04
(4,46)	1:B:121:LYS:HD2	1:B:113:PHE:HD1	8	12.96	0.67	13.04
(4,46)	1:B:121:LYS:HD2	1:B:113:PHE:HD2	8	12.96	0.67	13.04
(4,46)	1:B:121:LYS:HD3	1:B:113:PHE:HD1	8	12.96	0.67	13.04
(4,46)	1:B:121:LYS:HD3	1:B:113:PHE:HD2	8	12.96	0.67	13.04
(4,27)	1:A:116:ARG:HA	1:A:70:LEU:HD11	8	11.51	1.46	12.11
(4,27)	1:A:116:ARG:HA	1:A:70:LEU:HD12	8	11.51	1.46	12.11
(4,27)	1:A:116:ARG:HA	1:A:70:LEU:HD13	8	11.51	1.46	12.11
(4,27)	1:A:116:ARG:HA	1:A:70:LEU:HD21	8	11.51	1.46	12.11
(4,27)	1:A:116:ARG:HA	1:A:70:LEU:HD22	8	11.51	1.46	12.11
(4,27)	1:A:116:ARG:HA	1:A:70:LEU:HD23	8	11.51	1.46	12.11
(4,27)	1:B:116:ARG:HA	1:B:70:LEU:HD11	8	11.51	1.46	12.11
(4,27)	1:B:116:ARG:HA	1:B:70:LEU:HD12	8	11.51	1.46	12.11
(4,27)	1:B:116:ARG:HA	1:B:70:LEU:HD13	8	11.51	1.46	12.11
(4,27)	1:B:116:ARG:HA	1:B:70:LEU:HD21	8	11.51	1.46	12.11
(4,27)	1:B:116:ARG:HA	1:B:70:LEU:HD22	8	11.51	1.46	12.11
(4,27)	1:B:116:ARG:HA	1:B:70:LEU:HD23	8	11.51	1.46	12.11
(4,1)	1:A:77:VAL:HG11	1:A:114:ILE:HB	8	11.13	0.83	11.21
(4,1)	1:A:77:VAL:HG12	1:A:114:ILE:HB	8	11.13	0.83	11.21
(4,1)	1:A:77:VAL:HG13	1:A:114:ILE:HB	8	11.13	0.83	11.21
(4,1)	1:B:77:VAL:HG11	1:B:114:ILE:HB	8	11.13	0.83	11.21
(4,1)	1:B:77:VAL:HG12	1:B:114:ILE:HB	8	11.13	0.83	11.21
(4,1)	1:B:77:VAL:HG13	1:B:114:ILE:HB	8	11.13	0.83	11.21
(4,39)	1:A:120:GLY:HA2	1:A:114:ILE:HB	8	9.64	0.42	9.73
(4,39)	1:A:120:GLY:HA3	1:A:114:ILE:HB	8	9.64	0.42	9.73
(4,39)	1:B:120:GLY:HA2	1:B:114:ILE:HB	8	9.64	0.42	9.73
(4,39)	1:B:120:GLY:HA3	1:B:114:ILE:HB	8	9.64	0.42	9.73
(4,24)	1:A:114:ILE:HA	1:A:120:GLY:HA2	8	9.46	0.47	9.44
(4,24)	1:A:114:ILE:HA	1:A:120:GLY:HA3	8	9.46	0.47	9.44
(4,24)	1:B:114:ILE:HA	1:B:120:GLY:HA2	8	9.46	0.47	9.44
(4,24)	1:B:114:ILE:HA	1:B:120:GLY:HA3	8	9.46	0.47	9.44
(4,37)	1:A:120:GLY:HA2	1:A:114:ILE:HA	8	9.46	0.47	9.44
(4,37)	1:A:120:GLY:HA3	1:A:114:ILE:HA	8	9.46	0.47	9.44
(4,37)	1:B:120:GLY:HA2	1:B:114:ILE:HA	8	9.46	0.47	9.44
(4,37)	1:B:120:GLY:HA3	1:B:114:ILE:HA	8	9.46	0.47	9.44
(4,44)	1:A:120:GLY:HA2	1:A:114:ILE:HA	8	9.46	0.47	9.44
(4,44)	1:A:120:GLY:HA3	1:A:114:ILE:HA	8	9.46	0.47	9.44
(4,44)	1:B:120:GLY:HA2	1:B:114:ILE:HA	8	9.46	0.47	9.44
(4,44)	1:B:120:GLY:HA3	1:B:114:ILE:HA	8	9.46	0.47	9.44
(5,1)	1:B:82:LYS:HE2	1:B:67:GLU:HA	8	9.36	2.66	9.78
(5,1)	1:B:82:LYS:HE3	1:B:67:GLU:HA	8	9.36	2.66	9.78

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(5,1)	1:A:82:LYS:HE2	1:A:67:GLU:HA	8	9.36	2.66	9.78
(5,1)	1:A:82:LYS:HE3	1:A:67:GLU:HA	8	9.36	2.66	9.78
(4,40)	1:A:120:GLY:HA2	1:A:114:ILE:HG12	8	8.77	0.41	8.8
(4,40)	1:A:120:GLY:HA2	1:A:114:ILE:HG13	8	8.77	0.41	8.8
(4,40)	1:A:120:GLY:HA3	1:A:114:ILE:HG12	8	8.77	0.41	8.8
(4,40)	1:A:120:GLY:HA3	1:A:114:ILE:HG13	8	8.77	0.41	8.8
(4,40)	1:B:120:GLY:HA2	1:B:114:ILE:HG12	8	8.77	0.41	8.8
(4,40)	1:B:120:GLY:HA2	1:B:114:ILE:HG13	8	8.77	0.41	8.8
(4,40)	1:B:120:GLY:HA3	1:B:114:ILE:HG12	8	8.77	0.41	8.8
(4,40)	1:B:120:GLY:HA3	1:B:114:ILE:HG13	8	8.77	0.41	8.8
(4,18)	1:A:114:ILE:HG21	1:A:77:VAL:HG21	8	8.32	1.35	8.56
(4,18)	1:A:114:ILE:HG21	1:A:77:VAL:HG22	8	8.32	1.35	8.56
(4,18)	1:A:114:ILE:HG21	1:A:77:VAL:HG23	8	8.32	1.35	8.56
(4,18)	1:A:114:ILE:HG22	1:A:77:VAL:HG21	8	8.32	1.35	8.56
(4,18)	1:A:114:ILE:HG22	1:A:77:VAL:HG22	8	8.32	1.35	8.56
(4,18)	1:A:114:ILE:HG22	1:A:77:VAL:HG23	8	8.32	1.35	8.56
(4,18)	1:A:114:ILE:HG23	1:A:77:VAL:HG21	8	8.32	1.35	8.56
(4,18)	1:A:114:ILE:HG23	1:A:77:VAL:HG22	8	8.32	1.35	8.56
(4,18)	1:A:114:ILE:HG23	1:A:77:VAL:HG23	8	8.32	1.35	8.56
(4,18)	1:B:114:ILE:HG21	1:B:77:VAL:HG21	8	8.32	1.35	8.56
(4,18)	1:B:114:ILE:HG21	1:B:77:VAL:HG22	8	8.32	1.35	8.56
(4,18)	1:B:114:ILE:HG21	1:B:77:VAL:HG23	8	8.32	1.35	8.56
(4,18)	1:B:114:ILE:HG22	1:B:77:VAL:HG21	8	8.32	1.35	8.56
(4,18)	1:B:114:ILE:HG22	1:B:77:VAL:HG22	8	8.32	1.35	8.56
(4,18)	1:B:114:ILE:HG22	1:B:77:VAL:HG23	8	8.32	1.35	8.56
(4,18)	1:B:114:ILE:HG23	1:B:77:VAL:HG21	8	8.32	1.35	8.56
(4,18)	1:B:114:ILE:HG23	1:B:77:VAL:HG22	8	8.32	1.35	8.56
(4,18)	1:B:114:ILE:HG23	1:B:77:VAL:HG23	8	8.32	1.35	8.56
(4,19)	1:A:114:ILE:HG21	1:A:77:VAL:HG21	8	8.32	1.35	8.56
(4,19)	1:A:114:ILE:HG21	1:A:77:VAL:HG22	8	8.32	1.35	8.56
(4,19)	1:A:114:ILE:HG21	1:A:77:VAL:HG23	8	8.32	1.35	8.56
(4,19)	1:A:114:ILE:HG22	1:A:77:VAL:HG21	8	8.32	1.35	8.56
(4,19)	1:A:114:ILE:HG22	1:A:77:VAL:HG22	8	8.32	1.35	8.56
(4,19)	1:A:114:ILE:HG22	1:A:77:VAL:HG23	8	8.32	1.35	8.56
(4,19)	1:A:114:ILE:HG23	1:A:77:VAL:HG21	8	8.32	1.35	8.56
(4,19)	1:A:114:ILE:HG23	1:A:77:VAL:HG22	8	8.32	1.35	8.56
(4,19)	1:A:114:ILE:HG23	1:A:77:VAL:HG23	8	8.32	1.35	8.56
(4,19)	1:B:114:ILE:HG21	1:B:77:VAL:HG21	8	8.32	1.35	8.56
(4,19)	1:B:114:ILE:HG21	1:B:77:VAL:HG22	8	8.32	1.35	8.56
(4,19)	1:B:114:ILE:HG21	1:B:77:VAL:HG23	8	8.32	1.35	8.56
(4,19)	1:B:114:ILE:HG22	1:B:77:VAL:HG21	8	8.32	1.35	8.56
(4,19)	1:B:114:ILE:HG22	1:B:77:VAL:HG22	8	8.32	1.35	8.56

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(4,19)	1:B:114:ILE:HG22	1:B:77:VAL:HG23	8	8.32	1.35	8.56
(4,19)	1:B:114:ILE:HG23	1:B:77:VAL:HG21	8	8.32	1.35	8.56
(4,19)	1:B:114:ILE:HG23	1:B:77:VAL:HG22	8	8.32	1.35	8.56
(4,19)	1:B:114:ILE:HG23	1:B:77:VAL:HG23	8	8.32	1.35	8.56
(4,50)	1:A:115:SER:H	1:A:120:GLY:HA2	8	8.12	0.53	7.98
(4,50)	1:A:115:SER:H	1:A:120:GLY:HA3	8	8.12	0.53	7.98
(4,50)	1:B:115:SER:H	1:B:120:GLY:HA2	8	8.12	0.53	7.98
(4,50)	1:B:115:SER:H	1:B:120:GLY:HA3	8	8.12	0.53	7.98
(5,3)	1:B:82:LYS:H	1:B:66:SER:H	8	7.98	1.77	7.35
(5,3)	1:A:82:LYS:H	1:A:66:SER:H	8	7.98	1.77	7.35
(4,41)	1:A:120:GLY:HA2	1:A:114:ILE:HD11	8	7.65	0.45	7.62
(4,41)	1:A:120:GLY:HA2	1:A:114:ILE:HD12	8	7.65	0.45	7.62
(4,41)	1:A:120:GLY:HA2	1:A:114:ILE:HD13	8	7.65	0.45	7.62
(4,41)	1:A:120:GLY:HA3	1:A:114:ILE:HD11	8	7.65	0.45	7.62
(4,41)	1:A:120:GLY:HA3	1:A:114:ILE:HD12	8	7.65	0.45	7.62
(4,41)	1:A:120:GLY:HA3	1:A:114:ILE:HD13	8	7.65	0.45	7.62
(4,41)	1:B:120:GLY:HA2	1:B:114:ILE:HD11	8	7.65	0.45	7.62
(4,41)	1:B:120:GLY:HA2	1:B:114:ILE:HD12	8	7.65	0.45	7.62
(4,41)	1:B:120:GLY:HA2	1:B:114:ILE:HD13	8	7.65	0.45	7.62
(4,41)	1:B:120:GLY:HA3	1:B:114:ILE:HD11	8	7.65	0.45	7.62
(4,41)	1:B:120:GLY:HA3	1:B:114:ILE:HD12	8	7.65	0.45	7.62
(4,41)	1:B:120:GLY:HA3	1:B:114:ILE:HD13	8	7.65	0.45	7.62
(5,4)	1:B:82:LYS:H	1:B:66:SER:HA	8	7.03	1.25	7.12
(5,4)	1:A:82:LYS:H	1:A:66:SER:HA	8	7.03	1.25	7.12
(4,26)	1:A:115:SER:HB2	1:A:119:HIS:HD2	8	6.8	2.28	6.94
(4,26)	1:B:115:SER:HB2	1:B:119:HIS:HD2	8	6.8	2.28	6.94
(4,38)	1:A:120:GLY:HA2	1:A:114:ILE:HG21	8	5.76	0.39	5.85
(4,38)	1:A:120:GLY:HA2	1:A:114:ILE:HG22	8	5.76	0.39	5.85
(4,38)	1:A:120:GLY:HA2	1:A:114:ILE:HG23	8	5.76	0.39	5.85
(4,38)	1:A:120:GLY:HA3	1:A:114:ILE:HG21	8	5.76	0.39	5.85
(4,38)	1:A:120:GLY:HA3	1:A:114:ILE:HG22	8	5.76	0.39	5.85
(4,38)	1:A:120:GLY:HA3	1:A:114:ILE:HG23	8	5.76	0.39	5.85
(4,38)	1:B:120:GLY:HA2	1:B:114:ILE:HG21	8	5.76	0.39	5.85
(4,38)	1:B:120:GLY:HA2	1:B:114:ILE:HG22	8	5.76	0.39	5.85
(4,38)	1:B:120:GLY:HA2	1:B:114:ILE:HG23	8	5.76	0.39	5.85
(4,38)	1:B:120:GLY:HA3	1:B:114:ILE:HG21	8	5.76	0.39	5.85
(4,38)	1:B:120:GLY:HA3	1:B:114:ILE:HG22	8	5.76	0.39	5.85
(4,38)	1:B:120:GLY:HA3	1:B:114:ILE:HG23	8	5.76	0.39	5.85
(4,42)	1:A:120:GLY:HA2	1:A:114:ILE:HG21	8	5.76	0.39	5.85
(4,42)	1:A:120:GLY:HA2	1:A:114:ILE:HG22	8	5.76	0.39	5.85
(4,42)	1:A:120:GLY:HA2	1:A:114:ILE:HG23	8	5.76	0.39	5.85
(4,42)	1:A:120:GLY:HA3	1:A:114:ILE:HG21	8	5.76	0.39	5.85

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(4,42)	1:A:120:GLY:HA3	1:A:114:ILE:HG22	8	5.76	0.39	5.85
(4,42)	1:A:120:GLY:HA3	1:A:114:ILE:HG23	8	5.76	0.39	5.85
(4,42)	1:B:120:GLY:HA2	1:B:114:ILE:HG21	8	5.76	0.39	5.85
(4,42)	1:B:120:GLY:HA2	1:B:114:ILE:HG22	8	5.76	0.39	5.85
(4,42)	1:B:120:GLY:HA2	1:B:114:ILE:HG23	8	5.76	0.39	5.85
(4,42)	1:B:120:GLY:HA3	1:B:114:ILE:HG21	8	5.76	0.39	5.85
(4,42)	1:B:120:GLY:HA3	1:B:114:ILE:HG22	8	5.76	0.39	5.85
(4,42)	1:B:120:GLY:HA3	1:B:114:ILE:HG23	8	5.76	0.39	5.85
(4,43)	1:A:120:GLY:HA2	1:A:114:ILE:HG21	8	5.76	0.39	5.85
(4,43)	1:A:120:GLY:HA2	1:A:114:ILE:HG22	8	5.76	0.39	5.85
(4,43)	1:A:120:GLY:HA2	1:A:114:ILE:HG23	8	5.76	0.39	5.85
(4,43)	1:A:120:GLY:HA3	1:A:114:ILE:HG21	8	5.76	0.39	5.85
(4,43)	1:A:120:GLY:HA3	1:A:114:ILE:HG22	8	5.76	0.39	5.85
(4,43)	1:A:120:GLY:HA3	1:A:114:ILE:HG23	8	5.76	0.39	5.85
(4,43)	1:B:120:GLY:HA2	1:B:114:ILE:HG21	8	5.76	0.39	5.85
(4,43)	1:B:120:GLY:HA2	1:B:114:ILE:HG22	8	5.76	0.39	5.85
(4,43)	1:B:120:GLY:HA2	1:B:114:ILE:HG23	8	5.76	0.39	5.85
(4,43)	1:B:120:GLY:HA3	1:B:114:ILE:HG21	8	5.76	0.39	5.85
(4,43)	1:B:120:GLY:HA3	1:B:114:ILE:HG22	8	5.76	0.39	5.85
(4,43)	1:B:120:GLY:HA3	1:B:114:ILE:HG23	8	5.76	0.39	5.85
(4,25)	1:A:115:SER:HB2	1:A:119:HIS:HB3	8	5.55	0.86	5.3
(4,25)	1:B:115:SER:HB2	1:B:119:HIS:HB3	8	5.55	0.86	5.3
(4,35)	1:A:119:HIS:HB3	1:A:115:SER:HB2	8	5.55	0.86	5.3
(4,35)	1:B:119:HIS:HB3	1:B:115:SER:HB2	8	5.55	0.86	5.3
(4,36)	1:A:119:HIS:HB3	1:A:115:SER:HB2	8	5.55	0.86	5.3
(4,36)	1:B:119:HIS:HB3	1:B:115:SER:HB2	8	5.55	0.86	5.3
(4,34)	1:A:119:HIS:HB2	1:A:115:SER:HB2	8	5.36	1.57	4.82
(4,34)	1:B:119:HIS:HB2	1:B:115:SER:HB2	8	5.36	1.57	4.82
(4,23)	1:A:114:ILE:HG21	1:A:119:HIS:HA	8	5.0	0.64	4.98
(4,23)	1:A:114:ILE:HG22	1:A:119:HIS:HA	8	5.0	0.64	4.98
(4,23)	1:A:114:ILE:HG23	1:A:119:HIS:HA	8	5.0	0.64	4.98
(4,23)	1:B:114:ILE:HG21	1:B:119:HIS:HA	8	5.0	0.64	4.98
(4,23)	1:B:114:ILE:HG22	1:B:119:HIS:HA	8	5.0	0.64	4.98
(4,23)	1:B:114:ILE:HG23	1:B:119:HIS:HA	8	5.0	0.64	4.98
(4,51)	1:A:119:HIS:H	1:A:114:ILE:HG21	8	3.8	0.75	3.76
(4,51)	1:A:119:HIS:H	1:A:114:ILE:HG22	8	3.8	0.75	3.76
(4,51)	1:A:119:HIS:H	1:A:114:ILE:HG23	8	3.8	0.75	3.76
(4,51)	1:B:119:HIS:H	1:B:114:ILE:HG21	8	3.8	0.75	3.76
(4,51)	1:B:119:HIS:H	1:B:114:ILE:HG22	8	3.8	0.75	3.76
(4,51)	1:B:119:HIS:H	1:B:114:ILE:HG23	8	3.8	0.75	3.76
(5,10)	1:A:119:HIS:H	1:A:116:ARG:HA	8	3.15	0.45	3.22
(5,10)	1:B:119:HIS:H	1:B:116:ARG:HA	8	3.15	0.45	3.22

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(4,21)	1:A:114:ILE:HG21	1:A:118:PHE:HB2	8	1.33	0.55	1.52
(4,21)	1:A:114:ILE:HG21	1:A:118:PHE:HB3	8	1.33	0.55	1.52
(4,21)	1:A:114:ILE:HG22	1:A:118:PHE:HB2	8	1.33	0.55	1.52
(4,21)	1:A:114:ILE:HG22	1:A:118:PHE:HB3	8	1.33	0.55	1.52
(4,21)	1:A:114:ILE:HG23	1:A:118:PHE:HB2	8	1.33	0.55	1.52
(4,21)	1:A:114:ILE:HG23	1:A:118:PHE:HB3	8	1.33	0.55	1.52
(4,21)	1:B:114:ILE:HG21	1:B:118:PHE:HB2	8	1.33	0.55	1.52
(4,21)	1:B:114:ILE:HG21	1:B:118:PHE:HB3	8	1.33	0.55	1.52
(4,21)	1:B:114:ILE:HG22	1:B:118:PHE:HB2	8	1.33	0.55	1.52
(4,21)	1:B:114:ILE:HG22	1:B:118:PHE:HB3	8	1.33	0.55	1.52
(4,21)	1:B:114:ILE:HG23	1:B:118:PHE:HB2	8	1.33	0.55	1.52
(4,21)	1:B:114:ILE:HG23	1:B:118:PHE:HB3	8	1.33	0.55	1.52
(4,22)	1:A:114:ILE:HG21	1:A:118:PHE:HB2	8	1.33	0.55	1.52
(4,22)	1:A:114:ILE:HG21	1:A:118:PHE:HB3	8	1.33	0.55	1.52
(4,22)	1:A:114:ILE:HG22	1:A:118:PHE:HB2	8	1.33	0.55	1.52
(4,22)	1:A:114:ILE:HG22	1:A:118:PHE:HB3	8	1.33	0.55	1.52
(4,22)	1:A:114:ILE:HG23	1:A:118:PHE:HB2	8	1.33	0.55	1.52
(4,22)	1:A:114:ILE:HG23	1:A:118:PHE:HB3	8	1.33	0.55	1.52
(4,22)	1:B:114:ILE:HG21	1:B:118:PHE:HB2	8	1.33	0.55	1.52
(4,22)	1:B:114:ILE:HG21	1:B:118:PHE:HB3	8	1.33	0.55	1.52
(4,22)	1:B:114:ILE:HG22	1:B:118:PHE:HB2	8	1.33	0.55	1.52
(4,22)	1:B:114:ILE:HG22	1:B:118:PHE:HB3	8	1.33	0.55	1.52
(4,22)	1:B:114:ILE:HG23	1:B:118:PHE:HB2	8	1.33	0.55	1.52
(4,22)	1:B:114:ILE:HG23	1:B:118:PHE:HB3	8	1.33	0.55	1.52
(5,2)	1:A:116:ARG:HB2	1:A:118:PHE:HA	8	1.24	0.66	1.21
(5,2)	1:A:116:ARG:HB3	1:A:118:PHE:HA	8	1.24	0.66	1.21
(5,2)	1:B:116:ARG:HB2	1:B:118:PHE:HA	8	1.24	0.66	1.21
(5,2)	1:B:116:ARG:HB3	1:B:118:PHE:HA	8	1.24	0.66	1.21
(1,104)	1:A:92:LYS:H	1:A:100:VAL:HG11	8	0.74	0.27	0.76
(1,104)	1:A:92:LYS:H	1:A:100:VAL:HG12	8	0.74	0.27	0.76
(1,104)	1:A:92:LYS:H	1:A:100:VAL:HG13	8	0.74	0.27	0.76
(1,104)	1:B:92:LYS:H	1:B:100:VAL:HG11	8	0.74	0.27	0.76
(1,104)	1:B:92:LYS:H	1:B:100:VAL:HG12	8	0.74	0.27	0.76
(1,104)	1:B:92:LYS:H	1:B:100:VAL:HG13	8	0.74	0.27	0.76
(1,309)	1:A:146:ASN:H	1:A:133:ILE:HA	8	0.67	0.23	0.69
(1,309)	1:B:146:ASN:H	1:B:133:ILE:HA	8	0.67	0.23	0.69
(1,83)	1:B:85:SER:H	1:B:86:PRO:HA	8	0.46	0.08	0.48
(1,83)	1:A:85:SER:H	1:A:86:PRO:HA	8	0.46	0.08	0.48
(1,231)	1:A:127:ASP:H	1:A:128:VAL:HG11	7	1.14	0.28	1.22
(1,231)	1:A:127:ASP:H	1:A:128:VAL:HG12	7	1.14	0.28	1.22
(1,231)	1:A:127:ASP:H	1:A:128:VAL:HG13	7	1.14	0.28	1.22
(1,231)	1:B:127:ASP:H	1:B:128:VAL:HG11	7	1.14	0.28	1.22

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,231)	1:B:127:ASP:H	1:B:128:VAL:HG12	7	1.14	0.28	1.22
(1,231)	1:B:127:ASP:H	1:B:128:VAL:HG13	7	1.14	0.28	1.22
(1,290)	1:A:138:SER:H	1:A:137:LEU:HD21	7	0.43	0.04	0.41
(1,290)	1:A:138:SER:H	1:A:137:LEU:HD22	7	0.43	0.04	0.41
(1,290)	1:A:138:SER:H	1:A:137:LEU:HD23	7	0.43	0.04	0.41
(1,290)	1:B:138:SER:H	1:B:137:LEU:HD21	7	0.43	0.04	0.41
(1,290)	1:B:138:SER:H	1:B:137:LEU:HD22	7	0.43	0.04	0.41
(1,290)	1:B:138:SER:H	1:B:137:LEU:HD23	7	0.43	0.04	0.41
(1,222)	1:A:126:ALA:H	1:A:128:VAL:HG11	6	1.5	0.13	1.58
(1,222)	1:A:126:ALA:H	1:A:128:VAL:HG12	6	1.5	0.13	1.58
(1,222)	1:A:126:ALA:H	1:A:128:VAL:HG13	6	1.5	0.13	1.58
(1,222)	1:B:126:ALA:H	1:B:128:VAL:HG11	6	1.5	0.13	1.58
(1,222)	1:B:126:ALA:H	1:B:128:VAL:HG12	6	1.5	0.13	1.58
(1,222)	1:B:126:ALA:H	1:B:128:VAL:HG13	6	1.5	0.13	1.58
(1,258)	1:A:134:THR:H	1:A:133:ILE:HD11	6	0.74	0.05	0.75
(1,258)	1:A:134:THR:H	1:A:133:ILE:HD12	6	0.74	0.05	0.75
(1,258)	1:A:134:THR:H	1:A:133:ILE:HD13	6	0.74	0.05	0.75
(1,258)	1:B:134:THR:H	1:B:133:ILE:HD11	6	0.74	0.05	0.75
(1,258)	1:B:134:THR:H	1:B:133:ILE:HD12	6	0.74	0.05	0.75
(1,258)	1:B:134:THR:H	1:B:133:ILE:HD13	6	0.74	0.05	0.75
(1,3)	1:A:66:SER:HA	1:A:65:LEU:HD11	6	0.27	0.14	0.24
(1,3)	1:A:66:SER:HA	1:A:65:LEU:HD12	6	0.27	0.14	0.24
(1,3)	1:A:66:SER:HA	1:A:65:LEU:HD13	6	0.27	0.14	0.24
(1,3)	1:A:66:SER:HA	1:A:65:LEU:HD21	6	0.27	0.14	0.24
(1,3)	1:A:66:SER:HA	1:A:65:LEU:HD22	6	0.27	0.14	0.24
(1,3)	1:A:66:SER:HA	1:A:65:LEU:HD23	6	0.27	0.14	0.24
(1,3)	1:B:66:SER:HA	1:B:65:LEU:HD11	6	0.27	0.14	0.24
(1,3)	1:B:66:SER:HA	1:B:65:LEU:HD12	6	0.27	0.14	0.24
(1,3)	1:B:66:SER:HA	1:B:65:LEU:HD13	6	0.27	0.14	0.24
(1,3)	1:B:66:SER:HA	1:B:65:LEU:HD21	6	0.27	0.14	0.24
(1,3)	1:B:66:SER:HA	1:B:65:LEU:HD22	6	0.27	0.14	0.24
(1,3)	1:B:66:SER:HA	1:B:65:LEU:HD23	6	0.27	0.14	0.24
(4,30)	1:B:118:PHE:HA	1:B:116:ARG:HG2	4	0.68	0.32	0.53
(4,30)	1:B:118:PHE:HA	1:B:116:ARG:HG3	4	0.68	0.32	0.53
(4,30)	1:A:118:PHE:HA	1:A:116:ARG:HG2	4	0.68	0.32	0.53
(4,30)	1:A:118:PHE:HA	1:A:116:ARG:HG3	4	0.68	0.32	0.53
(1,49)	1:A:78:ASN:HA	1:A:79:LEU:HD11	4	0.26	0.11	0.26
(1,49)	1:A:78:ASN:HA	1:A:79:LEU:HD12	4	0.26	0.11	0.26
(1,49)	1:A:78:ASN:HA	1:A:79:LEU:HD13	4	0.26	0.11	0.26
(1,49)	1:A:78:ASN:HA	1:A:79:LEU:HD21	4	0.26	0.11	0.26
(1,49)	1:A:78:ASN:HA	1:A:79:LEU:HD22	4	0.26	0.11	0.26
(1,49)	1:A:78:ASN:HA	1:A:79:LEU:HD23	4	0.26	0.11	0.26

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,49)	1:B:78:ASN:HA	1:B:79:LEU:HD11	4	0.26	0.11	0.26
(1,49)	1:B:78:ASN:HA	1:B:79:LEU:HD12	4	0.26	0.11	0.26
(1,49)	1:B:78:ASN:HA	1:B:79:LEU:HD13	4	0.26	0.11	0.26
(1,49)	1:B:78:ASN:HA	1:B:79:LEU:HD21	4	0.26	0.11	0.26
(1,49)	1:B:78:ASN:HA	1:B:79:LEU:HD22	4	0.26	0.11	0.26
(1,49)	1:B:78:ASN:HA	1:B:79:LEU:HD23	4	0.26	0.11	0.26
(2,133)	1:B:118:PHE:HB2	1:B:81:VAL:HG21	3	0.83	0.29	0.83
(2,133)	1:B:118:PHE:HB2	1:B:81:VAL:HG22	3	0.83	0.29	0.83
(2,133)	1:B:118:PHE:HB2	1:B:81:VAL:HG23	3	0.83	0.29	0.83
(2,133)	1:B:118:PHE:HB3	1:B:81:VAL:HG21	3	0.83	0.29	0.83
(2,133)	1:B:118:PHE:HB3	1:B:81:VAL:HG22	3	0.83	0.29	0.83
(2,133)	1:B:118:PHE:HB3	1:B:81:VAL:HG23	3	0.83	0.29	0.83
(2,133)	1:A:118:PHE:HB2	1:A:81:VAL:HG21	3	0.83	0.29	0.83
(2,133)	1:A:118:PHE:HB2	1:A:81:VAL:HG22	3	0.83	0.29	0.83
(2,133)	1:A:118:PHE:HB2	1:A:81:VAL:HG23	3	0.83	0.29	0.83
(2,133)	1:A:118:PHE:HB3	1:A:81:VAL:HG21	3	0.83	0.29	0.83
(2,133)	1:A:118:PHE:HB3	1:A:81:VAL:HG22	3	0.83	0.29	0.83
(2,133)	1:A:118:PHE:HB3	1:A:81:VAL:HG23	3	0.83	0.29	0.83
(1,172)	1:A:113:PHE:HA	1:A:107:ARG:HA	3	0.59	0.42	0.36
(1,172)	1:B:113:PHE:HA	1:B:107:ARG:HA	3	0.59	0.42	0.36
(2,146)	1:A:127:ASP:H	1:A:124:ILE:HG21	3	0.47	0.31	0.26
(2,146)	1:A:127:ASP:H	1:A:124:ILE:HG22	3	0.47	0.31	0.26
(2,146)	1:A:127:ASP:H	1:A:124:ILE:HG23	3	0.47	0.31	0.26
(2,146)	1:B:127:ASP:H	1:B:124:ILE:HG21	3	0.47	0.31	0.26
(2,146)	1:B:127:ASP:H	1:B:124:ILE:HG22	3	0.47	0.31	0.26
(2,146)	1:B:127:ASP:H	1:B:124:ILE:HG23	3	0.47	0.31	0.26
(2,113)	1:A:113:PHE:H	1:A:111:HIS:HA	3	0.23	0.07	0.26
(2,113)	1:B:113:PHE:H	1:B:111:HIS:HA	3	0.23	0.07	0.26
(1,186)	1:A:115:SER:HA	1:A:105:GLU:HA	2	1.72	0.01	1.72
(1,186)	1:B:115:SER:HA	1:B:105:GLU:HA	2	1.72	0.01	1.72
(1,230)	1:A:127:ASP:H	1:A:128:VAL:HB	2	1.67	0.58	1.67
(1,230)	1:B:127:ASP:H	1:B:128:VAL:HB	2	1.67	0.58	1.67
(2,38)	1:B:82:LYS:HE2	1:B:83:HIS:HE1	2	1.42	0.72	1.42
(2,38)	1:B:82:LYS:HE3	1:B:83:HIS:HE1	2	1.42	0.72	1.42
(2,38)	1:A:82:LYS:HE2	1:A:83:HIS:HE1	2	1.42	0.72	1.42
(2,38)	1:A:82:LYS:HE3	1:A:83:HIS:HE1	2	1.42	0.72	1.42
(2,118)	1:A:114:ILE:HA	1:A:113:PHE:HE1	2	1.21	0.01	1.21
(2,118)	1:A:114:ILE:HA	1:A:113:PHE:HE2	2	1.21	0.01	1.21
(2,118)	1:B:114:ILE:HA	1:B:113:PHE:HE1	2	1.21	0.01	1.21
(2,118)	1:B:114:ILE:HA	1:B:113:PHE:HE2	2	1.21	0.01	1.21
(2,121)	1:A:115:SER:HA	1:A:105:GLU:HG2	2	1.0	0.01	1.0
(2,121)	1:A:115:SER:HA	1:A:105:GLU:HG3	2	1.0	0.01	1.0

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,121)	1:B:115:SER:HA	1:B:105:GLU:HG2	2	1.0	0.01	1.0
(2,121)	1:B:115:SER:HA	1:B:105:GLU:HG3	2	1.0	0.01	1.0
(2,108)	1:A:108:GLN:H	1:A:114:ILE:HD11	2	0.84	0.36	0.84
(2,108)	1:A:108:GLN:H	1:A:114:ILE:HD12	2	0.84	0.36	0.84
(2,108)	1:A:108:GLN:H	1:A:114:ILE:HD13	2	0.84	0.36	0.84
(2,108)	1:B:108:GLN:H	1:B:114:ILE:HD11	2	0.84	0.36	0.84
(2,108)	1:B:108:GLN:H	1:B:114:ILE:HD12	2	0.84	0.36	0.84
(2,108)	1:B:108:GLN:H	1:B:114:ILE:HD13	2	0.84	0.36	0.84
(2,7)	1:A:66:SER:HB2	1:A:77:VAL:HG11	2	0.75	0.2	0.75
(2,7)	1:A:66:SER:HB2	1:A:77:VAL:HG12	2	0.75	0.2	0.75
(2,7)	1:A:66:SER:HB2	1:A:77:VAL:HG13	2	0.75	0.2	0.75
(2,7)	1:A:66:SER:HB3	1:A:77:VAL:HG11	2	0.75	0.2	0.75
(2,7)	1:A:66:SER:HB3	1:A:77:VAL:HG12	2	0.75	0.2	0.75
(2,7)	1:A:66:SER:HB3	1:A:77:VAL:HG13	2	0.75	0.2	0.75
(2,7)	1:B:66:SER:HB2	1:B:77:VAL:HG11	2	0.75	0.2	0.75
(2,7)	1:B:66:SER:HB2	1:B:77:VAL:HG12	2	0.75	0.2	0.75
(2,7)	1:B:66:SER:HB2	1:B:77:VAL:HG13	2	0.75	0.2	0.75
(2,7)	1:B:66:SER:HB3	1:B:77:VAL:HG11	2	0.75	0.2	0.75
(2,7)	1:B:66:SER:HB3	1:B:77:VAL:HG12	2	0.75	0.2	0.75
(2,7)	1:B:66:SER:HB3	1:B:77:VAL:HG13	2	0.75	0.2	0.75
(2,95)	1:B:106:GLU:H	1:B:115:SER:HB2	2	0.64	0.15	0.64
(2,95)	1:B:106:GLU:H	1:B:115:SER:HB3	2	0.64	0.15	0.64
(2,95)	1:A:106:GLU:H	1:A:115:SER:HB2	2	0.64	0.15	0.64
(2,95)	1:A:106:GLU:H	1:A:115:SER:HB3	2	0.64	0.15	0.64
(2,8)	1:A:66:SER:HA	1:A:77:VAL:HG21	2	0.62	0.44	0.62
(2,8)	1:A:66:SER:HA	1:A:77:VAL:HG22	2	0.62	0.44	0.62
(2,8)	1:A:66:SER:HA	1:A:77:VAL:HG23	2	0.62	0.44	0.62
(2,8)	1:B:66:SER:HA	1:B:77:VAL:HG21	2	0.62	0.44	0.62
(2,8)	1:B:66:SER:HA	1:B:77:VAL:HG22	2	0.62	0.44	0.62
(2,8)	1:B:66:SER:HA	1:B:77:VAL:HG23	2	0.62	0.44	0.62
(2,92)	1:B:104:HIS:H	1:B:105:GLU:HG2	2	0.52	0.06	0.52
(2,92)	1:B:104:HIS:H	1:B:105:GLU:HG3	2	0.52	0.06	0.52
(2,92)	1:A:104:HIS:H	1:A:105:GLU:HG2	2	0.52	0.06	0.52
(2,92)	1:A:104:HIS:H	1:A:105:GLU:HG3	2	0.52	0.06	0.52
(4,31)	1:B:118:PHE:HB2	1:B:116:ARG:HA	2	0.4	0.0	0.4
(4,31)	1:B:118:PHE:HB3	1:B:116:ARG:HA	2	0.4	0.0	0.4
(4,31)	1:A:118:PHE:HB2	1:A:116:ARG:HA	2	0.4	0.0	0.4
(4,31)	1:A:118:PHE:HB3	1:A:116:ARG:HA	2	0.4	0.0	0.4
(1,209)	1:A:121:LYS:H	1:A:122:TYR:HA	2	0.36	0.01	0.36
(1,209)	1:B:121:LYS:H	1:B:122:TYR:HA	2	0.36	0.01	0.36
(1,69)	1:B:82:LYS:HE2	1:B:82:LYS:HA	2	0.29	0.17	0.29
(1,69)	1:B:82:LYS:HE3	1:B:82:LYS:HA	2	0.29	0.17	0.29

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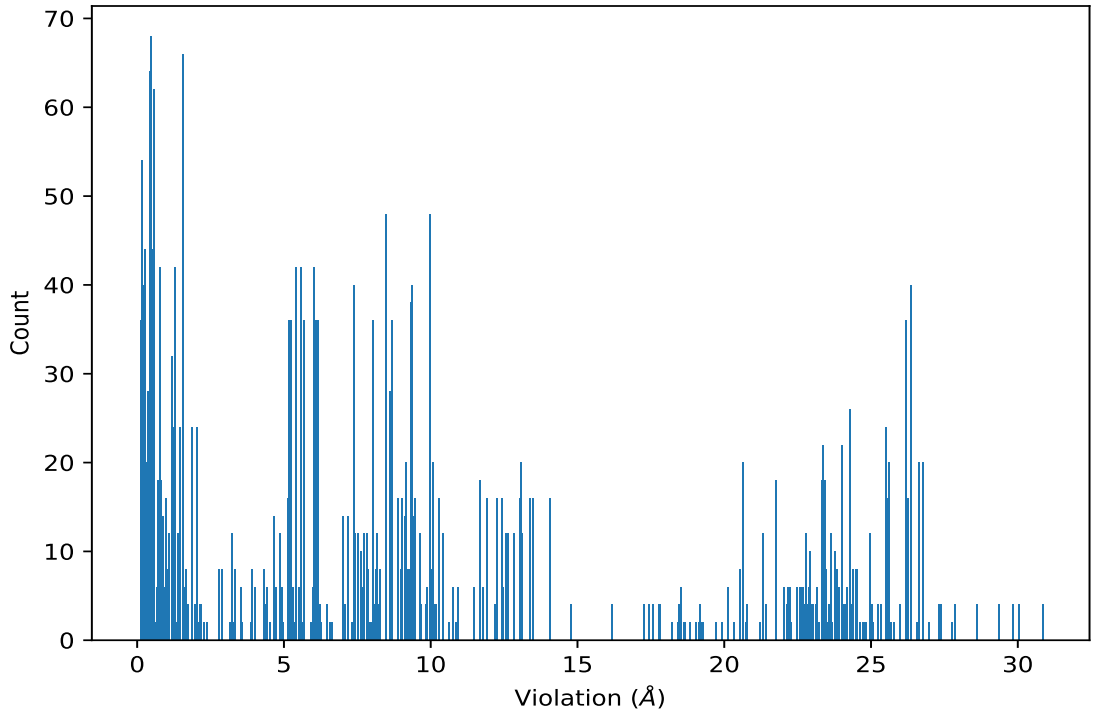
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,69)	1:A:82:LYS:HE2	1:A:82:LYS:HA	2	0.29	0.17	0.29
(1,69)	1:A:82:LYS:HE3	1:A:82:LYS:HA	2	0.29	0.17	0.29
(3,270)	1:B:110:GLU:H	1:B:109:ASP:HB2	2	0.27	0.0	0.27
(3,270)	1:B:110:GLU:H	1:B:109:ASP:HB3	2	0.27	0.0	0.27
(3,270)	1:A:110:GLU:H	1:A:109:ASP:HB2	2	0.27	0.0	0.27
(3,270)	1:A:110:GLU:H	1:A:109:ASP:HB3	2	0.27	0.0	0.27
(3,329)	1:B:118:PHE:HA	1:B:118:PHE:HD1	2	0.16	0.02	0.16
(3,329)	1:B:118:PHE:HA	1:B:118:PHE:HD2	2	0.16	0.02	0.16
(3,329)	1:A:118:PHE:HA	1:A:118:PHE:HD1	2	0.16	0.02	0.16
(3,329)	1:A:118:PHE:HA	1:A:118:PHE:HD2	2	0.16	0.02	0.16

[1]Number of violated models, [2]Standard 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)
(5,5)	1:B:110:GLU:H	1:B:123:ARG:HB2	4	30.9
(5,5)	1:B:110:GLU:H	1:B:123:ARG:HB3	4	30.9
(5,5)	1:A:110:GLU:H	1:A:123:ARG:HB2	4	30.9
(5,5)	1:A:110:GLU:H	1:A:123:ARG:HB3	4	30.9
(5,5)	1:B:110:GLU:H	1:B:123:ARG:HB2	3	30.02
(5,5)	1:B:110:GLU:H	1:B:123:ARG:HB3	3	30.02
(5,5)	1:A:110:GLU:H	1:A:123:ARG:HB2	3	30.02
(5,5)	1:A:110:GLU:H	1:A:123:ARG:HB3	3	30.02
(5,5)	1:B:110:GLU:H	1:B:123:ARG:HB2	5	29.84
(5,5)	1:B:110:GLU:H	1:B:123:ARG:HB3	5	29.84
(5,5)	1:A:110:GLU:H	1:A:123:ARG:HB2	5	29.84
(5,5)	1:A:110:GLU:H	1:A:123:ARG:HB3	5	29.84
(5,5)	1:B:110:GLU:H	1:B:123:ARG:HB2	2	29.35
