Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	8OX2 / pdb_00008ox2
BMRB ID	:	34813
Title	:	BRICHOS trimer
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Deposited on	:	2023-04-30

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 (i)) were used in the production of this report:

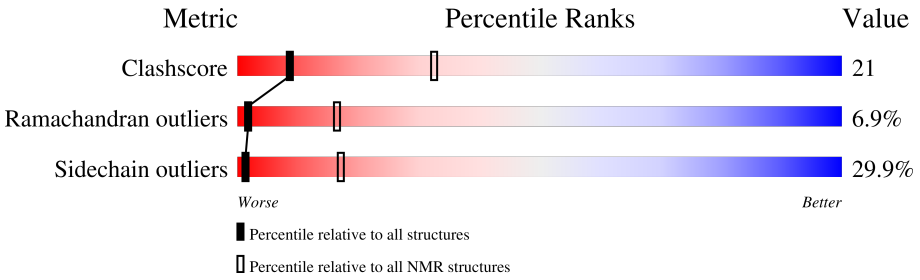
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance

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

The overall completeness of chemical shifts assignment is 23%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	114	36% 39% 7% 18%
1	B	114	38% 40% · 18%
1	C	114	38% 39% 5% 18%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 9 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:89-A:151, A:167-A:197, B:89-B:151, B:167-B:197, C:89-C:151, C:167-C:197 (282)	1.15	9

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

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

The models can be grouped into 3 clusters and 3 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 5022 atoms, of which 2505 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Pulmonary surfactant-associated protein C.

Mol	Chain	Residues	Atoms						Trace
1	A	114	Total	C	H	N	O	S	0
			1674	535	835	135	162	7	
1	B	114	Total	C	H	N	O	S	0
			1674	535	835	135	162	7	
1	C	114	Total	C	H	N	O	S	0
			1674	535	835	135	162	7	

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	84	GLY	-	expression tag	UNP E5RI64
B	84	GLY	-	expression tag	UNP E5RI64
C	84	GLY	-	expression tag	UNP E5RI64

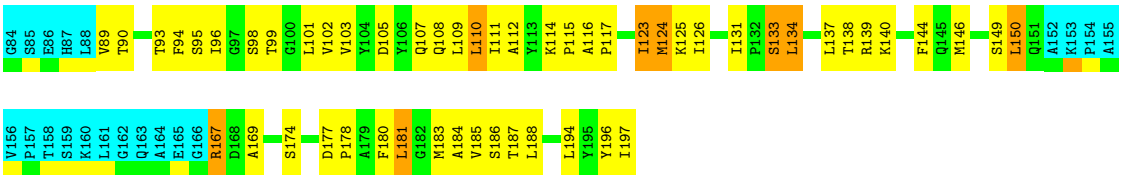
4 Residue-property plots (i)

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.

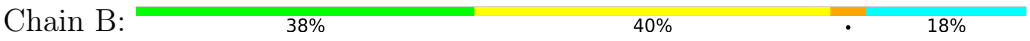
• Molecule 1: Pulmonary surfactant-associated protein C

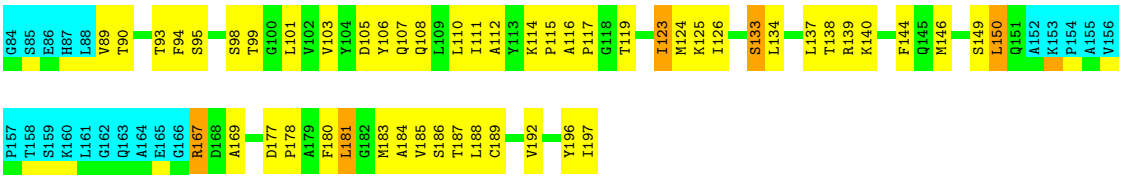
Chain A:



• Molecule 1: Pulmonary surfactant-associated protein C

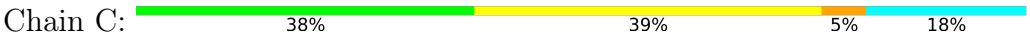
Chain B:

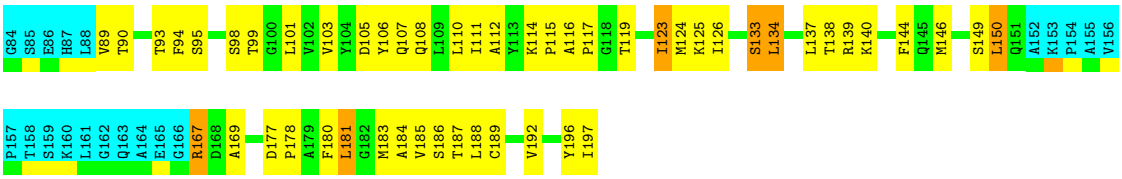




• Molecule 1: Pulmonary surfactant-associated protein C

Chain C:





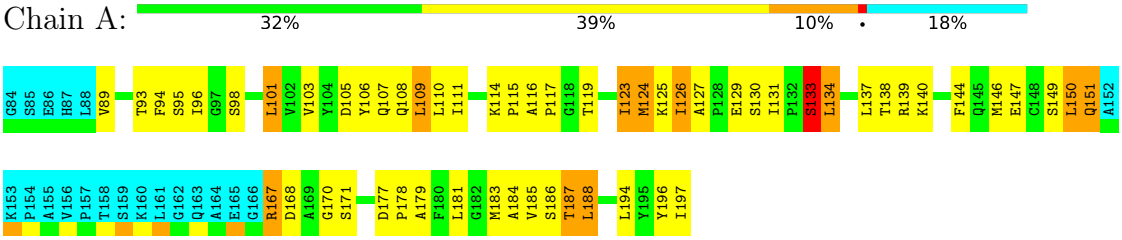
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

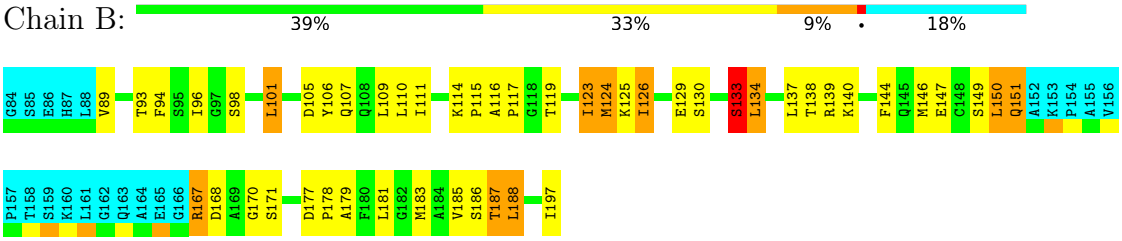
• Molecule 1: Pulmonary surfactant-associated protein C

Chain A:



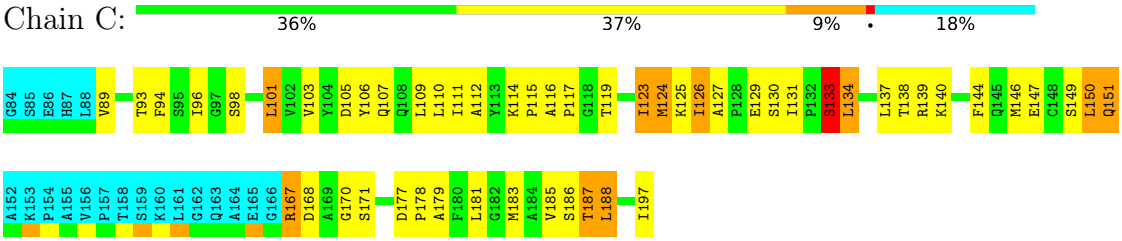
• Molecule 1: Pulmonary surfactant-associated protein C

Chain B:



• Molecule 1: Pulmonary surfactant-associated protein C

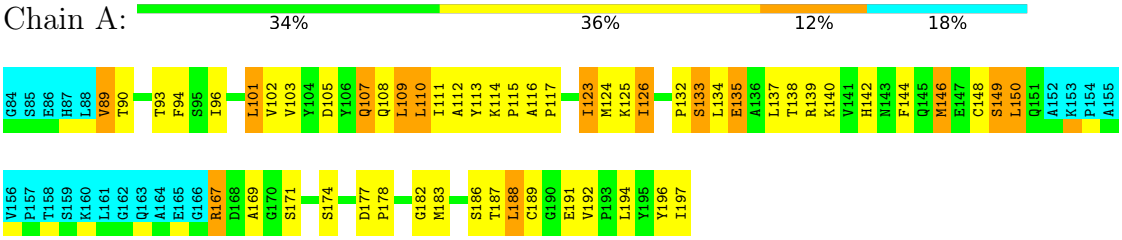
Chain C:



4.2.2 Score per residue for model 2

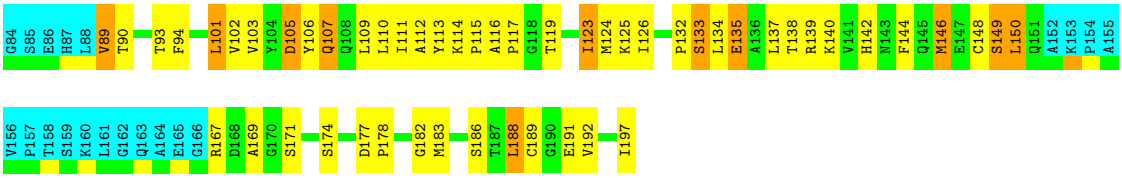
• Molecule 1: Pulmonary surfactant-associated protein C

Chain A:



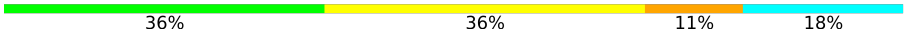
• Molecule 1: Pulmonary surfactant-associated protein C

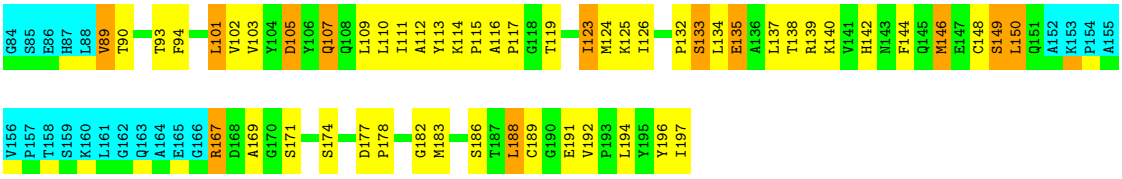
Chain B:



• Molecule 1: Pulmonary surfactant-associated protein C

Chain C:

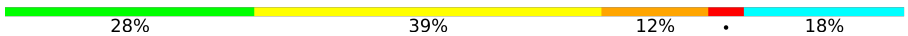


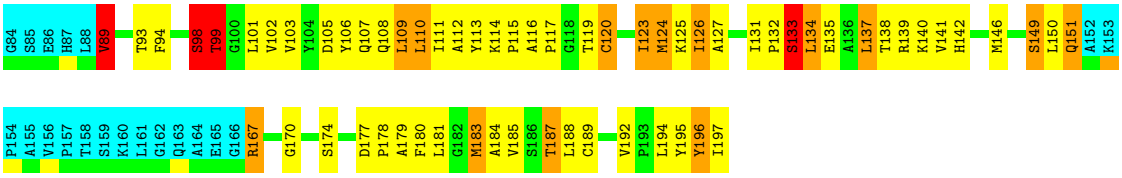


4.2.3 Score per residue for model 3

• Molecule 1: Pulmonary surfactant-associated protein C

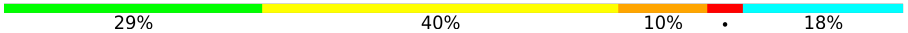
Chain A:

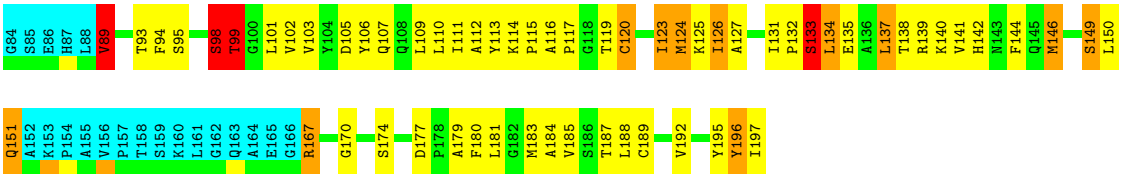




• Molecule 1: Pulmonary surfactant-associated protein C

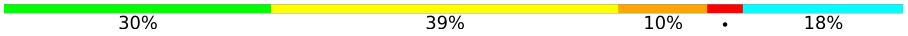
Chain B:

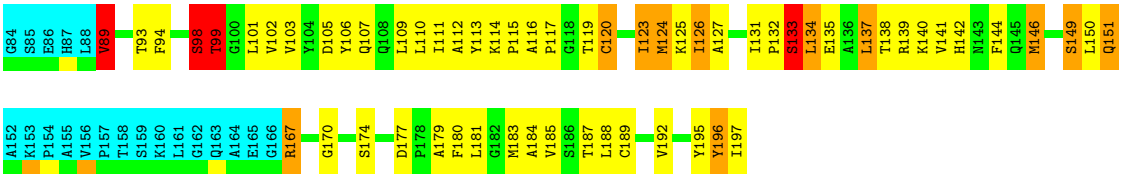




• Molecule 1: Pulmonary surfactant-associated protein C

Chain C:

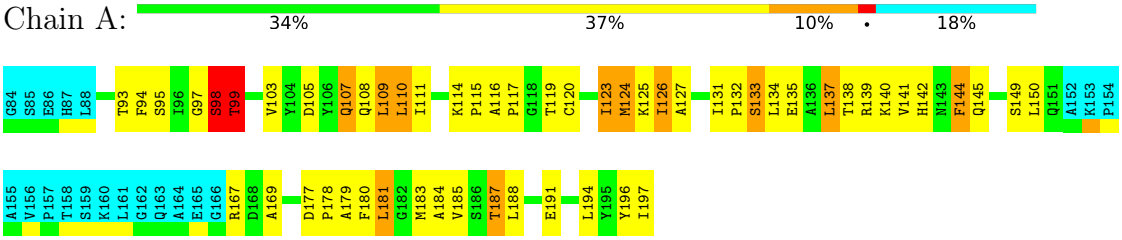




4.2.4 Score per residue for model 4

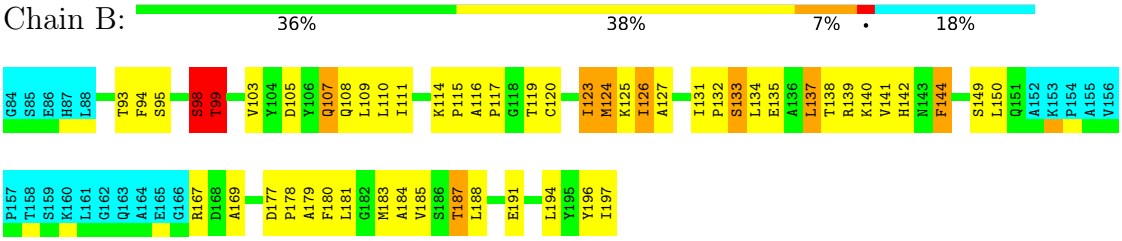
• Molecule 1: Pulmonary surfactant-associated protein C

Chain A:



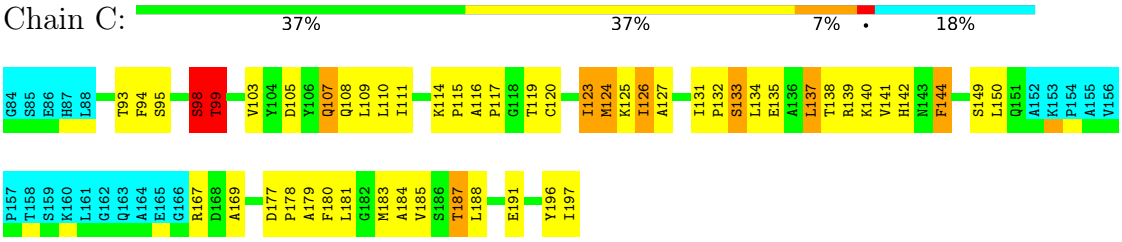
• Molecule 1: Pulmonary surfactant-associated protein C

Chain B:



• Molecule 1: Pulmonary surfactant-associated protein C

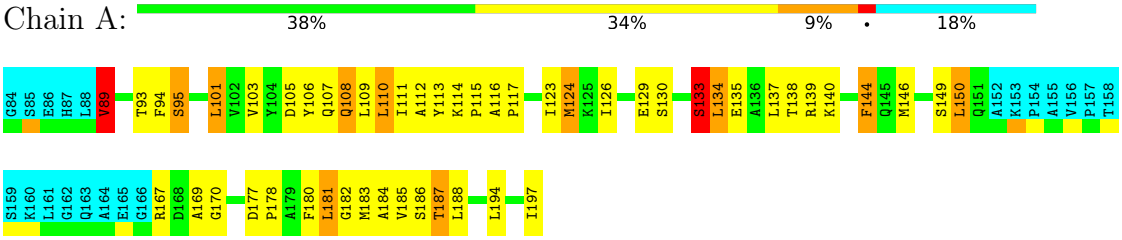
Chain C:



4.2.5 Score per residue for model 5

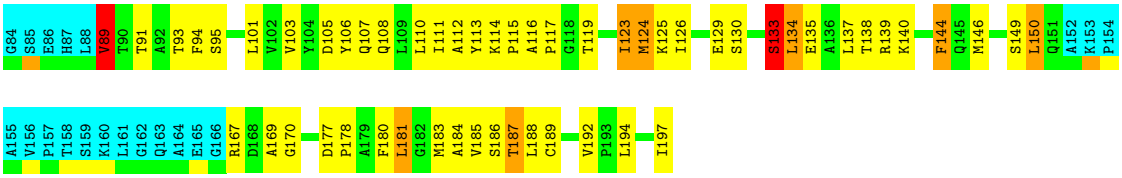
• Molecule 1: Pulmonary surfactant-associated protein C

Chain A:



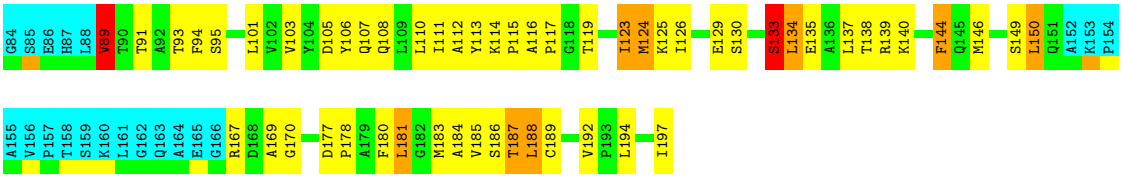
• Molecule 1: Pulmonary surfactant-associated protein C

Chain B:



• Molecule 1: Pulmonary surfactant-associated protein C

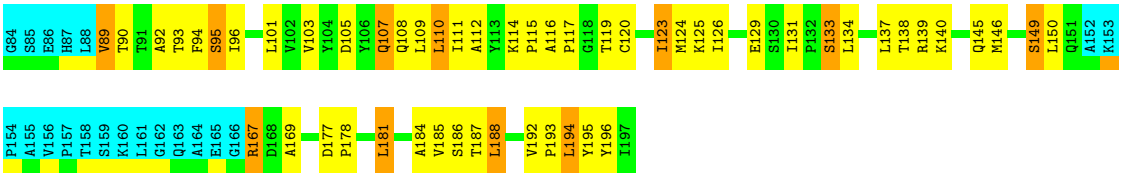
Chain C:



4.2.6 Score per residue for model 6

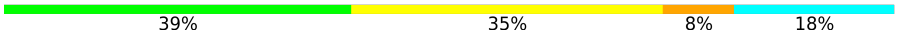
• Molecule 1: Pulmonary surfactant-associated protein C

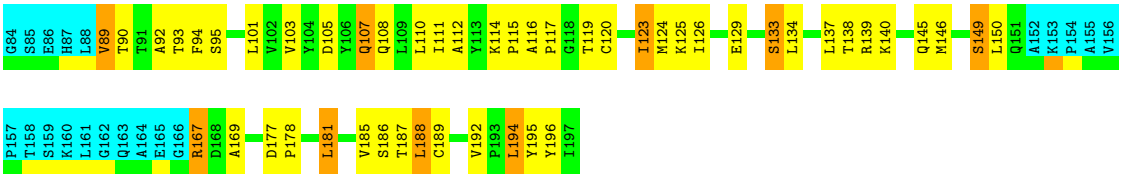
Chain A:



• Molecule 1: Pulmonary surfactant-associated protein C

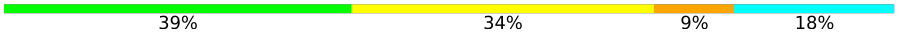
Chain B:

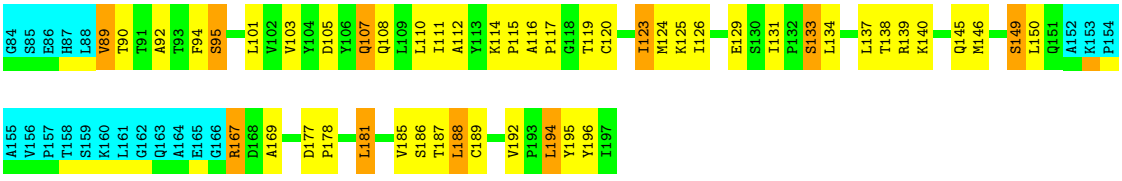




• Molecule 1: Pulmonary surfactant-associated protein C

Chain C:

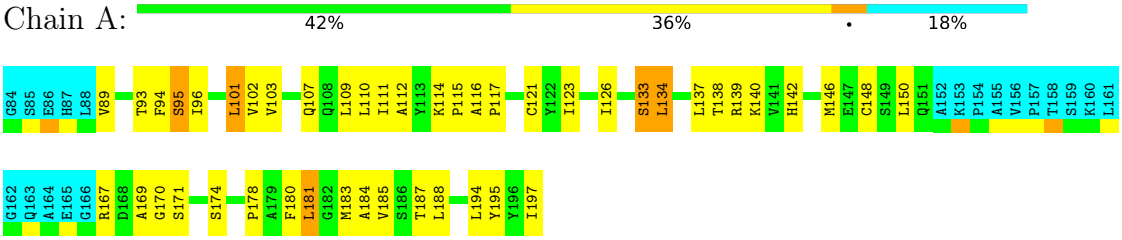




4.2.7 Score per residue for model 7

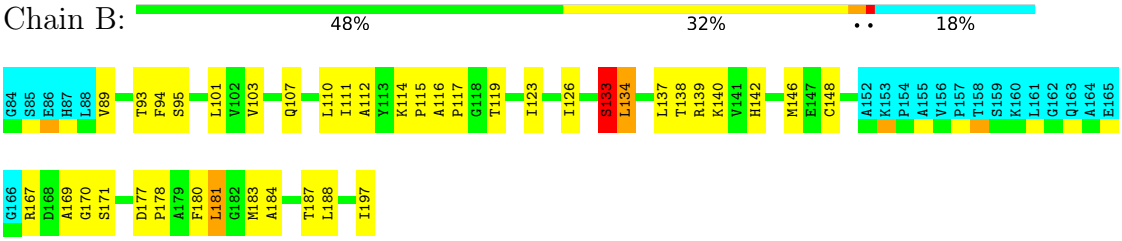
• Molecule 1: Pulmonary surfactant-associated protein C

Chain A:



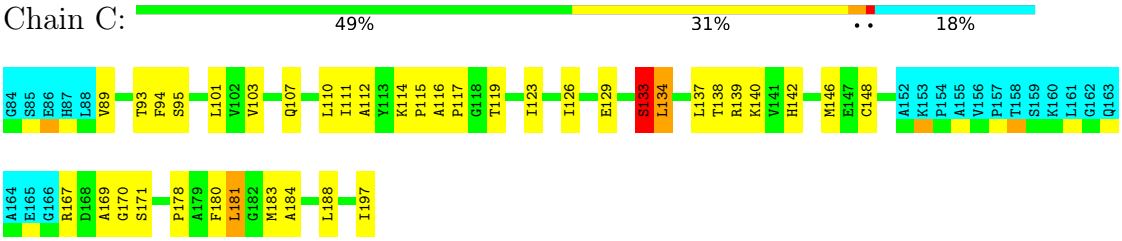
• Molecule 1: Pulmonary surfactant-associated protein C

Chain B:



• Molecule 1: Pulmonary surfactant-associated protein C

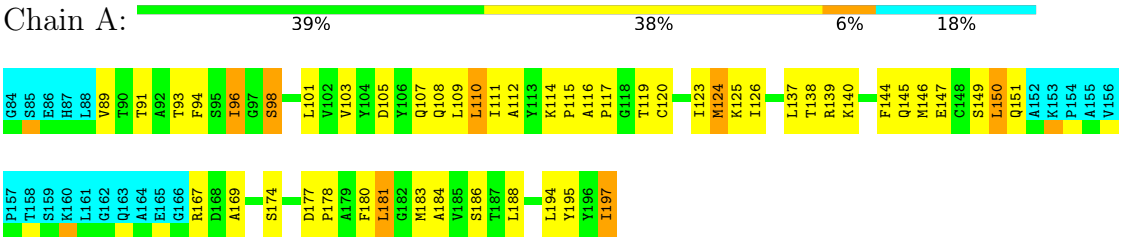
Chain C:



4.2.8 Score per residue for model 8

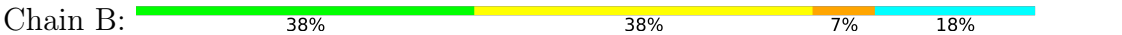
• Molecule 1: Pulmonary surfactant-associated protein C

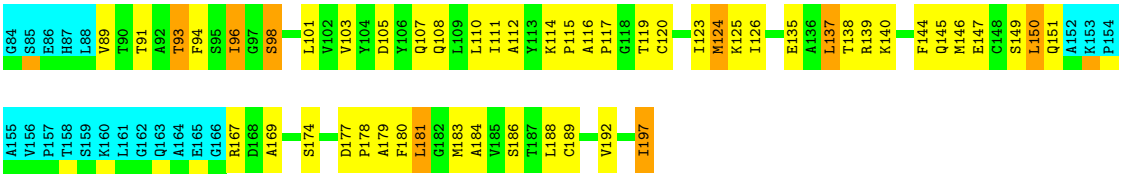
Chain A:



• Molecule 1: Pulmonary surfactant-associated protein C

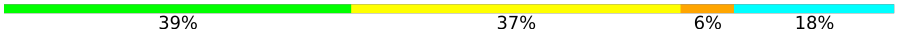
Chain B:

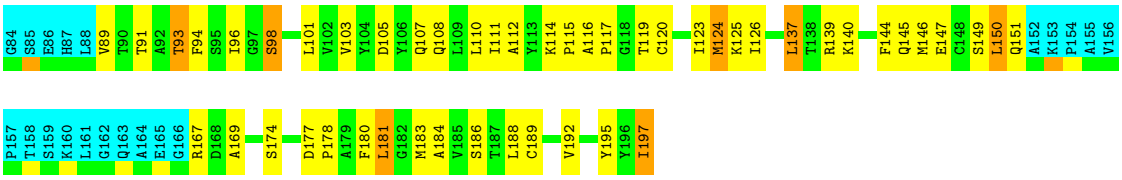




• Molecule 1: Pulmonary surfactant-associated protein C

Chain C:

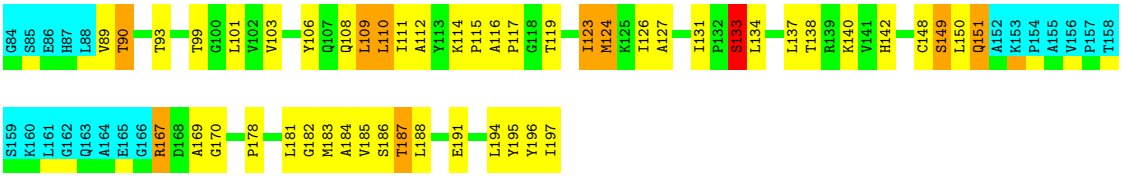




4.2.9 Score per residue for model 9 (medoid)

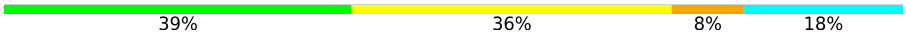
• Molecule 1: Pulmonary surfactant-associated protein C

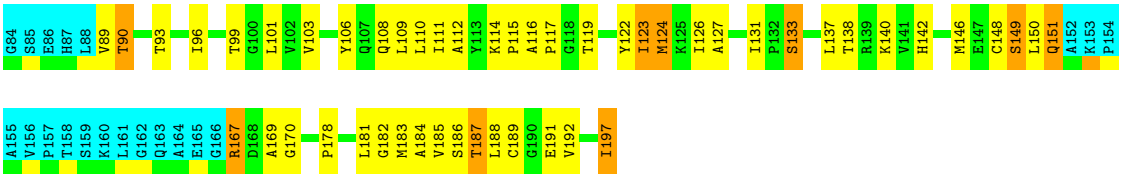
Chain A:



• Molecule 1: Pulmonary surfactant-associated protein C

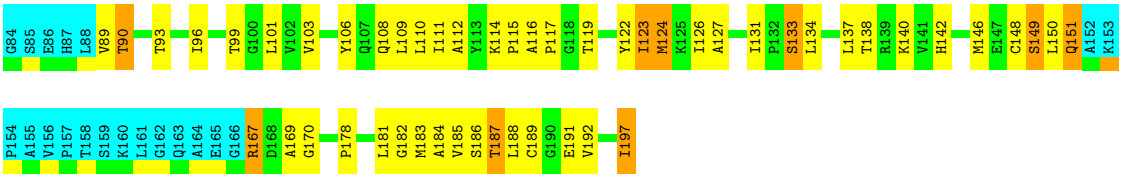
Chain B:





• Molecule 1: Pulmonary surfactant-associated protein C

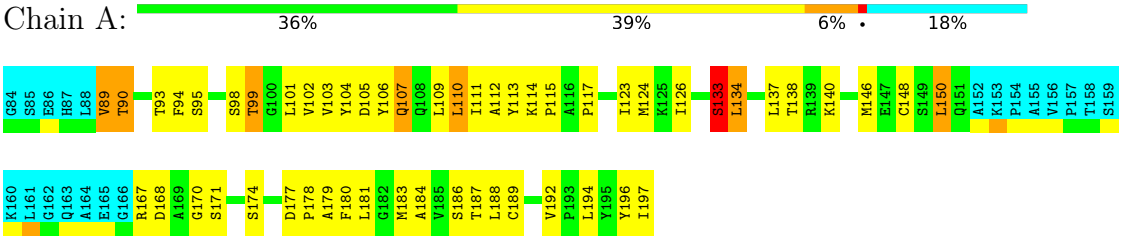
Chain C:



4.2.10 Score per residue for model 10

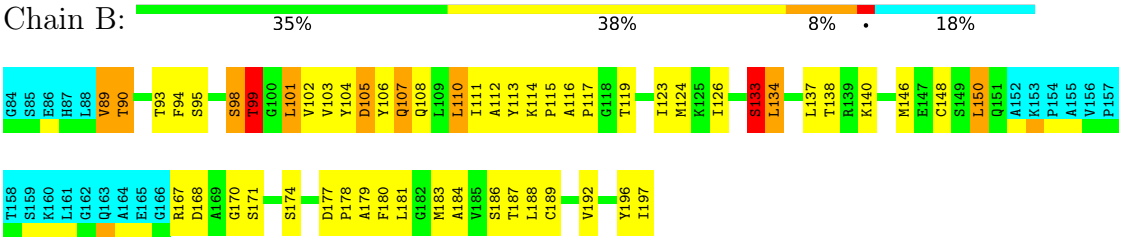
• Molecule 1: Pulmonary surfactant-associated protein C

Chain A:



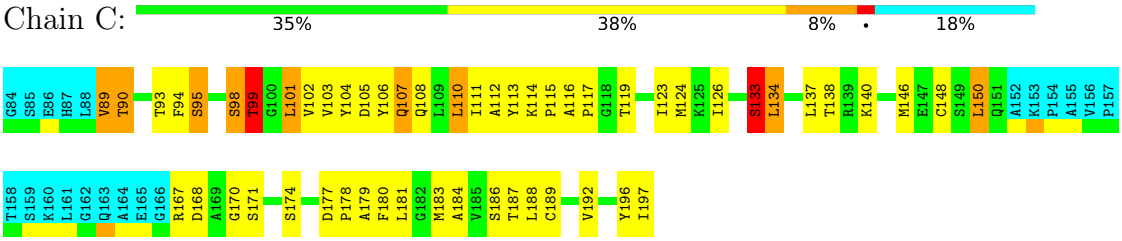
• Molecule 1: Pulmonary surfactant-associated protein C

Chain B:



• Molecule 1: Pulmonary surfactant-associated protein C

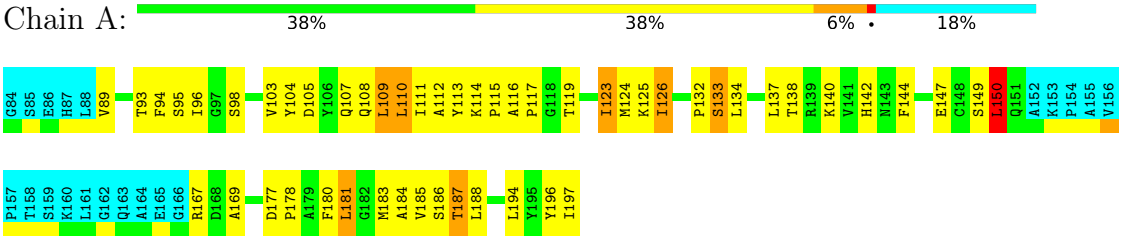
Chain C:



4.2.11 Score per residue for model 11

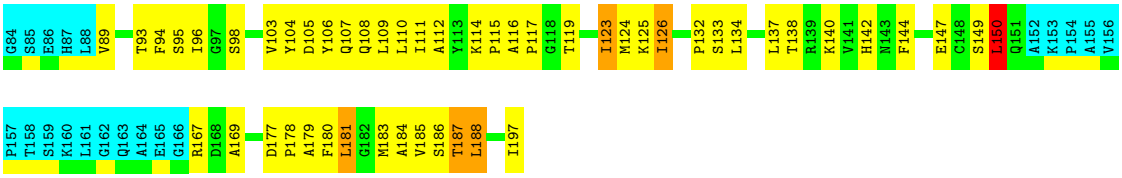
• Molecule 1: Pulmonary surfactant-associated protein C

Chain A:

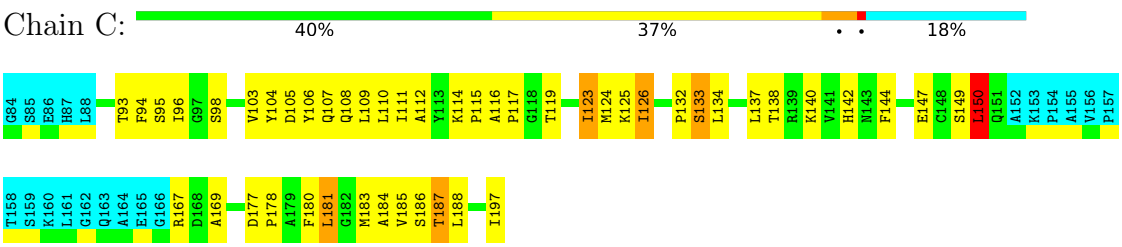


• Molecule 1: Pulmonary surfactant-associated protein C

Chain B:

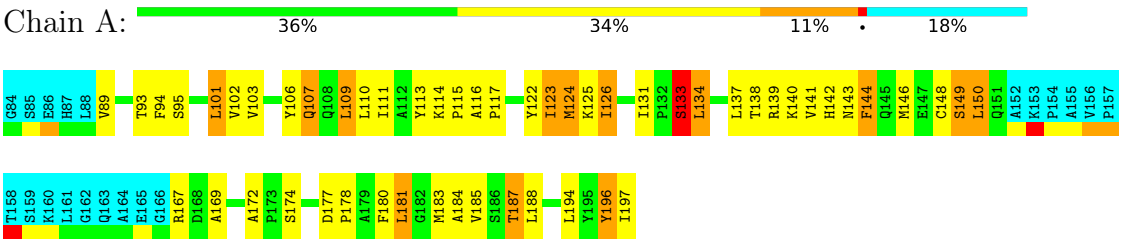


• Molecule 1: Pulmonary surfactant-associated protein C

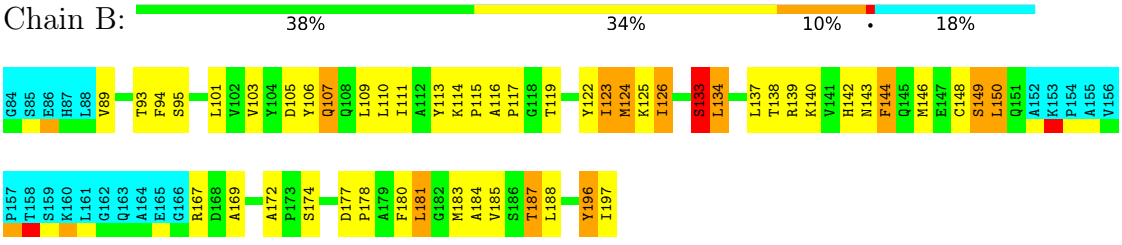


4.2.12 Score per residue for model 12

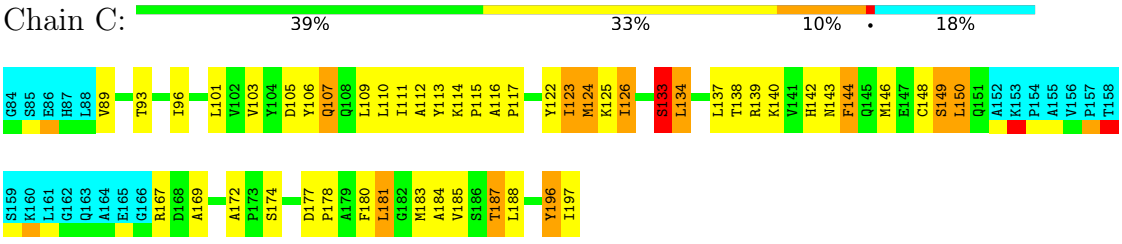
• Molecule 1: Pulmonary surfactant-associated protein C



• Molecule 1: Pulmonary surfactant-associated protein C



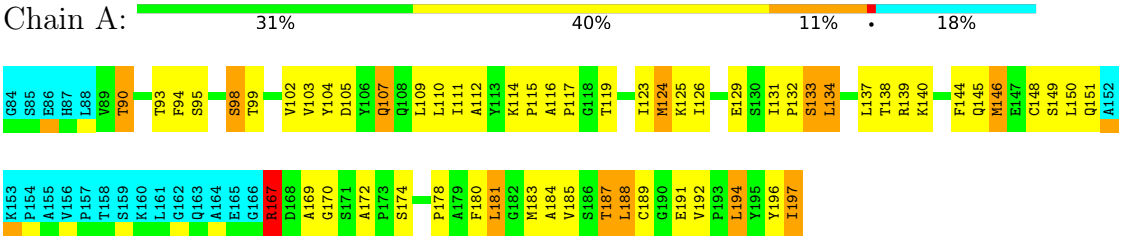
• Molecule 1: Pulmonary surfactant-associated protein C



4.2.13 Score per residue for model 13

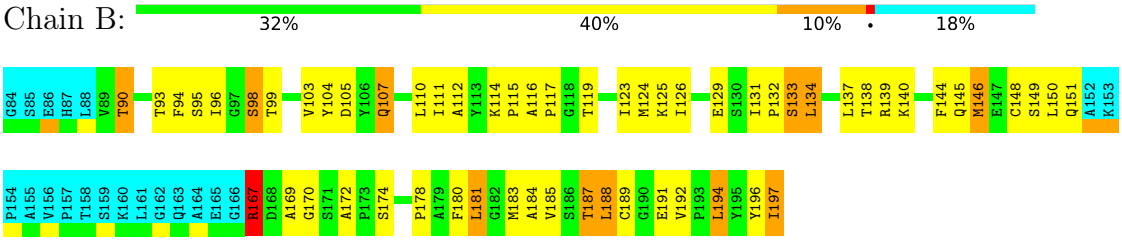
• Molecule 1: Pulmonary surfactant-associated protein C

Chain A:



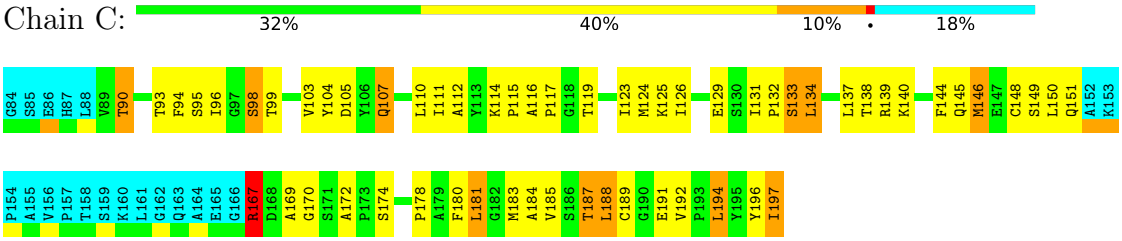
• Molecule 1: Pulmonary surfactant-associated protein C

Chain B:



• Molecule 1: Pulmonary surfactant-associated protein C

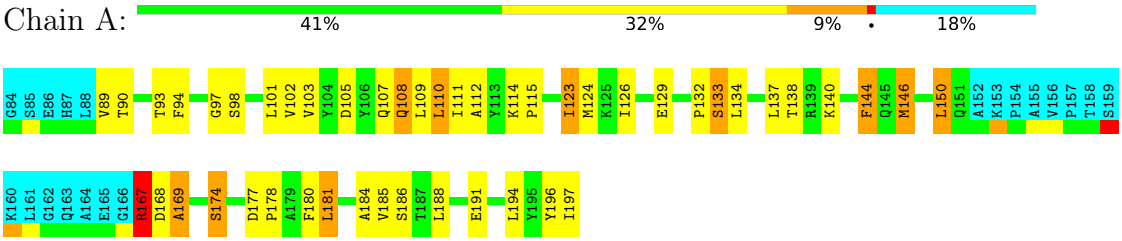
Chain C:



4.2.14 Score per residue for model 14

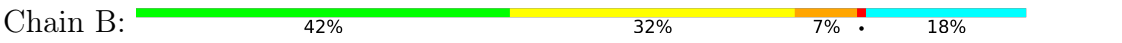
• Molecule 1: Pulmonary surfactant-associated protein C

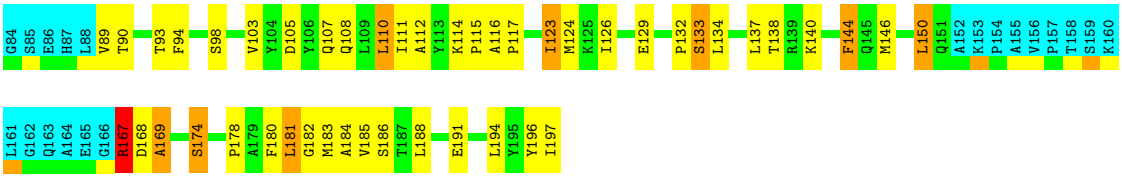
Chain A:



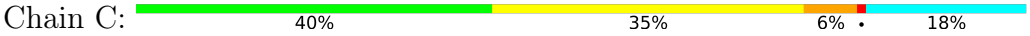
• Molecule 1: Pulmonary surfactant-associated protein C

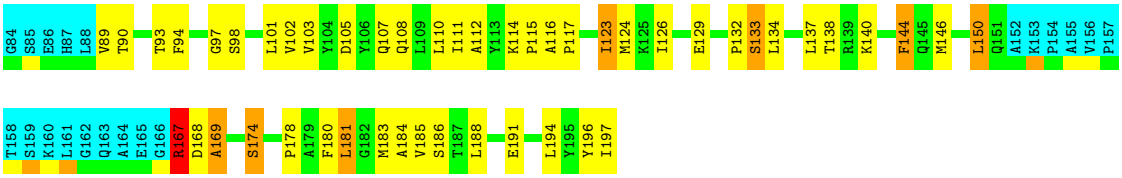
Chain B:





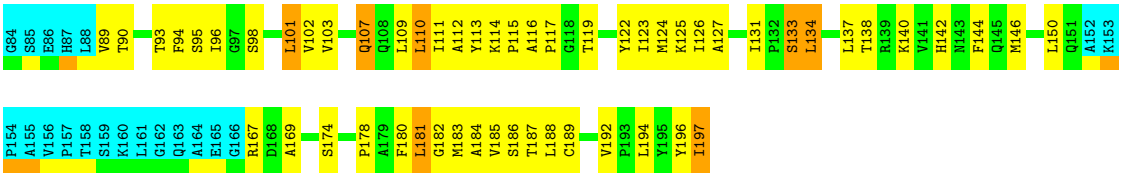
• Molecule 1: Pulmonary surfactant-associated protein C



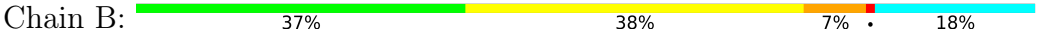


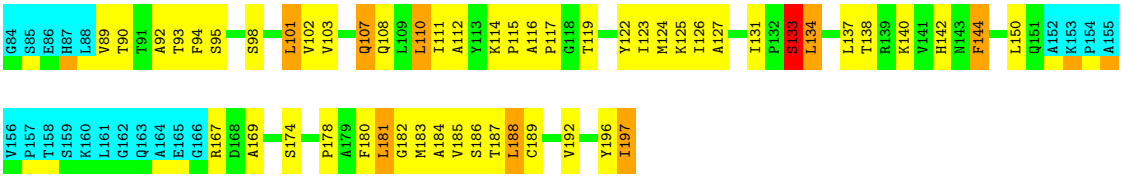
4.2.15 Score per residue for model 15

• Molecule 1: Pulmonary surfactant-associated protein C

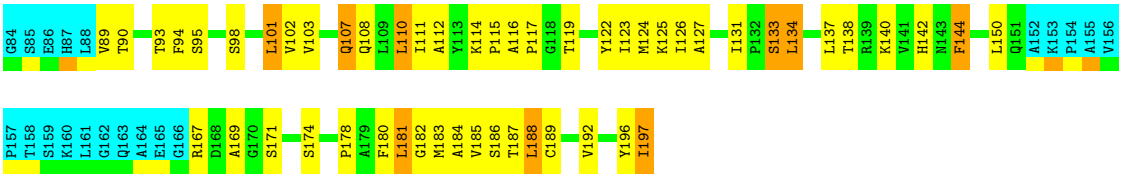


• Molecule 1: Pulmonary surfactant-associated protein C





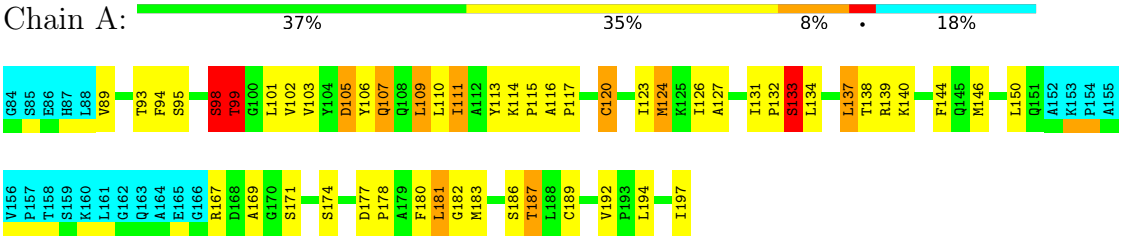
• Molecule 1: Pulmonary surfactant-associated protein C



4.2.16 Score per residue for model 16

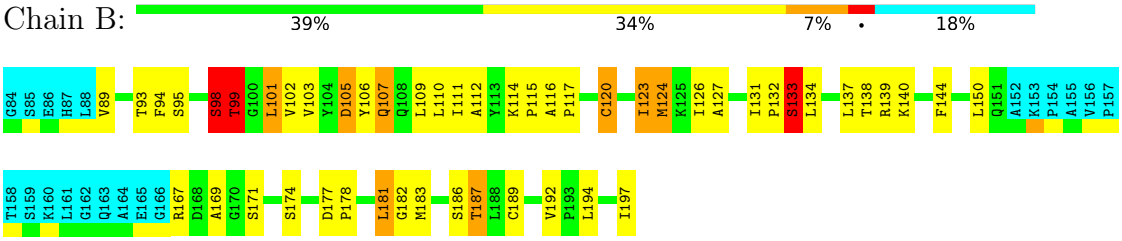
• Molecule 1: Pulmonary surfactant-associated protein C

Chain A:



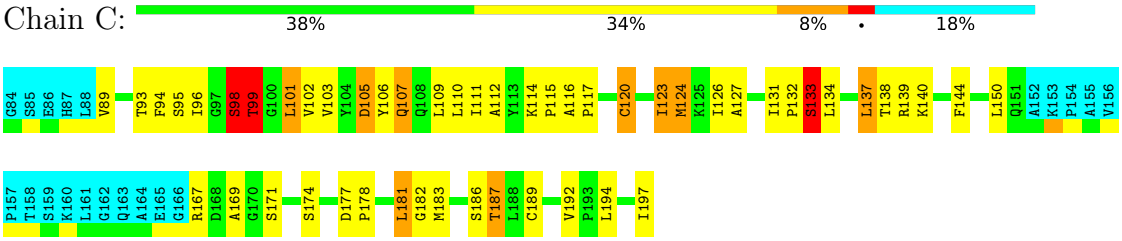
• Molecule 1: Pulmonary surfactant-associated protein C

Chain B:



• Molecule 1: Pulmonary surfactant-associated protein C

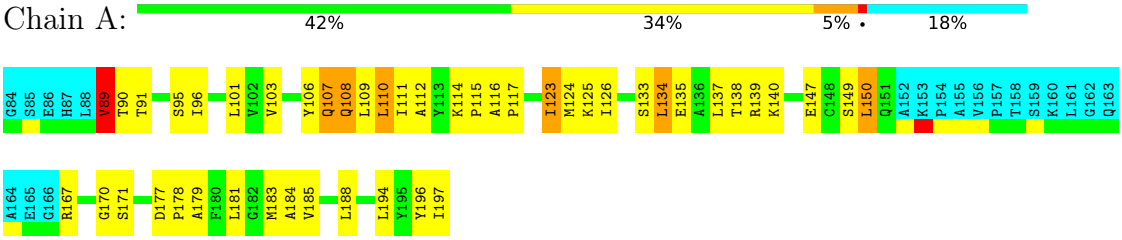
Chain C:



4.2.17 Score per residue for model 17

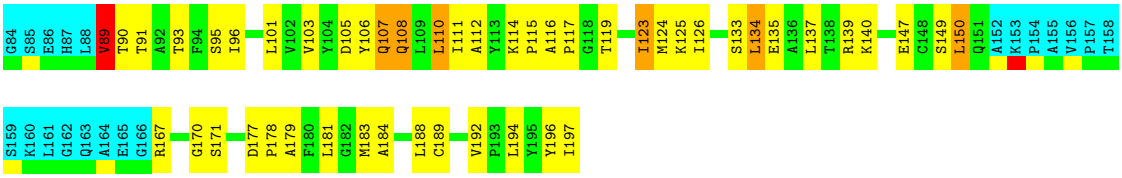
• Molecule 1: Pulmonary surfactant-associated protein C

Chain A:



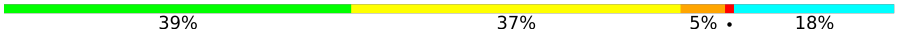
• Molecule 1: Pulmonary surfactant-associated protein C

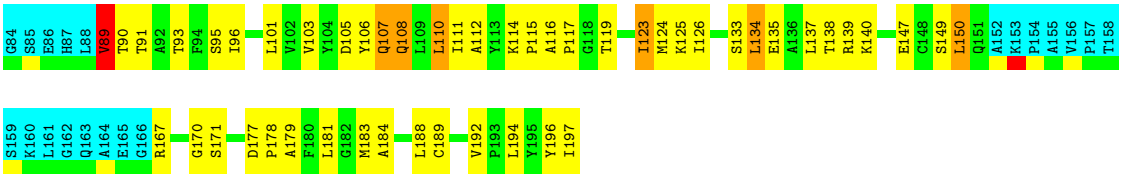
Chain B:



• Molecule 1: Pulmonary surfactant-associated protein C

Chain C:

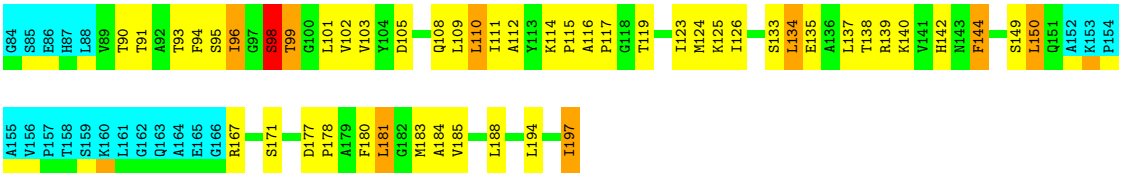




4.2.18 Score per residue for model 18

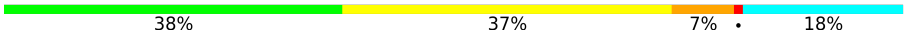
• Molecule 1: Pulmonary surfactant-associated protein C

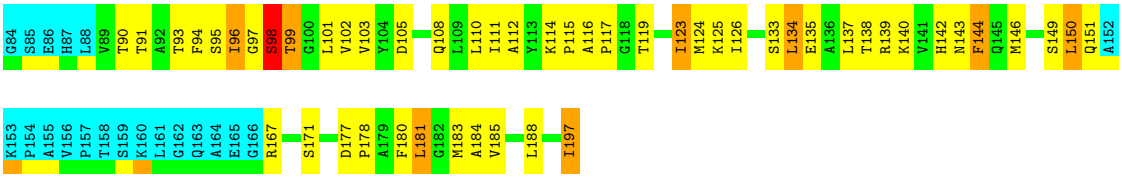
Chain A:



• Molecule 1: Pulmonary surfactant-associated protein C

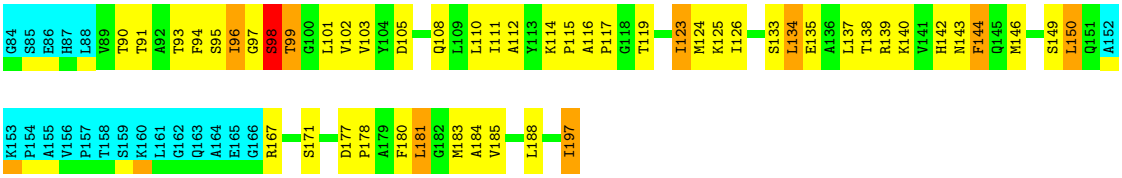
Chain B:





• Molecule 1: Pulmonary surfactant-associated protein C

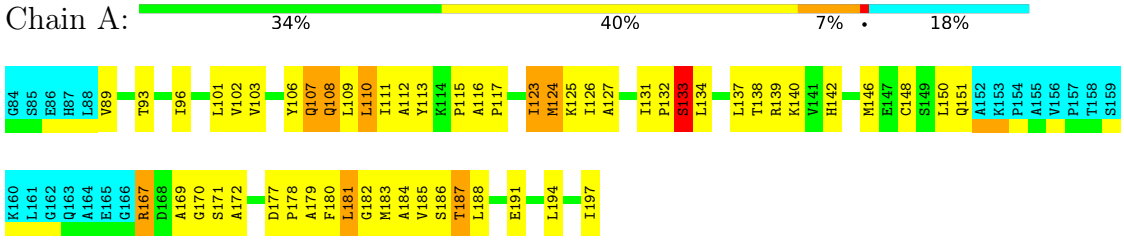
Chain C:



4.2.19 Score per residue for model 19

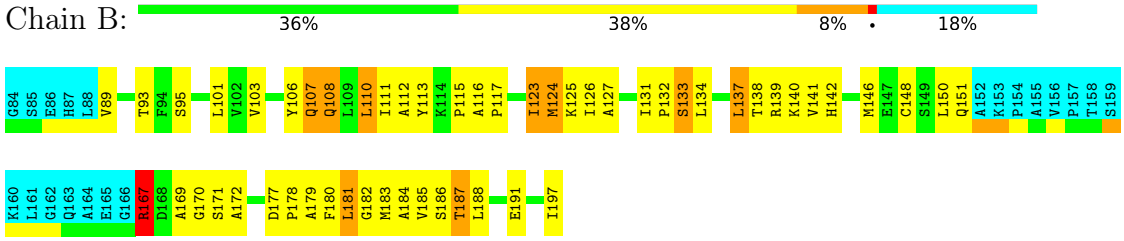
• Molecule 1: Pulmonary surfactant-associated protein C

Chain A:



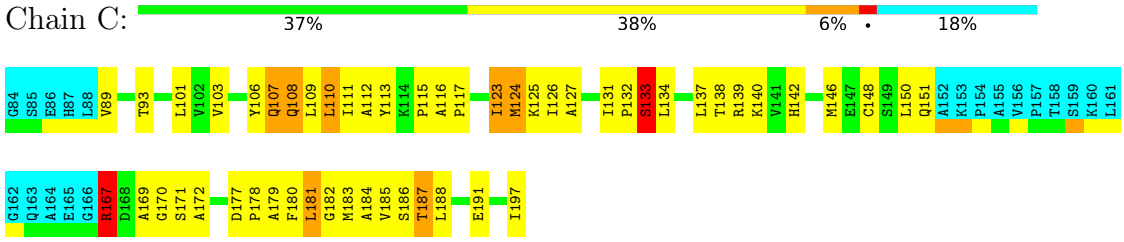
• Molecule 1: Pulmonary surfactant-associated protein C

Chain B:



• Molecule 1: Pulmonary surfactant-associated protein C

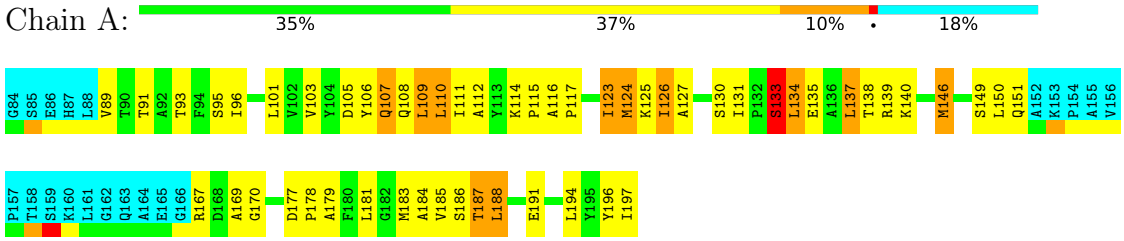
Chain C:



4.2.20 Score per residue for model 20

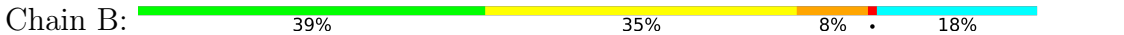
• Molecule 1: Pulmonary surfactant-associated protein C

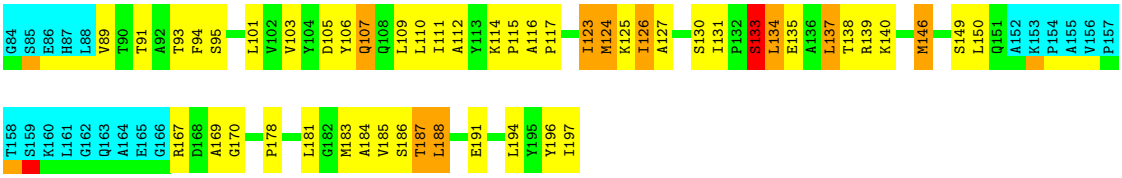
Chain A:



• Molecule 1: Pulmonary surfactant-associated protein C

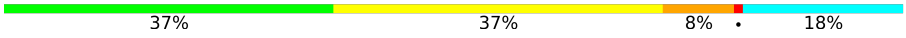
Chain B:

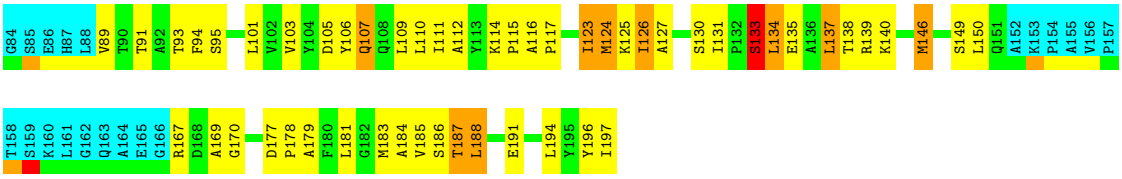




• Molecule 1: Pulmonary surfactant-associated protein C

Chain C:





5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics*.

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
CYANA	structure calculation	3.98.15

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	1001
Number of shifts mapped to atoms	1001
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	23%

6 Model quality

6.1 Standard geometry

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	701	696	696	35±6
1	B	701	696	696	34±5
1	C	701	696	696	34±5
All	All	42060	41760	41760	1779

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 21.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:111:ILE:HD11	1:A:126:ILE:HG23	1.09	1.23	4	11
1:B:111:ILE:HD11	1:B:126:ILE:HG23	1.06	1.24	4	10
1:C:111:ILE:HD11	1:C:126:ILE:HG23	1.03	1.22	3	10
1:A:112:ALA:HB2	1:A:185:VAL:HG12	0.96	1.34	18	10
1:C:112:ALA:HB2	1:C:185:VAL:HG12	0.87	1.43	18	8
1:B:112:ALA:HB2	1:B:185:VAL:HG12	0.86	1.44	18	8
1:A:110:LEU:HD21	1:A:181:LEU:HD12	0.84	1.49	15	6
1:C:110:LEU:HD21	1:C:181:LEU:HD12	0.83	1.50	19	4
1:C:116:ALA:HB3	1:C:119:THR:HG21	0.81	1.50	8	13
1:C:93:THR:HG22	1:C:103:VAL:HG12	0.81	1.52	11	8
1:A:116:ALA:HB3	1:A:119:THR:HG21	0.81	1.50	8	8
1:B:116:ALA:HB3	1:B:119:THR:HG21	0.81	1.51	8	14

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:93:THR:HG22	1:B:103:VAL:HG12	0.80	1.53	11	8
1:B:110:LEU:HD21	1:B:181:LEU:HD12	0.80	1.53	4	4
1:C:111:ILE:HD11	1:C:126:ILE:CG2	0.75	2.12	9	15
1:C:103:VAL:HG22	1:C:112:ALA:HB3	0.75	1.59	14	19
1:B:111:ILE:HD11	1:B:126:ILE:CG2	0.73	2.12	9	15
1:B:103:VAL:HG22	1:B:112:ALA:HB3	0.73	1.59	2	17
1:A:178:PRO:HA	1:A:181:LEU:HD21	0.73	1.60	12	14
1:A:111:ILE:HD11	1:A:126:ILE:CG2	0.71	2.14	9	18
1:A:103:VAL:HG22	1:A:112:ALA:HB3	0.71	1.60	2	15
1:C:113:TYR:CE1	1:C:146:MET:HE2	0.70	2.22	5	4
1:B:113:TYR:CE1	1:B:146:MET:HE2	0.69	2.23	5	4
1:B:94:PHE:HB2	1:B:134:LEU:HD21	0.69	1.65	6	2
1:A:113:TYR:CE1	1:A:146:MET:HE2	0.68	2.24	5	4
1:B:188:LEU:HD11	1:C:94:PHE:CZ	0.68	2.23	8	3
1:C:123:ILE:HD11	1:C:185:VAL:HG11	0.68	1.66	12	9
1:A:188:LEU:HD11	1:B:94:PHE:CZ	0.68	2.23	8	1
1:A:93:THR:HG22	1:A:103:VAL:HG12	0.68	1.66	11	6
1:B:123:ILE:HD11	1:B:185:VAL:HG11	0.68	1.65	20	10
1:A:123:ILE:HD11	1:A:185:VAL:HG11	0.67	1.67	3	9
1:A:187:THR:HG22	1:B:133:SER:CB	0.67	2.20	3	10
1:A:189:CYS:O	1:A:192:VAL:HG22	0.67	1.89	10	3
1:A:149:SER:O	1:A:150:LEU:HD23	0.67	1.90	3	3
1:B:111:ILE:HD12	1:B:124:MET:O	0.66	1.90	19	8
1:C:180:PHE:O	1:C:181:LEU:HD23	0.66	1.91	10	3
1:C:150:LEU:HD21	1:C:197:ILE:HG22	0.65	1.67	8	1
1:C:111:ILE:HD12	1:C:124:MET:O	0.65	1.90	19	8
1:C:113:TYR:CD1	1:C:146:MET:HE2	0.65	2.26	19	2
1:A:133:SER:CB	1:C:187:THR:HG22	0.65	2.21	1	9
1:B:187:THR:HG22	1:C:133:SER:CB	0.65	2.21	12	10
1:C:146:MET:HE3	1:C:197:ILE:HD12	0.65	1.67	12	1
1:A:180:PHE:C	1:A:181:LEU:HD23	0.65	2.17	12	11
1:A:101:LEU:HD23	1:A:102:VAL:N	0.65	2.07	3	2
1:B:180:PHE:O	1:B:181:LEU:HD23	0.65	1.92	3	3
1:A:183:MET:O	1:A:183:MET:HE3	0.65	1.92	17	5
1:C:178:PRO:HA	1:C:181:LEU:HD21	0.65	1.68	12	11
1:B:113:TYR:CD1	1:B:146:MET:HE2	0.65	2.27	19	2
1:C:110:LEU:HD12	1:C:123:ILE:HG12	0.64	1.68	9	14
1:B:110:LEU:HD12	1:B:123:ILE:HG12	0.64	1.69	9	14
1:C:109:LEU:O	1:C:110:LEU:HD22	0.64	1.93	16	7
1:A:178:PRO:HA	1:A:181:LEU:HD11	0.64	1.67	18	11
1:C:124:MET:HE1	1:C:137:LEU:HD11	0.64	1.69	3	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:126:ILE:HD12	1:C:131:ILE:HD12	0.64	1.68	15	4
1:B:146:MET:HE3	1:B:197:ILE:HD12	0.64	1.68	12	1
1:A:89:VAL:HG12	1:A:183:MET:CG	0.64	2.22	8	2
1:A:187:THR:HG22	1:B:133:SER:HB3	0.64	1.70	20	6
1:A:106:TYR:CE1	1:C:89:VAL:HG11	0.64	2.28	10	2
1:B:109:LEU:O	1:B:110:LEU:HD22	0.64	1.92	16	7
1:B:150:LEU:HD21	1:B:197:ILE:HG22	0.64	1.67	8	1
1:C:184:ALA:O	1:C:188:LEU:HD12	0.64	1.93	14	15
1:C:89:VAL:HG12	1:C:183:MET:CG	0.64	2.23	8	2
1:A:150:LEU:HD21	1:A:197:ILE:HG22	0.64	1.70	8	1
1:A:126:ILE:HD12	1:A:131:ILE:HD12	0.64	1.69	15	4
1:A:180:PHE:O	1:A:181:LEU:HD23	0.63	1.93	10	3
1:A:105:ASP:O	1:A:126:ILE:HD11	0.63	1.93	18	3
1:C:105:ASP:O	1:C:126:ILE:HD11	0.63	1.94	18	4
1:A:188:LEU:HD21	1:B:94:PHE:CE2	0.63	2.28	4	5
1:B:89:VAL:HG12	1:B:183:MET:CG	0.63	2.22	8	2
1:B:94:PHE:HB3	1:B:134:LEU:HD11	0.63	1.70	14	2
1:A:89:VAL:HG21	1:B:106:TYR:HB3	0.63	1.71	1	4
1:A:188:LEU:HD21	1:B:94:PHE:CD2	0.63	2.29	15	8
1:A:94:PHE:CE2	1:C:188:LEU:HD21	0.63	2.29	4	6
1:B:188:LEU:HD11	1:C:94:PHE:CE1	0.62	2.29	18	1
1:B:111:ILE:HD11	1:B:126:ILE:HG21	0.62	1.70	14	7
1:B:105:ASP:O	1:B:126:ILE:HD11	0.62	1.93	18	4
1:B:188:LEU:HD21	1:C:94:PHE:CD2	0.62	2.29	6	6
1:A:133:SER:HB3	1:C:187:THR:HG22	0.62	1.70	20	3
1:B:109:LEU:C	1:B:110:LEU:HD22	0.62	2.20	12	9
1:C:110:LEU:O	1:C:111:ILE:HD13	0.62	1.95	2	3
1:B:111:ILE:CG2	1:B:124:MET:HE3	0.62	2.24	6	3
1:B:110:LEU:O	1:B:111:ILE:HD13	0.62	1.94	2	3
1:A:111:ILE:HD12	1:A:124:MET:O	0.62	1.95	19	7
1:C:111:ILE:CG2	1:C:124:MET:HE3	0.62	2.24	6	3
1:A:89:VAL:HG11	1:B:106:TYR:CD1	0.62	2.30	10	1
1:C:109:LEU:C	1:C:110:LEU:HD22	0.62	2.19	12	9
1:C:110:LEU:HD12	1:C:123:ILE:CG1	0.62	2.24	20	11
1:B:178:PRO:HA	1:B:181:LEU:HD21	0.62	1.69	12	11
1:B:183:MET:O	1:B:183:MET:HE3	0.62	1.94	17	4
1:B:89:VAL:HG11	1:C:106:TYR:CE1	0.62	2.29	17	2
1:B:110:LEU:HD12	1:B:123:ILE:CG1	0.61	2.25	20	11
1:A:103:VAL:HG22	1:A:112:ALA:CB	0.61	2.24	8	8
1:A:145:GLN:O	1:A:150:LEU:HD23	0.61	1.95	8	1
1:A:184:ALA:O	1:A:188:LEU:HD12	0.61	1.95	17	18

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:101:LEU:HD13	1:A:102:VAL:N	0.61	2.09	16	4
1:A:111:ILE:CG2	1:A:124:MET:HE3	0.61	2.25	8	4
1:B:184:ALA:O	1:B:188:LEU:HD12	0.61	1.95	14	15
1:C:183:MET:O	1:C:183:MET:HE3	0.61	1.94	17	4
1:C:94:PHE:HB3	1:C:134:LEU:HD11	0.61	1.71	14	1
1:B:94:PHE:CB	1:B:134:LEU:HD11	0.61	2.26	14	1
1:A:94:PHE:CE1	1:C:188:LEU:HD11	0.61	2.30	18	1
1:C:111:ILE:HD13	1:C:124:MET:HG3	0.61	1.71	12	4
1:B:178:PRO:HA	1:B:181:LEU:HD11	0.61	1.73	16	8
1:C:112:ALA:HB2	1:C:185:VAL:CG1	0.61	2.24	18	1
1:B:134:LEU:O	1:B:138:THR:HG23	0.61	1.96	20	17
1:A:94:PHE:CZ	1:C:188:LEU:HD11	0.61	2.29	8	2
1:A:109:LEU:C	1:A:110:LEU:HD22	0.60	2.21	12	9
1:C:110:LEU:HD21	1:C:181:LEU:HD11	0.60	1.73	20	3
1:A:106:TYR:HB3	1:C:89:VAL:HG21	0.60	1.73	1	2
1:C:145:GLN:O	1:C:150:LEU:HD23	0.60	1.96	8	1
1:A:113:TYR:CE2	1:A:146:MET:HE2	0.60	2.31	2	3
1:A:89:VAL:HG11	1:B:106:TYR:CE1	0.60	2.31	10	2
1:A:113:TYR:CD1	1:A:146:MET:HE2	0.60	2.31	19	1
1:B:111:ILE:HD13	1:B:124:MET:HG3	0.60	1.72	12	4
1:C:189:CYS:O	1:C:192:VAL:HG13	0.60	1.97	10	7
1:A:123:ILE:HB	1:A:194:LEU:HD22	0.60	1.72	13	3
1:B:188:LEU:HD21	1:C:94:PHE:CE2	0.60	2.31	4	5
1:B:180:PHE:C	1:B:181:LEU:HD23	0.60	2.22	19	11
1:C:150:LEU:HD22	1:C:196:TYR:O	0.60	1.96	3	2
1:A:106:TYR:CD1	1:C:89:VAL:HG11	0.60	2.31	10	1
1:A:90:THR:CG2	1:C:90:THR:HG23	0.60	2.27	14	4
1:B:150:LEU:HD22	1:B:196:TYR:O	0.60	1.96	3	2
1:A:188:LEU:HD21	1:B:94:PHE:CD1	0.60	2.32	10	4
1:C:134:LEU:O	1:C:138:THR:HG23	0.59	1.97	20	19
1:C:111:ILE:HD11	1:C:126:ILE:HG21	0.59	1.71	14	7
1:B:145:GLN:O	1:B:150:LEU:HD23	0.59	1.96	8	1
1:A:94:PHE:CD2	1:C:188:LEU:HD21	0.59	2.32	15	5
1:B:113:TYR:CE2	1:B:146:MET:HE2	0.59	2.32	2	2
1:C:178:PRO:HA	1:C:181:LEU:HD11	0.59	1.74	16	10
1:A:187:THR:HG23	1:B:133:SER:HA	0.59	1.74	6	4
1:B:89:VAL:HG11	1:C:106:TYR:CD1	0.59	2.32	10	2
1:A:110:LEU:HD12	1:A:123:ILE:HG12	0.59	1.74	9	10
1:A:111:ILE:HD13	1:A:124:MET:HG3	0.59	1.75	12	4
1:B:89:VAL:HG21	1:C:106:TYR:HB3	0.59	1.73	1	4
1:C:180:PHE:C	1:C:181:LEU:HD23	0.59	2.22	19	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:187:THR:HG22	1:C:133:SER:HB3	0.59	1.73	20	3
1:A:134:LEU:O	1:A:138:THR:HG23	0.59	1.98	3	19
1:A:134:LEU:HD23	1:C:117:PRO:HB3	0.59	1.74	15	1
1:A:133:SER:HA	1:C:187:THR:HG23	0.59	1.74	15	4
1:B:187:THR:HG23	1:C:133:SER:HA	0.59	1.75	6	4
1:C:94:PHE:CB	1:C:134:LEU:HD11	0.59	2.28	14	1
1:B:90:THR:HG23	1:C:90:THR:CG2	0.59	2.27	14	4
1:C:113:TYR:CE2	1:C:146:MET:HE2	0.59	2.32	2	2
1:B:124:MET:HE1	1:B:137:LEU:HD11	0.59	1.75	3	3
1:A:111:ILE:HD11	1:A:126:ILE:HG21	0.59	1.75	17	8
1:B:189:CYS:O	1:B:192:VAL:HG13	0.58	1.97	15	6
1:A:94:PHE:CE1	1:C:188:LEU:HD21	0.58	2.33	11	2
1:A:113:TYR:HB2	1:A:124:MET:HE1	0.58	1.76	5	2
1:C:96:ILE:HB	1:C:138:THR:HG22	0.58	1.76	1	7
1:A:177:ASP:OD1	1:A:179:ALA:HB2	0.58	1.99	10	4
1:C:177:ASP:OD1	1:C:179:ALA:HB2	0.58	1.99	10	4
1:A:94:PHE:CD1	1:C:188:LEU:HD21	0.58	2.33	10	2
1:C:94:PHE:HB2	1:C:134:LEU:HD21	0.58	1.74	6	2
1:A:150:LEU:HD22	1:A:196:TYR:O	0.58	1.99	3	2
1:B:177:ASP:OD1	1:B:179:ALA:HB2	0.57	1.99	10	4
1:B:187:THR:HG22	1:C:133:SER:HB2	0.57	1.76	13	5
1:B:188:LEU:HD21	1:C:94:PHE:CD1	0.57	2.34	10	3
1:B:149:SER:C	1:B:150:LEU:HD23	0.57	2.25	12	3
1:B:110:LEU:HD21	1:B:181:LEU:HD11	0.57	1.75	20	3
1:A:187:THR:HG22	1:B:133:SER:HB2	0.57	1.77	13	5
1:A:90:THR:HG23	1:B:90:THR:HG22	0.57	1.76	15	2
1:B:90:THR:HG23	1:C:90:THR:HG22	0.57	1.76	15	3
1:A:194:LEU:HD12	1:A:194:LEU:O	0.57	1.99	4	7
1:B:188:LEU:HD21	1:C:94:PHE:CE1	0.57	2.34	11	2
1:A:188:LEU:HD21	1:B:94:PHE:CE1	0.56	2.35	11	3
1:A:126:ILE:HG22	1:A:132:PRO:CG	0.56	2.30	3	7
1:A:149:SER:C	1:A:150:LEU:HD23	0.56	2.26	3	4
1:A:104:TYR:CD2	1:A:111:ILE:HD12	0.56	2.35	11	2
1:B:123:ILE:CD1	1:B:185:VAL:HG11	0.56	2.30	20	6
1:B:126:ILE:HD12	1:B:131:ILE:HD12	0.56	1.77	15	4
1:A:89:VAL:HG21	1:B:106:TYR:CB	0.56	2.31	20	5
1:A:96:ILE:HB	1:A:138:THR:HG22	0.56	1.78	1	2
1:A:123:ILE:CD1	1:A:185:VAL:HG11	0.56	2.31	20	6
1:A:124:MET:HE1	1:A:137:LEU:HD11	0.56	1.76	3	3
1:A:124:MET:SD	1:A:197:ILE:HD11	0.56	2.41	17	10
1:A:133:SER:HB2	1:C:187:THR:HG22	0.56	1.78	13	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:111:ILE:HG21	1:B:124:MET:HE3	0.56	1.78	6	1
1:C:123:ILE:CD1	1:C:185:VAL:HG11	0.56	2.31	20	4
1:A:106:TYR:CB	1:C:89:VAL:HG21	0.56	2.31	20	5
1:B:101:LEU:HD13	1:B:102:VAL:N	0.56	2.16	10	4
1:C:149:SER:C	1:C:150:LEU:HD23	0.56	2.25	12	3
1:A:108:GLN:O	1:A:110:LEU:HD22	0.56	2.01	19	5
1:A:181:LEU:N	1:A:181:LEU:HD13	0.56	2.16	18	3
1:A:146:MET:HE3	1:A:197:ILE:HD12	0.56	1.77	12	1
1:A:90:THR:HG23	1:B:90:THR:CG2	0.55	2.30	14	4
1:B:126:ILE:HG22	1:B:132:PRO:CG	0.55	2.31	3	7
1:C:126:ILE:HG22	1:C:132:PRO:CG	0.55	2.32	3	7
1:A:108:GLN:CG	1:A:110:LEU:HD23	0.55	2.31	19	2
1:B:126:ILE:HG22	1:B:132:PRO:HG2	0.55	1.78	4	2
1:A:126:ILE:HD12	1:A:131:ILE:CD1	0.55	2.32	13	3
1:C:127:ALA:O	1:C:131:ILE:HD13	0.55	2.02	9	8
1:C:111:ILE:HD13	1:C:124:MET:CG	0.55	2.31	12	3
1:B:127:ALA:O	1:B:131:ILE:HD13	0.55	2.01	19	7
1:B:110:LEU:HD11	1:B:178:PRO:HB2	0.55	1.77	5	1
1:A:110:LEU:HD21	1:A:181:LEU:CD1	0.55	2.29	15	2
1:A:116:ALA:HB3	1:A:119:THR:OG1	0.55	2.01	3	2
1:C:101:LEU:HD23	1:C:102:VAL:N	0.55	2.17	3	2
1:A:94:PHE:CB	1:A:134:LEU:HD11	0.55	2.31	14	1
1:C:110:LEU:HD11	1:C:178:PRO:HB2	0.55	1.78	5	1
1:C:108:GLN:CG	1:C:110:LEU:HD23	0.55	2.32	17	2
1:A:126:ILE:HG22	1:A:132:PRO:HG2	0.55	1.77	3	2
1:B:149:SER:O	1:B:150:LEU:HD23	0.55	2.02	6	3
1:A:94:PHE:HB3	1:A:134:LEU:HD11	0.55	1.78	14	1
1:A:116:ALA:HB1	1:A:117:PRO:HD2	0.54	1.79	3	18
1:B:96:ILE:CD1	1:B:102:VAL:HG23	0.54	2.32	18	1
1:B:111:ILE:HD13	1:B:124:MET:CG	0.54	2.31	12	2
1:C:124:MET:SD	1:C:197:ILE:HD11	0.54	2.42	17	9
1:C:111:ILE:HG21	1:C:124:MET:HE3	0.54	1.78	6	1
1:C:111:ILE:HD11	1:C:126:ILE:HD13	0.54	1.79	8	5
1:C:95:SER:O	1:C:134:LEU:HD21	0.54	2.03	17	3
1:A:108:GLN:HG2	1:A:110:LEU:HD23	0.54	1.79	19	2
1:A:90:THR:HG22	1:C:90:THR:HG23	0.54	1.79	15	3
1:A:93:THR:HG21	1:B:93:THR:O	0.54	2.02	7	16
1:B:89:VAL:HG21	1:C:106:TYR:CD1	0.54	2.37	17	3
1:A:102:VAL:HG12	1:A:112:ALA:O	0.54	2.02	13	1
1:B:108:GLN:CG	1:B:110:LEU:HD23	0.54	2.33	17	2
1:B:124:MET:SD	1:B:197:ILE:HD11	0.54	2.43	17	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:101:LEU:HD13	1:C:102:VAL:N	0.54	2.17	16	4
1:A:134:LEU:HD12	1:C:117:PRO:HB3	0.54	1.80	3	1
1:C:149:SER:O	1:C:150:LEU:HD23	0.54	2.03	6	3
1:B:95:SER:O	1:B:134:LEU:HD21	0.54	2.03	15	3
1:B:112:ALA:HB2	1:B:185:VAL:CG1	0.54	2.24	18	1
1:C:181:LEU:HD13	1:C:181:LEU:N	0.54	2.18	16	3
1:A:172:ALA:HB1	1:A:177:ASP:OD1	0.54	2.03	12	1
1:C:123:ILE:HB	1:C:194:LEU:HD22	0.54	1.80	6	2
1:B:111:ILE:HD11	1:B:126:ILE:HD13	0.54	1.79	8	4
1:B:101:LEU:HD23	1:B:102:VAL:N	0.54	2.18	3	1
1:B:146:MET:HE3	1:B:197:ILE:HG13	0.54	1.79	9	1
1:A:89:VAL:HG12	1:A:184:ALA:HB2	0.54	1.79	10	1
1:C:150:LEU:HD21	1:C:195:TYR:CB	0.53	2.33	3	2
1:B:123:ILE:HB	1:B:194:LEU:HD22	0.53	1.80	6	2
1:C:146:MET:HE3	1:C:197:ILE:HG13	0.53	1.79	9	1
1:C:96:ILE:CD1	1:C:102:VAL:HG23	0.53	2.33	18	1
1:B:101:LEU:O	1:B:101:LEU:HD23	0.53	2.03	1	1
1:A:106:TYR:CD1	1:C:89:VAL:HG21	0.53	2.38	17	3
1:A:194:LEU:HD12	1:A:194:LEU:C	0.53	2.28	14	18
1:C:116:ALA:HB1	1:C:117:PRO:HD2	0.53	1.81	3	20
1:C:111:ILE:HB	1:C:124:MET:HE3	0.53	1.80	10	1
1:B:117:PRO:HB3	1:C:134:LEU:HD23	0.53	1.79	15	1
1:A:127:ALA:O	1:A:131:ILE:HD13	0.53	2.03	9	8
1:A:89:VAL:HG21	1:B:106:TYR:CD1	0.53	2.39	17	3
1:B:181:LEU:HD13	1:B:181:LEU:N	0.53	2.18	16	3
1:C:104:TYR:CD2	1:C:111:ILE:HD12	0.53	2.38	11	2
1:A:101:LEU:HD23	1:A:101:LEU:O	0.53	2.03	1	2
1:B:91:THR:HG23	1:B:105:ASP:CG	0.53	2.29	8	1
1:A:93:THR:O	1:C:93:THR:HG21	0.53	2.04	8	15
1:B:116:ALA:HB3	1:B:119:THR:OG1	0.53	2.04	3	2
1:A:117:PRO:HB3	1:B:134:LEU:HD23	0.53	1.81	15	2
1:A:110:LEU:HD12	1:A:123:ILE:CG1	0.52	2.33	2	6
1:C:126:ILE:HG22	1:C:132:PRO:HG2	0.52	1.81	4	2
1:A:91:THR:HG23	1:A:105:ASP:CG	0.52	2.28	8	1
1:B:104:TYR:CD2	1:B:111:ILE:HD12	0.52	2.39	11	2
1:C:101:LEU:HD23	1:C:101:LEU:O	0.52	2.04	1	1
1:B:134:LEU:HD12	1:B:135:GLU:N	0.52	2.19	2	1
1:C:93:THR:CG2	1:C:103:VAL:HG12	0.52	2.33	4	3
1:A:94:PHE:HB2	1:A:134:LEU:HD21	0.52	1.82	16	2
1:B:150:LEU:HD13	1:B:196:TYR:O	0.52	2.04	12	1
1:C:150:LEU:HD13	1:C:196:TYR:O	0.52	2.04	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:178:PRO:C	1:A:181:LEU:HD22	0.52	2.29	17	4
1:A:113:TYR:OH	1:A:141:VAL:HG13	0.52	2.04	3	2
1:A:150:LEU:HD21	1:A:195:TYR:HB3	0.52	1.80	3	1
1:A:188:LEU:HD11	1:B:94:PHE:CE1	0.52	2.40	18	1
1:C:91:THR:HG23	1:C:105:ASP:CG	0.52	2.30	8	1
1:A:111:ILE:HB	1:A:124:MET:HE3	0.52	1.79	10	3
1:B:111:ILE:HB	1:B:124:MET:HE3	0.52	1.81	10	1
1:B:150:LEU:HD21	1:B:195:TYR:CB	0.52	2.34	3	2
1:B:178:PRO:C	1:B:181:LEU:HD22	0.52	2.30	17	4
1:B:110:LEU:CD2	1:B:181:LEU:HD12	0.52	2.34	15	1
1:B:93:THR:HG21	1:C:93:THR:O	0.52	2.05	8	16
1:B:103:VAL:HG22	1:B:112:ALA:CB	0.52	2.34	2	3
1:C:103:VAL:HG22	1:C:112:ALA:CB	0.52	2.34	2	2
1:C:89:VAL:HG12	1:C:184:ALA:HB2	0.52	1.81	10	1
1:B:93:THR:CG2	1:B:103:VAL:HG12	0.52	2.34	4	2
1:B:172:ALA:HB1	1:B:177:ASP:OD1	0.52	2.05	12	1
1:C:110:LEU:HD11	1:C:181:LEU:HD12	0.51	1.82	8	2
1:B:116:ALA:HB1	1:B:117:PRO:HD2	0.51	1.81	3	20
1:A:150:LEU:HD21	1:A:195:TYR:CB	0.51	2.34	6	2
1:C:150:LEU:HD11	1:C:195:TYR:HB3	0.51	1.82	6	1
1:B:89:VAL:HG12	1:B:183:MET:HG3	0.51	1.80	8	2
1:B:89:VAL:HG12	1:B:184:ALA:HB2	0.51	1.82	10	1
1:C:111:ILE:CD1	1:C:126:ILE:HG23	0.51	2.25	1	6
1:C:116:ALA:HB3	1:C:119:THR:OG1	0.51	2.05	3	2
1:A:187:THR:HG22	1:B:133:SER:HA	0.51	1.82	11	1
1:B:90:THR:HG23	1:C:90:THR:HG23	0.51	1.81	13	1
1:A:124:MET:CG	1:A:197:ILE:HD11	0.51	2.36	18	1
1:A:110:LEU:HD21	1:A:181:LEU:HD11	0.51	1.81	20	3
1:A:111:ILE:HG21	1:A:124:MET:HE3	0.51	1.81	8	2
1:A:112:ALA:HB2	1:A:185:VAL:CG1	0.51	2.23	18	1
1:A:94:PHE:CB	1:A:134:LEU:HD21	0.51	2.36	16	2
1:A:95:SER:O	1:A:134:LEU:HD21	0.51	2.05	17	3
1:B:167:ARG:O	1:B:172:ALA:HB3	0.51	2.06	19	2
1:C:178:PRO:C	1:C:181:LEU:HD22	0.51	2.30	17	4
1:B:189:CYS:HB3	1:B:192:VAL:HG22	0.51	1.83	13	5
1:A:189:CYS:O	1:A:192:VAL:HG13	0.51	2.05	15	4
1:A:89:VAL:HG12	1:A:183:MET:HG3	0.51	1.82	8	2
1:C:98:SER:OG	1:C:99:THR:HG22	0.51	2.06	18	1
1:A:106:TYR:HB3	1:C:89:VAL:HG11	0.51	1.81	12	2
1:A:168:ASP:O	1:A:169:ALA:HB2	0.51	2.06	14	1
1:B:93:THR:HG22	1:B:103:VAL:CG1	0.51	2.36	3	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:150:LEU:HD11	1:B:195:TYR:HB3	0.51	1.83	6	1
1:C:89:VAL:HG12	1:C:183:MET:HG3	0.51	1.82	8	2
1:B:96:ILE:HB	1:B:138:THR:HG22	0.50	1.82	9	5
1:A:134:LEU:HD12	1:A:135:GLU:N	0.50	2.21	2	1
1:B:98:SER:OG	1:B:99:THR:HG22	0.50	2.06	18	1
1:C:172:ALA:HB1	1:C:177:ASP:OD1	0.50	2.06	12	1
1:C:110:LEU:CD2	1:C:181:LEU:HD12	0.50	2.32	15	1
1:B:89:VAL:HG21	1:C:106:TYR:CB	0.50	2.35	1	5
1:A:93:THR:CG2	1:A:103:VAL:HG12	0.50	2.36	11	3
1:C:124:MET:CG	1:C:197:ILE:HD11	0.50	2.37	18	4
1:C:168:ASP:O	1:C:169:ALA:HB2	0.50	2.06	14	1
1:A:178:PRO:CA	1:A:181:LEU:HD11	0.50	2.37	19	1
1:A:178:PRO:CB	1:A:181:LEU:HD11	0.50	2.36	19	1
1:A:108:GLN:HB3	1:A:110:LEU:HD23	0.50	1.83	4	7
1:B:124:MET:CG	1:B:197:ILE:HD11	0.50	2.36	18	4
1:C:189:CYS:O	1:C:192:VAL:HG22	0.50	2.07	2	3
1:B:91:THR:HG21	1:B:184:ALA:CB	0.50	2.37	5	2
1:B:108:GLN:HB3	1:B:110:LEU:HD23	0.50	1.83	9	2
1:B:95:SER:O	1:B:134:LEU:HD11	0.50	2.07	10	2
1:A:98:SER:OG	1:A:99:THR:HG22	0.50	2.06	18	1
1:C:194:LEU:HD12	1:C:194:LEU:O	0.50	2.06	20	2
1:A:93:THR:HG22	1:A:103:VAL:CG1	0.50	2.37	2	6
1:B:189:CYS:O	1:B:192:VAL:HG22	0.50	2.07	15	3
1:A:150:LEU:HD13	1:A:196:TYR:O	0.49	2.06	12	1
1:A:178:PRO:CA	1:A:181:LEU:HD21	0.49	2.37	18	2
1:B:194:LEU:HD12	1:B:194:LEU:O	0.49	2.06	20	3
1:A:110:LEU:O	1:A:111:ILE:HD13	0.49	2.07	10	1
1:A:167:ARG:O	1:A:172:ALA:HB3	0.49	2.07	19	2
1:C:167:ARG:O	1:C:172:ALA:HB3	0.49	2.06	19	2
1:A:177:ASP:OD2	1:A:179:ALA:HB2	0.49	2.07	19	3
1:C:189:CYS:HB3	1:C:192:VAL:HG22	0.49	1.83	13	4
1:A:89:VAL:HG11	1:B:106:TYR:CD2	0.49	2.43	5	1
1:A:110:LEU:CD2	1:A:181:LEU:HD12	0.49	2.36	6	3
1:C:93:THR:HG22	1:C:103:VAL:CG1	0.49	2.32	11	4
1:A:96:ILE:HA	1:A:134:LEU:HD11	0.49	1.85	17	1
1:A:133:SER:HA	1:C:187:THR:HG22	0.49	1.84	11	1
1:B:168:ASP:O	1:B:169:ALA:HB2	0.49	2.07	14	1
1:A:102:VAL:HG11	1:A:137:LEU:HG	0.49	1.85	16	1
1:A:111:ILE:HD13	1:A:124:MET:CG	0.49	2.37	12	2
1:C:134:LEU:HD12	1:C:135:GLU:N	0.49	2.22	2	1
1:B:123:ILE:HD13	1:B:194:LEU:CD2	0.49	2.38	16	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:106:TYR:CD2	1:C:89:VAL:HG11	0.49	2.43	5	1
1:C:94:PHE:CB	1:C:134:LEU:HD21	0.49	2.37	16	2
1:A:188:LEU:HA	1:B:134:LEU:HD13	0.49	1.83	14	1
1:A:189:CYS:HB3	1:A:192:VAL:HG22	0.49	1.84	13	2
1:C:108:GLN:HB3	1:C:110:LEU:HD23	0.49	1.83	9	2
1:A:96:ILE:CD1	1:A:102:VAL:HG23	0.49	2.37	18	1
1:C:123:ILE:HD13	1:C:194:LEU:CD2	0.48	2.38	16	2
1:B:108:GLN:O	1:B:110:LEU:HD22	0.48	2.08	19	2
1:A:149:SER:O	1:A:150:LEU:C	0.48	2.56	11	2
1:B:94:PHE:CB	1:B:134:LEU:HD21	0.48	2.38	6	2
1:C:108:GLN:O	1:C:110:LEU:HD22	0.48	2.08	19	2
1:A:146:MET:CB	1:A:197:ILE:HG21	0.48	2.38	13	1
1:A:90:THR:HG23	1:C:90:THR:HG23	0.48	1.86	13	2
1:C:91:THR:HG21	1:C:184:ALA:CB	0.48	2.39	5	2
1:C:150:LEU:HD21	1:C:195:TYR:HB2	0.48	1.85	6	1
1:C:111:ILE:HD12	1:C:124:MET:C	0.48	2.33	19	2
1:C:96:ILE:HA	1:C:134:LEU:HD11	0.48	1.86	17	1
1:B:111:ILE:CD1	1:B:126:ILE:HG23	0.48	2.32	5	6
1:B:89:VAL:HG13	1:B:183:MET:CG	0.48	2.39	17	1
1:B:149:SER:O	1:B:150:LEU:C	0.47	2.57	2	2
1:C:149:SER:O	1:C:150:LEU:C	0.47	2.57	2	2
1:C:95:SER:O	1:C:134:LEU:HD11	0.47	2.09	10	1
1:B:110:LEU:HD11	1:B:181:LEU:HD12	0.47	1.85	8	1
1:A:89:VAL:HG11	1:B:106:TYR:CG	0.47	2.44	9	1
1:B:89:VAL:HG11	1:C:106:TYR:HB3	0.47	1.86	12	2
1:C:89:VAL:HG13	1:C:183:MET:CG	0.47	2.39	17	1
1:A:187:THR:HG21	1:B:106:TYR:OH	0.47	2.10	2	1
1:C:126:ILE:HD12	1:C:131:ILE:CD1	0.47	2.40	13	2
1:A:134:LEU:HD21	1:C:188:LEU:HA	0.47	1.86	13	1
1:C:177:ASP:OD2	1:C:179:ALA:HB2	0.47	2.09	19	3
1:B:89:VAL:O	1:B:90:THR:C	0.47	2.58	10	2
1:B:187:THR:HG22	1:C:133:SER:HA	0.47	1.87	11	1
1:B:177:ASP:OD2	1:B:179:ALA:HB2	0.47	2.10	19	4
1:B:177:ASP:CG	1:B:178:PRO:HD2	0.47	2.35	16	8
1:B:117:PRO:HB3	1:C:134:LEU:HD12	0.47	1.86	3	1
1:B:89:VAL:HG11	1:C:106:TYR:CG	0.46	2.45	9	1
1:C:89:VAL:O	1:C:90:THR:C	0.46	2.58	10	2
1:A:89:VAL:HG11	1:B:106:TYR:HB3	0.46	1.86	12	2
1:C:177:ASP:CG	1:C:178:PRO:HD2	0.46	2.35	16	7
1:B:126:ILE:HD12	1:B:131:ILE:CD1	0.46	2.41	13	1
1:B:180:PHE:C	1:B:181:LEU:HD13	0.46	2.36	18	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:179:ALA:HA	1:A:194:LEU:HD11	0.46	1.88	10	1
1:A:89:VAL:HG13	1:A:183:MET:CG	0.46	2.41	17	1
1:C:150:LEU:O	1:C:150:LEU:HD12	0.46	2.11	18	1
1:B:150:LEU:HD12	1:B:150:LEU:O	0.46	2.11	18	1
1:A:150:LEU:HD11	1:A:195:TYR:CE2	0.46	2.46	7	1
1:B:116:ALA:HB3	1:B:119:THR:CG2	0.46	2.34	8	1
1:A:180:PHE:C	1:A:181:LEU:HD13	0.46	2.36	18	3
1:B:150:LEU:HD21	1:B:195:TYR:HB2	0.46	1.86	6	1
1:C:95:SER:O	1:C:134:LEU:HD22	0.46	2.10	6	1
1:C:110:LEU:HD21	1:C:181:LEU:CD1	0.46	2.35	15	2
1:A:150:LEU:O	1:A:150:LEU:HD23	0.46	2.11	5	1
1:C:89:VAL:HG12	1:C:183:MET:CB	0.46	2.41	8	1
1:C:180:PHE:C	1:C:181:LEU:HD13	0.45	2.36	18	2
1:A:106:TYR:CG	1:C:89:VAL:HG11	0.45	2.46	9	1
1:B:110:LEU:HD21	1:B:181:LEU:CD1	0.45	2.41	9	2
1:A:113:TYR:CD2	1:A:146:MET:HE2	0.45	2.46	16	1
1:B:111:ILE:HD12	1:B:124:MET:C	0.45	2.35	19	2
1:A:89:VAL:O	1:A:90:THR:C	0.45	2.58	9	2
1:C:122:TYR:HB3	1:C:197:ILE:HD12	0.45	1.88	15	2
1:A:106:TYR:CZ	1:C:89:VAL:HG11	0.45	2.45	17	1
1:A:116:ALA:HB3	1:A:119:THR:CG2	0.45	2.34	8	1
1:B:110:LEU:HD12	1:B:123:ILE:HG13	0.45	1.88	16	2
1:B:89:VAL:HG11	1:C:106:TYR:CD2	0.45	2.46	5	1
1:B:89:VAL:HG12	1:B:183:MET:CB	0.45	2.42	8	1
1:C:110:LEU:HD12	1:C:123:ILE:HG13	0.45	1.88	16	2
1:A:110:LEU:HD23	1:A:181:LEU:O	0.45	2.12	15	1
1:C:108:GLN:HG2	1:C:110:LEU:HD23	0.45	1.88	19	2
1:A:150:LEU:HD11	1:A:195:TYR:HB3	0.45	1.89	9	1
1:C:124:MET:HG2	1:C:197:ILE:HD11	0.45	1.89	18	2
1:A:150:LEU:HD12	1:A:150:LEU:O	0.45	2.12	18	1
1:A:90:THR:HG23	1:B:90:THR:HG23	0.45	1.87	13	1
1:A:177:ASP:CG	1:A:178:PRO:HD2	0.45	2.36	5	9
1:A:181:LEU:H	1:A:181:LEU:HD23	0.45	1.70	1	1
1:C:92:ALA:HB1	1:C:94:PHE:CE2	0.45	2.47	6	1
1:B:126:ILE:HG22	1:B:132:PRO:HG3	0.44	1.89	14	2
1:A:106:TYR:HB2	1:C:89:VAL:HG21	0.44	1.89	12	2
1:A:93:THR:CB	1:A:103:VAL:HG12	0.44	2.42	1	5
1:C:181:LEU:HD23	1:C:181:LEU:H	0.44	1.73	1	1
1:C:113:TYR:OH	1:C:141:VAL:HG13	0.44	2.13	3	1
1:A:178:PRO:C	1:A:181:LEU:HD21	0.44	2.38	18	2
1:A:96:ILE:HD13	1:A:102:VAL:CG2	0.44	2.42	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:106:TYR:CE2	1:C:89:VAL:HG11	0.44	2.48	5	1
1:A:95:SER:O	1:A:134:LEU:HD22	0.44	2.13	6	1
1:B:96:ILE:HA	1:B:134:LEU:HD11	0.44	1.88	17	1
1:A:98:SER:O	1:A:99:THR:HG23	0.44	2.13	4	3
1:A:89:VAL:HG21	1:B:106:TYR:HB2	0.44	1.90	16	2
1:C:178:PRO:CA	1:C:181:LEU:HD11	0.43	2.43	19	1
1:A:91:THR:HG21	1:A:184:ALA:CB	0.43	2.43	20	1
1:A:96:ILE:HD11	1:A:138:THR:HG23	0.43	1.89	8	1
1:B:137:LEU:O	1:B:141:VAL:HG23	0.43	2.13	4	3
1:B:124:MET:HG2	1:B:197:ILE:HD11	0.43	1.89	18	2
1:B:98:SER:O	1:B:99:THR:HG23	0.43	2.13	3	4
1:A:110:LEU:HD11	1:A:181:LEU:HD12	0.43	1.89	8	1
1:A:101:LEU:HD23	1:A:101:LEU:C	0.43	2.38	14	1
1:C:146:MET:CE	1:C:197:ILE:HD12	0.43	2.44	20	1
1:A:89:VAL:HG12	1:A:183:MET:CB	0.43	2.43	8	1
1:B:89:VAL:HG11	1:C:106:TYR:CE2	0.43	2.49	5	1
1:A:95:SER:CB	1:A:101:LEU:HD12	0.43	2.43	7	2
1:A:103:VAL:O	1:A:103:VAL:HG23	0.43	2.14	12	1
1:B:178:PRO:CA	1:B:181:LEU:HD21	0.43	2.44	18	1
1:C:98:SER:O	1:C:99:THR:HG23	0.43	2.13	3	4
1:C:104:TYR:CD1	1:C:111:ILE:HD12	0.43	2.49	10	1
1:C:126:ILE:HG22	1:C:132:PRO:HG3	0.43	1.90	14	1
1:B:89:VAL:HG21	1:C:106:TYR:CG	0.43	2.49	17	1
1:B:178:PRO:CA	1:B:181:LEU:HD11	0.43	2.43	19	1
1:A:104:TYR:CD1	1:A:111:ILE:HD12	0.42	2.49	10	1
1:A:93:THR:HB	1:A:103:VAL:HG12	0.42	1.90	1	1
1:A:134:LEU:HD13	1:C:117:PRO:CB	0.42	2.44	2	1
1:A:95:SER:HB3	1:A:101:LEU:HD12	0.42	1.89	7	1
1:B:122:TYR:HB3	1:B:197:ILE:HD12	0.42	1.91	15	2
1:B:89:VAL:HG11	1:C:106:TYR:CZ	0.42	2.48	17	1
1:A:150:LEU:HD21	1:A:195:TYR:HB2	0.42	1.90	9	1
1:A:146:MET:CG	1:A:197:ILE:HG21	0.42	2.45	14	1
1:A:89:VAL:HG11	1:B:106:TYR:CZ	0.42	2.49	17	1
1:C:178:PRO:CA	1:C:181:LEU:HD21	0.42	2.44	18	1
1:C:146:MET:CB	1:C:197:ILE:HG21	0.42	2.44	13	1
1:A:89:VAL:HG21	1:B:106:TYR:CG	0.42	2.49	17	1
1:C:91:THR:HG23	1:C:105:ASP:OD1	0.42	2.15	8	1
1:A:106:TYR:CG	1:C:89:VAL:HG21	0.42	2.49	17	1
1:B:89:VAL:HG12	1:B:183:MET:HB3	0.42	1.91	8	1
1:A:106:TYR:CD2	1:C:89:VAL:HG21	0.42	2.50	5	1
1:C:150:LEU:HD12	1:C:195:TYR:HB3	0.42	1.92	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:178:PRO:CB	1:C:181:LEU:HD11	0.42	2.45	12	1
1:A:124:MET:HG2	1:A:197:ILE:HD11	0.42	1.89	18	1
1:A:110:LEU:HG	1:A:181:LEU:HD23	0.42	1.91	18	1
1:A:89:VAL:HG11	1:B:106:TYR:CE2	0.42	2.49	5	1
1:B:146:MET:CB	1:B:197:ILE:HG21	0.42	2.45	13	1
1:B:146:MET:CE	1:B:197:ILE:HD12	0.42	2.45	20	1
1:B:108:GLN:HG2	1:B:110:LEU:HD23	0.41	1.91	19	2
1:B:91:THR:HG21	1:B:184:ALA:HB2	0.41	1.91	20	1
1:C:137:LEU:O	1:C:141:VAL:HG23	0.41	2.14	4	2
1:A:192:VAL:HB	1:A:193:PRO:HD2	0.41	1.92	6	1
1:C:146:MET:HE3	1:C:197:ILE:HG21	0.41	1.92	18	1
1:B:181:LEU:HD23	1:B:181:LEU:H	0.41	1.73	1	1
1:B:93:THR:CB	1:B:103:VAL:HG12	0.41	2.46	12	1
1:A:96:ILE:HD13	1:A:102:VAL:HG23	0.41	1.92	19	2
1:A:111:ILE:CD1	1:A:126:ILE:HG23	0.41	2.45	7	1
1:B:91:THR:HG23	1:B:105:ASP:OD1	0.41	2.16	8	1
1:B:194:LEU:C	1:B:194:LEU:HD12	0.41	2.40	14	1
1:C:194:LEU:C	1:C:194:LEU:HD12	0.41	2.40	14	2
1:A:92:ALA:HB1	1:A:94:PHE:CE2	0.41	2.50	6	1
1:B:92:ALA:HB1	1:B:94:PHE:CE2	0.41	2.51	6	2
1:B:178:PRO:CB	1:B:181:LEU:HD11	0.41	2.45	12	1
1:A:117:PRO:CB	1:B:134:LEU:HD13	0.41	2.45	2	1
1:A:150:LEU:HD12	1:A:195:TYR:HB3	0.41	1.91	8	1
1:B:96:ILE:HD11	1:B:138:THR:HG23	0.41	1.93	8	1
1:C:89:VAL:HG12	1:C:183:MET:HB3	0.41	1.90	8	1
1:C:116:ALA:HB3	1:C:119:THR:CG2	0.41	2.33	8	1
1:A:188:LEU:HA	1:B:134:LEU:HD21	0.41	1.92	13	1
1:A:122:TYR:HB3	1:A:197:ILE:HD12	0.41	1.92	15	1
1:B:134:LEU:HD12	1:B:134:LEU:C	0.41	2.41	2	1
1:A:150:LEU:O	1:A:151:GLN:C	0.41	2.63	20	1
1:B:89:VAL:HG21	1:C:106:TYR:CD2	0.41	2.51	5	1
1:B:104:TYR:CD1	1:B:111:ILE:HD12	0.41	2.51	10	1
1:A:126:ILE:HG22	1:A:132:PRO:HG3	0.41	1.93	14	2
1:B:194:LEU:HD12	1:B:194:LEU:C	0.41	2.41	17	1
1:C:194:LEU:HD12	1:C:194:LEU:C	0.41	2.41	17	1
1:A:146:MET:CE	1:A:197:ILE:HD12	0.41	2.46	20	1
1:B:89:VAL:HG21	1:C:106:TYR:HB2	0.40	1.93	16	1
1:B:146:MET:HE3	1:B:197:ILE:HG21	0.40	1.93	18	1
1:A:137:LEU:O	1:A:141:VAL:HG23	0.40	2.17	4	1
1:A:96:ILE:HD13	1:A:102:VAL:HG21	0.40	1.92	2	1
1:A:89:VAL:HG12	1:A:183:MET:HB3	0.40	1.92	8	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	93/114 (82%)	70±3 (75±3%)	17±3 (18±3%)	6±2 (7±2%)	2	16
1	B	93/114 (82%)	70±3 (75±3%)	17±3 (18±3%)	6±2 (7±2%)	2	17
1	C	93/114 (82%)	70±2 (75±3%)	17±3 (18±3%)	6±2 (7±2%)	2	16
All	All	5580/6840 (82%)	4177 (75%)	1020 (18%)	383 (7%)	2	16

All 56 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	115	PRO	20
1	B	115	PRO	20
1	C	115	PRO	20
1	A	133	SER	19
1	C	133	SER	18
1	A	107	GLN	16
1	B	107	GLN	16
1	B	133	SER	16
1	C	107	GLN	16
1	B	144	PHE	10
1	C	144	PHE	10
1	A	144	PHE	9
1	A	98	SER	9
1	B	98	SER	9
1	C	98	SER	9
1	A	89	VAL	7
1	B	89	VAL	7
1	C	89	VAL	7
1	A	150	LEU	6
1	A	170	GLY	6
1	B	150	LEU	6
1	B	170	GLY	6
1	C	150	LEU	6
1	C	170	GLY	6
1	A	99	THR	6

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Mol	Chain	Res	Type	Models (Total)
1	B	99	THR	6
1	C	99	THR	6
1	B	151	GLN	5
1	A	182	GLY	5
1	A	90	THR	5
1	B	90	THR	5
1	C	90	THR	5
1	A	169	ALA	5
1	B	169	ALA	5
1	C	169	ALA	5
1	A	151	GLN	4
1	C	151	GLN	4
1	B	182	GLY	4
1	C	182	GLY	4
1	A	120	CYS	3
1	B	120	CYS	3
1	C	120	CYS	3
1	A	174	SER	3
1	B	167	ARG	3
1	C	167	ARG	3
1	B	105	ASP	2
1	A	97	GLY	2
1	A	167	ARG	2
1	B	174	SER	2
1	C	97	GLY	2
1	C	174	SER	2
1	A	146	MET	1
1	B	146	MET	1
1	C	105	ASP	1
1	C	146	MET	1
1	B	97	GLY	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	77/91 (85%)	53±4 (69±5%)	24±4 (31±5%)	1 15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	77/91 (85%)	54±3 (71±5%)	23±3 (29±5%)	1 18
1	C	77/91 (85%)	54±3 (71±5%)	22±3 (29±5%)	1 18
All	All	4620/5460 (85%)	3239 (70%)	1381 (30%)	1 17

All 154 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	109	LEU	20
1	A	137	LEU	20
1	A	140	LYS	20
1	A	167	ARG	20
1	B	137	LEU	20
1	B	140	LYS	20
1	B	167	ARG	20
1	C	137	LEU	20
1	C	140	LYS	20
1	C	167	ARG	20
1	A	114	LYS	19
1	A	123	ILE	19
1	B	114	LYS	19
1	B	123	ILE	19
1	C	114	LYS	19
1	C	123	ILE	19
1	A	110	LEU	17
1	A	139	ARG	15
1	B	101	LEU	15
1	B	125	LYS	15
1	B	139	ARG	15
1	B	183	MET	15
1	C	101	LEU	15
1	C	125	LYS	15
1	C	139	ARG	15
1	C	183	MET	15
1	A	125	LYS	14
1	A	183	MET	14
1	A	101	LEU	13
1	A	149	SER	13
1	A	186	SER	13
1	A	196	TYR	13
1	B	105	ASP	13

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Mol	Chain	Res	Type	Models (Total)
1	B	133	SER	13
1	B	149	SER	13
1	B	186	SER	13
1	C	105	ASP	13
1	C	149	SER	13
1	C	186	SER	13
1	A	107	GLN	13
1	B	107	GLN	13
1	C	107	GLN	13
1	A	181	LEU	13
1	A	105	ASP	12
1	A	133	SER	12
1	C	133	SER	12
1	B	95	SER	12
1	B	181	LEU	12
1	C	181	LEU	12
1	A	95	SER	11
1	A	124	MET	11
1	A	134	LEU	11
1	A	187	THR	11
1	B	124	MET	11
1	B	134	LEU	11
1	C	124	MET	11
1	C	134	LEU	11
1	B	187	THR	10
1	C	187	THR	10
1	A	142	HIS	10
1	B	142	HIS	10
1	C	142	HIS	10
1	C	196	TYR	10
1	C	95	SER	10
1	A	150	LEU	9
1	B	150	LEU	9
1	C	150	LEU	9
1	C	171	SER	9
1	B	144	PHE	9
1	C	144	PHE	9
1	A	197	ILE	9
1	B	196	TYR	9
1	B	197	ILE	9
1	C	197	ILE	9
1	A	98	SER	8

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Mol	Chain	Res	Type	Models (Total)
1	A	146	MET	8
1	A	171	SER	8
1	B	98	SER	8
1	B	146	MET	8
1	B	171	SER	8
1	C	98	SER	8
1	C	146	MET	8
1	A	144	PHE	8
1	A	174	SER	8
1	B	135	GLU	8
1	B	174	SER	8
1	C	174	SER	8
1	B	108	GLN	8
1	C	108	GLN	8
1	A	126	ILE	7
1	B	188	LEU	7
1	C	188	LEU	7
1	A	135	GLU	7
1	A	148	CYS	7
1	A	191	GLU	7
1	B	148	CYS	7
1	B	191	GLU	7
1	C	135	GLU	7
1	C	148	CYS	7
1	C	191	GLU	7
1	A	108	GLN	7
1	B	110	LEU	7
1	B	126	ILE	6
1	C	126	ILE	6
1	C	129	GLU	6
1	C	110	LEU	6
1	A	129	GLU	5
1	A	151	GLN	5
1	A	188	LEU	5
1	B	129	GLU	5
1	B	151	GLN	5
1	C	151	GLN	5
1	A	99	THR	5
1	B	99	THR	5
1	C	99	THR	5
1	A	147	GLU	4
1	B	147	GLU	4