(5,5)	1:B:110:GLU:H	1:B:123:ARG:HB3	2	29.35
(5,5)	1:A:110:GLU:H	1:A:123:ARG:HB2	2	29.35
(5,5)	1:A:110:GLU:H	1:A:123:ARG:HB3	2	29.35
(5,5)	1:B:110:GLU:H	1:B:123:ARG:HB2	8	28.62
(5,5)	1:B:110:GLU:H	1:B:123:ARG:HB3	8	28.62
(5,5)	1:A:110:GLU:H	1:A:123:ARG:HB2	8	28.62
(5,5)	1:A:110:GLU:H	1:A:123:ARG:HB3	8	28.62
(5,5)	1:B:110:GLU:H	1:B:123:ARG:HB2	6	27.87
(5,5)	1:B:110:GLU:H	1:B:123:ARG:HB3	6	27.87
(5,5)	1:A:110:GLU:H	1:A:123:ARG:HB2	6	27.87
(5,5)	1:A:110:GLU:H	1:A:123:ARG:HB3	6	27.87
(4,49)	1:A:113:PHE:H	1:A:123:ARG:HG3	4	27.79
(4,49)	1:B:113:PHE:H	1:B:123:ARG:HG3	4	27.79
(5,5)	1:B:110:GLU:H	1:B:123:ARG:HB2	7	27.36
(5,5)	1:B:110:GLU:H	1:B:123:ARG:HB3	7	27.36
(5,5)	1:A:110:GLU:H	1:A:123:ARG:HB2	7	27.36
(5,5)	1:A:110:GLU:H	1:A:123:ARG:HB3	7	27.36
(5,5)	1:B:110:GLU:H	1:B:123:ARG:HB2	1	27.32
(5,5)	1:B:110:GLU:H	1:B:123:ARG:HB3	1	27.32
(5,5)	1:A:110:GLU:H	1:A:123:ARG:HB2	1	27.32
(5,5)	1:A:110:GLU:H	1:A:123:ARG:HB3	1	27.32
(4,49)	1:A:113:PHE:H	1:A:123:ARG:HG3	6	26.95
(4,49)	1:B:113:PHE:H	1:B:123:ARG:HG3	6	26.95
(4,9)	1:A:111:HIS:HB2	1:A:123:ARG:HB2	5	26.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,9)	1:A:111:HIS:HB2	1:A:123:ARG:HB3	5	26.78
(4,9)	1:B:111:HIS:HB2	1:B:123:ARG:HB2	5	26.78
(4,9)	1:B:111:HIS:HB2	1:B:123:ARG:HB3	5	26.78
(4,7)	1:A:111:HIS:HB2	1:A:123:ARG:HB2	5	26.78
(4,7)	1:A:111:HIS:HB2	1:A:123:ARG:HB3	5	26.78
(4,7)	1:B:111:HIS:HB2	1:B:123:ARG:HB2	5	26.78
(4,7)	1:B:111:HIS:HB2	1:B:123:ARG:HB3	5	26.78
(4,6)	1:A:111:HIS:HB2	1:A:123:ARG:HB2	5	26.78
(4,6)	1:A:111:HIS:HB2	1:A:123:ARG:HB3	5	26.78
(4,6)	1:B:111:HIS:HB2	1:B:123:ARG:HB2	5	26.78
(4,6)	1:B:111:HIS:HB2	1:B:123:ARG:HB3	5	26.78
(4,4)	1:A:111:HIS:HB2	1:A:123:ARG:HB2	5	26.78
(4,4)	1:A:111:HIS:HB2	1:A:123:ARG:HB3	5	26.78
(4,4)	1:B:111:HIS:HB2	1:B:123:ARG:HB2	5	26.78
(4,4)	1:B:111:HIS:HB2	1:B:123:ARG:HB3	5	26.78
(4,2)	1:A:111:HIS:HB2	1:A:123:ARG:HB2	5	26.78
(4,2)	1:A:111:HIS:HB2	1:A:123:ARG:HB3	5	26.78
(4,2)	1:B:111:HIS:HB2	1:B:123:ARG:HB2	5	26.78
(4,2)	1:B:111:HIS:HB2	1:B:123:ARG:HB3	5	26.78
(4,9)	1:A:111:HIS:HB2	1:A:123:ARG:HB2	3	26.61
(4,9)	1:A:111:HIS:HB2	1:A:123:ARG:HB3	3	26.61
(4,9)	1:B:111:HIS:HB2	1:B:123:ARG:HB2	3	26.61
(4,9)	1:B:111:HIS:HB2	1:B:123:ARG:HB3	3	26.61
(4,7)	1:A:111:HIS:HB2	1:A:123:ARG:HB2	3	26.61
(4,7)	1:A:111:HIS:HB2	1:A:123:ARG:HB3	3	26.61
(4,7)	1:B:111:HIS:HB2	1:B:123:ARG:HB2	3	26.61
(4,7)	1:B:111:HIS:HB2	1:B:123:ARG:HB3	3	26.61
(4,6)	1:A:111:HIS:HB2	1:A:123:ARG:HB2	3	26.61
(4,6)	1:A:111:HIS:HB2	1:A:123:ARG:HB3	3	26.61
(4,6)	1:B:111:HIS:HB2	1:B:123:ARG:HB2	3	26.61
(4,6)	1:B:111:HIS:HB2	1:B:123:ARG:HB3	3	26.61
(4,4)	1:A:111:HIS:HB2	1:A:123:ARG:HB2	3	26.61
(4,4)	1:A:111:HIS:HB2	1:A:123:ARG:HB3	3	26.61
(4,4)	1:B:111:HIS:HB2	1:B:123:ARG:HB2	3	26.61
(4,4)	1:B:111:HIS:HB2	1:B:123:ARG:HB3	3	26.61
(4,2)	1:A:111:HIS:HB2	1:A:123:ARG:HB2	3	26.61
(4,2)	1:A:111:HIS:HB2	1:A:123:ARG:HB3	3	26.61
(4,2)	1:B:111:HIS:HB2	1:B:123:ARG:HB2	3	26.61
(4,2)	1:B:111:HIS:HB2	1:B:123:ARG:HB3	3	26.61
(4,49)	1:A:113:PHE:H	1:A:123:ARG:HG3	5	26.56
(4,49)	1:B:113:PHE:H	1:B:123:ARG:HG3	5	26.56
(4,9)	1:A:111:HIS:HB2	1:A:123:ARG:HB2	2	26.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,9)	1:A:111:HIS:HB2	1:A:123:ARG:HB3	2	26.39
(4,9)	1:B:111:HIS:HB2	1:B:123:ARG:HB2	2	26.39
(4,9)	1:B:111:HIS:HB2	1:B:123:ARG:HB3	2	26.39
(4,7)	1:A:111:HIS:HB2	1:A:123:ARG:HB2	2	26.39
(4,7)	1:A:111:HIS:HB2	1:A:123:ARG:HB3	2	26.39
(4,7)	1:B:111:HIS:HB2	1:B:123:ARG:HB2	2	26.39
(4,7)	1:B:111:HIS:HB2	1:B:123:ARG:HB3	2	26.39
(4,6)	1:A:111:HIS:HB2	1:A:123:ARG:HB2	2	26.39
(4,6)	1:A:111:HIS:HB2	1:A:123:ARG:HB3	2	26.39
(4,6)	1:B:111:HIS:HB2	1:B:123:ARG:HB2	2	26.39
(4,6)	1:B:111:HIS:HB2	1:B:123:ARG:HB3	2	26.39
(4,4)	1:A:111:HIS:HB2	1:A:123:ARG:HB2	2	26.39
(4,4)	1:A:111:HIS:HB2	1:A:123:ARG:HB3	2	26.39
(4,4)	1:B:111:HIS:HB2	1:B:123:ARG:HB2	2	26.39
(4,4)	1:B:111:HIS:HB2	1:B:123:ARG:HB3	2	26.39
(4,2)	1:A:111:HIS:HB2	1:A:123:ARG:HB2	2	26.39
(4,2)	1:A:111:HIS:HB2	1:A:123:ARG:HB3	2	26.39
(4,2)	1:B:111:HIS:HB2	1:B:123:ARG:HB2	2	26.39
(4,2)	1:B:111:HIS:HB2	1:B:123:ARG:HB3	2	26.39
(4,9)	1:A:111:HIS:HB2	1:A:123:ARG:HB2	4	26.38
(4,9)	1:A:111:HIS:HB2	1:A:123:ARG:HB3	4	26.38
(4,9)	1:B:111:HIS:HB2	1:B:123:ARG:HB2	4	26.38
(4,9)	1:B:111:HIS:HB2	1:B:123:ARG:HB3	4	26.38
(4,7)	1:A:111:HIS:HB2	1:A:123:ARG:HB2	4	26.38
(4,7)	1:A:111:HIS:HB2	1:A:123:ARG:HB3	4	26.38
(4,7)	1:B:111:HIS:HB2	1:B:123:ARG:HB2	4	26.38
(4,7)	1:B:111:HIS:HB2	1:B:123:ARG:HB3	4	26.38
(4,6)	1:A:111:HIS:HB2	1:A:123:ARG:HB2	4	26.38
(4,6)	1:A:111:HIS:HB2	1:A:123:ARG:HB3	4	26.38
(4,6)	1:B:111:HIS:HB2	1:B:123:ARG:HB2	4	26.38
(4,6)	1:B:111:HIS:HB2	1:B:123:ARG:HB3	4	26.38
(4,4)	1:A:111:HIS:HB2	1:A:123:ARG:HB2	4	26.38
(4,4)	1:A:111:HIS:HB2	1:A:123:ARG:HB3	4	26.38
(4,4)	1:B:111:HIS:HB2	1:B:123:ARG:HB2	4	26.38
(4,4)	1:B:111:HIS:HB2	1:B:123:ARG:HB3	4	26.38
(4,2)	1:A:111:HIS:HB2	1:A:123:ARG:HB2	4	26.38
(4,2)	1:A:111:HIS:HB2	1:A:123:ARG:HB3	4	26.38
(4,2)	1:B:111:HIS:HB2	1:B:123:ARG:HB2	4	26.38
(4,2)	1:B:111:HIS:HB2	1:B:123:ARG:HB3	4	26.38
(4,8)	1:A:111:HIS:HB3	1:A:123:ARG:HB2	4	26.27
(4,8)	1:A:111:HIS:HB3	1:A:123:ARG:HB3	4	26.27
(4,8)	1:B:111:HIS:HB3	1:B:123:ARG:HB2	4	26.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,8)	1:B:111:HIS:HB3	1:B:123:ARG:HB3	4	26.27
(4,5)	1:A:111:HIS:HB3	1:A:123:ARG:HB2	4	26.27
(4,5)	1:A:111:HIS:HB3	1:A:123:ARG:HB3	4	26.27
(4,5)	1:B:111:HIS:HB3	1:B:123:ARG:HB2	4	26.27
(4,5)	1:B:111:HIS:HB3	1:B:123:ARG:HB3	4	26.27
(4,3)	1:A:111:HIS:HB3	1:A:123:ARG:HB2	4	26.27
(4,3)	1:A:111:HIS:HB3	1:A:123:ARG:HB3	4	26.27
(4,3)	1:B:111:HIS:HB3	1:B:123:ARG:HB2	4	26.27
(4,3)	1:B:111:HIS:HB3	1:B:123:ARG:HB3	4	26.27
(4,10)	1:A:111:HIS:HB3	1:A:123:ARG:HB2	4	26.27
(4,10)	1:A:111:HIS:HB3	1:A:123:ARG:HB3	4	26.27
(4,10)	1:B:111:HIS:HB3	1:B:123:ARG:HB2	4	26.27
(4,10)	1:B:111:HIS:HB3	1:B:123:ARG:HB3	4	26.27
(5,8)	1:A:113:PHE:H	1:A:123:ARG:H	4	26.22
(5,8)	1:B:113:PHE:H	1:B:123:ARG:H	4	26.22
(4,8)	1:A:111:HIS:HB3	1:A:123:ARG:HB2	5	26.17
(4,8)	1:A:111:HIS:HB3	1:A:123:ARG:HB3	5	26.17
(4,8)	1:B:111:HIS:HB3	1:B:123:ARG:HB2	5	26.17
(4,8)	1:B:111:HIS:HB3	1:B:123:ARG:HB3	5	26.17
(4,5)	1:A:111:HIS:HB3	1:A:123:ARG:HB2	5	26.17
(4,5)	1:A:111:HIS:HB3	1:A:123:ARG:HB3	5	26.17
(4,5)	1:B:111:HIS:HB3	1:B:123:ARG:HB2	5	26.17
(4,5)	1:B:111:HIS:HB3	1:B:123:ARG:HB3	5	26.17
(4,3)	1:A:111:HIS:HB3	1:A:123:ARG:HB2	5	26.17
(4,3)	1:A:111:HIS:HB3	1:A:123:ARG:HB3	5	26.17
(4,3)	1:B:111:HIS:HB3	1:B:123:ARG:HB2	5	26.17
(4,3)	1:B:111:HIS:HB3	1:B:123:ARG:HB3	5	26.17
(4,10)	1:A:111:HIS:HB3	1:A:123:ARG:HB2	5	26.17
(4,10)	1:A:111:HIS:HB3	1:A:123:ARG:HB3	5	26.17
(4,10)	1:B:111:HIS:HB3	1:B:123:ARG:HB2	5	26.17
(4,10)	1:B:111:HIS:HB3	1:B:123:ARG:HB3	5	26.17
(4,9)	1:A:111:HIS:HB2	1:A:123:ARG:HB2	8	26.16
(4,9)	1:A:111:HIS:HB2	1:A:123:ARG:HB3	8	26.16
(4,9)	1:B:111:HIS:HB2	1:B:123:ARG:HB2	8	26.16
(4,9)	1:B:111:HIS:HB2	1:B:123:ARG:HB3	8	26.16
(4,7)	1:A:111:HIS:HB2	1:A:123:ARG:HB2	8	26.16
(4,7)	1:A:111:HIS:HB2	1:A:123:ARG:HB3	8	26.16
(4,7)	1:B:111:HIS:HB2	1:B:123:ARG:HB2	8	26.16
(4,7)	1:B:111:HIS:HB2	1:B:123:ARG:HB3	8	26.16
(4,6)	1:A:111:HIS:HB2	1:A:123:ARG:HB2	8	26.16
(4,6)	1:A:111:HIS:HB2	1:A:123:ARG:HB3	8	26.16
(4,6)	1:B:111:HIS:HB2	1:B:123:ARG:HB2	8	26.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,6)	1:B:111:HIS:HB2	1:B:123:ARG:HB3	8	26.16
(4,4)	1:A:111:HIS:HB2	1:A:123:ARG:HB2	8	26.16
(4,4)	1:A:111:HIS:HB2	1:A:123:ARG:HB3	8	26.16
(4,4)	1:B:111:HIS:HB2	1:B:123:ARG:HB2	8	26.16
(4,4)	1:B:111:HIS:HB2	1:B:123:ARG:HB3	8	26.16
(4,2)	1:A:111:HIS:HB2	1:A:123:ARG:HB2	8	26.16
(4,2)	1:A:111:HIS:HB2	1:A:123:ARG:HB3	8	26.16
(4,2)	1:B:111:HIS:HB2	1:B:123:ARG:HB2	8	26.16
(4,2)	1:B:111:HIS:HB2	1:B:123:ARG:HB3	8	26.16
(5,9)	1:A:113:PHE:H	1:A:123:ARG:HG2	4	25.96
(5,9)	1:A:113:PHE:H	1:A:123:ARG:HG3	4	25.96
(5,9)	1:B:113:PHE:H	1:B:123:ARG:HG2	4	25.96
(5,9)	1:B:113:PHE:H	1:B:123:ARG:HG3	4	25.96
(5,8)	1:A:113:PHE:H	1:A:123:ARG:H	6	25.79
(5,8)	1:B:113:PHE:H	1:B:123:ARG:H	6	25.79
(4,49)	1:A:113:PHE:H	1:A:123:ARG:HG3	3	25.67
(4,49)	1:B:113:PHE:H	1:B:123:ARG:HG3	3	25.67
(5,8)	1:A:113:PHE:H	1:A:123:ARG:H	5	25.63
(5,8)	1:B:113:PHE:H	1:B:123:ARG:H	5	25.63
(4,49)	1:A:113:PHE:H	1:A:123:ARG:HG3	2	25.63
(4,49)	1:B:113:PHE:H	1:B:123:ARG:HG3	2	25.63
(4,8)	1:A:111:HIS:HB3	1:A:123:ARG:HB2	3	25.61
(4,8)	1:A:111:HIS:HB3	1:A:123:ARG:HB3	3	25.61
(4,8)	1:B:111:HIS:HB3	1:B:123:ARG:HB2	3	25.61
(4,8)	1:B:111:HIS:HB3	1:B:123:ARG:HB3	3	25.61
(4,5)	1:A:111:HIS:HB3	1:A:123:ARG:HB2	3	25.61
(4,5)	1:A:111:HIS:HB3	1:A:123:ARG:HB3	3	25.61
(4,5)	1:B:111:HIS:HB3	1:B:123:ARG:HB2	3	25.61
(4,5)	1:B:111:HIS:HB3	1:B:123:ARG:HB3	3	25.61
(4,3)	1:A:111:HIS:HB3	1:A:123:ARG:HB2	3	25.61
(4,3)	1:A:111:HIS:HB3	1:A:123:ARG:HB3	3	25.61
(4,3)	1:B:111:HIS:HB3	1:B:123:ARG:HB2	3	25.61
(4,3)	1:B:111:HIS:HB3	1:B:123:ARG:HB3	3	25.61
(4,10)	1:A:111:HIS:HB3	1:A:123:ARG:HB2	3	25.61
(4,10)	1:A:111:HIS:HB3	1:A:123:ARG:HB3	3	25.61
(4,10)	1:B:111:HIS:HB3	1:B:123:ARG:HB2	3	25.61
(4,10)	1:B:111:HIS:HB3	1:B:123:ARG:HB3	3	25.61
(4,8)	1:A:111:HIS:HB3	1:A:123:ARG:HB2	8	25.56
(4,8)	1:A:111:HIS:HB3	1:A:123:ARG:HB3	8	25.56
(4,8)	1:B:111:HIS:HB3	1:B:123:ARG:HB2	8	25.56
(4,8)	1:B:111:HIS:HB3	1:B:123:ARG:HB3	8	25.56
(4,5)	1:A:111:HIS:HB3	1:A:123:ARG:HB2	8	25.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,5)	1:A:111:HIS:HB3	1:A:123:ARG:HB3	8	25.56
(4,5)	1:B:111:HIS:HB3	1:B:123:ARG:HB2	8	25.56
(4,5)	1:B:111:HIS:HB3	1:B:123:ARG:HB3	8	25.56
(4,3)	1:A:111:HIS:HB3	1:A:123:ARG:HB2	8	25.56
(4,3)	1:A:111:HIS:HB3	1:A:123:ARG:HB3	8	25.56
(4,3)	1:B:111:HIS:HB3	1:B:123:ARG:HB2	8	25.56
(4,3)	1:B:111:HIS:HB3	1:B:123:ARG:HB3	8	25.56
(4,10)	1:A:111:HIS:HB3	1:A:123:ARG:HB2	8	25.56
(4,10)	1:A:111:HIS:HB3	1:A:123:ARG:HB3	8	25.56
(4,10)	1:B:111:HIS:HB3	1:B:123:ARG:HB2	8	25.56
(4,10)	1:B:111:HIS:HB3	1:B:123:ARG:HB3	8	25.56
(4,57)	1:A:122:TYR:H	1:A:110:GLU:HB2	4	25.54
(4,57)	1:A:122:TYR:H	1:A:110:GLU:HB3	4	25.54
(4,57)	1:B:122:TYR:H	1:B:110:GLU:HB2	4	25.54
(4,57)	1:B:122:TYR:H	1:B:110:GLU:HB3	4	25.54
(4,56)	1:A:122:TYR:H	1:A:110:GLU:HB2	4	25.54
(4,56)	1:A:122:TYR:H	1:A:110:GLU:HB3	4	25.54
(4,56)	1:B:122:TYR:H	1:B:110:GLU:HB2	4	25.54
(4,56)	1:B:122:TYR:H	1:B:110:GLU:HB3	4	25.54
(4,8)	1:A:111:HIS:HB3	1:A:123:ARG:HB2	2	25.52
(4,8)	1:A:111:HIS:HB3	1:A:123:ARG:HB3	2	25.52
(4,8)	1:B:111:HIS:HB3	1:B:123:ARG:HB2	2	25.52
(4,8)	1:B:111:HIS:HB3	1:B:123:ARG:HB3	2	25.52
(4,5)	1:A:111:HIS:HB3	1:A:123:ARG:HB2	2	25.52
(4,5)	1:A:111:HIS:HB3	1:A:123:ARG:HB3	2	25.52
(4,5)	1:B:111:HIS:HB3	1:B:123:ARG:HB2	2	25.52
(4,5)	1:B:111:HIS:HB3	1:B:123:ARG:HB3	2	25.52
(4,3)	1:A:111:HIS:HB3	1:A:123:ARG:HB2	2	25.52
(4,3)	1:A:111:HIS:HB3	1:A:123:ARG:HB3	2	25.52
(4,3)	1:B:111:HIS:HB3	1:B:123:ARG:HB2	2	25.52
(4,3)	1:B:111:HIS:HB3	1:B:123:ARG:HB3	2	25.52
(4,10)	1:A:111:HIS:HB3	1:A:123:ARG:HB2	2	25.52
(4,10)	1:A:111:HIS:HB3	1:A:123:ARG:HB3	2	25.52
(4,10)	1:B:111:HIS:HB3	1:B:123:ARG:HB2	2	25.52
(4,10)	1:B:111:HIS:HB3	1:B:123:ARG:HB3	2	25.52
(5,9)	1:A:113:PHE:H	1:A:123:ARG:HG2	6	25.32
(5,9)	1:A:113:PHE:H	1:A:123:ARG:HG3	6	25.32
(5,9)	1:B:113:PHE:H	1:B:123:ARG:HG2	6	25.32
(5,9)	1:B:113:PHE:H	1:B:123:ARG:HG3	6	25.32
(4,47)	1:A:122:TYR:HA	1:A:112:GLY:HA2	4	25.24
(4,47)	1:B:122:TYR:HA	1:B:112:GLY:HA2	4	25.24
(4,11)	1:A:112:GLY:HA2	1:A:122:TYR:HA	4	25.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,11)	1:B:112:GLY:HA2	1:B:122:TYR:HA	4	25.24
(4,14)	1:A:112:GLY:HA3	1:A:122:TYR:HB2	3	25.07
(4,14)	1:B:112:GLY:HA3	1:B:122:TYR:HB2	3	25.07
(4,49)	1:A:113:PHE:H	1:A:123:ARG:HG3	8	25.01
(4,49)	1:B:113:PHE:H	1:B:123:ARG:HG3	8	25.01
(4,13)	1:A:112:GLY:HA2	1:A:122:TYR:HB3	4	25.0
(4,13)	1:B:112:GLY:HA2	1:B:122:TYR:HB3	4	25.0
(5,9)	1:A:113:PHE:H	1:A:123:ARG:HG2	5	24.98
(5,9)	1:A:113:PHE:H	1:A:123:ARG:HG3	5	24.98
(5,9)	1:B:113:PHE:H	1:B:123:ARG:HG2	5	24.98
(5,9)	1:B:113:PHE:H	1:B:123:ARG:HG3	5	24.98
(4,57)	1:A:122:TYR:H	1:A:110:GLU:HB2	5	24.95
(4,57)	1:A:122:TYR:H	1:A:110:GLU:HB3	5	24.95
(4,57)	1:B:122:TYR:H	1:B:110:GLU:HB2	5	24.95
(4,57)	1:B:122:TYR:H	1:B:110:GLU:HB3	5	24.95
(4,56)	1:A:122:TYR:H	1:A:110:GLU:HB2	5	24.95
(4,56)	1:A:122:TYR:H	1:A:110:GLU:HB3	5	24.95
(4,56)	1:B:122:TYR:H	1:B:110:GLU:HB2	5	24.95
(4,56)	1:B:122:TYR:H	1:B:110:GLU:HB3	5	24.95
(5,7)	1:A:113:PHE:H	1:A:122:TYR:HA	4	24.84
(5,7)	1:B:113:PHE:H	1:B:122:TYR:HA	4	24.84
(4,49)	1:A:113:PHE:H	1:A:123:ARG:HG3	1	24.75
(4,49)	1:B:113:PHE:H	1:B:123:ARG:HG3	1	24.75
(5,8)	1:A:113:PHE:H	1:A:123:ARG:H	3	24.7
(5,8)	1:B:113:PHE:H	1:B:123:ARG:H	3	24.7
(5,7)	1:A:113:PHE:H	1:A:122:TYR:HA	6	24.64
(5,7)	1:B:113:PHE:H	1:B:122:TYR:HA	6	24.64
(4,57)	1:A:122:TYR:H	1:A:110:GLU:HB2	3	24.53
(4,57)	1:A:122:TYR:H	1:A:110:GLU:HB3	3	24.53
(4,57)	1:B:122:TYR:H	1:B:110:GLU:HB2	3	24.53
(4,57)	1:B:122:TYR:H	1:B:110:GLU:HB3	3	24.53
(4,56)	1:A:122:TYR:H	1:A:110:GLU:HB2	3	24.53
(4,56)	1:A:122:TYR:H	1:A:110:GLU:HB3	3	24.53
(4,56)	1:B:122:TYR:H	1:B:110:GLU:HB2	3	24.53
(4,56)	1:B:122:TYR:H	1:B:110:GLU:HB3	3	24.53
(5,7)	1:A:113:PHE:H	1:A:122:TYR:HA	5	24.49
(5,7)	1:B:113:PHE:H	1:B:122:TYR:HA	5	24.49
(4,49)	1:A:113:PHE:H	1:A:123:ARG:HG3	7	24.49
(4,49)	1:B:113:PHE:H	1:B:123:ARG:HG3	7	24.49
(4,48)	1:A:122:TYR:HA	1:A:112:GLY:HA3	4	24.46
(4,48)	1:B:122:TYR:HA	1:B:112:GLY:HA3	4	24.46
(4,12)	1:A:112:GLY:HA3	1:A:122:TYR:HA	4	24.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,12)	1:B:112:GLY:HA3	1:B:122:TYR:HA	4	24.46
(4,48)	1:A:122:TYR:HA	1:A:112:GLY:HA3	5	24.39
(4,48)	1:B:122:TYR:HA	1:B:112:GLY:HA3	5	24.39
(4,12)	1:A:112:GLY:HA3	1:A:122:TYR:HA	5	24.39
(4,12)	1:B:112:GLY:HA3	1:B:122:TYR:HA	5	24.39
(4,13)	1:A:112:GLY:HA2	1:A:122:TYR:HB3	5	24.38
(4,13)	1:B:112:GLY:HA2	1:B:122:TYR:HB3	5	24.38
(5,8)	1:A:113:PHE:H	1:A:123:ARG:H	2	24.36
(5,8)	1:B:113:PHE:H	1:B:123:ARG:H	2	24.36
(5,8)	1:A:113:PHE:H	1:A:123:ARG:H	1	24.32
(5,8)	1:B:113:PHE:H	1:B:123:ARG:H	1	24.32
(4,15)	1:A:112:GLY:HA2	1:A:122:TYR:HB2	4	24.31
(4,15)	1:B:112:GLY:HA2	1:B:122:TYR:HB2	4	24.31
(4,57)	1:A:122:TYR:H	1:A:110:GLU:HB2	2	24.29
(4,57)	1:A:122:TYR:H	1:A:110:GLU:HB3	2	24.29
(4,57)	1:B:122:TYR:H	1:B:110:GLU:HB2	2	24.29
(4,57)	1:B:122:TYR:H	1:B:110:GLU:HB3	2	24.29
(4,56)	1:A:122:TYR:H	1:A:110:GLU:HB2	2	24.29
(4,56)	1:A:122:TYR:H	1:A:110:GLU:HB3	2	24.29
(4,56)	1:B:122:TYR:H	1:B:110:GLU:HB2	2	24.29
(4,56)	1:B:122:TYR:H	1:B:110:GLU:HB3	2	24.29
(4,8)	1:A:111:HIS:HB3	1:A:123:ARG:HB2	7	24.27
(4,8)	1:A:111:HIS:HB3	1:A:123:ARG:HB3	7	24.27
(4,8)	1:B:111:HIS:HB3	1:B:123:ARG:HB2	7	24.27
(4,8)	1:B:111:HIS:HB3	1:B:123:ARG:HB3	7	24.27
(4,5)	1:A:111:HIS:HB3	1:A:123:ARG:HB2	7	24.27
(4,5)	1:A:111:HIS:HB3	1:A:123:ARG:HB3	7	24.27
(4,5)	1:B:111:HIS:HB3	1:B:123:ARG:HB2	7	24.27
(4,5)	1:B:111:HIS:HB3	1:B:123:ARG:HB3	7	24.27
(4,3)	1:A:111:HIS:HB3	1:A:123:ARG:HB2	7	24.27
(4,3)	1:A:111:HIS:HB3	1:A:123:ARG:HB3	7	24.27
(4,3)	1:B:111:HIS:HB3	1:B:123:ARG:HB2	7	24.27
(4,3)	1:B:111:HIS:HB3	1:B:123:ARG:HB3	7	24.27
(4,10)	1:A:111:HIS:HB3	1:A:123:ARG:HB2	7	24.27
(4,10)	1:A:111:HIS:HB3	1:A:123:ARG:HB3	7	24.27
(4,10)	1:B:111:HIS:HB3	1:B:123:ARG:HB2	7	24.27
(4,10)	1:B:111:HIS:HB3	1:B:123:ARG:HB3	7	24.27
(4,15)	1:A:112:GLY:HA2	1:A:122:TYR:HB2	3	24.25
(4,15)	1:B:112:GLY:HA2	1:B:122:TYR:HB2	3	24.25
(5,9)	1:A:113:PHE:H	1:A:123:ARG:HG2	3	24.17
(5,9)	1:A:113:PHE:H	1:A:123:ARG:HG3	3	24.17
(5,9)	1:B:113:PHE:H	1:B:123:ARG:HG2	3	24.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,9)	1:B:113:PHE:H	1:B:123:ARG:HG3	3	24.17
(4,13)	1:A:112:GLY:HA2	1:A:122:TYR:HB3	8	24.16
(4,13)	1:B:112:GLY:HA2	1:B:122:TYR:HB3	8	24.16
(5,9)	1:A:113:PHE:H	1:A:123:ARG:HG2	2	24.1
(5,9)	1:A:113:PHE:H	1:A:123:ARG:HG3	2	24.1
(5,9)	1:B:113:PHE:H	1:B:123:ARG:HG2	2	24.1
(5,9)	1:B:113:PHE:H	1:B:123:ARG:HG3	2	24.1
(4,47)	1:A:122:TYR:HA	1:A:112:GLY:HA2	5	24.09
(4,47)	1:B:122:TYR:HA	1:B:112:GLY:HA2	5	24.09
(4,11)	1:A:112:GLY:HA2	1:A:122:TYR:HA	5	24.09
(4,11)	1:B:112:GLY:HA2	1:B:122:TYR:HA	5	24.09
(4,9)	1:A:111:HIS:HB2	1:A:123:ARG:HB2	7	24.01
(4,9)	1:A:111:HIS:HB2	1:A:123:ARG:HB3	7	24.01
(4,9)	1:B:111:HIS:HB2	1:B:123:ARG:HB2	7	24.01
(4,9)	1:B:111:HIS:HB2	1:B:123:ARG:HB3	7	24.01
(4,7)	1:A:111:HIS:HB2	1:A:123:ARG:HB2	7	24.01
(4,7)	1:A:111:HIS:HB2	1:A:123:ARG:HB3	7	24.01
(4,7)	1:B:111:HIS:HB2	1:B:123:ARG:HB2	7	24.01
(4,7)	1:B:111:HIS:HB2	1:B:123:ARG:HB3	7	24.01
(4,6)	1:A:111:HIS:HB2	1:A:123:ARG:HB2	7	24.01
(4,6)	1:A:111:HIS:HB2	1:A:123:ARG:HB3	7	24.01
(4,6)	1:B:111:HIS:HB2	1:B:123:ARG:HB2	7	24.01
(4,6)	1:B:111:HIS:HB2	1:B:123:ARG:HB3	7	24.01
(4,4)	1:A:111:HIS:HB2	1:A:123:ARG:HB2	7	24.01
(4,4)	1:A:111:HIS:HB2	1:A:123:ARG:HB3	7	24.01
(4,4)	1:B:111:HIS:HB2	1:B:123:ARG:HB2	7	24.01
(4,4)	1:B:111:HIS:HB2	1:B:123:ARG:HB3	7	24.01
(4,2)	1:A:111:HIS:HB2	1:A:123:ARG:HB2	7	24.01
(4,2)	1:A:111:HIS:HB2	1:A:123:ARG:HB3	7	24.01
(4,2)	1:B:111:HIS:HB2	1:B:123:ARG:HB2	7	24.01
(4,2)	1:B:111:HIS:HB2	1:B:123:ARG:HB3	7	24.01
(5,8)	1:A:113:PHE:H	1:A:123:ARG:H	8	24.0
(5,8)	1:B:113:PHE:H	1:B:123:ARG:H	8	24.0
(4,17)	1:A:112:GLY:HA2	1:A:124:ILE:HD11	5	23.93
(4,17)	1:A:112:GLY:HA2	1:A:124:ILE:HD12	5	23.93
(4,17)	1:A:112:GLY:HA2	1:A:124:ILE:HD13	5	23.93
(4,17)	1:B:112:GLY:HA2	1:B:124:ILE:HD11	5	23.93
(4,17)	1:B:112:GLY:HA2	1:B:124:ILE:HD12	5	23.93
(4,17)	1:B:112:GLY:HA2	1:B:124:ILE:HD13	5	23.93
(4,57)	1:A:122:TYR:H	1:A:110:GLU:HB2	8	23.84
(4,57)	1:A:122:TYR:H	1:A:110:GLU:HB3	8	23.84
(4,57)	1:B:122:TYR:H	1:B:110:GLU:HB2	8	23.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,57)	1:B:122:TYR:H	1:B:110:GLU:HB3	8	23.84
(4,56)	1:A:122:TYR:H	1:A:110:GLU:HB2	8	23.84
(4,56)	1:A:122:TYR:H	1:A:110:GLU:HB3	8	23.84
(4,56)	1:B:122:TYR:H	1:B:110:GLU:HB2	8	23.84
(4,56)	1:B:122:TYR:H	1:B:110:GLU:HB3	8	23.84
(4,47)	1:A:122:TYR:HA	1:A:112:GLY:HA2	6	23.76
(4,47)	1:B:122:TYR:HA	1:B:112:GLY:HA2	6	23.76
(4,14)	1:A:112:GLY:HA3	1:A:122:TYR:HB2	5	23.76
(4,14)	1:B:112:GLY:HA3	1:B:122:TYR:HB2	5	23.76
(4,11)	1:A:112:GLY:HA2	1:A:122:TYR:HA	6	23.76
(4,11)	1:B:112:GLY:HA2	1:B:122:TYR:HA	6	23.76
(4,48)	1:A:122:TYR:HA	1:A:112:GLY:HA3	3	23.75
(4,48)	1:B:122:TYR:HA	1:B:112:GLY:HA3	3	23.75
(4,12)	1:A:112:GLY:HA3	1:A:122:TYR:HA	3	23.75
(4,12)	1:B:112:GLY:HA3	1:B:122:TYR:HA	3	23.75
(4,14)	1:A:112:GLY:HA3	1:A:122:TYR:HB2	8	23.68
(4,14)	1:B:112:GLY:HA3	1:B:122:TYR:HB2	8	23.68
(5,8)	1:A:113:PHE:H	1:A:123:ARG:H	7	23.64
(5,8)	1:B:113:PHE:H	1:B:123:ARG:H	7	23.64
(5,9)	1:A:113:PHE:H	1:A:123:ARG:HG2	8	23.62
(5,9)	1:A:113:PHE:H	1:A:123:ARG:HG3	8	23.62
(5,9)	1:B:113:PHE:H	1:B:123:ARG:HG2	8	23.62
(5,9)	1:B:113:PHE:H	1:B:123:ARG:HG3	8	23.62
(4,48)	1:A:122:TYR:HA	1:A:112:GLY:HA3	2	23.61
(4,48)	1:B:122:TYR:HA	1:B:112:GLY:HA3	2	23.61
(4,15)	1:A:112:GLY:HA2	1:A:122:TYR:HB2	8	23.61
(4,15)	1:B:112:GLY:HA2	1:B:122:TYR:HB2	8	23.61
(4,12)	1:A:112:GLY:HA3	1:A:122:TYR:HA	2	23.61
(4,12)	1:B:112:GLY:HA3	1:B:122:TYR:HA	2	23.61
(4,15)	1:A:112:GLY:HA2	1:A:122:TYR:HB2	5	23.56
(4,15)	1:B:112:GLY:HA2	1:B:122:TYR:HB2	5	23.56
(4,13)	1:A:112:GLY:HA2	1:A:122:TYR:HB3	2	23.56
(4,13)	1:B:112:GLY:HA2	1:B:122:TYR:HB3	2	23.56
(4,13)	1:A:112:GLY:HA2	1:A:122:TYR:HB3	7	23.51
(4,13)	1:B:112:GLY:HA2	1:B:122:TYR:HB3	7	23.51
(4,14)	1:A:112:GLY:HA3	1:A:122:TYR:HB2	4	23.49
(4,14)	1:B:112:GLY:HA3	1:B:122:TYR:HB2	4	23.49
(4,14)	1:A:112:GLY:HA3	1:A:122:TYR:HB2	2	23.47
(4,14)	1:B:112:GLY:HA3	1:B:122:TYR:HB2	2	23.47
(5,9)	1:A:113:PHE:H	1:A:123:ARG:HG2	1	23.45
(5,9)	1:A:113:PHE:H	1:A:123:ARG:HG3	1	23.45
(5,9)	1:B:113:PHE:H	1:B:123:ARG:HG2	1	23.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,9)	1:B:113:PHE:H	1:B:123:ARG:HG3	1	23.45
(4,8)	1:A:111:HIS:HB3	1:A:123:ARG:HB2	6	23.44
(4,8)	1:A:111:HIS:HB3	1:A:123:ARG:HB3	6	23.44
(4,8)	1:B:111:HIS:HB3	1:B:123:ARG:HB2	6	23.44
(4,8)	1:B:111:HIS:HB3	1:B:123:ARG:HB3	6	23.44
(4,5)	1:A:111:HIS:HB3	1:A:123:ARG:HB2	6	23.44
(4,5)	1:A:111:HIS:HB3	1:A:123:ARG:HB3	6	23.44
(4,5)	1:B:111:HIS:HB3	1:B:123:ARG:HB2	6	23.44
(4,5)	1:B:111:HIS:HB3	1:B:123:ARG:HB3	6	23.44
(4,3)	1:A:111:HIS:HB3	1:A:123:ARG:HB2	6	23.44
(4,3)	1:A:111:HIS:HB3	1:A:123:ARG:HB3	6	23.44
(4,3)	1:B:111:HIS:HB3	1:B:123:ARG:HB2	6	23.44
(4,3)	1:B:111:HIS:HB3	1:B:123:ARG:HB3	6	23.44
(4,10)	1:A:111:HIS:HB3	1:A:123:ARG:HB2	6	23.44
(4,10)	1:A:111:HIS:HB3	1:A:123:ARG:HB3	6	23.44
(4,10)	1:B:111:HIS:HB3	1:B:123:ARG:HB2	6	23.44
(4,10)	1:B:111:HIS:HB3	1:B:123:ARG:HB3	6	23.44
(5,7)	1:A:113:PHE:H	1:A:122:TYR:HA	1	23.4
(5,7)	1:B:113:PHE:H	1:B:122:TYR:HA	1	23.4
(4,9)	1:A:111:HIS:HB2	1:A:123:ARG:HB2	6	23.37
(4,9)	1:A:111:HIS:HB2	1:A:123:ARG:HB3	6	23.37
(4,9)	1:B:111:HIS:HB2	1:B:123:ARG:HB2	6	23.37
(4,9)	1:B:111:HIS:HB2	1:B:123:ARG:HB3	6	23.37
(4,7)	1:A:111:HIS:HB2	1:A:123:ARG:HB2	6	23.37
(4,7)	1:A:111:HIS:HB2	1:A:123:ARG:HB3	6	23.37
(4,7)	1:B:111:HIS:HB2	1:B:123:ARG:HB2	6	23.37
(4,7)	1:B:111:HIS:HB2	1:B:123:ARG:HB3	6	23.37
(4,6)	1:A:111:HIS:HB2	1:A:123:ARG:HB2	6	23.37
(4,6)	1:A:111:HIS:HB2	1:A:123:ARG:HB3	6	23.37
(4,6)	1:B:111:HIS:HB2	1:B:123:ARG:HB2	6	23.37
(4,6)	1:B:111:HIS:HB2	1:B:123:ARG:HB3	6	23.37
(4,4)	1:A:111:HIS:HB2	1:A:123:ARG:HB2	6	23.37