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Mol	Chain	Res	Type	Models (Total)
1	C	147	GLU	4
1	A	89	VAL	4
1	A	120	CYS	4
1	B	89	VAL	4
1	B	120	CYS	4
1	C	89	VAL	4
1	C	120	CYS	4
1	A	96	ILE	4
1	A	130	SER	3
1	B	130	SER	3
1	C	130	SER	3
1	A	145	GLN	3
1	A	168	ASP	2
1	B	168	ASP	2
1	C	168	ASP	2
1	A	194	LEU	2
1	B	145	GLN	2
1	B	194	LEU	2
1	C	145	GLN	2
1	C	194	LEU	2
1	B	96	ILE	2
1	C	96	ILE	2
1	B	143	ASN	2
1	C	143	ASN	2
1	A	91	THR	2
1	B	91	THR	2
1	C	91	THR	2
1	A	121	CYS	1
1	B	93	THR	1
1	C	93	THR	1
1	A	102	VAL	1
1	A	122	TYR	1
1	A	143	ASN	1
1	B	122	TYR	1
1	C	122	TYR	1
1	A	111	ILE	1
1	C	109	LEU	1

6.3.3 RNA

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates

There are no oligosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 23% for the well-defined parts and 23% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *nef_chemical_shift_list_C*

7.1.1 Bookkeeping

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

Total number of shifts	1001
Number of shifts mapped to atoms	1001
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	98	-0.03 ± 0.29	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	92	0.18 ± 0.26	None needed (< 0.5 ppm)
$^{13}C'$	0	—	None (insufficient data)
^{15}N	98	-0.06 ± 0.32	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 23%, i.e. 839 atoms were assigned a chemical shift out of a possible 3627. 0 out of 45 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	333/1392 (24%)	170/567 (30%)	81/564 (14%)	82/261 (31%)
Sidechain	475/1962 (24%)	324/1305 (25%)	151/615 (25%)	0/42 (0%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	31/273 (11%)	31/129 (24%)	0/141 (0%)	0/3 (0%)
Overall	839/3627 (23%)	525/2001 (26%)	232/1320 (18%)	82/306 (27%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 23%, i.e. 998 atoms were assigned a chemical shift out of a possible 4338. 0 out of 54 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	398/1689 (24%)	202/690 (29%)	98/684 (14%)	98/315 (31%)
Sidechain	569/2355 (24%)	387/1563 (25%)	182/741 (25%)	0/51 (0%)
Aromatic	31/294 (11%)	31/141 (22%)	0/147 (0%)	0/6 (0%)
Overall	998/4338 (23%)	620/2394 (26%)	280/1572 (18%)	98/372 (26%)

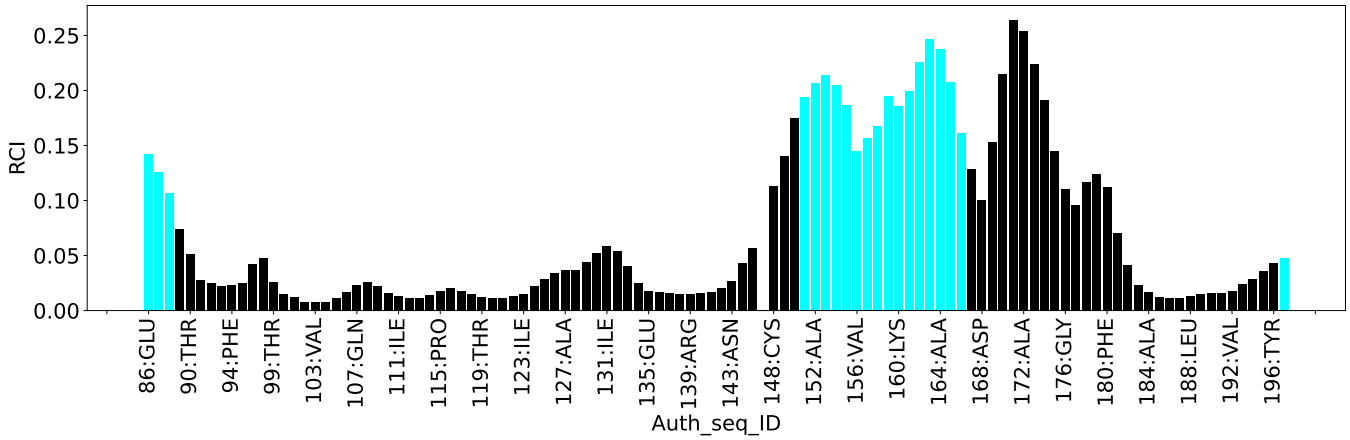
7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots (i)

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	2372
Intra-residue (|i-j|=0)	593
Sequential (|i-j|=1)	792
Medium range (|i-j|>1 and |i-j|<5)	349
Long range (|i-j|≥5)	573
Inter-chain	65
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	318
Number of unmapped restraints	0
Number of restraints per residue	7.9
Number of long range restraints per residue[1]	1.7

[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

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	97.3	0.2
0.2-0.5 (Medium)	62.5	0.5
>0.5 (Large)	4.2	0.75

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

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

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	46.3	9.89
10.0-20.0 (Medium)	0.8	18.54
>20.0 (Large)	4.2	48.12

9 Distance violation analysis (i)

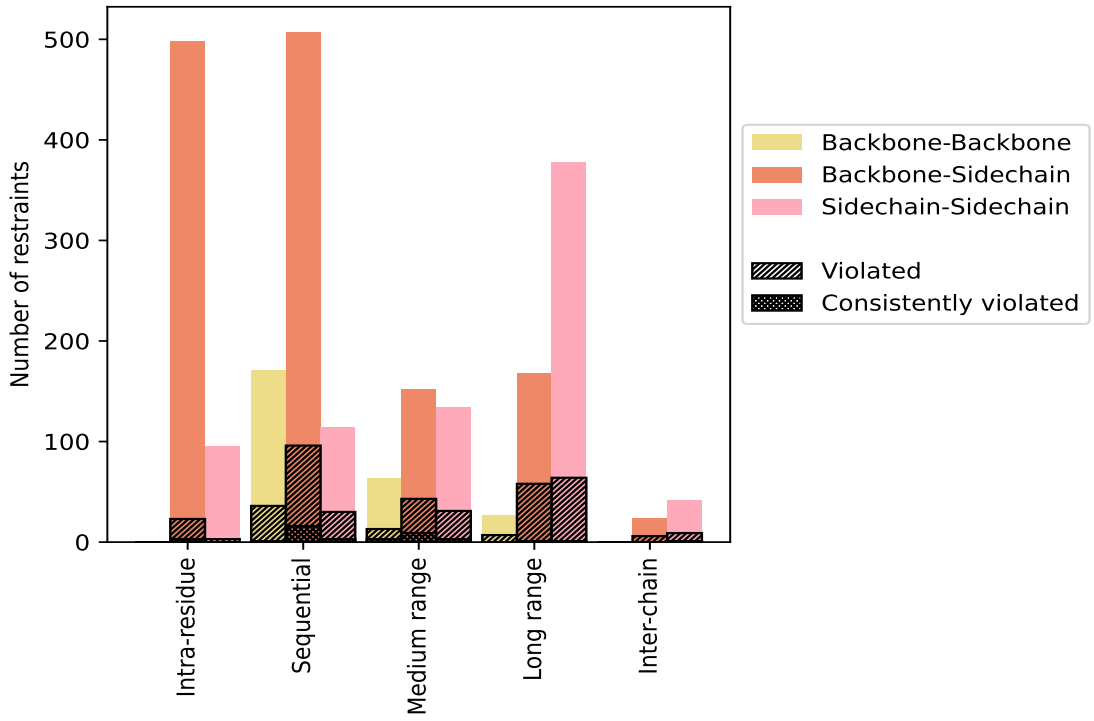
9.1 Summary of distance violations (i)

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)	593	25.0	26	4.4	1.1	3	0.5	0.1
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	498	21.0	23	4.6	1.0	3	0.6	0.1
Sidechain-Sidechain	95	4.0	3	3.2	0.1	0	0.0	0.0
Sequential (|i-j|=1)	792	33.4	162	20.5	6.8	20	2.5	0.8
Backbone-Backbone	171	7.2	36	21.1	1.5	1	0.6	0.0
Backbone-Sidechain	507	21.4	96	18.9	4.0	16	3.2	0.7
Sidechain-Sidechain	114	4.8	30	26.3	1.3	3	2.6	0.1
Medium range (|i-j|>1 & |i-j|<5)	349	14.7	87	24.9	3.7	15	4.3	0.6
Backbone-Backbone	63	2.7	13	20.6	0.5	3	4.8	0.1
Backbone-Sidechain	152	6.4	43	28.3	1.8	9	5.9	0.4
Sidechain-Sidechain	134	5.6	31	23.1	1.3	3	2.2	0.1
Long range (|i-j|≥5)	573	24.2	129	22.5	5.4	2	0.3	0.1
Backbone-Backbone	27	1.1	7	25.9	0.3	0	0.0	0.0
Backbone-Sidechain	168	7.1	58	34.5	2.4	1	0.6	0.0
Sidechain-Sidechain	378	15.9	64	16.9	2.7	1	0.3	0.0
Inter-chain	65	2.7	15	23.1	0.6	1	1.5	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	24	1.0	6	25.0	0.3	0	0.0	0.0
Sidechain-Sidechain	41	1.7	9	22.0	0.4	1	2.4	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	2372	100.0	419	17.7	17.7	41	1.7	1.7
Backbone-Backbone	261	11.0	56	21.5	2.4	4	1.5	0.2
Backbone-Sidechain	1349	56.9	226	16.8	9.5	29	2.1	1.2
Sidechain-Sidechain	762	32.1	137	18.0	5.8	8	1.0	0.3

[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



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

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	9	73	30	30	2	144	0.22	0.69	0.11	0.19
2	8	82	31	22	4	147	0.22	0.7	0.11	0.19
3	13	85	30	45	6	179	0.2	0.7	0.09	0.17
4	11	75	39	55	5	185	0.2	0.68	0.1	0.17
5	8	80	32	30	6	156	0.22	0.74	0.1	0.19
6	8	76	38	45	6	173	0.21	0.65	0.1	0.18
7	14	76	27	48	7	172	0.23	0.63	0.12	0.18
8	13	84	31	57	11	196	0.21	0.64	0.1	0.19
9	9	79	30	37	8	163	0.22	0.68	0.11	0.19
10	13	82	43	43	6	187	0.21	0.64	0.1	0.18

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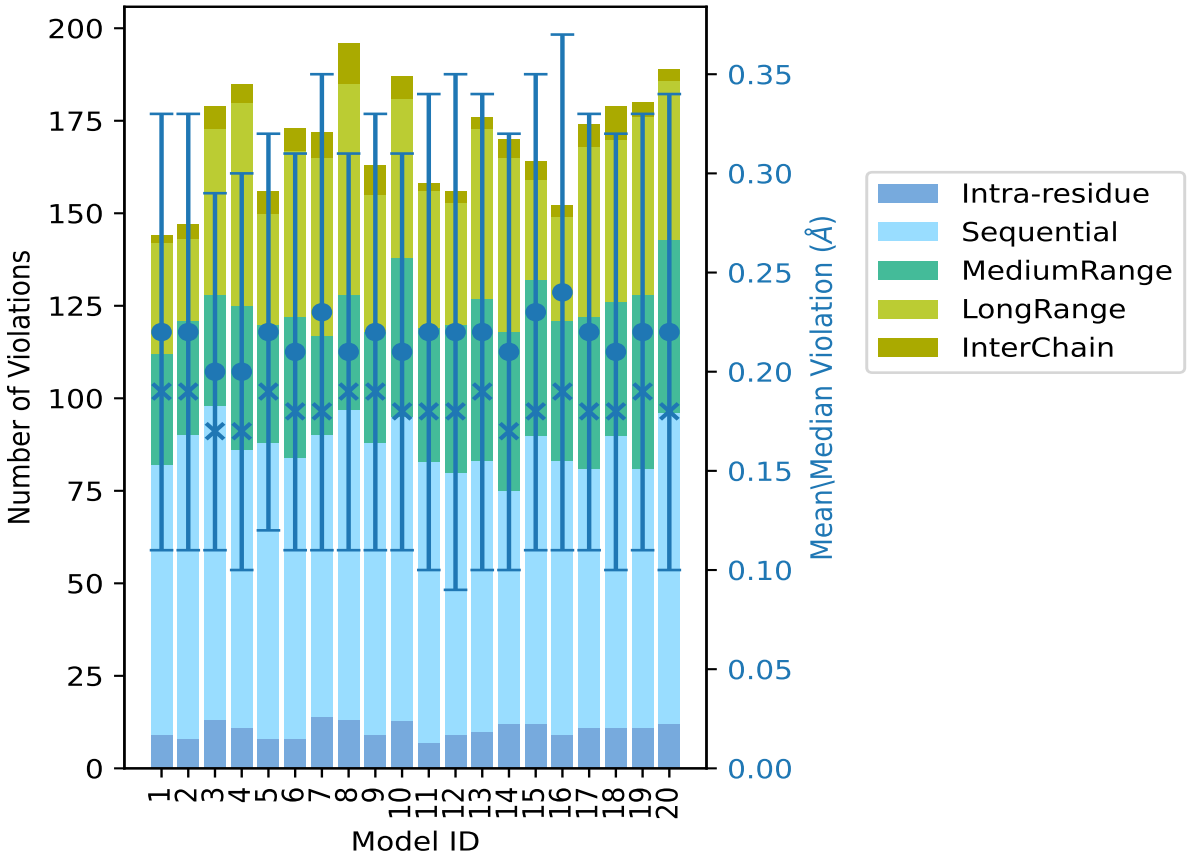
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
11	7	76	36	37	2	158	0.22	0.65	0.12	0.18
12	9	71	40	33	3	156	0.22	0.64	0.13	0.18
13	10	73	44	46	3	176	0.22	0.64	0.12	0.19
14	12	63	43	47	5	170	0.21	0.74	0.11	0.17
15	12	78	42	27	5	164	0.23	0.7	0.12	0.18
16	9	74	38	28	3	152	0.24	0.75	0.13	0.19
17	11	70	41	46	6	174	0.22	0.62	0.11	0.18
18	11	79	36	44	9	179	0.21	0.64	0.11	0.18
19	11	70	47	48	4	180	0.22	0.64	0.11	0.19
20	12	84	47	43	3	189	0.22	0.64	0.12	0.18

[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



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

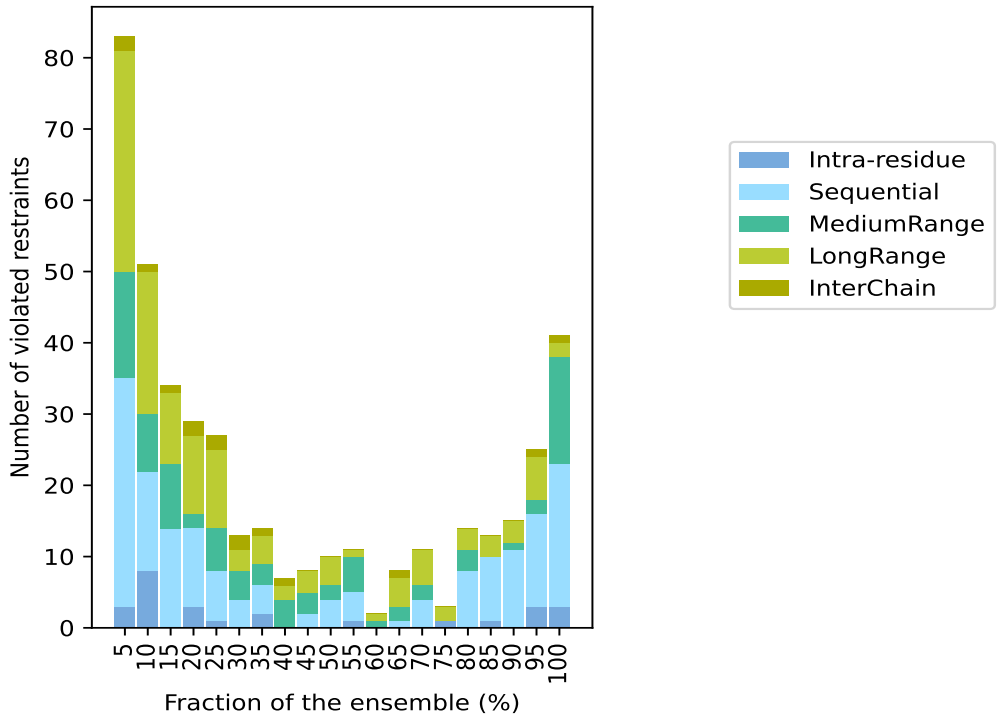
9.3 Distance violation statistics for the ensemble (i)

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, 1953(IR:567, SQ:630, MR:262, LR:444, IC:50) 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]	%
3	32	15	31	2	83	1	5.0
8	14	8	20	1	51	2	10.0
0	14	9	10	1	34	3	15.0
3	11	2	11	2	29	4	20.0
1	7	6	11	2	27	5	25.0
0	4	4	3	2	13	6	30.0
2	4	3	4	1	14	7	35.0
0	0	4	2	1	7	8	40.0
0	2	3	3	0	8	9	45.0
0	4	2	4	0	10	10	50.0
1	4	5	1	0	11	11	55.0
0	0	1	1	0	2	12	60.0
0	1	2	4	1	8	13	65.0
0	4	2	5	0	11	14	70.0
1	0	0	2	0	3	15	75.0
0	8	3	3	0	14	16	80.0
1	9	0	3	0	13	17	85.0
0	11	1	3	0	15	18	90.0
3	13	2	6	1	25	19	95.0
3	20	15	2	1	41	20	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

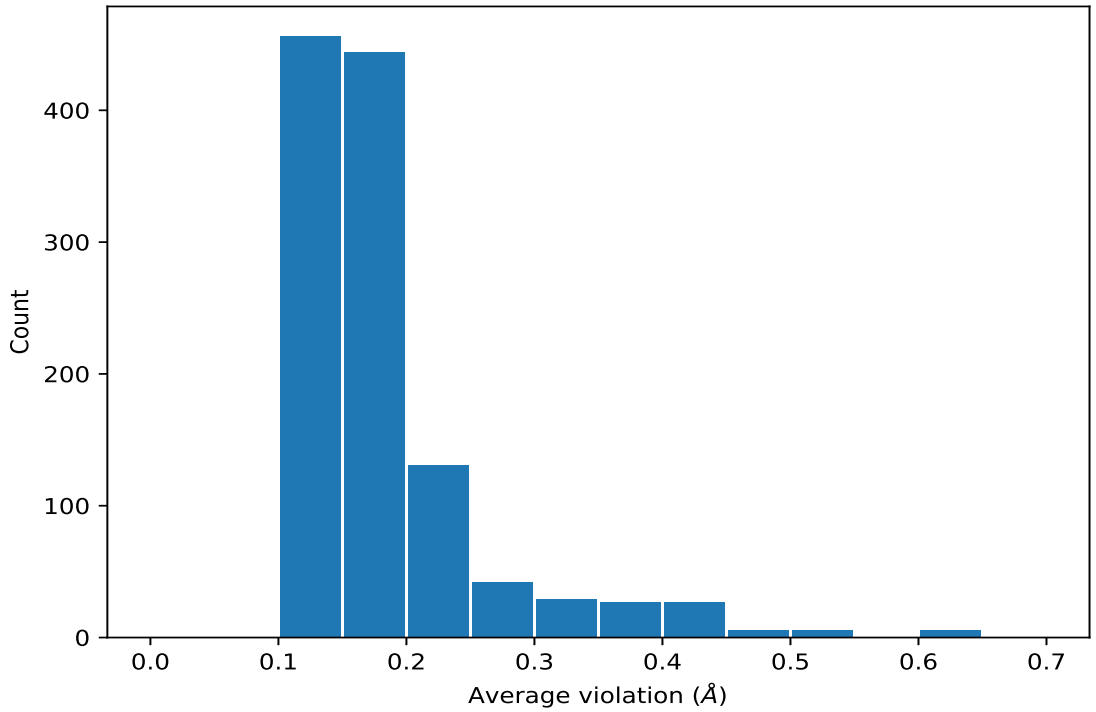
9.3.1 Bar graph : Distance violation statistics for the ensemble



9.4 Most violated distance restraints in the ensemble

9.4.1 Histogram : Distribution of mean distance violations

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



9.4.2 Table: Most violated distance restraints

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

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,26)	1:109:A:LEU:HD21	1:110:A:LEU:H	20	0.47	0.1	0.49
(1,26)	1:109:A:LEU:HD22	1:110:A:LEU:H	20	0.47	0.1	0.49
(1,26)	1:109:A:LEU:HD23	1:110:A:LEU:H	20	0.47	0.1	0.49
(1,845)	1:156:A:VAL:HB	1:157:A:PRO:HD3	20	0.44	0.06	0.44
(1,846)	1:156:B:VAL:HB	1:157:B:PRO:HD3	20	0.43	0.06	0.42
(1,847)	1:156:C:VAL:HB	1:157:C:PRO:HD3	20	0.43	0.06	0.41
(1,205)	1:111:A:ILE:HD11	1:137:A:LEU:HD11	20	0.41	0.08	0.42
(1,205)	1:111:A:ILE:HD11	1:137:A:LEU:HD12	20	0.41	0.08	0.42
(1,205)	1:111:A:ILE:HD11	1:137:A:LEU:HD13	20	0.41	0.08	0.42
(1,205)	1:111:A:ILE:HD12	1:137:A:LEU:HD11	20	0.41	0.08	0.42
(1,205)	1:111:A:ILE:HD12	1:137:A:LEU:HD12	20	0.41	0.08	0.42
(1,205)	1:111:A:ILE:HD12	1:137:A:LEU:HD13	20	0.41	0.08	0.42
(1,205)	1:111:A:ILE:HD13	1:137:A:LEU:HD11	20	0.41	0.08	0.42
(1,205)	1:111:A:ILE:HD13	1:137:A:LEU:HD12	20	0.41	0.08	0.42
(1,205)	1:111:A:ILE:HD13	1:137:A:LEU:HD13	20	0.41	0.08	0.42
(1,730)	1:155:C:ALA:HB1	1:157:C:PRO:HD2	20	0.39	0.08	0.37

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,730)	1:155:C:ALA:HB2	1:157:C:PRO:HD2	20	0.39	0.08	0.37
(1,730)	1:155:C:ALA:HB3	1:157:C:PRO:HD2	20	0.39	0.08	0.37
(1,729)	1:155:B:ALA:HB1	1:157:B:PRO:HD2	20	0.39	0.08	0.37
(1,729)	1:155:B:ALA:HB2	1:157:B:PRO:HD2	20	0.39	0.08	0.37
(1,729)	1:155:B:ALA:HB3	1:157:B:PRO:HD2	20	0.39	0.08	0.37
(1,1059)	1:178:A:PRO:HB3	1:179:A:ALA:H	20	0.38	0.04	0.4
(1,1060)	1:178:B:PRO:HB3	1:179:B:ALA:H	20	0.38	0.04	0.4
(1,1061)	1:178:C:PRO:HB3	1:179:C:ALA:H	20	0.38	0.04	0.4
(1,728)	1:155:A:ALA:HB1	1:157:A:PRO:HD2	20	0.36	0.1	0.34
(1,728)	1:155:A:ALA:HB2	1:157:A:PRO:HD2	20	0.36	0.1	0.34
(1,728)	1:155:A:ALA:HB3	1:157:A:PRO:HD2	20	0.36	0.1	0.34
(1,138)	1:192:A:VAL:HG21	1:135:B:GLU:HG2	20	0.34	0.07	0.34
(1,138)	1:192:A:VAL:HG21	1:135:B:GLU:HG3	20	0.34	0.07	0.34
(1,138)	1:192:A:VAL:HG22	1:135:B:GLU:HG2	20	0.34	0.07	0.34
(1,138)	1:192:A:VAL:HG22	1:135:B:GLU:HG3	20	0.34	0.07	0.34
(1,138)	1:192:A:VAL:HG23	1:135:B:GLU:HG2	20	0.34	0.07	0.34
(1,138)	1:192:A:VAL:HG23	1:135:B:GLU:HG3	20	0.34	0.07	0.34
(1,1910)	1:178:A:PRO:HB2	1:179:A:ALA:H	20	0.34	0.07	0.37
(1,1910)	1:178:A:PRO:HB3	1:179:A:ALA:H	20	0.34	0.07	0.37
(1,2103)	1:178:B:PRO:HB2	1:179:B:ALA:H	20	0.34	0.07	0.37
(1,2103)	1:178:B:PRO:HB3	1:179:B:ALA:H	20	0.34	0.07	0.37
(1,2329)	1:178:C:PRO:HB2	1:179:C:ALA:H	20	0.34	0.07	0.36
(1,2329)	1:178:C:PRO:HB3	1:179:C:ALA:H	20	0.34	0.07	0.36
(1,753)	1:189:A:CYS:H	1:192:A:VAL:HG11	20	0.3	0.04	0.3
(1,753)	1:189:A:CYS:H	1:192:A:VAL:HG12	20	0.3	0.04	0.3
(1,753)	1:189:A:CYS:H	1:192:A:VAL:HG13	20	0.3	0.04	0.3
(1,250)	1:118:B:GLY:HA2	1:119:B:THR:HG21	20	0.29	0.03	0.29
(1,250)	1:118:B:GLY:HA2	1:119:B:THR:HG22	20	0.29	0.03	0.29
(1,250)	1:118:B:GLY:HA2	1:119:B:THR:HG23	20	0.29	0.03	0.29
(1,251)	1:118:C:GLY:HA2	1:119:C:THR:HG21	20	0.29	0.03	0.29
(1,251)	1:118:C:GLY:HA2	1:119:C:THR:HG22	20	0.29	0.03	0.29
(1,251)	1:118:C:GLY:HA2	1:119:C:THR:HG23	20	0.29	0.03	0.29
(1,249)	1:118:A:GLY:HA2	1:119:A:THR:HG21	20	0.28	0.03	0.28
(1,249)	1:118:A:GLY:HA2	1:119:A:THR:HG22	20	0.28	0.03	0.28
(1,249)	1:118:A:GLY:HA2	1:119:A:THR:HG23	20	0.28	0.03	0.28
(1,1073)	1:139:C:ARG:H	1:141:C:VAL:HB	20	0.22	0.02	0.22
(1,1072)	1:139:B:ARG:H	1:141:B:VAL:HB	20	0.22	0.02	0.21
(1,755)	1:189:C:CYS:H	1:192:C:VAL:HG11	20	0.21	0.04	0.21
(1,755)	1:189:C:CYS:H	1:192:C:VAL:HG12	20	0.21	0.04	0.21
(1,755)	1:189:C:CYS:H	1:192:C:VAL:HG13	20	0.21	0.04	0.21
(1,754)	1:189:B:CYS:H	1:192:B:VAL:HG11	20	0.21	0.04	0.21
(1,754)	1:189:B:CYS:H	1:192:B:VAL:HG12	20	0.21	0.04	0.21

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,754)	1:189:B:CYS:H	1:192:B:VAL:HG13	20	0.21	0.04	0.21
(1,1049)	1:137:C:LEU:HG	1:138:C:THR:H	20	0.2	0.01	0.2
(1,1071)	1:139:A:ARG:H	1:141:A:VAL:HB	20	0.19	0.04	0.21
(1,1155)	1:167:A:ARG:HA	1:168:A:ASP:H	20	0.19	0.02	0.2
(1,1048)	1:137:B:LEU:HG	1:138:B:THR:H	20	0.19	0.01	0.19
(1,1047)	1:137:A:LEU:HG	1:138:A:THR:H	20	0.19	0.02	0.18
(1,1614)	1:116:A:ALA:H	1:119:A:THR:HB	20	0.18	0.03	0.18
(1,1533)	1:122:A:TYR:H	1:189:A:CYS:HB2	20	0.17	0.04	0.17
(1,1533)	1:122:A:TYR:H	1:189:A:CYS:HB3	20	0.17	0.04	0.17
(1,1548)	1:167:C:ARG:H	1:170:C:GLY:HA2	20	0.17	0.06	0.16
(1,1548)	1:167:C:ARG:H	1:170:C:GLY:HA3	20	0.17	0.06	0.16
(1,1546)	1:167:A:ARG:H	1:170:A:GLY:HA2	20	0.17	0.06	0.15
(1,1546)	1:167:A:ARG:H	1:170:A:GLY:HA3	20	0.17	0.06	0.15
(1,1547)	1:167:B:ARG:H	1:170:B:GLY:HA2	20	0.17	0.06	0.15
(1,1547)	1:167:B:ARG:H	1:170:B:GLY:HA3	20	0.17	0.06	0.15
(1,1615)	1:116:B:ALA:H	1:119:B:THR:HB	20	0.15	0.02	0.16
(1,1616)	1:116:C:ALA:H	1:119:C:THR:HB	20	0.15	0.02	0.16
(1,1099)	1:167:B:ARG:H	1:167:B:ARG:HB2	20	0.15	0.04	0.13
(1,1098)	1:167:A:ARG:H	1:167:A:ARG:HB2	20	0.15	0.04	0.13
(1,1100)	1:167:C:ARG:H	1:167:C:ARG:HB2	20	0.15	0.04	0.13
(1,1904)	1:176:A:GLY:H	1:177:A:ASP:HB2	20	0.14	0.01	0.14
(1,1904)	1:176:A:GLY:H	1:177:A:ASP:HB3	20	0.14	0.01	0.14
(1,2096)	1:176:B:GLY:H	1:177:B:ASP:HB2	20	0.14	0.01	0.14
(1,2096)	1:176:B:GLY:H	1:177:B:ASP:HB3	20	0.14	0.01	0.14
(1,2322)	1:176:C:GLY:H	1:177:C:ASP:HB2	20	0.14	0.01	0.14
(1,2322)	1:176:C:GLY:H	1:177:C:ASP:HB3	20	0.14	0.01	0.14
(1,1443)	1:155:A:ALA:HA	1:156:A:VAL:H	19	0.5	0.11	0.49
(1,1445)	1:155:C:ALA:HA	1:156:C:VAL:H	19	0.5	0.12	0.48
(1,1444)	1:155:B:ALA:HA	1:156:B:VAL:H	19	0.5	0.12	0.48
(1,1561)	1:167:C:ARG:H	1:167:C:ARG:HB3	19	0.36	0.02	0.36
(1,1560)	1:167:B:ARG:H	1:167:B:ARG:HB3	19	0.36	0.02	0.36
(1,1559)	1:167:A:ARG:H	1:167:A:ARG:HB3	19	0.35	0.02	0.36
(1,1887)	1:156:A:VAL:HB	1:157:A:PRO:HD2	19	0.33	0.1	0.31
(1,1887)	1:156:A:VAL:HB	1:157:A:PRO:HD3	19	0.33	0.1	0.31
(1,122)	1:113:A:TYR:HD1	1:137:A:LEU:HD21	19	0.29	0.06	0.28
(1,122)	1:113:A:TYR:HD1	1:137:A:LEU:HD22	19	0.29	0.06	0.28
(1,122)	1:113:A:TYR:HD1	1:137:A:LEU:HD23	19	0.29	0.06	0.28
(1,122)	1:113:A:TYR:HD2	1:137:A:LEU:HD21	19	0.29	0.06	0.28
(1,122)	1:113:A:TYR:HD2	1:137:A:LEU:HD22	19	0.29	0.06	0.28
(1,122)	1:113:A:TYR:HD2	1:137:A:LEU:HD23	19	0.29	0.06	0.28
(1,395)	1:109:A:LEU:HG	1:111:A:ILE:HD11	19	0.28	0.06	0.28
(1,395)	1:109:A:LEU:HG	1:111:A:ILE:HD12	19	0.28	0.06	0.28

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,395)	1:109:A:LEU:HG	1:111:A:ILE:HD13	19	0.28	0.06	0.28
(1,2072)	1:156:B:VAL:HB	1:157:B:PRO:HD2	19	0.27	0.1	0.27
(1,2072)	1:156:B:VAL:HB	1:157:B:PRO:HD3	19	0.27	0.1	0.27
(1,2298)	1:156:C:VAL:HB	1:157:C:PRO:HD2	19	0.27	0.1	0.26
(1,2298)	1:156:C:VAL:HB	1:157:C:PRO:HD3	19	0.27	0.1	0.26
(1,958)	1:187:A:THR:HA	1:188:A:LEU:HD11	19	0.25	0.08	0.24
(1,958)	1:187:A:THR:HA	1:188:A:LEU:HD12	19	0.25	0.08	0.24
(1,958)	1:187:A:THR:HA	1:188:A:LEU:HD13	19	0.25	0.08	0.24
(1,2094)	1:172:B:ALA:HA	1:178:B:PRO:HD2	19	0.22	0.06	0.19
(1,2094)	1:172:B:ALA:HA	1:178:B:PRO:HD3	19	0.22	0.06	0.19
(1,2320)	1:172:C:ALA:HA	1:178:C:PRO:HD2	19	0.22	0.06	0.19
(1,2320)	1:172:C:ALA:HA	1:178:C:PRO:HD3	19	0.22	0.06	0.19
(1,1036)	1:188:A:LEU:HD21	1:134:B:LEU:H	19	0.21	0.1	0.15
(1,1036)	1:188:A:LEU:HD22	1:134:B:LEU:H	19	0.21	0.1	0.15
(1,1036)	1:188:A:LEU:HD23	1:134:B:LEU:H	19	0.21	0.1	0.15
(1,1)	1:108:A:GLN:HA	1:109:A:LEU:HD21	19	0.21	0.04	0.21
(1,1)	1:108:A:GLN:HA	1:109:A:LEU:HD22	19	0.21	0.04	0.21
(1,1)	1:108:A:GLN:HA	1:109:A:LEU:HD23	19	0.21	0.04	0.21
(1,1842)	1:121:A:CYS:HB2	1:189:A:CYS:H	19	0.2	0.04	0.2
(1,1842)	1:121:A:CYS:HB3	1:189:A:CYS:H	19	0.2	0.04	0.2
(1,1156)	1:167:B:ARG:HA	1:168:B:ASP:H	19	0.2	0.0	0.2
(1,1157)	1:167:C:ARG:HA	1:168:C:ASP:H	19	0.19	0.0	0.19
(1,1818)	1:95:B:SER:HB2	1:101:B:LEU:H	19	0.19	0.06	0.18
(1,1818)	1:95:B:SER:HB3	1:101:B:LEU:H	19	0.19	0.06	0.18
(1,1902)	1:172:A:ALA:HA	1:178:A:PRO:HD2	19	0.19	0.06	0.17
(1,1902)	1:172:A:ALA:HA	1:178:A:PRO:HD3	19	0.19	0.06	0.17
(1,653)	1:172:A:ALA:HB1	1:173:A:PRO:HD3	19	0.18	0.01	0.18
(1,653)	1:172:A:ALA:HB2	1:173:A:PRO:HD3	19	0.18	0.01	0.18
(1,653)	1:172:A:ALA:HB3	1:173:A:PRO:HD3	19	0.18	0.01	0.18
(1,655)	1:172:C:ALA:HB1	1:173:C:PRO:HD3	19	0.18	0.01	0.18
(1,655)	1:172:C:ALA:HB2	1:173:C:PRO:HD3	19	0.18	0.01	0.18
(1,655)	1:172:C:ALA:HB3	1:173:C:PRO:HD3	19	0.18	0.01	0.18
(1,654)	1:172:B:ALA:HB1	1:173:B:PRO:HD3	19	0.17	0.01	0.18
(1,654)	1:172:B:ALA:HB2	1:173:B:PRO:HD3	19	0.17	0.01	0.18
(1,654)	1:172:B:ALA:HB3	1:173:B:PRO:HD3	19	0.17	0.01	0.18
(1,182)	1:137:A:LEU:HD11	1:141:A:VAL:HG11	19	0.16	0.03	0.15
(1,182)	1:137:A:LEU:HD11	1:141:A:VAL:HG12	19	0.16	0.03	0.15
(1,182)	1:137:A:LEU:HD11	1:141:A:VAL:HG13	19	0.16	0.03	0.15
(1,182)	1:137:A:LEU:HD12	1:141:A:VAL:HG11	19	0.16	0.03	0.15
(1,182)	1:137:A:LEU:HD12	1:141:A:VAL:HG12	19	0.16	0.03	0.15
(1,182)	1:137:A:LEU:HD12	1:141:A:VAL:HG13	19	0.16	0.03	0.15
(1,182)	1:137:A:LEU:HD13	1:141:A:VAL:HG11	19	0.16	0.03	0.15

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,182)	1:137:A:LEU:HD13	1:141:A:VAL:HG12	19	0.16	0.03	0.15
(1,182)	1:137:A:LEU:HD13	1:141:A:VAL:HG13	19	0.16	0.03	0.15
(1,1888)	1:156:A:VAL:HG11	1:157:A:PRO:HB2	18	0.62	0.15	0.64
(1,1888)	1:156:A:VAL:HG11	1:157:A:PRO:HB3	18	0.62	0.15	0.64
(1,1888)	1:156:A:VAL:HG12	1:157:A:PRO:HB2	18	0.62	0.15	0.64
(1,1888)	1:156:A:VAL:HG12	1:157:A:PRO:HB3	18	0.62	0.15	0.64
(1,1888)	1:156:A:VAL:HG13	1:157:A:PRO:HB2	18	0.62	0.15	0.64
(1,1888)	1:156:A:VAL:HG13	1:157:A:PRO:HB3	18	0.62	0.15	0.64
(1,861)	1:153:A:LYS:HA	1:154:A:PRO:HD3	18	0.46	0.01	0.46
(1,862)	1:153:B:LYS:HA	1:154:B:PRO:HD3	18	0.46	0.01	0.46
(1,863)	1:153:C:LYS:HA	1:154:C:PRO:HD3	18	0.46	0.01	0.46
(1,1881)	1:153:A:LYS:HA	1:154:A:PRO:HD2	18	0.32	0.01	0.32
(1,1881)	1:153:A:LYS:HA	1:154:A:PRO:HD3	18	0.32	0.01	0.32
(1,2063)	1:153:B:LYS:HA	1:154:B:PRO:HD2	18	0.32	0.01	0.32
(1,2063)	1:153:B:LYS:HA	1:154:B:PRO:HD3	18	0.32	0.01	0.32
(1,2289)	1:153:C:LYS:HA	1:154:C:PRO:HD2	18	0.32	0.01	0.32
(1,2289)	1:153:C:LYS:HA	1:154:C:PRO:HD3	18	0.32	0.01	0.32
(1,1737)	1:194:A:LEU:HD21	1:195:A:TYR:H	18	0.24	0.02	0.24
(1,1737)	1:194:A:LEU:HD22	1:195:A:TYR:H	18	0.24	0.02	0.24
(1,1737)	1:194:A:LEU:HD23	1:195:A:TYR:H	18	0.24	0.02	0.24
(1,175)	1:179:A:ALA:HB1	1:181:A:LEU:HD21	18	0.18	0.05	0.18
(1,175)	1:179:A:ALA:HB1	1:181:A:LEU:HD22	18	0.18	0.05	0.18
(1,175)	1:179:A:ALA:HB1	1:181:A:LEU:HD23	18	0.18	0.05	0.18
(1,175)	1:179:A:ALA:HB2	1:181:A:LEU:HD21	18	0.18	0.05	0.18
(1,175)	1:179:A:ALA:HB2	1:181:A:LEU:HD22	18	0.18	0.05	0.18
(1,175)	1:179:A:ALA:HB2	1:181:A:LEU:HD23	18	0.18	0.05	0.18
(1,175)	1:179:A:ALA:HB3	1:181:A:LEU:HD21	18	0.18	0.05	0.18
(1,175)	1:179:A:ALA:HB3	1:181:A:LEU:HD22	18	0.18	0.05	0.18
(1,175)	1:179:A:ALA:HB3	1:181:A:LEU:HD23	18	0.18	0.05	0.18
(1,864)	1:153:A:LYS:HA	1:154:A:PRO:HD2	18	0.18	0.01	0.18
(1,865)	1:153:B:LYS:HA	1:154:B:PRO:HD2	18	0.18	0.01	0.18
(1,866)	1:153:C:LYS:HA	1:154:C:PRO:HD2	18	0.18	0.01	0.18
(1,1819)	1:95:C:SER:HB2	1:101:C:LEU:H	18	0.17	0.05	0.17
(1,1819)	1:95:C:SER:HB3	1:101:C:LEU:H	18	0.17	0.05	0.17
(1,2010)	1:121:B:CYS:HB2	1:189:B:CYS:H	18	0.13	0.02	0.14
(1,2010)	1:121:B:CYS:HB3	1:189:B:CYS:H	18	0.13	0.02	0.14
(1,2236)	1:121:C:CYS:HB2	1:189:C:CYS:H	18	0.13	0.01	0.13
(1,2236)	1:121:C:CYS:HB3	1:189:C:CYS:H	18	0.13	0.01	0.13
(1,1768)	1:178:A:PRO:HD3	1:179:A:ALA:H	17	0.25	0.03	0.25
(1,1769)	1:178:B:PRO:HD3	1:179:B:ALA:H	17	0.24	0.03	0.24
(1,1770)	1:178:C:PRO:HD3	1:179:C:ALA:H	17	0.24	0.03	0.24
(1,1520)	1:178:A:PRO:HG2	1:179:A:ALA:H	17	0.23	0.03	0.24

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1520)	1:178:A:PRO:HG3	1:179:A:ALA:H	17	0.23	0.03	0.24
(1,1521)	1:178:B:PRO:HG2	1:179:B:ALA:H	17	0.23	0.03	0.23
(1,1521)	1:178:B:PRO:HG3	1:179:B:ALA:H	17	0.23	0.03	0.23
(1,1522)	1:178:C:PRO:HG2	1:179:C:ALA:H	17	0.23	0.03	0.23
(1,1522)	1:178:C:PRO:HG3	1:179:C:ALA:H	17	0.23	0.03	0.23
(1,890)	1:152:C:ALA:HA	1:157:C:PRO:HG2	17	0.21	0.07	0.2
(1,890)	1:152:C:ALA:HA	1:157:C:PRO:HG3	17	0.21	0.07	0.2
(1,889)	1:152:B:ALA:HA	1:157:B:PRO:HG2	17	0.21	0.07	0.21
(1,889)	1:152:B:ALA:HA	1:157:B:PRO:HG3	17	0.21	0.07	0.21
(1,1535)	1:122:C:TYR:H	1:189:C:CYS:HB2	17	0.14	0.03	0.14
(1,1535)	1:122:C:TYR:H	1:189:C:CYS:HB3	17	0.14	0.03	0.14
(1,1276)	1:109:A:LEU:H	1:109:A:LEU:HG	17	0.14	0.03	0.12
(1,1903)	1:172:A:ALA:HB1	1:173:A:PRO:HD2	17	0.14	0.02	0.13
(1,1903)	1:172:A:ALA:HB1	1:173:A:PRO:HD3	17	0.14	0.02	0.13
(1,1903)	1:172:A:ALA:HB2	1:173:A:PRO:HD2	17	0.14	0.02	0.13
(1,1903)	1:172:A:ALA:HB2	1:173:A:PRO:HD3	17	0.14	0.02	0.13
(1,1903)	1:172:A:ALA:HB3	1:173:A:PRO:HD2	17	0.14	0.02	0.13
(1,1903)	1:172:A:ALA:HB3	1:173:A:PRO:HD3	17	0.14	0.02	0.13
(1,2321)	1:172:C:ALA:HB1	1:173:C:PRO:HD2	17	0.13	0.01	0.13
(1,2321)	1:172:C:ALA:HB1	1:173:C:PRO:HD3	17	0.13	0.01	0.13
(1,2321)	1:172:C:ALA:HB2	1:173:C:PRO:HD2	17	0.13	0.01	0.13
(1,2321)	1:172:C:ALA:HB2	1:173:C:PRO:HD3	17	0.13	0.01	0.13
(1,2321)	1:172:C:ALA:HB3	1:173:C:PRO:HD2	17	0.13	0.01	0.13
(1,2321)	1:172:C:ALA:HB3	1:173:C:PRO:HD3	17	0.13	0.01	0.13
(1,2095)	1:172:B:ALA:HB1	1:173:B:PRO:HD2	17	0.13	0.01	0.12
(1,2095)	1:172:B:ALA:HB1	1:173:B:PRO:HD3	17	0.13	0.01	0.12
(1,2095)	1:172:B:ALA:HB2	1:173:B:PRO:HD2	17	0.13	0.01	0.12
(1,2095)	1:172:B:ALA:HB2	1:173:B:PRO:HD3	17	0.13	0.01	0.12
(1,2095)	1:172:B:ALA:HB3	1:173:B:PRO:HD2	17	0.13	0.01	0.12
(1,2095)	1:172:B:ALA:HB3	1:173:B:PRO:HD3	17	0.13	0.01	0.12
(1,124)	1:96:A:ILE:H	1:101:A:LEU:HD21	16	0.35	0.12	0.37
(1,124)	1:96:A:ILE:H	1:101:A:LEU:HD22	16	0.35	0.12	0.37
(1,124)	1:96:A:ILE:H	1:101:A:LEU:HD23	16	0.35	0.12	0.37
(1,1461)	1:180:A:PHE:H	1:181:A:LEU:HA	16	0.22	0.08	0.22
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG11	16	0.22	0.08	0.2
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG12	16	0.22	0.08	0.2
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG13	16	0.22	0.08	0.2
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG21	16	0.22	0.08	0.2
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG22	16	0.22	0.08	0.2
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG23	16	0.22	0.08	0.2
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG11	16	0.22	0.08	0.2
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG12	16	0.22	0.08	0.2

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG13	16	0.22	0.08	0.2
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG21	16	0.22	0.08	0.2
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG22	16	0.22	0.08	0.2
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG23	16	0.22	0.08	0.2
(1,1463)	1:180:C:PHE:H	1:181:C:LEU:HA	16	0.21	0.07	0.2
(1,1462)	1:180:B:PHE:H	1:181:B:LEU:HA	16	0.21	0.07	0.22
(1,435)	1:183:A:MET:HE1	1:186:A:SER:HA	16	0.21	0.03	0.2
(1,435)	1:183:A:MET:HE2	1:186:A:SER:HA	16	0.21	0.03	0.2
(1,435)	1:183:A:MET:HE3	1:186:A:SER:HA	16	0.21	0.03	0.2
(1,888)	1:152:A:ALA:HA	1:157:A:PRO:HG2	16	0.2	0.07	0.2
(1,888)	1:152:A:ALA:HA	1:157:A:PRO:HG3	16	0.2	0.07	0.2
(1,1889)	1:156:A:VAL:HG11	1:157:A:PRO:HD2	16	0.19	0.02	0.2
(1,1889)	1:156:A:VAL:HG11	1:157:A:PRO:HD3	16	0.19	0.02	0.2
(1,1889)	1:156:A:VAL:HG12	1:157:A:PRO:HD2	16	0.19	0.02	0.2
(1,1889)	1:156:A:VAL:HG12	1:157:A:PRO:HD3	16	0.19	0.02	0.2
(1,1889)	1:156:A:VAL:HG13	1:157:A:PRO:HD2	16	0.19	0.02	0.2
(1,1889)	1:156:A:VAL:HG13	1:157:A:PRO:HD3	16	0.19	0.02	0.2
(1,56)	1:156:A:VAL:HG11	1:157:A:PRO:HD3	16	0.18	0.06	0.18
(1,56)	1:156:A:VAL:HG12	1:157:A:PRO:HD3	16	0.18	0.06	0.18
(1,56)	1:156:A:VAL:HG13	1:157:A:PRO:HD3	16	0.18	0.06	0.18
(1,437)	1:183:C:MET:HE1	1:186:C:SER:HA	16	0.17	0.02	0.17
(1,437)	1:183:C:MET:HE2	1:186:C:SER:HA	16	0.17	0.02	0.17
(1,437)	1:183:C:MET:HE3	1:186:C:SER:HA	16	0.17	0.02	0.17
(1,436)	1:183:B:MET:HE1	1:186:B:SER:HA	16	0.17	0.02	0.17
(1,436)	1:183:B:MET:HE2	1:186:B:SER:HA	16	0.17	0.02	0.17
(1,436)	1:183:B:MET:HE3	1:186:B:SER:HA	16	0.17	0.02	0.17
(1,1534)	1:122:B:TYR:H	1:189:B:CYS:HB2	16	0.15	0.04	0.15
(1,1534)	1:122:B:TYR:H	1:189:B:CYS:HB3	16	0.15	0.04	0.15
(1,1387)	1:141:A:VAL:HG21	1:142:A:HIS:H	16	0.12	0.02	0.12
(1,1387)	1:141:A:VAL:HG22	1:142:A:HIS:H	16	0.12	0.02	0.12
(1,1387)	1:141:A:VAL:HG23	1:142:A:HIS:H	16	0.12	0.02	0.12
(1,965)	1:110:A:LEU:HD11	1:125:A:LYS:HB3	15	0.18	0.05	0.16
(1,965)	1:110:A:LEU:HD12	1:125:A:LYS:HB3	15	0.18	0.05	0.16
(1,965)	1:110:A:LEU:HD13	1:125:A:LYS:HB3	15	0.18	0.05	0.16
(1,1511)	1:137:A:LEU:H	1:137:A:LEU:HG	15	0.15	0.04	0.16
(1,1562)	1:145:A:GLN:HA	1:151:A:GLN:H	15	0.15	0.03	0.14
(1,1097)	1:157:C:PRO:HA	1:158:C:THR:H	14	0.19	0.03	0.18
(1,1096)	1:157:B:PRO:HA	1:158:B:THR:H	14	0.19	0.03	0.18
(1,2295)	1:155:C:ALA:HB1	1:157:C:PRO:HD2	14	0.19	0.06	0.18
(1,2295)	1:155:C:ALA:HB1	1:157:C:PRO:HD3	14	0.19	0.06	0.18
(1,2295)	1:155:C:ALA:HB2	1:157:C:PRO:HD2	14	0.19	0.06	0.18
(1,2295)	1:155:C:ALA:HB2	1:157:C:PRO:HD3	14	0.19	0.06	0.18

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2295)	1:155:C:ALA:HB3	1:157:C:PRO:HD2	14	0.19	0.06	0.18
(1,2295)	1:155:C:ALA:HB3	1:157:C:PRO:HD3	14	0.19	0.06	0.18
(1,2069)	1:155:B:ALA:HB1	1:157:B:PRO:HD2	14	0.19	0.06	0.18
(1,2069)	1:155:B:ALA:HB1	1:157:B:PRO:HD3	14	0.19	0.06	0.18
(1,2069)	1:155:B:ALA:HB2	1:157:B:PRO:HD2	14	0.19	0.06	0.18
(1,2069)	1:155:B:ALA:HB2	1:157:B:PRO:HD3	14	0.19	0.06	0.18
(1,2069)	1:155:B:ALA:HB3	1:157:B:PRO:HD2	14	0.19	0.06	0.18
(1,2069)	1:155:B:ALA:HB3	1:157:B:PRO:HD3	14	0.19	0.06	0.18
(1,1095)	1:157:A:PRO:HA	1:158:A:THR:H	14	0.18	0.03	0.18
(1,1610)	1:118:A:GLY:H	1:192:A:VAL:HG21	14	0.18	0.06	0.17
(1,1610)	1:118:A:GLY:H	1:192:A:VAL:HG22	14	0.18	0.06	0.17
(1,1610)	1:118:A:GLY:H	1:192:A:VAL:HG23	14	0.18	0.06	0.17
(1,749)	1:123:A:ILE:HG21	1:179:A:ALA:HB1	14	0.17	0.05	0.18
(1,749)	1:123:A:ILE:HG21	1:179:A:ALA:HB2	14	0.17	0.05	0.18
(1,749)	1:123:A:ILE:HG21	1:179:A:ALA:HB3	14	0.17	0.05	0.18
(1,749)	1:123:A:ILE:HG22	1:179:A:ALA:HB1	14	0.17	0.05	0.18
(1,749)	1:123:A:ILE:HG22	1:179:A:ALA:HB2	14	0.17	0.05	0.18
(1,749)	1:123:A:ILE:HG22	1:179:A:ALA:HB3	14	0.17	0.05	0.18
(1,749)	1:123:A:ILE:HG23	1:179:A:ALA:HB1	14	0.17	0.05	0.18
(1,749)	1:123:A:ILE:HG23	1:179:A:ALA:HB2	14	0.17	0.05	0.18
(1,749)	1:123:A:ILE:HG23	1:179:A:ALA:HB3	14	0.17	0.05	0.18
(1,1817)	1:95:A:SER:HB2	1:101:A:LEU:H	14	0.15	0.06	0.14
(1,1817)	1:95:A:SER:HB3	1:101:A:LEU:H	14	0.15	0.06	0.14
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD11	14	0.15	0.04	0.14
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD12	14	0.15	0.04	0.14
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD13	14	0.15	0.04	0.14
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD21	14	0.15	0.04	0.14
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD22	14	0.15	0.04	0.14
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD23	14	0.15	0.04	0.14
(1,1431)	1:111:B:ILE:H	1:123:B:ILE:HG21	14	0.14	0.03	0.14
(1,1431)	1:111:B:ILE:H	1:123:B:ILE:HG22	14	0.14	0.03	0.14
(1,1431)	1:111:B:ILE:H	1:123:B:ILE:HG23	14	0.14	0.03	0.14
(1,1432)	1:111:C:ILE:H	1:123:C:ILE:HG21	14	0.14	0.03	0.14
(1,1432)	1:111:C:ILE:H	1:123:C:ILE:HG22	14	0.14	0.03	0.14
(1,1432)	1:111:C:ILE:H	1:123:C:ILE:HG23	14	0.14	0.03	0.14
(1,451)	1:95:A:SER:HB2	1:101:A:LEU:HD21	13	0.28	0.11	0.3
(1,451)	1:95:A:SER:HB2	1:101:A:LEU:HD22	13	0.28	0.11	0.3
(1,451)	1:95:A:SER:HB2	1:101:A:LEU:HD23	13	0.28	0.11	0.3
(1,451)	1:95:A:SER:HB3	1:101:A:LEU:HD21	13	0.28	0.11	0.3
(1,451)	1:95:A:SER:HB3	1:101:A:LEU:HD22	13	0.28	0.11	0.3
(1,451)	1:95:A:SER:HB3	1:101:A:LEU:HD23	13	0.28	0.11	0.3
(1,635)	1:96:A:ILE:HG21	1:100:A:GLY:H	13	0.18	0.04	0.16

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,635)	1:96:A:ILE:HG22	1:100:A:GLY:H	13	0.18	0.04	0.16
(1,635)	1:96:A:ILE:HG23	1:100:A:GLY:H	13	0.18	0.04	0.16
(1,636)	1:96:B:ILE:HG21	1:100:B:GLY:H	13	0.16	0.04	0.16
(1,636)	1:96:B:ILE:HG22	1:100:B:GLY:H	13	0.16	0.04	0.16
(1,636)	1:96:B:ILE:HG23	1:100:B:GLY:H	13	0.16	0.04	0.16
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD11	13	0.15	0.04	0.13
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD12	13	0.15	0.04	0.13
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD13	13	0.15	0.04	0.13
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD21	13	0.15	0.04	0.13
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD22	13	0.15	0.04	0.13
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD23	13	0.15	0.04	0.13
(1,1430)	1:111:A:ILE:H	1:123:A:ILE:HG21	13	0.14	0.04	0.14
(1,1430)	1:111:A:ILE:H	1:123:A:ILE:HG22	13	0.14	0.04	0.14
(1,1430)	1:111:A:ILE:H	1:123:A:ILE:HG23	13	0.14	0.04	0.14
(1,1563)	1:145:B:GLN:HA	1:151:B:GLN:H	13	0.13	0.02	0.13
(1,361)	1:183:A:MET:HG2	1:131:B:ILE:HD11	13	0.13	0.03	0.12
(1,361)	1:183:A:MET:HG2	1:131:B:ILE:HD12	13	0.13	0.03	0.12
(1,361)	1:183:A:MET:HG2	1:131:B:ILE:HD13	13	0.13	0.03	0.12
(1,361)	1:183:A:MET:HG3	1:131:B:ILE:HD11	13	0.13	0.03	0.12
(1,361)	1:183:A:MET:HG3	1:131:B:ILE:HD12	13	0.13	0.03	0.12
(1,361)	1:183:A:MET:HG3	1:131:B:ILE:HD13	13	0.13	0.03	0.12
(1,1564)	1:145:C:GLN:HA	1:151:C:GLN:H	13	0.13	0.02	0.12
(1,219)	1:96:A:ILE:HG21	1:141:A:VAL:HG11	12	0.18	0.04	0.18
(1,219)	1:96:A:ILE:HG21	1:141:A:VAL:HG12	12	0.18	0.04	0.18
(1,219)	1:96:A:ILE:HG21	1:141:A:VAL:HG13	12	0.18	0.04	0.18
(1,219)	1:96:A:ILE:HG22	1:141:A:VAL:HG11	12	0.18	0.04	0.18
(1,219)	1:96:A:ILE:HG22	1:141:A:VAL:HG12	12	0.18	0.04	0.18
(1,219)	1:96:A:ILE:HG22	1:141:A:VAL:HG13	12	0.18	0.04	0.18
(1,219)	1:96:A:ILE:HG23	1:141:A:VAL:HG11	12	0.18	0.04	0.18
(1,219)	1:96:A:ILE:HG23	1:141:A:VAL:HG12	12	0.18	0.04	0.18
(1,219)	1:96:A:ILE:HG23	1:141:A:VAL:HG13	12	0.18	0.04	0.18
(1,637)	1:96:C:ILE:HG21	1:100:C:GLY:H	12	0.16	0.03	0.16
(1,637)	1:96:C:ILE:HG22	1:100:C:GLY:H	12	0.16	0.03	0.16
(1,637)	1:96:C:ILE:HG23	1:100:C:GLY:H	12	0.16	0.03	0.16
(1,928)	1:178:A:PRO:HG2	1:181:A:LEU:HD21	11	0.19	0.02	0.19
(1,928)	1:178:A:PRO:HG2	1:181:A:LEU:HD22	11	0.19	0.02	0.19
(1,928)	1:178:A:PRO:HG2	1:181:A:LEU:HD23	11	0.19	0.02	0.19
(1,928)	1:178:A:PRO:HG3	1:181:A:LEU:HD21	11	0.19	0.02	0.19
(1,928)	1:178:A:PRO:HG3	1:181:A:LEU:HD22	11	0.19	0.02	0.19
(1,928)	1:178:A:PRO:HG3	1:181:A:LEU:HD23	11	0.19	0.02	0.19
(1,1885)	1:155:A:ALA:HB1	1:157:A:PRO:HD2	11	0.19	0.08	0.17
(1,1885)	1:155:A:ALA:HB1	1:157:A:PRO:HD3	11	0.19	0.08	0.17

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1885)	1:155:A:ALA:HB2	1:157:A:PRO:HD2	11	0.19	0.08	0.17
(1,1885)	1:155:A:ALA:HB2	1:157:A:PRO:HD3	11	0.19	0.08	0.17
(1,1885)	1:155:A:ALA:HB3	1:157:A:PRO:HD2	11	0.19	0.08	0.17
(1,1885)	1:155:A:ALA:HB3	1:157:A:PRO:HD3	11	0.19	0.08	0.17
(1,1408)	1:152:A:ALA:HB1	1:153:A:LYS:H	11	0.17	0.03	0.17
(1,1408)	1:152:A:ALA:HB2	1:153:A:LYS:H	11	0.17	0.03	0.17
(1,1408)	1:152:A:ALA:HB3	1:153:A:LYS:H	11	0.17	0.03	0.17
(1,1409)	1:152:B:ALA:HB1	1:153:B:LYS:H	11	0.16	0.03	0.17
(1,1409)	1:152:B:ALA:HB2	1:153:B:LYS:H	11	0.16	0.03	0.17
(1,1409)	1:152:B:ALA:HB3	1:153:B:LYS:H	11	0.16	0.03	0.17
(1,1410)	1:152:C:ALA:HB1	1:153:C:LYS:H	11	0.16	0.03	0.17
(1,1410)	1:152:C:ALA:HB2	1:153:C:LYS:H	11	0.16	0.03	0.17
(1,1410)	1:152:C:ALA:HB3	1:153:C:LYS:H	11	0.16	0.03	0.17
(1,1549)	1:167:A:ARG:H	1:171:A:SER:HA	11	0.15	0.04	0.15
(1,1201)	1:196:A:TYR:H	1:196:A:TYR:HE1	11	0.15	0.04	0.14
(1,1201)	1:196:A:TYR:H	1:196:A:TYR:HE2	11	0.15	0.04	0.14
(1,2112)	1:179:B:ALA:HB1	1:181:B:LEU:HD11	11	0.15	0.03	0.14
(1,2112)	1:179:B:ALA:HB1	1:181:B:LEU:HD12	11	0.15	0.03	0.14
(1,2112)	1:179:B:ALA:HB1	1:181:B:LEU:HD13	11	0.15	0.03	0.14
(1,2112)	1:179:B:ALA:HB1	1:181:B:LEU:HD21	11	0.15	0.03	0.14
(1,2112)	1:179:B:ALA:HB1	1:181:B:LEU:HD22	11	0.15	0.03	0.14
(1,2112)	1:179:B:ALA:HB1	1:181:B:LEU:HD23	11	0.15	0.03	0.14
(1,2112)	1:179:B:ALA:HB2	1:181:B:LEU:HD11	11	0.15	0.03	0.14
(1,2112)	1:179:B:ALA:HB2	1:181:B:LEU:HD12	11	0.15	0.03	0.14
(1,2112)	1:179:B:ALA:HB2	1:181:B:LEU:HD13	11	0.15	0.03	0.14
(1,2112)	1:179:B:ALA:HB2	1:181:B:LEU:HD21	11	0.15	0.03	0.14
(1,2112)	1:179:B:ALA:HB2	1:181:B:LEU:HD22	11	0.15	0.03	0.14
(1,2112)	1:179:B:ALA:HB2	1:181:B:LEU:HD23	11	0.15	0.03	0.14
(1,2112)	1:179:B:ALA:HB3	1:181:B:LEU:HD11	11	0.15	0.03	0.14
(1,2112)	1:179:B:ALA:HB3	1:181:B:LEU:HD12	11	0.15	0.03	0.14
(1,2112)	1:179:B:ALA:HB3	1:181:B:LEU:HD13	11	0.15	0.03	0.14
(1,2112)	1:179:B:ALA:HB3	1:181:B:LEU:HD21	11	0.15	0.03	0.14
(1,2112)	1:179:B:ALA:HB3	1:181:B:LEU:HD22	11	0.15	0.03	0.14
(1,2112)	1:179:B:ALA:HB3	1:181:B:LEU:HD23	11	0.15	0.03	0.14
(1,2338)	1:179:C:ALA:HB1	1:181:C:LEU:HD11	11	0.14	0.03	0.13
(1,2338)	1:179:C:ALA:HB1	1:181:C:LEU:HD12	11	0.14	0.03	0.13
(1,2338)	1:179:C:ALA:HB1	1:181:C:LEU:HD13	11	0.14	0.03	0.13
(1,2338)	1:179:C:ALA:HB1	1:181:C:LEU:HD21	11	0.14	0.03	0.13
(1,2338)	1:179:C:ALA:HB1	1:181:C:LEU:HD22	11	0.14	0.03	0.13
(1,2338)	1:179:C:ALA:HB1	1:181:C:LEU:HD23	11	0.14	0.03	0.13
(1,2338)	1:179:C:ALA:HB2	1:181:C:LEU:HD11	11	0.14	0.03	0.13
(1,2338)	1:179:C:ALA:HB2	1:181:C:LEU:HD12	11	0.14	0.03	0.13

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2338)	1:179:C:ALA:HB2	1:181:C:LEU:HD13	11	0.14	0.03	0.13
(1,2338)	1:179:C:ALA:HB2	1:181:C:LEU:HD21	11	0.14	0.03	0.13
(1,2338)	1:179:C:ALA:HB2	1:181:C:LEU:HD22	11	0.14	0.03	0.13
(1,2338)	1:179:C:ALA:HB2	1:181:C:LEU:HD23	11	0.14	0.03	0.13
(1,2338)	1:179:C:ALA:HB3	1:181:C:LEU:HD11	11	0.14	0.03	0.13
(1,2338)	1:179:C:ALA:HB3	1:181:C:LEU:HD12	11	0.14	0.03	0.13
(1,2338)	1:179:C:ALA:HB3	1:181:C:LEU:HD13	11	0.14	0.03	0.13
(1,2338)	1:179:C:ALA:HB3	1:181:C:LEU:HD21	11	0.14	0.03	0.13
(1,2338)	1:179:C:ALA:HB3	1:181:C:LEU:HD22	11	0.14	0.03	0.13
(1,2338)	1:179:C:ALA:HB3	1:181:C:LEU:HD23	11	0.14	0.03	0.13
(1,665)	1:113:A:TYR:HE1	1:197:A:ILE:HG21	11	0.14	0.04	0.12
(1,665)	1:113:A:TYR:HE1	1:197:A:ILE:HG22	11	0.14	0.04	0.12
(1,665)	1:113:A:TYR:HE1	1:197:A:ILE:HG23	11	0.14	0.04	0.12
(1,665)	1:113:A:TYR:HE2	1:197:A:ILE:HG21	11	0.14	0.04	0.12
(1,665)	1:113:A:TYR:HE2	1:197:A:ILE:HG22	11	0.14	0.04	0.12
(1,665)	1:113:A:TYR:HE2	1:197:A:ILE:HG23	11	0.14	0.04	0.12
(1,815)	1:176:C:GLY:H	1:177:C:ASP:HB2	11	0.13	0.02	0.12
(1,228)	1:96:C:ILE:HD11	1:102:C:VAL:HG11	10	0.24	0.03	0.26
(1,228)	1:96:C:ILE:HD11	1:102:C:VAL:HG12	10	0.24	0.03	0.26
(1,228)	1:96:C:ILE:HD11	1:102:C:VAL:HG13	10	0.24	0.03	0.26
(1,228)	1:96:C:ILE:HD12	1:102:C:VAL:HG11	10	0.24	0.03	0.26
(1,228)	1:96:C:ILE:HD12	1:102:C:VAL:HG12	10	0.24	0.03	0.26
(1,228)	1:96:C:ILE:HD12	1:102:C:VAL:HG13	10	0.24	0.03	0.26
(1,228)	1:96:C:ILE:HD13	1:102:C:VAL:HG11	10	0.24	0.03	0.26
(1,228)	1:96:C:ILE:HD13	1:102:C:VAL:HG12	10	0.24	0.03	0.26
(1,228)	1:96:C:ILE:HD13	1:102:C:VAL:HG13	10	0.24	0.03	0.26
(1,226)	1:96:A:ILE:HD11	1:102:A:VAL:HG11	10	0.24	0.05	0.24
(1,226)	1:96:A:ILE:HD11	1:102:A:VAL:HG12	10	0.24	0.05	0.24
(1,226)	1:96:A:ILE:HD11	1:102:A:VAL:HG13	10	0.24	0.05	0.24
(1,226)	1:96:A:ILE:HD12	1:102:A:VAL:HG11	10	0.24	0.05	0.24
(1,226)	1:96:A:ILE:HD12	1:102:A:VAL:HG12	10	0.24	0.05	0.24
(1,226)	1:96:A:ILE:HD12	1:102:A:VAL:HG13	10	0.24	0.05	0.24
(1,226)	1:96:A:ILE:HD13	1:102:A:VAL:HG11	10	0.24	0.05	0.24
(1,226)	1:96:A:ILE:HD13	1:102:A:VAL:HG12	10	0.24	0.05	0.24
(1,226)	1:96:A:ILE:HD13	1:102:A:VAL:HG13	10	0.24	0.05	0.24
(1,227)	1:96:B:ILE:HD11	1:102:B:VAL:HG11	10	0.23	0.03	0.24
(1,227)	1:96:B:ILE:HD11	1:102:B:VAL:HG12	10	0.23	0.03	0.24
(1,227)	1:96:B:ILE:HD11	1:102:B:VAL:HG13	10	0.23	0.03	0.24
(1,227)	1:96:B:ILE:HD12	1:102:B:VAL:HG11	10	0.23	0.03	0.24
(1,227)	1:96:B:ILE:HD12	1:102:B:VAL:HG12	10	0.23	0.03	0.24
(1,227)	1:96:B:ILE:HD12	1:102:B:VAL:HG13	10	0.23	0.03	0.24
(1,227)	1:96:B:ILE:HD13	1:102:B:VAL:HG11	10	0.23	0.03	0.24

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,227)	1:96:B:ILE:HD13	1:102:B:VAL:HG12	10	0.23	0.03	0.24
(1,227)	1:96:B:ILE:HD13	1:102:B:VAL:HG13	10	0.23	0.03	0.24
(1,1551)	1:167:C:ARG:H	1:171:C:SER:HA	10	0.15	0.04	0.14
(1,1686)	1:90:A:THR:H	1:91:A:THR:HB	10	0.14	0.03	0.14
(1,1692)	1:120:A:CYS:H	1:192:A:VAL:HG11	10	0.14	0.02	0.14
(1,1692)	1:120:A:CYS:H	1:192:A:VAL:HG12	10	0.14	0.02	0.14
(1,1692)	1:120:A:CYS:H	1:192:A:VAL:HG13	10	0.14	0.02	0.14
(1,712)	1:141:A:VAL:HG21	1:144:A:PHE:HD1	10	0.14	0.03	0.12
(1,712)	1:141:A:VAL:HG21	1:144:A:PHE:HD2	10	0.14	0.03	0.12
(1,712)	1:141:A:VAL:HG22	1:144:A:PHE:HD1	10	0.14	0.03	0.12
(1,712)	1:141:A:VAL:HG22	1:144:A:PHE:HD2	10	0.14	0.03	0.12
(1,712)	1:141:A:VAL:HG23	1:144:A:PHE:HD1	10	0.14	0.03	0.12
(1,712)	1:141:A:VAL:HG23	1:144:A:PHE:HD2	10	0.14	0.03	0.12
(1,813)	1:176:A:GLY:H	1:177:A:ASP:HB2	10	0.13	0.02	0.13
(1,814)	1:176:B:GLY:H	1:177:B:ASP:HB2	10	0.13	0.02	0.12
(1,55)	1:156:A:VAL:HG11	1:157:A:PRO:HD2	10	0.11	0.01	0.11
(1,55)	1:156:A:VAL:HG12	1:157:A:PRO:HD2	10	0.11	0.01	0.11
(1,55)	1:156:A:VAL:HG13	1:157:A:PRO:HD2	10	0.11	0.01	0.11
(1,1676)	1:94:A:PHE:H	1:102:A:VAL:HG11	9	0.4	0.18	0.38
(1,1676)	1:94:A:PHE:H	1:102:A:VAL:HG12	9	0.4	0.18	0.38
(1,1676)	1:94:A:PHE:H	1:102:A:VAL:HG13	9	0.4	0.18	0.38
(1,301)	1:181:A:LEU:HD11	1:196:A:TYR:HE1	9	0.24	0.11	0.25
(1,301)	1:181:A:LEU:HD11	1:196:A:TYR:HE2	9	0.24	0.11	0.25
(1,301)	1:181:A:LEU:HD12	1:196:A:TYR:HE1	9	0.24	0.11	0.25
(1,301)	1:181:A:LEU:HD12	1:196:A:TYR:HE2	9	0.24	0.11	0.25
(1,301)	1:181:A:LEU:HD13	1:196:A:TYR:HE1	9	0.24	0.11	0.25
(1,301)	1:181:A:LEU:HD13	1:196:A:TYR:HE2	9	0.24	0.11	0.25
(1,539)	1:111:A:ILE:HG21	1:126:A:ILE:HG21	9	0.2	0.09	0.16
(1,539)	1:111:A:ILE:HG21	1:126:A:ILE:HG22	9	0.2	0.09	0.16
(1,539)	1:111:A:ILE:HG21	1:126:A:ILE:HG23	9	0.2	0.09	0.16
(1,539)	1:111:A:ILE:HG22	1:126:A:ILE:HG21	9	0.2	0.09	0.16
(1,539)	1:111:A:ILE:HG22	1:126:A:ILE:HG22	9	0.2	0.09	0.16
(1,539)	1:111:A:ILE:HG22	1:126:A:ILE:HG23	9	0.2	0.09	0.16
(1,539)	1:111:A:ILE:HG23	1:126:A:ILE:HG21	9	0.2	0.09	0.16
(1,539)	1:111:A:ILE:HG23	1:126:A:ILE:HG22	9	0.2	0.09	0.16
(1,539)	1:111:A:ILE:HG23	1:126:A:ILE:HG23	9	0.2	0.09	0.16
(1,1550)	1:167:B:ARG:H	1:171:B:SER:HA	9	0.15	0.04	0.13
(1,891)	1:165:A:GLU:HB2	1:167:A:ARG:HG2	9	0.15	0.04	0.14
(1,891)	1:165:A:GLU:HB2	1:167:A:ARG:HG3	9	0.15	0.04	0.14
(1,1688)	1:90:C:THR:H	1:91:C:THR:HB	9	0.15	0.03	0.16
(1,1687)	1:90:B:THR:H	1:91:B:THR:HB	9	0.14	0.03	0.14
(1,396)	1:109:B:LEU:HG	1:111:B:ILE:HD11	9	0.13	0.02	0.12

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,396)	1:109:B:LEU:HG	1:111:B:ILE:HD12	9	0.13	0.02	0.12
(1,396)	1:109:B:LEU:HG	1:111:B:ILE:HD13	9	0.13	0.02	0.12
(1,892)	1:165:B:GLU:HB2	1:167:B:ARG:HG2	8	0.15	0.04	0.14
(1,892)	1:165:B:GLU:HB2	1:167:B:ARG:HG3	8	0.15	0.04	0.14
(1,893)	1:165:C:GLU:HB2	1:167:C:ARG:HG2	8	0.14	0.04	0.13
(1,893)	1:165:C:GLU:HB2	1:167:C:ARG:HG3	8	0.14	0.04	0.13
(1,1554)	1:156:C:VAL:HB	1:167:C:ARG:H	8	0.14	0.03	0.12
(1,784)	1:167:B:ARG:HD2	1:169:B:ALA:HB1	8	0.14	0.03	0.13
(1,784)	1:167:B:ARG:HD2	1:169:B:ALA:HB2	8	0.14	0.03	0.13
(1,784)	1:167:B:ARG:HD2	1:169:B:ALA:HB3	8	0.14	0.03	0.13
(1,784)	1:167:B:ARG:HD3	1:169:B:ALA:HB1	8	0.14	0.03	0.13
(1,784)	1:167:B:ARG:HD3	1:169:B:ALA:HB2	8	0.14	0.03	0.13
(1,784)	1:167:B:ARG:HD3	1:169:B:ALA:HB3	8	0.14	0.03	0.13
(1,1553)	1:156:B:VAL:HB	1:167:B:ARG:H	8	0.14	0.03	0.12
(1,785)	1:167:C:ARG:HD2	1:169:C:ALA:HB1	8	0.14	0.04	0.12
(1,785)	1:167:C:ARG:HD2	1:169:C:ALA:HB2	8	0.14	0.04	0.12
(1,785)	1:167:C:ARG:HD2	1:169:C:ALA:HB3	8	0.14	0.04	0.12
(1,785)	1:167:C:ARG:HD3	1:169:C:ALA:HB1	8	0.14	0.04	0.12
(1,785)	1:167:C:ARG:HD3	1:169:C:ALA:HB2	8	0.14	0.04	0.12
(1,785)	1:167:C:ARG:HD3	1:169:C:ALA:HB3	8	0.14	0.04	0.12
(1,157)	1:101:A:LEU:HD21	1:95:B:SER:HB2	8	0.13	0.02	0.12
(1,157)	1:101:A:LEU:HD21	1:95:B:SER:HB3	8	0.13	0.02	0.12
(1,157)	1:101:A:LEU:HD22	1:95:B:SER:HB2	8	0.13	0.02	0.12
(1,157)	1:101:A:LEU:HD22	1:95:B:SER:HB3	8	0.13	0.02	0.12
(1,157)	1:101:A:LEU:HD23	1:95:B:SER:HB2	8	0.13	0.02	0.12
(1,157)	1:101:A:LEU:HD23	1:95:B:SER:HB3	8	0.13	0.02	0.12
(1,215)	1:101:A:LEU:HD21	1:103:A:VAL:HG11	7	0.41	0.09	0.43
(1,215)	1:101:A:LEU:HD21	1:103:A:VAL:HG12	7	0.41	0.09	0.43
(1,215)	1:101:A:LEU:HD21	1:103:A:VAL:HG13	7	0.41	0.09	0.43
(1,215)	1:101:A:LEU:HD22	1:103:A:VAL:HG11	7	0.41	0.09	0.43
(1,215)	1:101:A:LEU:HD22	1:103:A:VAL:HG12	7	0.41	0.09	0.43
(1,215)	1:101:A:LEU:HD22	1:103:A:VAL:HG13	7	0.41	0.09	0.43
(1,215)	1:101:A:LEU:HD23	1:103:A:VAL:HG11	7	0.41	0.09	0.43
(1,215)	1:101:A:LEU:HD23	1:103:A:VAL:HG12	7	0.41	0.09	0.43
(1,215)	1:101:A:LEU:HD23	1:103:A:VAL:HG13	7	0.41	0.09	0.43
(1,1830)	1:102:A:VAL:HG11	1:111:A:ILE:HG12	7	0.28	0.06	0.27
(1,1830)	1:102:A:VAL:HG11	1:111:A:ILE:HG13	7	0.28	0.06	0.27
(1,1830)	1:102:A:VAL:HG12	1:111:A:ILE:HG12	7	0.28	0.06	0.27
(1,1830)	1:102:A:VAL:HG12	1:111:A:ILE:HG13	7	0.28	0.06	0.27
(1,1830)	1:102:A:VAL:HG13	1:111:A:ILE:HG12	7	0.28	0.06	0.27
(1,1830)	1:102:A:VAL:HG13	1:111:A:ILE:HG13	7	0.28	0.06	0.27
(1,1774)	1:125:A:LYS:H	1:126:A:ILE:HG21	7	0.19	0.07	0.16

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1774)	1:125:A:LYS:H	1:126:A:ILE:HG22	7	0.19	0.07	0.16
(1,1774)	1:125:A:LYS:H	1:126:A:ILE:HG23	7	0.19	0.07	0.16
(1,1884)	1:154:A:PRO:HB2	1:167:A:ARG:H	7	0.18	0.05	0.21
(1,1884)	1:154:A:PRO:HB3	1:167:A:ARG:H	7	0.18	0.05	0.21
(1,365)	1:126:B:ILE:HG21	1:131:B:ILE:HD11	7	0.17	0.05	0.15
(1,365)	1:126:B:ILE:HG21	1:131:B:ILE:HD12	7	0.17	0.05	0.15
(1,365)	1:126:B:ILE:HG21	1:131:B:ILE:HD13	7	0.17	0.05	0.15
(1,365)	1:126:B:ILE:HG22	1:131:B:ILE:HD11	7	0.17	0.05	0.15
(1,365)	1:126:B:ILE:HG22	1:131:B:ILE:HD12	7	0.17	0.05	0.15
(1,365)	1:126:B:ILE:HG22	1:131:B:ILE:HD13	7	0.17	0.05	0.15
(1,365)	1:126:B:ILE:HG23	1:131:B:ILE:HD11	7	0.17	0.05	0.15
(1,365)	1:126:B:ILE:HG23	1:131:B:ILE:HD12	7	0.17	0.05	0.15
(1,365)	1:126:B:ILE:HG23	1:131:B:ILE:HD13	7	0.17	0.05	0.15
(1,769)	1:102:A:VAL:HG21	1:104:A:TYR:HE1	7	0.14	0.02	0.14
(1,769)	1:102:A:VAL:HG21	1:104:A:TYR:HE2	7	0.14	0.02	0.14
(1,769)	1:102:A:VAL:HG22	1:104:A:TYR:HE1	7	0.14	0.02	0.14
(1,769)	1:102:A:VAL:HG22	1:104:A:TYR:HE2	7	0.14	0.02	0.14
(1,769)	1:102:A:VAL:HG23	1:104:A:TYR:HE1	7	0.14	0.02	0.14
(1,769)	1:102:A:VAL:HG23	1:104:A:TYR:HE2	7	0.14	0.02	0.14
(1,363)	1:131:A:ILE:HD11	1:183:C:MET:HG2	7	0.14	0.02	0.15
(1,363)	1:131:A:ILE:HD11	1:183:C:MET:HG3	7	0.14	0.02	0.15
(1,363)	1:131:A:ILE:HD12	1:183:C:MET:HG2	7	0.14	0.02	0.15
(1,363)	1:131:A:ILE:HD12	1:183:C:MET:HG3	7	0.14	0.02	0.15
(1,363)	1:131:A:ILE:HD13	1:183:C:MET:HG2	7	0.14	0.02	0.15
(1,363)	1:131:A:ILE:HD13	1:183:C:MET:HG3	7	0.14	0.02	0.15
(1,783)	1:167:A:ARG:HD2	1:169:A:ALA:HB1	7	0.14	0.03	0.15
(1,783)	1:167:A:ARG:HD2	1:169:A:ALA:HB2	7	0.14	0.03	0.15
(1,783)	1:167:A:ARG:HD2	1:169:A:ALA:HB3	7	0.14	0.03	0.15
(1,783)	1:167:A:ARG:HD3	1:169:A:ALA:HB1	7	0.14	0.03	0.15
(1,783)	1:167:A:ARG:HD3	1:169:A:ALA:HB2	7	0.14	0.03	0.15
(1,783)	1:167:A:ARG:HD3	1:169:A:ALA:HB3	7	0.14	0.03	0.15
(1,134)	1:110:A:LEU:HD11	1:111:A:ILE:HD11	7	0.14	0.03	0.14
(1,134)	1:110:A:LEU:HD11	1:111:A:ILE:HD12	7	0.14	0.03	0.14
(1,134)	1:110:A:LEU:HD11	1:111:A:ILE:HD13	7	0.14	0.03	0.14
(1,134)	1:110:A:LEU:HD12	1:111:A:ILE:HD11	7	0.14	0.03	0.14
(1,134)	1:110:A:LEU:HD12	1:111:A:ILE:HD12	7	0.14	0.03	0.14
(1,134)	1:110:A:LEU:HD12	1:111:A:ILE:HD13	7	0.14	0.03	0.14
(1,134)	1:110:A:LEU:HD13	1:111:A:ILE:HD11	7	0.14	0.03	0.14
(1,134)	1:110:A:LEU:HD13	1:111:A:ILE:HD12	7	0.14	0.03	0.14
(1,134)	1:110:A:LEU:HD13	1:111:A:ILE:HD13	7	0.14	0.03	0.14
(1,1202)	1:196:B:TYR:H	1:196:B:TYR:HE1	7	0.13	0.02	0.14
(1,1202)	1:196:B:TYR:H	1:196:B:TYR:HE2	7	0.13	0.02	0.14

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1504)	1:92:A:ALA:H	1:103:A:VAL:HG21	7	0.13	0.01	0.12
(1,1504)	1:92:A:ALA:H	1:103:A:VAL:HG22	7	0.13	0.01	0.12
(1,1504)	1:92:A:ALA:H	1:103:A:VAL:HG23	7	0.13	0.01	0.12
(1,1512)	1:137:B:LEU:H	1:137:B:LEU:HG	7	0.12	0.01	0.11
(1,1077)	1:173:A:PRO:HB3	1:174:A:SER:H	7	0.11	0.01	0.11
(1,1079)	1:173:C:PRO:HB3	1:174:C:SER:H	7	0.11	0.01	0.12
(1,1030)	1:152:A:ALA:H	1:153:A:LYS:H	6	0.33	0.1	0.29
(1,1032)	1:152:C:ALA:H	1:153:C:LYS:H	6	0.32	0.1	0.27
(1,1031)	1:152:B:ALA:H	1:153:B:LYS:H	6	0.32	0.1	0.27
(1,364)	1:126:A:ILE:HG21	1:131:A:ILE:HD11	6	0.19	0.04	0.18
(1,364)	1:126:A:ILE:HG21	1:131:A:ILE:HD12	6	0.19	0.04	0.18
(1,364)	1:126:A:ILE:HG21	1:131:A:ILE:HD13	6	0.19	0.04	0.18
(1,364)	1:126:A:ILE:HG22	1:131:A:ILE:HD11	6	0.19	0.04	0.18
(1,364)	1:126:A:ILE:HG22	1:131:A:ILE:HD12	6	0.19	0.04	0.18
(1,364)	1:126:A:ILE:HG22	1:131:A:ILE:HD13	6	0.19	0.04	0.18
(1,364)	1:126:A:ILE:HG23	1:131:A:ILE:HD11	6	0.19	0.04	0.18
(1,364)	1:126:A:ILE:HG23	1:131:A:ILE:HD12	6	0.19	0.04	0.18
(1,364)	1:126:A:ILE:HG23	1:131:A:ILE:HD13	6	0.19	0.04	0.18
(1,2292)	1:154:C:PRO:HB2	1:167:C:ARG:H	6	0.19	0.05	0.19
(1,2292)	1:154:C:PRO:HB3	1:167:C:ARG:H	6	0.19	0.05	0.19
(1,371)	1:96:A:ILE:HD11	1:102:A:VAL:HB	6	0.16	0.03	0.15
(1,371)	1:96:A:ILE:HD12	1:102:A:VAL:HB	6	0.16	0.03	0.15
(1,371)	1:96:A:ILE:HD13	1:102:A:VAL:HB	6	0.16	0.03	0.15
(1,739)	1:175:C:GLY:HA2	1:179:C:ALA:HB1	6	0.14	0.05	0.12
(1,739)	1:175:C:GLY:HA2	1:179:C:ALA:HB2	6	0.14	0.05	0.12
(1,739)	1:175:C:GLY:HA2	1:179:C:ALA:HB3	6	0.14	0.05	0.12
(1,739)	1:175:C:GLY:HA3	1:179:C:ALA:HB1	6	0.14	0.05	0.12
(1,739)	1:175:C:GLY:HA3	1:179:C:ALA:HB2	6	0.14	0.05	0.12
(1,739)	1:175:C:GLY:HA3	1:179:C:ALA:HB3	6	0.14	0.05	0.12
(1,1507)	1:92:A:ALA:H	1:93:C:THR:HG21	6	0.14	0.05	0.13
(1,1507)	1:92:A:ALA:H	1:93:C:THR:HG22	6	0.14	0.05	0.13
(1,1507)	1:92:A:ALA:H	1:93:C:THR:HG23	6	0.14	0.05	0.13
(1,1350)	1:127:A:ALA:H	1:131:A:ILE:HG21	6	0.13	0.01	0.14
(1,1350)	1:127:A:ALA:H	1:131:A:ILE:HG22	6	0.13	0.01	0.14
(1,1350)	1:127:A:ALA:H	1:131:A:ILE:HG23	6	0.13	0.01	0.14
(1,42)	1:188:A:LEU:HD11	1:106:B:TYR:HE1	6	0.13	0.01	0.13
(1,42)	1:188:A:LEU:HD11	1:106:B:TYR:HE2	6	0.13	0.01	0.13
(1,42)	1:188:A:LEU:HD12	1:106:B:TYR:HE1	6	0.13	0.01	0.13
(1,42)	1:188:A:LEU:HD12	1:106:B:TYR:HE2	6	0.13	0.01	0.13
(1,42)	1:188:A:LEU:HD13	1:106:B:TYR:HE1	6	0.13	0.01	0.13
(1,42)	1:188:A:LEU:HD13	1:106:B:TYR:HE2	6	0.13	0.01	0.13
(1,397)	1:109:C:LEU:HG	1:111:C:ILE:HD11	6	0.13	0.02	0.12

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,397)	1:109:C:LEU:HG	1:111:C:ILE:HD12	6	0.13	0.02	0.12
(1,397)	1:109:C:LEU:HG	1:111:C:ILE:HD13	6	0.13	0.02	0.12
(1,1078)	1:173:B:PRO:HB3	1:174:B:SER:H	6	0.12	0.0	0.12
(1,895)	1:165:B:GLU:HB3	1:169:B:ALA:HB1	6	0.11	0.01	0.11
(1,895)	1:165:B:GLU:HB3	1:169:B:ALA:HB2	6	0.11	0.01	0.11
(1,895)	1:165:B:GLU:HB3	1:169:B:ALA:HB3	6	0.11	0.01	0.11
(1,2113)	1:180:B:PHE:H	1:181:B:LEU:HB2	5	0.23	0.09	0.29
(1,2113)	1:180:B:PHE:H	1:181:B:LEU:HB3	5	0.23	0.09	0.29
(1,2339)	1:180:C:PHE:H	1:181:C:LEU:HB2	5	0.23	0.09	0.29
(1,2339)	1:180:C:PHE:H	1:181:C:LEU:HB3	5	0.23	0.09	0.29
(1,1916)	1:180:A:PHE:H	1:181:A:LEU:HB2	5	0.22	0.09	0.28
(1,1916)	1:180:A:PHE:H	1:181:A:LEU:HB3	5	0.22	0.09	0.28
(1,573)	1:194:A:LEU:HD21	1:196:A:TYR:HE1	5	0.21	0.1	0.19
(1,573)	1:194:A:LEU:HD21	1:196:A:TYR:HE2	5	0.21	0.1	0.19
(1,573)	1:194:A:LEU:HD22	1:196:A:TYR:HE1	5	0.21	0.1	0.19
(1,573)	1:194:A:LEU:HD22	1:196:A:TYR:HE2	5	0.21	0.1	0.19
(1,573)	1:194:A:LEU:HD23	1:196:A:TYR:HE1	5	0.21	0.1	0.19
(1,573)	1:194:A:LEU:HD23	1:196:A:TYR:HE2	5	0.21	0.1	0.19
(1,2066)	1:154:B:PRO:HB2	1:167:B:ARG:H	5	0.2	0.04	0.22
(1,2066)	1:154:B:PRO:HB3	1:167:B:ARG:H	5	0.2	0.04	0.22
(1,1602)	1:89:A:VAL:HG21	1:91:A:THR:H	5	0.18	0.03	0.19
(1,1602)	1:89:A:VAL:HG22	1:91:A:THR:H	5	0.18	0.03	0.19
(1,1602)	1:89:A:VAL:HG23	1:91:A:THR:H	5	0.18	0.03	0.19
(1,239)	1:102:A:VAL:HG21	1:137:A:LEU:HD21	5	0.18	0.06	0.15
(1,239)	1:102:A:VAL:HG21	1:137:A:LEU:HD22	5	0.18	0.06	0.15
(1,239)	1:102:A:VAL:HG21	1:137:A:LEU:HD23	5	0.18	0.06	0.15
(1,239)	1:102:A:VAL:HG22	1:137:A:LEU:HD21	5	0.18	0.06	0.15
(1,239)	1:102:A:VAL:HG22	1:137:A:LEU:HD22	5	0.18	0.06	0.15
(1,239)	1:102:A:VAL:HG22	1:137:A:LEU:HD23	5	0.18	0.06	0.15
(1,239)	1:102:A:VAL:HG23	1:137:A:LEU:HD21	5	0.18	0.06	0.15
(1,239)	1:102:A:VAL:HG23	1:137:A:LEU:HD22	5	0.18	0.06	0.15
(1,239)	1:102:A:VAL:HG23	1:137:A:LEU:HD23	5	0.18	0.06	0.15
(1,366)	1:126:C:ILE:HG21	1:131:C:ILE:HD11	5	0.18	0.04	0.19
(1,366)	1:126:C:ILE:HG21	1:131:C:ILE:HD12	5	0.18	0.04	0.19
(1,366)	1:126:C:ILE:HG21	1:131:C:ILE:HD13	5	0.18	0.04	0.19
(1,366)	1:126:C:ILE:HG22	1:131:C:ILE:HD11	5	0.18	0.04	0.19
(1,366)	1:126:C:ILE:HG22	1:131:C:ILE:HD12	5	0.18	0.04	0.19
(1,366)	1:126:C:ILE:HG22	1:131:C:ILE:HD13	5	0.18	0.04	0.19
(1,366)	1:126:C:ILE:HG23	1:131:C:ILE:HD11	5	0.18	0.04	0.19
(1,366)	1:126:C:ILE:HG23	1:131:C:ILE:HD12	5	0.18	0.04	0.19
(1,366)	1:126:C:ILE:HG23	1:131:C:ILE:HD13	5	0.18	0.04	0.19
(1,572)	1:121:A:CYS:H	1:194:A:LEU:HD21	5	0.17	0.07	0.13

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,572)	1:121:A:CYS:H	1:194:A:LEU:HD22	5	0.17	0.07	0.13
(1,572)	1:121:A:CYS:H	1:194:A:LEU:HD23	5	0.17	0.07	0.13
(1,848)	1:150:A:LEU:HD11	1:167:A:ARG:HG2	5	0.17	0.06	0.14
(1,848)	1:150:A:LEU:HD11	1:167:A:ARG:HG3	5	0.17	0.06	0.14
(1,848)	1:150:A:LEU:HD12	1:167:A:ARG:HG2	5	0.17	0.06	0.14
(1,848)	1:150:A:LEU:HD12	1:167:A:ARG:HG3	5	0.17	0.06	0.14
(1,848)	1:150:A:LEU:HD13	1:167:A:ARG:HG2	5	0.17	0.06	0.14
(1,848)	1:150:A:LEU:HD13	1:167:A:ARG:HG3	5	0.17	0.06	0.14
(1,2283)	1:150:C:LEU:HD11	1:167:C:ARG:HG2	5	0.17	0.08	0.13
(1,2283)	1:150:C:LEU:HD11	1:167:C:ARG:HG3	5	0.17	0.08	0.13
(1,2283)	1:150:C:LEU:HD12	1:167:C:ARG:HG2	5	0.17	0.08	0.13
(1,2283)	1:150:C:LEU:HD12	1:167:C:ARG:HG3	5	0.17	0.08	0.13
(1,2283)	1:150:C:LEU:HD13	1:167:C:ARG:HG2	5	0.17	0.08	0.13
(1,2283)	1:150:C:LEU:HD13	1:167:C:ARG:HG3	5	0.17	0.08	0.13
(1,2283)	1:150:C:LEU:HD21	1:167:C:ARG:HG2	5	0.17	0.08	0.13
(1,2283)	1:150:C:LEU:HD21	1:167:C:ARG:HG3	5	0.17	0.08	0.13
(1,2283)	1:150:C:LEU:HD22	1:167:C:ARG:HG2	5	0.17	0.08	0.13
(1,2283)	1:150:C:LEU:HD22	1:167:C:ARG:HG3	5	0.17	0.08	0.13
(1,2283)	1:150:C:LEU:HD23	1:167:C:ARG:HG2	5	0.17	0.08	0.13
(1,2283)	1:150:C:LEU:HD23	1:167:C:ARG:HG3	5	0.17	0.08	0.13
(1,2057)	1:150:B:LEU:HD11	1:167:B:ARG:HG2	5	0.17	0.08	0.13
(1,2057)	1:150:B:LEU:HD11	1:167:B:ARG:HG3	5	0.17	0.08	0.13
(1,2057)	1:150:B:LEU:HD12	1:167:B:ARG:HG2	5	0.17	0.08	0.13
(1,2057)	1:150:B:LEU:HD12	1:167:B:ARG:HG3	5	0.17	0.08	0.13
(1,2057)	1:150:B:LEU:HD13	1:167:B:ARG:HG2	5	0.17	0.08	0.13
(1,2057)	1:150:B:LEU:HD13	1:167:B:ARG:HG3	5	0.17	0.08	0.13
(1,2057)	1:150:B:LEU:HD21	1:167:B:ARG:HG2	5	0.17	0.08	0.13
(1,2057)	1:150:B:LEU:HD21	1:167:B:ARG:HG3	5	0.17	0.08	0.13
(1,2057)	1:150:B:LEU:HD22	1:167:B:ARG:HG2	5	0.17	0.08	0.13
(1,2057)	1:150:B:LEU:HD22	1:167:B:ARG:HG3	5	0.17	0.08	0.13
(1,2057)	1:150:B:LEU:HD23	1:167:B:ARG:HG2	5	0.17	0.08	0.13
(1,2057)	1:150:B:LEU:HD23	1:167:B:ARG:HG3	5	0.17	0.08	0.13
(1,1835)	1:109:A:LEU:HB2	1:110:A:LEU:HD11	5	0.16	0.03	0.17
(1,1835)	1:109:A:LEU:HB2	1:110:A:LEU:HD12	5	0.16	0.03	0.17
(1,1835)	1:109:A:LEU:HB2	1:110:A:LEU:HD13	5	0.16	0.03	0.17
(1,1835)	1:109:A:LEU:HB3	1:110:A:LEU:HD11	5	0.16	0.03	0.17
(1,1835)	1:109:A:LEU:HB3	1:110:A:LEU:HD12	5	0.16	0.03	0.17
(1,1835)	1:109:A:LEU:HB3	1:110:A:LEU:HD13	5	0.16	0.03	0.17
(1,577)	1:178:A:PRO:HG2	1:194:A:LEU:HD21	5	0.16	0.04	0.16
(1,577)	1:178:A:PRO:HG2	1:194:A:LEU:HD22	5	0.16	0.04	0.16
(1,577)	1:178:A:PRO:HG2	1:194:A:LEU:HD23	5	0.16	0.04	0.16
(1,577)	1:178:A:PRO:HG3	1:194:A:LEU:HD21	5	0.16	0.04	0.16

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,577)	1:178:A:PRO:HG3	1:194:A:LEU:HD22	5	0.16	0.04	0.16
(1,577)	1:178:A:PRO:HG3	1:194:A:LEU:HD23	5	0.16	0.04	0.16
(1,737)	1:175:A:GLY:HA2	1:179:A:ALA:HB1	5	0.16	0.05	0.15
(1,737)	1:175:A:GLY:HA2	1:179:A:ALA:HB2	5	0.16	0.05	0.15
(1,737)	1:175:A:GLY:HA2	1:179:A:ALA:HB3	5	0.16	0.05	0.15
(1,737)	1:175:A:GLY:HA3	1:179:A:ALA:HB1	5	0.16	0.05	0.15
(1,737)	1:175:A:GLY:HA3	1:179:A:ALA:HB2	5	0.16	0.05	0.15
(1,737)	1:175:A:GLY:HA3	1:179:A:ALA:HB3	5	0.16	0.05	0.15
(1,198)	1:109:A:LEU:H	1:110:A:LEU:HD21	5	0.15	0.02	0.16
(1,198)	1:109:A:LEU:H	1:110:A:LEU:HD22	5	0.15	0.02	0.16
(1,198)	1:109:A:LEU:H	1:110:A:LEU:HD23	5	0.15	0.02	0.16
(1,738)	1:175:B:GLY:HA2	1:179:B:ALA:HB1	5	0.15	0.06	0.12
(1,738)	1:175:B:GLY:HA2	1:179:B:ALA:HB2	5	0.15	0.06	0.12
(1,738)	1:175:B:GLY:HA2	1:179:B:ALA:HB3	5	0.15	0.06	0.12
(1,738)	1:175:B:GLY:HA3	1:179:B:ALA:HB1	5	0.15	0.06	0.12
(1,738)	1:175:B:GLY:HA3	1:179:B:ALA:HB2	5	0.15	0.06	0.12
(1,738)	1:175:B:GLY:HA3	1:179:B:ALA:HB3	5	0.15	0.06	0.12
(1,1911)	1:178:A:PRO:HB2	1:180:A:PHE:H	5	0.15	0.02	0.15
(1,1911)	1:178:A:PRO:HB3	1:180:A:PHE:H	5	0.15	0.02	0.15
(1,1506)	1:93:B:THR:HG21	1:92:C:ALA:H	5	0.15	0.05	0.13
(1,1506)	1:93:B:THR:HG22	1:92:C:ALA:H	5	0.15	0.05	0.13
(1,1506)	1:93:B:THR:HG23	1:92:C:ALA:H	5	0.15	0.05	0.13
(1,425)	1:89:A:VAL:HG11	1:183:A:MET:HE1	5	0.15	0.04	0.14
(1,425)	1:89:A:VAL:HG11	1:183:A:MET:HE2	5	0.15	0.04	0.14
(1,425)	1:89:A:VAL:HG11	1:183:A:MET:HE3	5	0.15	0.04	0.14
(1,425)	1:89:A:VAL:HG12	1:183:A:MET:HE1	5	0.15	0.04	0.14
(1,425)	1:89:A:VAL:HG12	1:183:A:MET:HE2	5	0.15	0.04	0.14
(1,425)	1:89:A:VAL:HG12	1:183:A:MET:HE3	5	0.15	0.04	0.14
(1,425)	1:89:A:VAL:HG13	1:183:A:MET:HE1	5	0.15	0.04	0.14
(1,425)	1:89:A:VAL:HG13	1:183:A:MET:HE2	5	0.15	0.04	0.14
(1,425)	1:89:A:VAL:HG13	1:183:A:MET:HE3	5	0.15	0.04	0.14
(1,1203)	1:196:C:TYR:H	1:196:C:TYR:HE1	5	0.14	0.01	0.15
(1,1203)	1:196:C:TYR:H	1:196:C:TYR:HE2	5	0.14	0.01	0.15
(1,154)	1:187:A:THR:HG21	1:188:A:LEU:HD21	5	0.13	0.03	0.12
(1,154)	1:187:A:THR:HG21	1:188:A:LEU:HD22	5	0.13	0.03	0.12
(1,154)	1:187:A:THR:HG21	1:188:A:LEU:HD23	5	0.13	0.03	0.12
(1,154)	1:187:A:THR:HG22	1:188:A:LEU:HD21	5	0.13	0.03	0.12
(1,154)	1:187:A:THR:HG22	1:188:A:LEU:HD22	5	0.13	0.03	0.12
(1,154)	1:187:A:THR:HG22	1:188:A:LEU:HD23	5	0.13	0.03	0.12
(1,154)	1:187:A:THR:HG23	1:188:A:LEU:HD21	5	0.13	0.03	0.12
(1,154)	1:187:A:THR:HG23	1:188:A:LEU:HD22	5	0.13	0.03	0.12
(1,154)	1:187:A:THR:HG23	1:188:A:LEU:HD23	5	0.13	0.03	0.12

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,538)	1:111:C:ILE:HD11	1:131:C:ILE:HG21	5	0.13	0.02	0.13
(1,538)	1:111:C:ILE:HD11	1:131:C:ILE:HG22	5	0.13	0.02	0.13
(1,538)	1:111:C:ILE:HD11	1:131:C:ILE:HG23	5	0.13	0.02	0.13
(1,538)	1:111:C:ILE:HD12	1:131:C:ILE:HG21	5	0.13	0.02	0.13
(1,538)	1:111:C:ILE:HD12	1:131:C:ILE:HG22	5	0.13	0.02	0.13
(1,538)	1:111:C:ILE:HD12	1:131:C:ILE:HG23	5	0.13	0.02	0.13
(1,538)	1:111:C:ILE:HD13	1:131:C:ILE:HG21	5	0.13	0.02	0.13
(1,538)	1:111:C:ILE:HD13	1:131:C:ILE:HG22	5	0.13	0.02	0.13
(1,538)	1:111:C:ILE:HD13	1:131:C:ILE:HG23	5	0.13	0.02	0.13
(1,792)	1:153:A:LYS:HE2	1:154:A:PRO:HG2	5	0.13	0.03	0.13
(1,792)	1:153:A:LYS:HE2	1:154:A:PRO:HG3	5	0.13	0.03	0.13
(1,792)	1:153:A:LYS:HE3	1:154:A:PRO:HG2	5	0.13	0.03	0.13
(1,792)	1:153:A:LYS:HE3	1:154:A:PRO:HG3	5	0.13	0.03	0.13
(1,362)	1:183:B:MET:HG2	1:131:C:ILE:HD11	5	0.12	0.02	0.12
(1,362)	1:183:B:MET:HG2	1:131:C:ILE:HD12	5	0.12	0.02	0.12
(1,362)	1:183:B:MET:HG2	1:131:C:ILE:HD13	5	0.12	0.02	0.12
(1,362)	1:183:B:MET:HG3	1:131:C:ILE:HD11	5	0.12	0.02	0.12
(1,362)	1:183:B:MET:HG3	1:131:C:ILE:HD12	5	0.12	0.02	0.12
(1,362)	1:183:B:MET:HG3	1:131:C:ILE:HD13	5	0.12	0.02	0.12
(1,280)	1:123:A:ILE:HD11	1:189:A:CYS:HB2	5	0.11	0.0	0.11
(1,280)	1:123:A:ILE:HD11	1:189:A:CYS:HB3	5	0.11	0.0	0.11
(1,280)	1:123:A:ILE:HD12	1:189:A:CYS:HB2	5	0.11	0.0	0.11
(1,280)	1:123:A:ILE:HD12	1:189:A:CYS:HB3	5	0.11	0.0	0.11
(1,280)	1:123:A:ILE:HD13	1:189:A:CYS:HB2	5	0.11	0.0	0.11
(1,280)	1:123:A:ILE:HD13	1:189:A:CYS:HB3	5	0.11	0.0	0.11
(1,896)	1:165:C:GLU:HB3	1:169:C:ALA:HB1	5	0.11	0.01	0.1
(1,896)	1:165:C:GLU:HB3	1:169:C:ALA:HB2	5	0.11	0.01	0.1
(1,896)	1:165:C:GLU:HB3	1:169:C:ALA:HB3	5	0.11	0.01	0.1
(1,1374)	1:155:A:ALA:H	1:156:A:VAL:HG11	4	0.42	0.22	0.38
(1,1374)	1:155:A:ALA:H	1:156:A:VAL:HG12	4	0.42	0.22	0.38
(1,1374)	1:155:A:ALA:H	1:156:A:VAL:HG13	4	0.42	0.22	0.38
(1,935)	1:95:A:SER:H	1:101:A:LEU:HD11	4	0.39	0.05	0.38
(1,935)	1:95:A:SER:H	1:101:A:LEU:HD12	4	0.39	0.05	0.38
(1,935)	1:95:A:SER:H	1:101:A:LEU:HD13	4	0.39	0.05	0.38
(1,1362)	1:154:A:PRO:HA	1:155:A:ALA:H	4	0.35	0.09	0.34
(1,1363)	1:154:B:PRO:HA	1:155:B:ALA:H	4	0.35	0.1	0.34
(1,1364)	1:154:C:PRO:HA	1:155:C:ALA:H	4	0.35	0.1	0.34
(1,2060)	1:151:B:GLN:HB2	1:152:B:ALA:HA	4	0.17	0.04	0.16
(1,2060)	1:151:B:GLN:HB3	1:152:B:ALA:HA	4	0.17	0.04	0.16
(1,1892)	1:161:A:LEU:HD11	1:162:A:GLY:HA2	4	0.17	0.06	0.15
(1,1892)	1:161:A:LEU:HD11	1:162:A:GLY:HA3	4	0.17	0.06	0.15
(1,1892)	1:161:A:LEU:HD12	1:162:A:GLY:HA2	4	0.17	0.06	0.15

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1892)	1:161:A:LEU:HD12	1:162:A:GLY:HA3	4	0.17	0.06	0.15
(1,1892)	1:161:A:LEU:HD13	1:162:A:GLY:HA2	4	0.17	0.06	0.15
(1,1892)	1:161:A:LEU:HD13	1:162:A:GLY:HA3	4	0.17	0.06	0.15
(1,2286)	1:151:C:GLN:HB2	1:152:C:ALA:HA	4	0.17	0.04	0.16
(1,2286)	1:151:C:GLN:HB3	1:152:C:ALA:HA	4	0.17	0.04	0.16
(1,1918)	1:183:A:MET:HB2	1:183:A:MET:HE1	4	0.16	0.01	0.16
(1,1918)	1:183:A:MET:HB2	1:183:A:MET:HE2	4	0.16	0.01	0.16
(1,1918)	1:183:A:MET:HB2	1:183:A:MET:HE3	4	0.16	0.01	0.16
(1,1918)	1:183:A:MET:HB3	1:183:A:MET:HE1	4	0.16	0.01	0.16
(1,1918)	1:183:A:MET:HB3	1:183:A:MET:HE2	4	0.16	0.01	0.16
(1,1918)	1:183:A:MET:HB3	1:183:A:MET:HE3	4	0.16	0.01	0.16
(1,2119)	1:183:B:MET:HB2	1:183:B:MET:HE1	4	0.16	0.01	0.16
(1,2119)	1:183:B:MET:HB2	1:183:B:MET:HE2	4	0.16	0.01	0.16
(1,2119)	1:183:B:MET:HB2	1:183:B:MET:HE3	4	0.16	0.01	0.16
(1,2119)	1:183:B:MET:HB3	1:183:B:MET:HE1	4	0.16	0.01	0.16
(1,2119)	1:183:B:MET:HB3	1:183:B:MET:HE2	4	0.16	0.01	0.16
(1,2119)	1:183:B:MET:HB3	1:183:B:MET:HE3	4	0.16	0.01	0.16
(1,2345)	1:183:C:MET:HB2	1:183:C:MET:HE1	4	0.16	0.01	0.16
(1,2345)	1:183:C:MET:HB2	1:183:C:MET:HE2	4	0.16	0.01	0.16
(1,2345)	1:183:C:MET:HB2	1:183:C:MET:HE3	4	0.16	0.01	0.16
(1,2345)	1:183:C:MET:HB3	1:183:C:MET:HE1	4	0.16	0.01	0.16
(1,2345)	1:183:C:MET:HB3	1:183:C:MET:HE2	4	0.16	0.01	0.16
(1,2345)	1:183:C:MET:HB3	1:183:C:MET:HE3	4	0.16	0.01	0.16
(1,1867)	1:134:A:LEU:H	1:188:C:LEU:HD11	4	0.15	0.02	0.16
(1,1867)	1:134:A:LEU:H	1:188:C:LEU:HD12	4	0.15	0.02	0.16
(1,1867)	1:134:A:LEU:H	1:188:C:LEU:HD13	4	0.15	0.02	0.16
(1,1867)	1:134:A:LEU:H	1:188:C:LEU:HD21	4	0.15	0.02	0.16
(1,1867)	1:134:A:LEU:H	1:188:C:LEU:HD22	4	0.15	0.02	0.16
(1,1867)	1:134:A:LEU:H	1:188:C:LEU:HD23	4	0.15	0.02	0.16
(1,2138)	1:188:B:LEU:HD11	1:134:C:LEU:H	4	0.15	0.01	0.15
(1,2138)	1:188:B:LEU:HD12	1:134:C:LEU:H	4	0.15	0.01	0.15
(1,2138)	1:188:B:LEU:HD13	1:134:C:LEU:H	4	0.15	0.01	0.15
(1,2138)	1:188:B:LEU:HD21	1:134:C:LEU:H	4	0.15	0.01	0.15
(1,2138)	1:188:B:LEU:HD22	1:134:C:LEU:H	4	0.15	0.01	0.15
(1,2138)	1:188:B:LEU:HD23	1:134:C:LEU:H	4	0.15	0.01	0.15
(1,2163)	1:89:C:VAL:HG11	1:183:C:MET:HE1	4	0.14	0.04	0.14
(1,2163)	1:89:C:VAL:HG11	1:183:C:MET:HE2	4	0.14	0.04	0.14
(1,2163)	1:89:C:VAL:HG11	1:183:C:MET:HE3	4	0.14	0.04	0.14
(1,2163)	1:89:C:VAL:HG12	1:183:C:MET:HE1	4	0.14	0.04	0.14
(1,2163)	1:89:C:VAL:HG12	1:183:C:MET:HE2	4	0.14	0.04	0.14
(1,2163)	1:89:C:VAL:HG12	1:183:C:MET:HE3	4	0.14	0.04	0.14
(1,2163)	1:89:C:VAL:HG13	1:183:C:MET:HE1	4	0.14	0.04	0.14

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2163)	1:89:C:VAL:HG13	1:183:C:MET:HE2	4	0.14	0.04	0.14
(1,2163)	1:89:C:VAL:HG13	1:183:C:MET:HE3	4	0.14	0.04	0.14
(1,2163)	1:89:C:VAL:HG21	1:183:C:MET:HE1	4	0.14	0.04	0.14
(1,2163)	1:89:C:VAL:HG21	1:183:C:MET:HE2	4	0.14	0.04	0.14
(1,2163)	1:89:C:VAL:HG21	1:183:C:MET:HE3	4	0.14	0.04	0.14
(1,2163)	1:89:C:VAL:HG22	1:183:C:MET:HE1	4	0.14	0.04	0.14
(1,2163)	1:89:C:VAL:HG22	1:183:C:MET:HE2	4	0.14	0.04	0.14
(1,2163)	1:89:C:VAL:HG22	1:183:C:MET:HE3	4	0.14	0.04	0.14
(1,2163)	1:89:C:VAL:HG23	1:183:C:MET:HE1	4	0.14	0.04	0.14
(1,2163)	1:89:C:VAL:HG23	1:183:C:MET:HE2	4	0.14	0.04	0.14
(1,2163)	1:89:C:VAL:HG23	1:183:C:MET:HE3	4	0.14	0.04	0.14
(1,1935)	1:89:B:VAL:HG11	1:183:B:MET:HE1	4	0.14	0.03	0.14
(1,1935)	1:89:B:VAL:HG11	1:183:B:MET:HE2	4	0.14	0.03	0.14
(1,1935)	1:89:B:VAL:HG11	1:183:B:MET:HE3	4	0.14	0.03	0.14
(1,1935)	1:89:B:VAL:HG12	1:183:B:MET:HE1	4	0.14	0.03	0.14
(1,1935)	1:89:B:VAL:HG12	1:183:B:MET:HE2	4	0.14	0.03	0.14
(1,1935)	1:89:B:VAL:HG12	1:183:B:MET:HE3	4	0.14	0.03	0.14
(1,1935)	1:89:B:VAL:HG13	1:183:B:MET:HE1	4	0.14	0.03	0.14
(1,1935)	1:89:B:VAL:HG13	1:183:B:MET:HE2	4	0.14	0.03	0.14
(1,1935)	1:89:B:VAL:HG13	1:183:B:MET:HE3	4	0.14	0.03	0.14
(1,1935)	1:89:B:VAL:HG21	1:183:B:MET:HE1	4	0.14	0.03	0.14
(1,1935)	1:89:B:VAL:HG21	1:183:B:MET:HE2	4	0.14	0.03	0.14
(1,1935)	1:89:B:VAL:HG21	1:183:B:MET:HE3	4	0.14	0.03	0.14
(1,1935)	1:89:B:VAL:HG22	1:183:B:MET:HE1	4	0.14	0.03	0.14
(1,1935)	1:89:B:VAL:HG22	1:183:B:MET:HE2	4	0.14	0.03	0.14
(1,1935)	1:89:B:VAL:HG22	1:183:B:MET:HE3	4	0.14	0.03	0.14
(1,1935)	1:89:B:VAL:HG23	1:183:B:MET:HE1	4	0.14	0.03	0.14
(1,1935)	1:89:B:VAL:HG23	1:183:B:MET:HE2	4	0.14	0.03	0.14
(1,1935)	1:89:B:VAL:HG23	1:183:B:MET:HE3	4	0.14	0.03	0.14
(1,1552)	1:156:A:VAL:HB	1:167:A:ARG:H	4	0.14	0.04	0.12
(1,349)	1:123:A:ILE:HD11	1:196:A:TYR:HE1	4	0.13	0.01	0.13
(1,349)	1:123:A:ILE:HD11	1:196:A:TYR:HE2	4	0.13	0.01	0.13
(1,349)	1:123:A:ILE:HD12	1:196:A:TYR:HE1	4	0.13	0.01	0.13
(1,349)	1:123:A:ILE:HD12	1:196:A:TYR:HE2	4	0.13	0.01	0.13
(1,349)	1:123:A:ILE:HD13	1:196:A:TYR:HE1	4	0.13	0.01	0.13
(1,349)	1:123:A:ILE:HD13	1:196:A:TYR:HE2	4	0.13	0.01	0.13
(1,1489)	1:131:A:ILE:HA	1:133:A:SER:H	4	0.13	0.02	0.13
(1,751)	1:123:C:ILE:HG21	1:179:C:ALA:HB1	4	0.13	0.02	0.13
(1,751)	1:123:C:ILE:HG21	1:179:C:ALA:HB2	4	0.13	0.02	0.13
(1,751)	1:123:C:ILE:HG21	1:179:C:ALA:HB3	4	0.13	0.02	0.13
(1,751)	1:123:C:ILE:HG22	1:179:C:ALA:HB1	4	0.13	0.02	0.13
(1,751)	1:123:C:ILE:HG22	1:179:C:ALA:HB2	4	0.13	0.02	0.13