(4,4)	1:A:111:HIS:HB2	1:A:123:ARG:HB3	6	23.37
(4,4)	1:B:111:HIS:HB2	1:B:123:ARG:HB2	6	23.37
(4,4)	1:B:111:HIS:HB2	1:B:123:ARG:HB3	6	23.37
(4,2)	1:A:111:HIS:HB2	1:A:123:ARG:HB2	6	23.37
(4,2)	1:A:111:HIS:HB2	1:A:123:ARG:HB3	6	23.37
(4,2)	1:B:111:HIS:HB2	1:B:123:ARG:HB2	6	23.37
(4,2)	1:B:111:HIS:HB2	1:B:123:ARG:HB3	6	23.37
(5,7)	1:A:113:PHE:H	1:A:122:TYR:HA	3	23.36
(5,7)	1:B:113:PHE:H	1:B:122:TYR:HA	3	23.36
(5,7)	1:A:113:PHE:H	1:A:122:TYR:HA	2	23.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,7)	1:B:113:PHE:H	1:B:122:TYR:HA	2	23.33
(4,57)	1:A:122:TYR:H	1:A:110:GLU:HB2	7	23.32
(4,57)	1:A:122:TYR:H	1:A:110:GLU:HB3	7	23.32
(4,57)	1:B:122:TYR:H	1:B:110:GLU:HB2	7	23.32
(4,57)	1:B:122:TYR:H	1:B:110:GLU:HB3	7	23.32
(4,56)	1:A:122:TYR:H	1:A:110:GLU:HB2	7	23.32
(4,56)	1:A:122:TYR:H	1:A:110:GLU:HB3	7	23.32
(4,56)	1:B:122:TYR:H	1:B:110:GLU:HB2	7	23.32
(4,56)	1:B:122:TYR:H	1:B:110:GLU:HB3	7	23.32
(4,57)	1:A:122:TYR:H	1:A:110:GLU:HB2	6	23.31
(4,57)	1:A:122:TYR:H	1:A:110:GLU:HB3	6	23.31
(4,57)	1:B:122:TYR:H	1:B:110:GLU:HB2	6	23.31
(4,57)	1:B:122:TYR:H	1:B:110:GLU:HB3	6	23.31
(4,56)	1:A:122:TYR:H	1:A:110:GLU:HB2	6	23.31
(4,56)	1:A:122:TYR:H	1:A:110:GLU:HB3	6	23.31
(4,56)	1:B:122:TYR:H	1:B:110:GLU:HB2	6	23.31
(4,56)	1:B:122:TYR:H	1:B:110:GLU:HB3	6	23.31
(5,7)	1:A:113:PHE:H	1:A:122:TYR:HA	8	23.21
(5,7)	1:B:113:PHE:H	1:B:122:TYR:HA	8	23.21
(4,48)	1:A:122:TYR:HA	1:A:112:GLY:HA3	8	23.19
(4,48)	1:B:122:TYR:HA	1:B:112:GLY:HA3	8	23.19
(4,12)	1:A:112:GLY:HA3	1:A:122:TYR:HA	8	23.19
(4,12)	1:B:112:GLY:HA3	1:B:122:TYR:HA	8	23.19
(4,13)	1:A:112:GLY:HA2	1:A:122:TYR:HB3	6	23.16
(4,13)	1:B:112:GLY:HA2	1:B:122:TYR:HB3	6	23.16
(5,9)	1:A:113:PHE:H	1:A:123:ARG:HG2	7	23.14
(5,9)	1:A:113:PHE:H	1:A:123:ARG:HG3	7	23.14
(5,9)	1:B:113:PHE:H	1:B:123:ARG:HG2	7	23.14
(5,9)	1:B:113:PHE:H	1:B:123:ARG:HG3	7	23.14
(4,47)	1:A:122:TYR:HA	1:A:112:GLY:HA2	8	23.04
(4,47)	1:B:122:TYR:HA	1:B:112:GLY:HA2	8	23.04
(4,11)	1:A:112:GLY:HA2	1:A:122:TYR:HA	8	23.04
(4,11)	1:B:112:GLY:HA2	1:B:122:TYR:HA	8	23.04
(4,47)	1:A:122:TYR:HA	1:A:112:GLY:HA2	7	22.97
(4,47)	1:B:122:TYR:HA	1:B:112:GLY:HA2	7	22.97
(4,11)	1:A:112:GLY:HA2	1:A:122:TYR:HA	7	22.97
(4,11)	1:B:112:GLY:HA2	1:B:122:TYR:HA	7	22.97
(5,7)	1:A:113:PHE:H	1:A:122:TYR:HA	7	22.91
(5,7)	1:B:113:PHE:H	1:B:122:TYR:HA	7	22.91
(4,47)	1:A:122:TYR:HA	1:A:112:GLY:HA2	1	22.9
(4,47)	1:B:122:TYR:HA	1:B:112:GLY:HA2	1	22.9
(4,47)	1:A:122:TYR:HA	1:A:112:GLY:HA2	2	22.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,47)	1:B:122:TYR:HA	1:B:112:GLY:HA2	2	22.9
(4,11)	1:A:112:GLY:HA2	1:A:122:TYR:HA	1	22.9
(4,11)	1:B:112:GLY:HA2	1:B:122:TYR:HA	1	22.9
(4,11)	1:A:112:GLY:HA2	1:A:122:TYR:HA	2	22.9
(4,11)	1:B:112:GLY:HA2	1:B:122:TYR:HA	2	22.9
(4,15)	1:A:112:GLY:HA2	1:A:122:TYR:HB2	2	22.87
(4,15)	1:B:112:GLY:HA2	1:B:122:TYR:HB2	2	22.87
(4,47)	1:A:122:TYR:HA	1:A:112:GLY:HA2	3	22.86
(4,47)	1:B:122:TYR:HA	1:B:112:GLY:HA2	3	22.86
(4,11)	1:A:112:GLY:HA2	1:A:122:TYR:HA	3	22.86
(4,11)	1:B:112:GLY:HA2	1:B:122:TYR:HA	3	22.86
(4,15)	1:A:112:GLY:HA2	1:A:122:TYR:HB2	6	22.8
(4,15)	1:B:112:GLY:HA2	1:B:122:TYR:HB2	6	22.8
(4,13)	1:A:112:GLY:HA2	1:A:122:TYR:HB3	3	22.8
(4,13)	1:B:112:GLY:HA2	1:B:122:TYR:HB3	3	22.8
(4,17)	1:A:112:GLY:HA2	1:A:124:ILE:HD11	1	22.78
(4,17)	1:A:112:GLY:HA2	1:A:124:ILE:HD12	1	22.78
(4,17)	1:A:112:GLY:HA2	1:A:124:ILE:HD13	1	22.78
(4,17)	1:B:112:GLY:HA2	1:B:124:ILE:HD11	1	22.78
(4,17)	1:B:112:GLY:HA2	1:B:124:ILE:HD12	1	22.78
(4,17)	1:B:112:GLY:HA2	1:B:124:ILE:HD13	1	22.78
(4,16)	1:A:112:GLY:HA2	1:A:122:TYR:HD1	4	22.75
(4,16)	1:A:112:GLY:HA2	1:A:122:TYR:HD2	4	22.75
(4,16)	1:B:112:GLY:HA2	1:B:122:TYR:HD1	4	22.75
(4,16)	1:B:112:GLY:HA2	1:B:122:TYR:HD2	4	22.75
(4,15)	1:A:112:GLY:HA2	1:A:122:TYR:HB2	7	22.75
(4,15)	1:B:112:GLY:HA2	1:B:122:TYR:HB2	7	22.75
(4,48)	1:A:122:TYR:HA	1:A:112:GLY:HA3	6	22.73
(4,48)	1:B:122:TYR:HA	1:B:112:GLY:HA3	6	22.73
(4,12)	1:A:112:GLY:HA3	1:A:122:TYR:HA	6	22.73
(4,12)	1:B:112:GLY:HA3	1:B:122:TYR:HA	6	22.73
(4,17)	1:A:112:GLY:HA2	1:A:124:ILE:HD11	6	22.66
(4,17)	1:A:112:GLY:HA2	1:A:124:ILE:HD12	6	22.66
(4,17)	1:A:112:GLY:HA2	1:A:124:ILE:HD13	6	22.66
(4,17)	1:B:112:GLY:HA2	1:B:124:ILE:HD11	6	22.66
(4,17)	1:B:112:GLY:HA2	1:B:124:ILE:HD12	6	22.66
(4,17)	1:B:112:GLY:HA2	1:B:124:ILE:HD13	6	22.66
(4,17)	1:A:112:GLY:HA2	1:A:124:ILE:HD11	2	22.62
(4,17)	1:A:112:GLY:HA2	1:A:124:ILE:HD12	2	22.62
(4,17)	1:A:112:GLY:HA2	1:A:124:ILE:HD13	2	22.62
(4,17)	1:B:112:GLY:HA2	1:B:124:ILE:HD11	2	22.62
(4,17)	1:B:112:GLY:HA2	1:B:124:ILE:HD12	2	22.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,17)	1:B:112:GLY:HA2	1:B:124:ILE:HD13	2	22.62
(4,48)	1:A:122:TYR:HA	1:A:112:GLY:HA3	7	22.59
(4,48)	1:B:122:TYR:HA	1:B:112:GLY:HA3	7	22.59
(4,12)	1:A:112:GLY:HA3	1:A:122:TYR:HA	7	22.59
(4,12)	1:B:112:GLY:HA3	1:B:122:TYR:HA	7	22.59
(4,13)	1:A:112:GLY:HA2	1:A:122:TYR:HB3	1	22.58
(4,13)	1:B:112:GLY:HA2	1:B:122:TYR:HB3	1	22.58
(4,17)	1:A:112:GLY:HA2	1:A:124:ILE:HD11	7	22.49
(4,17)	1:A:112:GLY:HA2	1:A:124:ILE:HD12	7	22.49
(4,17)	1:A:112:GLY:HA2	1:A:124:ILE:HD13	7	22.49
(4,17)	1:B:112:GLY:HA2	1:B:124:ILE:HD11	7	22.49
(4,17)	1:B:112:GLY:HA2	1:B:124:ILE:HD12	7	22.49
(4,17)	1:B:112:GLY:HA2	1:B:124:ILE:HD13	7	22.49
(4,14)	1:A:112:GLY:HA3	1:A:122:TYR:HB2	7	22.29
(4,14)	1:B:112:GLY:HA3	1:B:122:TYR:HB2	7	22.29
(4,17)	1:A:112:GLY:HA2	1:A:124:ILE:HD11	4	22.22
(4,17)	1:A:112:GLY:HA2	1:A:124:ILE:HD12	4	22.22
(4,17)	1:A:112:GLY:HA2	1:A:124:ILE:HD13	4	22.22
(4,17)	1:B:112:GLY:HA2	1:B:124:ILE:HD11	4	22.22
(4,17)	1:B:112:GLY:HA2	1:B:124:ILE:HD12	4	22.22
(4,17)	1:B:112:GLY:HA2	1:B:124:ILE:HD13	4	22.22
(4,17)	1:A:112:GLY:HA2	1:A:124:ILE:HD11	8	22.19
(4,17)	1:A:112:GLY:HA2	1:A:124:ILE:HD12	8	22.19
(4,17)	1:A:112:GLY:HA2	1:A:124:ILE:HD13	8	22.19
(4,17)	1:B:112:GLY:HA2	1:B:124:ILE:HD11	8	22.19
(4,17)	1:B:112:GLY:HA2	1:B:124:ILE:HD12	8	22.19
(4,17)	1:B:112:GLY:HA2	1:B:124:ILE:HD13	8	22.19
(4,16)	1:A:112:GLY:HA2	1:A:122:TYR:HD1	5	22.11
(4,16)	1:A:112:GLY:HA2	1:A:122:TYR:HD2	5	22.11
(4,16)	1:B:112:GLY:HA2	1:B:122:TYR:HD1	5	22.11
(4,16)	1:B:112:GLY:HA2	1:B:122:TYR:HD2	5	22.11
(4,48)	1:A:122:TYR:HA	1:A:112:GLY:HA3	1	22.04
(4,48)	1:B:122:TYR:HA	1:B:112:GLY:HA3	1	22.04
(4,12)	1:A:112:GLY:HA3	1:A:122:TYR:HA	1	22.04
(4,12)	1:B:112:GLY:HA3	1:B:122:TYR:HA	1	22.04
(4,15)	1:A:112:GLY:HA2	1:A:122:TYR:HB2	1	22.03
(4,15)	1:B:112:GLY:HA2	1:B:122:TYR:HB2	1	22.03
(4,8)	1:A:111:HIS:HB3	1:A:123:ARG:HB2	1	21.76
(4,8)	1:A:111:HIS:HB3	1:A:123:ARG:HB3	1	21.76
(4,8)	1:B:111:HIS:HB3	1:B:123:ARG:HB2	1	21.76
(4,8)	1:B:111:HIS:HB3	1:B:123:ARG:HB3	1	21.76
(4,5)	1:A:111:HIS:HB3	1:A:123:ARG:HB2	1	21.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,5)	1:A:111:HIS:HB3	1:A:123:ARG:HB3	1	21.76
(4,5)	1:B:111:HIS:HB3	1:B:123:ARG:HB2	1	21.76
(4,5)	1:B:111:HIS:HB3	1:B:123:ARG:HB3	1	21.76
(4,3)	1:A:111:HIS:HB3	1:A:123:ARG:HB2	1	21.76
(4,3)	1:A:111:HIS:HB3	1:A:123:ARG:HB3	1	21.76
(4,3)	1:B:111:HIS:HB3	1:B:123:ARG:HB2	1	21.76
(4,3)	1:B:111:HIS:HB3	1:B:123:ARG:HB3	1	21.76
(4,14)	1:A:112:GLY:HA3	1:A:122:TYR:HB2	6	21.76
(4,14)	1:B:112:GLY:HA3	1:B:122:TYR:HB2	6	21.76
(4,10)	1:A:111:HIS:HB3	1:A:123:ARG:HB2	1	21.76
(4,10)	1:A:111:HIS:HB3	1:A:123:ARG:HB3	1	21.76
(4,10)	1:B:111:HIS:HB3	1:B:123:ARG:HB2	1	21.76
(4,10)	1:B:111:HIS:HB3	1:B:123:ARG:HB3	1	21.76
(4,16)	1:A:112:GLY:HA2	1:A:122:TYR:HD1	6	21.41
(4,16)	1:A:112:GLY:HA2	1:A:122:TYR:HD2	6	21.41
(4,16)	1:B:112:GLY:HA2	1:B:122:TYR:HD1	6	21.41
(4,16)	1:B:112:GLY:HA2	1:B:122:TYR:HD2	6	21.41
(4,57)	1:A:122:TYR:H	1:A:110:GLU:HB2	1	21.33
(4,57)	1:A:122:TYR:H	1:A:110:GLU:HB3	1	21.33
(4,57)	1:B:122:TYR:H	1:B:110:GLU:HB2	1	21.33
(4,57)	1:B:122:TYR:H	1:B:110:GLU:HB3	1	21.33
(4,56)	1:A:122:TYR:H	1:A:110:GLU:HB2	1	21.33
(4,56)	1:A:122:TYR:H	1:A:110:GLU:HB3	1	21.33
(4,56)	1:B:122:TYR:H	1:B:110:GLU:HB2	1	21.33
(4,56)	1:B:122:TYR:H	1:B:110:GLU:HB3	1	21.33
(4,16)	1:A:112:GLY:HA2	1:A:122:TYR:HD1	7	21.33
(4,16)	1:A:112:GLY:HA2	1:A:122:TYR:HD2	7	21.33
(4,16)	1:B:112:GLY:HA2	1:B:122:TYR:HD1	7	21.33
(4,16)	1:B:112:GLY:HA2	1:B:122:TYR:HD2	7	21.33
(4,14)	1:A:112:GLY:HA3	1:A:122:TYR:HB2	1	21.23
(4,14)	1:B:112:GLY:HA3	1:B:122:TYR:HB2	1	21.23
(4,16)	1:A:112:GLY:HA2	1:A:122:TYR:HD1	1	20.75
(4,16)	1:A:112:GLY:HA2	1:A:122:TYR:HD2	1	20.75
(4,16)	1:B:112:GLY:HA2	1:B:122:TYR:HD1	1	20.75
(4,16)	1:B:112:GLY:HA2	1:B:122:TYR:HD2	1	20.75
(5,6)	1:A:113:PHE:H	1:A:121:LYS:H	4	20.71
(5,6)	1:B:113:PHE:H	1:B:121:LYS:H	4	20.71
(4,9)	1:A:111:HIS:HB2	1:A:123:ARG:HB2	1	20.64
(4,9)	1:A:111:HIS:HB2	1:A:123:ARG:HB3	1	20.64
(4,9)	1:B:111:HIS:HB2	1:B:123:ARG:HB2	1	20.64
(4,9)	1:B:111:HIS:HB2	1:B:123:ARG:HB3	1	20.64
(4,7)	1:A:111:HIS:HB2	1:A:123:ARG:HB2	1	20.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,7)	1:A:111:HIS:HB2	1:A:123:ARG:HB3	1	20.64
(4,7)	1:B:111:HIS:HB2	1:B:123:ARG:HB2	1	20.64
(4,7)	1:B:111:HIS:HB2	1:B:123:ARG:HB3	1	20.64
(4,6)	1:A:111:HIS:HB2	1:A:123:ARG:HB2	1	20.64
(4,6)	1:A:111:HIS:HB2	1:A:123:ARG:HB3	1	20.64
(4,6)	1:B:111:HIS:HB2	1:B:123:ARG:HB2	1	20.64
(4,6)	1:B:111:HIS:HB2	1:B:123:ARG:HB3	1	20.64
(4,4)	1:A:111:HIS:HB2	1:A:123:ARG:HB2	1	20.64
(4,4)	1:A:111:HIS:HB2	1:A:123:ARG:HB3	1	20.64
(4,4)	1:B:111:HIS:HB2	1:B:123:ARG:HB2	1	20.64
(4,4)	1:B:111:HIS:HB2	1:B:123:ARG:HB3	1	20.64
(4,2)	1:A:111:HIS:HB2	1:A:123:ARG:HB2	1	20.64
(4,2)	1:A:111:HIS:HB2	1:A:123:ARG:HB3	1	20.64
(4,2)	1:B:111:HIS:HB2	1:B:123:ARG:HB2	1	20.64
(4,2)	1:B:111:HIS:HB2	1:B:123:ARG:HB3	1	20.64
(4,17)	1:A:112:GLY:HA2	1:A:124:ILE:HD11	3	20.54
(4,17)	1:A:112:GLY:HA2	1:A:124:ILE:HD12	3	20.54
(4,17)	1:A:112:GLY:HA2	1:A:124:ILE:HD13	3	20.54
(4,17)	1:B:112:GLY:HA2	1:B:124:ILE:HD11	3	20.54
(4,17)	1:B:112:GLY:HA2	1:B:124:ILE:HD12	3	20.54
(4,17)	1:B:112:GLY:HA2	1:B:124:ILE:HD13	3	20.54
(5,6)	1:A:113:PHE:H	1:A:121:LYS:H	6	20.53
(5,6)	1:B:113:PHE:H	1:B:121:LYS:H	6	20.53
(5,6)	1:A:113:PHE:H	1:A:121:LYS:H	5	20.33
(5,6)	1:B:113:PHE:H	1:B:121:LYS:H	5	20.33
(5,12)	1:A:121:LYS:H	1:A:113:PHE:H	4	20.11
(5,12)	1:B:121:LYS:H	1:B:113:PHE:H	4	20.11
(4,16)	1:A:112:GLY:HA2	1:A:122:TYR:HD1	3	20.11
(4,16)	1:A:112:GLY:HA2	1:A:122:TYR:HD2	3	20.11
(4,16)	1:B:112:GLY:HA2	1:B:122:TYR:HD1	3	20.11
(4,16)	1:B:112:GLY:HA2	1:B:122:TYR:HD2	3	20.11
(5,12)	1:A:121:LYS:H	1:A:113:PHE:H	6	19.93
(5,12)	1:B:121:LYS:H	1:B:113:PHE:H	6	19.93
(5,12)	1:A:121:LYS:H	1:A:113:PHE:H	5	19.73
(5,12)	1:B:121:LYS:H	1:B:113:PHE:H	5	19.73
(5,6)	1:A:113:PHE:H	1:A:121:LYS:H	1	19.26
(5,6)	1:B:113:PHE:H	1:B:121:LYS:H	1	19.26
(5,6)	1:A:113:PHE:H	1:A:121:LYS:H	3	19.22
(5,6)	1:B:113:PHE:H	1:B:121:LYS:H	3	19.22
(4,16)	1:A:112:GLY:HA2	1:A:122:TYR:HD1	8	19.17
(4,16)	1:A:112:GLY:HA2	1:A:122:TYR:HD2	8	19.17
(4,16)	1:B:112:GLY:HA2	1:B:122:TYR:HD1	8	19.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,16)	1:B:112:GLY:HA2	1:B:122:TYR:HD2	8	19.17
(5,6)	1:A:113:PHE:H	1:A:121:LYS:H	2	19.13
(5,6)	1:B:113:PHE:H	1:B:121:LYS:H	2	19.13
(5,6)	1:A:113:PHE:H	1:A:121:LYS:H	8	19.03
(5,6)	1:B:113:PHE:H	1:B:121:LYS:H	8	19.03
(5,6)	1:A:113:PHE:H	1:A:121:LYS:H	7	18.8
(5,6)	1:B:113:PHE:H	1:B:121:LYS:H	7	18.8
(5,12)	1:A:121:LYS:H	1:A:113:PHE:H	1	18.66
(5,12)	1:B:121:LYS:H	1:B:113:PHE:H	1	18.66
(5,12)	1:A:121:LYS:H	1:A:113:PHE:H	3	18.62
(5,12)	1:B:121:LYS:H	1:B:113:PHE:H	3	18.62
(5,12)	1:A:121:LYS:H	1:A:113:PHE:H	2	18.53
(5,12)	1:B:121:LYS:H	1:B:113:PHE:H	2	18.53
(4,16)	1:A:112:GLY:HA2	1:A:122:TYR:HD1	2	18.52
(4,16)	1:A:112:GLY:HA2	1:A:122:TYR:HD2	2	18.52
(4,16)	1:B:112:GLY:HA2	1:B:122:TYR:HD1	2	18.52
(4,16)	1:B:112:GLY:HA2	1:B:122:TYR:HD2	2	18.52
(4,28)	1:A:116:ARG:HA	1:A:71:GLU:HG2	4	18.48
(4,28)	1:A:116:ARG:HA	1:A:71:GLU:HG3	4	18.48
(4,28)	1:B:116:ARG:HA	1:B:71:GLU:HG2	4	18.48
(4,28)	1:B:116:ARG:HA	1:B:71:GLU:HG3	4	18.48
(5,12)	1:A:121:LYS:H	1:A:113:PHE:H	8	18.43
(5,12)	1:B:121:LYS:H	1:B:113:PHE:H	8	18.43
(5,12)	1:A:121:LYS:H	1:A:113:PHE:H	7	18.2
(5,12)	1:B:121:LYS:H	1:B:113:PHE:H	7	18.2
(4,28)	1:A:116:ARG:HA	1:A:71:GLU:HG2	6	17.8
(4,28)	1:A:116:ARG:HA	1:A:71:GLU:HG3	6	17.8
(4,28)	1:B:116:ARG:HA	1:B:71:GLU:HG2	6	17.8
(4,28)	1:B:116:ARG:HA	1:B:71:GLU:HG3	6	17.8
(4,28)	1:A:116:ARG:HA	1:A:71:GLU:HG2	2	17.76
(4,28)	1:A:116:ARG:HA	1:A:71:GLU:HG3	2	17.76
(4,28)	1:B:116:ARG:HA	1:B:71:GLU:HG2	2	17.76
(4,28)	1:B:116:ARG:HA	1:B:71:GLU:HG3	2	17.76
(4,28)	1:A:116:ARG:HA	1:A:71:GLU:HG2	8	17.57
(4,28)	1:A:116:ARG:HA	1:A:71:GLU:HG3	8	17.57
(4,28)	1:B:116:ARG:HA	1:B:71:GLU:HG2	8	17.57
(4,28)	1:B:116:ARG:HA	1:B:71:GLU:HG3	8	17.57
(4,28)	1:A:116:ARG:HA	1:A:71:GLU:HG2	5	17.41
(4,28)	1:A:116:ARG:HA	1:A:71:GLU:HG3	5	17.41
(4,28)	1:B:116:ARG:HA	1:B:71:GLU:HG2	5	17.41
(4,28)	1:B:116:ARG:HA	1:B:71:GLU:HG3	5	17.41
(4,28)	1:A:116:ARG:HA	1:A:71:GLU:HG2	1	17.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,28)	1:A:116:ARG:HA	1:A:71:GLU:HG3	1	17.25
(4,28)	1:B:116:ARG:HA	1:B:71:GLU:HG2	1	17.25
(4,28)	1:B:116:ARG:HA	1:B:71:GLU:HG3	1	17.25
(4,28)	1:A:116:ARG:HA	1:A:71:GLU:HG2	7	16.18
(4,28)	1:A:116:ARG:HA	1:A:71:GLU:HG3	7	16.18
(4,28)	1:B:116:ARG:HA	1:B:71:GLU:HG2	7	16.18
(4,28)	1:B:116:ARG:HA	1:B:71:GLU:HG3	7	16.18
(4,28)	1:A:116:ARG:HA	1:A:71:GLU:HG2	3	14.75
(4,28)	1:A:116:ARG:HA	1:A:71:GLU:HG3	3	14.75
(4,28)	1:B:116:ARG:HA	1:B:71:GLU:HG2	3	14.75
(4,28)	1:B:116:ARG:HA	1:B:71:GLU:HG3	3	14.75
(4,46)	1:A:121:LYS:HD2	1:A:113:PHE:HD1	6	14.08
(4,46)	1:A:121:LYS:HD2	1:A:113:PHE:HD2	6	14.08
(4,46)	1:A:121:LYS:HD3	1:A:113:PHE:HD1	6	14.08
(4,46)	1:A:121:LYS:HD3	1:A:113:PHE:HD2	6	14.08
(4,46)	1:B:121:LYS:HD2	1:B:113:PHE:HD1	6	14.08
(4,46)	1:B:121:LYS:HD2	1:B:113:PHE:HD2	6	14.08
(4,46)	1:B:121:LYS:HD3	1:B:113:PHE:HD1	6	14.08
(4,46)	1:B:121:LYS:HD3	1:B:113:PHE:HD2	6	14.08
(4,45)	1:A:121:LYS:HD2	1:A:113:PHE:HD1	6	14.08
(4,45)	1:A:121:LYS:HD2	1:A:113:PHE:HD2	6	14.08
(4,45)	1:A:121:LYS:HD3	1:A:113:PHE:HD1	6	14.08
(4,45)	1:A:121:LYS:HD3	1:A:113:PHE:HD2	6	14.08
(4,45)	1:B:121:LYS:HD2	1:B:113:PHE:HD1	6	14.08
(4,45)	1:B:121:LYS:HD2	1:B:113:PHE:HD2	6	14.08
(4,45)	1:B:121:LYS:HD3	1:B:113:PHE:HD1	6	14.08
(4,45)	1:B:121:LYS:HD3	1:B:113:PHE:HD2	6	14.08
(4,46)	1:A:121:LYS:HD2	1:A:113:PHE:HD1	4	13.48
(4,46)	1:A:121:LYS:HD2	1:A:113:PHE:HD2	4	13.48
(4,46)	1:A:121:LYS:HD3	1:A:113:PHE:HD1	4	13.48
(4,46)	1:A:121:LYS:HD3	1:A:113:PHE:HD2	4	13.48
(4,46)	1:B:121:LYS:HD2	1:B:113:PHE:HD1	4	13.48
(4,46)	1:B:121:LYS:HD2	1:B:113:PHE:HD2	4	13.48
(4,46)	1:B:121:LYS:HD3	1:B:113:PHE:HD1	4	13.48
(4,46)	1:B:121:LYS:HD3	1:B:113:PHE:HD2	4	13.48
(4,45)	1:A:121:LYS:HD2	1:A:113:PHE:HD1	4	13.48
(4,45)	1:A:121:LYS:HD2	1:A:113:PHE:HD2	4	13.48
(4,45)	1:A:121:LYS:HD3	1:A:113:PHE:HD1	4	13.48
(4,45)	1:A:121:LYS:HD3	1:A:113:PHE:HD2	4	13.48
(4,45)	1:B:121:LYS:HD2	1:B:113:PHE:HD1	4	13.48
(4,45)	1:B:121:LYS:HD2	1:B:113:PHE:HD2	4	13.48
(4,45)	1:B:121:LYS:HD3	1:B:113:PHE:HD1	4	13.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,45)	1:B:121:LYS:HD3	1:B:113:PHE:HD2	4	13.48
(4,46)	1:A:121:LYS:HD2	1:A:113:PHE:HD1	5	13.37
(4,46)	1:A:121:LYS:HD2	1:A:113:PHE:HD2	5	13.37
(4,46)	1:A:121:LYS:HD3	1:A:113:PHE:HD1	5	13.37
(4,46)	1:A:121:LYS:HD3	1:A:113:PHE:HD2	5	13.37
(4,46)	1:B:121:LYS:HD2	1:B:113:PHE:HD1	5	13.37
(4,46)	1:B:121:LYS:HD2	1:B:113:PHE:HD2	5	13.37
(4,46)	1:B:121:LYS:HD3	1:B:113:PHE:HD1	5	13.37
(4,46)	1:B:121:LYS:HD3	1:B:113:PHE:HD2	5	13.37
(4,45)	1:A:121:LYS:HD2	1:A:113:PHE:HD1	5	13.37
(4,45)	1:A:121:LYS:HD2	1:A:113:PHE:HD2	5	13.37
(4,45)	1:A:121:LYS:HD3	1:A:113:PHE:HD1	5	13.37
(4,45)	1:A:121:LYS:HD3	1:A:113:PHE:HD2	5	13.37
(4,45)	1:B:121:LYS:HD2	1:B:113:PHE:HD1	5	13.37
(4,45)	1:B:121:LYS:HD2	1:B:113:PHE:HD2	5	13.37
(4,45)	1:B:121:LYS:HD3	1:B:113:PHE:HD1	5	13.37
(4,45)	1:B:121:LYS:HD3	1:B:113:PHE:HD2	5	13.37
(4,27)	1:A:116:ARG:HA	1:A:70:LEU:HD11	8	13.14
(4,27)	1:A:116:ARG:HA	1:A:70:LEU:HD12	8	13.14
(4,27)	1:A:116:ARG:HA	1:A:70:LEU:HD13	8	13.14
(4,27)	1:A:116:ARG:HA	1:A:70:LEU:HD21	8	13.14
(4,27)	1:A:116:ARG:HA	1:A:70:LEU:HD22	8	13.14
(4,27)	1:A:116:ARG:HA	1:A:70:LEU:HD23	8	13.14
(4,27)	1:B:116:ARG:HA	1:B:70:LEU:HD11	8	13.14
(4,27)	1:B:116:ARG:HA	1:B:70:LEU:HD12	8	13.14
(4,27)	1:B:116:ARG:HA	1:B:70:LEU:HD13	8	13.14
(4,27)	1:B:116:ARG:HA	1:B:70:LEU:HD21	8	13.14
(4,27)	1:B:116:ARG:HA	1:B:70:LEU:HD22	8	13.14
(4,27)	1:B:116:ARG:HA	1:B:70:LEU:HD23	8	13.14
(5,1)	1:B:82:LYS:HE2	1:B:67:GLU:HA	2	13.07
(5,1)	1:B:82:LYS:HE3	1:B:67:GLU:HA	2	13.07
(5,1)	1:A:82:LYS:HE2	1:A:67:GLU:HA	2	13.07
(5,1)	1:A:82:LYS:HE3	1:A:67:GLU:HA	2	13.07
(4,46)	1:A:121:LYS:HD2	1:A:113:PHE:HD1	7	13.07
(4,46)	1:A:121:LYS:HD2	1:A:113:PHE:HD2	7	13.07
(4,46)	1:A:121:LYS:HD3	1:A:113:PHE:HD1	7	13.07
(4,46)	1:A:121:LYS:HD3	1:A:113:PHE:HD2	7	13.07
(4,46)	1:B:121:LYS:HD2	1:B:113:PHE:HD1	7	13.07
(4,46)	1:B:121:LYS:HD2	1:B:113:PHE:HD2	7	13.07
(4,46)	1:B:121:LYS:HD3	1:B:113:PHE:HD1	7	13.07
(4,46)	1:B:121:LYS:HD3	1:B:113:PHE:HD2	7	13.07
(4,45)	1:A:121:LYS:HD2	1:A:113:PHE:HD1	7	13.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,45)	1:A:121:LYS:HD2	1:A:113:PHE:HD2	7	13.07
(4,45)	1:A:121:LYS:HD3	1:A:113:PHE:HD1	7	13.07
(4,45)	1:A:121:LYS:HD3	1:A:113:PHE:HD2	7	13.07
(4,45)	1:B:121:LYS:HD2	1:B:113:PHE:HD1	7	13.07
(4,45)	1:B:121:LYS:HD2	1:B:113:PHE:HD2	7	13.07
(4,45)	1:B:121:LYS:HD3	1:B:113:PHE:HD1	7	13.07
(4,45)	1:B:121:LYS:HD3	1:B:113:PHE:HD2	7	13.07
(4,46)	1:A:121:LYS:HD2	1:A:113:PHE:HD1	1	13.02
(4,46)	1:A:121:LYS:HD2	1:A:113:PHE:HD2	1	13.02
(4,46)	1:A:121:LYS:HD3	1:A:113:PHE:HD1	1	13.02
(4,46)	1:A:121:LYS:HD3	1:A:113:PHE:HD2	1	13.02
(4,46)	1:B:121:LYS:HD2	1:B:113:PHE:HD1	1	13.02
(4,46)	1:B:121:LYS:HD2	1:B:113:PHE:HD2	1	13.02
(4,46)	1:B:121:LYS:HD3	1:B:113:PHE:HD1	1	13.02
(4,46)	1:B:121:LYS:HD3	1:B:113:PHE:HD2	1	13.02
(4,45)	1:A:121:LYS:HD2	1:A:113:PHE:HD1	1	13.02
(4,45)	1:A:121:LYS:HD2	1:A:113:PHE:HD2	1	13.02
(4,45)	1:A:121:LYS:HD3	1:A:113:PHE:HD1	1	13.02
(4,45)	1:A:121:LYS:HD3	1:A:113:PHE:HD2	1	13.02
(4,45)	1:B:121:LYS:HD2	1:B:113:PHE:HD1	1	13.02
(4,45)	1:B:121:LYS:HD2	1:B:113:PHE:HD2	1	13.02
(4,45)	1:B:121:LYS:HD3	1:B:113:PHE:HD1	1	13.02
(4,45)	1:B:121:LYS:HD3	1:B:113:PHE:HD2	1	13.02
(4,27)	1:A:116:ARG:HA	1:A:70:LEU:HD11	6	12.81
(4,27)	1:A:116:ARG:HA	1:A:70:LEU:HD12	6	12.81
(4,27)	1:A:116:ARG:HA	1:A:70:LEU:HD13	6	12.81
(4,27)	1:A:116:ARG:HA	1:A:70:LEU:HD21	6	12.81
(4,27)	1:A:116:ARG:HA	1:A:70:LEU:HD22	6	12.81
(4,27)	1:A:116:ARG:HA	1:A:70:LEU:HD23	6	12.81
(4,27)	1:B:116:ARG:HA	1:B:70:LEU:HD11	6	12.81
(4,27)	1:B:116:ARG:HA	1:B:70:LEU:HD12	6	12.81
(4,27)	1:B:116:ARG:HA	1:B:70:LEU:HD13	6	12.81
(4,27)	1:B:116:ARG:HA	1:B:70:LEU:HD21	6	12.81
(4,27)	1:B:116:ARG:HA	1:B:70:LEU:HD22	6	12.81
(4,27)	1:B:116:ARG:HA	1:B:70:LEU:HD23	6	12.81
(4,27)	1:A:116:ARG:HA	1:A:70:LEU:HD11	5	12.61
(4,27)	1:A:116:ARG:HA	1:A:70:LEU:HD12	5	12.61
(4,27)	1:A:116:ARG:HA	1:A:70:LEU:HD13	5	12.61
(4,27)	1:A:116:ARG:HA	1:A:70:LEU:HD21	5	12.61
(4,27)	1:A:116:ARG:HA	1:A:70:LEU:HD22	5	12.61
(4,27)	1:A:116:ARG:HA	1:A:70:LEU:HD23	5	12.61
(4,27)	1:B:116:ARG:HA	1:B:70:LEU:HD11	5	12.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,27)	1:B:116:ARG:HA	1:B:70:LEU:HD12	5	12.61
(4,27)	1:B:116:ARG:HA	1:B:70:LEU:HD13	5	12.61
(4,27)	1:B:116:ARG:HA	1:B:70:LEU:HD21	5	12.61
(4,27)	1:B:116:ARG:HA	1:B:70:LEU:HD22	5	12.61
(4,27)	1:B:116:ARG:HA	1:B:70:LEU:HD23	5	12.61
(4,27)	1:A:116:ARG:HA	1:A:70:LEU:HD11	2	12.56
(4,27)	1:A:116:ARG:HA	1:A:70:LEU:HD12	2	12.56
(4,27)	1:A:116:ARG:HA	1:A:70:LEU:HD13	2	12.56
(4,27)	1:A:116:ARG:HA	1:A:70:LEU:HD21	2	12.56
(4,27)	1:A:116:ARG:HA	1:A:70:LEU:HD22	2	12.56
(4,27)	1:A:116:ARG:HA	1:A:70:LEU:HD23	2	12.56
(4,27)	1:B:116:ARG:HA	1:B:70:LEU:HD11	2	12.56
(4,27)	1:B:116:ARG:HA	1:B:70:LEU:HD12	2	12.56
(4,27)	1:B:116:ARG:HA	1:B:70:LEU:HD13	2	12.56
(4,27)	1:B:116:ARG:HA	1:B:70:LEU:HD21	2	12.56
(4,27)	1:B:116:ARG:HA	1:B:70:LEU:HD22	2	12.56
(4,27)	1:B:116:ARG:HA	1:B:70:LEU:HD23	2	12.56
(4,1)	1:A:77:VAL:HG11	1:A:114:ILE:HB	6	12.48
(4,1)	1:A:77:VAL:HG12	1:A:114:ILE:HB	6	12.48
(4,1)	1:A:77:VAL:HG13	1:A:114:ILE:HB	6	12.48
(4,1)	1:B:77:VAL:HG11	1:B:114:ILE:HB	6	12.48
(4,1)	1:B:77:VAL:HG12	1:B:114:ILE:HB	6	12.48
(4,1)	1:B:77:VAL:HG13	1:B:114:ILE:HB	6	12.48
(4,46)	1:A:121:LYS:HD2	1:A:113:PHE:HD1	8	12.43
(4,46)	1:A:121:LYS:HD2	1:A:113:PHE:HD2	8	12.43
(4,46)	1:A:121:LYS:HD3	1:A:113:PHE:HD1	8	12.43
(4,46)	1:A:121:LYS:HD3	1:A:113:PHE:HD2	8	12.43
(4,46)	1:B:121:LYS:HD2	1:B:113:PHE:HD1	8	12.43
(4,46)	1:B:121:LYS:HD2	1:B:113:PHE:HD2	8	12.43
(4,46)	1:B:121:LYS:HD3	1:B:113:PHE:HD1	8	12.43
(4,46)	1:B:121:LYS:HD3	1:B:113:PHE:HD2	8	12.43
(4,45)	1:A:121:LYS:HD2	1:A:113:PHE:HD1	8	12.43
(4,45)	1:A:121:LYS:HD2	1:A:113:PHE:HD2	8	12.43
(4,45)	1:A:121:LYS:HD3	1:A:113:PHE:HD1	8	12.43
(4,45)	1:A:121:LYS:HD3	1:A:113:PHE:HD2	8	12.43
(4,45)	1:B:121:LYS:HD2	1:B:113:PHE:HD1	8	12.43
(4,45)	1:B:121:LYS:HD2	1:B:113:PHE:HD2	8	12.43
(4,45)	1:B:121:LYS:HD3	1:B:113:PHE:HD1	8	12.43
(4,45)	1:B:121:LYS:HD3	1:B:113:PHE:HD2	8	12.43
(4,46)	1:A:121:LYS:HD2	1:A:113:PHE:HD1	2	12.28
(4,46)	1:A:121:LYS:HD2	1:A:113:PHE:HD2	2	12.28