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,751)	1:123:C:ILE:HG22	1:179:C:ALA:HB3	4	0.13	0.02	0.13
(1,751)	1:123:C:ILE:HG23	1:179:C:ALA:HB1	4	0.13	0.02	0.13
(1,751)	1:123:C:ILE:HG23	1:179:C:ALA:HB2	4	0.13	0.02	0.13
(1,751)	1:123:C:ILE:HG23	1:179:C:ALA:HB3	4	0.13	0.02	0.13
(1,1161)	1:94:A:PHE:H	1:101:A:LEU:HD11	4	0.13	0.04	0.11
(1,1161)	1:94:A:PHE:H	1:101:A:LEU:HD12	4	0.13	0.04	0.11
(1,1161)	1:94:A:PHE:H	1:101:A:LEU:HD13	4	0.13	0.04	0.11
(1,1799)	1:151:A:GLN:HA	1:152:A:ALA:H	4	0.13	0.0	0.13
(1,1801)	1:151:C:GLN:HA	1:152:C:ALA:H	4	0.13	0.0	0.13
(1,750)	1:123:B:ILE:HG21	1:179:B:ALA:HB1	4	0.12	0.02	0.12
(1,750)	1:123:B:ILE:HG21	1:179:B:ALA:HB2	4	0.12	0.02	0.12
(1,750)	1:123:B:ILE:HG21	1:179:B:ALA:HB3	4	0.12	0.02	0.12
(1,750)	1:123:B:ILE:HG22	1:179:B:ALA:HB1	4	0.12	0.02	0.12
(1,750)	1:123:B:ILE:HG22	1:179:B:ALA:HB2	4	0.12	0.02	0.12
(1,750)	1:123:B:ILE:HG22	1:179:B:ALA:HB3	4	0.12	0.02	0.12
(1,750)	1:123:B:ILE:HG23	1:179:B:ALA:HB1	4	0.12	0.02	0.12
(1,750)	1:123:B:ILE:HG23	1:179:B:ALA:HB2	4	0.12	0.02	0.12
(1,750)	1:123:B:ILE:HG23	1:179:B:ALA:HB3	4	0.12	0.02	0.12
(1,1800)	1:151:B:GLN:HA	1:152:B:ALA:H	4	0.12	0.01	0.13
(1,373)	1:96:C:ILE:HD11	1:102:C:VAL:HB	4	0.12	0.02	0.12
(1,373)	1:96:C:ILE:HD12	1:102:C:VAL:HB	4	0.12	0.02	0.12
(1,373)	1:96:C:ILE:HD13	1:102:C:VAL:HB	4	0.12	0.02	0.12
(1,51)	1:185:A:VAL:HB	1:188:A:LEU:HD11	4	0.12	0.01	0.12
(1,51)	1:185:A:VAL:HB	1:188:A:LEU:HD12	4	0.12	0.01	0.12
(1,51)	1:185:A:VAL:HB	1:188:A:LEU:HD13	4	0.12	0.01	0.12
(1,351)	1:123:C:ILE:HD11	1:196:C:TYR:HE1	4	0.11	0.0	0.11
(1,351)	1:123:C:ILE:HD11	1:196:C:TYR:HE2	4	0.11	0.0	0.11
(1,351)	1:123:C:ILE:HD12	1:196:C:TYR:HE1	4	0.11	0.0	0.11
(1,351)	1:123:C:ILE:HD12	1:196:C:TYR:HE2	4	0.11	0.0	0.11
(1,351)	1:123:C:ILE:HD13	1:196:C:TYR:HE1	4	0.11	0.0	0.11
(1,351)	1:123:C:ILE:HD13	1:196:C:TYR:HE2	4	0.11	0.0	0.11
(1,350)	1:123:B:ILE:HD11	1:196:B:TYR:HE1	4	0.11	0.0	0.11
(1,350)	1:123:B:ILE:HD11	1:196:B:TYR:HE2	4	0.11	0.0	0.11
(1,350)	1:123:B:ILE:HD12	1:196:B:TYR:HE1	4	0.11	0.0	0.11
(1,350)	1:123:B:ILE:HD12	1:196:B:TYR:HE2	4	0.11	0.0	0.11
(1,350)	1:123:B:ILE:HD13	1:196:B:TYR:HE1	4	0.11	0.0	0.11
(1,350)	1:123:B:ILE:HD13	1:196:B:TYR:HE2	4	0.11	0.0	0.11
(1,976)	1:196:A:TYR:H	1:197:A:ILE:HG21	4	0.1	0.0	0.1
(1,976)	1:196:A:TYR:H	1:197:A:ILE:HG22	4	0.1	0.0	0.1
(1,976)	1:196:A:TYR:H	1:197:A:ILE:HG23	4	0.1	0.0	0.1
(1,1369)	1:154:B:PRO:HB3	1:155:B:ALA:H	3	0.33	0.11	0.39
(1,1370)	1:154:C:PRO:HB3	1:155:C:ALA:H	3	0.33	0.11	0.39

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1368)	1:154:A:PRO:HB3	1:155:A:ALA:H	3	0.33	0.1	0.39
(1,1775)	1:125:B:LYS:H	1:126:B:ILE:HG21	3	0.21	0.03	0.21
(1,1775)	1:125:B:LYS:H	1:126:B:ILE:HG22	3	0.21	0.03	0.21
(1,1775)	1:125:B:LYS:H	1:126:B:ILE:HG23	3	0.21	0.03	0.21
(1,1776)	1:125:C:LYS:H	1:126:C:ILE:HG21	3	0.21	0.03	0.21
(1,1776)	1:125:C:LYS:H	1:126:C:ILE:HG22	3	0.21	0.03	0.21
(1,1776)	1:125:C:LYS:H	1:126:C:ILE:HG23	3	0.21	0.03	0.21
(1,1912)	1:178:A:PRO:HB2	1:194:A:LEU:HD21	3	0.2	0.07	0.21
(1,1912)	1:178:A:PRO:HB2	1:194:A:LEU:HD22	3	0.2	0.07	0.21
(1,1912)	1:178:A:PRO:HB2	1:194:A:LEU:HD23	3	0.2	0.07	0.21
(1,1912)	1:178:A:PRO:HB3	1:194:A:LEU:HD21	3	0.2	0.07	0.21
(1,1912)	1:178:A:PRO:HB3	1:194:A:LEU:HD22	3	0.2	0.07	0.21
(1,1912)	1:178:A:PRO:HB3	1:194:A:LEU:HD23	3	0.2	0.07	0.21
(1,1878)	1:151:A:GLN:HB2	1:152:A:ALA:HA	3	0.19	0.03	0.19
(1,1878)	1:151:A:GLN:HB3	1:152:A:ALA:HA	3	0.19	0.03	0.19
(1,810)	1:176:A:GLY:H	1:177:A:ASP:HB3	3	0.18	0.03	0.17
(1,812)	1:176:C:GLY:H	1:177:C:ASP:HB3	3	0.18	0.02	0.18
(1,216)	1:96:A:ILE:HG21	1:102:A:VAL:HG11	3	0.18	0.07	0.15
(1,216)	1:96:A:ILE:HG21	1:102:A:VAL:HG12	3	0.18	0.07	0.15
(1,216)	1:96:A:ILE:HG21	1:102:A:VAL:HG13	3	0.18	0.07	0.15
(1,216)	1:96:A:ILE:HG22	1:102:A:VAL:HG11	3	0.18	0.07	0.15
(1,216)	1:96:A:ILE:HG22	1:102:A:VAL:HG12	3	0.18	0.07	0.15
(1,216)	1:96:A:ILE:HG22	1:102:A:VAL:HG13	3	0.18	0.07	0.15
(1,216)	1:96:A:ILE:HG23	1:102:A:VAL:HG11	3	0.18	0.07	0.15
(1,216)	1:96:A:ILE:HG23	1:102:A:VAL:HG12	3	0.18	0.07	0.15
(1,216)	1:96:A:ILE:HG23	1:102:A:VAL:HG13	3	0.18	0.07	0.15
(1,811)	1:176:B:GLY:H	1:177:B:ASP:HB3	3	0.18	0.02	0.17
(1,942)	1:101:A:LEU:HD11	1:188:A:LEU:HD21	3	0.18	0.0	0.18
(1,942)	1:101:A:LEU:HD11	1:188:A:LEU:HD22	3	0.18	0.0	0.18
(1,942)	1:101:A:LEU:HD11	1:188:A:LEU:HD23	3	0.18	0.0	0.18
(1,942)	1:101:A:LEU:HD12	1:188:A:LEU:HD21	3	0.18	0.0	0.18
(1,942)	1:101:A:LEU:HD12	1:188:A:LEU:HD22	3	0.18	0.0	0.18
(1,942)	1:101:A:LEU:HD12	1:188:A:LEU:HD23	3	0.18	0.0	0.18
(1,942)	1:101:A:LEU:HD13	1:188:A:LEU:HD21	3	0.18	0.0	0.18
(1,942)	1:101:A:LEU:HD13	1:188:A:LEU:HD22	3	0.18	0.0	0.18
(1,942)	1:101:A:LEU:HD13	1:188:A:LEU:HD23	3	0.18	0.0	0.18
(1,1204)	1:149:A:SER:HB2	1:151:A:GLN:H	3	0.17	0.06	0.13
(1,1204)	1:149:A:SER:HB3	1:151:A:GLN:H	3	0.17	0.06	0.13
(1,1458)	1:179:A:ALA:HA	1:180:A:PHE:H	3	0.17	0.0	0.17
(1,1459)	1:179:B:ALA:HA	1:180:B:PHE:H	3	0.17	0.0	0.17
(1,1460)	1:179:C:ALA:HA	1:180:C:PHE:H	3	0.16	0.0	0.16
(1,1526)	1:179:A:ALA:H	1:181:A:LEU:HD11	3	0.16	0.05	0.14

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1526)	1:179:A:ALA:H	1:181:A:LEU:HD12	3	0.16	0.05	0.14
(1,1526)	1:179:A:ALA:H	1:181:A:LEU:HD13	3	0.16	0.05	0.14
(1,537)	1:111:B:ILE:HD11	1:131:B:ILE:HG21	3	0.15	0.02	0.16
(1,537)	1:111:B:ILE:HD11	1:131:B:ILE:HG22	3	0.15	0.02	0.16
(1,537)	1:111:B:ILE:HD11	1:131:B:ILE:HG23	3	0.15	0.02	0.16
(1,537)	1:111:B:ILE:HD12	1:131:B:ILE:HG21	3	0.15	0.02	0.16
(1,537)	1:111:B:ILE:HD12	1:131:B:ILE:HG22	3	0.15	0.02	0.16
(1,537)	1:111:B:ILE:HD12	1:131:B:ILE:HG23	3	0.15	0.02	0.16
(1,537)	1:111:B:ILE:HD13	1:131:B:ILE:HG21	3	0.15	0.02	0.16
(1,537)	1:111:B:ILE:HD13	1:131:B:ILE:HG22	3	0.15	0.02	0.16
(1,537)	1:111:B:ILE:HD13	1:131:B:ILE:HG23	3	0.15	0.02	0.16
(1,793)	1:153:B:LYS:HE2	1:154:B:PRO:HG2	3	0.15	0.01	0.15
(1,793)	1:153:B:LYS:HE2	1:154:B:PRO:HG3	3	0.15	0.01	0.15
(1,793)	1:153:B:LYS:HE3	1:154:B:PRO:HG2	3	0.15	0.01	0.15
(1,793)	1:153:B:LYS:HE3	1:154:B:PRO:HG3	3	0.15	0.01	0.15
(1,1505)	1:93:A:THR:HG21	1:92:B:ALA:H	3	0.15	0.05	0.12
(1,1505)	1:93:A:THR:HG22	1:92:B:ALA:H	3	0.15	0.05	0.12
(1,1505)	1:93:A:THR:HG23	1:92:B:ALA:H	3	0.15	0.05	0.12
(1,794)	1:153:C:LYS:HE2	1:154:C:PRO:HG2	3	0.14	0.01	0.14
(1,794)	1:153:C:LYS:HE2	1:154:C:PRO:HG3	3	0.14	0.01	0.14
(1,794)	1:153:C:LYS:HE3	1:154:C:PRO:HG2	3	0.14	0.01	0.14
(1,794)	1:153:C:LYS:HE3	1:154:C:PRO:HG3	3	0.14	0.01	0.14
(1,1540)	1:136:B:ALA:HB1	1:140:B:LYS:H	3	0.14	0.02	0.13
(1,1540)	1:136:B:ALA:HB2	1:140:B:LYS:H	3	0.14	0.02	0.13
(1,1540)	1:136:B:ALA:HB3	1:140:B:LYS:H	3	0.14	0.02	0.13
(1,1620)	1:129:A:GLU:H	1:131:A:ILE:H	3	0.14	0.02	0.14
(1,795)	1:150:A:LEU:HD11	1:153:A:LYS:HE2	3	0.14	0.04	0.12
(1,795)	1:150:A:LEU:HD11	1:153:A:LYS:HE3	3	0.14	0.04	0.12
(1,795)	1:150:A:LEU:HD12	1:153:A:LYS:HE2	3	0.14	0.04	0.12
(1,795)	1:150:A:LEU:HD12	1:153:A:LYS:HE3	3	0.14	0.04	0.12
(1,795)	1:150:A:LEU:HD13	1:153:A:LYS:HE2	3	0.14	0.04	0.12
(1,795)	1:150:A:LEU:HD13	1:153:A:LYS:HE3	3	0.14	0.04	0.12
(1,1621)	1:129:B:GLU:H	1:131:B:ILE:H	3	0.14	0.03	0.13
(1,36)	1:102:A:VAL:HG21	1:112:A:ALA:H	3	0.13	0.02	0.14
(1,36)	1:102:A:VAL:HG22	1:112:A:ALA:H	3	0.13	0.02	0.14
(1,36)	1:102:A:VAL:HG23	1:112:A:ALA:H	3	0.13	0.02	0.14
(1,1556)	1:155:A:ALA:HB1	1:167:A:ARG:H	3	0.13	0.02	0.12
(1,1556)	1:155:A:ALA:HB2	1:167:A:ARG:H	3	0.13	0.02	0.12
(1,1556)	1:155:A:ALA:HB3	1:167:A:ARG:H	3	0.13	0.02	0.12
(1,1787)	1:96:A:ILE:HG21	1:101:A:LEU:H	3	0.13	0.02	0.13
(1,1787)	1:96:A:ILE:HG22	1:101:A:LEU:H	3	0.13	0.02	0.13
(1,1787)	1:96:A:ILE:HG23	1:101:A:LEU:H	3	0.13	0.02	0.13

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1848)	1:124:A:MET:HB2	1:197:A:ILE:HD11	3	0.13	0.02	0.12
(1,1848)	1:124:A:MET:HB2	1:197:A:ILE:HD12	3	0.13	0.02	0.12
(1,1848)	1:124:A:MET:HB2	1:197:A:ILE:HD13	3	0.13	0.02	0.12
(1,1848)	1:124:A:MET:HB3	1:197:A:ILE:HD11	3	0.13	0.02	0.12
(1,1848)	1:124:A:MET:HB3	1:197:A:ILE:HD12	3	0.13	0.02	0.12
(1,1848)	1:124:A:MET:HB3	1:197:A:ILE:HD13	3	0.13	0.02	0.12
(1,372)	1:96:B:ILE:HD11	1:102:B:VAL:HB	3	0.12	0.01	0.12
(1,372)	1:96:B:ILE:HD12	1:102:B:VAL:HB	3	0.12	0.01	0.12
(1,372)	1:96:B:ILE:HD13	1:102:B:VAL:HB	3	0.12	0.01	0.12
(1,1541)	1:136:C:ALA:HB1	1:140:C:LYS:H	3	0.12	0.02	0.11
(1,1541)	1:136:C:ALA:HB2	1:140:C:LYS:H	3	0.12	0.02	0.11
(1,1541)	1:136:C:ALA:HB3	1:140:C:LYS:H	3	0.12	0.02	0.11
(1,1574)	1:119:A:THR:H	1:192:A:VAL:HG11	3	0.11	0.01	0.11
(1,1574)	1:119:A:THR:H	1:192:A:VAL:HG12	3	0.11	0.01	0.11
(1,1574)	1:119:A:THR:H	1:192:A:VAL:HG13	3	0.11	0.01	0.11
(1,1491)	1:131:C:ILE:HA	1:133:C:SER:H	3	0.11	0.01	0.11
(1,1040)	1:137:A:LEU:HD11	1:140:A:LYS:H	3	0.11	0.0	0.11
(1,1040)	1:137:A:LEU:HD12	1:140:A:LYS:H	3	0.11	0.0	0.11
(1,1040)	1:137:A:LEU:HD13	1:140:A:LYS:H	3	0.11	0.0	0.11
(1,1442)	1:156:A:VAL:H	1:156:A:VAL:HG11	2	0.53	0.01	0.53
(1,1442)	1:156:A:VAL:H	1:156:A:VAL:HG12	2	0.53	0.01	0.53
(1,1442)	1:156:A:VAL:H	1:156:A:VAL:HG13	2	0.53	0.01	0.53
(1,1402)	1:153:A:LYS:H	1:153:A:LYS:HB3	2	0.38	0.01	0.38
(1,1403)	1:153:B:LYS:H	1:153:B:LYS:HB3	2	0.38	0.01	0.38
(1,1404)	1:153:C:LYS:H	1:153:C:LYS:HB3	2	0.38	0.01	0.38
(1,842)	1:156:A:VAL:HB	1:157:A:PRO:HD2	2	0.26	0.02	0.26
(1,1555)	1:156:A:VAL:HG11	1:167:A:ARG:H	2	0.25	0.06	0.25
(1,1555)	1:156:A:VAL:HG12	1:167:A:ARG:H	2	0.25	0.06	0.25
(1,1555)	1:156:A:VAL:HG13	1:167:A:ARG:H	2	0.25	0.06	0.25
(1,623)	1:96:A:ILE:HG21	1:138:A:THR:HB	2	0.24	0.13	0.24
(1,623)	1:96:A:ILE:HG22	1:138:A:THR:HB	2	0.24	0.13	0.24
(1,623)	1:96:A:ILE:HG23	1:138:A:THR:HB	2	0.24	0.13	0.24
(1,302)	1:161:A:LEU:HA	1:161:A:LEU:HD11	2	0.22	0.04	0.22
(1,302)	1:161:A:LEU:HA	1:161:A:LEU:HD12	2	0.22	0.04	0.22
(1,302)	1:161:A:LEU:HA	1:161:A:LEU:HD13	2	0.22	0.04	0.22
(1,1154)	1:156:A:VAL:HG11	1:158:A:THR:H	2	0.19	0.02	0.19
(1,1154)	1:156:A:VAL:HG12	1:158:A:THR:H	2	0.19	0.02	0.19
(1,1154)	1:156:A:VAL:HG13	1:158:A:THR:H	2	0.19	0.02	0.19
(1,1205)	1:149:B:SER:HB2	1:151:B:GLN:H	2	0.18	0.07	0.18
(1,1205)	1:149:B:SER:HB3	1:151:B:GLN:H	2	0.18	0.07	0.18
(1,624)	1:96:B:ILE:HG21	1:138:B:THR:HB	2	0.18	0.04	0.18
(1,624)	1:96:B:ILE:HG22	1:138:B:THR:HB	2	0.18	0.04	0.18

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,624)	1:96:B:ILE:HG23	1:138:B:THR:HB	2	0.18	0.04	0.18
(1,1206)	1:149:C:SER:HB2	1:151:C:GLN:H	2	0.18	0.06	0.18
(1,1206)	1:149:C:SER:HB3	1:151:C:GLN:H	2	0.18	0.06	0.18
(1,1528)	1:91:B:THR:HG21	1:106:B:TYR:H	2	0.17	0.04	0.17
(1,1528)	1:91:B:THR:HG22	1:106:B:TYR:H	2	0.17	0.04	0.17
(1,1528)	1:91:B:THR:HG23	1:106:B:TYR:H	2	0.17	0.04	0.17
(1,1529)	1:91:C:THR:HG21	1:106:C:TYR:H	2	0.17	0.04	0.17
(1,1529)	1:91:C:THR:HG22	1:106:C:TYR:H	2	0.17	0.04	0.17
(1,1529)	1:91:C:THR:HG23	1:106:C:TYR:H	2	0.17	0.04	0.17
(1,575)	1:193:A:PRO:HA	1:194:A:LEU:HD21	2	0.16	0.01	0.16
(1,575)	1:193:A:PRO:HA	1:194:A:LEU:HD22	2	0.16	0.01	0.16
(1,575)	1:193:A:PRO:HA	1:194:A:LEU:HD23	2	0.16	0.01	0.16
(1,1527)	1:91:A:THR:HG21	1:106:A:TYR:H	2	0.16	0.04	0.16
(1,1527)	1:91:A:THR:HG22	1:106:A:TYR:H	2	0.16	0.04	0.16
(1,1527)	1:91:A:THR:HG23	1:106:A:TYR:H	2	0.16	0.04	0.16
(1,625)	1:96:C:ILE:HG21	1:138:C:THR:HB	2	0.16	0.05	0.16
(1,625)	1:96:C:ILE:HG22	1:138:C:THR:HB	2	0.16	0.05	0.16
(1,625)	1:96:C:ILE:HG23	1:138:C:THR:HB	2	0.16	0.05	0.16
(1,1880)	1:153:A:LYS:H	1:154:A:PRO:HD2	2	0.16	0.01	0.16
(1,1880)	1:153:A:LYS:H	1:154:A:PRO:HD3	2	0.16	0.01	0.16
(1,2062)	1:153:B:LYS:H	1:154:B:PRO:HD2	2	0.16	0.01	0.16
(1,2062)	1:153:B:LYS:H	1:154:B:PRO:HD3	2	0.16	0.01	0.16
(1,2288)	1:153:C:LYS:H	1:154:C:PRO:HD2	2	0.15	0.0	0.15
(1,2288)	1:153:C:LYS:H	1:154:C:PRO:HD3	2	0.15	0.0	0.15
(1,540)	1:111:B:ILE:HG21	1:126:B:ILE:HG21	2	0.15	0.0	0.15
(1,540)	1:111:B:ILE:HG21	1:126:B:ILE:HG22	2	0.15	0.0	0.15
(1,540)	1:111:B:ILE:HG21	1:126:B:ILE:HG23	2	0.15	0.0	0.15
(1,540)	1:111:B:ILE:HG22	1:126:B:ILE:HG21	2	0.15	0.0	0.15
(1,540)	1:111:B:ILE:HG22	1:126:B:ILE:HG22	2	0.15	0.0	0.15
(1,540)	1:111:B:ILE:HG22	1:126:B:ILE:HG23	2	0.15	0.0	0.15
(1,540)	1:111:B:ILE:HG23	1:126:B:ILE:HG21	2	0.15	0.0	0.15
(1,540)	1:111:B:ILE:HG23	1:126:B:ILE:HG22	2	0.15	0.0	0.15
(1,540)	1:111:B:ILE:HG23	1:126:B:ILE:HG23	2	0.15	0.0	0.15
(1,541)	1:111:C:ILE:HG21	1:126:C:ILE:HG21	2	0.15	0.0	0.15
(1,541)	1:111:C:ILE:HG21	1:126:C:ILE:HG22	2	0.15	0.0	0.15
(1,541)	1:111:C:ILE:HG21	1:126:C:ILE:HG23	2	0.15	0.0	0.15
(1,541)	1:111:C:ILE:HG22	1:126:C:ILE:HG21	2	0.15	0.0	0.15
(1,541)	1:111:C:ILE:HG22	1:126:C:ILE:HG22	2	0.15	0.0	0.15
(1,541)	1:111:C:ILE:HG22	1:126:C:ILE:HG23	2	0.15	0.0	0.15
(1,541)	1:111:C:ILE:HG23	1:126:C:ILE:HG21	2	0.15	0.0	0.15
(1,541)	1:111:C:ILE:HG23	1:126:C:ILE:HG22	2	0.15	0.0	0.15
(1,541)	1:111:C:ILE:HG23	1:126:C:ILE:HG23	2	0.15	0.0	0.15

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,576)	1:189:A:CYS:HB2	1:194:A:LEU:HD21	2	0.14	0.02	0.14
(1,576)	1:189:A:CYS:HB2	1:194:A:LEU:HD22	2	0.14	0.02	0.14
(1,576)	1:189:A:CYS:HB2	1:194:A:LEU:HD23	2	0.14	0.02	0.14
(1,576)	1:189:A:CYS:HB3	1:194:A:LEU:HD21	2	0.14	0.02	0.14
(1,576)	1:189:A:CYS:HB3	1:194:A:LEU:HD22	2	0.14	0.02	0.14
(1,576)	1:189:A:CYS:HB3	1:194:A:LEU:HD23	2	0.14	0.02	0.14
(1,1622)	1:129:C:GLU:H	1:131:C:ILE:H	2	0.14	0.01	0.14
(1,63)	1:110:A:LEU:HD11	1:123:A:ILE:HD11	2	0.14	0.02	0.14
(1,63)	1:110:A:LEU:HD11	1:123:A:ILE:HD12	2	0.14	0.02	0.14
(1,63)	1:110:A:LEU:HD11	1:123:A:ILE:HD13	2	0.14	0.02	0.14
(1,63)	1:110:A:LEU:HD12	1:123:A:ILE:HD11	2	0.14	0.02	0.14
(1,63)	1:110:A:LEU:HD12	1:123:A:ILE:HD12	2	0.14	0.02	0.14
(1,63)	1:110:A:LEU:HD12	1:123:A:ILE:HD13	2	0.14	0.02	0.14
(1,63)	1:110:A:LEU:HD13	1:123:A:ILE:HD11	2	0.14	0.02	0.14
(1,63)	1:110:A:LEU:HD13	1:123:A:ILE:HD12	2	0.14	0.02	0.14
(1,63)	1:110:A:LEU:HD13	1:123:A:ILE:HD13	2	0.14	0.02	0.14
(1,1788)	1:96:B:ILE:HG21	1:101:B:LEU:H	2	0.14	0.02	0.14
(1,1788)	1:96:B:ILE:HG22	1:101:B:LEU:H	2	0.14	0.02	0.14
(1,1788)	1:96:B:ILE:HG23	1:101:B:LEU:H	2	0.14	0.02	0.14
(1,1789)	1:96:C:ILE:HG21	1:101:C:LEU:H	2	0.14	0.02	0.14
(1,1789)	1:96:C:ILE:HG22	1:101:C:LEU:H	2	0.14	0.02	0.14
(1,1789)	1:96:C:ILE:HG23	1:101:C:LEU:H	2	0.14	0.02	0.14
(1,536)	1:111:A:ILE:HD11	1:131:A:ILE:HG21	2	0.12	0.02	0.12
(1,536)	1:111:A:ILE:HD11	1:131:A:ILE:HG22	2	0.12	0.02	0.12
(1,536)	1:111:A:ILE:HD11	1:131:A:ILE:HG23	2	0.12	0.02	0.12
(1,536)	1:111:A:ILE:HD12	1:131:A:ILE:HG21	2	0.12	0.02	0.12
(1,536)	1:111:A:ILE:HD12	1:131:A:ILE:HG22	2	0.12	0.02	0.12
(1,536)	1:111:A:ILE:HD12	1:131:A:ILE:HG23	2	0.12	0.02	0.12
(1,536)	1:111:A:ILE:HD13	1:131:A:ILE:HG21	2	0.12	0.02	0.12
(1,536)	1:111:A:ILE:HD13	1:131:A:ILE:HG22	2	0.12	0.02	0.12
(1,536)	1:111:A:ILE:HD13	1:131:A:ILE:HG23	2	0.12	0.02	0.12
(1,650)	1:94:A:PHE:HE1	1:131:A:ILE:HG21	2	0.12	0.01	0.12
(1,650)	1:94:A:PHE:HE1	1:131:A:ILE:HG22	2	0.12	0.01	0.12
(1,650)	1:94:A:PHE:HE1	1:131:A:ILE:HG23	2	0.12	0.01	0.12
(1,650)	1:94:A:PHE:HE2	1:131:A:ILE:HG21	2	0.12	0.01	0.12
(1,650)	1:94:A:PHE:HE2	1:131:A:ILE:HG22	2	0.12	0.01	0.12
(1,650)	1:94:A:PHE:HE2	1:131:A:ILE:HG23	2	0.12	0.01	0.12
(1,693)	1:123:A:ILE:H	1:124:A:MET:HE1	2	0.12	0.02	0.12
(1,693)	1:123:A:ILE:H	1:124:A:MET:HE2	2	0.12	0.02	0.12
(1,693)	1:123:A:ILE:H	1:124:A:MET:HE3	2	0.12	0.02	0.12
(1,1237)	1:96:A:ILE:H	1:100:A:GLY:H	2	0.12	0.02	0.12
(1,1513)	1:137:C:LEU:H	1:137:C:LEU:HG	2	0.12	0.01	0.12

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1539)	1:136:A:ALA:HB1	1:140:A:LYS:H	2	0.12	0.02	0.12
(1,1539)	1:136:A:ALA:HB2	1:140:A:LYS:H	2	0.12	0.02	0.12
(1,1539)	1:136:A:ALA:HB3	1:140:A:LYS:H	2	0.12	0.02	0.12
(1,1670)	1:101:A:LEU:HD11	1:102:A:VAL:H	2	0.12	0.02	0.12
(1,1670)	1:101:A:LEU:HD12	1:102:A:VAL:H	2	0.12	0.02	0.12
(1,1670)	1:101:A:LEU:HD13	1:102:A:VAL:H	2	0.12	0.02	0.12
(1,894)	1:165:A:GLU:HB3	1:169:A:ALA:HB1	2	0.12	0.02	0.12
(1,894)	1:165:A:GLU:HB3	1:169:A:ALA:HB2	2	0.12	0.02	0.12
(1,894)	1:165:A:GLU:HB3	1:169:A:ALA:HB3	2	0.12	0.02	0.12
(1,568)	1:156:A:VAL:HB	1:161:A:LEU:HD11	2	0.12	0.01	0.12
(1,568)	1:156:A:VAL:HB	1:161:A:LEU:HD12	2	0.12	0.01	0.12
(1,568)	1:156:A:VAL:HB	1:161:A:LEU:HD13	2	0.12	0.01	0.12
(1,694)	1:123:B:ILE:H	1:124:B:MET:HE1	2	0.12	0.01	0.12
(1,694)	1:123:B:ILE:H	1:124:B:MET:HE2	2	0.12	0.01	0.12
(1,694)	1:123:B:ILE:H	1:124:B:MET:HE3	2	0.12	0.01	0.12
(1,695)	1:123:C:ILE:H	1:124:C:MET:HE1	2	0.12	0.01	0.12
(1,695)	1:123:C:ILE:H	1:124:C:MET:HE2	2	0.12	0.01	0.12
(1,695)	1:123:C:ILE:H	1:124:C:MET:HE3	2	0.12	0.01	0.12
(1,843)	1:156:B:VAL:HB	1:157:B:PRO:HD2	2	0.12	0.01	0.12
(1,844)	1:156:C:VAL:HB	1:157:C:PRO:HD2	2	0.12	0.01	0.12
(1,948)	1:185:A:VAL:HG11	1:189:A:CYS:HB2	2	0.12	0.01	0.12
(1,948)	1:185:A:VAL:HG11	1:189:A:CYS:HB3	2	0.12	0.01	0.12
(1,948)	1:185:A:VAL:HG12	1:189:A:CYS:HB2	2	0.12	0.01	0.12
(1,948)	1:185:A:VAL:HG12	1:189:A:CYS:HB3	2	0.12	0.01	0.12
(1,948)	1:185:A:VAL:HG13	1:189:A:CYS:HB2	2	0.12	0.01	0.12
(1,948)	1:185:A:VAL:HG13	1:189:A:CYS:HB3	2	0.12	0.01	0.12
(1,1734)	1:194:A:LEU:HG	1:195:A:TYR:H	2	0.12	0.01	0.12
(1,1832)	1:108:A:GLN:H	1:108:A:GLN:HG2	2	0.12	0.0	0.12
(1,1832)	1:108:A:GLN:H	1:108:A:GLN:HG3	2	0.12	0.0	0.12
(1,256)	1:111:B:ILE:H	1:124:B:MET:HE1	2	0.11	0.0	0.11
(1,256)	1:111:B:ILE:H	1:124:B:MET:HE2	2	0.11	0.0	0.11
(1,256)	1:111:B:ILE:H	1:124:B:MET:HE3	2	0.11	0.0	0.11
(1,1831)	1:106:A:TYR:HE1	1:188:C:LEU:HD11	2	0.11	0.0	0.11
(1,1831)	1:106:A:TYR:HE1	1:188:C:LEU:HD12	2	0.11	0.0	0.11
(1,1831)	1:106:A:TYR:HE1	1:188:C:LEU:HD13	2	0.11	0.0	0.11
(1,1831)	1:106:A:TYR:HE1	1:188:C:LEU:HD21	2	0.11	0.0	0.11
(1,1831)	1:106:A:TYR:HE1	1:188:C:LEU:HD22	2	0.11	0.0	0.11
(1,1831)	1:106:A:TYR:HE1	1:188:C:LEU:HD23	2	0.11	0.0	0.11
(1,1831)	1:106:A:TYR:HE2	1:188:C:LEU:HD11	2	0.11	0.0	0.11
(1,1831)	1:106:A:TYR:HE2	1:188:C:LEU:HD12	2	0.11	0.0	0.11
(1,1831)	1:106:A:TYR:HE2	1:188:C:LEU:HD13	2	0.11	0.0	0.11
(1,1831)	1:106:A:TYR:HE2	1:188:C:LEU:HD21	2	0.11	0.0	0.11

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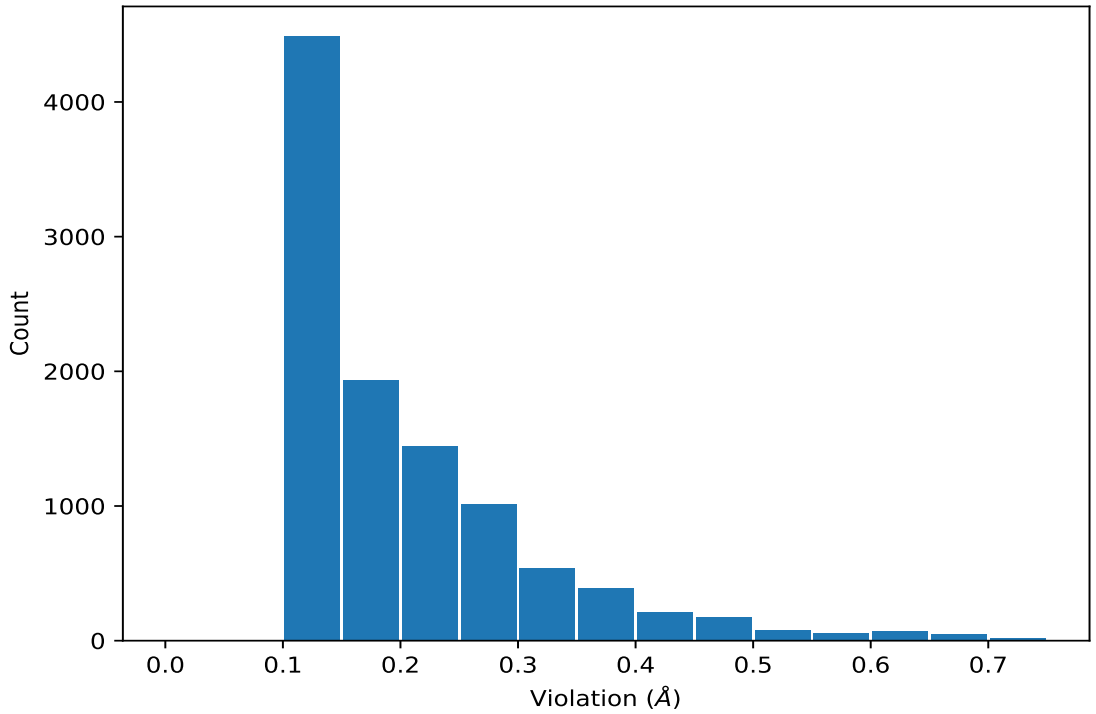
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1831)	1:106:A:TYR:HE2	1:188:C:LEU:HD22	2	0.11	0.0	0.11
(1,1831)	1:106:A:TYR:HE2	1:188:C:LEU:HD23	2	0.11	0.0	0.11
(1,257)	1:111:C:ILE:H	1:124:C:MET:HE1	2	0.11	0.0	0.11
(1,257)	1:111:C:ILE:H	1:124:C:MET:HE2	2	0.11	0.0	0.11
(1,257)	1:111:C:ILE:H	1:124:C:MET:HE3	2	0.11	0.0	0.11
(1,512)	1:102:A:VAL:HG11	1:103:A:VAL:H	2	0.11	0.0	0.11
(1,512)	1:102:A:VAL:HG12	1:103:A:VAL:H	2	0.11	0.0	0.11
(1,512)	1:102:A:VAL:HG13	1:103:A:VAL:H	2	0.11	0.0	0.11
(1,910)	1:140:B:LYS:HD2	1:197:B:ILE:HG21	2	0.11	0.0	0.11
(1,910)	1:140:B:LYS:HD2	1:197:B:ILE:HG22	2	0.11	0.0	0.11
(1,910)	1:140:B:LYS:HD2	1:197:B:ILE:HG23	2	0.11	0.0	0.11
(1,910)	1:140:B:LYS:HD3	1:197:B:ILE:HG21	2	0.11	0.0	0.11
(1,910)	1:140:B:LYS:HD3	1:197:B:ILE:HG22	2	0.11	0.0	0.11
(1,910)	1:140:B:LYS:HD3	1:197:B:ILE:HG23	2	0.11	0.0	0.11
(1,1471)	1:181:A:LEU:H	1:181:A:LEU:HD11	2	0.11	0.0	0.11
(1,1471)	1:181:A:LEU:H	1:181:A:LEU:HD12	2	0.11	0.0	0.11
(1,1471)	1:181:A:LEU:H	1:181:A:LEU:HD13	2	0.11	0.0	0.11
(1,651)	1:94:B:PHE:HE1	1:131:B:ILE:HG21	2	0.1	0.0	0.1
(1,651)	1:94:B:PHE:HE1	1:131:B:ILE:HG22	2	0.1	0.0	0.1
(1,651)	1:94:B:PHE:HE1	1:131:B:ILE:HG23	2	0.1	0.0	0.1
(1,651)	1:94:B:PHE:HE2	1:131:B:ILE:HG21	2	0.1	0.0	0.1
(1,651)	1:94:B:PHE:HE2	1:131:B:ILE:HG22	2	0.1	0.0	0.1
(1,651)	1:94:B:PHE:HE2	1:131:B:ILE:HG23	2	0.1	0.0	0.1
(1,1125)	1:153:A:LYS:H	1:154:A:PRO:HD2	2	0.1	0.0	0.1