(4,46)	1:A:121:LYS:HD3	1:A:113:PHE:HD1	2	12.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,46)	1:A:121:LYS:HD3	1:A:113:PHE:HD2	2	12.28
(4,46)	1:B:121:LYS:HD2	1:B:113:PHE:HD1	2	12.28
(4,46)	1:B:121:LYS:HD2	1:B:113:PHE:HD2	2	12.28
(4,46)	1:B:121:LYS:HD3	1:B:113:PHE:HD1	2	12.28
(4,46)	1:B:121:LYS:HD3	1:B:113:PHE:HD2	2	12.28
(4,45)	1:A:121:LYS:HD2	1:A:113:PHE:HD1	2	12.28
(4,45)	1:A:121:LYS:HD2	1:A:113:PHE:HD2	2	12.28
(4,45)	1:A:121:LYS:HD3	1:A:113:PHE:HD1	2	12.28
(4,45)	1:A:121:LYS:HD3	1:A:113:PHE:HD2	2	12.28
(4,45)	1:B:121:LYS:HD2	1:B:113:PHE:HD1	2	12.28
(4,45)	1:B:121:LYS:HD2	1:B:113:PHE:HD2	2	12.28
(4,45)	1:B:121:LYS:HD3	1:B:113:PHE:HD1	2	12.28
(4,45)	1:B:121:LYS:HD3	1:B:113:PHE:HD2	2	12.28
(5,1)	1:B:82:LYS:HE2	1:B:67:GLU:HA	5	12.15
(5,1)	1:B:82:LYS:HE3	1:B:67:GLU:HA	5	12.15
(5,1)	1:A:82:LYS:HE2	1:A:67:GLU:HA	5	12.15
(5,1)	1:A:82:LYS:HE3	1:A:67:GLU:HA	5	12.15
(4,46)	1:A:121:LYS:HD2	1:A:113:PHE:HD1	3	11.91
(4,46)	1:A:121:LYS:HD2	1:A:113:PHE:HD2	3	11.91
(4,46)	1:A:121:LYS:HD3	1:A:113:PHE:HD1	3	11.91
(4,46)	1:A:121:LYS:HD3	1:A:113:PHE:HD2	3	11.91
(4,46)	1:B:121:LYS:HD2	1:B:113:PHE:HD1	3	11.91
(4,46)	1:B:121:LYS:HD2	1:B:113:PHE:HD2	3	11.91
(4,46)	1:B:121:LYS:HD3	1:B:113:PHE:HD1	3	11.91
(4,46)	1:B:121:LYS:HD3	1:B:113:PHE:HD2	3	11.91
(4,45)	1:A:121:LYS:HD2	1:A:113:PHE:HD1	3	11.91
(4,45)	1:A:121:LYS:HD2	1:A:113:PHE:HD2	3	11.91
(4,45)	1:A:121:LYS:HD3	1:A:113:PHE:HD1	3	11.91
(4,45)	1:A:121:LYS:HD3	1:A:113:PHE:HD2	3	11.91
(4,45)	1:B:121:LYS:HD2	1:B:113:PHE:HD1	3	11.91
(4,45)	1:B:121:LYS:HD2	1:B:113:PHE:HD2	3	11.91
(4,45)	1:B:121:LYS:HD3	1:B:113:PHE:HD1	3	11.91
(4,45)	1:B:121:LYS:HD3	1:B:113:PHE:HD2	3	11.91
(4,1)	1:A:77:VAL:HG11	1:A:114:ILE:HB	2	11.77
(4,1)	1:A:77:VAL:HG12	1:A:114:ILE:HB	2	11.77
(4,1)	1:A:77:VAL:HG13	1:A:114:ILE:HB	2	11.77
(4,1)	1:B:77:VAL:HG11	1:B:114:ILE:HB	2	11.77
(4,1)	1:B:77:VAL:HG12	1:B:114:ILE:HB	2	11.77
(4,1)	1:B:77:VAL:HG13	1:B:114:ILE:HB	2	11.77
(4,27)	1:A:116:ARG:HA	1:A:70:LEU:HD11	4	11.66
(4,27)	1:A:116:ARG:HA	1:A:70:LEU:HD12	4	11.66
(4,27)	1:A:116:ARG:HA	1:A:70:LEU:HD13	4	11.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,27)	1:A:116:ARG:HA	1:A:70:LEU:HD21	4	11.66
(4,27)	1:A:116:ARG:HA	1:A:70:LEU:HD22	4	11.66
(4,27)	1:A:116:ARG:HA	1:A:70:LEU:HD23	4	11.66
(4,27)	1:B:116:ARG:HA	1:B:70:LEU:HD11	4	11.66
(4,27)	1:B:116:ARG:HA	1:B:70:LEU:HD12	4	11.66
(4,27)	1:B:116:ARG:HA	1:B:70:LEU:HD13	4	11.66
(4,27)	1:B:116:ARG:HA	1:B:70:LEU:HD21	4	11.66
(4,27)	1:B:116:ARG:HA	1:B:70:LEU:HD22	4	11.66
(4,27)	1:B:116:ARG:HA	1:B:70:LEU:HD23	4	11.66
(4,1)	1:A:77:VAL:HG11	1:A:114:ILE:HB	5	11.66
(4,1)	1:A:77:VAL:HG12	1:A:114:ILE:HB	5	11.66
(4,1)	1:A:77:VAL:HG13	1:A:114:ILE:HB	5	11.66
(4,1)	1:B:77:VAL:HG11	1:B:114:ILE:HB	5	11.66
(4,1)	1:B:77:VAL:HG12	1:B:114:ILE:HB	5	11.66
(4,1)	1:B:77:VAL:HG13	1:B:114:ILE:HB	5	11.66
(4,1)	1:A:77:VAL:HG11	1:A:114:ILE:HB	8	11.48
(4,1)	1:A:77:VAL:HG12	1:A:114:ILE:HB	8	11.48
(4,1)	1:A:77:VAL:HG13	1:A:114:ILE:HB	8	11.48
(4,1)	1:B:77:VAL:HG11	1:B:114:ILE:HB	8	11.48
(4,1)	1:B:77:VAL:HG12	1:B:114:ILE:HB	8	11.48
(4,1)	1:B:77:VAL:HG13	1:B:114:ILE:HB	8	11.48
(4,1)	1:A:77:VAL:HG11	1:A:114:ILE:HB	7	10.94
(4,1)	1:A:77:VAL:HG12	1:A:114:ILE:HB	7	10.94
(4,1)	1:A:77:VAL:HG13	1:A:114:ILE:HB	7	10.94
(4,1)	1:B:77:VAL:HG11	1:B:114:ILE:HB	7	10.94
(4,1)	1:B:77:VAL:HG12	1:B:114:ILE:HB	7	10.94
(4,1)	1:B:77:VAL:HG13	1:B:114:ILE:HB	7	10.94
(5,3)	1:B:82:LYS:H	1:B:66:SER:H	3	10.86
(5,3)	1:A:82:LYS:H	1:A:66:SER:H	3	10.86
(4,1)	1:A:77:VAL:HG11	1:A:114:ILE:HB	1	10.77
(4,1)	1:A:77:VAL:HG12	1:A:114:ILE:HB	1	10.77
(4,1)	1:A:77:VAL:HG13	1:A:114:ILE:HB	1	10.77
(4,1)	1:B:77:VAL:HG11	1:B:114:ILE:HB	1	10.77
(4,1)	1:B:77:VAL:HG12	1:B:114:ILE:HB	1	10.77
(4,1)	1:B:77:VAL:HG13	1:B:114:ILE:HB	1	10.77
(4,26)	1:A:115:SER:HB2	1:A:119:HIS:HD2	4	10.62
(4,26)	1:B:115:SER:HB2	1:B:119:HIS:HD2	4	10.62
(4,27)	1:A:116:ARG:HA	1:A:70:LEU:HD11	1	10.41
(4,27)	1:A:116:ARG:HA	1:A:70:LEU:HD12	1	10.41
(4,27)	1:A:116:ARG:HA	1:A:70:LEU:HD13	1	10.41
(4,27)	1:A:116:ARG:HA	1:A:70:LEU:HD21	1	10.41
(4,27)	1:A:116:ARG:HA	1:A:70:LEU:HD22	1	10.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,27)	1:A:116:ARG:HA	1:A:70:LEU:HD23	1	10.41
(4,27)	1:B:116:ARG:HA	1:B:70:LEU:HD11	1	10.41
(4,27)	1:B:116:ARG:HA	1:B:70:LEU:HD12	1	10.41
(4,27)	1:B:116:ARG:HA	1:B:70:LEU:HD13	1	10.41
(4,27)	1:B:116:ARG:HA	1:B:70:LEU:HD21	1	10.41
(4,27)	1:B:116:ARG:HA	1:B:70:LEU:HD22	1	10.41
(4,27)	1:B:116:ARG:HA	1:B:70:LEU:HD23	1	10.41
(5,1)	1:B:82:LYS:HE2	1:B:67:GLU:HA	3	10.27
(5,1)	1:B:82:LYS:HE3	1:B:67:GLU:HA	3	10.27
(5,1)	1:A:82:LYS:HE2	1:A:67:GLU:HA	3	10.27
(5,1)	1:A:82:LYS:HE3	1:A:67:GLU:HA	3	10.27
(4,44)	1:A:120:GLY:HA2	1:A:114:ILE:HA	4	10.26
(4,44)	1:A:120:GLY:HA3	1:A:114:ILE:HA	4	10.26
(4,44)	1:B:120:GLY:HA2	1:B:114:ILE:HA	4	10.26
(4,44)	1:B:120:GLY:HA3	1:B:114:ILE:HA	4	10.26
(4,37)	1:A:120:GLY:HA2	1:A:114:ILE:HA	4	10.26
(4,37)	1:A:120:GLY:HA3	1:A:114:ILE:HA	4	10.26
(4,37)	1:B:120:GLY:HA2	1:B:114:ILE:HA	4	10.26
(4,37)	1:B:120:GLY:HA3	1:B:114:ILE:HA	4	10.26
(4,24)	1:A:114:ILE:HA	1:A:120:GLY:HA2	4	10.26
(4,24)	1:A:114:ILE:HA	1:A:120:GLY:HA3	4	10.26
(4,24)	1:B:114:ILE:HA	1:B:120:GLY:HA2	4	10.26
(4,24)	1:B:114:ILE:HA	1:B:120:GLY:HA3	4	10.26
(5,1)	1:B:82:LYS:HE2	1:B:67:GLU:HA	7	10.19
(5,1)	1:B:82:LYS:HE3	1:B:67:GLU:HA	7	10.19
(5,1)	1:A:82:LYS:HE2	1:A:67:GLU:HA	7	10.19
(5,1)	1:A:82:LYS:HE3	1:A:67:GLU:HA	7	10.19
(4,39)	1:A:120:GLY:HA2	1:A:114:ILE:HB	5	10.14
(4,39)	1:A:120:GLY:HA3	1:A:114:ILE:HB	5	10.14
(4,39)	1:B:120:GLY:HA2	1:B:114:ILE:HB	5	10.14
(4,39)	1:B:120:GLY:HA3	1:B:114:ILE:HB	5	10.14
(5,3)	1:B:82:LYS:H	1:B:66:SER:H	7	10.09
(5,3)	1:A:82:LYS:H	1:A:66:SER:H	7	10.09
(4,1)	1:A:77:VAL:HG11	1:A:114:ILE:HB	3	10.06
(4,1)	1:A:77:VAL:HG12	1:A:114:ILE:HB	3	10.06
(4,1)	1:A:77:VAL:HG13	1:A:114:ILE:HB	3	10.06
(4,1)	1:B:77:VAL:HG11	1:B:114:ILE:HB	3	10.06
(4,1)	1:B:77:VAL:HG12	1:B:114:ILE:HB	3	10.06
(4,1)	1:B:77:VAL:HG13	1:B:114:ILE:HB	3	10.06
(4,27)	1:A:116:ARG:HA	1:A:70:LEU:HD11	7	10.05
(4,27)	1:A:116:ARG:HA	1:A:70:LEU:HD12	7	10.05
(4,27)	1:A:116:ARG:HA	1:A:70:LEU:HD13	7	10.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,27)	1:A:116:ARG:HA	1:A:70:LEU:HD21	7	10.05
(4,27)	1:A:116:ARG:HA	1:A:70:LEU:HD22	7	10.05
(4,27)	1:A:116:ARG:HA	1:A:70:LEU:HD23	7	10.05
(4,27)	1:B:116:ARG:HA	1:B:70:LEU:HD11	7	10.05
(4,27)	1:B:116:ARG:HA	1:B:70:LEU:HD12	7	10.05
(4,27)	1:B:116:ARG:HA	1:B:70:LEU:HD13	7	10.05
(4,27)	1:B:116:ARG:HA	1:B:70:LEU:HD21	7	10.05
(4,27)	1:B:116:ARG:HA	1:B:70:LEU:HD22	7	10.05
(4,27)	1:B:116:ARG:HA	1:B:70:LEU:HD23	7	10.05
(4,39)	1:A:120:GLY:HA2	1:A:114:ILE:HB	6	10.03
(4,39)	1:A:120:GLY:HA3	1:A:114:ILE:HB	6	10.03
(4,39)	1:B:120:GLY:HA2	1:B:114:ILE:HB	6	10.03
(4,39)	1:B:120:GLY:HA3	1:B:114:ILE:HB	6	10.03
(4,39)	1:A:120:GLY:HA2	1:A:114:ILE:HB	4	10.02
(4,39)	1:A:120:GLY:HA3	1:A:114:ILE:HB	4	10.02
(4,39)	1:B:120:GLY:HA2	1:B:114:ILE:HB	4	10.02
(4,39)	1:B:120:GLY:HA3	1:B:114:ILE:HB	4	10.02
(4,44)	1:A:120:GLY:HA2	1:A:114:ILE:HA	5	9.98
(4,44)	1:A:120:GLY:HA3	1:A:114:ILE:HA	5	9.98
(4,44)	1:B:120:GLY:HA2	1:B:114:ILE:HA	5	9.98
(4,44)	1:B:120:GLY:HA3	1:B:114:ILE:HA	5	9.98
(4,37)	1:A:120:GLY:HA2	1:A:114:ILE:HA	5	9.98
(4,37)	1:A:120:GLY:HA3	1:A:114:ILE:HA	5	9.98
(4,37)	1:B:120:GLY:HA2	1:B:114:ILE:HA	5	9.98
(4,37)	1:B:120:GLY:HA3	1:B:114:ILE:HA	5	9.98
(4,24)	1:A:114:ILE:HA	1:A:120:GLY:HA2	5	9.98
(4,24)	1:A:114:ILE:HA	1:A:120:GLY:HA3	5	9.98
(4,24)	1:B:114:ILE:HA	1:B:120:GLY:HA2	5	9.98
(4,24)	1:B:114:ILE:HA	1:B:120:GLY:HA3	5	9.98
(4,19)	1:A:114:ILE:HG21	1:A:77:VAL:HG21	6	9.98
(4,19)	1:A:114:ILE:HG21	1:A:77:VAL:HG22	6	9.98
(4,19)	1:A:114:ILE:HG21	1:A:77:VAL:HG23	6	9.98
(4,19)	1:A:114:ILE:HG22	1:A:77:VAL:HG21	6	9.98
(4,19)	1:A:114:ILE:HG22	1:A:77:VAL:HG22	6	9.98
(4,19)	1:A:114:ILE:HG22	1:A:77:VAL:HG23	6	9.98
(4,19)	1:A:114:ILE:HG23	1:A:77:VAL:HG21	6	9.98
(4,19)	1:A:114:ILE:HG23	1:A:77:VAL:HG22	6	9.98
(4,19)	1:A:114:ILE:HG23	1:A:77:VAL:HG23	6	9.98
(4,19)	1:B:114:ILE:HG21	1:B:77:VAL:HG21	6	9.98
(4,19)	1:B:114:ILE:HG21	1:B:77:VAL:HG22	6	9.98
(4,19)	1:B:114:ILE:HG21	1:B:77:VAL:HG23	6	9.98
(4,19)	1:B:114:ILE:HG22	1:B:77:VAL:HG21	6	9.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,19)	1:B:114:ILE:HG22	1:B:77:VAL:HG22	6	9.98
(4,19)	1:B:114:ILE:HG22	1:B:77:VAL:HG23	6	9.98
(4,19)	1:B:114:ILE:HG23	1:B:77:VAL:HG21	6	9.98
(4,19)	1:B:114:ILE:HG23	1:B:77:VAL:HG22	6	9.98
(4,19)	1:B:114:ILE:HG23	1:B:77:VAL:HG23	6	9.98
(4,18)	1:A:114:ILE:HG21	1:A:77:VAL:HG21	6	9.98
(4,18)	1:A:114:ILE:HG21	1:A:77:VAL:HG22	6	9.98
(4,18)	1:A:114:ILE:HG21	1:A:77:VAL:HG23	6	9.98
(4,18)	1:A:114:ILE:HG22	1:A:77:VAL:HG21	6	9.98
(4,18)	1:A:114:ILE:HG22	1:A:77:VAL:HG22	6	9.98
(4,18)	1:A:114:ILE:HG22	1:A:77:VAL:HG23	6	9.98
(4,18)	1:A:114:ILE:HG23	1:A:77:VAL:HG21	6	9.98
(4,18)	1:A:114:ILE:HG23	1:A:77:VAL:HG22	6	9.98
(4,18)	1:A:114:ILE:HG23	1:A:77:VAL:HG23	6	9.98
(4,18)	1:B:114:ILE:HG21	1:B:77:VAL:HG21	6	9.98
(4,18)	1:B:114:ILE:HG21	1:B:77:VAL:HG22	6	9.98
(4,18)	1:B:114:ILE:HG21	1:B:77:VAL:HG23	6	9.98
(4,18)	1:B:114:ILE:HG22	1:B:77:VAL:HG21	6	9.98
(4,18)	1:B:114:ILE:HG22	1:B:77:VAL:HG22	6	9.98
(4,18)	1:B:114:ILE:HG22	1:B:77:VAL:HG23	6	9.98
(4,18)	1:B:114:ILE:HG23	1:B:77:VAL:HG21	6	9.98
(4,18)	1:B:114:ILE:HG23	1:B:77:VAL:HG22	6	9.98
(4,18)	1:B:114:ILE:HG23	1:B:77:VAL:HG23	6	9.98
(4,1)	1:A:77:VAL:HG11	1:A:114:ILE:HB	4	9.86
(4,1)	1:A:77:VAL:HG12	1:A:114:ILE:HB	4	9.86
(4,1)	1:A:77:VAL:HG13	1:A:114:ILE:HB	4	9.86
(4,1)	1:B:77:VAL:HG11	1:B:114:ILE:HB	4	9.86
(4,1)	1:B:77:VAL:HG12	1:B:114:ILE:HB	4	9.86
(4,1)	1:B:77:VAL:HG13	1:B:114:ILE:HB	4	9.86
(4,39)	1:A:120:GLY:HA2	1:A:114:ILE:HB	7	9.81
(4,39)	1:A:120:GLY:HA3	1:A:114:ILE:HB	7	9.81
(4,39)	1:B:120:GLY:HA2	1:B:114:ILE:HB	7	9.81
(4,39)	1:B:120:GLY:HA3	1:B:114:ILE:HB	7	9.81
(4,39)	1:A:120:GLY:HA2	1:A:114:ILE:HB	3	9.65
(4,39)	1:A:120:GLY:HA3	1:A:114:ILE:HB	3	9.65
(4,39)	1:B:120:GLY:HA2	1:B:114:ILE:HB	3	9.65
(4,39)	1:B:120:GLY:HA3	1:B:114:ILE:HB	3	9.65
(4,44)	1:A:120:GLY:HA2	1:A:114:ILE:HA	6	9.61
(4,44)	1:A:120:GLY:HA3	1:A:114:ILE:HA	6	9.61
(4,44)	1:B:120:GLY:HA2	1:B:114:ILE:HA	6	9.61
(4,44)	1:B:120:GLY:HA3	1:B:114:ILE:HA	6	9.61
(4,37)	1:A:120:GLY:HA2	1:A:114:ILE:HA	6	9.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,37)	1:A:120:GLY:HA3	1:A:114:ILE:HA	6	9.61
(4,37)	1:B:120:GLY:HA2	1:B:114:ILE:HA	6	9.61
(4,37)	1:B:120:GLY:HA3	1:B:114:ILE:HA	6	9.61
(4,24)	1:A:114:ILE:HA	1:A:120:GLY:HA2	6	9.61
(4,24)	1:A:114:ILE:HA	1:A:120:GLY:HA3	6	9.61
(4,24)	1:B:114:ILE:HA	1:B:120:GLY:HA2	6	9.61
(4,24)	1:B:114:ILE:HA	1:B:120:GLY:HA3	6	9.61
(4,44)	1:A:120:GLY:HA2	1:A:114:ILE:HA	3	9.48
(4,44)	1:A:120:GLY:HA3	1:A:114:ILE:HA	3	9.48
(4,44)	1:B:120:GLY:HA2	1:B:114:ILE:HA	3	9.48
(4,44)	1:B:120:GLY:HA3	1:B:114:ILE:HA	3	9.48
(4,37)	1:A:120:GLY:HA2	1:A:114:ILE:HA	3	9.48
(4,37)	1:A:120:GLY:HA3	1:A:114:ILE:HA	3	9.48
(4,37)	1:B:120:GLY:HA2	1:B:114:ILE:HA	3	9.48
(4,37)	1:B:120:GLY:HA3	1:B:114:ILE:HA	3	9.48
(4,24)	1:A:114:ILE:HA	1:A:120:GLY:HA2	3	9.48
(4,24)	1:A:114:ILE:HA	1:A:120:GLY:HA3	3	9.48
(4,24)	1:B:114:ILE:HA	1:B:120:GLY:HA2	3	9.48
(4,24)	1:B:114:ILE:HA	1:B:120:GLY:HA3	3	9.48
(4,39)	1:A:120:GLY:HA2	1:A:114:ILE:HB	2	9.47
(4,39)	1:A:120:GLY:HA3	1:A:114:ILE:HB	2	9.47
(4,39)	1:B:120:GLY:HA2	1:B:114:ILE:HB	2	9.47
(4,39)	1:B:120:GLY:HA3	1:B:114:ILE:HB	2	9.47
(5,3)	1:B:82:LYS:H	1:B:66:SER:H	6	9.41
(5,3)	1:A:82:LYS:H	1:A:66:SER:H	6	9.41
(4,44)	1:A:120:GLY:HA2	1:A:114:ILE:HA	2	9.4
(4,44)	1:A:120:GLY:HA3	1:A:114:ILE:HA	2	9.4
(4,44)	1:B:120:GLY:HA2	1:B:114:ILE:HA	2	9.4
(4,44)	1:B:120:GLY:HA3	1:B:114:ILE:HA	2	9.4
(4,37)	1:A:120:GLY:HA2	1:A:114:ILE:HA	2	9.4
(4,37)	1:A:120:GLY:HA3	1:A:114:ILE:HA	2	9.4
(4,37)	1:B:120:GLY:HA2	1:B:114:ILE:HA	2	9.4
(4,37)	1:B:120:GLY:HA3	1:B:114:ILE:HA	2	9.4
(4,24)	1:A:114:ILE:HA	1:A:120:GLY:HA2	2	9.4
(4,24)	1:A:114:ILE:HA	1:A:120:GLY:HA3	2	9.4
(4,24)	1:B:114:ILE:HA	1:B:120:GLY:HA2	2	9.4
(4,24)	1:B:114:ILE:HA	1:B:120:GLY:HA3	2	9.4
(4,19)	1:A:114:ILE:HG21	1:A:77:VAL:HG21	5	9.39
(4,19)	1:A:114:ILE:HG21	1:A:77:VAL:HG22	5	9.39
(4,19)	1:A:114:ILE:HG21	1:A:77:VAL:HG23	5	9.39
(4,19)	1:A:114:ILE:HG22	1:A:77:VAL:HG21	5	9.39
(4,19)	1:A:114:ILE:HG22	1:A:77:VAL:HG22	5	9.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,19)	1:A:114:ILE:HG22	1:A:77:VAL:HG23	5	9.39
(4,19)	1:A:114:ILE:HG23	1:A:77:VAL:HG21	5	9.39
(4,19)	1:A:114:ILE:HG23	1:A:77:VAL:HG22	5	9.39
(4,19)	1:A:114:ILE:HG23	1:A:77:VAL:HG23	5	9.39
(4,19)	1:B:114:ILE:HG21	1:B:77:VAL:HG21	5	9.39
(4,19)	1:B:114:ILE:HG21	1:B:77:VAL:HG22	5	9.39
(4,19)	1:B:114:ILE:HG21	1:B:77:VAL:HG23	5	9.39
(4,19)	1:B:114:ILE:HG22	1:B:77:VAL:HG21	5	9.39
(4,19)	1:B:114:ILE:HG22	1:B:77:VAL:HG22	5	9.39
(4,19)	1:B:114:ILE:HG22	1:B:77:VAL:HG23	5	9.39
(4,19)	1:B:114:ILE:HG23	1:B:77:VAL:HG21	5	9.39
(4,19)	1:B:114:ILE:HG23	1:B:77:VAL:HG22	5	9.39
(4,19)	1:B:114:ILE:HG23	1:B:77:VAL:HG23	5	9.39
(4,18)	1:A:114:ILE:HG21	1:A:77:VAL:HG21	5	9.39
(4,18)	1:A:114:ILE:HG21	1:A:77:VAL:HG22	5	9.39
(4,18)	1:A:114:ILE:HG21	1:A:77:VAL:HG23	5	9.39
(4,18)	1:A:114:ILE:HG22	1:A:77:VAL:HG21	5	9.39
(4,18)	1:A:114:ILE:HG22	1:A:77:VAL:HG22	5	9.39
(4,18)	1:A:114:ILE:HG22	1:A:77:VAL:HG23	5	9.39
(4,18)	1:A:114:ILE:HG23	1:A:77:VAL:HG21	5	9.39
(4,18)	1:A:114:ILE:HG23	1:A:77:VAL:HG22	5	9.39
(4,18)	1:A:114:ILE:HG23	1:A:77:VAL:HG23	5	9.39
(4,18)	1:B:114:ILE:HG21	1:B:77:VAL:HG21	5	9.39
(4,18)	1:B:114:ILE:HG21	1:B:77:VAL:HG22	5	9.39
(4,18)	1:B:114:ILE:HG21	1:B:77:VAL:HG23	5	9.39
(4,18)	1:B:114:ILE:HG22	1:B:77:VAL:HG21	5	9.39
(4,18)	1:B:114:ILE:HG22	1:B:77:VAL:HG22	5	9.39
(4,18)	1:B:114:ILE:HG22	1:B:77:VAL:HG23	5	9.39
(4,18)	1:B:114:ILE:HG23	1:B:77:VAL:HG21	5	9.39
(4,18)	1:B:114:ILE:HG23	1:B:77:VAL:HG22	5	9.39
(4,18)	1:B:114:ILE:HG23	1:B:77:VAL:HG23	5	9.39
(5,1)	1:B:82:LYS:HE2	1:B:67:GLU:HA	1	9.38
(5,1)	1:B:82:LYS:HE3	1:B:67:GLU:HA	1	9.38
(5,1)	1:A:82:LYS:HE2	1:A:67:GLU:HA	1	9.38
(5,1)	1:A:82:LYS:HE3	1:A:67:GLU:HA	1	9.38
(5,4)	1:B:82:LYS:H	1:B:66:SER:HA	3	9.34
(5,4)	1:A:82:LYS:H	1:A:66:SER:HA	3	9.34
(4,19)	1:A:114:ILE:HG21	1:A:77:VAL:HG21	8	9.33
(4,19)	1:A:114:ILE:HG21	1:A:77:VAL:HG22	8	9.33
(4,19)	1:A:114:ILE:HG21	1:A:77:VAL:HG23	8	9.33
(4,19)	1:A:114:ILE:HG22	1:A:77:VAL:HG21	8	9.33
(4,19)	1:A:114:ILE:HG22	1:A:77:VAL:HG22	8	9.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,19)	1:A:114:ILE:HG22	1:A:77:VAL:HG23	8	9.33
(4,19)	1:A:114:ILE:HG23	1:A:77:VAL:HG21	8	9.33
(4,19)	1:A:114:ILE:HG23	1:A:77:VAL:HG22	8	9.33
(4,19)	1:A:114:ILE:HG23	1:A:77:VAL:HG23	8	9.33
(4,19)	1:B:114:ILE:HG21	1:B:77:VAL:HG21	8	9.33
(4,19)	1:B:114:ILE:HG21	1:B:77:VAL:HG22	8	9.33
(4,19)	1:B:114:ILE:HG21	1:B:77:VAL:HG23	8	9.33
(4,19)	1:B:114:ILE:HG22	1:B:77:VAL:HG21	8	9.33
(4,19)	1:B:114:ILE:HG22	1:B:77:VAL:HG22	8	9.33
(4,19)	1:B:114:ILE:HG22	1:B:77:VAL:HG23	8	9.33
(4,19)	1:B:114:ILE:HG23	1:B:77:VAL:HG21	8	9.33
(4,19)	1:B:114:ILE:HG23	1:B:77:VAL:HG22	8	9.33
(4,19)	1:B:114:ILE:HG23	1:B:77:VAL:HG23	8	9.33
(4,18)	1:A:114:ILE:HG21	1:A:77:VAL:HG21	8	9.33
(4,18)	1:A:114:ILE:HG21	1:A:77:VAL:HG22	8	9.33
(4,18)	1:A:114:ILE:HG21	1:A:77:VAL:HG23	8	9.33
(4,18)	1:A:114:ILE:HG22	1:A:77:VAL:HG21	8	9.33
(4,18)	1:A:114:ILE:HG22	1:A:77:VAL:HG22	8	9.33
(4,18)	1:A:114:ILE:HG22	1:A:77:VAL:HG23	8	9.33
(4,18)	1:A:114:ILE:HG23	1:A:77:VAL:HG21	8	9.33
(4,18)	1:A:114:ILE:HG23	1:A:77:VAL:HG22	8	9.33
(4,18)	1:A:114:ILE:HG23	1:A:77:VAL:HG23	8	9.33
(4,18)	1:B:114:ILE:HG21	1:B:77:VAL:HG21	8	9.33
(4,18)	1:B:114:ILE:HG21	1:B:77:VAL:HG22	8	9.33
(4,18)	1:B:114:ILE:HG21	1:B:77:VAL:HG23	8	9.33
(4,18)	1:B:114:ILE:HG22	1:B:77:VAL:HG21	8	9.33
(4,18)	1:B:114:ILE:HG22	1:B:77:VAL:HG22	8	9.33
(4,18)	1:B:114:ILE:HG22	1:B:77:VAL:HG23	8	9.33
(4,18)	1:B:114:ILE:HG23	1:B:77:VAL:HG21	8	9.33
(4,18)	1:B:114:ILE:HG23	1:B:77:VAL:HG22	8	9.33
(4,18)	1:B:114:ILE:HG23	1:B:77:VAL:HG23	8	9.33
(4,40)	1:A:120:GLY:HA2	1:A:114:ILE:HG12	5	9.25
(4,40)	1:A:120:GLY:HA2	1:A:114:ILE:HG13	5	9.25
(4,40)	1:A:120:GLY:HA3	1:A:114:ILE:HG12	5	9.25
(4,40)	1:A:120:GLY:HA3	1:A:114:ILE:HG13	5	9.25
(4,40)	1:B:120:GLY:HA2	1:B:114:ILE:HG12	5	9.25
(4,40)	1:B:120:GLY:HA2	1:B:114:ILE:HG13	5	9.25
(4,40)	1:B:120:GLY:HA3	1:B:114:ILE:HG12	5	9.25
(4,40)	1:B:120:GLY:HA3	1:B:114:ILE:HG13	5	9.25
(4,40)	1:A:120:GLY:HA2	1:A:114:ILE:HG12	6	9.2
(4,40)	1:A:120:GLY:HA2	1:A:114:ILE:HG13	6	9.2
(4,40)	1:A:120:GLY:HA3	1:A:114:ILE:HG12	6	9.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,40)	1:A:120:GLY:HA3	1:A:114:ILE:HG13	6	9.2
(4,40)	1:B:120:GLY:HA2	1:B:114:ILE:HG12	6	9.2
(4,40)	1:B:120:GLY:HA2	1:B:114:ILE:HG13	6	9.2
(4,40)	1:B:120:GLY:HA3	1:B:114:ILE:HG12	6	9.2
(4,40)	1:B:120:GLY:HA3	1:B:114:ILE:HG13	6	9.2
(4,44)	1:A:120:GLY:HA2	1:A:114:ILE:HA	8	9.18
(4,44)	1:A:120:GLY:HA3	1:A:114:ILE:HA	8	9.18
(4,44)	1:B:120:GLY:HA2	1:B:114:ILE:HA	8	9.18
(4,44)	1:B:120:GLY:HA3	1:B:114:ILE:HA	8	9.18
(4,37)	1:A:120:GLY:HA2	1:A:114:ILE:HA	8	9.18
(4,37)	1:A:120:GLY:HA3	1:A:114:ILE:HA	8	9.18
(4,37)	1:B:120:GLY:HA2	1:B:114:ILE:HA	8	9.18
(4,37)	1:B:120:GLY:HA3	1:B:114:ILE:HA	8	9.18
(4,24)	1:A:114:ILE:HA	1:A:120:GLY:HA2	8	9.18
(4,24)	1:A:114:ILE:HA	1:A:120:GLY:HA3	8	9.18
(4,24)	1:B:114:ILE:HA	1:B:120:GLY:HA2	8	9.18
(4,24)	1:B:114:ILE:HA	1:B:120:GLY:HA3	8	9.18
(4,40)	1:A:120:GLY:HA2	1:A:114:ILE:HG12	4	9.16
(4,40)	1:A:120:GLY:HA2	1:A:114:ILE:HG13	4	9.16
(4,40)	1:A:120:GLY:HA3	1:A:114:ILE:HG12	4	9.16
(4,40)	1:A:120:GLY:HA3	1:A:114:ILE:HG13	4	9.16
(4,40)	1:B:120:GLY:HA2	1:B:114:ILE:HG12	4	9.16
(4,40)	1:B:120:GLY:HA2	1:B:114:ILE:HG13	4	9.16
(4,40)	1:B:120:GLY:HA3	1:B:114:ILE:HG12	4	9.16
(4,40)	1:B:120:GLY:HA3	1:B:114:ILE:HG13	4	9.16
(4,34)	1:A:119:HIS:HB2	1:A:115:SER:HB2	4	9.14
(4,34)	1:B:119:HIS:HB2	1:B:115:SER:HB2	4	9.14
(4,44)	1:A:120:GLY:HA2	1:A:114:ILE:HA	7	9.13
(4,44)	1:A:120:GLY:HA3	1:A:114:ILE:HA	7	9.13
(4,44)	1:B:120:GLY:HA2	1:B:114:ILE:HA	7	9.13
(4,44)	1:B:120:GLY:HA3	1:B:114:ILE:HA	7	9.13
(4,37)	1:A:120:GLY:HA2	1:A:114:ILE:HA	7	9.13
(4,37)	1:A:120:GLY:HA3	1:A:114:ILE:HA	7	9.13
(4,37)	1:B:120:GLY:HA2	1:B:114:ILE:HA	7	9.13
(4,37)	1:B:120:GLY:HA3	1:B:114:ILE:HA	7	9.13
(4,24)	1:A:114:ILE:HA	1:A:120:GLY:HA2	7	9.13
(4,24)	1:A:114:ILE:HA	1:A:120:GLY:HA3	7	9.13
(4,24)	1:B:114:ILE:HA	1:B:120:GLY:HA2	7	9.13
(4,24)	1:B:114:ILE:HA	1:B:120:GLY:HA3	7	9.13
(4,50)	1:A:115:SER:H	1:A:120:GLY:HA2	4	9.03
(4,50)	1:A:115:SER:H	1:A:120:GLY:HA3	4	9.03
(4,50)	1:B:115:SER:H	1:B:120:GLY:HA2	4	9.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,50)	1:B:115:SER:H	1:B:120:GLY:HA3	4	9.03
(4,39)	1:A:120:GLY:HA2	1:A:114:ILE:HB	8	9.01
(4,39)	1:A:120:GLY:HA3	1:A:114:ILE:HB	8	9.01
(4,39)	1:B:120:GLY:HA2	1:B:114:ILE:HB	8	9.01
(4,39)	1:B:120:GLY:HA3	1:B:114:ILE:HB	8	9.01
(4,40)	1:A:120:GLY:HA2	1:A:114:ILE:HG12	7	9.0
(4,40)	1:A:120:GLY:HA2	1:A:114:ILE:HG13	7	9.0
(4,40)	1:A:120:GLY:HA3	1:A:114:ILE:HG12	7	9.0
(4,40)	1:A:120:GLY:HA3	1:A:114:ILE:HG13	7	9.0
(4,40)	1:B:120:GLY:HA2	1:B:114:ILE:HG12	7	9.0
(4,40)	1:B:120:GLY:HA2	1:B:114:ILE:HG13	7	9.0
(4,40)	1:B:120:GLY:HA3	1:B:114:ILE:HG12	7	9.0
(4,40)	1:B:120:GLY:HA3	1:B:114:ILE:HG13	7	9.0
(4,39)	1:A:120:GLY:HA2	1:A:114:ILE:HB	1	8.99
(4,39)	1:A:120:GLY:HA3	1:A:114:ILE:HB	1	8.99
(4,39)	1:B:120:GLY:HA2	1:B:114:ILE:HB	1	8.99
(4,39)	1:B:120:GLY:HA3	1:B:114:ILE:HB	1	8.99
(5,1)	1:B:82:LYS:HE2	1:B:67:GLU:HA	4	8.97
(5,1)	1:B:82:LYS:HE3	1:B:67:GLU:HA	4	8.97
(5,1)	1:A:82:LYS:HE2	1:A:67:GLU:HA	4	8.97
(5,1)	1:A:82:LYS:HE3	1:A:67:GLU:HA	4	8.97
(4,50)	1:A:115:SER:H	1:A:120:GLY:HA2	5	8.85
(4,50)	1:A:115:SER:H	1:A:120:GLY:HA3	5	8.85
(4,50)	1:B:115:SER:H	1:B:120:GLY:HA2	5	8.85
(4,50)	1:B:115:SER:H	1:B:120:GLY:HA3	5	8.85
(4,27)	1:A:116:ARG:HA	1:A:70:LEU:HD11	3	8.85
(4,27)	1:A:116:ARG:HA	1:A:70:LEU:HD12	3	8.85
(4,27)	1:A:116:ARG:HA	1:A:70:LEU:HD13	3	8.85
(4,27)	1:A:116:ARG:HA	1:A:70:LEU:HD21	3	8.85
(4,27)	1:A:116:ARG:HA	1:A:70:LEU:HD22	3	8.85
(4,27)	1:A:116:ARG:HA	1:A:70:LEU:HD23	3	8.85
(4,27)	1:B:116:ARG:HA	1:B:70:LEU:HD11	3	8.85
(4,27)	1:B:116:ARG:HA	1:B:70:LEU:HD12	3	8.85
(4,27)	1:B:116:ARG:HA	1:B:70:LEU:HD13	3	8.85
(4,27)	1:B:116:ARG:HA	1:B:70:LEU:HD21	3	8.85
(4,27)	1:B:116:ARG:HA	1:B:70:LEU:HD22	3	8.85
(4,27)	1:B:116:ARG:HA	1:B:70:LEU:HD23	3	8.85
(4,19)	1:A:114:ILE:HG21	1:A:77:VAL:HG21	7	8.66
(4,19)	1:A:114:ILE:HG21	1:A:77:VAL:HG22	7	8.66
(4,19)	1:A:114:ILE:HG21	1:A:77:VAL:HG23	7	8.66
(4,19)	1:A:114:ILE:HG22	1:A:77:VAL:HG21	7	8.66
(4,19)	1:A:114:ILE:HG22	1:A:77:VAL:HG22	7	8.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,19)	1:A:114:ILE:HG22	1:A:77:VAL:HG23	7	8.66
(4,19)	1:A:114:ILE:HG23	1:A:77:VAL:HG21	7	8.66
(4,19)	1:A:114:ILE:HG23	1:A:77:VAL:HG22	7	8.66
(4,19)	1:A:114:ILE:HG23	1:A:77:VAL:HG23	7	8.66
(4,19)	1:B:114:ILE:HG21	1:B:77:VAL:HG21	7	8.66
(4,19)	1:B:114:ILE:HG21	1:B:77:VAL:HG22	7	8.66
(4,19)	1:B:114:ILE:HG21	1:B:77:VAL:HG23	7	8.66
(4,19)	1:B:114:ILE:HG22	1:B:77:VAL:HG21	7	8.66
(4,19)	1:B:114:ILE:HG22	1:B:77:VAL:HG22	7	8.66
(4,19)	1:B:114:ILE:HG22	1:B:77:VAL:HG23	7	8.66
(4,19)	1:B:114:ILE:HG23	1:B:77:VAL:HG21	7	8.66
(4,19)	1:B:114:ILE:HG23	1:B:77:VAL:HG22	7	8.66
(4,19)	1:B:114:ILE:HG23	1:B:77:VAL:HG23	7	8.66
(4,18)	1:A:114:ILE:HG21	1:A:77:VAL:HG21	7	8.66
(4,18)	1:A:114:ILE:HG21	1:A:77:VAL:HG22	7	8.66
(4,18)	1:A:114:ILE:HG21	1:A:77:VAL:HG23	7	8.66
(4,18)	1:A:114:ILE:HG22	1:A:77:VAL:HG21	7	8.66
(4,18)	1:A:114:ILE:HG22	1:A:77:VAL:HG22	7	8.66
(4,18)	1:A:114:ILE:HG22	1:A:77:VAL:HG23	7	8.66
(4,18)	1:A:114:ILE:HG23	1:A:77:VAL:HG21	7	8.66
(4,18)	1:A:114:ILE:HG23	1:A:77:VAL:HG22	7	8.66
(4,18)	1:A:114:ILE:HG23	1:A:77:VAL:HG23	7	8.66
(4,18)	1:B:114:ILE:HG21	1:B:77:VAL:HG21	7	8.66
(4,18)	1:B:114:ILE:HG21	1:B:77:VAL:HG22	7	8.66
(4,18)	1:B:114:ILE:HG21	1:B:77:VAL:HG23	7	8.66
(4,18)	1:B:114:ILE:HG22	1:B:77:VAL:HG21	7	8.66
(4,18)	1:B:114:ILE:HG22	1:B:77:VAL:HG22	7	8.66
(4,18)	1:B:114:ILE:HG22	1:B:77:VAL:HG23	7	8.66
(4,18)	1:B:114:ILE:HG23	1:B:77:VAL:HG21	7	8.66
(4,18)	1:B:114:ILE:HG23	1:B:77:VAL:HG22	7	8.66
(4,18)	1:B:114:ILE:HG23	1:B:77:VAL:HG23	7	8.66
(4,44)	1:A:120:GLY:HA2	1:A:114:ILE:HA	1	8.64
(4,44)	1:A:120:GLY:HA3	1:A:114:ILE:HA	1	8.64
(4,44)	1:B:120:GLY:HA2	1:B:114:ILE:HA	1	8.64
(4,44)	1:B:120:GLY:HA3	1:B:114:ILE:HA	1	8.64
(4,37)	1:A:120:GLY:HA2	1:A:114:ILE:HA	1	8.64
(4,37)	1:A:120:GLY:HA3	1:A:114:ILE:HA	1	8.64
(4,37)	1:B:120:GLY:HA2	1:B:114:ILE:HA	1	8.64
(4,37)	1:B:120:GLY:HA3	1:B:114:ILE:HA	1	8.64
(4,24)	1:A:114:ILE:HA	1:A:120:GLY:HA2	1	8.64
(4,24)	1:A:114:ILE:HA	1:A:120:GLY:HA3	1	8.64
(4,24)	1:B:114:ILE:HA	1:B:120:GLY:HA2	1	8.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,24)	1:B:114:ILE:HA	1:B:120:GLY:HA3	1	8.64
(4,40)	1:A:120:GLY:HA2	1:A:114:ILE:HG12	3	8.61
(4,40)	1:A:120:GLY:HA2	1:A:114:ILE:HG13	3	8.61
(4,40)	1:A:120:GLY:HA3	1:A:114:ILE:HG12	3	8.61
(4,40)	1:A:120:GLY:HA3	1:A:114:ILE:HG13	3	8.61
(4,40)	1:B:120:GLY:HA2	1:B:114:ILE:HG12	3	8.61
(4,40)	1:B:120:GLY:HA2	1:B:114:ILE:HG13	3	8.61
(4,40)	1:B:120:GLY:HA3	1:B:114:ILE:HG12	3	8.61
(4,40)	1:B:120:GLY:HA3	1:B:114:ILE:HG13	3	8.61
(4,40)	1:A:120:GLY:HA2	1:A:114:ILE:HG12	2	8.6
(4,40)	1:A:120:GLY:HA2	1:A:114:ILE:HG13	2	8.6
(4,40)	1:A:120:GLY:HA3	1:A:114:ILE:HG12	2	8.6
(4,40)	1:A:120:GLY:HA3	1:A:114:ILE:HG13	2	8.6
(4,40)	1:B:120:GLY:HA2	1:B:114:ILE:HG12	2	8.6
(4,40)	1:B:120:GLY:HA2	1:B:114:ILE:HG13	2	8.6
(4,40)	1:B:120:GLY:HA3	1:B:114:ILE:HG12	2	8.6
(4,40)	1:B:120:GLY:HA3	1:B:114:ILE:HG13	2	8.6
(4,41)	1:A:120:GLY:HA2	1:A:114:ILE:HD11	7	8.45
(4,41)	1:A:120:GLY:HA2	1:A:114:ILE:HD12	7	8.45
(4,41)	1:A:120:GLY:HA2	1:A:114:ILE:HD13	7	8.45
(4,41)	1:A:120:GLY:HA3	1:A:114:ILE:HD11	7	8.45
(4,41)	1:A:120:GLY:HA3	1:A:114:ILE:HD12	7	8.45
(4,41)	1:A:120:GLY:HA3	1:A:114:ILE:HD13	7	8.45
(4,41)	1:B:120:GLY:HA2	1:B:114:ILE:HD11	7	8.45
(4,41)	1:B:120:GLY:HA2	1:B:114:ILE:HD12	7	8.45
(4,41)	1:B:120:GLY:HA2	1:B:114:ILE:HD13	7	8.45
(4,41)	1:B:120:GLY:HA3	1:B:114:ILE:HD11	7	8.45
(4,41)	1:B:120:GLY:HA3	1:B:114:ILE:HD12	7	8.45
(4,41)	1:B:120:GLY:HA3	1:B:114:ILE:HD13	7	8.45
(4,19)	1:A:114:ILE:HG21	1:A:77:VAL:HG21	1	8.45
(4,19)	1:A:114:ILE:HG21	1:A:77:VAL:HG22	1	8.45
(4,19)	1:A:114:ILE:HG21	1:A:77:VAL:HG23	1	8.45
(4,19)	1:A:114:ILE:HG22	1:A:77:VAL:HG21	1	8.45
(4,19)	1:A:114:ILE:HG22	1:A:77:VAL:HG22	1	8.45
(4,19)	1:A:114:ILE:HG22	1:A:77:VAL:HG23	1	8.45
(4,19)	1:A:114:ILE:HG23	1:A:77:VAL:HG21	1	8.45
(4,19)	1:A:114:ILE:HG23	1:A:77:VAL:HG22	1	8.45
(4,19)	1:A:114:ILE:HG23	1:A:77:VAL:HG23	1	8.45
(4,19)	1:B:114:ILE:HG21	1:B:77:VAL:HG21	1	8.45
(4,19)	1:B:114:ILE:HG21	1:B:77:VAL:HG22	1	8.45
(4,19)	1:B:114:ILE:HG21	1:B:77:VAL:HG23	1	8.45
(4,19)	1:B:114:ILE:HG22	1:B:77:VAL:HG21	1	8.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,19)	1:B:114:ILE:HG22	1:B:77:VAL:HG22	1	8.45
(4,19)	1:B:114:ILE:HG22	1:B:77:VAL:HG23	1	8.45
(4,19)	1:B:114:ILE:HG23	1:B:77:VAL:HG21	1	8.45
(4,19)	1:B:114:ILE:HG23	1:B:77:VAL:HG22	1	8.45
(4,19)	1:B:114:ILE:HG23	1:B:77:VAL:HG23	1	8.45
(4,18)	1:A:114:ILE:HG21	1:A:77:VAL:HG21	1	8.45
(4,18)	1:A:114:ILE:HG21	1:A:77:VAL:HG22	1	8.45
(4,18)	1:A:114:ILE:HG21	1:A:77:VAL:HG23	1	8.45
(4,18)	1:A:114:ILE:HG22	1:A:77:VAL:HG21	1	8.45
(4,18)	1:A:114:ILE:HG22	1:A:77:VAL:HG22	1	8.45
(4,18)	1:A:114:ILE:HG22	1:A:77:VAL:HG23	1	8.45
(4,18)	1:A:114:ILE:HG23	1:A:77:VAL:HG21	1	8.45
(4,18)	1:A:114:ILE:HG23	1:A:77:VAL:HG22	1	8.45
(4,18)	1:A:114:ILE:HG23	1:A:77:VAL:HG23	1	8.45
(4,18)	1:B:114:ILE:HG21	1:B:77:VAL:HG21	1	8.45
(4,18)	1:B:114:ILE:HG21	1:B:77:VAL:HG22	1	8.45
(4,18)	1:B:114:ILE:HG21	1:B:77:VAL:HG23	1	8.45
(4,18)	1:B:114:ILE:HG22	1:B:77:VAL:HG21	1	8.45
(4,18)	1:B:114:ILE:HG22	1:B:77:VAL:HG22	1	8.45
(4,18)	1:B:114:ILE:HG22	1:B:77:VAL:HG23	1	8.45
(4,18)	1:B:114:ILE:HG23	1:B:77:VAL:HG21	1	8.45
(4,18)	1:B:114:ILE:HG23	1:B:77:VAL:HG22	1	8.45
(4,18)	1:B:114:ILE:HG23	1:B:77:VAL:HG23	1	8.45
(4,40)	1:A:120:GLY:HA2	1:A:114:ILE:HG12	8	8.26
(4,40)	1:A:120:GLY:HA2	1:A:114:ILE:HG13	8	8.26
(4,40)	1:A:120:GLY:HA3	1:A:114:ILE:HG12	8	8.26
(4,40)	1:A:120:GLY:HA3	1:A:114:ILE:HG13	8	8.26
(4,40)	1:B:120:GLY:HA2	1:B:114:ILE:HG12	8	8.26
(4,40)	1:B:120:GLY:HA2	1:B:114:ILE:HG13	8	8.26
(4,40)	1:B:120:GLY:HA3	1:B:114:ILE:HG12	8	8.26
(4,40)	1:B:120:GLY:HA3	1:B:114:ILE:HG13	8	8.26
(4,50)	1:A:115:SER:H	1:A:120:GLY:HA2	2	8.23
(4,50)	1:A:115:SER:H	1:A:120:GLY:HA3	2	8.23
(4,50)	1:B:115:SER:H	1:B:120:GLY:HA2	2	8.23
(4,50)	1:B:115:SER:H	1:B:120:GLY:HA3	2	8.23
(4,41)	1:A:120:GLY:HA2	1:A:114:ILE:HD11	5	8.16
(4,41)	1:A:120:GLY:HA2	1:A:114:ILE:HD12	5	8.16
(4,41)	1:A:120:GLY:HA2	1:A:114:ILE:HD13	5	8.16
(4,41)	1:A:120:GLY:HA3	1:A:114:ILE:HD11	5	8.16
(4,41)	1:A:120:GLY:HA3	1:A:114:ILE:HD12	5	8.16
(4,41)	1:A:120:GLY:HA3	1:A:114:ILE:HD13	5	8.16
(4,41)	1:B:120:GLY:HA2	1:B:114:ILE:HD11	5	8.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,41)	1:B:120:GLY:HA2	1:B:114:ILE:HD12	5	8.16
(4,41)	1:B:120:GLY:HA2	1:B:114:ILE:HD13	5	8.16
(4,41)	1:B:120:GLY:HA3	1:B:114:ILE:HD11	5	8.16
(4,41)	1:B:120:GLY:HA3	1:B:114:ILE:HD12	5	8.16
(4,41)	1:B:120:GLY:HA3	1:B:114:ILE:HD13	5	8.16
(4,40)	1:A:120:GLY:HA2	1:A:114:ILE:HG12	1	8.11
(4,40)	1:A:120:GLY:HA2	1:A:114:ILE:HG13	1	8.11
(4,40)	1:A:120:GLY:HA3	1:A:114:ILE:HG12	1	8.11
(4,40)	1:A:120:GLY:HA3	1:A:114:ILE:HG13	1	8.11
(4,40)	1:B:120:GLY:HA2	1:B:114:ILE:HG12	1	8.11
(4,40)	1:B:120:GLY:HA2	1:B:114:ILE:HG13	1	8.11
(4,40)	1:B:120:GLY:HA3	1:B:114:ILE:HG12	1	8.11
(4,40)	1:B:120:GLY:HA3	1:B:114:ILE:HG13	1	8.11
(4,50)	1:A:115:SER:H	1:A:120:GLY:HA2	6	8.07
(4,50)	1:A:115:SER:H	1:A:120:GLY:HA3	6	8.07
(4,50)	1:B:115:SER:H	1:B:120:GLY:HA2	6	8.07
(4,50)	1:B:115:SER:H	1:B:120:GLY:HA3	6	8.07
(4,19)	1:A:114:ILE:HG21	1:A:77:VAL:HG21	4	8.0
(4,19)	1:A:114:ILE:HG21	1:A:77:VAL:HG22	4	8.0
(4,19)	1:A:114:ILE:HG21	1:A:77:VAL:HG23	4	8.0
(4,19)	1:A:114:ILE:HG22	1:A:77:VAL:HG21	4	8.0
(4,19)	1:A:114:ILE:HG22	1:A:77:VAL:HG22	4	8.0
(4,19)	1:A:114:ILE:HG22	1:A:77:VAL:HG23	4	8.0
(4,19)	1:A:114:ILE:HG23	1:A:77:VAL:HG21	4	8.0
(4,19)	1:A:114:ILE:HG23	1:A:77:VAL:HG22	4	8.0
(4,19)	1:A:114:ILE:HG23	1:A:77:VAL:HG23	4	8.0
(4,19)	1:B:114:ILE:HG21	1:B:77:VAL:HG21	4	8.0
(4,19)	1:B:114:ILE:HG21	1:B:77:VAL:HG22	4	8.0
(4,19)	1:B:114:ILE:HG21	1:B:77:VAL:HG23	4	8.0
(4,19)	1:B:114:ILE:HG22	1:B:77:VAL:HG21	4	8.0
(4,19)	1:B:114:ILE:HG22	1:B:77:VAL:HG22	4	8.0
(4,19)	1:B:114:ILE:HG22	1:B:77:VAL:HG23	4	8.0
(4,19)	1:B:114:ILE:HG23	1:B:77:VAL:HG21	4	8.0
(4,19)	1:B:114:ILE:HG23	1:B:77:VAL:HG22	4	8.0
(4,19)	1:B:114:ILE:HG23	1:B:77:VAL:HG23	4	8.0
(4,18)	1:A:114:ILE:HG21	1:A:77:VAL:HG21	4	8.0
(4,18)	1:A:114:ILE:HG21	1:A:77:VAL:HG22	4	8.0
(4,18)	1:A:114:ILE:HG21	1:A:77:VAL:HG23	4	8.0
(4,18)	1:A:114:ILE:HG22	1:A:77:VAL:HG21	4	8.0
(4,18)	1:A:114:ILE:HG22	1:A:77:VAL:HG22	4	8.0
(4,18)	1:A:114:ILE:HG22	1:A:77:VAL:HG23	4	8.0
(4,18)	1:A:114:ILE:HG23	1:A:77:VAL:HG21	4	8.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,18)	1:A:114:ILE:HG23	1:A:77:VAL:HG22	4	8.0
(4,18)	1:A:114:ILE:HG23	1:A:77:VAL:HG23	4	8.0
(4,18)	1:B:114:ILE:HG21	1:B:77:VAL:HG21	4	8.0
(4,18)	1:B:114:ILE:HG21	1:B:77:VAL:HG22	4	8.0
(4,18)	1:B:114:ILE:HG21	1:B:77:VAL:HG23	4	8.0
(4,18)	1:B:114:ILE:HG22	1:B:77:VAL:HG21	4	8.0
(4,18)	1:B:114:ILE:HG22	1:B:77:VAL:HG22	4	8.0
(4,18)	1:B:114:ILE:HG22	1:B:77:VAL:HG23	4	8.0
(4,18)	1:B:114:ILE:HG23	1:B:77:VAL:HG21	4	8.0
(4,18)	1:B:114:ILE:HG23	1:B:77:VAL:HG22	4	8.0
(4,18)	1:B:114:ILE:HG23	1:B:77:VAL:HG23	4	8.0
(4,26)	1:A:115:SER:HB2	1:A:119:HIS:HD2	2	7.98
(4,26)	1:B:115:SER:HB2	1:B:119:HIS:HD2	2	7.98
(4,26)	1:A:115:SER:HB2	1:A:119:HIS:HD2	7	7.91
(4,26)	1:B:115:SER:HB2	1:B:119:HIS:HD2	7	7.91
(4,50)	1:A:115:SER:H	1:A:120:GLY:HA2	8	7.89
(4,50)	1:A:115:SER:H	1:A:120:GLY:HA3	8	7.89
(4,50)	1:B:115:SER:H	1:B:120:GLY:HA2	8	7.89
(4,50)	1:B:115:SER:H	1:B:120:GLY:HA3	8	7.89
(4,50)	1:A:115:SER:H	1:A:120:GLY:HA2	3	7.85
(4,50)	1:A:115:SER:H	1:A:120:GLY:HA3	3	7.85
(4,50)	1:B:115:SER:H	1:B:120:GLY:HA2	3	7.85
(4,50)	1:B:115:SER:H	1:B:120:GLY:HA3	3	7.85
(4,41)	1:A:120:GLY:HA2	1:A:114:ILE:HD11	4	7.81
(4,41)	1:A:120:GLY:HA2	1:A:114:ILE:HD12	4	7.81
(4,41)	1:A:120:GLY:HA2	1:A:114:ILE:HD13	4	7.81
(4,41)	1:A:120:GLY:HA3	1:A:114:ILE:HD11	4	7.81
(4,41)	1:A:120:GLY:HA3	1:A:114:ILE:HD12	4	7.81
(4,41)	1:A:120:GLY:HA3	1:A:114:ILE:HD13	4	7.81
(4,41)	1:B:120:GLY:HA2	1:B:114:ILE:HD11	4	7.81
(4,41)	1:B:120:GLY:HA2	1:B:114:ILE:HD12	4	7.81
(4,41)	1:B:120:GLY:HA2	1:B:114:ILE:HD13	4	7.81
(4,41)	1:B:120:GLY:HA3	1:B:114:ILE:HD11	4	7.81
(4,41)	1:B:120:GLY:HA3	1:B:114:ILE:HD12	4	7.81
(4,41)	1:B:120:GLY:HA3	1:B:114:ILE:HD13	4	7.81
(4,41)	1:A:120:GLY:HA2	1:A:114:ILE:HD11	6	7.7
(4,41)	1:A:120:GLY:HA2	1:A:114:ILE:HD12	6	7.7
(4,41)	1:A:120:GLY:HA2	1:A:114:ILE:HD13	6	7.7
(4,41)	1:A:120:GLY:HA3	1:A:114:ILE:HD11	6	7.7
(4,41)	1:A:120:GLY:HA3	1:A:114:ILE:HD12	6	7.7
(4,41)	1:A:120:GLY:HA3	1:A:114:ILE:HD13	6	7.7
(4,41)	1:B:120:GLY:HA2	1:B:114:ILE:HD11	6	7.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,41)	1:B:120:GLY:HA2	1:B:114:ILE:HD12	6	7.7
(4,41)	1:B:120:GLY:HA2	1:B:114:ILE:HD13	6	7.7
(4,41)	1:B:120:GLY:HA3	1:B:114:ILE:HD11	6	7.7
(4,41)	1:B:120:GLY:HA3	1:B:114:ILE:HD12	6	7.7
(4,41)	1:B:120:GLY:HA3	1:B:114:ILE:HD13	6	7.7
(4,50)	1:A:115:SER:H	1:A:120:GLY:HA2	7	7.69
(4,50)	1:A:115:SER:H	1:A:120:GLY:HA3	7	7.69
(4,50)	1:B:115:SER:H	1:B:120:GLY:HA2	7	7.69
(4,50)	1:B:115:SER:H	1:B:120:GLY:HA3	7	7.69
(5,3)	1:B:82:LYS:H	1:B:66:SER:H	5	7.65
(5,3)	1:A:82:LYS:H	1:A:66:SER:H	5	7.65
(4,36)	1:A:119:HIS:HB3	1:A:115:SER:HB2	4	7.63
(4,36)	1:B:119:HIS:HB3	1:B:115:SER:HB2	4	7.63
(4,35)	1:A:119:HIS:HB3	1:A:115:SER:HB2	4	7.63
(4,35)	1:B:119:HIS:HB3	1:B:115:SER:HB2	4	7.63
(4,25)	1:A:115:SER:HB2	1:A:119:HIS:HB3	4	7.63
(4,25)	1:B:115:SER:HB2	1:B:119:HIS:HB3	4	7.63
(5,4)	1:B:82:LYS:H	1:B:66:SER:HA	7	7.62
(5,4)	1:A:82:LYS:H	1:A:66:SER:HA	7	7.62
(5,4)	1:B:82:LYS:H	1:B:66:SER:HA	2	7.6
(5,4)	1:A:82:LYS:H	1:A:66:SER:HA	2	7.6
(4,41)	1:A:120:GLY:HA2	1:A:114:ILE:HD11	3	7.54
(4,41)	1:A:120:GLY:HA2	1:A:114:ILE:HD12	3	7.54
(4,41)	1:A:120:GLY:HA2	1:A:114:ILE:HD13	3	7.54
(4,41)	1:A:120:GLY:HA3	1:A:114:ILE:HD11	3	7.54
(4,41)	1:A:120:GLY:HA3	1:A:114:ILE:HD12	3	7.54
(4,41)	1:A:120:GLY:HA3	1:A:114:ILE:HD13	3	7.54
(4,41)	1:B:120:GLY:HA2	1:B:114:ILE:HD11	3	7.54
(4,41)	1:B:120:GLY:HA2	1:B:114:ILE:HD12	3	7.54
(4,41)	1:B:120:GLY:HA2	1:B:114:ILE:HD13	3	7.54
(4,41)	1:B:120:GLY:HA3	1:B:114:ILE:HD11	3	7.54
(4,41)	1:B:120:GLY:HA3	1:B:114:ILE:HD12	3	7.54
(4,41)	1:B:120:GLY:HA3	1:B:114:ILE:HD13	3	7.54
(4,41)	1:A:120:GLY:HA2	1:A:114:ILE:HD11	2	7.4
(4,41)	1:A:120:GLY:HA2	1:A:114:ILE:HD12	2	7.4
(4,41)	1:A:120:GLY:HA2	1:A:114:ILE:HD13	2	7.4
(4,41)	1:A:120:GLY:HA3	1:A:114:ILE:HD11	2	7.4
(4,41)	1:A:120:GLY:HA3	1:A:114:ILE:HD12	2	7.4
(4,41)	1:A:120:GLY:HA3	1:A:114:ILE:HD13	2	7.4
(4,41)	1:B:120:GLY:HA2	1:B:114:ILE:HD11	2	7.4
(4,41)	1:B:120:GLY:HA2	1:B:114:ILE:HD12	2	7.4
(4,41)	1:B:120:GLY:HA2	1:B:114:ILE:HD13	2	7.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,41)	1:B:120:GLY:HA3	1:B:114:ILE:HD11	2	7.4
(4,41)	1:B:120:GLY:HA3	1:B:114:ILE:HD12	2	7.4
(4,41)	1:B:120:GLY:HA3	1:B:114:ILE:HD13	2	7.4
(4,50)	1:A:115:SER:H	1:A:120:GLY:HA2	1	7.38
(4,50)	1:A:115:SER:H	1:A:120:GLY:HA3	1	7.38
(4,50)	1:B:115:SER:H	1:B:120:GLY:HA2	1	7.38
(4,50)	1:B:115:SER:H	1:B:120:GLY:HA3	1	7.38
(4,19)	1:A:114:ILE:HG21	1:A:77:VAL:HG21	2	7.35
(4,19)	1:A:114:ILE:HG21	1:A:77:VAL:HG22	2	7.35
(4,19)	1:A:114:ILE:HG21	1:A:77:VAL:HG23	2	7.35
(4,19)	1:A:114:ILE:HG22	1:A:77:VAL:HG21	2	7.35
(4,19)	1:A:114:ILE:HG22	1:A:77:VAL:HG22	2	7.35
(4,19)	1:A:114:ILE:HG22	1:A:77:VAL:HG23	2	7.35
(4,19)	1:A:114:ILE:HG23	1:A:77:VAL:HG21	2	7.35
(4,19)	1:A:114:ILE:HG23	1:A:77:VAL:HG22	2	7.35
(4,19)	1:A:114:ILE:HG23	1:A:77:VAL:HG23	2	7.35
(4,19)	1:B:114:ILE:HG21	1:B:77:VAL:HG21	2	7.35
(4,19)	1:B:114:ILE:HG21	1:B:77:VAL:HG22	2	7.35
(4,19)	1:B:114:ILE:HG21	1:B:77:VAL:HG23	2	7.35
(4,19)	1:B:114:ILE:HG22	1:B:77:VAL:HG21	2	7.35
(4,19)	1:B:114:ILE:HG22	1:B:77:VAL:HG22	2	7.35
(4,19)	1:B:114:ILE:HG22	1:B:77:VAL:HG23	2	7.35
(4,19)	1:B:114:ILE:HG23	1:B:77:VAL:HG21	2	7.35
(4,19)	1:B:114:ILE:HG23	1:B:77:VAL:HG22	2	7.35
(4,19)	1:B:114:ILE:HG23	1:B:77:VAL:HG23	2	7.35
(4,18)	1:A:114:ILE:HG21	1:A:77:VAL:HG21	2	7.35
(4,18)	1:A:114:ILE:HG21	1:A:77:VAL:HG22	2	7.35
(4,18)	1:A:114:ILE:HG21	1:A:77:VAL:HG23	2	7.35
(4,18)	1:A:114:ILE:HG22	1:A:77:VAL:HG21	2	7.35
(4,18)	1:A:114:ILE:HG22	1:A:77:VAL:HG22	2	7.35
(4,18)	1:A:114:ILE:HG22	1:A:77:VAL:HG23	2	7.35
(4,18)	1:A:114:ILE:HG23	1:A:77:VAL:HG21	2	7.35
(4,18)	1:A:114:ILE:HG23	1:A:77:VAL:HG22	2	7.35
(4,18)	1:A:114:ILE:HG23	1:A:77:VAL:HG23	2	7.35
(4,18)	1:B:114:ILE:HG21	1:B:77:VAL:HG21	2	7.35
(4,18)	1:B:114:ILE:HG21	1:B:77:VAL:HG22	2	7.35
(4,18)	1:B:114:ILE:HG21	1:B:77:VAL:HG23	2	7.35
(4,18)	1:B:114:ILE:HG22	1:B:77:VAL:HG21	2	7.35
(4,18)	1:B:114:ILE:HG22	1:B:77:VAL:HG22	2	7.35
(4,18)	1:B:114:ILE:HG22	1:B:77:VAL:HG23	2	7.35
(4,18)	1:B:114:ILE:HG23	1:B:77:VAL:HG21	2	7.35
(4,18)	1:B:114:ILE:HG23	1:B:77:VAL:HG22	2	7.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,18)	1:B:114:ILE:HG23	1:B:77:VAL:HG23	2	7.35
(4,26)	1:A:115:SER:HB2	1:A:119:HIS:HD2	6	7.32
(4,26)	1:B:115:SER:HB2	1:B:119:HIS:HD2	6	7.32
(5,4)	1:B:82:LYS:H	1:B:66:SER:HA	5	7.16
(5,4)	1:A:82:LYS:H	1:A:66:SER:HA	5	7.16
(4,41)	1:A:120:GLY:HA2	1:A:114:ILE:HD11	1	7.16
(4,41)	1:A:120:GLY:HA2	1:A:114:ILE:HD12	1	7.16
(4,41)	1:A:120:GLY:HA2	1:A:114:ILE:HD13	1	7.16
(4,41)	1:A:120:GLY:HA3	1:A:114:ILE:HD11	1	7.16
(4,41)	1:A:120:GLY:HA3	1:A:114:ILE:HD12	1	7.16
(4,41)	1:A:120:GLY:HA3	1:A:114:ILE:HD13	1	7.16
(4,41)	1:B:120:GLY:HA2	1:B:114:ILE:HD11	1	7.16
(4,41)	1:B:120:GLY:HA2	1:B:114:ILE:HD12	1	7.16
(4,41)	1:B:120:GLY:HA2	1:B:114:ILE:HD13	1	7.16
(4,41)	1:B:120:GLY:HA3	1:B:114:ILE:HD11	1	7.16
(4,41)	1:B:120:GLY:HA3	1:B:114:ILE:HD12	1	7.16
(4,41)	1:B:120:GLY:HA3	1:B:114:ILE:HD13	1	7.16
(5,4)	1:B:82:LYS:H	1:B:66:SER:HA	6	7.07
(5,4)	1:A:82:LYS:H	1:A:66:SER:HA	6	7.07
(5,3)	1:B:82:LYS:H	1:B:66:SER:H	2	7.05
(5,3)	1:A:82:LYS:H	1:A:66:SER:H	2	7.05
(4,41)	1:A:120:GLY:HA2	1:A:114:ILE:HD11	8	7.01
(4,41)	1:A:120:GLY:HA2	1:A:114:ILE:HD12	8	7.01
(4,41)	1:A:120:GLY:HA2	1:A:114:ILE:HD13	8	7.01
(4,41)	1:A:120:GLY:HA3	1:A:114:ILE:HD11	8	7.01
(4,41)	1:A:120:GLY:HA3	1:A:114:ILE:HD12	8	7.01
(4,41)	1:A:120:GLY:HA3	1:A:114:ILE:HD13	8	7.01
(4,41)	1:B:120:GLY:HA2	1:B:114:ILE:HD11	8	7.01
(4,41)	1:B:120:GLY:HA2	1:B:114:ILE:HD12	8	7.01
(4,41)	1:B:120:GLY:HA2	1:B:114:ILE:HD13	8	7.01
(4,41)	1:B:120:GLY:HA3	1:B:114:ILE:HD11	8	7.01
(4,41)	1:B:120:GLY:HA3	1:B:114:ILE:HD12	8	7.01
(4,41)	1:B:120:GLY:HA3	1:B:114:ILE:HD13	8	7.01
(5,4)	1:B:82:LYS:H	1:B:66:SER:HA	1	7.0
(5,4)	1:A:82:LYS:H	1:A:66:SER:HA	1	7.0
(5,3)	1:B:82:LYS:H	1:B:66:SER:H	1	6.61
(5,3)	1:A:82:LYS:H	1:A:66:SER:H	1	6.61
(4,26)	1:A:115:SER:HB2	1:A:119:HIS:HD2	8	6.57
(4,26)	1:B:115:SER:HB2	1:B:119:HIS:HD2	8	6.57
(5,1)	1:B:82:LYS:HE2	1:B:67:GLU:HA	6	6.48
(5,1)	1:B:82:LYS:HE3	1:B:67:GLU:HA	6	6.48
(5,1)	1:A:82:LYS:HE2	1:A:67:GLU:HA	6	6.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,1)	1:A:82:LYS:HE3	1:A:67:GLU:HA	6	6.48
(4,26)	1:A:115:SER:HB2	1:A:119:HIS:HD2	1	6.27
(4,26)	1:B:115:SER:HB2	1:B:119:HIS:HD2	1	6.27
(5,3)	1:B:82:LYS:H	1:B:66:SER:H	8	6.24
(5,3)	1:A:82:LYS:H	1:A:66:SER:H	8	6.24
(4,34)	1:A:119:HIS:HB2	1:A:115:SER:HB2	1	6.23
(4,34)	1:B:119:HIS:HB2	1:B:115:SER:HB2	1	6.23
(4,43)	1:A:120:GLY:HA2	1:A:114:ILE:HG21	5	6.18
(4,43)	1:A:120:GLY:HA2	1:A:114:ILE:HG22	5	6.18
(4,43)	1:A:120:GLY:HA2	1:A:114:ILE:HG23	5	6.18
(4,43)	1:A:120:GLY:HA3	1:A:114:ILE:HG21	5	6.18
(4,43)	1:A:120:GLY:HA3	1:A:114:ILE:HG22	5	6.18
(4,43)	1:A:120:GLY:HA3	1:A:114:ILE:HG23	5	6.18
(4,43)	1:B:120:GLY:HA2	1:B:114:ILE:HG21	5	6.18
(4,43)	1:B:120:GLY:HA2	1:B:114:ILE:HG22	5	6.18
(4,43)	1:B:120:GLY:HA2	1:B:114:ILE:HG23	5	6.18
(4,43)	1:B:120:GLY:HA3	1:B:114:ILE:HG21	5	6.18
(4,43)	1:B:120:GLY:HA3	1:B:114:ILE:HG22	5	6.18
(4,43)	1:B:120:GLY:HA3	1:B:114:ILE:HG23	5	6.18
(4,42)	1:A:120:GLY:HA2	1:A:114:ILE:HG21	5	6.18
(4,42)	1:A:120:GLY:HA2	1:A:114:ILE:HG22	5	6.18
(4,42)	1:A:120:GLY:HA2	1:A:114:ILE:HG23	5	6.18
(4,42)	1:A:120:GLY:HA3	1:A:114:ILE:HG21	5	6.18
(4,42)	1:A:120:GLY:HA3	1:A:114:ILE:HG22	5	6.18
(4,42)	1:A:120:GLY:HA3	1:A:114:ILE:HG23	5	6.18
(4,42)	1:B:120:GLY:HA2	1:B:114:ILE:HG21	5	6.18
(4,42)	1:B:120:GLY:HA2	1:B:114:ILE:HG22	5	6.18
(4,42)	1:B:120:GLY:HA2	1:B:114:ILE:HG23	5	6.18
(4,42)	1:B:120:GLY:HA3	1:B:114:ILE:HG21	5	6.18
(4,42)	1:B:120:GLY:HA3	1:B:114:ILE:HG22	5	6.18
(4,42)	1:B:120:GLY:HA3	1:B:114:ILE:HG23	5	6.18
(4,38)	1:A:120:GLY:HA2	1:A:114:ILE:HG21	5	6.18
(4,38)	1:A:120:GLY:HA2	1:A:114:ILE:HG22	5	6.18
(4,38)	1:A:120:GLY:HA2	1:A:114:ILE:HG23	5	6.18
(4,38)	1:A:120:GLY:HA3	1:A:114:ILE:HG21	5	6.18
(4,38)	1:A:120:GLY:HA3	1:A:114:ILE:HG22	5	6.18
(4,38)	1:A:120:GLY:HA3	1:A:114:ILE:HG23	5	6.18
(4,38)	1:B:120:GLY:HA2	1:B:114:ILE:HG21	5	6.18
(4,38)	1:B:120:GLY:HA2	1:B:114:ILE:HG22	5	6.18
(4,38)	1:B:120:GLY:HA2	1:B:114:ILE:HG23	5	6.18
(4,38)	1:B:120:GLY:HA3	1:B:114:ILE:HG21	5	6.18
(4,38)	1:B:120:GLY:HA3	1:B:114:ILE:HG22	5	6.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,38)	1:B:120:GLY:HA3	1:B:114:ILE:HG23	5	6.18
(4,43)	1:A:120:GLY:HA2	1:A:114:ILE:HG21	7	6.14
(4,43)	1:A:120:GLY:HA2	1:A:114:ILE:HG22	7	6.14
(4,43)	1:A:120:GLY:HA2	1:A:114:ILE:HG23	7	6.14
(4,43)	1:A:120:GLY:HA3	1:A:114:ILE:HG21	7	6.14
(4,43)	1:A:120:GLY:HA3	1:A:114:ILE:HG22	7	6.14
(4,43)	1:A:120:GLY:HA3	1:A:114:ILE:HG23	7	6.14
(4,43)	1:B:120:GLY:HA2	1:B:114:ILE:HG21	7	6.14
(4,43)	1:B:120:GLY:HA2	1:B:114:ILE:HG22	7	6.14
(4,43)	1:B:120:GLY:HA2	1:B:114:ILE:HG23	7	6.14
(4,43)	1:B:120:GLY:HA3	1:B:114:ILE:HG21	7	6.14
(4,43)	1:B:120:GLY:HA3	1:B:114:ILE:HG22	7	6.14
(4,43)	1:B:120:GLY:HA3	1:B:114:ILE:HG23	7	6.14
(4,42)	1:A:120:GLY:HA2	1:A:114:ILE:HG21	7	6.14
(4,42)	1:A:120:GLY:HA2	1:A:114:ILE:HG22	7	6.14
(4,42)	1:A:120:GLY:HA2	1:A:114:ILE:HG23	7	6.14
(4,42)	1:A:120:GLY:HA3	1:A:114:ILE:HG21	7	6.14
(4,42)	1:A:120:GLY:HA3	1:A:114:ILE:HG22	7	6.14
(4,42)	1:A:120:GLY:HA3	1:A:114:ILE:HG23	7	6.14
(4,42)	1:B:120:GLY:HA2	1:B:114:ILE:HG21	7	6.14
(4,42)	1:B:120:GLY:HA2	1:B:114:ILE:HG22	7	6.14
(4,42)	1:B:120:GLY:HA2	1:B:114:ILE:HG23	7	6.14
(4,42)	1:B:120:GLY:HA3	1:B:114:ILE:HG21	7	6.14
(4,42)	1:B:120:GLY:HA3	1:B:114:ILE:HG22	7	6.14
(4,42)	1:B:120:GLY:HA3	1:B:114:ILE:HG23	7	6.14
(4,38)	1:A:120:GLY:HA2	1:A:114:ILE:HG21	7	6.14
(4,38)	1:A:120:GLY:HA2	1:A:114:ILE:HG22	7	6.14
(4,38)	1:A:120:GLY:HA2	1:A:114:ILE:HG23	7	6.14
(4,38)	1:A:120:GLY:HA3	1:A:114:ILE:HG21	7	6.14
(4,38)	1:A:120:GLY:HA3	1:A:114:ILE:HG22	7	6.14
(4,38)	1:A:120:GLY:HA3	1:A:114:ILE:HG23	7	6.14
(4,38)	1:B:120:GLY:HA2	1:B:114:ILE:HG21	7	6.14
(4,38)	1:B:120:GLY:HA2	1:B:114:ILE:HG22	7	6.14
(4,38)	1:B:120:GLY:HA2	1:B:114:ILE:HG23	7	6.14
(4,38)	1:B:120:GLY:HA3	1:B:114:ILE:HG21	7	6.14
(4,38)	1:B:120:GLY:HA3	1:B:114:ILE:HG22	7	6.14
(4,38)	1:B:120:GLY:HA3	1:B:114:ILE:HG23	7	6.14
(4,43)	1:A:120:GLY:HA2	1:A:114:ILE:HG21	4	6.09
(4,43)	1:A:120:GLY:HA2	1:A:114:ILE:HG22	4	6.09
(4,43)	1:A:120:GLY:HA2	1:A:114:ILE:HG23	4	6.09
(4,43)	1:A:120:GLY:HA3	1:A:114:ILE:HG21	4	6.09
(4,43)	1:A:120:GLY:HA3	1:A:114:ILE:HG22	4	6.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,43)	1:A:120:GLY:HA3	1:A:114:ILE:HG23	4	6.09
(4,43)	1:B:120:GLY:HA2	1:B:114:ILE:HG21	4	6.09
(4,43)	1:B:120:GLY:HA2	1:B:114:ILE:HG22	4	6.09
(4,43)	1:B:120:GLY:HA2	1:B:114:ILE:HG23	4	6.09
(4,43)	1:B:120:GLY:HA3	1:B:114:ILE:HG21	4	6.09
(4,43)	1:B:120:GLY:HA3	1:B:114:ILE:HG22	4	6.09
(4,43)	1:B:120:GLY:HA3	1:B:114:ILE:HG23	4	6.09
(4,42)	1:A:120:GLY:HA2	1:A:114:ILE:HG21	4	6.09
(4,42)	1:A:120:GLY:HA2	1:A:114:ILE:HG22	4	6.09
(4,42)	1:A:120:GLY:HA2	1:A:114:ILE:HG23	4	6.09
(4,42)	1:A:120:GLY:HA3	1:A:114:ILE:HG21	4	6.09
(4,42)	1:A:120:GLY:HA3	1:A:114:ILE:HG22	4	6.09
(4,42)	1:A:120:GLY:HA3	1:A:114:ILE:HG23	4	6.09
(4,42)	1:B:120:GLY:HA2	1:B:114:ILE:HG21	4	6.09
(4,42)	1:B:120:GLY:HA2	1:B:114:ILE:HG22	4	6.09
(4,42)	1:B:120:GLY:HA2	1:B:114:ILE:HG23	4	6.09
(4,42)	1:B:120:GLY:HA3	1:B:114:ILE:HG21	4	6.09
(4,42)	1:B:120:GLY:HA3	1:B:114:ILE:HG22	4	6.09
(4,42)	1:B:120:GLY:HA3	1:B:114:ILE:HG23	4	6.09
(4,38)	1:A:120:GLY:HA2	1:A:114:ILE:HG21	4	6.09