[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)
(1,1374)	1:155:A:ALA:H	1:156:A:VAL:HG11	16	0.75
(1,1374)	1:155:A:ALA:H	1:156:A:VAL:HG12	16	0.75
(1,1374)	1:155:A:ALA:H	1:156:A:VAL:HG13	16	0.75
(1,1888)	1:156:A:VAL:HG11	1:157:A:PRO:HB2	5	0.74
(1,1888)	1:156:A:VAL:HG11	1:157:A:PRO:HB3	5	0.74
(1,1888)	1:156:A:VAL:HG12	1:157:A:PRO:HB2	5	0.74
(1,1888)	1:156:A:VAL:HG12	1:157:A:PRO:HB3	5	0.74
(1,1888)	1:156:A:VAL:HG13	1:157:A:PRO:HB2	5	0.74
(1,1888)	1:156:A:VAL:HG13	1:157:A:PRO:HB3	5	0.74
(1,1888)	1:156:A:VAL:HG11	1:157:A:PRO:HB2	14	0.74
(1,1888)	1:156:A:VAL:HG11	1:157:A:PRO:HB3	14	0.74
(1,1888)	1:156:A:VAL:HG12	1:157:A:PRO:HB2	14	0.74
(1,1888)	1:156:A:VAL:HG12	1:157:A:PRO:HB3	14	0.74
(1,1888)	1:156:A:VAL:HG13	1:157:A:PRO:HB2	14	0.74
(1,1888)	1:156:A:VAL:HG13	1:157:A:PRO:HB3	14	0.74
(1,1888)	1:156:A:VAL:HG11	1:157:A:PRO:HB2	2	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1888)	1:156:A:VAL:HG11	1:157:A:PRO:HB3	2	0.7
(1,1888)	1:156:A:VAL:HG12	1:157:A:PRO:HB2	2	0.7
(1,1888)	1:156:A:VAL:HG12	1:157:A:PRO:HB3	2	0.7
(1,1888)	1:156:A:VAL:HG13	1:157:A:PRO:HB2	2	0.7
(1,1888)	1:156:A:VAL:HG13	1:157:A:PRO:HB3	2	0.7
(1,1888)	1:156:A:VAL:HG11	1:157:A:PRO:HB2	3	0.7
(1,1888)	1:156:A:VAL:HG11	1:157:A:PRO:HB3	3	0.7
(1,1888)	1:156:A:VAL:HG12	1:157:A:PRO:HB2	3	0.7
(1,1888)	1:156:A:VAL:HG12	1:157:A:PRO:HB3	3	0.7
(1,1888)	1:156:A:VAL:HG13	1:157:A:PRO:HB2	3	0.7
(1,1888)	1:156:A:VAL:HG13	1:157:A:PRO:HB3	3	0.7
(1,1888)	1:156:A:VAL:HG11	1:157:A:PRO:HB2	15	0.7
(1,1888)	1:156:A:VAL:HG11	1:157:A:PRO:HB3	15	0.7
(1,1888)	1:156:A:VAL:HG12	1:157:A:PRO:HB2	15	0.7
(1,1888)	1:156:A:VAL:HG12	1:157:A:PRO:HB3	15	0.7
(1,1888)	1:156:A:VAL:HG13	1:157:A:PRO:HB2	15	0.7
(1,1888)	1:156:A:VAL:HG13	1:157:A:PRO:HB3	15	0.7
(1,1888)	1:156:A:VAL:HG11	1:157:A:PRO:HB2	1	0.69
(1,1888)	1:156:A:VAL:HG11	1:157:A:PRO:HB3	1	0.69
(1,1888)	1:156:A:VAL:HG12	1:157:A:PRO:HB2	1	0.69
(1,1888)	1:156:A:VAL:HG12	1:157:A:PRO:HB3	1	0.69
(1,1888)	1:156:A:VAL:HG13	1:157:A:PRO:HB2	1	0.69
(1,1888)	1:156:A:VAL:HG13	1:157:A:PRO:HB3	1	0.69
(1,1676)	1:94:A:PHE:H	1:102:A:VAL:HG11	1	0.69
(1,1676)	1:94:A:PHE:H	1:102:A:VAL:HG12	1	0.69
(1,1676)	1:94:A:PHE:H	1:102:A:VAL:HG13	1	0.69
(1,1888)	1:156:A:VAL:HG11	1:157:A:PRO:HB2	4	0.68
(1,1888)	1:156:A:VAL:HG11	1:157:A:PRO:HB3	4	0.68
(1,1888)	1:156:A:VAL:HG12	1:157:A:PRO:HB2	4	0.68
(1,1888)	1:156:A:VAL:HG12	1:157:A:PRO:HB3	4	0.68
(1,1888)	1:156:A:VAL:HG13	1:157:A:PRO:HB2	4	0.68
(1,1888)	1:156:A:VAL:HG13	1:157:A:PRO:HB3	4	0.68
(1,1888)	1:156:A:VAL:HG11	1:157:A:PRO:HB2	9	0.68
(1,1888)	1:156:A:VAL:HG11	1:157:A:PRO:HB3	9	0.68
(1,1888)	1:156:A:VAL:HG12	1:157:A:PRO:HB2	9	0.68
(1,1888)	1:156:A:VAL:HG12	1:157:A:PRO:HB3	9	0.68
(1,1888)	1:156:A:VAL:HG13	1:157:A:PRO:HB2	9	0.68
(1,1888)	1:156:A:VAL:HG13	1:157:A:PRO:HB3	9	0.68
(1,1888)	1:156:A:VAL:HG11	1:157:A:PRO:HB2	6	0.65
(1,1888)	1:156:A:VAL:HG11	1:157:A:PRO:HB3	6	0.65
(1,1888)	1:156:A:VAL:HG12	1:157:A:PRO:HB2	6	0.65
(1,1888)	1:156:A:VAL:HG12	1:157:A:PRO:HB3	6	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1888)	1:156:A:VAL:HG13	1:157:A:PRO:HB2	6	0.65
(1,1888)	1:156:A:VAL:HG13	1:157:A:PRO:HB3	6	0.65
(1,1445)	1:155:C:ALA:HA	1:156:C:VAL:H	11	0.65
(1,1444)	1:155:B:ALA:HA	1:156:B:VAL:H	11	0.65
(1,1443)	1:155:A:ALA:HA	1:156:A:VAL:H	11	0.65
(1,1888)	1:156:A:VAL:HG11	1:157:A:PRO:HB2	8	0.64
(1,1888)	1:156:A:VAL:HG11	1:157:A:PRO:HB3	8	0.64
(1,1888)	1:156:A:VAL:HG12	1:157:A:PRO:HB2	8	0.64
(1,1888)	1:156:A:VAL:HG12	1:157:A:PRO:HB3	8	0.64
(1,1888)	1:156:A:VAL:HG13	1:157:A:PRO:HB2	8	0.64
(1,1888)	1:156:A:VAL:HG13	1:157:A:PRO:HB3	8	0.64
(1,1888)	1:156:A:VAL:HG11	1:157:A:PRO:HB2	10	0.64
(1,1888)	1:156:A:VAL:HG11	1:157:A:PRO:HB3	10	0.64
(1,1888)	1:156:A:VAL:HG12	1:157:A:PRO:HB2	10	0.64
(1,1888)	1:156:A:VAL:HG12	1:157:A:PRO:HB3	10	0.64
(1,1888)	1:156:A:VAL:HG13	1:157:A:PRO:HB2	10	0.64
(1,1888)	1:156:A:VAL:HG13	1:157:A:PRO:HB3	10	0.64
(1,1888)	1:156:A:VAL:HG11	1:157:A:PRO:HB2	13	0.64
(1,1888)	1:156:A:VAL:HG11	1:157:A:PRO:HB3	13	0.64
(1,1888)	1:156:A:VAL:HG12	1:157:A:PRO:HB2	13	0.64
(1,1888)	1:156:A:VAL:HG12	1:157:A:PRO:HB3	13	0.64
(1,1888)	1:156:A:VAL:HG13	1:157:A:PRO:HB2	13	0.64
(1,1888)	1:156:A:VAL:HG13	1:157:A:PRO:HB3	13	0.64
(1,1888)	1:156:A:VAL:HG11	1:157:A:PRO:HB2	18	0.64
(1,1888)	1:156:A:VAL:HG11	1:157:A:PRO:HB3	18	0.64
(1,1888)	1:156:A:VAL:HG12	1:157:A:PRO:HB2	18	0.64
(1,1888)	1:156:A:VAL:HG12	1:157:A:PRO:HB3	18	0.64
(1,1888)	1:156:A:VAL:HG13	1:157:A:PRO:HB2	18	0.64
(1,1888)	1:156:A:VAL:HG13	1:157:A:PRO:HB3	18	0.64
(1,1888)	1:156:A:VAL:HG11	1:157:A:PRO:HB2	19	0.64
(1,1888)	1:156:A:VAL:HG11	1:157:A:PRO:HB3	19	0.64
(1,1888)	1:156:A:VAL:HG12	1:157:A:PRO:HB2	19	0.64
(1,1888)	1:156:A:VAL:HG12	1:157:A:PRO:HB3	19	0.64
(1,1888)	1:156:A:VAL:HG13	1:157:A:PRO:HB2	19	0.64
(1,1888)	1:156:A:VAL:HG13	1:157:A:PRO:HB3	19	0.64
(1,1888)	1:156:A:VAL:HG11	1:157:A:PRO:HB2	20	0.64
(1,1888)	1:156:A:VAL:HG11	1:157:A:PRO:HB3	20	0.64
(1,1888)	1:156:A:VAL:HG12	1:157:A:PRO:HB2	20	0.64
(1,1888)	1:156:A:VAL:HG12	1:157:A:PRO:HB3	20	0.64
(1,1888)	1:156:A:VAL:HG13	1:157:A:PRO:HB2	20	0.64
(1,1888)	1:156:A:VAL:HG13	1:157:A:PRO:HB3	20	0.64
(1,1676)	1:94:A:PHE:H	1:102:A:VAL:HG11	12	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1676)	1:94:A:PHE:H	1:102:A:VAL:HG12	12	0.64
(1,1676)	1:94:A:PHE:H	1:102:A:VAL:HG13	12	0.64
(1,1445)	1:155:C:ALA:HA	1:156:C:VAL:H	12	0.64
(1,1444)	1:155:B:ALA:HA	1:156:B:VAL:H	12	0.64
(1,1443)	1:155:A:ALA:HA	1:156:A:VAL:H	12	0.64
(1,1445)	1:155:C:ALA:HA	1:156:C:VAL:H	7	0.63
(1,1444)	1:155:B:ALA:HA	1:156:B:VAL:H	7	0.63
(1,1888)	1:156:A:VAL:HG11	1:157:A:PRO:HB2	17	0.62
(1,1888)	1:156:A:VAL:HG11	1:157:A:PRO:HB3	17	0.62
(1,1888)	1:156:A:VAL:HG12	1:157:A:PRO:HB2	17	0.62
(1,1888)	1:156:A:VAL:HG12	1:157:A:PRO:HB3	17	0.62
(1,1888)	1:156:A:VAL:HG13	1:157:A:PRO:HB2	17	0.62
(1,1888)	1:156:A:VAL:HG13	1:157:A:PRO:HB3	17	0.62
(1,1445)	1:155:C:ALA:HA	1:156:C:VAL:H	13	0.62
(1,1445)	1:155:C:ALA:HA	1:156:C:VAL:H	19	0.62
(1,1445)	1:155:C:ALA:HA	1:156:C:VAL:H	20	0.62
(1,1444)	1:155:B:ALA:HA	1:156:B:VAL:H	13	0.62
(1,1443)	1:155:A:ALA:HA	1:156:A:VAL:H	13	0.62
(1,1887)	1:156:A:VAL:HB	1:157:A:PRO:HD2	7	0.61
(1,1887)	1:156:A:VAL:HB	1:157:A:PRO:HD3	7	0.61
(1,1445)	1:155:C:ALA:HA	1:156:C:VAL:H	17	0.61
(1,1444)	1:155:B:ALA:HA	1:156:B:VAL:H	17	0.61
(1,1444)	1:155:B:ALA:HA	1:156:B:VAL:H	19	0.61
(1,1444)	1:155:B:ALA:HA	1:156:B:VAL:H	20	0.61
(1,1443)	1:155:A:ALA:HA	1:156:A:VAL:H	7	0.61
(1,1443)	1:155:A:ALA:HA	1:156:A:VAL:H	17	0.61
(1,730)	1:155:C:ALA:HB1	1:157:C:PRO:HD2	14	0.61
(1,730)	1:155:C:ALA:HB2	1:157:C:PRO:HD2	14	0.61
(1,730)	1:155:C:ALA:HB3	1:157:C:PRO:HD2	14	0.61
(1,729)	1:155:B:ALA:HB1	1:157:B:PRO:HD2	14	0.61
(1,729)	1:155:B:ALA:HB2	1:157:B:PRO:HD2	14	0.61
(1,729)	1:155:B:ALA:HB3	1:157:B:PRO:HD2	14	0.61
(1,728)	1:155:A:ALA:HB1	1:157:A:PRO:HD2	14	0.61
(1,728)	1:155:A:ALA:HB2	1:157:A:PRO:HD2	14	0.61
(1,728)	1:155:A:ALA:HB3	1:157:A:PRO:HD2	14	0.61
(1,1887)	1:156:A:VAL:HB	1:157:A:PRO:HD2	16	0.6
(1,1887)	1:156:A:VAL:HB	1:157:A:PRO:HD3	16	0.6
(1,1443)	1:155:A:ALA:HA	1:156:A:VAL:H	19	0.6
(1,1443)	1:155:A:ALA:HA	1:156:A:VAL:H	20	0.6
(1,845)	1:156:A:VAL:HB	1:157:A:PRO:HD3	16	0.59
(1,1445)	1:155:C:ALA:HA	1:156:C:VAL:H	15	0.58
(1,1444)	1:155:B:ALA:HA	1:156:B:VAL:H	15	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1443)	1:155:A:ALA:HA	1:156:A:VAL:H	15	0.58
(1,26)	1:109:A:LEU:HD21	1:110:A:LEU:H	11	0.58
(1,26)	1:109:A:LEU:HD22	1:110:A:LEU:H	11	0.58
(1,26)	1:109:A:LEU:HD23	1:110:A:LEU:H	11	0.58
(1,26)	1:109:A:LEU:HD21	1:110:A:LEU:H	2	0.57
(1,26)	1:109:A:LEU:HD22	1:110:A:LEU:H	2	0.57
(1,26)	1:109:A:LEU:HD23	1:110:A:LEU:H	2	0.57
(1,26)	1:109:A:LEU:HD21	1:110:A:LEU:H	3	0.57
(1,26)	1:109:A:LEU:HD22	1:110:A:LEU:H	3	0.57
(1,26)	1:109:A:LEU:HD23	1:110:A:LEU:H	3	0.57
(1,26)	1:109:A:LEU:HD21	1:110:A:LEU:H	4	0.57
(1,26)	1:109:A:LEU:HD22	1:110:A:LEU:H	4	0.57
(1,26)	1:109:A:LEU:HD23	1:110:A:LEU:H	4	0.57
(1,26)	1:109:A:LEU:HD21	1:110:A:LEU:H	9	0.57
(1,26)	1:109:A:LEU:HD22	1:110:A:LEU:H	9	0.57
(1,26)	1:109:A:LEU:HD23	1:110:A:LEU:H	9	0.57
(1,845)	1:156:A:VAL:HB	1:157:A:PRO:HD3	7	0.56
(1,728)	1:155:A:ALA:HB1	1:157:A:PRO:HD2	12	0.56
(1,728)	1:155:A:ALA:HB2	1:157:A:PRO:HD2	12	0.56
(1,728)	1:155:A:ALA:HB3	1:157:A:PRO:HD2	12	0.56
(1,26)	1:109:A:LEU:HD21	1:110:A:LEU:H	1	0.56
(1,26)	1:109:A:LEU:HD22	1:110:A:LEU:H	1	0.56
(1,26)	1:109:A:LEU:HD23	1:110:A:LEU:H	1	0.56
(1,26)	1:109:A:LEU:HD21	1:110:A:LEU:H	12	0.56
(1,26)	1:109:A:LEU:HD22	1:110:A:LEU:H	12	0.56
(1,26)	1:109:A:LEU:HD23	1:110:A:LEU:H	12	0.56
(1,26)	1:109:A:LEU:HD21	1:110:A:LEU:H	20	0.56
(1,26)	1:109:A:LEU:HD22	1:110:A:LEU:H	20	0.56
(1,26)	1:109:A:LEU:HD23	1:110:A:LEU:H	20	0.56
(1,1445)	1:155:C:ALA:HA	1:156:C:VAL:H	16	0.55
(1,1444)	1:155:B:ALA:HA	1:156:B:VAL:H	16	0.55
(1,847)	1:156:C:VAL:HB	1:157:C:PRO:HD3	16	0.55
(1,846)	1:156:B:VAL:HB	1:157:B:PRO:HD3	16	0.55
(1,215)	1:101:A:LEU:HD21	1:103:A:VAL:HG11	2	0.55
(1,215)	1:101:A:LEU:HD21	1:103:A:VAL:HG12	2	0.55
(1,215)	1:101:A:LEU:HD21	1:103:A:VAL:HG13	2	0.55
(1,215)	1:101:A:LEU:HD22	1:103:A:VAL:HG11	2	0.55
(1,215)	1:101:A:LEU:HD22	1:103:A:VAL:HG12	2	0.55
(1,215)	1:101:A:LEU:HD22	1:103:A:VAL:HG13	2	0.55
(1,215)	1:101:A:LEU:HD23	1:103:A:VAL:HG11	2	0.55
(1,215)	1:101:A:LEU:HD23	1:103:A:VAL:HG12	2	0.55
(1,215)	1:101:A:LEU:HD23	1:103:A:VAL:HG13	2	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,26)	1:109:A:LEU:HD21	1:110:A:LEU:H	13	0.55
(1,26)	1:109:A:LEU:HD22	1:110:A:LEU:H	13	0.55
(1,26)	1:109:A:LEU:HD23	1:110:A:LEU:H	13	0.55
(1,26)	1:109:A:LEU:HD21	1:110:A:LEU:H	16	0.55
(1,26)	1:109:A:LEU:HD22	1:110:A:LEU:H	16	0.55
(1,26)	1:109:A:LEU:HD23	1:110:A:LEU:H	16	0.55
(1,1443)	1:155:A:ALA:HA	1:156:A:VAL:H	16	0.54
(1,1442)	1:156:A:VAL:H	1:156:A:VAL:HG11	7	0.54
(1,1442)	1:156:A:VAL:H	1:156:A:VAL:HG12	7	0.54
(1,1442)	1:156:A:VAL:H	1:156:A:VAL:HG13	7	0.54
(1,847)	1:156:C:VAL:HB	1:157:C:PRO:HD3	7	0.54
(1,846)	1:156:B:VAL:HB	1:157:B:PRO:HD3	7	0.54
(1,205)	1:111:A:ILE:HD11	1:137:A:LEU:HD11	8	0.54
(1,205)	1:111:A:ILE:HD11	1:137:A:LEU:HD12	8	0.54
(1,205)	1:111:A:ILE:HD11	1:137:A:LEU:HD13	8	0.54
(1,205)	1:111:A:ILE:HD12	1:137:A:LEU:HD11	8	0.54
(1,205)	1:111:A:ILE:HD12	1:137:A:LEU:HD12	8	0.54
(1,205)	1:111:A:ILE:HD12	1:137:A:LEU:HD13	8	0.54
(1,205)	1:111:A:ILE:HD13	1:137:A:LEU:HD11	8	0.54
(1,205)	1:111:A:ILE:HD13	1:137:A:LEU:HD12	8	0.54
(1,205)	1:111:A:ILE:HD13	1:137:A:LEU:HD13	8	0.54
(1,2298)	1:156:C:VAL:HB	1:157:C:PRO:HD2	7	0.53
(1,2298)	1:156:C:VAL:HB	1:157:C:PRO:HD3	7	0.53
(1,2072)	1:156:B:VAL:HB	1:157:B:PRO:HD2	7	0.53
(1,2072)	1:156:B:VAL:HB	1:157:B:PRO:HD3	7	0.53
(1,2298)	1:156:C:VAL:HB	1:157:C:PRO:HD2	16	0.52
(1,2298)	1:156:C:VAL:HB	1:157:C:PRO:HD3	16	0.52
(1,2072)	1:156:B:VAL:HB	1:157:B:PRO:HD2	16	0.52
(1,2072)	1:156:B:VAL:HB	1:157:B:PRO:HD3	16	0.52
(1,1442)	1:156:A:VAL:H	1:156:A:VAL:HG11	16	0.52
(1,1442)	1:156:A:VAL:H	1:156:A:VAL:HG12	16	0.52
(1,1442)	1:156:A:VAL:H	1:156:A:VAL:HG13	16	0.52
(1,847)	1:156:C:VAL:HB	1:157:C:PRO:HD3	11	0.52
(1,847)	1:156:C:VAL:HB	1:157:C:PRO:HD3	12	0.52
(1,846)	1:156:B:VAL:HB	1:157:B:PRO:HD3	11	0.52
(1,846)	1:156:B:VAL:HB	1:157:B:PRO:HD3	12	0.52
(1,730)	1:155:C:ALA:HB1	1:157:C:PRO:HD2	12	0.51
(1,730)	1:155:C:ALA:HB2	1:157:C:PRO:HD2	12	0.51
(1,730)	1:155:C:ALA:HB3	1:157:C:PRO:HD2	12	0.51
(1,729)	1:155:B:ALA:HB1	1:157:B:PRO:HD2	12	0.51
(1,729)	1:155:B:ALA:HB2	1:157:B:PRO:HD2	12	0.51
(1,729)	1:155:B:ALA:HB3	1:157:B:PRO:HD2	12	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,728)	1:155:A:ALA:HB1	1:157:A:PRO:HD2	11	0.51
(1,728)	1:155:A:ALA:HB2	1:157:A:PRO:HD2	11	0.51
(1,728)	1:155:A:ALA:HB3	1:157:A:PRO:HD2	11	0.51
(1,215)	1:101:A:LEU:HD21	1:103:A:VAL:HG11	15	0.5
(1,215)	1:101:A:LEU:HD21	1:103:A:VAL:HG12	15	0.5
(1,215)	1:101:A:LEU:HD21	1:103:A:VAL:HG13	15	0.5
(1,215)	1:101:A:LEU:HD22	1:103:A:VAL:HG11	15	0.5
(1,215)	1:101:A:LEU:HD22	1:103:A:VAL:HG12	15	0.5
(1,215)	1:101:A:LEU:HD22	1:103:A:VAL:HG13	15	0.5
(1,215)	1:101:A:LEU:HD23	1:103:A:VAL:HG11	15	0.5
(1,215)	1:101:A:LEU:HD23	1:103:A:VAL:HG12	15	0.5
(1,215)	1:101:A:LEU:HD23	1:103:A:VAL:HG13	15	0.5
(1,205)	1:111:A:ILE:HD11	1:137:A:LEU:HD11	2	0.5
(1,205)	1:111:A:ILE:HD11	1:137:A:LEU:HD12	2	0.5
(1,205)	1:111:A:ILE:HD11	1:137:A:LEU:HD13	2	0.5
(1,205)	1:111:A:ILE:HD12	1:137:A:LEU:HD11	2	0.5
(1,205)	1:111:A:ILE:HD12	1:137:A:LEU:HD12	2	0.5
(1,205)	1:111:A:ILE:HD12	1:137:A:LEU:HD13	2	0.5
(1,205)	1:111:A:ILE:HD13	1:137:A:LEU:HD11	2	0.5
(1,205)	1:111:A:ILE:HD13	1:137:A:LEU:HD12	2	0.5
(1,205)	1:111:A:ILE:HD13	1:137:A:LEU:HD13	2	0.5
(1,205)	1:111:A:ILE:HD11	1:137:A:LEU:HD11	9	0.5
(1,205)	1:111:A:ILE:HD11	1:137:A:LEU:HD12	9	0.5
(1,205)	1:111:A:ILE:HD11	1:137:A:LEU:HD13	9	0.5
(1,205)	1:111:A:ILE:HD12	1:137:A:LEU:HD11	9	0.5
(1,205)	1:111:A:ILE:HD12	1:137:A:LEU:HD12	9	0.5
(1,205)	1:111:A:ILE:HD12	1:137:A:LEU:HD13	9	0.5
(1,205)	1:111:A:ILE:HD13	1:137:A:LEU:HD11	9	0.5
(1,205)	1:111:A:ILE:HD13	1:137:A:LEU:HD12	9	0.5
(1,205)	1:111:A:ILE:HD13	1:137:A:LEU:HD13	9	0.5
(1,205)	1:111:A:ILE:HD11	1:137:A:LEU:HD11	11	0.5
(1,205)	1:111:A:ILE:HD11	1:137:A:LEU:HD12	11	0.5
(1,205)	1:111:A:ILE:HD11	1:137:A:LEU:HD13	11	0.5
(1,205)	1:111:A:ILE:HD12	1:137:A:LEU:HD11	11	0.5
(1,205)	1:111:A:ILE:HD12	1:137:A:LEU:HD12	11	0.5
(1,205)	1:111:A:ILE:HD12	1:137:A:LEU:HD13	11	0.5
(1,205)	1:111:A:ILE:HD13	1:137:A:LEU:HD11	11	0.5
(1,205)	1:111:A:ILE:HD13	1:137:A:LEU:HD12	11	0.5
(1,205)	1:111:A:ILE:HD13	1:137:A:LEU:HD13	11	0.5
(1,124)	1:96:A:ILE:H	1:101:A:LEU:HD21	9	0.5
(1,124)	1:96:A:ILE:H	1:101:A:LEU:HD22	9	0.5
(1,124)	1:96:A:ILE:H	1:101:A:LEU:HD23	9	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,124)	1:96:A:ILE:H	1:101:A:LEU:HD21	19	0.5
(1,124)	1:96:A:ILE:H	1:101:A:LEU:HD22	19	0.5
(1,124)	1:96:A:ILE:H	1:101:A:LEU:HD23	19	0.5
(1,1443)	1:155:A:ALA:HA	1:156:A:VAL:H	10	0.49
(1,863)	1:153:C:LYS:HA	1:154:C:PRO:HD3	9	0.49
(1,863)	1:153:C:LYS:HA	1:154:C:PRO:HD3	16	0.49
(1,862)	1:153:B:LYS:HA	1:154:B:PRO:HD3	9	0.49
(1,862)	1:153:B:LYS:HA	1:154:B:PRO:HD3	16	0.49
(1,861)	1:153:A:LYS:HA	1:154:A:PRO:HD3	9	0.49
(1,861)	1:153:A:LYS:HA	1:154:A:PRO:HD3	16	0.49
(1,205)	1:111:A:ILE:HD11	1:137:A:LEU:HD11	17	0.49
(1,205)	1:111:A:ILE:HD11	1:137:A:LEU:HD12	17	0.49
(1,205)	1:111:A:ILE:HD11	1:137:A:LEU:HD13	17	0.49
(1,205)	1:111:A:ILE:HD12	1:137:A:LEU:HD11	17	0.49
(1,205)	1:111:A:ILE:HD12	1:137:A:LEU:HD12	17	0.49
(1,205)	1:111:A:ILE:HD12	1:137:A:LEU:HD13	17	0.49
(1,205)	1:111:A:ILE:HD13	1:137:A:LEU:HD11	17	0.49
(1,205)	1:111:A:ILE:HD13	1:137:A:LEU:HD12	17	0.49
(1,205)	1:111:A:ILE:HD13	1:137:A:LEU:HD13	17	0.49
(1,138)	1:192:A:VAL:HG21	1:135:B:GLU:HG2	13	0.49
(1,138)	1:192:A:VAL:HG21	1:135:B:GLU:HG3	13	0.49
(1,138)	1:192:A:VAL:HG22	1:135:B:GLU:HG2	13	0.49
(1,138)	1:192:A:VAL:HG22	1:135:B:GLU:HG3	13	0.49
(1,138)	1:192:A:VAL:HG23	1:135:B:GLU:HG2	13	0.49
(1,138)	1:192:A:VAL:HG23	1:135:B:GLU:HG3	13	0.49
(1,1445)	1:155:C:ALA:HA	1:156:C:VAL:H	10	0.48
(1,1445)	1:155:C:ALA:HA	1:156:C:VAL:H	18	0.48
(1,1444)	1:155:B:ALA:HA	1:156:B:VAL:H	10	0.48
(1,1364)	1:154:C:PRO:HA	1:155:C:ALA:H	15	0.48
(1,1363)	1:154:B:PRO:HA	1:155:B:ALA:H	15	0.48
(1,1362)	1:154:A:PRO:HA	1:155:A:ALA:H	15	0.48
(1,1032)	1:152:C:ALA:H	1:153:C:LYS:H	15	0.48
(1,1031)	1:152:B:ALA:H	1:153:B:LYS:H	15	0.48
(1,1030)	1:152:A:ALA:H	1:153:A:LYS:H	15	0.48
(1,205)	1:111:A:ILE:HD11	1:137:A:LEU:HD11	18	0.48
(1,205)	1:111:A:ILE:HD11	1:137:A:LEU:HD12	18	0.48
(1,205)	1:111:A:ILE:HD11	1:137:A:LEU:HD13	18	0.48
(1,205)	1:111:A:ILE:HD12	1:137:A:LEU:HD11	18	0.48
(1,205)	1:111:A:ILE:HD12	1:137:A:LEU:HD12	18	0.48
(1,205)	1:111:A:ILE:HD12	1:137:A:LEU:HD13	18	0.48
(1,205)	1:111:A:ILE:HD13	1:137:A:LEU:HD11	18	0.48
(1,205)	1:111:A:ILE:HD13	1:137:A:LEU:HD12	18	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,205)	1:111:A:ILE:HD13	1:137:A:LEU:HD13	18	0.48
(1,124)	1:96:A:ILE:H	1:101:A:LEU:HD21	7	0.48
(1,124)	1:96:A:ILE:H	1:101:A:LEU:HD22	7	0.48
(1,124)	1:96:A:ILE:H	1:101:A:LEU:HD23	7	0.48
(1,1444)	1:155:B:ALA:HA	1:156:B:VAL:H	18	0.47
(1,1443)	1:155:A:ALA:HA	1:156:A:VAL:H	18	0.47
(1,958)	1:187:A:THR:HA	1:188:A:LEU:HD11	6	0.47
(1,958)	1:187:A:THR:HA	1:188:A:LEU:HD12	6	0.47
(1,958)	1:187:A:THR:HA	1:188:A:LEU:HD13	6	0.47
(1,863)	1:153:C:LYS:HA	1:154:C:PRO:HD3	8	0.47
(1,862)	1:153:B:LYS:HA	1:154:B:PRO:HD3	1	0.47
(1,862)	1:153:B:LYS:HA	1:154:B:PRO:HD3	8	0.47
(1,861)	1:153:A:LYS:HA	1:154:A:PRO:HD3	1	0.47
(1,861)	1:153:A:LYS:HA	1:154:A:PRO:HD3	8	0.47
(1,861)	1:153:A:LYS:HA	1:154:A:PRO:HD3	11	0.47
(1,124)	1:96:A:ILE:H	1:101:A:LEU:HD21	5	0.47
(1,124)	1:96:A:ILE:H	1:101:A:LEU:HD22	5	0.47
(1,124)	1:96:A:ILE:H	1:101:A:LEU:HD23	5	0.47
(1,124)	1:96:A:ILE:H	1:101:A:LEU:HD21	20	0.47
(1,124)	1:96:A:ILE:H	1:101:A:LEU:HD22	20	0.47
(1,124)	1:96:A:ILE:H	1:101:A:LEU:HD23	20	0.47
(1,1676)	1:94:A:PHE:H	1:102:A:VAL:HG11	13	0.46
(1,1676)	1:94:A:PHE:H	1:102:A:VAL:HG12	13	0.46
(1,1676)	1:94:A:PHE:H	1:102:A:VAL:HG13	13	0.46
(1,1445)	1:155:C:ALA:HA	1:156:C:VAL:H	2	0.46
(1,1444)	1:155:B:ALA:HA	1:156:B:VAL:H	2	0.46
(1,1443)	1:155:A:ALA:HA	1:156:A:VAL:H	2	0.46
(1,863)	1:153:C:LYS:HA	1:154:C:PRO:HD3	1	0.46
(1,863)	1:153:C:LYS:HA	1:154:C:PRO:HD3	2	0.46
(1,863)	1:153:C:LYS:HA	1:154:C:PRO:HD3	3	0.46
(1,863)	1:153:C:LYS:HA	1:154:C:PRO:HD3	4	0.46
(1,863)	1:153:C:LYS:HA	1:154:C:PRO:HD3	6	0.46
(1,863)	1:153:C:LYS:HA	1:154:C:PRO:HD3	10	0.46
(1,863)	1:153:C:LYS:HA	1:154:C:PRO:HD3	11	0.46
(1,863)	1:153:C:LYS:HA	1:154:C:PRO:HD3	12	0.46
(1,863)	1:153:C:LYS:HA	1:154:C:PRO:HD3	13	0.46
(1,863)	1:153:C:LYS:HA	1:154:C:PRO:HD3	18	0.46
(1,863)	1:153:C:LYS:HA	1:154:C:PRO:HD3	19	0.46
(1,862)	1:153:B:LYS:HA	1:154:B:PRO:HD3	2	0.46
(1,862)	1:153:B:LYS:HA	1:154:B:PRO:HD3	3	0.46
(1,862)	1:153:B:LYS:HA	1:154:B:PRO:HD3	4	0.46
(1,862)	1:153:B:LYS:HA	1:154:B:PRO:HD3	6	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,862)	1:153:B:LYS:HA	1:154:B:PRO:HD3	10	0.46
(1,862)	1:153:B:LYS:HA	1:154:B:PRO:HD3	11	0.46
(1,862)	1:153:B:LYS:HA	1:154:B:PRO:HD3	12	0.46
(1,862)	1:153:B:LYS:HA	1:154:B:PRO:HD3	13	0.46
(1,862)	1:153:B:LYS:HA	1:154:B:PRO:HD3	18	0.46
(1,862)	1:153:B:LYS:HA	1:154:B:PRO:HD3	19	0.46
(1,861)	1:153:A:LYS:HA	1:154:A:PRO:HD3	2	0.46
(1,861)	1:153:A:LYS:HA	1:154:A:PRO:HD3	3	0.46
(1,861)	1:153:A:LYS:HA	1:154:A:PRO:HD3	4	0.46
(1,861)	1:153:A:LYS:HA	1:154:A:PRO:HD3	6	0.46
(1,861)	1:153:A:LYS:HA	1:154:A:PRO:HD3	10	0.46
(1,861)	1:153:A:LYS:HA	1:154:A:PRO:HD3	12	0.46
(1,861)	1:153:A:LYS:HA	1:154:A:PRO:HD3	13	0.46
(1,861)	1:153:A:LYS:HA	1:154:A:PRO:HD3	18	0.46
(1,861)	1:153:A:LYS:HA	1:154:A:PRO:HD3	19	0.46
(1,845)	1:156:A:VAL:HB	1:157:A:PRO:HD3	12	0.46
(1,730)	1:155:C:ALA:HB1	1:157:C:PRO:HD2	13	0.46
(1,730)	1:155:C:ALA:HB2	1:157:C:PRO:HD2	13	0.46
(1,730)	1:155:C:ALA:HB3	1:157:C:PRO:HD2	13	0.46
(1,730)	1:155:C:ALA:HB1	1:157:C:PRO:HD2	19	0.46
(1,730)	1:155:C:ALA:HB2	1:157:C:PRO:HD2	19	0.46
(1,730)	1:155:C:ALA:HB3	1:157:C:PRO:HD2	19	0.46
(1,730)	1:155:C:ALA:HB1	1:157:C:PRO:HD2	20	0.46
(1,730)	1:155:C:ALA:HB2	1:157:C:PRO:HD2	20	0.46
(1,730)	1:155:C:ALA:HB3	1:157:C:PRO:HD2	20	0.46
(1,729)	1:155:B:ALA:HB1	1:157:B:PRO:HD2	13	0.46
(1,729)	1:155:B:ALA:HB2	1:157:B:PRO:HD2	13	0.46
(1,729)	1:155:B:ALA:HB3	1:157:B:PRO:HD2	13	0.46
(1,729)	1:155:B:ALA:HB1	1:157:B:PRO:HD2	19	0.46
(1,729)	1:155:B:ALA:HB2	1:157:B:PRO:HD2	19	0.46
(1,729)	1:155:B:ALA:HB3	1:157:B:PRO:HD2	19	0.46
(1,215)	1:101:A:LEU:HD21	1:103:A:VAL:HG11	16	0.46
(1,215)	1:101:A:LEU:HD21	1:103:A:VAL:HG12	16	0.46
(1,215)	1:101:A:LEU:HD21	1:103:A:VAL:HG13	16	0.46
(1,215)	1:101:A:LEU:HD22	1:103:A:VAL:HG11	16	0.46
(1,215)	1:101:A:LEU:HD22	1:103:A:VAL:HG12	16	0.46
(1,215)	1:101:A:LEU:HD22	1:103:A:VAL:HG13	16	0.46
(1,215)	1:101:A:LEU:HD23	1:103:A:VAL:HG11	16	0.46
(1,215)	1:101:A:LEU:HD23	1:103:A:VAL:HG12	16	0.46
(1,215)	1:101:A:LEU:HD23	1:103:A:VAL:HG13	16	0.46
(1,205)	1:111:A:ILE:HD11	1:137:A:LEU:HD11	10	0.46
(1,205)	1:111:A:ILE:HD11	1:137:A:LEU:HD12	10	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,205)	1:111:A:ILE:HD11	1:137:A:LEU:HD13	10	0.46
(1,205)	1:111:A:ILE:HD12	1:137:A:LEU:HD11	10	0.46
(1,205)	1:111:A:ILE:HD12	1:137:A:LEU:HD12	10	0.46
(1,205)	1:111:A:ILE:HD12	1:137:A:LEU:HD13	10	0.46
(1,205)	1:111:A:ILE:HD13	1:137:A:LEU:HD11	10	0.46
(1,205)	1:111:A:ILE:HD13	1:137:A:LEU:HD12	10	0.46
(1,205)	1:111:A:ILE:HD13	1:137:A:LEU:HD13	10	0.46
(1,138)	1:192:A:VAL:HG21	1:135:B:GLU:HG2	6	0.46
(1,138)	1:192:A:VAL:HG21	1:135:B:GLU:HG3	6	0.46
(1,138)	1:192:A:VAL:HG22	1:135:B:GLU:HG2	6	0.46
(1,138)	1:192:A:VAL:HG22	1:135:B:GLU:HG3	6	0.46
(1,138)	1:192:A:VAL:HG23	1:135:B:GLU:HG2	6	0.46
(1,138)	1:192:A:VAL:HG23	1:135:B:GLU:HG3	6	0.46
(1,1676)	1:94:A:PHE:H	1:102:A:VAL:HG11	14	0.45
(1,1676)	1:94:A:PHE:H	1:102:A:VAL:HG12	14	0.45
(1,1676)	1:94:A:PHE:H	1:102:A:VAL:HG13	14	0.45
(1,1032)	1:152:C:ALA:H	1:153:C:LYS:H	20	0.45
(1,935)	1:95:A:SER:H	1:101:A:LEU:HD11	2	0.45
(1,935)	1:95:A:SER:H	1:101:A:LEU:HD12	2	0.45
(1,935)	1:95:A:SER:H	1:101:A:LEU:HD13	2	0.45
(1,863)	1:153:C:LYS:HA	1:154:C:PRO:HD3	5	0.45
(1,863)	1:153:C:LYS:HA	1:154:C:PRO:HD3	15	0.45
(1,863)	1:153:C:LYS:HA	1:154:C:PRO:HD3	20	0.45
(1,862)	1:153:B:LYS:HA	1:154:B:PRO:HD3	5	0.45
(1,862)	1:153:B:LYS:HA	1:154:B:PRO:HD3	15	0.45
(1,862)	1:153:B:LYS:HA	1:154:B:PRO:HD3	20	0.45
(1,861)	1:153:A:LYS:HA	1:154:A:PRO:HD3	5	0.45
(1,861)	1:153:A:LYS:HA	1:154:A:PRO:HD3	15	0.45
(1,861)	1:153:A:LYS:HA	1:154:A:PRO:HD3	20	0.45
(1,845)	1:156:A:VAL:HB	1:157:A:PRO:HD3	10	0.45
(1,845)	1:156:A:VAL:HB	1:157:A:PRO:HD3	11	0.45
(1,845)	1:156:A:VAL:HB	1:157:A:PRO:HD3	13	0.45
(1,845)	1:156:A:VAL:HB	1:157:A:PRO:HD3	17	0.45
(1,845)	1:156:A:VAL:HB	1:157:A:PRO:HD3	19	0.45
(1,845)	1:156:A:VAL:HB	1:157:A:PRO:HD3	20	0.45
(1,729)	1:155:B:ALA:HB1	1:157:B:PRO:HD2	20	0.45
(1,729)	1:155:B:ALA:HB2	1:157:B:PRO:HD2	20	0.45
(1,729)	1:155:B:ALA:HB3	1:157:B:PRO:HD2	20	0.45
(1,205)	1:111:A:ILE:HD11	1:137:A:LEU:HD11	7	0.45
(1,205)	1:111:A:ILE:HD11	1:137:A:LEU:HD12	7	0.45
(1,205)	1:111:A:ILE:HD11	1:137:A:LEU:HD13	7	0.45
(1,205)	1:111:A:ILE:HD12	1:137:A:LEU:HD11	7	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,205)	1:111:A:ILE:HD12	1:137:A:LEU:HD12	7	0.45
(1,205)	1:111:A:ILE:HD12	1:137:A:LEU:HD13	7	0.45
(1,205)	1:111:A:ILE:HD13	1:137:A:LEU:HD11	7	0.45
(1,205)	1:111:A:ILE:HD13	1:137:A:LEU:HD12	7	0.45
(1,205)	1:111:A:ILE:HD13	1:137:A:LEU:HD13	7	0.45
(1,124)	1:96:A:ILE:H	1:101:A:LEU:HD21	18	0.45
(1,124)	1:96:A:ILE:H	1:101:A:LEU:HD22	18	0.45
(1,124)	1:96:A:ILE:H	1:101:A:LEU:HD23	18	0.45
(1,1443)	1:155:A:ALA:HA	1:156:A:VAL:H	3	0.44
(1,1036)	1:188:A:LEU:HD21	1:134:B:LEU:H	14	0.44
(1,1036)	1:188:A:LEU:HD22	1:134:B:LEU:H	14	0.44
(1,1036)	1:188:A:LEU:HD23	1:134:B:LEU:H	14	0.44
(1,1031)	1:152:B:ALA:H	1:153:B:LYS:H	20	0.44
(1,1030)	1:152:A:ALA:H	1:153:A:LYS:H	20	0.44
(1,863)	1:153:C:LYS:HA	1:154:C:PRO:HD3	17	0.44
(1,862)	1:153:B:LYS:HA	1:154:B:PRO:HD3	17	0.44
(1,861)	1:153:A:LYS:HA	1:154:A:PRO:HD3	17	0.44
(1,847)	1:156:C:VAL:HB	1:157:C:PRO:HD3	17	0.44
(1,846)	1:156:B:VAL:HB	1:157:B:PRO:HD3	17	0.44
(1,845)	1:156:A:VAL:HB	1:157:A:PRO:HD3	6	0.44
(1,845)	1:156:A:VAL:HB	1:157:A:PRO:HD3	8	0.44
(1,845)	1:156:A:VAL:HB	1:157:A:PRO:HD3	18	0.44
(1,730)	1:155:C:ALA:HB1	1:157:C:PRO:HD2	11	0.44
(1,730)	1:155:C:ALA:HB2	1:157:C:PRO:HD2	11	0.44
(1,730)	1:155:C:ALA:HB3	1:157:C:PRO:HD2	11	0.44
(1,729)	1:155:B:ALA:HB1	1:157:B:PRO:HD2	11	0.44
(1,729)	1:155:B:ALA:HB2	1:157:B:PRO:HD2	11	0.44
(1,729)	1:155:B:ALA:HB3	1:157:B:PRO:HD2	11	0.44
(1,847)	1:156:C:VAL:HB	1:157:C:PRO:HD3	10	0.43
(1,847)	1:156:C:VAL:HB	1:157:C:PRO:HD3	13	0.43
(1,847)	1:156:C:VAL:HB	1:157:C:PRO:HD3	19	0.43
(1,846)	1:156:B:VAL:HB	1:157:B:PRO:HD3	10	0.43
(1,846)	1:156:B:VAL:HB	1:157:B:PRO:HD3	13	0.43
(1,846)	1:156:B:VAL:HB	1:157:B:PRO:HD3	18	0.43
(1,846)	1:156:B:VAL:HB	1:157:B:PRO:HD3	19	0.43
(1,846)	1:156:B:VAL:HB	1:157:B:PRO:HD3	20	0.43
(1,845)	1:156:A:VAL:HB	1:157:A:PRO:HD3	4	0.43
(1,845)	1:156:A:VAL:HB	1:157:A:PRO:HD3	9	0.43
(1,301)	1:181:A:LEU:HD11	1:196:A:TYR:HE1	18	0.43
(1,301)	1:181:A:LEU:HD11	1:196:A:TYR:HE2	18	0.43
(1,301)	1:181:A:LEU:HD12	1:196:A:TYR:HE1	18	0.43
(1,301)	1:181:A:LEU:HD12	1:196:A:TYR:HE2	18	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,301)	1:181:A:LEU:HD13	1:196:A:TYR:HE1	18	0.43
(1,301)	1:181:A:LEU:HD13	1:196:A:TYR:HE2	18	0.43
(1,215)	1:101:A:LEU:HD21	1:103:A:VAL:HG11	10	0.43
(1,215)	1:101:A:LEU:HD21	1:103:A:VAL:HG12	10	0.43
(1,215)	1:101:A:LEU:HD21	1:103:A:VAL:HG13	10	0.43
(1,215)	1:101:A:LEU:HD22	1:103:A:VAL:HG11	10	0.43
(1,215)	1:101:A:LEU:HD22	1:103:A:VAL:HG12	10	0.43
(1,215)	1:101:A:LEU:HD22	1:103:A:VAL:HG13	10	0.43
(1,215)	1:101:A:LEU:HD23	1:103:A:VAL:HG11	10	0.43
(1,215)	1:101:A:LEU:HD23	1:103:A:VAL:HG12	10	0.43
(1,215)	1:101:A:LEU:HD23	1:103:A:VAL:HG13	10	0.43
(1,205)	1:111:A:ILE:HD11	1:137:A:LEU:HD11	5	0.43
(1,205)	1:111:A:ILE:HD11	1:137:A:LEU:HD12	5	0.43
(1,205)	1:111:A:ILE:HD11	1:137:A:LEU:HD13	5	0.43
(1,205)	1:111:A:ILE:HD12	1:137:A:LEU:HD11	5	0.43
(1,205)	1:111:A:ILE:HD12	1:137:A:LEU:HD12	5	0.43
(1,205)	1:111:A:ILE:HD12	1:137:A:LEU:HD13	5	0.43
(1,205)	1:111:A:ILE:HD13	1:137:A:LEU:HD11	5	0.43
(1,205)	1:111:A:ILE:HD13	1:137:A:LEU:HD12	5	0.43
(1,205)	1:111:A:ILE:HD13	1:137:A:LEU:HD13	5	0.43
(1,205)	1:111:A:ILE:HD11	1:137:A:LEU:HD11	14	0.43
(1,205)	1:111:A:ILE:HD11	1:137:A:LEU:HD12	14	0.43
(1,205)	1:111:A:ILE:HD11	1:137:A:LEU:HD13	14	0.43
(1,205)	1:111:A:ILE:HD12	1:137:A:LEU:HD11	14	0.43
(1,205)	1:111:A:ILE:HD12	1:137:A:LEU:HD12	14	0.43
(1,205)	1:111:A:ILE:HD12	1:137:A:LEU:HD13	14	0.43
(1,205)	1:111:A:ILE:HD13	1:137:A:LEU:HD11	14	0.43
(1,205)	1:111:A:ILE:HD13	1:137:A:LEU:HD12	14	0.43
(1,205)	1:111:A:ILE:HD13	1:137:A:LEU:HD13	14	0.43
(1,26)	1:109:A:LEU:HD21	1:110:A:LEU:H	10	0.43
(1,26)	1:109:A:LEU:HD22	1:110:A:LEU:H	10	0.43
(1,26)	1:109:A:LEU:HD23	1:110:A:LEU:H	10	0.43
(1,1370)	1:154:C:PRO:HB3	1:155:C:ALA:H	18	0.42
(1,1369)	1:154:B:PRO:HB3	1:155:B:ALA:H	18	0.42
(1,847)	1:156:C:VAL:HB	1:157:C:PRO:HD3	18	0.42
(1,847)	1:156:C:VAL:HB	1:157:C:PRO:HD3	20	0.42
(1,845)	1:156:A:VAL:HB	1:157:A:PRO:HD3	1	0.42
(1,451)	1:95:A:SER:HB2	1:101:A:LEU:HD21	11	0.42
(1,451)	1:95:A:SER:HB2	1:101:A:LEU:HD22	11	0.42
(1,451)	1:95:A:SER:HB2	1:101:A:LEU:HD23	11	0.42
(1,451)	1:95:A:SER:HB3	1:101:A:LEU:HD21	11	0.42
(1,451)	1:95:A:SER:HB3	1:101:A:LEU:HD22	11	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,451)	1:95:A:SER:HB3	1:101:A:LEU:HD23	11	0.42
(1,124)	1:96:A:ILE:H	1:101:A:LEU:HD21	17	0.42
(1,124)	1:96:A:ILE:H	1:101:A:LEU:HD22	17	0.42
(1,124)	1:96:A:ILE:H	1:101:A:LEU:HD23	17	0.42
(1,122)	1:113:A:TYR:HD1	1:137:A:LEU:HD21	9	0.42
(1,122)	1:113:A:TYR:HD1	1:137:A:LEU:HD22	9	0.42
(1,122)	1:113:A:TYR:HD1	1:137:A:LEU:HD23	9	0.42
(1,122)	1:113:A:TYR:HD2	1:137:A:LEU:HD21	9	0.42
(1,122)	1:113:A:TYR:HD2	1:137:A:LEU:HD22	9	0.42
(1,122)	1:113:A:TYR:HD2	1:137:A:LEU:HD23	9	0.42
(1,1445)	1:155:C:ALA:HA	1:156:C:VAL:H	3	0.41
(1,1444)	1:155:B:ALA:HA	1:156:B:VAL:H	3	0.41
(1,1368)	1:154:A:PRO:HB3	1:155:A:ALA:H	18	0.41
(1,935)	1:95:A:SER:H	1:101:A:LEU:HD11	15	0.41
(1,935)	1:95:A:SER:H	1:101:A:LEU:HD12	15	0.41
(1,935)	1:95:A:SER:H	1:101:A:LEU:HD13	15	0.41
(1,845)	1:156:A:VAL:HB	1:157:A:PRO:HD3	2	0.41
(1,845)	1:156:A:VAL:HB	1:157:A:PRO:HD3	3	0.41
(1,845)	1:156:A:VAL:HB	1:157:A:PRO:HD3	5	0.41
(1,845)	1:156:A:VAL:HB	1:157:A:PRO:HD3	15	0.41
(1,730)	1:155:C:ALA:HB1	1:157:C:PRO:HD2	17	0.41
(1,730)	1:155:C:ALA:HB2	1:157:C:PRO:HD2	17	0.41
(1,730)	1:155:C:ALA:HB3	1:157:C:PRO:HD2	17	0.41
(1,729)	1:155:B:ALA:HB1	1:157:B:PRO:HD2	17	0.41
(1,729)	1:155:B:ALA:HB2	1:157:B:PRO:HD2	17	0.41
(1,729)	1:155:B:ALA:HB3	1:157:B:PRO:HD2	17	0.41
(1,728)	1:155:A:ALA:HB1	1:157:A:PRO:HD2	13	0.41
(1,728)	1:155:A:ALA:HB2	1:157:A:PRO:HD2	13	0.41
(1,728)	1:155:A:ALA:HB3	1:157:A:PRO:HD2	13	0.41
(1,451)	1:95:A:SER:HB2	1:101:A:LEU:HD21	13	0.41
(1,451)	1:95:A:SER:HB2	1:101:A:LEU:HD22	13	0.41
(1,451)	1:95:A:SER:HB2	1:101:A:LEU:HD23	13	0.41
(1,451)	1:95:A:SER:HB3	1:101:A:LEU:HD21	13	0.41
(1,451)	1:95:A:SER:HB3	1:101:A:LEU:HD22	13	0.41
(1,451)	1:95:A:SER:HB3	1:101:A:LEU:HD23	13	0.41
(1,395)	1:109:A:LEU:HG	1:111:A:ILE:HD11	19	0.41
(1,395)	1:109:A:LEU:HG	1:111:A:ILE:HD12	19	0.41
(1,395)	1:109:A:LEU:HG	1:111:A:ILE:HD13	19	0.41
(1,122)	1:113:A:TYR:HD1	1:137:A:LEU:HD21	7	0.41
(1,122)	1:113:A:TYR:HD1	1:137:A:LEU:HD22	7	0.41
(1,122)	1:113:A:TYR:HD1	1:137:A:LEU:HD23	7	0.41
(1,122)	1:113:A:TYR:HD2	1:137:A:LEU:HD21	7	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,122)	1:113:A:TYR:HD2	1:137:A:LEU:HD22	7	0.41
(1,122)	1:113:A:TYR:HD2	1:137:A:LEU:HD23	7	0.41
(1,26)	1:109:A:LEU:HD21	1:110:A:LEU:H	15	0.41
(1,26)	1:109:A:LEU:HD22	1:110:A:LEU:H	15	0.41
(1,26)	1:109:A:LEU:HD23	1:110:A:LEU:H	15	0.41
(1,1443)	1:155:A:ALA:HA	1:156:A:VAL:H	6	0.4
(1,1364)	1:154:C:PRO:HA	1:155:C:ALA:H	7	0.4
(1,1363)	1:154:B:PRO:HA	1:155:B:ALA:H	7	0.4
(1,1362)	1:154:A:PRO:HA	1:155:A:ALA:H	7	0.4
(1,1061)	1:178:C:PRO:HB3	1:179:C:ALA:H	1	0.4
(1,1061)	1:178:C:PRO:HB3	1:179:C:ALA:H	2	0.4
(1,1061)	1:178:C:PRO:HB3	1:179:C:ALA:H	5	0.4
(1,1061)	1:178:C:PRO:HB3	1:179:C:ALA:H	6	0.4
(1,1061)	1:178:C:PRO:HB3	1:179:C:ALA:H	7	0.4
(1,1061)	1:178:C:PRO:HB3	1:179:C:ALA:H	8	0.4
(1,1061)	1:178:C:PRO:HB3	1:179:C:ALA:H	9	0.4
(1,1061)	1:178:C:PRO:HB3	1:179:C:ALA:H	11	0.4
(1,1061)	1:178:C:PRO:HB3	1:179:C:ALA:H	13	0.4
(1,1061)	1:178:C:PRO:HB3	1:179:C:ALA:H	14	0.4
(1,1061)	1:178:C:PRO:HB3	1:179:C:ALA:H	15	0.4
(1,1061)	1:178:C:PRO:HB3	1:179:C:ALA:H	16	0.4
(1,1061)	1:178:C:PRO:HB3	1:179:C:ALA:H	17	0.4
(1,1061)	1:178:C:PRO:HB3	1:179:C:ALA:H	18	0.4
(1,1061)	1:178:C:PRO:HB3	1:179:C:ALA:H	19	0.4
(1,1061)	1:178:C:PRO:HB3	1:179:C:ALA:H	20	0.4
(1,1060)	1:178:B:PRO:HB3	1:179:B:ALA:H	1	0.4
(1,1060)	1:178:B:PRO:HB3	1:179:B:ALA:H	2	0.4
(1,1060)	1:178:B:PRO:HB3	1:179:B:ALA:H	5	0.4
(1,1060)	1:178:B:PRO:HB3	1:179:B:ALA:H	6	0.4
(1,1060)	1:178:B:PRO:HB3	1:179:B:ALA:H	7	0.4
(1,1060)	1:178:B:PRO:HB3	1:179:B:ALA:H	8	0.4
(1,1060)	1:178:B:PRO:HB3	1:179:B:ALA:H	9	0.4
(1,1060)	1:178:B:PRO:HB3	1:179:B:ALA:H	11	0.4
(1,1060)	1:178:B:PRO:HB3	1:179:B:ALA:H	12	0.4
(1,1060)	1:178:B:PRO:HB3	1:179:B:ALA:H	13	0.4
(1,1060)	1:178:B:PRO:HB3	1:179:B:ALA:H	14	0.4
(1,1060)	1:178:B:PRO:HB3	1:179:B:ALA:H	15	0.4
(1,1060)	1:178:B:PRO:HB3	1:179:B:ALA:H	16	0.4
(1,1060)	1:178:B:PRO:HB3	1:179:B:ALA:H	17	0.4
(1,1060)	1:178:B:PRO:HB3	1:179:B:ALA:H	18	0.4
(1,1060)	1:178:B:PRO:HB3	1:179:B:ALA:H	19	0.4
(1,1060)	1:178:B:PRO:HB3	1:179:B:ALA:H	20	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1059)	1:178:A:PRO:HB3	1:179:A:ALA:H	1	0.4
(1,1059)	1:178:A:PRO:HB3	1:179:A:ALA:H	2	0.4
(1,1059)	1:178:A:PRO:HB3	1:179:A:ALA:H	5	0.4
(1,1059)	1:178:A:PRO:HB3	1:179:A:ALA:H	6	0.4
(1,1059)	1:178:A:PRO:HB3	1:179:A:ALA:H	7	0.4
(1,1059)	1:178:A:PRO:HB3	1:179:A:ALA:H	8	0.4
(1,1059)	1:178:A:PRO:HB3	1:179:A:ALA:H	9	0.4
(1,1059)	1:178:A:PRO:HB3	1:179:A:ALA:H	11	0.4
(1,1059)	1:178:A:PRO:HB3	1:179:A:ALA:H	12	0.4
(1,1059)	1:178:A:PRO:HB3	1:179:A:ALA:H	13	0.4
(1,1059)	1:178:A:PRO:HB3	1:179:A:ALA:H	14	0.4
(1,1059)	1:178:A:PRO:HB3	1:179:A:ALA:H	15	0.4
(1,1059)	1:178:A:PRO:HB3	1:179:A:ALA:H	16	0.4
(1,1059)	1:178:A:PRO:HB3	1:179:A:ALA:H	17	0.4
(1,1059)	1:178:A:PRO:HB3	1:179:A:ALA:H	18	0.4
(1,1059)	1:178:A:PRO:HB3	1:179:A:ALA:H	19	0.4
(1,1059)	1:178:A:PRO:HB3	1:179:A:ALA:H	20	0.4
(1,847)	1:156:C:VAL:HB	1:157:C:PRO:HD3	4	0.4
(1,847)	1:156:C:VAL:HB	1:157:C:PRO:HD3	8	0.4
(1,847)	1:156:C:VAL:HB	1:157:C:PRO:HD3	9	0.4
(1,846)	1:156:B:VAL:HB	1:157:B:PRO:HD3	8	0.4
(1,846)	1:156:B:VAL:HB	1:157:B:PRO:HD3	9	0.4
(1,728)	1:155:A:ALA:HB1	1:157:A:PRO:HD2	19	0.4
(1,728)	1:155:A:ALA:HB2	1:157:A:PRO:HD2	19	0.4
(1,728)	1:155:A:ALA:HB3	1:157:A:PRO:HD2	19	0.4
(1,451)	1:95:A:SER:HB2	1:101:A:LEU:HD21	1	0.4
(1,451)	1:95:A:SER:HB2	1:101:A:LEU:HD22	1	0.4
(1,451)	1:95:A:SER:HB2	1:101:A:LEU:HD23	1	0.4
(1,451)	1:95:A:SER:HB3	1:101:A:LEU:HD21	1	0.4
(1,451)	1:95:A:SER:HB3	1:101:A:LEU:HD22	1	0.4
(1,451)	1:95:A:SER:HB3	1:101:A:LEU:HD23	1	0.4
(1,205)	1:111:A:ILE:HD11	1:137:A:LEU:HD11	15	0.4
(1,205)	1:111:A:ILE:HD11	1:137:A:LEU:HD12	15	0.4
(1,205)	1:111:A:ILE:HD11	1:137:A:LEU:HD13	15	0.4
(1,205)	1:111:A:ILE:HD12	1:137:A:LEU:HD11	15	0.4
(1,205)	1:111:A:ILE:HD12	1:137:A:LEU:HD12	15	0.4
(1,205)	1:111:A:ILE:HD12	1:137:A:LEU:HD13	15	0.4
(1,205)	1:111:A:ILE:HD13	1:137:A:LEU:HD11	15	0.4
(1,205)	1:111:A:ILE:HD13	1:137:A:LEU:HD12	15	0.4
(1,205)	1:111:A:ILE:HD13	1:137:A:LEU:HD13	15	0.4
(1,26)	1:109:A:LEU:HD21	1:110:A:LEU:H	6	0.4
(1,26)	1:109:A:LEU:HD22	1:110:A:LEU:H	6	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,26)	1:109:A:LEU:HD23	1:110:A:LEU:H	6	0.4
(1,26)	1:109:A:LEU:HD21	1:110:A:LEU:H	7	0.4
(1,26)	1:109:A:LEU:HD22	1:110:A:LEU:H	7	0.4
(1,26)	1:109:A:LEU:HD23	1:110:A:LEU:H	7	0.4
(1,26)	1:109:A:LEU:HD21	1:110:A:LEU:H	17	0.4
(1,26)	1:109:A:LEU:HD22	1:110:A:LEU:H	17	0.4
(1,26)	1:109:A:LEU:HD23	1:110:A:LEU:H	17	0.4
(1,1885)	1:155:A:ALA:HB1	1:157:A:PRO:HD2	12	0.39
(1,1885)	1:155:A:ALA:HB1	1:157:A:PRO:HD3	12	0.39
(1,1885)	1:155:A:ALA:HB2	1:157:A:PRO:HD2	12	0.39
(1,1885)	1:155:A:ALA:HB2	1:157:A:PRO:HD3	12	0.39
(1,1885)	1:155:A:ALA:HB3	1:157:A:PRO:HD2	12	0.39
(1,1885)	1:155:A:ALA:HB3	1:157:A:PRO:HD3	12	0.39
(1,1443)	1:155:A:ALA:HA	1:156:A:VAL:H	8	0.39
(1,1404)	1:153:C:LYS:H	1:153:C:LYS:HB3	7	0.39
(1,1403)	1:153:B:LYS:H	1:153:B:LYS:HB3	7	0.39
(1,1402)	1:153:A:LYS:H	1:153:A:LYS:HB3	7	0.39
(1,1370)	1:154:C:PRO:HB3	1:155:C:ALA:H	10	0.39
(1,1369)	1:154:B:PRO:HB3	1:155:B:ALA:H	10	0.39
(1,1368)	1:154:A:PRO:HB3	1:155:A:ALA:H	10	0.39
(1,1061)	1:178:C:PRO:HB3	1:179:C:ALA:H	12	0.39
(1,847)	1:156:C:VAL:HB	1:157:C:PRO:HD3	1	0.39
(1,847)	1:156:C:VAL:HB	1:157:C:PRO:HD3	3	0.39
(1,847)	1:156:C:VAL:HB	1:157:C:PRO:HD3	6	0.39
(1,846)	1:156:B:VAL:HB	1:157:B:PRO:HD3	1	0.39
(1,846)	1:156:B:VAL:HB	1:157:B:PRO:HD3	3	0.39
(1,846)	1:156:B:VAL:HB	1:157:B:PRO:HD3	4	0.39
(1,846)	1:156:B:VAL:HB	1:157:B:PRO:HD3	6	0.39
(1,730)	1:155:C:ALA:HB1	1:157:C:PRO:HD2	10	0.39
(1,730)	1:155:C:ALA:HB2	1:157:C:PRO:HD2	10	0.39
(1,730)	1:155:C:ALA:HB3	1:157:C:PRO:HD2	10	0.39
(1,729)	1:155:B:ALA:HB1	1:157:B:PRO:HD2	10	0.39
(1,729)	1:155:B:ALA:HB2	1:157:B:PRO:HD2	10	0.39
(1,729)	1:155:B:ALA:HB3	1:157:B:PRO:HD2	10	0.39
(1,539)	1:111:A:ILE:HG21	1:126:A:ILE:HG21	6	0.39
(1,539)	1:111:A:ILE:HG21	1:126:A:ILE:HG22	6	0.39
(1,539)	1:111:A:ILE:HG21	1:126:A:ILE:HG23	6	0.39
(1,539)	1:111:A:ILE:HG22	1:126:A:ILE:HG21	6	0.39
(1,539)	1:111:A:ILE:HG22	1:126:A:ILE:HG22	6	0.39
(1,539)	1:111:A:ILE:HG22	1:126:A:ILE:HG23	6	0.39
(1,539)	1:111:A:ILE:HG23	1:126:A:ILE:HG21	6	0.39