(4,38)	1:A:120:GLY:HA2	1:A:114:ILE:HG22	4	6.09
(4,38)	1:A:120:GLY:HA2	1:A:114:ILE:HG23	4	6.09
(4,38)	1:A:120:GLY:HA3	1:A:114:ILE:HG21	4	6.09
(4,38)	1:A:120:GLY:HA3	1:A:114:ILE:HG22	4	6.09
(4,38)	1:A:120:GLY:HA3	1:A:114:ILE:HG23	4	6.09
(4,38)	1:B:120:GLY:HA2	1:B:114:ILE:HG21	4	6.09
(4,38)	1:B:120:GLY:HA2	1:B:114:ILE:HG22	4	6.09
(4,38)	1:B:120:GLY:HA2	1:B:114:ILE:HG23	4	6.09
(4,38)	1:B:120:GLY:HA3	1:B:114:ILE:HG21	4	6.09
(4,38)	1:B:120:GLY:HA3	1:B:114:ILE:HG22	4	6.09
(4,38)	1:B:120:GLY:HA3	1:B:114:ILE:HG23	4	6.09
(4,43)	1:A:120:GLY:HA2	1:A:114:ILE:HG21	6	6.04
(4,43)	1:A:120:GLY:HA2	1:A:114:ILE:HG22	6	6.04
(4,43)	1:A:120:GLY:HA2	1:A:114:ILE:HG23	6	6.04
(4,43)	1:A:120:GLY:HA3	1:A:114:ILE:HG21	6	6.04
(4,43)	1:A:120:GLY:HA3	1:A:114:ILE:HG22	6	6.04
(4,43)	1:A:120:GLY:HA3	1:A:114:ILE:HG23	6	6.04
(4,43)	1:B:120:GLY:HA2	1:B:114:ILE:HG21	6	6.04
(4,43)	1:B:120:GLY:HA2	1:B:114:ILE:HG22	6	6.04
(4,43)	1:B:120:GLY:HA2	1:B:114:ILE:HG23	6	6.04
(4,43)	1:B:120:GLY:HA3	1:B:114:ILE:HG21	6	6.04
(4,43)	1:B:120:GLY:HA3	1:B:114:ILE:HG22	6	6.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,43)	1:B:120:GLY:HA3	1:B:114:ILE:HG23	6	6.04
(4,42)	1:A:120:GLY:HA2	1:A:114:ILE:HG21	6	6.04
(4,42)	1:A:120:GLY:HA2	1:A:114:ILE:HG22	6	6.04
(4,42)	1:A:120:GLY:HA2	1:A:114:ILE:HG23	6	6.04
(4,42)	1:A:120:GLY:HA3	1:A:114:ILE:HG21	6	6.04
(4,42)	1:A:120:GLY:HA3	1:A:114:ILE:HG22	6	6.04
(4,42)	1:A:120:GLY:HA3	1:A:114:ILE:HG23	6	6.04
(4,42)	1:B:120:GLY:HA2	1:B:114:ILE:HG21	6	6.04
(4,42)	1:B:120:GLY:HA2	1:B:114:ILE:HG22	6	6.04
(4,42)	1:B:120:GLY:HA2	1:B:114:ILE:HG23	6	6.04
(4,42)	1:B:120:GLY:HA3	1:B:114:ILE:HG21	6	6.04
(4,42)	1:B:120:GLY:HA3	1:B:114:ILE:HG22	6	6.04
(4,42)	1:B:120:GLY:HA3	1:B:114:ILE:HG23	6	6.04
(4,38)	1:A:120:GLY:HA2	1:A:114:ILE:HG21	6	6.04
(4,38)	1:A:120:GLY:HA2	1:A:114:ILE:HG22	6	6.04
(4,38)	1:A:120:GLY:HA2	1:A:114:ILE:HG23	6	6.04
(4,38)	1:A:120:GLY:HA3	1:A:114:ILE:HG21	6	6.04
(4,38)	1:A:120:GLY:HA3	1:A:114:ILE:HG22	6	6.04
(4,38)	1:A:120:GLY:HA3	1:A:114:ILE:HG23	6	6.04
(4,38)	1:B:120:GLY:HA2	1:B:114:ILE:HG21	6	6.04
(4,38)	1:B:120:GLY:HA2	1:B:114:ILE:HG22	6	6.04
(4,38)	1:B:120:GLY:HA2	1:B:114:ILE:HG23	6	6.04
(4,38)	1:B:120:GLY:HA3	1:B:114:ILE:HG21	6	6.04
(4,38)	1:B:120:GLY:HA3	1:B:114:ILE:HG22	6	6.04
(4,38)	1:B:120:GLY:HA3	1:B:114:ILE:HG23	6	6.04
(4,23)	1:A:114:ILE:HG21	1:A:119:HIS:HA	6	6.04
(4,23)	1:A:114:ILE:HG22	1:A:119:HIS:HA	6	6.04
(4,23)	1:A:114:ILE:HG23	1:A:119:HIS:HA	6	6.04
(4,23)	1:B:114:ILE:HG21	1:B:119:HIS:HA	6	6.04
(4,23)	1:B:114:ILE:HG22	1:B:119:HIS:HA	6	6.04
(4,23)	1:B:114:ILE:HG23	1:B:119:HIS:HA	6	6.04
(4,36)	1:A:119:HIS:HB3	1:A:115:SER:HB2	7	5.96
(4,36)	1:B:119:HIS:HB3	1:B:115:SER:HB2	7	5.96
(4,35)	1:A:119:HIS:HB3	1:A:115:SER:HB2	7	5.96
(4,35)	1:B:119:HIS:HB3	1:B:115:SER:HB2	7	5.96
(4,25)	1:A:115:SER:HB2	1:A:119:HIS:HB3	7	5.96
(4,25)	1:B:115:SER:HB2	1:B:119:HIS:HB3	7	5.96
(5,3)	1:B:82:LYS:H	1:B:66:SER:H	4	5.91
(5,3)	1:A:82:LYS:H	1:A:66:SER:H	4	5.91
(4,43)	1:A:120:GLY:HA2	1:A:114:ILE:HG21	3	5.65
(4,43)	1:A:120:GLY:HA2	1:A:114:ILE:HG22	3	5.65
(4,43)	1:A:120:GLY:HA2	1:A:114:ILE:HG23	3	5.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,43)	1:A:120:GLY:HA3	1:A:114:ILE:HG21	3	5.65
(4,43)	1:A:120:GLY:HA3	1:A:114:ILE:HG22	3	5.65
(4,43)	1:A:120:GLY:HA3	1:A:114:ILE:HG23	3	5.65
(4,43)	1:B:120:GLY:HA2	1:B:114:ILE:HG21	3	5.65
(4,43)	1:B:120:GLY:HA2	1:B:114:ILE:HG22	3	5.65
(4,43)	1:B:120:GLY:HA2	1:B:114:ILE:HG23	3	5.65
(4,43)	1:B:120:GLY:HA3	1:B:114:ILE:HG21	3	5.65
(4,43)	1:B:120:GLY:HA3	1:B:114:ILE:HG22	3	5.65
(4,43)	1:B:120:GLY:HA3	1:B:114:ILE:HG23	3	5.65
(4,42)	1:A:120:GLY:HA2	1:A:114:ILE:HG21	3	5.65
(4,42)	1:A:120:GLY:HA2	1:A:114:ILE:HG22	3	5.65
(4,42)	1:A:120:GLY:HA2	1:A:114:ILE:HG23	3	5.65
(4,42)	1:A:120:GLY:HA3	1:A:114:ILE:HG21	3	5.65
(4,42)	1:A:120:GLY:HA3	1:A:114:ILE:HG22	3	5.65
(4,42)	1:A:120:GLY:HA3	1:A:114:ILE:HG23	3	5.65
(4,42)	1:B:120:GLY:HA2	1:B:114:ILE:HG21	3	5.65
(4,42)	1:B:120:GLY:HA2	1:B:114:ILE:HG22	3	5.65
(4,42)	1:B:120:GLY:HA2	1:B:114:ILE:HG23	3	5.65
(4,42)	1:B:120:GLY:HA3	1:B:114:ILE:HG21	3	5.65
(4,42)	1:B:120:GLY:HA3	1:B:114:ILE:HG22	3	5.65
(4,42)	1:B:120:GLY:HA3	1:B:114:ILE:HG23	3	5.65
(4,38)	1:A:120:GLY:HA2	1:A:114:ILE:HG21	3	5.65
(4,38)	1:A:120:GLY:HA2	1:A:114:ILE:HG22	3	5.65
(4,38)	1:A:120:GLY:HA2	1:A:114:ILE:HG23	3	5.65
(4,38)	1:A:120:GLY:HA3	1:A:114:ILE:HG21	3	5.65
(4,38)	1:A:120:GLY:HA3	1:A:114:ILE:HG22	3	5.65
(4,38)	1:A:120:GLY:HA3	1:A:114:ILE:HG23	3	5.65
(4,38)	1:B:120:GLY:HA2	1:B:114:ILE:HG21	3	5.65
(4,38)	1:B:120:GLY:HA2	1:B:114:ILE:HG22	3	5.65
(4,38)	1:B:120:GLY:HA2	1:B:114:ILE:HG23	3	5.65
(4,38)	1:B:120:GLY:HA3	1:B:114:ILE:HG21	3	5.65
(4,38)	1:B:120:GLY:HA3	1:B:114:ILE:HG22	3	5.65
(4,38)	1:B:120:GLY:HA3	1:B:114:ILE:HG23	3	5.65
(4,26)	1:A:115:SER:HB2	1:A:119:HIS:HD2	3	5.63
(4,26)	1:B:115:SER:HB2	1:B:119:HIS:HD2	3	5.63
(4,43)	1:A:120:GLY:HA2	1:A:114:ILE:HG21	2	5.57
(4,43)	1:A:120:GLY:HA2	1:A:114:ILE:HG22	2	5.57
(4,43)	1:A:120:GLY:HA2	1:A:114:ILE:HG23	2	5.57
(4,43)	1:A:120:GLY:HA3	1:A:114:ILE:HG21	2	5.57
(4,43)	1:A:120:GLY:HA3	1:A:114:ILE:HG22	2	5.57
(4,43)	1:A:120:GLY:HA3	1:A:114:ILE:HG23	2	5.57
(4,43)	1:B:120:GLY:HA2	1:B:114:ILE:HG21	2	5.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,43)	1:B:120:GLY:HA2	1:B:114:ILE:HG22	2	5.57
(4,43)	1:B:120:GLY:HA2	1:B:114:ILE:HG23	2	5.57
(4,43)	1:B:120:GLY:HA3	1:B:114:ILE:HG21	2	5.57
(4,43)	1:B:120:GLY:HA3	1:B:114:ILE:HG22	2	5.57
(4,43)	1:B:120:GLY:HA3	1:B:114:ILE:HG23	2	5.57
(4,42)	1:A:120:GLY:HA2	1:A:114:ILE:HG21	2	5.57
(4,42)	1:A:120:GLY:HA2	1:A:114:ILE:HG22	2	5.57
(4,42)	1:A:120:GLY:HA2	1:A:114:ILE:HG23	2	5.57
(4,42)	1:A:120:GLY:HA3	1:A:114:ILE:HG21	2	5.57
(4,42)	1:A:120:GLY:HA3	1:A:114:ILE:HG22	2	5.57
(4,42)	1:A:120:GLY:HA3	1:A:114:ILE:HG23	2	5.57
(4,42)	1:B:120:GLY:HA2	1:B:114:ILE:HG21	2	5.57
(4,42)	1:B:120:GLY:HA2	1:B:114:ILE:HG22	2	5.57
(4,42)	1:B:120:GLY:HA2	1:B:114:ILE:HG23	2	5.57
(4,42)	1:B:120:GLY:HA3	1:B:114:ILE:HG21	2	5.57
(4,42)	1:B:120:GLY:HA3	1:B:114:ILE:HG22	2	5.57
(4,42)	1:B:120:GLY:HA3	1:B:114:ILE:HG23	2	5.57
(4,38)	1:A:120:GLY:HA2	1:A:114:ILE:HG21	2	5.57
(4,38)	1:A:120:GLY:HA2	1:A:114:ILE:HG22	2	5.57
(4,38)	1:A:120:GLY:HA2	1:A:114:ILE:HG23	2	5.57
(4,38)	1:A:120:GLY:HA3	1:A:114:ILE:HG21	2	5.57
(4,38)	1:A:120:GLY:HA3	1:A:114:ILE:HG22	2	5.57
(4,38)	1:A:120:GLY:HA3	1:A:114:ILE:HG23	2	5.57
(4,38)	1:B:120:GLY:HA2	1:B:114:ILE:HG21	2	5.57
(4,38)	1:B:120:GLY:HA2	1:B:114:ILE:HG22	2	5.57
(4,38)	1:B:120:GLY:HA2	1:B:114:ILE:HG23	2	5.57
(4,38)	1:B:120:GLY:HA3	1:B:114:ILE:HG21	2	5.57
(4,38)	1:B:120:GLY:HA3	1:B:114:ILE:HG22	2	5.57
(4,38)	1:B:120:GLY:HA3	1:B:114:ILE:HG23	2	5.57
(4,23)	1:A:114:ILE:HG21	1:A:119:HIS:HA	7	5.55
(4,23)	1:A:114:ILE:HG22	1:A:119:HIS:HA	7	5.55
(4,23)	1:A:114:ILE:HG23	1:A:119:HIS:HA	7	5.55
(4,23)	1:B:114:ILE:HG21	1:B:119:HIS:HA	7	5.55
(4,23)	1:B:114:ILE:HG22	1:B:119:HIS:HA	7	5.55
(4,23)	1:B:114:ILE:HG23	1:B:119:HIS:HA	7	5.55
(4,36)	1:A:119:HIS:HB3	1:A:115:SER:HB2	2	5.54
(4,36)	1:B:119:HIS:HB3	1:B:115:SER:HB2	2	5.54
(4,35)	1:A:119:HIS:HB3	1:A:115:SER:HB2	2	5.54
(4,35)	1:B:119:HIS:HB3	1:B:115:SER:HB2	2	5.54
(4,25)	1:A:115:SER:HB2	1:A:119:HIS:HB3	2	5.54
(4,25)	1:B:115:SER:HB2	1:B:119:HIS:HB3	2	5.54
(4,23)	1:A:114:ILE:HG21	1:A:119:HIS:HA	5	5.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,23)	1:A:114:ILE:HG22	1:A:119:HIS:HA	5	5.44
(4,23)	1:A:114:ILE:HG23	1:A:119:HIS:HA	5	5.44
(4,23)	1:B:114:ILE:HG21	1:B:119:HIS:HA	5	5.44
(4,23)	1:B:114:ILE:HG22	1:B:119:HIS:HA	5	5.44
(4,23)	1:B:114:ILE:HG23	1:B:119:HIS:HA	5	5.44
(4,19)	1:A:114:ILE:HG21	1:A:77:VAL:HG21	3	5.41
(4,19)	1:A:114:ILE:HG21	1:A:77:VAL:HG22	3	5.41
(4,19)	1:A:114:ILE:HG21	1:A:77:VAL:HG23	3	5.41
(4,19)	1:A:114:ILE:HG22	1:A:77:VAL:HG21	3	5.41
(4,19)	1:A:114:ILE:HG22	1:A:77:VAL:HG22	3	5.41
(4,19)	1:A:114:ILE:HG22	1:A:77:VAL:HG23	3	5.41
(4,19)	1:A:114:ILE:HG23	1:A:77:VAL:HG21	3	5.41
(4,19)	1:A:114:ILE:HG23	1:A:77:VAL:HG22	3	5.41
(4,19)	1:A:114:ILE:HG23	1:A:77:VAL:HG23	3	5.41
(4,19)	1:B:114:ILE:HG21	1:B:77:VAL:HG21	3	5.41
(4,19)	1:B:114:ILE:HG21	1:B:77:VAL:HG22	3	5.41
(4,19)	1:B:114:ILE:HG21	1:B:77:VAL:HG23	3	5.41
(4,19)	1:B:114:ILE:HG22	1:B:77:VAL:HG21	3	5.41
(4,19)	1:B:114:ILE:HG22	1:B:77:VAL:HG22	3	5.41
(4,19)	1:B:114:ILE:HG22	1:B:77:VAL:HG23	3	5.41
(4,19)	1:B:114:ILE:HG23	1:B:77:VAL:HG21	3	5.41
(4,19)	1:B:114:ILE:HG23	1:B:77:VAL:HG22	3	5.41
(4,19)	1:B:114:ILE:HG23	1:B:77:VAL:HG23	3	5.41
(4,18)	1:A:114:ILE:HG21	1:A:77:VAL:HG21	3	5.41
(4,18)	1:A:114:ILE:HG21	1:A:77:VAL:HG22	3	5.41
(4,18)	1:A:114:ILE:HG21	1:A:77:VAL:HG23	3	5.41
(4,18)	1:A:114:ILE:HG22	1:A:77:VAL:HG21	3	5.41
(4,18)	1:A:114:ILE:HG22	1:A:77:VAL:HG22	3	5.41
(4,18)	1:A:114:ILE:HG22	1:A:77:VAL:HG23	3	5.41
(4,18)	1:A:114:ILE:HG23	1:A:77:VAL:HG21	3	5.41
(4,18)	1:A:114:ILE:HG23	1:A:77:VAL:HG22	3	5.41
(4,18)	1:A:114:ILE:HG23	1:A:77:VAL:HG23	3	5.41
(4,18)	1:B:114:ILE:HG21	1:B:77:VAL:HG21	3	5.41
(4,18)	1:B:114:ILE:HG21	1:B:77:VAL:HG22	3	5.41
(4,18)	1:B:114:ILE:HG21	1:B:77:VAL:HG23	3	5.41
(4,18)	1:B:114:ILE:HG22	1:B:77:VAL:HG21	3	5.41
(4,18)	1:B:114:ILE:HG22	1:B:77:VAL:HG22	3	5.41
(4,18)	1:B:114:ILE:HG22	1:B:77:VAL:HG23	3	5.41
(4,18)	1:B:114:ILE:HG23	1:B:77:VAL:HG21	3	5.41
(4,18)	1:B:114:ILE:HG23	1:B:77:VAL:HG22	3	5.41
(4,18)	1:B:114:ILE:HG23	1:B:77:VAL:HG23	3	5.41
(5,4)	1:B:82:LYS:H	1:B:66:SER:HA	8	5.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,4)	1:A:82:LYS:H	1:A:66:SER:HA	8	5.37
(4,36)	1:A:119:HIS:HB3	1:A:115:SER:HB2	5	5.32
(4,36)	1:B:119:HIS:HB3	1:B:115:SER:HB2	5	5.32
(4,35)	1:A:119:HIS:HB3	1:A:115:SER:HB2	5	5.32
(4,35)	1:B:119:HIS:HB3	1:B:115:SER:HB2	5	5.32
(4,25)	1:A:115:SER:HB2	1:A:119:HIS:HB3	5	5.32
(4,25)	1:B:115:SER:HB2	1:B:119:HIS:HB3	5	5.32
(4,36)	1:A:119:HIS:HB3	1:A:115:SER:HB2	6	5.28
(4,36)	1:B:119:HIS:HB3	1:B:115:SER:HB2	6	5.28
(4,35)	1:A:119:HIS:HB3	1:A:115:SER:HB2	6	5.28
(4,35)	1:B:119:HIS:HB3	1:B:115:SER:HB2	6	5.28
(4,25)	1:A:115:SER:HB2	1:A:119:HIS:HB3	6	5.28
(4,25)	1:B:115:SER:HB2	1:B:119:HIS:HB3	6	5.28
(4,43)	1:A:120:GLY:HA2	1:A:114:ILE:HG21	8	5.24
(4,43)	1:A:120:GLY:HA2	1:A:114:ILE:HG22	8	5.24
(4,43)	1:A:120:GLY:HA2	1:A:114:ILE:HG23	8	5.24
(4,43)	1:A:120:GLY:HA3	1:A:114:ILE:HG21	8	5.24
(4,43)	1:A:120:GLY:HA3	1:A:114:ILE:HG22	8	5.24
(4,43)	1:A:120:GLY:HA3	1:A:114:ILE:HG23	8	5.24
(4,43)	1:B:120:GLY:HA2	1:B:114:ILE:HG21	8	5.24
(4,43)	1:B:120:GLY:HA2	1:B:114:ILE:HG22	8	5.24
(4,43)	1:B:120:GLY:HA2	1:B:114:ILE:HG23	8	5.24
(4,43)	1:B:120:GLY:HA3	1:B:114:ILE:HG21	8	5.24
(4,43)	1:B:120:GLY:HA3	1:B:114:ILE:HG22	8	5.24
(4,43)	1:B:120:GLY:HA3	1:B:114:ILE:HG23	8	5.24
(4,42)	1:A:120:GLY:HA2	1:A:114:ILE:HG21	8	5.24
(4,42)	1:A:120:GLY:HA2	1:A:114:ILE:HG22	8	5.24
(4,42)	1:A:120:GLY:HA2	1:A:114:ILE:HG23	8	5.24
(4,42)	1:A:120:GLY:HA3	1:A:114:ILE:HG21	8	5.24
(4,42)	1:A:120:GLY:HA3	1:A:114:ILE:HG22	8	5.24
(4,42)	1:A:120:GLY:HA3	1:A:114:ILE:HG23	8	5.24
(4,42)	1:B:120:GLY:HA2	1:B:114:ILE:HG21	8	5.24
(4,42)	1:B:120:GLY:HA2	1:B:114:ILE:HG22	8	5.24
(4,42)	1:B:120:GLY:HA2	1:B:114:ILE:HG23	8	5.24
(4,42)	1:B:120:GLY:HA3	1:B:114:ILE:HG21	8	5.24
(4,42)	1:B:120:GLY:HA3	1:B:114:ILE:HG22	8	5.24
(4,42)	1:B:120:GLY:HA3	1:B:114:ILE:HG23	8	5.24
(4,38)	1:A:120:GLY:HA2	1:A:114:ILE:HG21	8	5.24
(4,38)	1:A:120:GLY:HA2	1:A:114:ILE:HG22	8	5.24
(4,38)	1:A:120:GLY:HA2	1:A:114:ILE:HG23	8	5.24
(4,38)	1:A:120:GLY:HA3	1:A:114:ILE:HG21	8	5.24
(4,38)	1:A:120:GLY:HA3	1:A:114:ILE:HG22	8	5.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,38)	1:A:120:GLY:HA3	1:A:114:ILE:HG23	8	5.24
(4,38)	1:B:120:GLY:HA2	1:B:114:ILE:HG21	8	5.24
(4,38)	1:B:120:GLY:HA2	1:B:114:ILE:HG22	8	5.24
(4,38)	1:B:120:GLY:HA2	1:B:114:ILE:HG23	8	5.24
(4,38)	1:B:120:GLY:HA3	1:B:114:ILE:HG21	8	5.24
(4,38)	1:B:120:GLY:HA3	1:B:114:ILE:HG22	8	5.24
(4,38)	1:B:120:GLY:HA3	1:B:114:ILE:HG23	8	5.24
(4,43)	1:A:120:GLY:HA2	1:A:114:ILE:HG21	1	5.16
(4,43)	1:A:120:GLY:HA2	1:A:114:ILE:HG22	1	5.16
(4,43)	1:A:120:GLY:HA2	1:A:114:ILE:HG23	1	5.16
(4,43)	1:A:120:GLY:HA3	1:A:114:ILE:HG21	1	5.16
(4,43)	1:A:120:GLY:HA3	1:A:114:ILE:HG22	1	5.16
(4,43)	1:A:120:GLY:HA3	1:A:114:ILE:HG23	1	5.16
(4,43)	1:B:120:GLY:HA2	1:B:114:ILE:HG21	1	5.16
(4,43)	1:B:120:GLY:HA2	1:B:114:ILE:HG22	1	5.16
(4,43)	1:B:120:GLY:HA2	1:B:114:ILE:HG23	1	5.16
(4,43)	1:B:120:GLY:HA3	1:B:114:ILE:HG21	1	5.16
(4,43)	1:B:120:GLY:HA3	1:B:114:ILE:HG22	1	5.16
(4,43)	1:B:120:GLY:HA3	1:B:114:ILE:HG23	1	5.16
(4,42)	1:A:120:GLY:HA2	1:A:114:ILE:HG21	1	5.16
(4,42)	1:A:120:GLY:HA2	1:A:114:ILE:HG22	1	5.16
(4,42)	1:A:120:GLY:HA2	1:A:114:ILE:HG23	1	5.16
(4,42)	1:A:120:GLY:HA3	1:A:114:ILE:HG21	1	5.16
(4,42)	1:A:120:GLY:HA3	1:A:114:ILE:HG22	1	5.16
(4,42)	1:A:120:GLY:HA3	1:A:114:ILE:HG23	1	5.16
(4,42)	1:B:120:GLY:HA2	1:B:114:ILE:HG21	1	5.16
(4,42)	1:B:120:GLY:HA2	1:B:114:ILE:HG22	1	5.16
(4,42)	1:B:120:GLY:HA2	1:B:114:ILE:HG23	1	5.16
(4,42)	1:B:120:GLY:HA3	1:B:114:ILE:HG21	1	5.16
(4,42)	1:B:120:GLY:HA3	1:B:114:ILE:HG22	1	5.16
(4,42)	1:B:120:GLY:HA3	1:B:114:ILE:HG23	1	5.16
(4,38)	1:A:120:GLY:HA2	1:A:114:ILE:HG21	1	5.16
(4,38)	1:A:120:GLY:HA2	1:A:114:ILE:HG22	1	5.16
(4,38)	1:A:120:GLY:HA2	1:A:114:ILE:HG23	1	5.16
(4,38)	1:A:120:GLY:HA3	1:A:114:ILE:HG21	1	5.16
(4,38)	1:A:120:GLY:HA3	1:A:114:ILE:HG22	1	5.16
(4,38)	1:A:120:GLY:HA3	1:A:114:ILE:HG23	1	5.16
(4,38)	1:B:120:GLY:HA2	1:B:114:ILE:HG21	1	5.16
(4,38)	1:B:120:GLY:HA2	1:B:114:ILE:HG22	1	5.16
(4,38)	1:B:120:GLY:HA2	1:B:114:ILE:HG23	1	5.16
(4,38)	1:B:120:GLY:HA3	1:B:114:ILE:HG21	1	5.16
(4,38)	1:B:120:GLY:HA3	1:B:114:ILE:HG22	1	5.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,38)	1:B:120:GLY:HA3	1:B:114:ILE:HG23	1	5.16
(4,34)	1:A:119:HIS:HB2	1:A:115:SER:HB2	7	5.14
(4,34)	1:B:119:HIS:HB2	1:B:115:SER:HB2	7	5.14
(5,4)	1:B:82:LYS:H	1:B:66:SER:HA	4	5.11
(5,4)	1:A:82:LYS:H	1:A:66:SER:HA	4	5.11
(4,36)	1:A:119:HIS:HB3	1:A:115:SER:HB2	8	5.11
(4,36)	1:B:119:HIS:HB3	1:B:115:SER:HB2	8	5.11
(4,35)	1:A:119:HIS:HB3	1:A:115:SER:HB2	8	5.11
(4,35)	1:B:119:HIS:HB3	1:B:115:SER:HB2	8	5.11
(4,25)	1:A:115:SER:HB2	1:A:119:HIS:HB3	8	5.11
(4,25)	1:B:115:SER:HB2	1:B:119:HIS:HB3	8	5.11
(4,23)	1:A:114:ILE:HG21	1:A:119:HIS:HA	4	5.1
(4,23)	1:A:114:ILE:HG22	1:A:119:HIS:HA	4	5.1
(4,23)	1:A:114:ILE:HG23	1:A:119:HIS:HA	4	5.1
(4,23)	1:B:114:ILE:HG21	1:B:119:HIS:HA	4	5.1
(4,23)	1:B:114:ILE:HG22	1:B:119:HIS:HA	4	5.1
(4,23)	1:B:114:ILE:HG23	1:B:119:HIS:HA	4	5.1
(4,34)	1:A:119:HIS:HB2	1:A:115:SER:HB2	2	4.99
(4,34)	1:B:119:HIS:HB2	1:B:115:SER:HB2	2	4.99
(4,36)	1:A:119:HIS:HB3	1:A:115:SER:HB2	1	4.91
(4,36)	1:B:119:HIS:HB3	1:B:115:SER:HB2	1	4.91
(4,35)	1:A:119:HIS:HB3	1:A:115:SER:HB2	1	4.91
(4,35)	1:B:119:HIS:HB3	1:B:115:SER:HB2	1	4.91
(4,25)	1:A:115:SER:HB2	1:A:119:HIS:HB3	1	4.91
(4,25)	1:B:115:SER:HB2	1:B:119:HIS:HB3	1	4.91
(4,51)	1:A:119:HIS:H	1:A:114:ILE:HG21	7	4.88
(4,51)	1:A:119:HIS:H	1:A:114:ILE:HG22	7	4.88
(4,51)	1:A:119:HIS:H	1:A:114:ILE:HG23	7	4.88
(4,51)	1:B:119:HIS:H	1:B:114:ILE:HG21	7	4.88
(4,51)	1:B:119:HIS:H	1:B:114:ILE:HG22	7	4.88
(4,51)	1:B:119:HIS:H	1:B:114:ILE:HG23	7	4.88
(4,23)	1:A:114:ILE:HG21	1:A:119:HIS:HA	2	4.87
(4,23)	1:A:114:ILE:HG22	1:A:119:HIS:HA	2	4.87
(4,23)	1:A:114:ILE:HG23	1:A:119:HIS:HA	2	4.87
(4,23)	1:B:114:ILE:HG21	1:B:119:HIS:HA	2	4.87
(4,23)	1:B:114:ILE:HG22	1:B:119:HIS:HA	2	4.87
(4,23)	1:B:114:ILE:HG23	1:B:119:HIS:HA	2	4.87
(4,23)	1:A:114:ILE:HG21	1:A:119:HIS:HA	3	4.72
(4,23)	1:A:114:ILE:HG22	1:A:119:HIS:HA	3	4.72
(4,23)	1:A:114:ILE:HG23	1:A:119:HIS:HA	3	4.72
(4,23)	1:B:114:ILE:HG21	1:B:119:HIS:HA	3	4.72
(4,23)	1:B:114:ILE:HG22	1:B:119:HIS:HA	3	4.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,23)	1:B:114:ILE:HG23	1:B:119:HIS:HA	3	4.72
(4,51)	1:A:119:HIS:H	1:A:114:ILE:HG21	6	4.69
(4,51)	1:A:119:HIS:H	1:A:114:ILE:HG22	6	4.69
(4,51)	1:A:119:HIS:H	1:A:114:ILE:HG23	6	4.69
(4,51)	1:B:119:HIS:H	1:B:114:ILE:HG21	6	4.69
(4,51)	1:B:119:HIS:H	1:B:114:ILE:HG22	6	4.69
(4,51)	1:B:119:HIS:H	1:B:114:ILE:HG23	6	4.69
(4,36)	1:A:119:HIS:HB3	1:A:115:SER:HB2	3	4.68
(4,36)	1:B:119:HIS:HB3	1:B:115:SER:HB2	3	4.68
(4,35)	1:A:119:HIS:HB3	1:A:115:SER:HB2	3	4.68
(4,35)	1:B:119:HIS:HB3	1:B:115:SER:HB2	3	4.68
(4,25)	1:A:115:SER:HB2	1:A:119:HIS:HB3	3	4.68
(4,25)	1:B:115:SER:HB2	1:B:119:HIS:HB3	3	4.68
(4,34)	1:A:119:HIS:HB2	1:A:115:SER:HB2	8	4.66
(4,34)	1:B:119:HIS:HB2	1:B:115:SER:HB2	8	4.66
(4,34)	1:A:119:HIS:HB2	1:A:115:SER:HB2	5	4.52
(4,34)	1:B:119:HIS:HB2	1:B:115:SER:HB2	5	4.52
(4,23)	1:A:114:ILE:HG21	1:A:119:HIS:HA	8	4.4
(4,23)	1:A:114:ILE:HG22	1:A:119:HIS:HA	8	4.4
(4,23)	1:A:114:ILE:HG23	1:A:119:HIS:HA	8	4.4
(4,23)	1:B:114:ILE:HG21	1:B:119:HIS:HA	8	4.4
(4,23)	1:B:114:ILE:HG22	1:B:119:HIS:HA	8	4.4
(4,23)	1:B:114:ILE:HG23	1:B:119:HIS:HA	8	4.4
(5,1)	1:B:82:LYS:HE2	1:B:67:GLU:HA	8	4.36
(5,1)	1:B:82:LYS:HE3	1:B:67:GLU:HA	8	4.36
(5,1)	1:A:82:LYS:HE2	1:A:67:GLU:HA	8	4.36
(5,1)	1:A:82:LYS:HE3	1:A:67:GLU:HA	8	4.36
(4,51)	1:A:119:HIS:H	1:A:114:ILE:HG21	4	4.34
(4,51)	1:A:119:HIS:H	1:A:114:ILE:HG22	4	4.34
(4,51)	1:A:119:HIS:H	1:A:114:ILE:HG23	4	4.34
(4,51)	1:B:119:HIS:H	1:B:114:ILE:HG21	4	4.34
(4,51)	1:B:119:HIS:H	1:B:114:ILE:HG22	4	4.34
(4,51)	1:B:119:HIS:H	1:B:114:ILE:HG23	4	4.34
(4,34)	1:A:119:HIS:HB2	1:A:115:SER:HB2	6	4.34
(4,34)	1:B:119:HIS:HB2	1:B:115:SER:HB2	6	4.34
(4,51)	1:A:119:HIS:H	1:A:114:ILE:HG21	5	4.0
(4,51)	1:A:119:HIS:H	1:A:114:ILE:HG22	5	4.0
(4,51)	1:A:119:HIS:H	1:A:114:ILE:HG23	5	4.0
(4,51)	1:B:119:HIS:H	1:B:114:ILE:HG21	5	4.0
(4,51)	1:B:119:HIS:H	1:B:114:ILE:HG22	5	4.0
(4,51)	1:B:119:HIS:H	1:B:114:ILE:HG23	5	4.0
(4,34)	1:A:119:HIS:HB2	1:A:115:SER:HB2	3	3.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,34)	1:B:119:HIS:HB2	1:B:115:SER:HB2	3	3.9
(4,23)	1:A:114:ILE:HG21	1:A:119:HIS:HA	1	3.9
(4,23)	1:A:114:ILE:HG22	1:A:119:HIS:HA	1	3.9
(4,23)	1:A:114:ILE:HG23	1:A:119:HIS:HA	1	3.9
(4,23)	1:B:114:ILE:HG21	1:B:119:HIS:HA	1	3.9
(4,23)	1:B:114:ILE:HG22	1:B:119:HIS:HA	1	3.9
(4,23)	1:B:114:ILE:HG23	1:B:119:HIS:HA	1	3.9
(5,10)	1:A:119:HIS:H	1:A:116:ARG:HA	4	3.89
(5,10)	1:B:119:HIS:H	1:B:116:ARG:HA	4	3.89
(5,10)	1:A:119:HIS:H	1:A:116:ARG:HA	7	3.57
(5,10)	1:B:119:HIS:H	1:B:116:ARG:HA	7	3.57
(4,51)	1:A:119:HIS:H	1:A:114:ILE:HG21	2	3.53
(4,51)	1:A:119:HIS:H	1:A:114:ILE:HG22	2	3.53
(4,51)	1:A:119:HIS:H	1:A:114:ILE:HG23	2	3.53
(4,51)	1:B:119:HIS:H	1:B:114:ILE:HG21	2	3.53
(4,51)	1:B:119:HIS:H	1:B:114:ILE:HG22	2	3.53
(4,51)	1:B:119:HIS:H	1:B:114:ILE:HG23	2	3.53
(4,51)	1:A:119:HIS:H	1:A:114:ILE:HG21	3	3.33
(4,51)	1:A:119:HIS:H	1:A:114:ILE:HG22	3	3.33
(4,51)	1:A:119:HIS:H	1:A:114:ILE:HG23	3	3.33
(4,51)	1:B:119:HIS:H	1:B:114:ILE:HG21	3	3.33
(4,51)	1:B:119:HIS:H	1:B:114:ILE:HG22	3	3.33
(4,51)	1:B:119:HIS:H	1:B:114:ILE:HG23	3	3.33
(5,10)	1:A:119:HIS:H	1:A:116:ARG:HA	6	3.31
(5,10)	1:B:119:HIS:H	1:B:116:ARG:HA	6	3.31
(5,10)	1:A:119:HIS:H	1:A:116:ARG:HA	5	3.28
(5,10)	1:B:119:HIS:H	1:B:116:ARG:HA	5	3.28
(2,85)	1:B:102:GLY:HA2	1:B:81:VAL:HG21	6	3.22
(2,85)	1:B:102:GLY:HA2	1:B:81:VAL:HG22	6	3.22
(2,85)	1:B:102:GLY:HA2	1:B:81:VAL:HG23	6	3.22
(2,85)	1:B:102:GLY:HA3	1:B:81:VAL:HG21	6	3.22
(2,85)	1:B:102:GLY:HA3	1:B:81:VAL:HG22	6	3.22
(2,85)	1:B:102:GLY:HA3	1:B:81:VAL:HG23	6	3.22
(2,85)	1:A:102:GLY:HA2	1:A:81:VAL:HG21	6	3.22
(2,85)	1:A:102:GLY:HA2	1:A:81:VAL:HG22	6	3.22
(2,85)	1:A:102:GLY:HA2	1:A:81:VAL:HG23	6	3.22
(2,85)	1:A:102:GLY:HA3	1:A:81:VAL:HG21	6	3.22
(2,85)	1:A:102:GLY:HA3	1:A:81:VAL:HG22	6	3.22
(2,85)	1:A:102:GLY:HA3	1:A:81:VAL:HG23	6	3.22
(5,10)	1:A:119:HIS:H	1:A:116:ARG:HA	2	3.15
(5,10)	1:B:119:HIS:H	1:B:116:ARG:HA	2	3.15
(4,51)	1:A:119:HIS:H	1:A:114:ILE:HG21	8	2.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,51)	1:A:119:HIS:H	1:A:114:ILE:HG22	8	2.87
(4,51)	1:A:119:HIS:H	1:A:114:ILE:HG23	8	2.87
(4,51)	1:B:119:HIS:H	1:B:114:ILE:HG21	8	2.87
(4,51)	1:B:119:HIS:H	1:B:114:ILE:HG22	8	2.87
(4,51)	1:B:119:HIS:H	1:B:114:ILE:HG23	8	2.87
(5,10)	1:A:119:HIS:H	1:A:116:ARG:HA	8	2.86
(5,10)	1:B:119:HIS:H	1:B:116:ARG:HA	8	2.86
(5,10)	1:A:119:HIS:H	1:A:116:ARG:HA	3	2.77
(5,10)	1:B:119:HIS:H	1:B:116:ARG:HA	3	2.77
(4,51)	1:A:119:HIS:H	1:A:114:ILE:HG21	1	2.77
(4,51)	1:A:119:HIS:H	1:A:114:ILE:HG22	1	2.77
(4,51)	1:A:119:HIS:H	1:A:114:ILE:HG23	1	2.77
(4,51)	1:B:119:HIS:H	1:B:114:ILE:HG21	1	2.77
(4,51)	1:B:119:HIS:H	1:B:114:ILE:HG22	1	2.77
(4,51)	1:B:119:HIS:H	1:B:114:ILE:HG23	1	2.77
(5,10)	1:A:119:HIS:H	1:A:116:ARG:HA	1	2.37
(5,10)	1:B:119:HIS:H	1:B:116:ARG:HA	1	2.37
(1,230)	1:A:127:ASP:H	1:A:128:VAL:HB	7	2.26
(1,230)	1:B:127:ASP:H	1:B:128:VAL:HB	7	2.26
(5,2)	1:A:116:ARG:HB2	1:A:118:PHE:HA	4	2.17
(5,2)	1:A:116:ARG:HB3	1:A:118:PHE:HA	4	2.17
(5,2)	1:B:116:ARG:HB2	1:B:118:PHE:HA	4	2.17
(5,2)	1:B:116:ARG:HB3	1:B:118:PHE:HA	4	2.17
(2,38)	1:B:82:LYS:HE2	1:B:83:HIS:HE1	6	2.13
(2,38)	1:B:82:LYS:HE3	1:B:83:HIS:HE1	6	2.13
(2,38)	1:A:82:LYS:HE2	1:A:83:HIS:HE1	6	2.13
(2,38)	1:A:82:LYS:HE3	1:A:83:HIS:HE1	6	2.13
(4,26)	1:A:115:SER:HB2	1:A:119:HIS:HD2	5	2.07
(4,26)	1:B:115:SER:HB2	1:B:119:HIS:HD2	5	2.07
(4,22)	1:A:114:ILE:HG21	1:A:118:PHE:HB2	7	2.02
(4,22)	1:A:114:ILE:HG21	1:A:118:PHE:HB3	7	2.02
(4,22)	1:A:114:ILE:HG22	1:A:118:PHE:HB2	7	2.02
(4,22)	1:A:114:ILE:HG22	1:A:118:PHE:HB3	7	2.02
(4,22)	1:A:114:ILE:HG23	1:A:118:PHE:HB2	7	2.02
(4,22)	1:A:114:ILE:HG23	1:A:118:PHE:HB3	7	2.02
(4,22)	1:B:114:ILE:HG21	1:B:118:PHE:HB2	7	2.02
(4,22)	1:B:114:ILE:HG21	1:B:118:PHE:HB3	7	2.02
(4,22)	1:B:114:ILE:HG22	1:B:118:PHE:HB2	7	2.02
(4,22)	1:B:114:ILE:HG22	1:B:118:PHE:HB3	7	2.02
(4,22)	1:B:114:ILE:HG23	1:B:118:PHE:HB2	7	2.02
(4,22)	1:B:114:ILE:HG23	1:B:118:PHE:HB3	7	2.02
(4,21)	1:A:114:ILE:HG21	1:A:118:PHE:HB2	7	2.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,21)	1:A:114:ILE:HG21	1:A:118:PHE:HB3	7	2.02
(4,21)	1:A:114:ILE:HG22	1:A:118:PHE:HB2	7	2.02
(4,21)	1:A:114:ILE:HG22	1:A:118:PHE:HB3	7	2.02
(4,21)	1:A:114:ILE:HG23	1:A:118:PHE:HB2	7	2.02
(4,21)	1:A:114:ILE:HG23	1:A:118:PHE:HB3	7	2.02
(4,21)	1:B:114:ILE:HG21	1:B:118:PHE:HB2	7	2.02
(4,21)	1:B:114:ILE:HG21	1:B:118:PHE:HB3	7	2.02
(4,21)	1:B:114:ILE:HG22	1:B:118:PHE:HB2	7	2.02
(4,21)	1:B:114:ILE:HG22	1:B:118:PHE:HB3	7	2.02
(4,21)	1:B:114:ILE:HG23	1:B:118:PHE:HB2	7	2.02
(4,21)	1:B:114:ILE:HG23	1:B:118:PHE:HB3	7	2.02
(5,2)	1:A:116:ARG:HB2	1:A:118:PHE:HA	5	1.96
(5,2)	1:A:116:ARG:HB3	1:A:118:PHE:HA	5	1.96
(5,2)	1:B:116:ARG:HB2	1:B:118:PHE:HA	5	1.96
(5,2)	1:B:116:ARG:HB3	1:B:118:PHE:HA	5	1.96
(4,22)	1:A:114:ILE:HG21	1:A:118:PHE:HB2	6	1.85
(4,22)	1:A:114:ILE:HG21	1:A:118:PHE:HB3	6	1.85
(4,22)	1:A:114:ILE:HG22	1:A:118:PHE:HB2	6	1.85
(4,22)	1:A:114:ILE:HG22	1:A:118:PHE:HB3	6	1.85
(4,22)	1:A:114:ILE:HG23	1:A:118:PHE:HB2	6	1.85
(4,22)	1:A:114:ILE:HG23	1:A:118:PHE:HB3	6	1.85
(4,22)	1:B:114:ILE:HG21	1:B:118:PHE:HB2	6	1.85
(4,22)	1:B:114:ILE:HG21	1:B:118:PHE:HB3	6	1.85
(4,22)	1:B:114:ILE:HG22	1:B:118:PHE:HB2	6	1.85
(4,22)	1:B:114:ILE:HG22	1:B:118:PHE:HB3	6	1.85
(4,22)	1:B:114:ILE:HG23	1:B:118:PHE:HB2	6	1.85
(4,22)	1:B:114:ILE:HG23	1:B:118:PHE:HB3	6	1.85
(4,21)	1:A:114:ILE:HG21	1:A:118:PHE:HB2	6	1.85
(4,21)	1:A:114:ILE:HG21	1:A:118:PHE:HB3	6	1.85
(4,21)	1:A:114:ILE:HG22	1:A:118:PHE:HB2	6	1.85
(4,21)	1:A:114:ILE:HG22	1:A:118:PHE:HB3	6	1.85
(4,21)	1:A:114:ILE:HG23	1:A:118:PHE:HB2	6	1.85
(4,21)	1:A:114:ILE:HG23	1:A:118:PHE:HB3	6	1.85
(4,21)	1:B:114:ILE:HG21	1:B:118:PHE:HB2	6	1.85
(4,21)	1:B:114:ILE:HG21	1:B:118:PHE:HB3	6	1.85
(4,21)	1:B:114:ILE:HG22	1:B:118:PHE:HB2	6	1.85
(4,21)	1:B:114:ILE:HG22	1:B:118:PHE:HB3	6	1.85
(4,21)	1:B:114:ILE:HG23	1:B:118:PHE:HB2	6	1.85
(4,21)	1:B:114:ILE:HG23	1:B:118:PHE:HB3	6	1.85
(1,186)	1:A:115:SER:HA	1:A:105:GLU:HA	7	1.73
(1,186)	1:B:115:SER:HA	1:B:105:GLU:HA	7	1.73
(1,186)	1:A:115:SER:HA	1:A:105:GLU:HA	1	1.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,186)	1:B:115:SER:HA	1:B:105:GLU:HA	1	1.71
(5,2)	1:A:116:ARG:HB2	1:A:118:PHE:HA	2	1.68
(5,2)	1:A:116:ARG:HB3	1:A:118:PHE:HA	2	1.68
(5,2)	1:B:116:ARG:HB2	1:B:118:PHE:HA	2	1.68
(5,2)	1:B:116:ARG:HB3	1:B:118:PHE:HA	2	1.68
(5,2)	1:A:116:ARG:HB2	1:A:118:PHE:HA	7	1.67
(5,2)	1:A:116:ARG:HB3	1:A:118:PHE:HA	7	1.67
(5,2)	1:B:116:ARG:HB2	1:B:118:PHE:HA	7	1.67
(5,2)	1:B:116:ARG:HB3	1:B:118:PHE:HA	7	1.67
(1,222)	1:A:126:ALA:H	1:A:128:VAL:HG11	1	1.62
(1,222)	1:A:126:ALA:H	1:A:128:VAL:HG12	1	1.62
(1,222)	1:A:126:ALA:H	1:A:128:VAL:HG13	1	1.62
(1,222)	1:B:126:ALA:H	1:B:128:VAL:HG11	1	1.62
(1,222)	1:B:126:ALA:H	1:B:128:VAL:HG12	1	1.62
(1,222)	1:B:126:ALA:H	1:B:128:VAL:HG13	1	1.62
(1,222)	1:A:126:ALA:H	1:A:128:VAL:HG11	2	1.59
(1,222)	1:A:126:ALA:H	1:A:128:VAL:HG12	2	1.59
(1,222)	1:A:126:ALA:H	1:A:128:VAL:HG13	2	1.59
(1,222)	1:B:126:ALA:H	1:B:128:VAL:HG11	2	1.59
(1,222)	1:B:126:ALA:H	1:B:128:VAL:HG12	2	1.59
(1,222)	1:B:126:ALA:H	1:B:128:VAL:HG13	2	1.59
(4,22)	1:A:114:ILE:HG21	1:A:118:PHE:HB2	3	1.58
(4,22)	1:A:114:ILE:HG21	1:A:118:PHE:HB3	3	1.58
(4,22)	1:A:114:ILE:HG22	1:A:118:PHE:HB2	3	1.58
(4,22)	1:A:114:ILE:HG22	1:A:118:PHE:HB3	3	1.58
(4,22)	1:A:114:ILE:HG23	1:A:118:PHE:HB2	3	1.58
(4,22)	1:A:114:ILE:HG23	1:A:118:PHE:HB3	3	1.58
(4,22)	1:B:114:ILE:HG21	1:B:118:PHE:HB2	3	1.58
(4,22)	1:B:114:ILE:HG21	1:B:118:PHE:HB3	3	1.58
(4,22)	1:B:114:ILE:HG22	1:B:118:PHE:HB2	3	1.58
(4,22)	1:B:114:ILE:HG22	1:B:118:PHE:HB3	3	1.58
(4,22)	1:B:114:ILE:HG23	1:B:118:PHE:HB2	3	1.58
(4,22)	1:B:114:ILE:HG23	1:B:118:PHE:HB3	3	1.58
(4,21)	1:A:114:ILE:HG21	1:A:118:PHE:HB2	3	1.58
(4,21)	1:A:114:ILE:HG21	1:A:118:PHE:HB3	3	1.58
(4,21)	1:A:114:ILE:HG22	1:A:118:PHE:HB2	3	1.58
(4,21)	1:A:114:ILE:HG22	1:A:118:PHE:HB3	3	1.58
(4,21)	1:A:114:ILE:HG23	1:A:118:PHE:HB2	3	1.58
(4,21)	1:A:114:ILE:HG23	1:A:118:PHE:HB3	3	1.58
(4,21)	1:B:114:ILE:HG21	1:B:118:PHE:HB2	3	1.58
(4,21)	1:B:114:ILE:HG21	1:B:118:PHE:HB3	3	1.58
(4,21)	1:B:114:ILE:HG22	1:B:118:PHE:HB2	3	1.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,21)	1:B:114:ILE:HG22	1:B:118:PHE:HB3	3	1.58
(4,21)	1:B:114:ILE:HG23	1:B:118:PHE:HB2	3	1.58
(4,21)	1:B:114:ILE:HG23	1:B:118:PHE:HB3	3	1.58
(1,222)	1:A:126:ALA:H	1:A:128:VAL:HG11	4	1.58
(1,222)	1:A:126:ALA:H	1:A:128:VAL:HG12	4	1.58
(1,222)	1:A:126:ALA:H	1:A:128:VAL:HG13	4	1.58
(1,222)	1:B:126:ALA:H	1:B:128:VAL:HG11	4	1.58
(1,222)	1:B:126:ALA:H	1:B:128:VAL:HG12	4	1.58
(1,222)	1:B:126:ALA:H	1:B:128:VAL:HG13	4	1.58
(1,222)	1:A:126:ALA:H	1:A:128:VAL:HG11	6	1.58
(1,222)	1:A:126:ALA:H	1:A:128:VAL:HG12	6	1.58
(1,222)	1:A:126:ALA:H	1:A:128:VAL:HG13	6	1.58
(1,222)	1:B:126:ALA:H	1:B:128:VAL:HG11	6	1.58
(1,222)	1:B:126:ALA:H	1:B:128:VAL:HG12	6	1.58
(1,222)	1:B:126:ALA:H	1:B:128:VAL:HG13	6	1.58
(4,22)	1:A:114:ILE:HG21	1:A:118:PHE:HB2	2	1.57
(4,22)	1:A:114:ILE:HG21	1:A:118:PHE:HB3	2	1.57
(4,22)	1:A:114:ILE:HG22	1:A:118:PHE:HB2	2	1.57
(4,22)	1:A:114:ILE:HG22	1:A:118:PHE:HB3	2	1.57
(4,22)	1:A:114:ILE:HG23	1:A:118:PHE:HB2	2	1.57
(4,22)	1:A:114:ILE:HG23	1:A:118:PHE:HB3	2	1.57
(4,22)	1:B:114:ILE:HG21	1:B:118:PHE:HB2	2	1.57
(4,22)	1:B:114:ILE:HG21	1:B:118:PHE:HB3	2	1.57
(4,22)	1:B:114:ILE:HG22	1:B:118:PHE:HB2	2	1.57
(4,22)	1:B:114:ILE:HG22	1:B:118:PHE:HB3	2	1.57
(4,22)	1:B:114:ILE:HG23	1:B:118:PHE:HB2	2	1.57
(4,22)	1:B:114:ILE:HG23	1:B:118:PHE:HB3	2	1.57
(4,21)	1:A:114:ILE:HG21	1:A:118:PHE:HB2	2	1.57
(4,21)	1:A:114:ILE:HG21	1:A:118:PHE:HB3	2	1.57
(4,21)	1:A:114:ILE:HG22	1:A:118:PHE:HB2	2	1.57
(4,21)	1:A:114:ILE:HG22	1:A:118:PHE:HB3	2	1.57
(4,21)	1:A:114:ILE:HG23	1:A:118:PHE:HB2	2	1.57
(4,21)	1:A:114:ILE:HG23	1:A:118:PHE:HB3	2	1.57
(4,21)	1:B:114:ILE:HG21	1:B:118:PHE:HB2	2	1.57
(4,21)	1:B:114:ILE:HG21	1:B:118:PHE:HB3	2	1.57
(4,21)	1:B:114:ILE:HG22	1:B:118:PHE:HB2	2	1.57
(4,21)	1:B:114:ILE:HG22	1:B:118:PHE:HB3	2	1.57
(4,21)	1:B:114:ILE:HG23	1:B:118:PHE:HB2	2	1.57
(4,21)	1:B:114:ILE:HG23	1:B:118:PHE:HB3	2	1.57
(4,22)	1:A:114:ILE:HG21	1:A:118:PHE:HB2	4	1.48
(4,22)	1:A:114:ILE:HG21	1:A:118:PHE:HB3	4	1.48
(4,22)	1:A:114:ILE:HG22	1:A:118:PHE:HB2	4	1.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,22)	1:A:114:ILE:HG22	1:A:118:PHE:HB3	4	1.48
(4,22)	1:A:114:ILE:HG23	1:A:118:PHE:HB2	4	1.48
(4,22)	1:A:114:ILE:HG23	1:A:118:PHE:HB3	4	1.48
(4,22)	1:B:114:ILE:HG21	1:B:118:PHE:HB2	4	1.48
(4,22)	1:B:114:ILE:HG21	1:B:118:PHE:HB3	4	1.48
(4,22)	1:B:114:ILE:HG22	1:B:118:PHE:HB2	4	1.48
(4,22)	1:B:114:ILE:HG22	1:B:118:PHE:HB3	4	1.48
(4,22)	1:B:114:ILE:HG23	1:B:118:PHE:HB2	4	1.48
(4,22)	1:B:114:ILE:HG23	1:B:118:PHE:HB3	4	1.48
(4,21)	1:A:114:ILE:HG21	1:A:118:PHE:HB2	4	1.48
(4,21)	1:A:114:ILE:HG21	1:A:118:PHE:HB3	4	1.48
(4,21)	1:A:114:ILE:HG22	1:A:118:PHE:HB2	4	1.48
(4,21)	1:A:114:ILE:HG22	1:A:118:PHE:HB3	4	1.48
(4,21)	1:A:114:ILE:HG23	1:A:118:PHE:HB2	4	1.48
(4,21)	1:A:114:ILE:HG23	1:A:118:PHE:HB3	4	1.48
(4,21)	1:B:114:ILE:HG21	1:B:118:PHE:HB2	4	1.48
(4,21)	1:B:114:ILE:HG21	1:B:118:PHE:HB3	4	1.48
(4,21)	1:B:114:ILE:HG22	1:B:118:PHE:HB2	4	1.48
(4,21)	1:B:114:ILE:HG22	1:B:118:PHE:HB3	4	1.48
(4,21)	1:B:114:ILE:HG23	1:B:118:PHE:HB2	4	1.48
(4,21)	1:B:114:ILE:HG23	1:B:118:PHE:HB3	4	1.48
(1,222)	1:A:126:ALA:H	1:A:128:VAL:HG11	3	1.39
(1,222)	1:A:126:ALA:H	1:A:128:VAL:HG12	3	1.39
(1,222)	1:A:126:ALA:H	1:A:128:VAL:HG13	3	1.39
(1,222)	1:B:126:ALA:H	1:B:128:VAL:HG11	3	1.39
(1,222)	1:B:126:ALA:H	1:B:128:VAL:HG12	3	1.39
(1,222)	1:B:126:ALA:H	1:B:128:VAL:HG13	3	1.39
(1,231)	1:A:127:ASP:H	1:A:128:VAL:HG11	2	1.38
(1,231)	1:A:127:ASP:H	1:A:128:VAL:HG12	2	1.38
(1,231)	1:A:127:ASP:H	1:A:128:VAL:HG13	2	1.38
(1,231)	1:B:127:ASP:H	1:B:128:VAL:HG11	2	1.38
(1,231)	1:B:127:ASP:H	1:B:128:VAL:HG12	2	1.38
(1,231)	1:B:127:ASP:H	1:B:128:VAL:HG13	2	1.38
(2,134)	1:A:119:HIS:HB2	1:A:101:HIS:HD2	5	1.33
(2,134)	1:B:119:HIS:HB2	1:B:101:HIS:HD2	5	1.33
(1,231)	1:A:127:ASP:H	1:A:128:VAL:HG11	6	1.29
(1,231)	1:A:127:ASP:H	1:A:128:VAL:HG12	6	1.29
(1,231)	1:A:127:ASP:H	1:A:128:VAL:HG13	6	1.29
(1,231)	1:B:127:ASP:H	1:B:128:VAL:HG11	6	1.29
(1,231)	1:B:127:ASP:H	1:B:128:VAL:HG12	6	1.29
(1,231)	1:B:127:ASP:H	1:B:128:VAL:HG13	6	1.29
(4,22)	1:A:114:ILE:HG21	1:A:118:PHE:HB2	5	1.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,22)	1:A:114:ILE:HG21	1:A:118:PHE:HB3	5	1.26
(4,22)	1:A:114:ILE:HG22	1:A:118:PHE:HB2	5	1.26
(4,22)	1:A:114:ILE:HG22	1:A:118:PHE:HB3	5	1.26
(4,22)	1:A:114:ILE:HG23	1:A:118:PHE:HB2	5	1.26
(4,22)	1:A:114:ILE:HG23	1:A:118:PHE:HB3	5	1.26
(4,22)	1:B:114:ILE:HG21	1:B:118:PHE:HB2	5	1.26
(4,22)	1:B:114:ILE:HG21	1:B:118:PHE:HB3	5	1.26
(4,22)	1:B:114:ILE:HG22	1:B:118:PHE:HB2	5	1.26
(4,22)	1:B:114:ILE:HG22	1:B:118:PHE:HB3	5	1.26
(4,22)	1:B:114:ILE:HG23	1:B:118:PHE:HB2	5	1.26
(4,22)	1:B:114:ILE:HG23	1:B:118:PHE:HB3	5	1.26
(4,21)	1:A:114:ILE:HG21	1:A:118:PHE:HB2	5	1.26
(4,21)	1:A:114:ILE:HG21	1:A:118:PHE:HB3	5	1.26
(4,21)	1:A:114:ILE:HG22	1:A:118:PHE:HB2	5	1.26
(4,21)	1:A:114:ILE:HG22	1:A:118:PHE:HB3	5	1.26
(4,21)	1:A:114:ILE:HG23	1:A:118:PHE:HB2	5	1.26
(4,21)	1:A:114:ILE:HG23	1:A:118:PHE:HB3	5	1.26
(4,21)	1:B:114:ILE:HG21	1:B:118:PHE:HB2	5	1.26
(4,21)	1:B:114:ILE:HG21	1:B:118:PHE:HB3	5	1.26
(4,21)	1:B:114:ILE:HG22	1:B:118:PHE:HB2	5	1.26
(4,21)	1:B:114:ILE:HG22	1:B:118:PHE:HB3	5	1.26
(4,21)	1:B:114:ILE:HG23	1:B:118:PHE:HB2	5	1.26
(4,21)	1:B:114:ILE:HG23	1:B:118:PHE:HB3	5	1.26
(1,222)	1:A:126:ALA:H	1:A:128:VAL:HG11	8	1.26
(1,222)	1:A:126:ALA:H	1:A:128:VAL:HG12	8	1.26
(1,222)	1:A:126:ALA:H	1:A:128:VAL:HG13	8	1.26
(1,222)	1:B:126:ALA:H	1:B:128:VAL:HG11	8	1.26
(1,222)	1:B:126:ALA:H	1:B:128:VAL:HG12	8	1.26
(1,222)	1:B:126:ALA:H	1:B:128:VAL:HG13	8	1.26
(1,231)	1:A:127:ASP:H	1:A:128:VAL:HG11	4	1.25
(1,231)	1:A:127:ASP:H	1:A:128:VAL:HG12	4	1.25
(1,231)	1:A:127:ASP:H	1:A:128:VAL:HG13	4	1.25
(1,231)	1:B:127:ASP:H	1:B:128:VAL:HG11	4	1.25
(1,231)	1:B:127:ASP:H	1:B:128:VAL:HG12	4	1.25
(1,231)	1:B:127:ASP:H	1:B:128:VAL:HG13	4	1.25
(4,30)	1:B:118:PHE:HA	1:B:116:ARG:HG2	7	1.23
(4,30)	1:B:118:PHE:HA	1:B:116:ARG:HG3	7	1.23
(4,30)	1:A:118:PHE:HA	1:A:116:ARG:HG2	7	1.23
(4,30)	1:A:118:PHE:HA	1:A:116:ARG:HG3	7	1.23
(2,118)	1:A:114:ILE:HA	1:A:113:PHE:HE1	7	1.22
(2,118)	1:A:114:ILE:HA	1:A:113:PHE:HE2	7	1.22
(2,118)	1:B:114:ILE:HA	1:B:113:PHE:HE1	7	1.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,118)	1:B:114:ILE:HA	1:B:113:PHE:HE2	7	1.22
(1,231)	1:A:127:ASP:H	1:A:128:VAL:HG11	1	1.22
(1,231)	1:A:127:ASP:H	1:A:128:VAL:HG12	1	1.22
(1,231)	1:A:127:ASP:H	1:A:128:VAL:HG13	1	1.22
(1,231)	1:B:127:ASP:H	1:B:128:VAL:HG11	1	1.22
(1,231)	1:B:127:ASP:H	1:B:128:VAL:HG12	1	1.22
(1,231)	1:B:127:ASP:H	1:B:128:VAL:HG13	1	1.22
(2,108)	1:A:108:GLN:H	1:A:114:ILE:HD11	4	1.21
(2,108)	1:A:108:GLN:H	1:A:114:ILE:HD12	4	1.21
(2,108)	1:A:108:GLN:H	1:A:114:ILE:HD13	4	1.21
(2,108)	1:B:108:GLN:H	1:B:114:ILE:HD11	4	1.21
(2,108)	1:B:108:GLN:H	1:B:114:ILE:HD12	4	1.21
(2,108)	1:B:108:GLN:H	1:B:114:ILE:HD13	4	1.21
(2,118)	1:A:114:ILE:HA	1:A:113:PHE:HE1	1	1.2
(2,118)	1:A:114:ILE:HA	1:A:113:PHE:HE2	1	1.2
(2,118)	1:B:114:ILE:HA	1:B:113:PHE:HE1	1	1.2
(2,118)	1:B:114:ILE:HA	1:B:113:PHE:HE2	1	1.2
(2,133)	1:B:118:PHE:HB2	1:B:81:VAL:HG21	6	1.18
(2,133)	1:B:118:PHE:HB2	1:B:81:VAL:HG22	6	1.18
(2,133)	1:B:118:PHE:HB2	1:B:81:VAL:HG23	6	1.18
(2,133)	1:B:118:PHE:HB3	1:B:81:VAL:HG21	6	1.18
(2,133)	1:B:118:PHE:HB3	1:B:81:VAL:HG22	6	1.18
(2,133)	1:B:118:PHE:HB3	1:B:81:VAL:HG23	6	1.18
(2,133)	1:A:118:PHE:HB2	1:A:81:VAL:HG21	6	1.18
(2,133)	1:A:118:PHE:HB2	1:A:81:VAL:HG22	6	1.18
(2,133)	1:A:118:PHE:HB2	1:A:81:VAL:HG23	6	1.18
(2,133)	1:A:118:PHE:HB3	1:A:81:VAL:HG21	6	1.18
(2,133)	1:A:118:PHE:HB3	1:A:81:VAL:HG22	6	1.18
(2,133)	1:A:118:PHE:HB3	1:A:81:VAL:HG23	6	1.18
(1,172)	1:A:113:PHE:HA	1:A:107:ARG:HA	7	1.18
(1,172)	1:B:113:PHE:HA	1:B:107:ARG:HA	7	1.18
(1,231)	1:A:127:ASP:H	1:A:128:VAL:HG11	8	1.17
(1,231)	1:A:127:ASP:H	1:A:128:VAL:HG12	8	1.17
(1,231)	1:A:127:ASP:H	1:A:128:VAL:HG13	8	1.17
(1,231)	1:B:127:ASP:H	1:B:128:VAL:HG11	8	1.17
(1,231)	1:B:127:ASP:H	1:B:128:VAL:HG12	8	1.17
(1,231)	1:B:127:ASP:H	1:B:128:VAL:HG13	8	1.17
(1,231)	1:A:127:ASP:H	1:A:128:VAL:HG11	3	1.16
(1,231)	1:A:127:ASP:H	1:A:128:VAL:HG12	3	1.16
(1,231)	1:A:127:ASP:H	1:A:128:VAL:HG13	3	1.16
(1,231)	1:B:127:ASP:H	1:B:128:VAL:HG11	3	1.16
(1,231)	1:B:127:ASP:H	1:B:128:VAL:HG12	3	1.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,231)	1:B:127:ASP:H	1:B:128:VAL:HG13	3	1.16
(1,104)	1:A:92:LYS:H	1:A:100:VAL:HG11	5	1.16
(1,104)	1:A:92:LYS:H	1:A:100:VAL:HG12	5	1.16
(1,104)	1:A:92:LYS:H	1:A:100:VAL:HG13	5	1.16
(1,104)	1:B:92:LYS:H	1:B:100:VAL:HG11	5	1.16
(1,104)	1:B:92:LYS:H	1:B:100:VAL:HG12	5	1.16
(1,104)	1:B:92:LYS:H	1:B:100:VAL:HG13	5	1.16
(2,16)	1:B:74:ARG:HA	1:B:75:PHE:HE1	8	1.09
(2,16)	1:B:74:ARG:HA	1:B:75:PHE:HE2	8	1.09
(2,16)	1:A:74:ARG:HA	1:A:75:PHE:HE1	8	1.09
(2,16)	1:A:74:ARG:HA	1:A:75:PHE:HE2	8	1.09
(1,230)	1:A:127:ASP:H	1:A:128:VAL:HB	5	1.09
(1,230)	1:B:127:ASP:H	1:B:128:VAL:HB	5	1.09
(2,8)	1:A:66:SER:HA	1:A:77:VAL:HG21	7	1.05
(2,8)	1:A:66:SER:HA	1:A:77:VAL:HG22	7	1.05
(2,8)	1:A:66:SER:HA	1:A:77:VAL:HG23	7	1.05
(2,8)	1:B:66:SER:HA	1:B:77:VAL:HG21	7	1.05
(2,8)	1:B:66:SER:HA	1:B:77:VAL:HG22	7	1.05
(2,8)	1:B:66:SER:HA	1:B:77:VAL:HG23	7	1.05
(2,121)	1:A:115:SER:HA	1:A:105:GLU:HG2	1	1.01
(2,121)	1:A:115:SER:HA	1:A:105:GLU:HG3	1	1.01
(2,121)	1:B:115:SER:HA	1:B:105:GLU:HG2	1	1.01
(2,121)	1:B:115:SER:HA	1:B:105:GLU:HG3	1	1.01
(2,121)	1:A:115:SER:HA	1:A:105:GLU:HG2	7	1.0
(2,121)	1:A:115:SER:HA	1:A:105:GLU:HG3	7	1.0
(2,121)	1:B:115:SER:HA	1:B:105:GLU:HG2	7	1.0
(2,121)	1:B:115:SER:HA	1:B:105:GLU:HG3	7	1.0
(1,309)	1:A:146:ASN:H	1:A:133:ILE:HA	6	0.96
(1,309)	1:B:146:ASN:H	1:B:133:ILE:HA	6	0.96
(2,7)	1:A:66:SER:HB2	1:A:77:VAL:HG11	2	0.95
(2,7)	1:A:66:SER:HB2	1:A:77:VAL:HG12	2	0.95
(2,7)	1:A:66:SER:HB2	1:A:77:VAL:HG13	2	0.95
(2,7)	1:A:66:SER:HB3	1:A:77:VAL:HG11	2	0.95
(2,7)	1:A:66:SER:HB3	1:A:77:VAL:HG12	2	0.95
(2,7)	1:A:66:SER:HB3	1:A:77:VAL:HG13	2	0.95
(2,7)	1:B:66:SER:HB2	1:B:77:VAL:HG11	2	0.95
(2,7)	1:B:66:SER:HB2	1:B:77:VAL:HG12	2	0.95
(2,7)	1:B:66:SER:HB2	1:B:77:VAL:HG13	2	0.95
(2,7)	1:B:66:SER:HB3	1:B:77:VAL:HG11	2	0.95
(2,7)	1:B:66:SER:HB3	1:B:77:VAL:HG12	2	0.95
(2,7)	1:B:66:SER:HB3	1:B:77:VAL:HG13	2	0.95
(1,309)	1:A:146:ASN:H	1:A:133:ILE:HA	1	0.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,309)	1:B:146:ASN:H	1:B:133:ILE:HA	1	0.95
(2,146)	1:A:127:ASP:H	1:A:124:ILE:HG21	5	0.91
(2,146)	1:A:127:ASP:H	1:A:124:ILE:HG22	5	0.91
(2,146)	1:A:127:ASP:H	1:A:124:ILE:HG23	5	0.91
(2,146)	1:B:127:ASP:H	1:B:124:ILE:HG21	5	0.91
(2,146)	1:B:127:ASP:H	1:B:124:ILE:HG22	5	0.91
(2,146)	1:B:127:ASP:H	1:B:124:ILE:HG23	5	0.91
(1,104)	1:A:92:LYS:H	1:A:100:VAL:HG11	2	0.89
(1,104)	1:A:92:LYS:H	1:A:100:VAL:HG12	2	0.89
(1,104)	1:A:92:LYS:H	1:A:100:VAL:HG13	2	0.89
(1,104)	1:B:92:LYS:H	1:B:100:VAL:HG11	2	0.89
(1,104)	1:B:92:LYS:H	1:B:100:VAL:HG12	2	0.89
(1,104)	1:B:92:LYS:H	1:B:100:VAL:HG13	2	0.89
(1,309)	1:A:146:ASN:H	1:A:133:ILE:HA	5	0.88
(1,309)	1:B:146:ASN:H	1:B:133:ILE:HA	5	0.88
(1,104)	1:A:92:LYS:H	1:A:100:VAL:HG11	6	0.85
(1,104)	1:A:92:LYS:H	1:A:100:VAL:HG12	6	0.85
(1,104)	1:A:92:LYS:H	1:A:100:VAL:HG13	6	0.85
(1,104)	1:B:92:LYS:H	1:B:100:VAL:HG11	6	0.85
(1,104)	1:B:92:LYS:H	1:B:100:VAL:HG12	6	0.85
(1,104)	1:B:92:LYS:H	1:B:100:VAL:HG13	6	0.85
(2,133)	1:B:118:PHE:HB2	1:B:81:VAL:HG21	4	0.83
(2,133)	1:B:118:PHE:HB2	1:B:81:VAL:HG22	4	0.83
(2,133)	1:B:118:PHE:HB2	1:B:81:VAL:HG23	4	0.83
(2,133)	1:B:118:PHE:HB3	1:B:81:VAL:HG21	4	0.83
(2,133)	1:B:118:PHE:HB3	1:B:81:VAL:HG22	4	0.83
(2,133)	1:B:118:PHE:HB3	1:B:81:VAL:HG23	4	0.83
(2,133)	1:A:118:PHE:HB2	1:A:81:VAL:HG21	4	0.83
(2,133)	1:A:118:PHE:HB2	1:A:81:VAL:HG22	4	0.83
(2,133)	1:A:118:PHE:HB2	1:A:81:VAL:HG23	4	0.83
(2,133)	1:A:118:PHE:HB3	1:A:81:VAL:HG21	4	0.83
(2,133)	1:A:118:PHE:HB3	1:A:81:VAL:HG22	4	0.83
(2,133)	1:A:118:PHE:HB3	1:A:81:VAL:HG23	4	0.83
(1,258)	1:A:134:THR:H	1:A:133:ILE:HD11	5	0.8
(1,258)	1:A:134:THR:H	1:A:133:ILE:HD12	5	0.8
(1,258)	1:A:134:THR:H	1:A:133:ILE:HD13	5	0.8
(1,258)	1:B:134:THR:H	1:B:133:ILE:HD11	5	0.8
(1,258)	1:B:134:THR:H	1:B:133:ILE:HD12	5	0.8
(1,258)	1:B:134:THR:H	1:B:133:ILE:HD13	5	0.8
(2,95)	1:B:106:GLU:H	1:B:115:SER:HB2	7	0.79
(2,95)	1:B:106:GLU:H	1:B:115:SER:HB3	7	0.79
(2,95)	1:A:106:GLU:H	1:A:115:SER:HB2	7	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,95)	1:A:106:GLU:H	1:A:115:SER:HB3	7	0.79
(1,258)	1:A:134:THR:H	1:A:133:ILE:HD11	7	0.79
(1,258)	1:A:134:THR:H	1:A:133:ILE:HD12	7	0.79
(1,258)	1:A:134:THR:H	1:A:133:ILE:HD13	7	0.79
(1,258)	1:B:134:THR:H	1:B:133:ILE:HD11	7	0.79
(1,258)	1:B:134:THR:H	1:B:133:ILE:HD12	7	0.79
(1,258)	1:B:134:THR:H	1:B:133:ILE:HD13	7	0.79
(5,2)	1:A:116:ARG:HB2	1:A:118:PHE:HA	8	0.76
(5,2)	1:A:116:ARG:HB3	1:A:118:PHE:HA	8	0.76
(5,2)	1:B:116:ARG:HB2	1:B:118:PHE:HA	8	0.76
(5,2)	1:B:116:ARG:HB3	1:B:118:PHE:HA	8	0.76
(1,104)	1:A:92:LYS:H	1:A:100:VAL:HG11	3	0.76
(1,104)	1:A:92:LYS:H	1:A:100:VAL:HG12	3	0.76
(1,104)	1:A:92:LYS:H	1:A:100:VAL:HG13	3	0.76
(1,104)	1:B:92:LYS:H	1:B:100:VAL:HG11	3	0.76
(1,104)	1:B:92:LYS:H	1:B:100:VAL:HG12	3	0.76
(1,104)	1:B:92:LYS:H	1:B:100:VAL:HG13	3	0.76
(1,104)	1:A:92:LYS:H	1:A:100:VAL:HG11	8	0.76
(1,104)	1:A:92:LYS:H	1:A:100:VAL:HG12	8	0.76
(1,104)	1:A:92:LYS:H	1:A:100:VAL:HG13	8	0.76
(1,104)	1:B:92:LYS:H	1:B:100:VAL:HG11	8	0.76
(1,104)	1:B:92:LYS:H	1:B:100:VAL:HG12	8	0.76
(1,104)	1:B:92:LYS:H	1:B:100:VAL:HG13	8	0.76
(5,2)	1:A:116:ARG:HB2	1:A:118:PHE:HA	6	0.75
(5,2)	1:A:116:ARG:HB3	1:A:118:PHE:HA	6	0.75
(5,2)	1:B:116:ARG:HB2	1:B:118:PHE:HA	6	0.75
(5,2)	1:B:116:ARG:HB3	1:B:118:PHE:HA	6	0.75
(1,258)	1:A:134:THR:H	1:A:133:ILE:HD11	1	0.75
(1,258)	1:A:134:THR:H	1:A:133:ILE:HD12	1	0.75
(1,258)	1:A:134:THR:H	1:A:133:ILE:HD13	1	0.75
(1,258)	1:B:134:THR:H	1:B:133:ILE:HD11	1	0.75
(1,258)	1:B:134:THR:H	1:B:133:ILE:HD12	1	0.75
(1,258)	1:B:134:THR:H	1:B:133:ILE:HD13	1	0.75
(1,258)	1:A:134:THR:H	1:A:133:ILE:HD11	2	0.75
(1,258)	1:A:134:THR:H	1:A:133:ILE:HD12	2	0.75
(1,258)	1:A:134:THR:H	1:A:133:ILE:HD13	2	0.75
(1,258)	1:B:134:THR:H	1:B:133:ILE:HD11	2	0.75
(1,258)	1:B:134:THR:H	1:B:133:ILE:HD12	2	0.75
(1,258)	1:B:134:THR:H	1:B:133:ILE:HD13	2	0.75
(1,309)	1:A:146:ASN:H	1:A:133:ILE:HA	8	0.74
(1,309)	1:B:146:ASN:H	1:B:133:ILE:HA	8	0.74
(1,258)	1:A:134:THR:H	1:A:133:ILE:HD11	4	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,258)	1:A:134:THR:H	1:A:133:ILE:HD12	4	0.72
(1,258)	1:A:134:THR:H	1:A:133:ILE:HD13	4	0.72
(1,258)	1:B:134:THR:H	1:B:133:ILE:HD11	4	0.72
(1,258)	1:B:134:THR:H	1:B:133:ILE:HD12	4	0.72
(1,258)	1:B:134:THR:H	1:B:133:ILE:HD13	4	0.72
(1,104)	1:A:92:LYS:H	1:A:100:VAL:HG11	7	0.72
(1,104)	1:A:92:LYS:H	1:A:100:VAL:HG12	7	0.72
(1,104)	1:A:92:LYS:H	1:A:100:VAL:HG13	7	0.72
(1,104)	1:B:92:LYS:H	1:B:100:VAL:HG11	7	0.72
(1,104)	1:B:92:LYS:H	1:B:100:VAL:HG12	7	0.72
(1,104)	1:B:92:LYS:H	1:B:100:VAL:HG13	7	0.72
(2,38)	1:B:82:LYS:HE2	1:B:83:HIS:HE1	8	0.7
(2,38)	1:B:82:LYS:HE3	1:B:83:HIS:HE1	8	0.7
(2,38)	1:A:82:LYS:HE2	1:A:83:HIS:HE1	8	0.7
(2,38)	1:A:82:LYS:HE3	1:A:83:HIS:HE1	8	0.7
(1,258)	1:A:134:THR:H	1:A:133:ILE:HD11	3	0.66
(1,258)	1:A:134:THR:H	1:A:133:ILE:HD12	3	0.66
(1,258)	1:A:134:THR:H	1:A:133:ILE:HD13	3	0.66
(1,258)	1:B:134:THR:H	1:B:133:ILE:HD11	3	0.66
(1,258)	1:B:134:THR:H	1:B:133:ILE:HD12	3	0.66
(1,258)	1:B:134:THR:H	1:B:133:ILE:HD13	3	0.66
(1,309)	1:A:146:ASN:H	1:A:133:ILE:HA	3	0.64
(1,309)	1:B:146:ASN:H	1:B:133:ILE:HA	3	0.64
(1,83)	1:B:85:SER:H	1:B:86:PRO:HA	8	0.59
(1,83)	1:A:85:SER:H	1:A:86:PRO:HA	8	0.59
(1,104)	1:A:92:LYS:H	1:A:100:VAL:HG11	1	0.59
(1,104)	1:A:92:LYS:H	1:A:100:VAL:HG12	1	0.59
(1,104)	1:A:92:LYS:H	1:A:100:VAL:HG13	1	0.59
(1,104)	1:B:92:LYS:H	1:B:100:VAL:HG11	1	0.59
(1,104)	1:B:92:LYS:H	1:B:100:VAL:HG12	1	0.59
(1,104)	1:B:92:LYS:H	1:B:100:VAL:HG13	1	0.59
(2,92)	1:B:104:HIS:H	1:B:105:GLU:HG2	7	0.58
(2,92)	1:B:104:HIS:H	1:B:105:GLU:HG3	7	0.58
(2,92)	1:A:104:HIS:H	1:A:105:GLU:HG2	7	0.58
(2,92)	1:A:104:HIS:H	1:A:105:GLU:HG3	7	0.58
(2,102)	1:A:108:GLN:H	1:A:113:PHE:H	7	0.58
(2,102)	1:B:108:GLN:H	1:B:113:PHE:H	7	0.58
(5,2)	1:A:116:ARG:HB2	1:A:118:PHE:HA	3	0.57
(5,2)	1:A:116:ARG:HB3	1:A:118:PHE:HA	3	0.57
(5,2)	1:B:116:ARG:HB2	1:B:118:PHE:HA	3	0.57
(5,2)	1:B:116:ARG:HB3	1:B:118:PHE:HA	3	0.57