(1,539)	1:111:A:ILE:HG23	1:126:A:ILE:HG22	6	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,539)	1:111:A:ILE:HG23	1:126:A:ILE:HG23	6	0.39
(1,301)	1:181:A:LEU:HD11	1:196:A:TYR:HE1	7	0.39
(1,301)	1:181:A:LEU:HD11	1:196:A:TYR:HE2	7	0.39
(1,301)	1:181:A:LEU:HD12	1:196:A:TYR:HE1	7	0.39
(1,301)	1:181:A:LEU:HD12	1:196:A:TYR:HE2	7	0.39
(1,301)	1:181:A:LEU:HD13	1:196:A:TYR:HE1	7	0.39
(1,301)	1:181:A:LEU:HD13	1:196:A:TYR:HE2	7	0.39
(1,251)	1:118:C:GLY:HA2	1:119:C:THR:HG21	8	0.39
(1,251)	1:118:C:GLY:HA2	1:119:C:THR:HG22	8	0.39
(1,251)	1:118:C:GLY:HA2	1:119:C:THR:HG23	8	0.39
(1,249)	1:118:A:GLY:HA2	1:119:A:THR:HG21	8	0.39
(1,249)	1:118:A:GLY:HA2	1:119:A:THR:HG22	8	0.39
(1,249)	1:118:A:GLY:HA2	1:119:A:THR:HG23	8	0.39
(1,205)	1:111:A:ILE:HD11	1:137:A:LEU:HD11	12	0.39
(1,205)	1:111:A:ILE:HD11	1:137:A:LEU:HD12	12	0.39
(1,205)	1:111:A:ILE:HD11	1:137:A:LEU:HD13	12	0.39
(1,205)	1:111:A:ILE:HD12	1:137:A:LEU:HD11	12	0.39
(1,205)	1:111:A:ILE:HD12	1:137:A:LEU:HD12	12	0.39
(1,205)	1:111:A:ILE:HD12	1:137:A:LEU:HD13	12	0.39
(1,205)	1:111:A:ILE:HD13	1:137:A:LEU:HD11	12	0.39
(1,205)	1:111:A:ILE:HD13	1:137:A:LEU:HD12	12	0.39
(1,205)	1:111:A:ILE:HD13	1:137:A:LEU:HD13	12	0.39
(1,138)	1:192:A:VAL:HG21	1:135:B:GLU:HG2	3	0.39
(1,138)	1:192:A:VAL:HG21	1:135:B:GLU:HG3	3	0.39
(1,138)	1:192:A:VAL:HG22	1:135:B:GLU:HG2	3	0.39
(1,138)	1:192:A:VAL:HG22	1:135:B:GLU:HG3	3	0.39
(1,138)	1:192:A:VAL:HG23	1:135:B:GLU:HG2	3	0.39
(1,138)	1:192:A:VAL:HG23	1:135:B:GLU:HG3	3	0.39
(1,138)	1:192:A:VAL:HG21	1:135:B:GLU:HG2	20	0.39
(1,138)	1:192:A:VAL:HG21	1:135:B:GLU:HG3	20	0.39
(1,138)	1:192:A:VAL:HG22	1:135:B:GLU:HG2	20	0.39
(1,138)	1:192:A:VAL:HG22	1:135:B:GLU:HG3	20	0.39
(1,138)	1:192:A:VAL:HG23	1:135:B:GLU:HG2	20	0.39
(1,138)	1:192:A:VAL:HG23	1:135:B:GLU:HG3	20	0.39
(1,1676)	1:94:A:PHE:H	1:102:A:VAL:HG11	11	0.38
(1,1676)	1:94:A:PHE:H	1:102:A:VAL:HG12	11	0.38
(1,1676)	1:94:A:PHE:H	1:102:A:VAL:HG13	11	0.38
(1,1561)	1:167:C:ARG:H	1:167:C:ARG:HB3	4	0.38
(1,1561)	1:167:C:ARG:H	1:167:C:ARG:HB3	17	0.38
(1,1561)	1:167:C:ARG:H	1:167:C:ARG:HB3	18	0.38
(1,1560)	1:167:B:ARG:H	1:167:B:ARG:HB3	4	0.38
(1,1560)	1:167:B:ARG:H	1:167:B:ARG:HB3	17	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1560)	1:167:B:ARG:H	1:167:B:ARG:HB3	18	0.38
(1,1559)	1:167:A:ARG:H	1:167:A:ARG:HB3	17	0.38
(1,1559)	1:167:A:ARG:H	1:167:A:ARG:HB3	18	0.38
(1,1547)	1:167:B:ARG:H	1:170:B:GLY:HA2	14	0.38
(1,1547)	1:167:B:ARG:H	1:170:B:GLY:HA3	14	0.38
(1,1404)	1:153:C:LYS:H	1:153:C:LYS:HB3	14	0.38
(1,1403)	1:153:B:LYS:H	1:153:B:LYS:HB3	14	0.38
(1,1402)	1:153:A:LYS:H	1:153:A:LYS:HB3	14	0.38
(1,1374)	1:155:A:ALA:H	1:156:A:VAL:HG11	7	0.38
(1,1374)	1:155:A:ALA:H	1:156:A:VAL:HG12	7	0.38
(1,1374)	1:155:A:ALA:H	1:156:A:VAL:HG13	7	0.38
(1,1374)	1:155:A:ALA:H	1:156:A:VAL:HG11	14	0.38
(1,1374)	1:155:A:ALA:H	1:156:A:VAL:HG12	14	0.38
(1,1374)	1:155:A:ALA:H	1:156:A:VAL:HG13	14	0.38
(1,1036)	1:188:A:LEU:HD21	1:134:B:LEU:H	10	0.38
(1,1036)	1:188:A:LEU:HD22	1:134:B:LEU:H	10	0.38
(1,1036)	1:188:A:LEU:HD23	1:134:B:LEU:H	10	0.38
(1,958)	1:187:A:THR:HA	1:188:A:LEU:HD11	2	0.38
(1,958)	1:187:A:THR:HA	1:188:A:LEU:HD12	2	0.38
(1,958)	1:187:A:THR:HA	1:188:A:LEU:HD13	2	0.38
(1,847)	1:156:C:VAL:HB	1:157:C:PRO:HD3	2	0.38
(1,847)	1:156:C:VAL:HB	1:157:C:PRO:HD3	5	0.38
(1,847)	1:156:C:VAL:HB	1:157:C:PRO:HD3	15	0.38
(1,846)	1:156:B:VAL:HB	1:157:B:PRO:HD3	2	0.38
(1,846)	1:156:B:VAL:HB	1:157:B:PRO:HD3	5	0.38
(1,846)	1:156:B:VAL:HB	1:157:B:PRO:HD3	15	0.38
(1,730)	1:155:C:ALA:HB1	1:157:C:PRO:HD2	15	0.38
(1,730)	1:155:C:ALA:HB2	1:157:C:PRO:HD2	15	0.38
(1,730)	1:155:C:ALA:HB3	1:157:C:PRO:HD2	15	0.38
(1,730)	1:155:C:ALA:HB1	1:157:C:PRO:HD2	18	0.38
(1,730)	1:155:C:ALA:HB2	1:157:C:PRO:HD2	18	0.38
(1,730)	1:155:C:ALA:HB3	1:157:C:PRO:HD2	18	0.38
(1,729)	1:155:B:ALA:HB1	1:157:B:PRO:HD2	15	0.38
(1,729)	1:155:B:ALA:HB2	1:157:B:PRO:HD2	15	0.38
(1,729)	1:155:B:ALA:HB3	1:157:B:PRO:HD2	15	0.38
(1,729)	1:155:B:ALA:HB1	1:157:B:PRO:HD2	18	0.38
(1,729)	1:155:B:ALA:HB2	1:157:B:PRO:HD2	18	0.38
(1,729)	1:155:B:ALA:HB3	1:157:B:PRO:HD2	18	0.38
(1,728)	1:155:A:ALA:HB1	1:157:A:PRO:HD2	10	0.38
(1,728)	1:155:A:ALA:HB2	1:157:A:PRO:HD2	10	0.38
(1,728)	1:155:A:ALA:HB3	1:157:A:PRO:HD2	10	0.38
(1,728)	1:155:A:ALA:HB1	1:157:A:PRO:HD2	20	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,728)	1:155:A:ALA:HB2	1:157:A:PRO:HD2	20	0.38
(1,728)	1:155:A:ALA:HB3	1:157:A:PRO:HD2	20	0.38
(1,451)	1:95:A:SER:HB2	1:101:A:LEU:HD21	6	0.38
(1,451)	1:95:A:SER:HB2	1:101:A:LEU:HD22	6	0.38
(1,451)	1:95:A:SER:HB2	1:101:A:LEU:HD23	6	0.38
(1,451)	1:95:A:SER:HB3	1:101:A:LEU:HD21	6	0.38
(1,451)	1:95:A:SER:HB3	1:101:A:LEU:HD22	6	0.38
(1,451)	1:95:A:SER:HB3	1:101:A:LEU:HD23	6	0.38
(1,451)	1:95:A:SER:HB2	1:101:A:LEU:HD21	12	0.38
(1,451)	1:95:A:SER:HB2	1:101:A:LEU:HD22	12	0.38
(1,451)	1:95:A:SER:HB2	1:101:A:LEU:HD23	12	0.38
(1,451)	1:95:A:SER:HB3	1:101:A:LEU:HD21	12	0.38
(1,451)	1:95:A:SER:HB3	1:101:A:LEU:HD22	12	0.38
(1,451)	1:95:A:SER:HB3	1:101:A:LEU:HD23	12	0.38
(1,367)	1:96:A:ILE:HD11	1:141:A:VAL:HG11	8	0.38
(1,367)	1:96:A:ILE:HD11	1:141:A:VAL:HG12	8	0.38
(1,367)	1:96:A:ILE:HD11	1:141:A:VAL:HG13	8	0.38
(1,367)	1:96:A:ILE:HD12	1:141:A:VAL:HG11	8	0.38
(1,367)	1:96:A:ILE:HD12	1:141:A:VAL:HG12	8	0.38
(1,367)	1:96:A:ILE:HD12	1:141:A:VAL:HG13	8	0.38
(1,367)	1:96:A:ILE:HD13	1:141:A:VAL:HG11	8	0.38
(1,367)	1:96:A:ILE:HD13	1:141:A:VAL:HG12	8	0.38
(1,367)	1:96:A:ILE:HD13	1:141:A:VAL:HG13	8	0.38
(1,250)	1:118:B:GLY:HA2	1:119:B:THR:HG21	8	0.38
(1,250)	1:118:B:GLY:HA2	1:119:B:THR:HG22	8	0.38
(1,250)	1:118:B:GLY:HA2	1:119:B:THR:HG23	8	0.38
(1,205)	1:111:A:ILE:HD11	1:137:A:LEU:HD11	16	0.38
(1,205)	1:111:A:ILE:HD11	1:137:A:LEU:HD12	16	0.38
(1,205)	1:111:A:ILE:HD11	1:137:A:LEU:HD13	16	0.38
(1,205)	1:111:A:ILE:HD12	1:137:A:LEU:HD11	16	0.38
(1,205)	1:111:A:ILE:HD12	1:137:A:LEU:HD12	16	0.38
(1,205)	1:111:A:ILE:HD12	1:137:A:LEU:HD13	16	0.38
(1,205)	1:111:A:ILE:HD13	1:137:A:LEU:HD11	16	0.38
(1,205)	1:111:A:ILE:HD13	1:137:A:LEU:HD12	16	0.38
(1,205)	1:111:A:ILE:HD13	1:137:A:LEU:HD13	16	0.38
(1,138)	1:192:A:VAL:HG21	1:135:B:GLU:HG2	4	0.38
(1,138)	1:192:A:VAL:HG21	1:135:B:GLU:HG3	4	0.38
(1,138)	1:192:A:VAL:HG22	1:135:B:GLU:HG2	4	0.38
(1,138)	1:192:A:VAL:HG22	1:135:B:GLU:HG3	4	0.38
(1,138)	1:192:A:VAL:HG23	1:135:B:GLU:HG2	4	0.38
(1,138)	1:192:A:VAL:HG23	1:135:B:GLU:HG3	4	0.38
(1,138)	1:192:A:VAL:HG21	1:135:B:GLU:HG2	15	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,138)	1:192:A:VAL:HG21	1:135:B:GLU:HG3	15	0.38
(1,138)	1:192:A:VAL:HG22	1:135:B:GLU:HG2	15	0.38
(1,138)	1:192:A:VAL:HG22	1:135:B:GLU:HG3	15	0.38
(1,138)	1:192:A:VAL:HG23	1:135:B:GLU:HG2	15	0.38
(1,138)	1:192:A:VAL:HG23	1:135:B:GLU:HG3	15	0.38
(1,138)	1:192:A:VAL:HG21	1:135:B:GLU:HG2	17	0.38
(1,138)	1:192:A:VAL:HG21	1:135:B:GLU:HG3	17	0.38
(1,138)	1:192:A:VAL:HG22	1:135:B:GLU:HG2	17	0.38
(1,138)	1:192:A:VAL:HG22	1:135:B:GLU:HG3	17	0.38
(1,138)	1:192:A:VAL:HG23	1:135:B:GLU:HG2	17	0.38
(1,138)	1:192:A:VAL:HG23	1:135:B:GLU:HG3	17	0.38
(1,124)	1:96:A:ILE:H	1:101:A:LEU:HD21	6	0.38
(1,124)	1:96:A:ILE:H	1:101:A:LEU:HD22	6	0.38
(1,124)	1:96:A:ILE:H	1:101:A:LEU:HD23	6	0.38
(1,26)	1:109:A:LEU:HD21	1:110:A:LEU:H	8	0.38
(1,26)	1:109:A:LEU:HD22	1:110:A:LEU:H	8	0.38
(1,26)	1:109:A:LEU:HD23	1:110:A:LEU:H	8	0.38
(1,2329)	1:178:C:PRO:HB2	1:179:C:ALA:H	5	0.37
(1,2329)	1:178:C:PRO:HB3	1:179:C:ALA:H	5	0.37
(1,2329)	1:178:C:PRO:HB2	1:179:C:ALA:H	6	0.37
(1,2329)	1:178:C:PRO:HB3	1:179:C:ALA:H	6	0.37
(1,2329)	1:178:C:PRO:HB2	1:179:C:ALA:H	7	0.37
(1,2329)	1:178:C:PRO:HB3	1:179:C:ALA:H	7	0.37
(1,2329)	1:178:C:PRO:HB2	1:179:C:ALA:H	8	0.37
(1,2329)	1:178:C:PRO:HB3	1:179:C:ALA:H	8	0.37
(1,2329)	1:178:C:PRO:HB2	1:179:C:ALA:H	9	0.37
(1,2329)	1:178:C:PRO:HB3	1:179:C:ALA:H	9	0.37
(1,2329)	1:178:C:PRO:HB2	1:179:C:ALA:H	14	0.37
(1,2329)	1:178:C:PRO:HB3	1:179:C:ALA:H	14	0.37
(1,2329)	1:178:C:PRO:HB2	1:179:C:ALA:H	15	0.37
(1,2329)	1:178:C:PRO:HB3	1:179:C:ALA:H	15	0.37
(1,2329)	1:178:C:PRO:HB2	1:179:C:ALA:H	18	0.37
(1,2329)	1:178:C:PRO:HB3	1:179:C:ALA:H	18	0.37
(1,2329)	1:178:C:PRO:HB2	1:179:C:ALA:H	19	0.37
(1,2329)	1:178:C:PRO:HB3	1:179:C:ALA:H	19	0.37
(1,2329)	1:178:C:PRO:HB2	1:179:C:ALA:H	20	0.37
(1,2329)	1:178:C:PRO:HB3	1:179:C:ALA:H	20	0.37
(1,2103)	1:178:B:PRO:HB2	1:179:B:ALA:H	5	0.37
(1,2103)	1:178:B:PRO:HB3	1:179:B:ALA:H	5	0.37
(1,2103)	1:178:B:PRO:HB2	1:179:B:ALA:H	6	0.37
(1,2103)	1:178:B:PRO:HB3	1:179:B:ALA:H	6	0.37
(1,2103)	1:178:B:PRO:HB2	1:179:B:ALA:H	7	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2103)	1:178:B:PRO:HB3	1:179:B:ALA:H	7	0.37
(1,2103)	1:178:B:PRO:HB2	1:179:B:ALA:H	8	0.37
(1,2103)	1:178:B:PRO:HB3	1:179:B:ALA:H	8	0.37
(1,2103)	1:178:B:PRO:HB2	1:179:B:ALA:H	9	0.37
(1,2103)	1:178:B:PRO:HB3	1:179:B:ALA:H	9	0.37
(1,2103)	1:178:B:PRO:HB2	1:179:B:ALA:H	13	0.37
(1,2103)	1:178:B:PRO:HB3	1:179:B:ALA:H	13	0.37
(1,2103)	1:178:B:PRO:HB2	1:179:B:ALA:H	14	0.37
(1,2103)	1:178:B:PRO:HB3	1:179:B:ALA:H	14	0.37
(1,2103)	1:178:B:PRO:HB2	1:179:B:ALA:H	16	0.37
(1,2103)	1:178:B:PRO:HB3	1:179:B:ALA:H	16	0.37
(1,2103)	1:178:B:PRO:HB2	1:179:B:ALA:H	18	0.37
(1,2103)	1:178:B:PRO:HB3	1:179:B:ALA:H	18	0.37
(1,2103)	1:178:B:PRO:HB2	1:179:B:ALA:H	19	0.37
(1,2103)	1:178:B:PRO:HB3	1:179:B:ALA:H	19	0.37
(1,2103)	1:178:B:PRO:HB2	1:179:B:ALA:H	20	0.37
(1,2103)	1:178:B:PRO:HB3	1:179:B:ALA:H	20	0.37
(1,1910)	1:178:A:PRO:HB2	1:179:A:ALA:H	2	0.37
(1,1910)	1:178:A:PRO:HB3	1:179:A:ALA:H	2	0.37
(1,1910)	1:178:A:PRO:HB2	1:179:A:ALA:H	5	0.37
(1,1910)	1:178:A:PRO:HB3	1:179:A:ALA:H	5	0.37
(1,1910)	1:178:A:PRO:HB2	1:179:A:ALA:H	7	0.37
(1,1910)	1:178:A:PRO:HB3	1:179:A:ALA:H	7	0.37
(1,1910)	1:178:A:PRO:HB2	1:179:A:ALA:H	8	0.37
(1,1910)	1:178:A:PRO:HB3	1:179:A:ALA:H	8	0.37
(1,1910)	1:178:A:PRO:HB2	1:179:A:ALA:H	9	0.37
(1,1910)	1:178:A:PRO:HB3	1:179:A:ALA:H	9	0.37
(1,1910)	1:178:A:PRO:HB2	1:179:A:ALA:H	14	0.37
(1,1910)	1:178:A:PRO:HB3	1:179:A:ALA:H	14	0.37
(1,1910)	1:178:A:PRO:HB2	1:179:A:ALA:H	15	0.37
(1,1910)	1:178:A:PRO:HB3	1:179:A:ALA:H	15	0.37
(1,1910)	1:178:A:PRO:HB2	1:179:A:ALA:H	16	0.37
(1,1910)	1:178:A:PRO:HB3	1:179:A:ALA:H	16	0.37
(1,1910)	1:178:A:PRO:HB2	1:179:A:ALA:H	17	0.37
(1,1910)	1:178:A:PRO:HB3	1:179:A:ALA:H	17	0.37
(1,1910)	1:178:A:PRO:HB2	1:179:A:ALA:H	18	0.37
(1,1910)	1:178:A:PRO:HB3	1:179:A:ALA:H	18	0.37
(1,1910)	1:178:A:PRO:HB2	1:179:A:ALA:H	19	0.37
(1,1910)	1:178:A:PRO:HB3	1:179:A:ALA:H	19	0.37
(1,1910)	1:178:A:PRO:HB2	1:179:A:ALA:H	20	0.37
(1,1910)	1:178:A:PRO:HB3	1:179:A:ALA:H	20	0.37
(1,1561)	1:167:C:ARG:H	1:167:C:ARG:HB3	2	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1561)	1:167:C:ARG:H	1:167:C:ARG:HB3	3	0.37
(1,1561)	1:167:C:ARG:H	1:167:C:ARG:HB3	10	0.37
(1,1561)	1:167:C:ARG:H	1:167:C:ARG:HB3	11	0.37
(1,1561)	1:167:C:ARG:H	1:167:C:ARG:HB3	16	0.37
(1,1560)	1:167:B:ARG:H	1:167:B:ARG:HB3	2	0.37
(1,1560)	1:167:B:ARG:H	1:167:B:ARG:HB3	10	0.37
(1,1560)	1:167:B:ARG:H	1:167:B:ARG:HB3	11	0.37
(1,1560)	1:167:B:ARG:H	1:167:B:ARG:HB3	16	0.37
(1,1559)	1:167:A:ARG:H	1:167:A:ARG:HB3	2	0.37
(1,1559)	1:167:A:ARG:H	1:167:A:ARG:HB3	4	0.37
(1,1559)	1:167:A:ARG:H	1:167:A:ARG:HB3	10	0.37
(1,1548)	1:167:C:ARG:H	1:170:C:GLY:HA2	14	0.37
(1,1548)	1:167:C:ARG:H	1:170:C:GLY:HA3	14	0.37
(1,1546)	1:167:A:ARG:H	1:170:A:GLY:HA2	14	0.37
(1,1546)	1:167:A:ARG:H	1:170:A:GLY:HA3	14	0.37
(1,1445)	1:155:C:ALA:HA	1:156:C:VAL:H	1	0.37
(1,1444)	1:155:B:ALA:HA	1:156:B:VAL:H	1	0.37
(1,1443)	1:155:A:ALA:HA	1:156:A:VAL:H	1	0.37
(1,1443)	1:155:A:ALA:HA	1:156:A:VAL:H	4	0.37
(1,1036)	1:188:A:LEU:HD21	1:134:B:LEU:H	6	0.37
(1,1036)	1:188:A:LEU:HD22	1:134:B:LEU:H	6	0.37
(1,1036)	1:188:A:LEU:HD23	1:134:B:LEU:H	6	0.37
(1,623)	1:96:A:ILE:HG21	1:138:A:THR:HB	8	0.37
(1,623)	1:96:A:ILE:HG22	1:138:A:THR:HB	8	0.37
(1,623)	1:96:A:ILE:HG23	1:138:A:THR:HB	8	0.37
(1,451)	1:95:A:SER:HB2	1:101:A:LEU:HD21	4	0.37
(1,451)	1:95:A:SER:HB2	1:101:A:LEU:HD22	4	0.37
(1,451)	1:95:A:SER:HB2	1:101:A:LEU:HD23	4	0.37
(1,451)	1:95:A:SER:HB3	1:101:A:LEU:HD21	4	0.37
(1,451)	1:95:A:SER:HB3	1:101:A:LEU:HD22	4	0.37
(1,451)	1:95:A:SER:HB3	1:101:A:LEU:HD23	4	0.37
(1,205)	1:111:A:ILE:HD11	1:137:A:LEU:HD11	1	0.37
(1,205)	1:111:A:ILE:HD11	1:137:A:LEU:HD12	1	0.37
(1,205)	1:111:A:ILE:HD11	1:137:A:LEU:HD13	1	0.37
(1,205)	1:111:A:ILE:HD12	1:137:A:LEU:HD11	1	0.37
(1,205)	1:111:A:ILE:HD12	1:137:A:LEU:HD12	1	0.37
(1,205)	1:111:A:ILE:HD12	1:137:A:LEU:HD13	1	0.37
(1,205)	1:111:A:ILE:HD13	1:137:A:LEU:HD11	1	0.37
(1,205)	1:111:A:ILE:HD13	1:137:A:LEU:HD12	1	0.37
(1,205)	1:111:A:ILE:HD13	1:137:A:LEU:HD13	1	0.37
(1,205)	1:111:A:ILE:HD11	1:137:A:LEU:HD11	4	0.37
(1,205)	1:111:A:ILE:HD11	1:137:A:LEU:HD12	4	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,205)	1:111:A:ILE:HD11	1:137:A:LEU:HD13	4	0.37
(1,205)	1:111:A:ILE:HD12	1:137:A:LEU:HD11	4	0.37
(1,205)	1:111:A:ILE:HD12	1:137:A:LEU:HD12	4	0.37
(1,205)	1:111:A:ILE:HD12	1:137:A:LEU:HD13	4	0.37
(1,205)	1:111:A:ILE:HD13	1:137:A:LEU:HD11	4	0.37
(1,205)	1:111:A:ILE:HD13	1:137:A:LEU:HD12	4	0.37
(1,205)	1:111:A:ILE:HD13	1:137:A:LEU:HD13	4	0.37
(1,205)	1:111:A:ILE:HD11	1:137:A:LEU:HD11	13	0.37
(1,205)	1:111:A:ILE:HD11	1:137:A:LEU:HD12	13	0.37
(1,205)	1:111:A:ILE:HD11	1:137:A:LEU:HD13	13	0.37
(1,205)	1:111:A:ILE:HD12	1:137:A:LEU:HD11	13	0.37
(1,205)	1:111:A:ILE:HD12	1:137:A:LEU:HD12	13	0.37
(1,205)	1:111:A:ILE:HD12	1:137:A:LEU:HD13	13	0.37
(1,205)	1:111:A:ILE:HD13	1:137:A:LEU:HD11	13	0.37
(1,205)	1:111:A:ILE:HD13	1:137:A:LEU:HD12	13	0.37
(1,205)	1:111:A:ILE:HD13	1:137:A:LEU:HD13	13	0.37
(1,26)	1:109:A:LEU:HD21	1:110:A:LEU:H	14	0.37
(1,26)	1:109:A:LEU:HD22	1:110:A:LEU:H	14	0.37
(1,26)	1:109:A:LEU:HD23	1:110:A:LEU:H	14	0.37
(1,26)	1:109:A:LEU:HD21	1:110:A:LEU:H	18	0.37
(1,26)	1:109:A:LEU:HD22	1:110:A:LEU:H	18	0.37
(1,26)	1:109:A:LEU:HD23	1:110:A:LEU:H	18	0.37
(1,2329)	1:178:C:PRO:HB2	1:179:C:ALA:H	1	0.36
(1,2329)	1:178:C:PRO:HB3	1:179:C:ALA:H	1	0.36
(1,2329)	1:178:C:PRO:HB2	1:179:C:ALA:H	2	0.36
(1,2329)	1:178:C:PRO:HB3	1:179:C:ALA:H	2	0.36
(1,2329)	1:178:C:PRO:HB2	1:179:C:ALA:H	11	0.36
(1,2329)	1:178:C:PRO:HB3	1:179:C:ALA:H	11	0.36
(1,2329)	1:178:C:PRO:HB2	1:179:C:ALA:H	13	0.36
(1,2329)	1:178:C:PRO:HB3	1:179:C:ALA:H	13	0.36
(1,2329)	1:178:C:PRO:HB2	1:179:C:ALA:H	16	0.36
(1,2329)	1:178:C:PRO:HB3	1:179:C:ALA:H	16	0.36
(1,2329)	1:178:C:PRO:HB2	1:179:C:ALA:H	17	0.36
(1,2329)	1:178:C:PRO:HB3	1:179:C:ALA:H	17	0.36
(1,2103)	1:178:B:PRO:HB2	1:179:B:ALA:H	1	0.36
(1,2103)	1:178:B:PRO:HB3	1:179:B:ALA:H	1	0.36
(1,2103)	1:178:B:PRO:HB2	1:179:B:ALA:H	2	0.36
(1,2103)	1:178:B:PRO:HB3	1:179:B:ALA:H	2	0.36
(1,2103)	1:178:B:PRO:HB2	1:179:B:ALA:H	11	0.36
(1,2103)	1:178:B:PRO:HB3	1:179:B:ALA:H	11	0.36
(1,2103)	1:178:B:PRO:HB2	1:179:B:ALA:H	15	0.36
(1,2103)	1:178:B:PRO:HB3	1:179:B:ALA:H	15	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2103)	1:178:B:PRO:HB2	1:179:B:ALA:H	17	0.36
(1,2103)	1:178:B:PRO:HB3	1:179:B:ALA:H	17	0.36
(1,2072)	1:156:B:VAL:HB	1:157:B:PRO:HD2	12	0.36
(1,2072)	1:156:B:VAL:HB	1:157:B:PRO:HD3	12	0.36
(1,1910)	1:178:A:PRO:HB2	1:179:A:ALA:H	1	0.36
(1,1910)	1:178:A:PRO:HB3	1:179:A:ALA:H	1	0.36
(1,1910)	1:178:A:PRO:HB2	1:179:A:ALA:H	6	0.36
(1,1910)	1:178:A:PRO:HB3	1:179:A:ALA:H	6	0.36
(1,1910)	1:178:A:PRO:HB2	1:179:A:ALA:H	11	0.36
(1,1910)	1:178:A:PRO:HB3	1:179:A:ALA:H	11	0.36
(1,1910)	1:178:A:PRO:HB2	1:179:A:ALA:H	12	0.36
(1,1910)	1:178:A:PRO:HB3	1:179:A:ALA:H	12	0.36
(1,1910)	1:178:A:PRO:HB2	1:179:A:ALA:H	13	0.36
(1,1910)	1:178:A:PRO:HB3	1:179:A:ALA:H	13	0.36
(1,1676)	1:94:A:PHE:H	1:102:A:VAL:HG11	4	0.36
(1,1676)	1:94:A:PHE:H	1:102:A:VAL:HG12	4	0.36
(1,1676)	1:94:A:PHE:H	1:102:A:VAL:HG13	4	0.36
(1,1561)	1:167:C:ARG:H	1:167:C:ARG:HB3	1	0.36
(1,1561)	1:167:C:ARG:H	1:167:C:ARG:HB3	5	0.36
(1,1561)	1:167:C:ARG:H	1:167:C:ARG:HB3	6	0.36
(1,1561)	1:167:C:ARG:H	1:167:C:ARG:HB3	7	0.36
(1,1561)	1:167:C:ARG:H	1:167:C:ARG:HB3	8	0.36
(1,1561)	1:167:C:ARG:H	1:167:C:ARG:HB3	9	0.36
(1,1560)	1:167:B:ARG:H	1:167:B:ARG:HB3	1	0.36
(1,1560)	1:167:B:ARG:H	1:167:B:ARG:HB3	3	0.36
(1,1560)	1:167:B:ARG:H	1:167:B:ARG:HB3	5	0.36
(1,1560)	1:167:B:ARG:H	1:167:B:ARG:HB3	6	0.36
(1,1560)	1:167:B:ARG:H	1:167:B:ARG:HB3	7	0.36
(1,1560)	1:167:B:ARG:H	1:167:B:ARG:HB3	8	0.36
(1,1560)	1:167:B:ARG:H	1:167:B:ARG:HB3	9	0.36
(1,1559)	1:167:A:ARG:H	1:167:A:ARG:HB3	1	0.36
(1,1559)	1:167:A:ARG:H	1:167:A:ARG:HB3	3	0.36
(1,1559)	1:167:A:ARG:H	1:167:A:ARG:HB3	8	0.36
(1,1559)	1:167:A:ARG:H	1:167:A:ARG:HB3	9	0.36
(1,1559)	1:167:A:ARG:H	1:167:A:ARG:HB3	11	0.36
(1,1559)	1:167:A:ARG:H	1:167:A:ARG:HB3	16	0.36
(1,1445)	1:155:C:ALA:HA	1:156:C:VAL:H	8	0.36
(1,1444)	1:155:B:ALA:HA	1:156:B:VAL:H	6	0.36
(1,1444)	1:155:B:ALA:HA	1:156:B:VAL:H	8	0.36
(1,935)	1:95:A:SER:H	1:101:A:LEU:HD11	16	0.36
(1,935)	1:95:A:SER:H	1:101:A:LEU:HD12	16	0.36
(1,935)	1:95:A:SER:H	1:101:A:LEU:HD13	16	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,888)	1:152:A:ALA:HA	1:157:A:PRO:HG2	14	0.36
(1,888)	1:152:A:ALA:HA	1:157:A:PRO:HG3	14	0.36
(1,730)	1:155:C:ALA:HB1	1:157:C:PRO:HD2	7	0.36
(1,730)	1:155:C:ALA:HB2	1:157:C:PRO:HD2	7	0.36
(1,730)	1:155:C:ALA:HB3	1:157:C:PRO:HD2	7	0.36
(1,729)	1:155:B:ALA:HB1	1:157:B:PRO:HD2	7	0.36
(1,729)	1:155:B:ALA:HB2	1:157:B:PRO:HD2	7	0.36
(1,729)	1:155:B:ALA:HB3	1:157:B:PRO:HD2	7	0.36
(1,215)	1:101:A:LEU:HD21	1:103:A:VAL:HG11	13	0.36
(1,215)	1:101:A:LEU:HD21	1:103:A:VAL:HG12	13	0.36
(1,215)	1:101:A:LEU:HD21	1:103:A:VAL:HG13	13	0.36
(1,215)	1:101:A:LEU:HD22	1:103:A:VAL:HG11	13	0.36
(1,215)	1:101:A:LEU:HD22	1:103:A:VAL:HG12	13	0.36
(1,215)	1:101:A:LEU:HD22	1:103:A:VAL:HG13	13	0.36
(1,215)	1:101:A:LEU:HD23	1:103:A:VAL:HG11	13	0.36
(1,215)	1:101:A:LEU:HD23	1:103:A:VAL:HG12	13	0.36
(1,215)	1:101:A:LEU:HD23	1:103:A:VAL:HG13	13	0.36
(1,124)	1:96:A:ILE:H	1:101:A:LEU:HD21	8	0.36
(1,124)	1:96:A:ILE:H	1:101:A:LEU:HD22	8	0.36
(1,124)	1:96:A:ILE:H	1:101:A:LEU:HD23	8	0.36
(1,2329)	1:178:C:PRO:HB2	1:179:C:ALA:H	12	0.35
(1,2329)	1:178:C:PRO:HB3	1:179:C:ALA:H	12	0.35
(1,2320)	1:172:C:ALA:HA	1:178:C:PRO:HD2	4	0.35
(1,2320)	1:172:C:ALA:HA	1:178:C:PRO:HD3	4	0.35
(1,2298)	1:156:C:VAL:HB	1:157:C:PRO:HD2	12	0.35
(1,2298)	1:156:C:VAL:HB	1:157:C:PRO:HD3	12	0.35
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG11	17	0.35
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG12	17	0.35
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG13	17	0.35
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG21	17	0.35
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG22	17	0.35
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG23	17	0.35
(1,2103)	1:178:B:PRO:HB2	1:179:B:ALA:H	12	0.35
(1,2103)	1:178:B:PRO:HB3	1:179:B:ALA:H	12	0.35
(1,2094)	1:172:B:ALA:HA	1:178:B:PRO:HD2	4	0.35
(1,2094)	1:172:B:ALA:HA	1:178:B:PRO:HD3	4	0.35
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG11	17	0.35
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG12	17	0.35
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG13	17	0.35
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG21	17	0.35
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG22	17	0.35
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG23	17	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1830)	1:102:A:VAL:HG11	1:111:A:ILE:HG12	13	0.35
(1,1830)	1:102:A:VAL:HG11	1:111:A:ILE:HG13	13	0.35
(1,1830)	1:102:A:VAL:HG12	1:111:A:ILE:HG12	13	0.35
(1,1830)	1:102:A:VAL:HG12	1:111:A:ILE:HG13	13	0.35
(1,1830)	1:102:A:VAL:HG13	1:111:A:ILE:HG12	13	0.35
(1,1830)	1:102:A:VAL:HG13	1:111:A:ILE:HG13	13	0.35
(1,1830)	1:102:A:VAL:HG11	1:111:A:ILE:HG12	14	0.35
(1,1830)	1:102:A:VAL:HG11	1:111:A:ILE:HG13	14	0.35
(1,1830)	1:102:A:VAL:HG12	1:111:A:ILE:HG12	14	0.35
(1,1830)	1:102:A:VAL:HG12	1:111:A:ILE:HG13	14	0.35
(1,1830)	1:102:A:VAL:HG13	1:111:A:ILE:HG12	14	0.35
(1,1830)	1:102:A:VAL:HG13	1:111:A:ILE:HG13	14	0.35
(1,1561)	1:167:C:ARG:H	1:167:C:ARG:HB3	12	0.35
(1,1560)	1:167:B:ARG:H	1:167:B:ARG:HB3	12	0.35
(1,1559)	1:167:A:ARG:H	1:167:A:ARG:HB3	5	0.35
(1,1559)	1:167:A:ARG:H	1:167:A:ARG:HB3	6	0.35
(1,1559)	1:167:A:ARG:H	1:167:A:ARG:HB3	7	0.35
(1,1559)	1:167:A:ARG:H	1:167:A:ARG:HB3	12	0.35
(1,1461)	1:180:A:PHE:H	1:181:A:LEU:HA	18	0.35
(1,1445)	1:155:C:ALA:HA	1:156:C:VAL:H	5	0.35
(1,1445)	1:155:C:ALA:HA	1:156:C:VAL:H	6	0.35
(1,1445)	1:155:C:ALA:HA	1:156:C:VAL:H	9	0.35
(1,1444)	1:155:B:ALA:HA	1:156:B:VAL:H	5	0.35
(1,1444)	1:155:B:ALA:HA	1:156:B:VAL:H	9	0.35
(1,753)	1:189:A:CYS:H	1:192:A:VAL:HG11	8	0.35
(1,753)	1:189:A:CYS:H	1:192:A:VAL:HG12	8	0.35
(1,753)	1:189:A:CYS:H	1:192:A:VAL:HG13	8	0.35
(1,728)	1:155:A:ALA:HB1	1:157:A:PRO:HD2	7	0.35
(1,728)	1:155:A:ALA:HB2	1:157:A:PRO:HD2	7	0.35
(1,728)	1:155:A:ALA:HB3	1:157:A:PRO:HD2	7	0.35
(1,728)	1:155:A:ALA:HB1	1:157:A:PRO:HD2	15	0.35
(1,728)	1:155:A:ALA:HB2	1:157:A:PRO:HD2	15	0.35
(1,728)	1:155:A:ALA:HB3	1:157:A:PRO:HD2	15	0.35
(1,395)	1:109:A:LEU:HG	1:111:A:ILE:HD11	17	0.35
(1,395)	1:109:A:LEU:HG	1:111:A:ILE:HD12	17	0.35
(1,395)	1:109:A:LEU:HG	1:111:A:ILE:HD13	17	0.35
(1,138)	1:192:A:VAL:HG21	1:135:B:GLU:HG2	1	0.35
(1,138)	1:192:A:VAL:HG21	1:135:B:GLU:HG3	1	0.35
(1,138)	1:192:A:VAL:HG22	1:135:B:GLU:HG2	1	0.35
(1,138)	1:192:A:VAL:HG22	1:135:B:GLU:HG3	1	0.35
(1,138)	1:192:A:VAL:HG23	1:135:B:GLU:HG2	1	0.35
(1,138)	1:192:A:VAL:HG23	1:135:B:GLU:HG3	1	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2298)	1:156:C:VAL:HB	1:157:C:PRO:HD2	11	0.34
(1,2298)	1:156:C:VAL:HB	1:157:C:PRO:HD3	11	0.34
(1,2072)	1:156:B:VAL:HB	1:157:B:PRO:HD2	11	0.34
(1,2072)	1:156:B:VAL:HB	1:157:B:PRO:HD3	11	0.34
(1,1887)	1:156:A:VAL:HB	1:157:A:PRO:HD2	10	0.34
(1,1887)	1:156:A:VAL:HB	1:157:A:PRO:HD3	10	0.34
(1,1887)	1:156:A:VAL:HB	1:157:A:PRO:HD2	17	0.34
(1,1887)	1:156:A:VAL:HB	1:157:A:PRO:HD3	17	0.34
(1,1818)	1:95:B:SER:HB2	1:101:B:LEU:H	3	0.34
(1,1818)	1:95:B:SER:HB3	1:101:B:LEU:H	3	0.34
(1,1559)	1:167:A:ARG:H	1:167:A:ARG:HB3	15	0.34
(1,1463)	1:180:C:PHE:H	1:181:C:LEU:HA	19	0.34
(1,1445)	1:155:C:ALA:HA	1:156:C:VAL:H	4	0.34
(1,1444)	1:155:B:ALA:HA	1:156:B:VAL:H	4	0.34
(1,1443)	1:155:A:ALA:HA	1:156:A:VAL:H	9	0.34
(1,753)	1:189:A:CYS:H	1:192:A:VAL:HG11	1	0.34
(1,753)	1:189:A:CYS:H	1:192:A:VAL:HG12	1	0.34
(1,753)	1:189:A:CYS:H	1:192:A:VAL:HG13	1	0.34
(1,753)	1:189:A:CYS:H	1:192:A:VAL:HG11	5	0.34
(1,753)	1:189:A:CYS:H	1:192:A:VAL:HG12	5	0.34
(1,753)	1:189:A:CYS:H	1:192:A:VAL:HG13	5	0.34
(1,730)	1:155:C:ALA:HB1	1:157:C:PRO:HD2	4	0.34
(1,730)	1:155:C:ALA:HB2	1:157:C:PRO:HD2	4	0.34
(1,730)	1:155:C:ALA:HB3	1:157:C:PRO:HD2	4	0.34
(1,730)	1:155:C:ALA:HB1	1:157:C:PRO:HD2	9	0.34
(1,730)	1:155:C:ALA:HB2	1:157:C:PRO:HD2	9	0.34
(1,730)	1:155:C:ALA:HB3	1:157:C:PRO:HD2	9	0.34
(1,730)	1:155:C:ALA:HB1	1:157:C:PRO:HD2	16	0.34
(1,730)	1:155:C:ALA:HB2	1:157:C:PRO:HD2	16	0.34
(1,730)	1:155:C:ALA:HB3	1:157:C:PRO:HD2	16	0.34
(1,729)	1:155:B:ALA:HB1	1:157:B:PRO:HD2	4	0.34
(1,729)	1:155:B:ALA:HB2	1:157:B:PRO:HD2	4	0.34
(1,729)	1:155:B:ALA:HB3	1:157:B:PRO:HD2	4	0.34
(1,729)	1:155:B:ALA:HB1	1:157:B:PRO:HD2	9	0.34
(1,729)	1:155:B:ALA:HB2	1:157:B:PRO:HD2	9	0.34
(1,729)	1:155:B:ALA:HB3	1:157:B:PRO:HD2	9	0.34
(1,729)	1:155:B:ALA:HB1	1:157:B:PRO:HD2	16	0.34
(1,729)	1:155:B:ALA:HB2	1:157:B:PRO:HD2	16	0.34
(1,729)	1:155:B:ALA:HB3	1:157:B:PRO:HD2	16	0.34
(1,728)	1:155:A:ALA:HB1	1:157:A:PRO:HD2	17	0.34
(1,728)	1:155:A:ALA:HB2	1:157:A:PRO:HD2	17	0.34
(1,728)	1:155:A:ALA:HB3	1:157:A:PRO:HD2	17	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,728)	1:155:A:ALA:HB1	1:157:A:PRO:HD2	18	0.34
(1,728)	1:155:A:ALA:HB2	1:157:A:PRO:HD2	18	0.34
(1,728)	1:155:A:ALA:HB3	1:157:A:PRO:HD2	18	0.34
(1,573)	1:194:A:LEU:HD21	1:196:A:TYR:HE1	13	0.34
(1,573)	1:194:A:LEU:HD21	1:196:A:TYR:HE2	13	0.34
(1,573)	1:194:A:LEU:HD22	1:196:A:TYR:HE1	13	0.34
(1,573)	1:194:A:LEU:HD22	1:196:A:TYR:HE2	13	0.34
(1,573)	1:194:A:LEU:HD23	1:196:A:TYR:HE1	13	0.34
(1,573)	1:194:A:LEU:HD23	1:196:A:TYR:HE2	13	0.34
(1,138)	1:192:A:VAL:HG21	1:135:B:GLU:HG2	5	0.34
(1,138)	1:192:A:VAL:HG21	1:135:B:GLU:HG3	5	0.34
(1,138)	1:192:A:VAL:HG22	1:135:B:GLU:HG2	5	0.34
(1,138)	1:192:A:VAL:HG22	1:135:B:GLU:HG3	5	0.34
(1,138)	1:192:A:VAL:HG23	1:135:B:GLU:HG2	5	0.34
(1,138)	1:192:A:VAL:HG23	1:135:B:GLU:HG3	5	0.34
(1,138)	1:192:A:VAL:HG21	1:135:B:GLU:HG2	8	0.34
(1,138)	1:192:A:VAL:HG21	1:135:B:GLU:HG3	8	0.34
(1,138)	1:192:A:VAL:HG22	1:135:B:GLU:HG2	8	0.34
(1,138)	1:192:A:VAL:HG22	1:135:B:GLU:HG3	8	0.34
(1,138)	1:192:A:VAL:HG23	1:135:B:GLU:HG2	8	0.34
(1,138)	1:192:A:VAL:HG23	1:135:B:GLU:HG3	8	0.34
(1,138)	1:192:A:VAL:HG21	1:135:B:GLU:HG2	11	0.34
(1,138)	1:192:A:VAL:HG21	1:135:B:GLU:HG3	11	0.34
(1,138)	1:192:A:VAL:HG22	1:135:B:GLU:HG2	11	0.34
(1,138)	1:192:A:VAL:HG22	1:135:B:GLU:HG3	11	0.34
(1,138)	1:192:A:VAL:HG23	1:135:B:GLU:HG2	11	0.34
(1,138)	1:192:A:VAL:HG23	1:135:B:GLU:HG3	11	0.34
(1,138)	1:192:A:VAL:HG21	1:135:B:GLU:HG2	19	0.34
(1,138)	1:192:A:VAL:HG21	1:135:B:GLU:HG3	19	0.34
(1,138)	1:192:A:VAL:HG22	1:135:B:GLU:HG2	19	0.34
(1,138)	1:192:A:VAL:HG22	1:135:B:GLU:HG3	19	0.34
(1,138)	1:192:A:VAL:HG23	1:135:B:GLU:HG2	19	0.34
(1,138)	1:192:A:VAL:HG23	1:135:B:GLU:HG3	19	0.34
(1,122)	1:113:A:TYR:HD1	1:137:A:LEU:HD21	16	0.34
(1,122)	1:113:A:TYR:HD1	1:137:A:LEU:HD22	16	0.34
(1,122)	1:113:A:TYR:HD1	1:137:A:LEU:HD23	16	0.34
(1,122)	1:113:A:TYR:HD2	1:137:A:LEU:HD21	16	0.34
(1,122)	1:113:A:TYR:HD2	1:137:A:LEU:HD22	16	0.34
(1,122)	1:113:A:TYR:HD2	1:137:A:LEU:HD23	16	0.34
(1,56)	1:156:A:VAL:HG11	1:157:A:PRO:HD3	14	0.34
(1,56)	1:156:A:VAL:HG12	1:157:A:PRO:HD3	14	0.34
(1,56)	1:156:A:VAL:HG13	1:157:A:PRO:HD3	14	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2283)	1:150:C:LEU:HD11	1:167:C:ARG:HG2	17	0.33
(1,2283)	1:150:C:LEU:HD11	1:167:C:ARG:HG3	17	0.33
(1,2283)	1:150:C:LEU:HD12	1:167:C:ARG:HG2	17	0.33
(1,2283)	1:150:C:LEU:HD12	1:167:C:ARG:HG3	17	0.33
(1,2283)	1:150:C:LEU:HD13	1:167:C:ARG:HG2	17	0.33
(1,2283)	1:150:C:LEU:HD13	1:167:C:ARG:HG3	17	0.33
(1,2283)	1:150:C:LEU:HD21	1:167:C:ARG:HG2	17	0.33
(1,2283)	1:150:C:LEU:HD21	1:167:C:ARG:HG3	17	0.33
(1,2283)	1:150:C:LEU:HD22	1:167:C:ARG:HG2	17	0.33
(1,2283)	1:150:C:LEU:HD22	1:167:C:ARG:HG3	17	0.33
(1,2283)	1:150:C:LEU:HD23	1:167:C:ARG:HG2	17	0.33
(1,2283)	1:150:C:LEU:HD23	1:167:C:ARG:HG3	17	0.33
(1,1887)	1:156:A:VAL:HB	1:157:A:PRO:HD2	13	0.33
(1,1887)	1:156:A:VAL:HB	1:157:A:PRO:HD3	13	0.33
(1,1887)	1:156:A:VAL:HB	1:157:A:PRO:HD2	19	0.33
(1,1887)	1:156:A:VAL:HB	1:157:A:PRO:HD3	19	0.33
(1,1561)	1:167:C:ARG:H	1:167:C:ARG:HB3	13	0.33
(1,1561)	1:167:C:ARG:H	1:167:C:ARG:HB3	15	0.33
(1,1561)	1:167:C:ARG:H	1:167:C:ARG:HB3	19	0.33
(1,1560)	1:167:B:ARG:H	1:167:B:ARG:HB3	13	0.33
(1,1560)	1:167:B:ARG:H	1:167:B:ARG:HB3	15	0.33
(1,1559)	1:167:A:ARG:H	1:167:A:ARG:HB3	19	0.33
(1,1462)	1:180:B:PHE:H	1:181:B:LEU:HA	19	0.33
(1,1443)	1:155:A:ALA:HA	1:156:A:VAL:H	5	0.33
(1,1036)	1:188:A:LEU:HD21	1:134:B:LEU:H	15	0.33
(1,1036)	1:188:A:LEU:HD22	1:134:B:LEU:H	15	0.33
(1,1036)	1:188:A:LEU:HD23	1:134:B:LEU:H	15	0.33
(1,935)	1:95:A:SER:H	1:101:A:LEU:HD11	10	0.33
(1,935)	1:95:A:SER:H	1:101:A:LEU:HD12	10	0.33
(1,935)	1:95:A:SER:H	1:101:A:LEU:HD13	10	0.33
(1,890)	1:152:C:ALA:HA	1:157:C:PRO:HG2	14	0.33
(1,890)	1:152:C:ALA:HA	1:157:C:PRO:HG3	14	0.33
(1,890)	1:152:C:ALA:HA	1:157:C:PRO:HG2	20	0.33
(1,890)	1:152:C:ALA:HA	1:157:C:PRO:HG3	20	0.33
(1,889)	1:152:B:ALA:HA	1:157:B:PRO:HG2	14	0.33
(1,889)	1:152:B:ALA:HA	1:157:B:PRO:HG3	14	0.33
(1,753)	1:189:A:CYS:H	1:192:A:VAL:HG11	11	0.33
(1,753)	1:189:A:CYS:H	1:192:A:VAL:HG12	11	0.33
(1,753)	1:189:A:CYS:H	1:192:A:VAL:HG13	11	0.33
(1,728)	1:155:A:ALA:HB1	1:157:A:PRO:HD2	16	0.33
(1,728)	1:155:A:ALA:HB2	1:157:A:PRO:HD2	16	0.33
(1,728)	1:155:A:ALA:HB3	1:157:A:PRO:HD2	16	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,395)	1:109:A:LEU:HG	1:111:A:ILE:HD11	11	0.33
(1,395)	1:109:A:LEU:HG	1:111:A:ILE:HD12	11	0.33
(1,395)	1:109:A:LEU:HG	1:111:A:ILE:HD13	11	0.33
(1,395)	1:109:A:LEU:HG	1:111:A:ILE:HD11	14	0.33
(1,395)	1:109:A:LEU:HG	1:111:A:ILE:HD12	14	0.33
(1,395)	1:109:A:LEU:HG	1:111:A:ILE:HD13	14	0.33
(1,138)	1:192:A:VAL:HG21	1:135:B:GLU:HG2	16	0.33
(1,138)	1:192:A:VAL:HG21	1:135:B:GLU:HG3	16	0.33
(1,138)	1:192:A:VAL:HG22	1:135:B:GLU:HG2	16	0.33
(1,138)	1:192:A:VAL:HG22	1:135:B:GLU:HG3	16	0.33
(1,138)	1:192:A:VAL:HG23	1:135:B:GLU:HG2	16	0.33
(1,138)	1:192:A:VAL:HG23	1:135:B:GLU:HG3	16	0.33
(1,26)	1:109:A:LEU:HD21	1:110:A:LEU:H	19	0.33
(1,26)	1:109:A:LEU:HD22	1:110:A:LEU:H	19	0.33
(1,26)	1:109:A:LEU:HD23	1:110:A:LEU:H	19	0.33
(1,2295)	1:155:C:ALA:HB1	1:157:C:PRO:HD2	12	0.32
(1,2295)	1:155:C:ALA:HB1	1:157:C:PRO:HD3	12	0.32
(1,2295)	1:155:C:ALA:HB2	1:157:C:PRO:HD2	12	0.32
(1,2295)	1:155:C:ALA:HB2	1:157:C:PRO:HD3	12	0.32
(1,2295)	1:155:C:ALA:HB3	1:157:C:PRO:HD2	12	0.32
(1,2295)	1:155:C:ALA:HB3	1:157:C:PRO:HD3	12	0.32
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG11	13	0.32
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG12	13	0.32
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG13	13	0.32
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG21	13	0.32
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG22	13	0.32
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG23	13	0.32
(1,2289)	1:153:C:LYS:HA	1:154:C:PRO:HD2	1	0.32
(1,2289)	1:153:C:LYS:HA	1:154:C:PRO:HD3	1	0.32
(1,2289)	1:153:C:LYS:HA	1:154:C:PRO:HD2	2	0.32
(1,2289)	1:153:C:LYS:HA	1:154:C:PRO:HD3	2	0.32
(1,2289)	1:153:C:LYS:HA	1:154:C:PRO:HD2	3	0.32
(1,2289)	1:153:C:LYS:HA	1:154:C:PRO:HD3	3	0.32
(1,2289)	1:153:C:LYS:HA	1:154:C:PRO:HD2	4	0.32
(1,2289)	1:153:C:LYS:HA	1:154:C:PRO:HD3	4	0.32
(1,2289)	1:153:C:LYS:HA	1:154:C:PRO:HD2	5	0.32
(1,2289)	1:153:C:LYS:HA	1:154:C:PRO:HD3	5	0.32
(1,2289)	1:153:C:LYS:HA	1:154:C:PRO:HD2	6	0.32
(1,2289)	1:153:C:LYS:HA	1:154:C:PRO:HD3	6	0.32
(1,2289)	1:153:C:LYS:HA	1:154:C:PRO:HD2	8	0.32
(1,2289)	1:153:C:LYS:HA	1:154:C:PRO:HD3	8	0.32
(1,2289)	1:153:C:LYS:HA	1:154:C:PRO:HD2	10	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2289)	1:153:C:LYS:HA	1:154:C:PRO:HD3	10	0.32
(1,2289)	1:153:C:LYS:HA	1:154:C:PRO:HD2	11	0.32
(1,2289)	1:153:C:LYS:HA	1:154:C:PRO:HD3	11	0.32
(1,2289)	1:153:C:LYS:HA	1:154:C:PRO:HD2	12	0.32
(1,2289)	1:153:C:LYS:HA	1:154:C:PRO:HD3	12	0.32
(1,2289)	1:153:C:LYS:HA	1:154:C:PRO:HD2	13	0.32
(1,2289)	1:153:C:LYS:HA	1:154:C:PRO:HD3	13	0.32
(1,2289)	1:153:C:LYS:HA	1:154:C:PRO:HD2	15	0.32
(1,2289)	1:153:C:LYS:HA	1:154:C:PRO:HD3	15	0.32
(1,2289)	1:153:C:LYS:HA	1:154:C:PRO:HD2	17	0.32
(1,2289)	1:153:C:LYS:HA	1:154:C:PRO:HD3	17	0.32
(1,2289)	1:153:C:LYS:HA	1:154:C:PRO:HD2	18	0.32
(1,2289)	1:153:C:LYS:HA	1:154:C:PRO:HD3	18	0.32
(1,2289)	1:153:C:LYS:HA	1:154:C:PRO:HD2	19	0.32
(1,2289)	1:153:C:LYS:HA	1:154:C:PRO:HD3	19	0.32
(1,2289)	1:153:C:LYS:HA	1:154:C:PRO:HD2	20	0.32
(1,2289)	1:153:C:LYS:HA	1:154:C:PRO:HD3	20	0.32
(1,2069)	1:155:B:ALA:HB1	1:157:B:PRO:HD2	12	0.32
(1,2069)	1:155:B:ALA:HB1	1:157:B:PRO:HD3	12	0.32
(1,2069)	1:155:B:ALA:HB2	1:157:B:PRO:HD2	12	0.32
(1,2069)	1:155:B:ALA:HB2	1:157:B:PRO:HD3	12	0.32
(1,2069)	1:155:B:ALA:HB3	1:157:B:PRO:HD2	12	0.32
(1,2069)	1:155:B:ALA:HB3	1:157:B:PRO:HD3	12	0.32
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG11	13	0.32
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG12	13	0.32
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG13	13	0.32
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG21	13	0.32
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG22	13	0.32
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG23	13	0.32
(1,2063)	1:153:B:LYS:HA	1:154:B:PRO:HD2	1	0.32
(1,2063)	1:153:B:LYS:HA	1:154:B:PRO:HD3	1	0.32
(1,2063)	1:153:B:LYS:HA	1:154:B:PRO:HD2	2	0.32
(1,2063)	1:153:B:LYS:HA	1:154:B:PRO:HD3	2	0.32
(1,2063)	1:153:B:LYS:HA	1:154:B:PRO:HD2	3	0.32
(1,2063)	1:153:B:LYS:HA	1:154:B:PRO:HD3	3	0.32
(1,2063)	1:153:B:LYS:HA	1:154:B:PRO:HD2	4	0.32
(1,2063)	1:153:B:LYS:HA	1:154:B:PRO:HD3	4	0.32
(1,2063)	1:153:B:LYS:HA	1:154:B:PRO:HD2	5	0.32
(1,2063)	1:153:B:LYS:HA	1:154:B:PRO:HD3	5	0.32
(1,2063)	1:153:B:LYS:HA	1:154:B:PRO:HD2	6	0.32
(1,2063)	1:153:B:LYS:HA	1:154:B:PRO:HD3	6	0.32
(1,2063)	1:153:B:LYS:HA	1:154:B:PRO:HD2	8	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2063)	1:153:B:LYS:HA	1:154:B:PRO:HD3	8	0.32
(1,2063)	1:153:B:LYS:HA	1:154:B:PRO:HD2	10	0.32
(1,2063)	1:153:B:LYS:HA	1:154:B:PRO:HD3	10	0.32
(1,2063)	1:153:B:LYS:HA	1:154:B:PRO:HD2	11	0.32
(1,2063)	1:153:B:LYS:HA	1:154:B:PRO:HD3	11	0.32
(1,2063)	1:153:B:LYS:HA	1:154:B:PRO:HD2	12	0.32
(1,2063)	1:153:B:LYS:HA	1:154:B:PRO:HD3	12	0.32
(1,2063)	1:153:B:LYS:HA	1:154:B:PRO:HD2	13	0.32
(1,2063)	1:153:B:LYS:HA	1:154:B:PRO:HD3	13	0.32
(1,2063)	1:153:B:LYS:HA	1:154:B:PRO:HD2	15	0.32
(1,2063)	1:153:B:LYS:HA	1:154:B:PRO:HD3	15	0.32
(1,2063)	1:153:B:LYS:HA	1:154:B:PRO:HD2	17	0.32
(1,2063)	1:153:B:LYS:HA	1:154:B:PRO:HD3	17	0.32
(1,2063)	1:153:B:LYS:HA	1:154:B:PRO:HD2	18	0.32
(1,2063)	1:153:B:LYS:HA	1:154:B:PRO:HD3	18	0.32
(1,2063)	1:153:B:LYS:HA	1:154:B:PRO:HD2	19	0.32
(1,2063)	1:153:B:LYS:HA	1:154:B:PRO:HD3	19	0.32
(1,2063)	1:153:B:LYS:HA	1:154:B:PRO:HD2	20	0.32
(1,2063)	1:153:B:LYS:HA	1:154:B:PRO:HD3	20	0.32
(1,2057)	1:150:B:LEU:HD11	1:167:B:ARG:HG2	17	0.32
(1,2057)	1:150:B:LEU:HD11	1:167:B:ARG:HG3	17	0.32
(1,2057)	1:150:B:LEU:HD12	1:167:B:ARG:HG2	17	0.32
(1,2057)	1:150:B:LEU:HD12	1:167:B:ARG:HG3	17	0.32
(1,2057)	1:150:B:LEU:HD13	1:167:B:ARG:HG2	17	0.32
(1,2057)	1:150:B:LEU:HD13	1:167:B:ARG:HG3	17	0.32
(1,2057)	1:150:B:LEU:HD21	1:167:B:ARG:HG2	17	0.32
(1,2057)	1:150:B:LEU:HD21	1:167:B:ARG:HG3	17	0.32
(1,2057)	1:150:B:LEU:HD22	1:167:B:ARG:HG2	17	0.32
(1,2057)	1:150:B:LEU:HD22	1:167:B:ARG:HG3	17	0.32
(1,2057)	1:150:B:LEU:HD23	1:167:B:ARG:HG2	17	0.32
(1,2057)	1:150:B:LEU:HD23	1:167:B:ARG:HG3	17	0.32
(1,1902)	1:172:A:ALA:HA	1:178:A:PRO:HD2	4	0.32
(1,1902)	1:172:A:ALA:HA	1:178:A:PRO:HD3	4	0.32
(1,1887)	1:156:A:VAL:HB	1:157:A:PRO:HD2	18	0.32
(1,1887)	1:156:A:VAL:HB	1:157:A:PRO:HD3	18	0.32
(1,1887)	1:156:A:VAL:HB	1:157:A:PRO:HD2	20	0.32
(1,1887)	1:156:A:VAL:HB	1:157:A:PRO:HD3	20	0.32
(1,1885)	1:155:A:ALA:HB1	1:157:A:PRO:HD2	11	0.32
(1,1885)	1:155:A:ALA:HB1	1:157:A:PRO:HD3	11	0.32
(1,1885)	1:155:A:ALA:HB2	1:157:A:PRO:HD2	11	0.32
(1,1885)	1:155:A:ALA:HB2	1:157:A:PRO:HD3	11	0.32
(1,1885)	1:155:A:ALA:HB3	1:157:A:PRO:HD2	11	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1885)	1:155:A:ALA:HB3	1:157:A:PRO:HD3	11	0.32
(1,1881)	1:153:A:LYS:HA	1:154:A:PRO:HD2	1	0.32
(1,1881)	1:153:A:LYS:HA	1:154:A:PRO:HD3	1	0.32
(1,1881)	1:153:A:LYS:HA	1:154:A:PRO:HD2	2	0.32