(2,57)	1:B:89:LEU:HD21	1:B:81:VAL:HG11	6	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,57)	1:B:89:LEU:HD21	1:B:81:VAL:HG12	6	0.57
(2,57)	1:B:89:LEU:HD21	1:B:81:VAL:HG13	6	0.57
(2,57)	1:B:89:LEU:HD22	1:B:81:VAL:HG11	6	0.57
(2,57)	1:B:89:LEU:HD22	1:B:81:VAL:HG12	6	0.57
(2,57)	1:B:89:LEU:HD22	1:B:81:VAL:HG13	6	0.57
(2,57)	1:B:89:LEU:HD23	1:B:81:VAL:HG11	6	0.57
(2,57)	1:B:89:LEU:HD23	1:B:81:VAL:HG12	6	0.57
(2,57)	1:B:89:LEU:HD23	1:B:81:VAL:HG13	6	0.57
(2,57)	1:A:89:LEU:HD21	1:A:81:VAL:HG11	6	0.57
(2,57)	1:A:89:LEU:HD21	1:A:81:VAL:HG12	6	0.57
(2,57)	1:A:89:LEU:HD21	1:A:81:VAL:HG13	6	0.57
(2,57)	1:A:89:LEU:HD22	1:A:81:VAL:HG11	6	0.57
(2,57)	1:A:89:LEU:HD22	1:A:81:VAL:HG12	6	0.57
(2,57)	1:A:89:LEU:HD22	1:A:81:VAL:HG13	6	0.57
(2,57)	1:A:89:LEU:HD23	1:A:81:VAL:HG11	6	0.57
(2,57)	1:A:89:LEU:HD23	1:A:81:VAL:HG12	6	0.57
(2,57)	1:A:89:LEU:HD23	1:A:81:VAL:HG13	6	0.57
(1,3)	1:A:66:SER:HA	1:A:65:LEU:HD11	3	0.57
(1,3)	1:A:66:SER:HA	1:A:65:LEU:HD12	3	0.57
(1,3)	1:A:66:SER:HA	1:A:65:LEU:HD13	3	0.57
(1,3)	1:A:66:SER:HA	1:A:65:LEU:HD21	3	0.57
(1,3)	1:A:66:SER:HA	1:A:65:LEU:HD22	3	0.57
(1,3)	1:A:66:SER:HA	1:A:65:LEU:HD23	3	0.57
(1,3)	1:B:66:SER:HA	1:B:65:LEU:HD11	3	0.57
(1,3)	1:B:66:SER:HA	1:B:65:LEU:HD12	3	0.57
(1,3)	1:B:66:SER:HA	1:B:65:LEU:HD13	3	0.57
(1,3)	1:B:66:SER:HA	1:B:65:LEU:HD21	3	0.57
(1,3)	1:B:66:SER:HA	1:B:65:LEU:HD22	3	0.57
(1,3)	1:B:66:SER:HA	1:B:65:LEU:HD23	3	0.57
(2,7)	1:A:66:SER:HB2	1:A:77:VAL:HG11	3	0.55
(2,7)	1:A:66:SER:HB2	1:A:77:VAL:HG12	3	0.55
(2,7)	1:A:66:SER:HB2	1:A:77:VAL:HG13	3	0.55
(2,7)	1:A:66:SER:HB3	1:A:77:VAL:HG11	3	0.55
(2,7)	1:A:66:SER:HB3	1:A:77:VAL:HG12	3	0.55
(2,7)	1:A:66:SER:HB3	1:A:77:VAL:HG13	3	0.55
(2,7)	1:B:66:SER:HB2	1:B:77:VAL:HG11	3	0.55
(2,7)	1:B:66:SER:HB2	1:B:77:VAL:HG12	3	0.55
(2,7)	1:B:66:SER:HB2	1:B:77:VAL:HG13	3	0.55
(2,7)	1:B:66:SER:HB3	1:B:77:VAL:HG11	3	0.55
(2,7)	1:B:66:SER:HB3	1:B:77:VAL:HG12	3	0.55
(2,7)	1:B:66:SER:HB3	1:B:77:VAL:HG13	3	0.55
(1,83)	1:B:85:SER:H	1:B:86:PRO:HA	7	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,83)	1:A:85:SER:H	1:A:86:PRO:HA	7	0.55
(4,30)	1:B:118:PHE:HA	1:B:116:ARG:HG2	6	0.54
(4,30)	1:B:118:PHE:HA	1:B:116:ARG:HG3	6	0.54
(4,30)	1:A:118:PHE:HA	1:A:116:ARG:HG2	6	0.54
(4,30)	1:A:118:PHE:HA	1:A:116:ARG:HG3	6	0.54
(4,30)	1:B:118:PHE:HA	1:B:116:ARG:HG2	8	0.52
(4,30)	1:B:118:PHE:HA	1:B:116:ARG:HG3	8	0.52
(4,30)	1:A:118:PHE:HA	1:A:116:ARG:HG2	8	0.52
(4,30)	1:A:118:PHE:HA	1:A:116:ARG:HG3	8	0.52
(4,22)	1:A:114:ILE:HG21	1:A:118:PHE:HB2	1	0.51
(4,22)	1:A:114:ILE:HG21	1:A:118:PHE:HB3	1	0.51
(4,22)	1:A:114:ILE:HG22	1:A:118:PHE:HB2	1	0.51
(4,22)	1:A:114:ILE:HG22	1:A:118:PHE:HB3	1	0.51
(4,22)	1:A:114:ILE:HG23	1:A:118:PHE:HB2	1	0.51
(4,22)	1:A:114:ILE:HG23	1:A:118:PHE:HB3	1	0.51
(4,22)	1:B:114:ILE:HG21	1:B:118:PHE:HB2	1	0.51
(4,22)	1:B:114:ILE:HG21	1:B:118:PHE:HB3	1	0.51
(4,22)	1:B:114:ILE:HG22	1:B:118:PHE:HB2	1	0.51
(4,22)	1:B:114:ILE:HG22	1:B:118:PHE:HB3	1	0.51
(4,22)	1:B:114:ILE:HG23	1:B:118:PHE:HB2	1	0.51
(4,22)	1:B:114:ILE:HG23	1:B:118:PHE:HB3	1	0.51
(4,21)	1:A:114:ILE:HG21	1:A:118:PHE:HB2	1	0.51
(4,21)	1:A:114:ILE:HG21	1:A:118:PHE:HB3	1	0.51
(4,21)	1:A:114:ILE:HG22	1:A:118:PHE:HB2	1	0.51
(4,21)	1:A:114:ILE:HG22	1:A:118:PHE:HB3	1	0.51
(4,21)	1:A:114:ILE:HG23	1:A:118:PHE:HB2	1	0.51
(4,21)	1:A:114:ILE:HG23	1:A:118:PHE:HB3	1	0.51
(4,21)	1:B:114:ILE:HG21	1:B:118:PHE:HB2	1	0.51
(4,21)	1:B:114:ILE:HG21	1:B:118:PHE:HB3	1	0.51
(4,21)	1:B:114:ILE:HG22	1:B:118:PHE:HB2	1	0.51
(4,21)	1:B:114:ILE:HG22	1:B:118:PHE:HB3	1	0.51
(4,21)	1:B:114:ILE:HG23	1:B:118:PHE:HB2	1	0.51
(4,21)	1:B:114:ILE:HG23	1:B:118:PHE:HB3	1	0.51
(2,6)	1:A:66:SER:HB2	1:A:77:VAL:HG21	1	0.51
(2,6)	1:A:66:SER:HB2	1:A:77:VAL:HG22	1	0.51
(2,6)	1:A:66:SER:HB2	1:A:77:VAL:HG23	1	0.51
(2,6)	1:A:66:SER:HB3	1:A:77:VAL:HG21	1	0.51
(2,6)	1:A:66:SER:HB3	1:A:77:VAL:HG22	1	0.51
(2,6)	1:A:66:SER:HB3	1:A:77:VAL:HG23	1	0.51
(2,6)	1:B:66:SER:HB2	1:B:77:VAL:HG21	1	0.51
(2,6)	1:B:66:SER:HB2	1:B:77:VAL:HG22	1	0.51
(2,6)	1:B:66:SER:HB2	1:B:77:VAL:HG23	1	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,6)	1:B:66:SER:HB3	1:B:77:VAL:HG21	1	0.51
(2,6)	1:B:66:SER:HB3	1:B:77:VAL:HG22	1	0.51
(2,6)	1:B:66:SER:HB3	1:B:77:VAL:HG23	1	0.51
(2,95)	1:B:106:GLU:H	1:B:115:SER:HB2	1	0.49
(2,95)	1:B:106:GLU:H	1:B:115:SER:HB3	1	0.49
(2,95)	1:A:106:GLU:H	1:A:115:SER:HB2	1	0.49
(2,95)	1:A:106:GLU:H	1:A:115:SER:HB3	1	0.49
(1,83)	1:B:85:SER:H	1:B:86:PRO:HA	1	0.49
(1,83)	1:A:85:SER:H	1:A:86:PRO:HA	1	0.49
(1,290)	1:A:138:SER:H	1:A:137:LEU:HD21	7	0.49
(1,290)	1:A:138:SER:H	1:A:137:LEU:HD22	7	0.49
(1,290)	1:A:138:SER:H	1:A:137:LEU:HD23	7	0.49
(1,290)	1:B:138:SER:H	1:B:137:LEU:HD21	7	0.49
(1,290)	1:B:138:SER:H	1:B:137:LEU:HD22	7	0.49
(1,290)	1:B:138:SER:H	1:B:137:LEU:HD23	7	0.49
(2,133)	1:B:118:PHE:HB2	1:B:81:VAL:HG21	7	0.48
(2,133)	1:B:118:PHE:HB2	1:B:81:VAL:HG22	7	0.48
(2,133)	1:B:118:PHE:HB2	1:B:81:VAL:HG23	7	0.48
(2,133)	1:B:118:PHE:HB3	1:B:81:VAL:HG21	7	0.48
(2,133)	1:B:118:PHE:HB3	1:B:81:VAL:HG22	7	0.48
(2,133)	1:B:118:PHE:HB3	1:B:81:VAL:HG23	7	0.48
(2,133)	1:A:118:PHE:HB2	1:A:81:VAL:HG21	7	0.48
(2,133)	1:A:118:PHE:HB2	1:A:81:VAL:HG22	7	0.48
(2,133)	1:A:118:PHE:HB2	1:A:81:VAL:HG23	7	0.48
(2,133)	1:A:118:PHE:HB3	1:A:81:VAL:HG21	7	0.48
(2,133)	1:A:118:PHE:HB3	1:A:81:VAL:HG22	7	0.48
(2,133)	1:A:118:PHE:HB3	1:A:81:VAL:HG23	7	0.48
(2,108)	1:A:108:GLN:H	1:A:114:ILE:HD11	6	0.48
(2,108)	1:A:108:GLN:H	1:A:114:ILE:HD12	6	0.48
(2,108)	1:A:108:GLN:H	1:A:114:ILE:HD13	6	0.48
(2,108)	1:B:108:GLN:H	1:B:114:ILE:HD11	6	0.48
(2,108)	1:B:108:GLN:H	1:B:114:ILE:HD12	6	0.48
(2,108)	1:B:108:GLN:H	1:B:114:ILE:HD13	6	0.48
(1,83)	1:B:85:SER:H	1:B:86:PRO:HA	2	0.48
(1,83)	1:A:85:SER:H	1:A:86:PRO:HA	2	0.48
(1,231)	1:A:127:ASP:H	1:A:128:VAL:HG11	7	0.48
(1,231)	1:A:127:ASP:H	1:A:128:VAL:HG12	7	0.48
(1,231)	1:A:127:ASP:H	1:A:128:VAL:HG13	7	0.48
(1,231)	1:B:127:ASP:H	1:B:128:VAL:HG11	7	0.48
(1,231)	1:B:127:ASP:H	1:B:128:VAL:HG12	7	0.48
(1,231)	1:B:127:ASP:H	1:B:128:VAL:HG13	7	0.48
(1,83)	1:B:85:SER:H	1:B:86:PRO:HA	5	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,83)	1:A:85:SER:H	1:A:86:PRO:HA	5	0.47
(1,290)	1:A:138:SER:H	1:A:137:LEU:HD21	4	0.47
(1,290)	1:A:138:SER:H	1:A:137:LEU:HD22	4	0.47
(1,290)	1:A:138:SER:H	1:A:137:LEU:HD23	4	0.47
(1,290)	1:B:138:SER:H	1:B:137:LEU:HD21	4	0.47
(1,290)	1:B:138:SER:H	1:B:137:LEU:HD22	4	0.47
(1,290)	1:B:138:SER:H	1:B:137:LEU:HD23	4	0.47
(2,92)	1:B:104:HIS:H	1:B:105:GLU:HG2	1	0.46
(2,92)	1:B:104:HIS:H	1:B:105:GLU:HG3	1	0.46
(2,92)	1:A:104:HIS:H	1:A:105:GLU:HG2	1	0.46
(2,92)	1:A:104:HIS:H	1:A:105:GLU:HG3	1	0.46
(1,69)	1:B:82:LYS:HE2	1:B:82:LYS:HA	6	0.46
(1,69)	1:B:82:LYS:HE3	1:B:82:LYS:HA	6	0.46
(1,69)	1:A:82:LYS:HE2	1:A:82:LYS:HA	6	0.46
(1,69)	1:A:82:LYS:HE3	1:A:82:LYS:HA	6	0.46
(1,290)	1:A:138:SER:H	1:A:137:LEU:HD21	2	0.46
(1,290)	1:A:138:SER:H	1:A:137:LEU:HD22	2	0.46
(1,290)	1:A:138:SER:H	1:A:137:LEU:HD23	2	0.46
(1,290)	1:B:138:SER:H	1:B:137:LEU:HD21	2	0.46
(1,290)	1:B:138:SER:H	1:B:137:LEU:HD22	2	0.46
(1,290)	1:B:138:SER:H	1:B:137:LEU:HD23	2	0.46
(1,83)	1:B:85:SER:H	1:B:86:PRO:HA	6	0.45
(1,83)	1:A:85:SER:H	1:A:86:PRO:HA	6	0.45
(1,309)	1:A:146:ASN:H	1:A:133:ILE:HA	2	0.45
(1,309)	1:B:146:ASN:H	1:B:133:ILE:HA	2	0.45
(1,27)	1:B:73:ASP:H	1:B:74:ARG:HB2	4	0.45
(1,27)	1:B:73:ASP:H	1:B:74:ARG:HB3	4	0.45
(1,27)	1:A:73:ASP:H	1:A:74:ARG:HB2	4	0.45
(1,27)	1:A:73:ASP:H	1:A:74:ARG:HB3	4	0.45
(4,31)	1:B:118:PHE:HB2	1:B:116:ARG:HA	2	0.41
(4,31)	1:B:118:PHE:HB3	1:B:116:ARG:HA	2	0.41
(4,31)	1:A:118:PHE:HB2	1:A:116:ARG:HA	2	0.41
(4,31)	1:A:118:PHE:HB3	1:A:116:ARG:HA	2	0.41
(4,30)	1:B:118:PHE:HA	1:B:116:ARG:HG2	3	0.41
(4,30)	1:B:118:PHE:HA	1:B:116:ARG:HG3	3	0.41
(4,30)	1:A:118:PHE:HA	1:A:116:ARG:HG2	3	0.41
(4,30)	1:A:118:PHE:HA	1:A:116:ARG:HG3	3	0.41
(1,49)	1:A:78:ASN:HA	1:A:79:LEU:HD11	4	0.41
(1,49)	1:A:78:ASN:HA	1:A:79:LEU:HD12	4	0.41
(1,49)	1:A:78:ASN:HA	1:A:79:LEU:HD13	4	0.41
(1,49)	1:A:78:ASN:HA	1:A:79:LEU:HD21	4	0.41
(1,49)	1:A:78:ASN:HA	1:A:79:LEU:HD22	4	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,49)	1:A:78:ASN:HA	1:A:79:LEU:HD23	4	0.41
(1,49)	1:B:78:ASN:HA	1:B:79:LEU:HD11	4	0.41
(1,49)	1:B:78:ASN:HA	1:B:79:LEU:HD12	4	0.41
(1,49)	1:B:78:ASN:HA	1:B:79:LEU:HD13	4	0.41
(1,49)	1:B:78:ASN:HA	1:B:79:LEU:HD21	4	0.41
(1,49)	1:B:78:ASN:HA	1:B:79:LEU:HD22	4	0.41
(1,49)	1:B:78:ASN:HA	1:B:79:LEU:HD23	4	0.41
(1,290)	1:A:138:SER:H	1:A:137:LEU:HD21	3	0.41
(1,290)	1:A:138:SER:H	1:A:137:LEU:HD22	3	0.41
(1,290)	1:A:138:SER:H	1:A:137:LEU:HD23	3	0.41
(1,290)	1:B:138:SER:H	1:B:137:LEU:HD21	3	0.41
(1,290)	1:B:138:SER:H	1:B:137:LEU:HD22	3	0.41
(1,290)	1:B:138:SER:H	1:B:137:LEU:HD23	3	0.41
(4,31)	1:B:118:PHE:HB2	1:B:116:ARG:HA	3	0.4
(4,31)	1:B:118:PHE:HB3	1:B:116:ARG:HA	3	0.4
(4,31)	1:A:118:PHE:HB2	1:A:116:ARG:HA	3	0.4
(4,31)	1:A:118:PHE:HB3	1:A:116:ARG:HA	3	0.4
(4,22)	1:A:114:ILE:HG21	1:A:118:PHE:HB2	8	0.4
(4,22)	1:A:114:ILE:HG21	1:A:118:PHE:HB3	8	0.4
(4,22)	1:A:114:ILE:HG22	1:A:118:PHE:HB2	8	0.4
(4,22)	1:A:114:ILE:HG22	1:A:118:PHE:HB3	8	0.4
(4,22)	1:A:114:ILE:HG23	1:A:118:PHE:HB2	8	0.4
(4,22)	1:A:114:ILE:HG23	1:A:118:PHE:HB3	8	0.4
(4,22)	1:B:114:ILE:HG21	1:B:118:PHE:HB2	8	0.4
(4,22)	1:B:114:ILE:HG21	1:B:118:PHE:HB3	8	0.4
(4,22)	1:B:114:ILE:HG22	1:B:118:PHE:HB2	8	0.4
(4,22)	1:B:114:ILE:HG22	1:B:118:PHE:HB3	8	0.4
(4,22)	1:B:114:ILE:HG23	1:B:118:PHE:HB2	8	0.4
(4,22)	1:B:114:ILE:HG23	1:B:118:PHE:HB3	8	0.4
(4,21)	1:A:114:ILE:HG21	1:A:118:PHE:HB2	8	0.4
(4,21)	1:A:114:ILE:HG21	1:A:118:PHE:HB3	8	0.4
(4,21)	1:A:114:ILE:HG22	1:A:118:PHE:HB2	8	0.4
(4,21)	1:A:114:ILE:HG22	1:A:118:PHE:HB3	8	0.4
(4,21)	1:A:114:ILE:HG23	1:A:118:PHE:HB2	8	0.4
(4,21)	1:A:114:ILE:HG23	1:A:118:PHE:HB3	8	0.4
(4,21)	1:B:114:ILE:HG21	1:B:118:PHE:HB2	8	0.4
(4,21)	1:B:114:ILE:HG21	1:B:118:PHE:HB3	8	0.4
(4,21)	1:B:114:ILE:HG22	1:B:118:PHE:HB2	8	0.4
(4,21)	1:B:114:ILE:HG22	1:B:118:PHE:HB3	8	0.4
(4,21)	1:B:114:ILE:HG23	1:B:118:PHE:HB2	8	0.4
(4,21)	1:B:114:ILE:HG23	1:B:118:PHE:HB3	8	0.4
(2,107)	1:A:108:GLN:HG2	1:A:113:PHE:HB2	2	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,107)	1:A:108:GLN:HG3	1:A:113:PHE:HB2	2	0.4
(2,107)	1:B:108:GLN:HG2	1:B:113:PHE:HB2	2	0.4
(2,107)	1:B:108:GLN:HG3	1:B:113:PHE:HB2	2	0.4
(1,290)	1:A:138:SER:H	1:A:137:LEU:HD21	5	0.4
(1,290)	1:A:138:SER:H	1:A:137:LEU:HD22	5	0.4
(1,290)	1:A:138:SER:H	1:A:137:LEU:HD23	5	0.4
(1,290)	1:B:138:SER:H	1:B:137:LEU:HD21	5	0.4
(1,290)	1:B:138:SER:H	1:B:137:LEU:HD22	5	0.4
(1,290)	1:B:138:SER:H	1:B:137:LEU:HD23	5	0.4
(1,309)	1:A:146:ASN:H	1:A:133:ILE:HA	4	0.39
(1,309)	1:B:146:ASN:H	1:B:133:ILE:HA	4	0.39
(1,290)	1:A:138:SER:H	1:A:137:LEU:HD21	8	0.39
(1,290)	1:A:138:SER:H	1:A:137:LEU:HD22	8	0.39
(1,290)	1:A:138:SER:H	1:A:137:LEU:HD23	8	0.39
(1,290)	1:B:138:SER:H	1:B:137:LEU:HD21	8	0.39
(1,290)	1:B:138:SER:H	1:B:137:LEU:HD22	8	0.39
(1,290)	1:B:138:SER:H	1:B:137:LEU:HD23	8	0.39
(3,115)	1:A:83:HIS:H	1:A:82:LYS:H	6	0.38
(3,115)	1:B:83:HIS:H	1:B:82:LYS:H	6	0.38
(1,83)	1:B:85:SER:H	1:B:86:PRO:HA	3	0.38
(1,83)	1:A:85:SER:H	1:A:86:PRO:HA	3	0.38
(1,309)	1:A:146:ASN:H	1:A:133:ILE:HA	7	0.37
(1,309)	1:B:146:ASN:H	1:B:133:ILE:HA	7	0.37
(1,290)	1:A:138:SER:H	1:A:137:LEU:HD21	1	0.37
(1,290)	1:A:138:SER:H	1:A:137:LEU:HD22	1	0.37
(1,290)	1:A:138:SER:H	1:A:137:LEU:HD23	1	0.37
(1,290)	1:B:138:SER:H	1:B:137:LEU:HD21	1	0.37
(1,290)	1:B:138:SER:H	1:B:137:LEU:HD22	1	0.37
(1,290)	1:B:138:SER:H	1:B:137:LEU:HD23	1	0.37
(1,209)	1:A:121:LYS:H	1:A:122:TYR:HA	8	0.37
(1,209)	1:B:121:LYS:H	1:B:122:TYR:HA	8	0.37
(5,2)	1:A:116:ARG:HB2	1:A:118:PHE:HA	1	0.36
(5,2)	1:A:116:ARG:HB3	1:A:118:PHE:HA	1	0.36
(5,2)	1:B:116:ARG:HB2	1:B:118:PHE:HA	1	0.36
(5,2)	1:B:116:ARG:HB3	1:B:118:PHE:HA	1	0.36
(1,172)	1:A:113:PHE:HA	1:A:107:ARG:HA	4	0.36
(1,172)	1:B:113:PHE:HA	1:B:107:ARG:HA	4	0.36
(2,4)	1:A:66:SER:HA	1:A:65:LEU:HG	4	0.34
(2,4)	1:B:66:SER:HA	1:B:65:LEU:HG	4	0.34
(1,209)	1:A:121:LYS:H	1:A:122:TYR:HA	2	0.34
(1,209)	1:B:121:LYS:H	1:B:122:TYR:HA	2	0.34
(2,100)	1:A:108:GLN:H	1:A:112:GLY:H	4	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,100)	1:B:108:GLN:H	1:B:112:GLY:H	4	0.33
(1,83)	1:B:85:SER:H	1:B:86:PRO:HA	4	0.31
(1,83)	1:A:85:SER:H	1:A:86:PRO:HA	4	0.31
(1,49)	1:A:78:ASN:HA	1:A:79:LEU:HD11	1	0.31
(1,49)	1:A:78:ASN:HA	1:A:79:LEU:HD12	1	0.31
(1,49)	1:A:78:ASN:HA	1:A:79:LEU:HD13	1	0.31
(1,49)	1:A:78:ASN:HA	1:A:79:LEU:HD21	1	0.31
(1,49)	1:A:78:ASN:HA	1:A:79:LEU:HD22	1	0.31
(1,49)	1:A:78:ASN:HA	1:A:79:LEU:HD23	1	0.31
(1,49)	1:B:78:ASN:HA	1:B:79:LEU:HD11	1	0.31
(1,49)	1:B:78:ASN:HA	1:B:79:LEU:HD12	1	0.31
(1,49)	1:B:78:ASN:HA	1:B:79:LEU:HD13	1	0.31
(1,49)	1:B:78:ASN:HA	1:B:79:LEU:HD21	1	0.31
(1,49)	1:B:78:ASN:HA	1:B:79:LEU:HD22	1	0.31
(1,49)	1:B:78:ASN:HA	1:B:79:LEU:HD23	1	0.31
(2,113)	1:A:113:PHE:H	1:A:111:HIS:HA	7	0.29
(2,113)	1:B:113:PHE:H	1:B:111:HIS:HA	7	0.29
(1,326)	1:B:151:GLN:H	1:B:152:VAL:H	2	0.29
(1,326)	1:A:151:GLN:H	1:A:152:VAL:H	2	0.29
(1,324)	1:B:151:GLN:H	1:B:150:LYS:H	1	0.29
(1,324)	1:A:151:GLN:H	1:A:150:LYS:H	1	0.29
(4,33)	1:B:118:PHE:HA	1:B:116:ARG:HA	4	0.27
(4,33)	1:A:118:PHE:HA	1:A:116:ARG:HA	4	0.27
(4,29)	1:A:116:ARG:HA	1:A:118:PHE:HA	4	0.27
(4,29)	1:B:116:ARG:HA	1:B:118:PHE:HA	4	0.27
(3,270)	1:B:110:GLU:H	1:B:109:ASP:HB2	2	0.27
(3,270)	1:B:110:GLU:H	1:B:109:ASP:HB3	2	0.27
(3,270)	1:A:110:GLU:H	1:A:109:ASP:HB2	2	0.27
(3,270)	1:A:110:GLU:H	1:A:109:ASP:HB3	2	0.27
(3,270)	1:B:110:GLU:H	1:B:109:ASP:HB2	6	0.27
(3,270)	1:B:110:GLU:H	1:B:109:ASP:HB3	6	0.27
(3,270)	1:A:110:GLU:H	1:A:109:ASP:HB2	6	0.27
(3,270)	1:A:110:GLU:H	1:A:109:ASP:HB3	6	0.27
(2,146)	1:A:127:ASP:H	1:A:124:ILE:HG21	2	0.26
(2,146)	1:A:127:ASP:H	1:A:124:ILE:HG22	2	0.26
(2,146)	1:A:127:ASP:H	1:A:124:ILE:HG23	2	0.26
(2,146)	1:B:127:ASP:H	1:B:124:ILE:HG21	2	0.26
(2,146)	1:B:127:ASP:H	1:B:124:ILE:HG22	2	0.26
(2,146)	1:B:127:ASP:H	1:B:124:ILE:HG23	2	0.26
(2,113)	1:A:113:PHE:H	1:A:111:HIS:HA	6	0.26
(2,113)	1:B:113:PHE:H	1:B:111:HIS:HA	6	0.26
(2,146)	1:A:127:ASP:H	1:A:124:ILE:HG21	1	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,146)	1:A:127:ASP:H	1:A:124:ILE:HG22	1	0.25
(2,146)	1:A:127:ASP:H	1:A:124:ILE:HG23	1	0.25
(2,146)	1:B:127:ASP:H	1:B:124:ILE:HG21	1	0.25
(2,146)	1:B:127:ASP:H	1:B:124:ILE:HG22	1	0.25
(2,146)	1:B:127:ASP:H	1:B:124:ILE:HG23	1	0.25
(1,3)	1:A:66:SER:HA	1:A:65:LEU:HD11	1	0.25
(1,3)	1:A:66:SER:HA	1:A:65:LEU:HD12	1	0.25
(1,3)	1:A:66:SER:HA	1:A:65:LEU:HD13	1	0.25
(1,3)	1:A:66:SER:HA	1:A:65:LEU:HD21	1	0.25
(1,3)	1:A:66:SER:HA	1:A:65:LEU:HD22	1	0.25
(1,3)	1:A:66:SER:HA	1:A:65:LEU:HD23	1	0.25
(1,3)	1:B:66:SER:HA	1:B:65:LEU:HD11	1	0.25
(1,3)	1:B:66:SER:HA	1:B:65:LEU:HD12	1	0.25
(1,3)	1:B:66:SER:HA	1:B:65:LEU:HD13	1	0.25
(1,3)	1:B:66:SER:HA	1:B:65:LEU:HD21	1	0.25
(1,3)	1:B:66:SER:HA	1:B:65:LEU:HD22	1	0.25
(1,3)	1:B:66:SER:HA	1:B:65:LEU:HD23	1	0.25
(1,3)	1:A:66:SER:HA	1:A:65:LEU:HD11	4	0.24
(1,3)	1:A:66:SER:HA	1:A:65:LEU:HD12	4	0.24
(1,3)	1:A:66:SER:HA	1:A:65:LEU:HD13	4	0.24
(1,3)	1:A:66:SER:HA	1:A:65:LEU:HD21	4	0.24
(1,3)	1:A:66:SER:HA	1:A:65:LEU:HD22	4	0.24
(1,3)	1:A:66:SER:HA	1:A:65:LEU:HD23	4	0.24
(1,3)	1:B:66:SER:HA	1:B:65:LEU:HD11	4	0.24
(1,3)	1:B:66:SER:HA	1:B:65:LEU:HD12	4	0.24
(1,3)	1:B:66:SER:HA	1:B:65:LEU:HD13	4	0.24
(1,3)	1:B:66:SER:HA	1:B:65:LEU:HD21	4	0.24
(1,3)	1:B:66:SER:HA	1:B:65:LEU:HD22	4	0.24
(1,3)	1:B:66:SER:HA	1:B:65:LEU:HD23	4	0.24
(1,172)	1:A:113:PHE:HA	1:A:107:ARG:HA	1	0.24
(1,172)	1:B:113:PHE:HA	1:B:107:ARG:HA	1	0.24
(1,3)	1:A:66:SER:HA	1:A:65:LEU:HD11	6	0.23
(1,3)	1:A:66:SER:HA	1:A:65:LEU:HD12	6	0.23
(1,3)	1:A:66:SER:HA	1:A:65:LEU:HD13	6	0.23
(1,3)	1:A:66:SER:HA	1:A:65:LEU:HD21	6	0.23
(1,3)	1:A:66:SER:HA	1:A:65:LEU:HD22	6	0.23
(1,3)	1:A:66:SER:HA	1:A:65:LEU:HD23	6	0.23
(1,3)	1:B:66:SER:HA	1:B:65:LEU:HD11	6	0.23
(1,3)	1:B:66:SER:HA	1:B:65:LEU:HD12	6	0.23
(1,3)	1:B:66:SER:HA	1:B:65:LEU:HD13	6	0.23
(1,3)	1:B:66:SER:HA	1:B:65:LEU:HD21	6	0.23
(1,3)	1:B:66:SER:HA	1:B:65:LEU:HD22	6	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3)	1:B:66:SER:HA	1:B:65:LEU:HD23	6	0.23
(1,49)	1:A:78:ASN:HA	1:A:79:LEU:HD11	2	0.21
(1,49)	1:A:78:ASN:HA	1:A:79:LEU:HD12	2	0.21
(1,49)	1:A:78:ASN:HA	1:A:79:LEU:HD13	2	0.21
(1,49)	1:A:78:ASN:HA	1:A:79:LEU:HD21	2	0.21
(1,49)	1:A:78:ASN:HA	1:A:79:LEU:HD22	2	0.21
(1,49)	1:A:78:ASN:HA	1:A:79:LEU:HD23	2	0.21
(1,49)	1:B:78:ASN:HA	1:B:79:LEU:HD11	2	0.21
(1,49)	1:B:78:ASN:HA	1:B:79:LEU:HD12	2	0.21
(1,49)	1:B:78:ASN:HA	1:B:79:LEU:HD13	2	0.21
(1,49)	1:B:78:ASN:HA	1:B:79:LEU:HD21	2	0.21
(1,49)	1:B:78:ASN:HA	1:B:79:LEU:HD22	2	0.21
(1,49)	1:B:78:ASN:HA	1:B:79:LEU:HD23	2	0.21
(3,283)	1:A:111:HIS:H	1:A:112:GLY:H	6	0.2
(3,283)	1:B:111:HIS:H	1:B:112:GLY:H	6	0.2
(2,9)	1:A:66:SER:HA	1:A:77:VAL:HG11	3	0.19
(2,9)	1:A:66:SER:HA	1:A:77:VAL:HG12	3	0.19
(2,9)	1:A:66:SER:HA	1:A:77:VAL:HG13	3	0.19
(2,9)	1:B:66:SER:HA	1:B:77:VAL:HG11	3	0.19
(2,9)	1:B:66:SER:HA	1:B:77:VAL:HG12	3	0.19
(2,9)	1:B:66:SER:HA	1:B:77:VAL:HG13	3	0.19
(3,329)	1:B:118:PHE:HA	1:B:118:PHE:HD1	8	0.18
(3,329)	1:B:118:PHE:HA	1:B:118:PHE:HD2	8	0.18
(3,329)	1:A:118:PHE:HA	1:A:118:PHE:HD1	8	0.18
(3,329)	1:A:118:PHE:HA	1:A:118:PHE:HD2	8	0.18
(2,8)	1:A:66:SER:HA	1:A:77:VAL:HG21	1	0.18
(2,8)	1:A:66:SER:HA	1:A:77:VAL:HG22	1	0.18
(2,8)	1:A:66:SER:HA	1:A:77:VAL:HG23	1	0.18
(2,8)	1:B:66:SER:HA	1:B:77:VAL:HG21	1	0.18
(2,8)	1:B:66:SER:HA	1:B:77:VAL:HG22	1	0.18
(2,8)	1:B:66:SER:HA	1:B:77:VAL:HG23	1	0.18
(1,3)	1:A:66:SER:HA	1:A:65:LEU:HD11	2	0.17
(1,3)	1:A:66:SER:HA	1:A:65:LEU:HD12	2	0.17
(1,3)	1:A:66:SER:HA	1:A:65:LEU:HD13	2	0.17
(1,3)	1:A:66:SER:HA	1:A:65:LEU:HD21	2	0.17
(1,3)	1:A:66:SER:HA	1:A:65:LEU:HD22	2	0.17
(1,3)	1:A:66:SER:HA	1:A:65:LEU:HD23	2	0.17
(1,3)	1:B:66:SER:HA	1:B:65:LEU:HD11	2	0.17
(1,3)	1:B:66:SER:HA	1:B:65:LEU:HD12	2	0.17
(1,3)	1:B:66:SER:HA	1:B:65:LEU:HD13	2	0.17
(1,3)	1:B:66:SER:HA	1:B:65:LEU:HD21	2	0.17
(1,3)	1:B:66:SER:HA	1:B:65:LEU:HD22	2	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3)	1:B:66:SER:HA	1:B:65:LEU:HD23	2	0.17
(1,3)	1:A:66:SER:HA	1:A:65:LEU:HD11	5	0.17
(1,3)	1:A:66:SER:HA	1:A:65:LEU:HD12	5	0.17
(1,3)	1:A:66:SER:HA	1:A:65:LEU:HD13	5	0.17
(1,3)	1:A:66:SER:HA	1:A:65:LEU:HD21	5	0.17
(1,3)	1:A:66:SER:HA	1:A:65:LEU:HD22	5	0.17
(1,3)	1:A:66:SER:HA	1:A:65:LEU:HD23	5	0.17
(1,3)	1:B:66:SER:HA	1:B:65:LEU:HD11	5	0.17
(1,3)	1:B:66:SER:HA	1:B:65:LEU:HD12	5	0.17
(1,3)	1:B:66:SER:HA	1:B:65:LEU:HD13	5	0.17
(1,3)	1:B:66:SER:HA	1:B:65:LEU:HD21	5	0.17
(1,3)	1:B:66:SER:HA	1:B:65:LEU:HD22	5	0.17
(1,3)	1:B:66:SER:HA	1:B:65:LEU:HD23	5	0.17
(3,31)	1:A:72:LYS:H	1:A:71:GLU:HB2	1	0.16
(3,31)	1:A:72:LYS:H	1:A:71:GLU:HB3	1	0.16
(3,31)	1:B:72:LYS:H	1:B:71:GLU:HB2	1	0.16
(3,31)	1:B:72:LYS:H	1:B:71:GLU:HB3	1	0.16
(1,104)	1:A:92:LYS:H	1:A:100:VAL:HG11	4	0.16
(1,104)	1:A:92:LYS:H	1:A:100:VAL:HG12	4	0.16
(1,104)	1:A:92:LYS:H	1:A:100:VAL:HG13	4	0.16
(1,104)	1:B:92:LYS:H	1:B:100:VAL:HG11	4	0.16
(1,104)	1:B:92:LYS:H	1:B:100:VAL:HG12	4	0.16
(1,104)	1:B:92:LYS:H	1:B:100:VAL:HG13	4	0.16
(3,329)	1:B:118:PHE:HA	1:B:118:PHE:HD1	2	0.15
(3,329)	1:B:118:PHE:HA	1:B:118:PHE:HD2	2	0.15
(3,329)	1:A:118:PHE:HA	1:A:118:PHE:HD1	2	0.15
(3,329)	1:A:118:PHE:HA	1:A:118:PHE:HD2	2	0.15
(2,144)	1:B:123:ARG:H	1:B:124:ILE:HG21	3	0.13
(2,144)	1:B:123:ARG:H	1:B:124:ILE:HG22	3	0.13
(2,144)	1:B:123:ARG:H	1:B:124:ILE:HG23	3	0.13
(2,144)	1:A:123:ARG:H	1:A:124:ILE:HG21	3	0.13
(2,144)	1:A:123:ARG:H	1:A:124:ILE:HG22	3	0.13
(2,144)	1:A:123:ARG:H	1:A:124:ILE:HG23	3	0.13
(2,113)	1:A:113:PHE:H	1:A:111:HIS:HA	4	0.13
(2,113)	1:B:113:PHE:H	1:B:111:HIS:HA	4	0.13
(2,211)	1:B:150:LYS:HE2	1:B:127:ASP:HB3	1	0.12
(2,211)	1:B:150:LYS:HE3	1:B:127:ASP:HB3	1	0.12
(2,211)	1:A:150:LYS:HE2	1:A:127:ASP:HB3	1	0.12
(2,211)	1:A:150:LYS:HE3	1:A:127:ASP:HB3	1	0.12
(1,69)	1:B:82:LYS:HE2	1:B:82:LYS:HA	3	0.12
(1,69)	1:B:82:LYS:HE3	1:B:82:LYS:HA	3	0.12
(1,69)	1:A:82:LYS:HE2	1:A:82:LYS:HA	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,69)	1:A:82:LYS:HE3	1:A:82:LYS:HA	3	0.12
(1,49)	1:A:78:ASN:HA	1:A:79:LEU:HD11	8	0.12
(1,49)	1:A:78:ASN:HA	1:A:79:LEU:HD12	8	0.12
(1,49)	1:A:78:ASN:HA	1:A:79:LEU:HD13	8	0.12
(1,49)	1:A:78:ASN:HA	1:A:79:LEU:HD21	8	0.12
(1,49)	1:A:78:ASN:HA	1:A:79:LEU:HD22	8	0.12
(1,49)	1:A:78:ASN:HA	1:A:79:LEU:HD23	8	0.12
(1,49)	1:B:78:ASN:HA	1:B:79:LEU:HD11	8	0.12
(1,49)	1:B:78:ASN:HA	1:B:79:LEU:HD12	8	0.12
(1,49)	1:B:78:ASN:HA	1:B:79:LEU:HD13	8	0.12
(1,49)	1:B:78:ASN:HA	1:B:79:LEU:HD21	8	0.12
(1,49)	1:B:78:ASN:HA	1:B:79:LEU:HD22	8	0.12
(1,49)	1:B:78:ASN:HA	1:B:79:LEU:HD23	8	0.12
(3,152)	1:B:90:LYS:HB2	1:B:101:HIS:HB2	1	0.11
(3,152)	1:B:90:LYS:HB2	1:B:101:HIS:HB3	1	0.11
(3,152)	1:B:90:LYS:HB3	1:B:101:HIS:HB2	1	0.11
(3,152)	1:B:90:LYS:HB3	1:B:101:HIS:HB3	1	0.11
(3,152)	1:A:90:LYS:HB2	1:A:101:HIS:HB2	1	0.11
(3,152)	1:A:90:LYS:HB2	1:A:101:HIS:HB3	1	0.11
(3,152)	1:A:90:LYS:HB3	1:A:101:HIS:HB2	1	0.11
(3,152)	1:A:90:LYS:HB3	1:A:101:HIS:HB3	1	0.11

10 Dihedral-angle violation analysis (i)

No dihedral-angle restraints found