(1,1881)	1:153:A:LYS:HA	1:154:A:PRO:HD3	2	0.32
(1,1881)	1:153:A:LYS:HA	1:154:A:PRO:HD2	3	0.32
(1,1881)	1:153:A:LYS:HA	1:154:A:PRO:HD3	3	0.32
(1,1881)	1:153:A:LYS:HA	1:154:A:PRO:HD2	4	0.32
(1,1881)	1:153:A:LYS:HA	1:154:A:PRO:HD3	4	0.32
(1,1881)	1:153:A:LYS:HA	1:154:A:PRO:HD2	5	0.32
(1,1881)	1:153:A:LYS:HA	1:154:A:PRO:HD3	5	0.32
(1,1881)	1:153:A:LYS:HA	1:154:A:PRO:HD2	6	0.32
(1,1881)	1:153:A:LYS:HA	1:154:A:PRO:HD3	6	0.32
(1,1881)	1:153:A:LYS:HA	1:154:A:PRO:HD2	8	0.32
(1,1881)	1:153:A:LYS:HA	1:154:A:PRO:HD3	8	0.32
(1,1881)	1:153:A:LYS:HA	1:154:A:PRO:HD2	10	0.32
(1,1881)	1:153:A:LYS:HA	1:154:A:PRO:HD3	10	0.32
(1,1881)	1:153:A:LYS:HA	1:154:A:PRO:HD2	11	0.32
(1,1881)	1:153:A:LYS:HA	1:154:A:PRO:HD3	11	0.32
(1,1881)	1:153:A:LYS:HA	1:154:A:PRO:HD2	12	0.32
(1,1881)	1:153:A:LYS:HA	1:154:A:PRO:HD3	12	0.32
(1,1881)	1:153:A:LYS:HA	1:154:A:PRO:HD2	13	0.32
(1,1881)	1:153:A:LYS:HA	1:154:A:PRO:HD3	13	0.32
(1,1881)	1:153:A:LYS:HA	1:154:A:PRO:HD2	15	0.32
(1,1881)	1:153:A:LYS:HA	1:154:A:PRO:HD3	15	0.32
(1,1881)	1:153:A:LYS:HA	1:154:A:PRO:HD2	17	0.32
(1,1881)	1:153:A:LYS:HA	1:154:A:PRO:HD3	17	0.32
(1,1881)	1:153:A:LYS:HA	1:154:A:PRO:HD2	18	0.32
(1,1881)	1:153:A:LYS:HA	1:154:A:PRO:HD3	18	0.32
(1,1881)	1:153:A:LYS:HA	1:154:A:PRO:HD2	19	0.32
(1,1881)	1:153:A:LYS:HA	1:154:A:PRO:HD3	19	0.32
(1,1881)	1:153:A:LYS:HA	1:154:A:PRO:HD2	20	0.32
(1,1881)	1:153:A:LYS:HA	1:154:A:PRO:HD3	20	0.32
(1,1817)	1:95:A:SER:HB2	1:101:A:LEU:H	3	0.32
(1,1817)	1:95:A:SER:HB3	1:101:A:LEU:H	3	0.32
(1,1560)	1:167:B:ARG:H	1:167:B:ARG:HB3	19	0.32
(1,1559)	1:167:A:ARG:H	1:167:A:ARG:HB3	13	0.32
(1,1559)	1:167:A:ARG:H	1:167:A:ARG:HB3	20	0.32
(1,1461)	1:180:A:PHE:H	1:181:A:LEU:HA	15	0.32
(1,889)	1:152:B:ALA:HA	1:157:B:PRO:HG2	20	0.32
(1,889)	1:152:B:ALA:HA	1:157:B:PRO:HG3	20	0.32
(1,753)	1:189:A:CYS:H	1:192:A:VAL:HG11	6	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,753)	1:189:A:CYS:H	1:192:A:VAL:HG12	6	0.32
(1,753)	1:189:A:CYS:H	1:192:A:VAL:HG13	6	0.32
(1,753)	1:189:A:CYS:H	1:192:A:VAL:HG11	7	0.32
(1,753)	1:189:A:CYS:H	1:192:A:VAL:HG12	7	0.32
(1,753)	1:189:A:CYS:H	1:192:A:VAL:HG13	7	0.32
(1,753)	1:189:A:CYS:H	1:192:A:VAL:HG11	9	0.32
(1,753)	1:189:A:CYS:H	1:192:A:VAL:HG12	9	0.32
(1,753)	1:189:A:CYS:H	1:192:A:VAL:HG13	9	0.32
(1,753)	1:189:A:CYS:H	1:192:A:VAL:HG11	12	0.32
(1,753)	1:189:A:CYS:H	1:192:A:VAL:HG12	12	0.32
(1,753)	1:189:A:CYS:H	1:192:A:VAL:HG13	12	0.32
(1,753)	1:189:A:CYS:H	1:192:A:VAL:HG11	19	0.32
(1,753)	1:189:A:CYS:H	1:192:A:VAL:HG12	19	0.32
(1,753)	1:189:A:CYS:H	1:192:A:VAL:HG13	19	0.32
(1,730)	1:155:C:ALA:HB1	1:157:C:PRO:HD2	1	0.32
(1,730)	1:155:C:ALA:HB2	1:157:C:PRO:HD2	1	0.32
(1,730)	1:155:C:ALA:HB3	1:157:C:PRO:HD2	1	0.32
(1,730)	1:155:C:ALA:HB1	1:157:C:PRO:HD2	6	0.32
(1,730)	1:155:C:ALA:HB2	1:157:C:PRO:HD2	6	0.32
(1,730)	1:155:C:ALA:HB3	1:157:C:PRO:HD2	6	0.32
(1,729)	1:155:B:ALA:HB1	1:157:B:PRO:HD2	1	0.32
(1,729)	1:155:B:ALA:HB2	1:157:B:PRO:HD2	1	0.32
(1,729)	1:155:B:ALA:HB3	1:157:B:PRO:HD2	1	0.32
(1,729)	1:155:B:ALA:HB1	1:157:B:PRO:HD2	6	0.32
(1,729)	1:155:B:ALA:HB2	1:157:B:PRO:HD2	6	0.32
(1,729)	1:155:B:ALA:HB3	1:157:B:PRO:HD2	6	0.32
(1,573)	1:194:A:LEU:HD21	1:196:A:TYR:HE1	6	0.32
(1,573)	1:194:A:LEU:HD21	1:196:A:TYR:HE2	6	0.32
(1,573)	1:194:A:LEU:HD22	1:196:A:TYR:HE1	6	0.32
(1,573)	1:194:A:LEU:HD22	1:196:A:TYR:HE2	6	0.32
(1,573)	1:194:A:LEU:HD23	1:196:A:TYR:HE1	6	0.32
(1,573)	1:194:A:LEU:HD23	1:196:A:TYR:HE2	6	0.32
(1,539)	1:111:A:ILE:HG21	1:126:A:ILE:HG21	7	0.32
(1,539)	1:111:A:ILE:HG21	1:126:A:ILE:HG22	7	0.32
(1,539)	1:111:A:ILE:HG21	1:126:A:ILE:HG23	7	0.32
(1,539)	1:111:A:ILE:HG22	1:126:A:ILE:HG21	7	0.32
(1,539)	1:111:A:ILE:HG22	1:126:A:ILE:HG22	7	0.32
(1,539)	1:111:A:ILE:HG22	1:126:A:ILE:HG23	7	0.32
(1,539)	1:111:A:ILE:HG23	1:126:A:ILE:HG21	7	0.32
(1,539)	1:111:A:ILE:HG23	1:126:A:ILE:HG22	7	0.32
(1,539)	1:111:A:ILE:HG23	1:126:A:ILE:HG23	7	0.32
(1,395)	1:109:A:LEU:HG	1:111:A:ILE:HD11	2	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,395)	1:109:A:LEU:HG	1:111:A:ILE:HD12	2	0.32
(1,395)	1:109:A:LEU:HG	1:111:A:ILE:HD13	2	0.32
(1,395)	1:109:A:LEU:HG	1:111:A:ILE:HD11	10	0.32
(1,395)	1:109:A:LEU:HG	1:111:A:ILE:HD12	10	0.32
(1,395)	1:109:A:LEU:HG	1:111:A:ILE:HD13	10	0.32
(1,138)	1:192:A:VAL:HG21	1:135:B:GLU:HG2	2	0.32
(1,138)	1:192:A:VAL:HG21	1:135:B:GLU:HG3	2	0.32
(1,138)	1:192:A:VAL:HG22	1:135:B:GLU:HG2	2	0.32
(1,138)	1:192:A:VAL:HG22	1:135:B:GLU:HG3	2	0.32
(1,138)	1:192:A:VAL:HG23	1:135:B:GLU:HG2	2	0.32
(1,138)	1:192:A:VAL:HG23	1:135:B:GLU:HG3	2	0.32
(1,122)	1:113:A:TYR:HD1	1:137:A:LEU:HD21	8	0.32
(1,122)	1:113:A:TYR:HD1	1:137:A:LEU:HD22	8	0.32
(1,122)	1:113:A:TYR:HD1	1:137:A:LEU:HD23	8	0.32
(1,122)	1:113:A:TYR:HD2	1:137:A:LEU:HD21	8	0.32
(1,122)	1:113:A:TYR:HD2	1:137:A:LEU:HD22	8	0.32
(1,122)	1:113:A:TYR:HD2	1:137:A:LEU:HD23	8	0.32
(1,2339)	1:180:C:PHE:H	1:181:C:LEU:HB2	10	0.31
(1,2339)	1:180:C:PHE:H	1:181:C:LEU:HB3	10	0.31
(1,2320)	1:172:C:ALA:HA	1:178:C:PRO:HD2	10	0.31
(1,2320)	1:172:C:ALA:HA	1:178:C:PRO:HD3	10	0.31
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG11	15	0.31
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG12	15	0.31
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG13	15	0.31
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG21	15	0.31
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG22	15	0.31
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG23	15	0.31
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG11	19	0.31
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG12	19	0.31
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG13	19	0.31
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG21	19	0.31
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG22	19	0.31
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG23	19	0.31
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG11	20	0.31
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG12	20	0.31
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG13	20	0.31
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG21	20	0.31
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG22	20	0.31
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG23	20	0.31
(1,2289)	1:153:C:LYS:HA	1:154:C:PRO:HD2	9	0.31
(1,2289)	1:153:C:LYS:HA	1:154:C:PRO:HD3	9	0.31
(1,2113)	1:180:B:PHE:H	1:181:B:LEU:HB2	10	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2113)	1:180:B:PHE:H	1:181:B:LEU:HB3	10	0.31
(1,2094)	1:172:B:ALA:HA	1:178:B:PRO:HD2	10	0.31
(1,2094)	1:172:B:ALA:HA	1:178:B:PRO:HD3	10	0.31
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG11	15	0.31
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG12	15	0.31
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG13	15	0.31
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG21	15	0.31
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG22	15	0.31
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG23	15	0.31
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG11	19	0.31
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG12	19	0.31
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG13	19	0.31
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG21	19	0.31
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG22	19	0.31
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG23	19	0.31
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG11	20	0.31
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG12	20	0.31
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG13	20	0.31
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG21	20	0.31
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG22	20	0.31
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG23	20	0.31
(1,2063)	1:153:B:LYS:HA	1:154:B:PRO:HD2	9	0.31
(1,2063)	1:153:B:LYS:HA	1:154:B:PRO:HD3	9	0.31
(1,1916)	1:180:A:PHE:H	1:181:A:LEU:HB2	10	0.31
(1,1916)	1:180:A:PHE:H	1:181:A:LEU:HB3	10	0.31
(1,1887)	1:156:A:VAL:HB	1:157:A:PRO:HD2	6	0.31
(1,1887)	1:156:A:VAL:HB	1:157:A:PRO:HD3	6	0.31
(1,1887)	1:156:A:VAL:HB	1:157:A:PRO:HD2	8	0.31
(1,1887)	1:156:A:VAL:HB	1:157:A:PRO:HD3	8	0.31
(1,1881)	1:153:A:LYS:HA	1:154:A:PRO:HD2	9	0.31
(1,1881)	1:153:A:LYS:HA	1:154:A:PRO:HD3	9	0.31
(1,1830)	1:102:A:VAL:HG11	1:111:A:ILE:HG12	1	0.31
(1,1830)	1:102:A:VAL:HG11	1:111:A:ILE:HG13	1	0.31
(1,1830)	1:102:A:VAL:HG12	1:111:A:ILE:HG12	1	0.31
(1,1830)	1:102:A:VAL:HG12	1:111:A:ILE:HG13	1	0.31
(1,1830)	1:102:A:VAL:HG13	1:111:A:ILE:HG12	1	0.31
(1,1830)	1:102:A:VAL:HG13	1:111:A:ILE:HG13	1	0.31
(1,1561)	1:167:C:ARG:H	1:167:C:ARG:HB3	20	0.31
(1,1560)	1:167:B:ARG:H	1:167:B:ARG:HB3	20	0.31
(1,1555)	1:156:A:VAL:HG11	1:167:A:ARG:H	7	0.31
(1,1555)	1:156:A:VAL:HG12	1:167:A:ARG:H	7	0.31
(1,1555)	1:156:A:VAL:HG13	1:167:A:ARG:H	7	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1463)	1:180:C:PHE:H	1:181:C:LEU:HA	15	0.31
(1,1462)	1:180:B:PHE:H	1:181:B:LEU:HA	15	0.31
(1,1461)	1:180:A:PHE:H	1:181:A:LEU:HA	19	0.31
(1,1100)	1:167:C:ARG:H	1:167:C:ARG:HB2	14	0.31
(1,1099)	1:167:B:ARG:H	1:167:B:ARG:HB2	14	0.31
(1,1098)	1:167:A:ARG:H	1:167:A:ARG:HB2	14	0.31
(1,1036)	1:188:A:LEU:HD21	1:134:B:LEU:H	9	0.31
(1,1036)	1:188:A:LEU:HD22	1:134:B:LEU:H	9	0.31
(1,1036)	1:188:A:LEU:HD23	1:134:B:LEU:H	9	0.31
(1,888)	1:152:A:ALA:HA	1:157:A:PRO:HG2	20	0.31
(1,888)	1:152:A:ALA:HA	1:157:A:PRO:HG3	20	0.31
(1,753)	1:189:A:CYS:H	1:192:A:VAL:HG11	18	0.31
(1,753)	1:189:A:CYS:H	1:192:A:VAL:HG12	18	0.31
(1,753)	1:189:A:CYS:H	1:192:A:VAL:HG13	18	0.31
(1,730)	1:155:C:ALA:HB1	1:157:C:PRO:HD2	3	0.31
(1,730)	1:155:C:ALA:HB2	1:157:C:PRO:HD2	3	0.31
(1,730)	1:155:C:ALA:HB3	1:157:C:PRO:HD2	3	0.31
(1,729)	1:155:B:ALA:HB1	1:157:B:PRO:HD2	3	0.31
(1,729)	1:155:B:ALA:HB2	1:157:B:PRO:HD2	3	0.31
(1,729)	1:155:B:ALA:HB3	1:157:B:PRO:HD2	3	0.31
(1,728)	1:155:A:ALA:HB1	1:157:A:PRO:HD2	4	0.31
(1,728)	1:155:A:ALA:HB2	1:157:A:PRO:HD2	4	0.31
(1,728)	1:155:A:ALA:HB3	1:157:A:PRO:HD2	4	0.31
(1,250)	1:118:B:GLY:HA2	1:119:B:THR:HG21	1	0.31
(1,250)	1:118:B:GLY:HA2	1:119:B:THR:HG22	1	0.31
(1,250)	1:118:B:GLY:HA2	1:119:B:THR:HG23	1	0.31
(1,205)	1:111:A:ILE:HD11	1:137:A:LEU:HD11	19	0.31
(1,205)	1:111:A:ILE:HD11	1:137:A:LEU:HD12	19	0.31
(1,205)	1:111:A:ILE:HD11	1:137:A:LEU:HD13	19	0.31
(1,205)	1:111:A:ILE:HD12	1:137:A:LEU:HD11	19	0.31
(1,205)	1:111:A:ILE:HD12	1:137:A:LEU:HD12	19	0.31
(1,205)	1:111:A:ILE:HD12	1:137:A:LEU:HD13	19	0.31
(1,205)	1:111:A:ILE:HD13	1:137:A:LEU:HD11	19	0.31
(1,205)	1:111:A:ILE:HD13	1:137:A:LEU:HD12	19	0.31
(1,205)	1:111:A:ILE:HD13	1:137:A:LEU:HD13	19	0.31
(1,138)	1:192:A:VAL:HG21	1:135:B:GLU:HG2	7	0.31
(1,138)	1:192:A:VAL:HG21	1:135:B:GLU:HG3	7	0.31
(1,138)	1:192:A:VAL:HG22	1:135:B:GLU:HG2	7	0.31
(1,138)	1:192:A:VAL:HG22	1:135:B:GLU:HG3	7	0.31
(1,138)	1:192:A:VAL:HG23	1:135:B:GLU:HG2	7	0.31
(1,138)	1:192:A:VAL:HG23	1:135:B:GLU:HG3	7	0.31
(1,124)	1:96:A:ILE:H	1:101:A:LEU:HD21	12	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,124)	1:96:A:ILE:H	1:101:A:LEU:HD22	12	0.31
(1,124)	1:96:A:ILE:H	1:101:A:LEU:HD23	12	0.31
(1,122)	1:113:A:TYR:HD1	1:137:A:LEU:HD21	1	0.31
(1,122)	1:113:A:TYR:HD1	1:137:A:LEU:HD22	1	0.31
(1,122)	1:113:A:TYR:HD1	1:137:A:LEU:HD23	1	0.31
(1,122)	1:113:A:TYR:HD2	1:137:A:LEU:HD21	1	0.31
(1,122)	1:113:A:TYR:HD2	1:137:A:LEU:HD22	1	0.31
(1,122)	1:113:A:TYR:HD2	1:137:A:LEU:HD23	1	0.31
(1,122)	1:113:A:TYR:HD1	1:137:A:LEU:HD21	5	0.31
(1,122)	1:113:A:TYR:HD1	1:137:A:LEU:HD22	5	0.31
(1,122)	1:113:A:TYR:HD1	1:137:A:LEU:HD23	5	0.31
(1,122)	1:113:A:TYR:HD2	1:137:A:LEU:HD21	5	0.31
(1,122)	1:113:A:TYR:HD2	1:137:A:LEU:HD22	5	0.31
(1,122)	1:113:A:TYR:HD2	1:137:A:LEU:HD23	5	0.31
(1,2298)	1:156:C:VAL:HB	1:157:C:PRO:HD2	17	0.3
(1,2298)	1:156:C:VAL:HB	1:157:C:PRO:HD3	17	0.3
(1,2289)	1:153:C:LYS:HA	1:154:C:PRO:HD2	16	0.3
(1,2289)	1:153:C:LYS:HA	1:154:C:PRO:HD3	16	0.3
(1,2072)	1:156:B:VAL:HB	1:157:B:PRO:HD2	17	0.3
(1,2072)	1:156:B:VAL:HB	1:157:B:PRO:HD3	17	0.3
(1,2063)	1:153:B:LYS:HA	1:154:B:PRO:HD2	16	0.3
(1,2063)	1:153:B:LYS:HA	1:154:B:PRO:HD3	16	0.3
(1,1881)	1:153:A:LYS:HA	1:154:A:PRO:HD2	16	0.3
(1,1881)	1:153:A:LYS:HA	1:154:A:PRO:HD3	16	0.3
(1,1774)	1:125:A:LYS:H	1:126:A:ILE:HG21	4	0.3
(1,1774)	1:125:A:LYS:H	1:126:A:ILE:HG22	4	0.3
(1,1774)	1:125:A:LYS:H	1:126:A:ILE:HG23	4	0.3
(1,1463)	1:180:C:PHE:H	1:181:C:LEU:HA	18	0.3
(1,1462)	1:180:B:PHE:H	1:181:B:LEU:HA	18	0.3
(1,1461)	1:180:A:PHE:H	1:181:A:LEU:HA	5	0.3
(1,1030)	1:152:A:ALA:H	1:153:A:LYS:H	10	0.3
(1,848)	1:150:A:LEU:HD11	1:167:A:ARG:HG2	17	0.3
(1,848)	1:150:A:LEU:HD11	1:167:A:ARG:HG3	17	0.3
(1,848)	1:150:A:LEU:HD12	1:167:A:ARG:HG2	17	0.3
(1,848)	1:150:A:LEU:HD12	1:167:A:ARG:HG3	17	0.3
(1,848)	1:150:A:LEU:HD13	1:167:A:ARG:HG2	17	0.3
(1,848)	1:150:A:LEU:HD13	1:167:A:ARG:HG3	17	0.3
(1,845)	1:156:A:VAL:HB	1:157:A:PRO:HD3	14	0.3
(1,753)	1:189:A:CYS:H	1:192:A:VAL:HG11	14	0.3
(1,753)	1:189:A:CYS:H	1:192:A:VAL:HG12	14	0.3
(1,753)	1:189:A:CYS:H	1:192:A:VAL:HG13	14	0.3
(1,753)	1:189:A:CYS:H	1:192:A:VAL:HG11	16	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,753)	1:189:A:CYS:H	1:192:A:VAL:HG12	16	0.3
(1,753)	1:189:A:CYS:H	1:192:A:VAL:HG13	16	0.3
(1,730)	1:155:C:ALA:HB1	1:157:C:PRO:HD2	5	0.3
(1,730)	1:155:C:ALA:HB2	1:157:C:PRO:HD2	5	0.3
(1,730)	1:155:C:ALA:HB3	1:157:C:PRO:HD2	5	0.3
(1,730)	1:155:C:ALA:HB1	1:157:C:PRO:HD2	8	0.3
(1,730)	1:155:C:ALA:HB2	1:157:C:PRO:HD2	8	0.3
(1,730)	1:155:C:ALA:HB3	1:157:C:PRO:HD2	8	0.3
(1,729)	1:155:B:ALA:HB1	1:157:B:PRO:HD2	5	0.3
(1,729)	1:155:B:ALA:HB2	1:157:B:PRO:HD2	5	0.3
(1,729)	1:155:B:ALA:HB3	1:157:B:PRO:HD2	5	0.3
(1,729)	1:155:B:ALA:HB1	1:157:B:PRO:HD2	8	0.3
(1,729)	1:155:B:ALA:HB2	1:157:B:PRO:HD2	8	0.3
(1,729)	1:155:B:ALA:HB3	1:157:B:PRO:HD2	8	0.3
(1,728)	1:155:A:ALA:HB1	1:157:A:PRO:HD2	9	0.3
(1,728)	1:155:A:ALA:HB2	1:157:A:PRO:HD2	9	0.3
(1,728)	1:155:A:ALA:HB3	1:157:A:PRO:HD2	9	0.3
(1,451)	1:95:A:SER:HB2	1:101:A:LEU:HD21	8	0.3
(1,451)	1:95:A:SER:HB2	1:101:A:LEU:HD22	8	0.3
(1,451)	1:95:A:SER:HB2	1:101:A:LEU:HD23	8	0.3
(1,451)	1:95:A:SER:HB3	1:101:A:LEU:HD21	8	0.3
(1,451)	1:95:A:SER:HB3	1:101:A:LEU:HD22	8	0.3
(1,451)	1:95:A:SER:HB3	1:101:A:LEU:HD23	8	0.3
(1,251)	1:118:C:GLY:HA2	1:119:C:THR:HG21	1	0.3
(1,251)	1:118:C:GLY:HA2	1:119:C:THR:HG22	1	0.3
(1,251)	1:118:C:GLY:HA2	1:119:C:THR:HG23	1	0.3
(1,251)	1:118:C:GLY:HA2	1:119:C:THR:HG21	11	0.3
(1,251)	1:118:C:GLY:HA2	1:119:C:THR:HG22	11	0.3
(1,251)	1:118:C:GLY:HA2	1:119:C:THR:HG23	11	0.3
(1,251)	1:118:C:GLY:HA2	1:119:C:THR:HG21	12	0.3
(1,251)	1:118:C:GLY:HA2	1:119:C:THR:HG22	12	0.3
(1,251)	1:118:C:GLY:HA2	1:119:C:THR:HG23	12	0.3
(1,251)	1:118:C:GLY:HA2	1:119:C:THR:HG21	14	0.3
(1,251)	1:118:C:GLY:HA2	1:119:C:THR:HG22	14	0.3
(1,251)	1:118:C:GLY:HA2	1:119:C:THR:HG23	14	0.3
(1,250)	1:118:B:GLY:HA2	1:119:B:THR:HG21	9	0.3
(1,250)	1:118:B:GLY:HA2	1:119:B:THR:HG22	9	0.3
(1,250)	1:118:B:GLY:HA2	1:119:B:THR:HG23	9	0.3
(1,250)	1:118:B:GLY:HA2	1:119:B:THR:HG21	11	0.3
(1,250)	1:118:B:GLY:HA2	1:119:B:THR:HG22	11	0.3
(1,250)	1:118:B:GLY:HA2	1:119:B:THR:HG23	11	0.3
(1,250)	1:118:B:GLY:HA2	1:119:B:THR:HG21	12	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,250)	1:118:B:GLY:HA2	1:119:B:THR:HG22	12	0.3
(1,250)	1:118:B:GLY:HA2	1:119:B:THR:HG23	12	0.3
(1,250)	1:118:B:GLY:HA2	1:119:B:THR:HG21	14	0.3
(1,250)	1:118:B:GLY:HA2	1:119:B:THR:HG22	14	0.3
(1,250)	1:118:B:GLY:HA2	1:119:B:THR:HG23	14	0.3
(1,249)	1:118:A:GLY:HA2	1:119:A:THR:HG21	1	0.3
(1,249)	1:118:A:GLY:HA2	1:119:A:THR:HG22	1	0.3
(1,249)	1:118:A:GLY:HA2	1:119:A:THR:HG23	1	0.3
(1,249)	1:118:A:GLY:HA2	1:119:A:THR:HG21	11	0.3
(1,249)	1:118:A:GLY:HA2	1:119:A:THR:HG22	11	0.3
(1,249)	1:118:A:GLY:HA2	1:119:A:THR:HG23	11	0.3
(1,215)	1:101:A:LEU:HD21	1:103:A:VAL:HG11	4	0.3
(1,215)	1:101:A:LEU:HD21	1:103:A:VAL:HG12	4	0.3
(1,215)	1:101:A:LEU:HD21	1:103:A:VAL:HG13	4	0.3
(1,215)	1:101:A:LEU:HD22	1:103:A:VAL:HG11	4	0.3
(1,215)	1:101:A:LEU:HD22	1:103:A:VAL:HG12	4	0.3
(1,215)	1:101:A:LEU:HD22	1:103:A:VAL:HG13	4	0.3
(1,215)	1:101:A:LEU:HD23	1:103:A:VAL:HG11	4	0.3
(1,215)	1:101:A:LEU:HD23	1:103:A:VAL:HG12	4	0.3
(1,215)	1:101:A:LEU:HD23	1:103:A:VAL:HG13	4	0.3
(1,215)	1:101:A:LEU:HD21	1:103:A:VAL:HG11	11	0.3
(1,215)	1:101:A:LEU:HD21	1:103:A:VAL:HG12	11	0.3
(1,215)	1:101:A:LEU:HD21	1:103:A:VAL:HG13	11	0.3
(1,215)	1:101:A:LEU:HD22	1:103:A:VAL:HG11	11	0.3
(1,215)	1:101:A:LEU:HD22	1:103:A:VAL:HG12	11	0.3
(1,215)	1:101:A:LEU:HD22	1:103:A:VAL:HG13	11	0.3
(1,215)	1:101:A:LEU:HD23	1:103:A:VAL:HG11	11	0.3
(1,215)	1:101:A:LEU:HD23	1:103:A:VAL:HG12	11	0.3
(1,215)	1:101:A:LEU:HD23	1:103:A:VAL:HG13	11	0.3
(1,138)	1:192:A:VAL:HG21	1:135:B:GLU:HG2	10	0.3
(1,138)	1:192:A:VAL:HG21	1:135:B:GLU:HG3	10	0.3
(1,138)	1:192:A:VAL:HG22	1:135:B:GLU:HG2	10	0.3
(1,138)	1:192:A:VAL:HG22	1:135:B:GLU:HG3	10	0.3
(1,138)	1:192:A:VAL:HG23	1:135:B:GLU:HG2	10	0.3
(1,138)	1:192:A:VAL:HG23	1:135:B:GLU:HG3	10	0.3
(1,122)	1:113:A:TYR:HD1	1:137:A:LEU:HD21	13	0.3
(1,122)	1:113:A:TYR:HD1	1:137:A:LEU:HD22	13	0.3
(1,122)	1:113:A:TYR:HD1	1:137:A:LEU:HD23	13	0.3
(1,122)	1:113:A:TYR:HD2	1:137:A:LEU:HD21	13	0.3
(1,122)	1:113:A:TYR:HD2	1:137:A:LEU:HD22	13	0.3
(1,122)	1:113:A:TYR:HD2	1:137:A:LEU:HD23	13	0.3
(1,122)	1:113:A:TYR:HD1	1:137:A:LEU:HD21	14	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,122)	1:113:A:TYR:HD1	1:137:A:LEU:HD22	14	0.3
(1,122)	1:113:A:TYR:HD1	1:137:A:LEU:HD23	14	0.3
(1,122)	1:113:A:TYR:HD2	1:137:A:LEU:HD21	14	0.3
(1,122)	1:113:A:TYR:HD2	1:137:A:LEU:HD22	14	0.3
(1,122)	1:113:A:TYR:HD2	1:137:A:LEU:HD23	14	0.3
(1,26)	1:109:A:LEU:HD21	1:110:A:LEU:H	5	0.3
(1,26)	1:109:A:LEU:HD22	1:110:A:LEU:H	5	0.3
(1,26)	1:109:A:LEU:HD23	1:110:A:LEU:H	5	0.3
(1,2339)	1:180:C:PHE:H	1:181:C:LEU:HB2	3	0.29
(1,2339)	1:180:C:PHE:H	1:181:C:LEU:HB3	3	0.29
(1,2339)	1:180:C:PHE:H	1:181:C:LEU:HB2	4	0.29
(1,2339)	1:180:C:PHE:H	1:181:C:LEU:HB3	4	0.29
(1,2320)	1:172:C:ALA:HA	1:178:C:PRO:HD2	3	0.29
(1,2320)	1:172:C:ALA:HA	1:178:C:PRO:HD3	3	0.29
(1,2113)	1:180:B:PHE:H	1:181:B:LEU:HB2	3	0.29
(1,2113)	1:180:B:PHE:H	1:181:B:LEU:HB3	3	0.29
(1,2113)	1:180:B:PHE:H	1:181:B:LEU:HB2	4	0.29
(1,2113)	1:180:B:PHE:H	1:181:B:LEU:HB3	4	0.29
(1,2094)	1:172:B:ALA:HA	1:178:B:PRO:HD2	8	0.29
(1,2094)	1:172:B:ALA:HA	1:178:B:PRO:HD3	8	0.29
(1,2072)	1:156:B:VAL:HB	1:157:B:PRO:HD2	10	0.29
(1,2072)	1:156:B:VAL:HB	1:157:B:PRO:HD3	10	0.29
(1,1916)	1:180:A:PHE:H	1:181:A:LEU:HB2	3	0.29
(1,1916)	1:180:A:PHE:H	1:181:A:LEU:HB3	3	0.29
(1,1887)	1:156:A:VAL:HB	1:157:A:PRO:HD2	4	0.29
(1,1887)	1:156:A:VAL:HB	1:157:A:PRO:HD3	4	0.29
(1,1887)	1:156:A:VAL:HB	1:157:A:PRO:HD2	12	0.29
(1,1887)	1:156:A:VAL:HB	1:157:A:PRO:HD3	12	0.29
(1,1819)	1:95:C:SER:HB2	1:101:C:LEU:H	3	0.29
(1,1819)	1:95:C:SER:HB3	1:101:C:LEU:H	3	0.29
(1,1768)	1:178:A:PRO:HD3	1:179:A:ALA:H	7	0.29
(1,1768)	1:178:A:PRO:HD3	1:179:A:ALA:H	9	0.29
(1,1676)	1:94:A:PHE:H	1:102:A:VAL:HG11	3	0.29
(1,1676)	1:94:A:PHE:H	1:102:A:VAL:HG12	3	0.29
(1,1676)	1:94:A:PHE:H	1:102:A:VAL:HG13	3	0.29
(1,1061)	1:178:C:PRO:HB3	1:179:C:ALA:H	4	0.29
(1,1060)	1:178:B:PRO:HB3	1:179:B:ALA:H	4	0.29
(1,1059)	1:178:A:PRO:HB3	1:179:A:ALA:H	4	0.29
(1,1032)	1:152:C:ALA:H	1:153:C:LYS:H	10	0.29
(1,1031)	1:152:B:ALA:H	1:153:B:LYS:H	10	0.29
(1,958)	1:187:A:THR:HA	1:188:A:LEU:HD11	10	0.29
(1,958)	1:187:A:THR:HA	1:188:A:LEU:HD12	10	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,958)	1:187:A:THR:HA	1:188:A:LEU:HD13	10	0.29
(1,958)	1:187:A:THR:HA	1:188:A:LEU:HD11	15	0.29
(1,958)	1:187:A:THR:HA	1:188:A:LEU:HD12	15	0.29
(1,958)	1:187:A:THR:HA	1:188:A:LEU:HD13	15	0.29
(1,847)	1:156:C:VAL:HB	1:157:C:PRO:HD3	14	0.29
(1,846)	1:156:B:VAL:HB	1:157:B:PRO:HD3	14	0.29
(1,755)	1:189:C:CYS:H	1:192:C:VAL:HG11	5	0.29
(1,755)	1:189:C:CYS:H	1:192:C:VAL:HG12	5	0.29
(1,755)	1:189:C:CYS:H	1:192:C:VAL:HG13	5	0.29
(1,754)	1:189:B:CYS:H	1:192:B:VAL:HG11	5	0.29
(1,754)	1:189:B:CYS:H	1:192:B:VAL:HG12	5	0.29
(1,754)	1:189:B:CYS:H	1:192:B:VAL:HG13	5	0.29
(1,753)	1:189:A:CYS:H	1:192:A:VAL:HG11	4	0.29
(1,753)	1:189:A:CYS:H	1:192:A:VAL:HG12	4	0.29
(1,753)	1:189:A:CYS:H	1:192:A:VAL:HG13	4	0.29
(1,753)	1:189:A:CYS:H	1:192:A:VAL:HG11	20	0.29
(1,753)	1:189:A:CYS:H	1:192:A:VAL:HG12	20	0.29
(1,753)	1:189:A:CYS:H	1:192:A:VAL:HG13	20	0.29
(1,730)	1:155:C:ALA:HB1	1:157:C:PRO:HD2	2	0.29
(1,730)	1:155:C:ALA:HB2	1:157:C:PRO:HD2	2	0.29
(1,730)	1:155:C:ALA:HB3	1:157:C:PRO:HD2	2	0.29
(1,729)	1:155:B:ALA:HB1	1:157:B:PRO:HD2	2	0.29
(1,729)	1:155:B:ALA:HB2	1:157:B:PRO:HD2	2	0.29
(1,729)	1:155:B:ALA:HB3	1:157:B:PRO:HD2	2	0.29
(1,728)	1:155:A:ALA:HB1	1:157:A:PRO:HD2	1	0.29
(1,728)	1:155:A:ALA:HB2	1:157:A:PRO:HD2	1	0.29
(1,728)	1:155:A:ALA:HB3	1:157:A:PRO:HD2	1	0.29
(1,572)	1:121:A:CYS:H	1:194:A:LEU:HD21	6	0.29
(1,572)	1:121:A:CYS:H	1:194:A:LEU:HD22	6	0.29
(1,572)	1:121:A:CYS:H	1:194:A:LEU:HD23	6	0.29
(1,251)	1:118:C:GLY:HA2	1:119:C:THR:HG21	2	0.29
(1,251)	1:118:C:GLY:HA2	1:119:C:THR:HG22	2	0.29
(1,251)	1:118:C:GLY:HA2	1:119:C:THR:HG23	2	0.29
(1,251)	1:118:C:GLY:HA2	1:119:C:THR:HG21	9	0.29
(1,251)	1:118:C:GLY:HA2	1:119:C:THR:HG22	9	0.29
(1,251)	1:118:C:GLY:HA2	1:119:C:THR:HG23	9	0.29
(1,251)	1:118:C:GLY:HA2	1:119:C:THR:HG21	13	0.29
(1,251)	1:118:C:GLY:HA2	1:119:C:THR:HG22	13	0.29
(1,251)	1:118:C:GLY:HA2	1:119:C:THR:HG23	13	0.29
(1,251)	1:118:C:GLY:HA2	1:119:C:THR:HG21	15	0.29
(1,251)	1:118:C:GLY:HA2	1:119:C:THR:HG22	15	0.29
(1,251)	1:118:C:GLY:HA2	1:119:C:THR:HG23	15	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,251)	1:118:C:GLY:HA2	1:119:C:THR:HG21	17	0.29
(1,251)	1:118:C:GLY:HA2	1:119:C:THR:HG22	17	0.29
(1,251)	1:118:C:GLY:HA2	1:119:C:THR:HG23	17	0.29
(1,251)	1:118:C:GLY:HA2	1:119:C:THR:HG21	18	0.29
(1,251)	1:118:C:GLY:HA2	1:119:C:THR:HG22	18	0.29
(1,251)	1:118:C:GLY:HA2	1:119:C:THR:HG23	18	0.29
(1,251)	1:118:C:GLY:HA2	1:119:C:THR:HG21	20	0.29
(1,251)	1:118:C:GLY:HA2	1:119:C:THR:HG22	20	0.29
(1,251)	1:118:C:GLY:HA2	1:119:C:THR:HG23	20	0.29
(1,250)	1:118:B:GLY:HA2	1:119:B:THR:HG21	2	0.29
(1,250)	1:118:B:GLY:HA2	1:119:B:THR:HG22	2	0.29
(1,250)	1:118:B:GLY:HA2	1:119:B:THR:HG23	2	0.29
(1,250)	1:118:B:GLY:HA2	1:119:B:THR:HG21	6	0.29
(1,250)	1:118:B:GLY:HA2	1:119:B:THR:HG22	6	0.29
(1,250)	1:118:B:GLY:HA2	1:119:B:THR:HG23	6	0.29
(1,250)	1:118:B:GLY:HA2	1:119:B:THR:HG21	13	0.29
(1,250)	1:118:B:GLY:HA2	1:119:B:THR:HG22	13	0.29
(1,250)	1:118:B:GLY:HA2	1:119:B:THR:HG23	13	0.29
(1,250)	1:118:B:GLY:HA2	1:119:B:THR:HG21	15	0.29
(1,250)	1:118:B:GLY:HA2	1:119:B:THR:HG22	15	0.29
(1,250)	1:118:B:GLY:HA2	1:119:B:THR:HG23	15	0.29
(1,250)	1:118:B:GLY:HA2	1:119:B:THR:HG21	17	0.29
(1,250)	1:118:B:GLY:HA2	1:119:B:THR:HG22	17	0.29
(1,250)	1:118:B:GLY:HA2	1:119:B:THR:HG23	17	0.29
(1,250)	1:118:B:GLY:HA2	1:119:B:THR:HG21	18	0.29
(1,250)	1:118:B:GLY:HA2	1:119:B:THR:HG22	18	0.29
(1,250)	1:118:B:GLY:HA2	1:119:B:THR:HG23	18	0.29
(1,250)	1:118:B:GLY:HA2	1:119:B:THR:HG21	20	0.29
(1,250)	1:118:B:GLY:HA2	1:119:B:THR:HG22	20	0.29
(1,250)	1:118:B:GLY:HA2	1:119:B:THR:HG23	20	0.29
(1,249)	1:118:A:GLY:HA2	1:119:A:THR:HG21	2	0.29
(1,249)	1:118:A:GLY:HA2	1:119:A:THR:HG22	2	0.29
(1,249)	1:118:A:GLY:HA2	1:119:A:THR:HG23	2	0.29
(1,249)	1:118:A:GLY:HA2	1:119:A:THR:HG21	6	0.29
(1,249)	1:118:A:GLY:HA2	1:119:A:THR:HG22	6	0.29
(1,249)	1:118:A:GLY:HA2	1:119:A:THR:HG23	6	0.29
(1,249)	1:118:A:GLY:HA2	1:119:A:THR:HG21	9	0.29
(1,249)	1:118:A:GLY:HA2	1:119:A:THR:HG22	9	0.29
(1,249)	1:118:A:GLY:HA2	1:119:A:THR:HG23	9	0.29
(1,249)	1:118:A:GLY:HA2	1:119:A:THR:HG21	14	0.29
(1,249)	1:118:A:GLY:HA2	1:119:A:THR:HG22	14	0.29
(1,249)	1:118:A:GLY:HA2	1:119:A:THR:HG23	14	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,226)	1:96:A:ILE:HD11	1:102:A:VAL:HG11	7	0.29
(1,226)	1:96:A:ILE:HD11	1:102:A:VAL:HG12	7	0.29
(1,226)	1:96:A:ILE:HD11	1:102:A:VAL:HG13	7	0.29
(1,226)	1:96:A:ILE:HD12	1:102:A:VAL:HG11	7	0.29
(1,226)	1:96:A:ILE:HD12	1:102:A:VAL:HG12	7	0.29
(1,226)	1:96:A:ILE:HD12	1:102:A:VAL:HG13	7	0.29
(1,226)	1:96:A:ILE:HD13	1:102:A:VAL:HG11	7	0.29
(1,226)	1:96:A:ILE:HD13	1:102:A:VAL:HG12	7	0.29
(1,226)	1:96:A:ILE:HD13	1:102:A:VAL:HG13	7	0.29
(1,226)	1:96:A:ILE:HD11	1:102:A:VAL:HG11	19	0.29
(1,226)	1:96:A:ILE:HD11	1:102:A:VAL:HG12	19	0.29
(1,226)	1:96:A:ILE:HD11	1:102:A:VAL:HG13	19	0.29
(1,226)	1:96:A:ILE:HD12	1:102:A:VAL:HG11	19	0.29
(1,226)	1:96:A:ILE:HD12	1:102:A:VAL:HG12	19	0.29
(1,226)	1:96:A:ILE:HD12	1:102:A:VAL:HG13	19	0.29
(1,226)	1:96:A:ILE:HD13	1:102:A:VAL:HG11	19	0.29
(1,226)	1:96:A:ILE:HD13	1:102:A:VAL:HG12	19	0.29
(1,226)	1:96:A:ILE:HD13	1:102:A:VAL:HG13	19	0.29
(1,219)	1:96:A:ILE:HG21	1:141:A:VAL:HG11	6	0.29
(1,219)	1:96:A:ILE:HG21	1:141:A:VAL:HG12	6	0.29
(1,219)	1:96:A:ILE:HG21	1:141:A:VAL:HG13	6	0.29
(1,219)	1:96:A:ILE:HG22	1:141:A:VAL:HG11	6	0.29
(1,219)	1:96:A:ILE:HG22	1:141:A:VAL:HG12	6	0.29
(1,219)	1:96:A:ILE:HG22	1:141:A:VAL:HG13	6	0.29
(1,219)	1:96:A:ILE:HG23	1:141:A:VAL:HG11	6	0.29
(1,219)	1:96:A:ILE:HG23	1:141:A:VAL:HG12	6	0.29
(1,219)	1:96:A:ILE:HG23	1:141:A:VAL:HG13	6	0.29
(1,138)	1:192:A:VAL:HG21	1:135:B:GLU:HG2	9	0.29
(1,138)	1:192:A:VAL:HG21	1:135:B:GLU:HG3	9	0.29
(1,138)	1:192:A:VAL:HG22	1:135:B:GLU:HG2	9	0.29
(1,138)	1:192:A:VAL:HG22	1:135:B:GLU:HG3	9	0.29
(1,138)	1:192:A:VAL:HG23	1:135:B:GLU:HG2	9	0.29
(1,138)	1:192:A:VAL:HG23	1:135:B:GLU:HG3	9	0.29
(1,138)	1:192:A:VAL:HG21	1:135:B:GLU:HG2	12	0.29
(1,138)	1:192:A:VAL:HG21	1:135:B:GLU:HG3	12	0.29
(1,138)	1:192:A:VAL:HG22	1:135:B:GLU:HG2	12	0.29
(1,138)	1:192:A:VAL:HG22	1:135:B:GLU:HG3	12	0.29
(1,138)	1:192:A:VAL:HG23	1:135:B:GLU:HG2	12	0.29
(1,138)	1:192:A:VAL:HG23	1:135:B:GLU:HG3	12	0.29
(1,2320)	1:172:C:ALA:HA	1:178:C:PRO:HD2	8	0.28
(1,2320)	1:172:C:ALA:HA	1:178:C:PRO:HD3	8	0.28
(1,2298)	1:156:C:VAL:HB	1:157:C:PRO:HD2	10	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2298)	1:156:C:VAL:HB	1:157:C:PRO:HD3	10	0.28
(1,2298)	1:156:C:VAL:HB	1:157:C:PRO:HD2	13	0.28
(1,2298)	1:156:C:VAL:HB	1:157:C:PRO:HD3	13	0.28
(1,2094)	1:172:B:ALA:HA	1:178:B:PRO:HD2	3	0.28
(1,2094)	1:172:B:ALA:HA	1:178:B:PRO:HD3	3	0.28
(1,2072)	1:156:B:VAL:HB	1:157:B:PRO:HD2	13	0.28
(1,2072)	1:156:B:VAL:HB	1:157:B:PRO:HD3	13	0.28
(1,1916)	1:180:A:PHE:H	1:181:A:LEU:HB2	4	0.28
(1,1916)	1:180:A:PHE:H	1:181:A:LEU:HB3	4	0.28
(1,1912)	1:178:A:PRO:HB2	1:194:A:LEU:HD21	19	0.28
(1,1912)	1:178:A:PRO:HB2	1:194:A:LEU:HD22	19	0.28
(1,1912)	1:178:A:PRO:HB2	1:194:A:LEU:HD23	19	0.28
(1,1912)	1:178:A:PRO:HB3	1:194:A:LEU:HD21	19	0.28
(1,1912)	1:178:A:PRO:HB3	1:194:A:LEU:HD22	19	0.28
(1,1912)	1:178:A:PRO:HB3	1:194:A:LEU:HD23	19	0.28
(1,1902)	1:172:A:ALA:HA	1:178:A:PRO:HD2	10	0.28
(1,1902)	1:172:A:ALA:HA	1:178:A:PRO:HD3	10	0.28
(1,1887)	1:156:A:VAL:HB	1:157:A:PRO:HD2	9	0.28
(1,1887)	1:156:A:VAL:HB	1:157:A:PRO:HD3	9	0.28
(1,1770)	1:178:C:PRO:HD3	1:179:C:ALA:H	7	0.28
(1,1770)	1:178:C:PRO:HD3	1:179:C:ALA:H	9	0.28
(1,1769)	1:178:B:PRO:HD3	1:179:B:ALA:H	9	0.28
(1,1768)	1:178:A:PRO:HD3	1:179:A:ALA:H	8	0.28
(1,1610)	1:118:A:GLY:H	1:192:A:VAL:HG21	12	0.28
(1,1610)	1:118:A:GLY:H	1:192:A:VAL:HG22	12	0.28
(1,1610)	1:118:A:GLY:H	1:192:A:VAL:HG23	12	0.28
(1,1533)	1:122:A:TYR:H	1:189:A:CYS:HB2	6	0.28
(1,1533)	1:122:A:TYR:H	1:189:A:CYS:HB3	6	0.28
(1,1520)	1:178:A:PRO:HG2	1:179:A:ALA:H	7	0.28
(1,1520)	1:178:A:PRO:HG3	1:179:A:ALA:H	7	0.28
(1,1520)	1:178:A:PRO:HG2	1:179:A:ALA:H	9	0.28
(1,1520)	1:178:A:PRO:HG3	1:179:A:ALA:H	9	0.28
(1,1461)	1:180:A:PHE:H	1:181:A:LEU:HA	16	0.28
(1,1061)	1:178:C:PRO:HB3	1:179:C:ALA:H	10	0.28
(1,1060)	1:178:B:PRO:HB3	1:179:B:ALA:H	10	0.28
(1,1059)	1:178:A:PRO:HB3	1:179:A:ALA:H	10	0.28
(1,958)	1:187:A:THR:HA	1:188:A:LEU:HD11	9	0.28
(1,958)	1:187:A:THR:HA	1:188:A:LEU:HD12	9	0.28
(1,958)	1:187:A:THR:HA	1:188:A:LEU:HD13	9	0.28
(1,890)	1:152:C:ALA:HA	1:157:C:PRO:HG2	17	0.28
(1,890)	1:152:C:ALA:HA	1:157:C:PRO:HG3	17	0.28
(1,889)	1:152:B:ALA:HA	1:157:B:PRO:HG2	17	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,889)	1:152:B:ALA:HA	1:157:B:PRO:HG3	17	0.28
(1,888)	1:152:A:ALA:HA	1:157:A:PRO:HG2	19	0.28
(1,888)	1:152:A:ALA:HA	1:157:A:PRO:HG3	19	0.28
(1,754)	1:189:B:CYS:H	1:192:B:VAL:HG11	16	0.28
(1,754)	1:189:B:CYS:H	1:192:B:VAL:HG12	16	0.28
(1,754)	1:189:B:CYS:H	1:192:B:VAL:HG13	16	0.28
(1,728)	1:155:A:ALA:HB1	1:157:A:PRO:HD2	5	0.28
(1,728)	1:155:A:ALA:HB2	1:157:A:PRO:HD2	5	0.28
(1,728)	1:155:A:ALA:HB3	1:157:A:PRO:HD2	5	0.28
(1,728)	1:155:A:ALA:HB1	1:157:A:PRO:HD2	6	0.28
(1,728)	1:155:A:ALA:HB2	1:157:A:PRO:HD2	6	0.28
(1,728)	1:155:A:ALA:HB3	1:157:A:PRO:HD2	6	0.28
(1,395)	1:109:A:LEU:HG	1:111:A:ILE:HD11	3	0.28
(1,395)	1:109:A:LEU:HG	1:111:A:ILE:HD12	3	0.28
(1,395)	1:109:A:LEU:HG	1:111:A:ILE:HD13	3	0.28
(1,395)	1:109:A:LEU:HG	1:111:A:ILE:HD11	8	0.28
(1,395)	1:109:A:LEU:HG	1:111:A:ILE:HD12	8	0.28
(1,395)	1:109:A:LEU:HG	1:111:A:ILE:HD13	8	0.28
(1,395)	1:109:A:LEU:HG	1:111:A:ILE:HD11	13	0.28
(1,395)	1:109:A:LEU:HG	1:111:A:ILE:HD12	13	0.28
(1,395)	1:109:A:LEU:HG	1:111:A:ILE:HD13	13	0.28
(1,395)	1:109:A:LEU:HG	1:111:A:ILE:HD11	18	0.28
(1,395)	1:109:A:LEU:HG	1:111:A:ILE:HD12	18	0.28
(1,395)	1:109:A:LEU:HG	1:111:A:ILE:HD13	18	0.28
(1,395)	1:109:A:LEU:HG	1:111:A:ILE:HD11	20	0.28
(1,395)	1:109:A:LEU:HG	1:111:A:ILE:HD12	20	0.28
(1,395)	1:109:A:LEU:HG	1:111:A:ILE:HD13	20	0.28
(1,251)	1:118:C:GLY:HA2	1:119:C:THR:HG21	5	0.28
(1,251)	1:118:C:GLY:HA2	1:119:C:THR:HG22	5	0.28
(1,251)	1:118:C:GLY:HA2	1:119:C:THR:HG23	5	0.28
(1,251)	1:118:C:GLY:HA2	1:119:C:THR:HG21	6	0.28
(1,251)	1:118:C:GLY:HA2	1:119:C:THR:HG22	6	0.28
(1,251)	1:118:C:GLY:HA2	1:119:C:THR:HG23	6	0.28
(1,251)	1:118:C:GLY:HA2	1:119:C:THR:HG21	7	0.28
(1,251)	1:118:C:GLY:HA2	1:119:C:THR:HG22	7	0.28
(1,251)	1:118:C:GLY:HA2	1:119:C:THR:HG23	7	0.28
(1,251)	1:118:C:GLY:HA2	1:119:C:THR:HG21	10	0.28
(1,251)	1:118:C:GLY:HA2	1:119:C:THR:HG22	10	0.28
(1,251)	1:118:C:GLY:HA2	1:119:C:THR:HG23	10	0.28
(1,251)	1:118:C:GLY:HA2	1:119:C:THR:HG21	19	0.28
(1,251)	1:118:C:GLY:HA2	1:119:C:THR:HG22	19	0.28
(1,251)	1:118:C:GLY:HA2	1:119:C:THR:HG23	19	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,250)	1:118:B:GLY:HA2	1:119:B:THR:HG21	5	0.28
(1,250)	1:118:B:GLY:HA2	1:119:B:THR:HG22	5	0.28
(1,250)	1:118:B:GLY:HA2	1:119:B:THR:HG23	5	0.28
(1,250)	1:118:B:GLY:HA2	1:119:B:THR:HG21	7	0.28
(1,250)	1:118:B:GLY:HA2	1:119:B:THR:HG22	7	0.28
(1,250)	1:118:B:GLY:HA2	1:119:B:THR:HG23	7	0.28
(1,250)	1:118:B:GLY:HA2	1:119:B:THR:HG21	10	0.28
(1,250)	1:118:B:GLY:HA2	1:119:B:THR:HG22	10	0.28
(1,250)	1:118:B:GLY:HA2	1:119:B:THR:HG23	10	0.28
(1,250)	1:118:B:GLY:HA2	1:119:B:THR:HG21	19	0.28
(1,250)	1:118:B:GLY:HA2	1:119:B:THR:HG22	19	0.28
(1,250)	1:118:B:GLY:HA2	1:119:B:THR:HG23	19	0.28
(1,249)	1:118:A:GLY:HA2	1:119:A:THR:HG21	7	0.28
(1,249)	1:118:A:GLY:HA2	1:119:A:THR:HG22	7	0.28
(1,249)	1:118:A:GLY:HA2	1:119:A:THR:HG23	7	0.28
(1,249)	1:118:A:GLY:HA2	1:119:A:THR:HG21	10	0.28
(1,249)	1:118:A:GLY:HA2	1:119:A:THR:HG22	10	0.28
(1,249)	1:118:A:GLY:HA2	1:119:A:THR:HG23	10	0.28
(1,249)	1:118:A:GLY:HA2	1:119:A:THR:HG21	12	0.28
(1,249)	1:118:A:GLY:HA2	1:119:A:THR:HG22	12	0.28
(1,249)	1:118:A:GLY:HA2	1:119:A:THR:HG23	12	0.28
(1,249)	1:118:A:GLY:HA2	1:119:A:THR:HG21	13	0.28
(1,249)	1:118:A:GLY:HA2	1:119:A:THR:HG22	13	0.28
(1,249)	1:118:A:GLY:HA2	1:119:A:THR:HG23	13	0.28
(1,249)	1:118:A:GLY:HA2	1:119:A:THR:HG21	15	0.28
(1,249)	1:118:A:GLY:HA2	1:119:A:THR:HG22	15	0.28
(1,249)	1:118:A:GLY:HA2	1:119:A:THR:HG23	15	0.28
(1,249)	1:118:A:GLY:HA2	1:119:A:THR:HG21	17	0.28
(1,249)	1:118:A:GLY:HA2	1:119:A:THR:HG22	17	0.28
(1,249)	1:118:A:GLY:HA2	1:119:A:THR:HG23	17	0.28
(1,249)	1:118:A:GLY:HA2	1:119:A:THR:HG21	18	0.28
(1,249)	1:118:A:GLY:HA2	1:119:A:THR:HG22	18	0.28
(1,249)	1:118:A:GLY:HA2	1:119:A:THR:HG23	18	0.28
(1,249)	1:118:A:GLY:HA2	1:119:A:THR:HG21	20	0.28
(1,249)	1:118:A:GLY:HA2	1:119:A:THR:HG22	20	0.28
(1,249)	1:118:A:GLY:HA2	1:119:A:THR:HG23	20	0.28
(1,228)	1:96:C:ILE:HD11	1:102:C:VAL:HG11	9	0.28
(1,228)	1:96:C:ILE:HD11	1:102:C:VAL:HG12	9	0.28
(1,228)	1:96:C:ILE:HD11	1:102:C:VAL:HG13	9	0.28
(1,228)	1:96:C:ILE:HD12	1:102:C:VAL:HG11	9	0.28
(1,228)	1:96:C:ILE:HD12	1:102:C:VAL:HG12	9	0.28
(1,228)	1:96:C:ILE:HD12	1:102:C:VAL:HG13	9	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,228)	1:96:C:ILE:HD13	1:102:C:VAL:HG11	9	0.28
(1,228)	1:96:C:ILE:HD13	1:102:C:VAL:HG12	9	0.28
(1,228)	1:96:C:ILE:HD13	1:102:C:VAL:HG13	9	0.28
(1,226)	1:96:A:ILE:HD11	1:102:A:VAL:HG11	9	0.28
(1,226)	1:96:A:ILE:HD11	1:102:A:VAL:HG12	9	0.28
(1,226)	1:96:A:ILE:HD11	1:102:A:VAL:HG13	9	0.28
(1,226)	1:96:A:ILE:HD12	1:102:A:VAL:HG11	9	0.28
(1,226)	1:96:A:ILE:HD12	1:102:A:VAL:HG12	9	0.28
(1,226)	1:96:A:ILE:HD12	1:102:A:VAL:HG13	9	0.28
(1,226)	1:96:A:ILE:HD13	1:102:A:VAL:HG11	9	0.28
(1,226)	1:96:A:ILE:HD13	1:102:A:VAL:HG12	9	0.28
(1,226)	1:96:A:ILE:HD13	1:102:A:VAL:HG13	9	0.28
(1,216)	1:96:A:ILE:HG21	1:102:A:VAL:HG11	8	0.28
(1,216)	1:96:A:ILE:HG21	1:102:A:VAL:HG12	8	0.28
(1,216)	1:96:A:ILE:HG21	1:102:A:VAL:HG13	8	0.28
(1,216)	1:96:A:ILE:HG22	1:102:A:VAL:HG11	8	0.28
(1,216)	1:96:A:ILE:HG22	1:102:A:VAL:HG12	8	0.28
(1,216)	1:96:A:ILE:HG22	1:102:A:VAL:HG13	8	0.28
(1,216)	1:96:A:ILE:HG23	1:102:A:VAL:HG11	8	0.28
(1,216)	1:96:A:ILE:HG23	1:102:A:VAL:HG12	8	0.28
(1,216)	1:96:A:ILE:HG23	1:102:A:VAL:HG13	8	0.28
(1,205)	1:111:A:ILE:HD11	1:137:A:LEU:HD11	3	0.28
(1,205)	1:111:A:ILE:HD11	1:137:A:LEU:HD12	3	0.28
(1,205)	1:111:A:ILE:HD11	1:137:A:LEU:HD13	3	0.28
(1,205)	1:111:A:ILE:HD12	1:137:A:LEU:HD11	3	0.28
(1,205)	1:111:A:ILE:HD12	1:137:A:LEU:HD12	3	0.28
(1,205)	1:111:A:ILE:HD12	1:137:A:LEU:HD13	3	0.28
(1,205)	1:111:A:ILE:HD13	1:137:A:LEU:HD11	3	0.28
(1,205)	1:111:A:ILE:HD13	1:137:A:LEU:HD12	3	0.28
(1,205)	1:111:A:ILE:HD13	1:137:A:LEU:HD13	3	0.28
(1,205)	1:111:A:ILE:HD11	1:137:A:LEU:HD11	6	0.28
(1,205)	1:111:A:ILE:HD11	1:137:A:LEU:HD12	6	0.28
(1,205)	1:111:A:ILE:HD11	1:137:A:LEU:HD13	6	0.28
(1,205)	1:111:A:ILE:HD12	1:137:A:LEU:HD11	6	0.28
(1,205)	1:111:A:ILE:HD12	1:137:A:LEU:HD12	6	0.28
(1,205)	1:111:A:ILE:HD12	1:137:A:LEU:HD13	6	0.28
(1,205)	1:111:A:ILE:HD13	1:137:A:LEU:HD11	6	0.28
(1,205)	1:111:A:ILE:HD13	1:137:A:LEU:HD12	6	0.28
(1,205)	1:111:A:ILE:HD13	1:137:A:LEU:HD13	6	0.28
(1,122)	1:113:A:TYR:HD1	1:137:A:LEU:HD21	12	0.28
(1,122)	1:113:A:TYR:HD1	1:137:A:LEU:HD22	12	0.28
(1,122)	1:113:A:TYR:HD1	1:137:A:LEU:HD23	12	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,122)	1:113:A:TYR:HD2	1:137:A:LEU:HD21	12	0.28
(1,122)	1:113:A:TYR:HD2	1:137:A:LEU:HD22	12	0.28
(1,122)	1:113:A:TYR:HD2	1:137:A:LEU:HD23	12	0.28
(1,122)	1:113:A:TYR:HD1	1:137:A:LEU:HD21	17	0.28
(1,122)	1:113:A:TYR:HD1	1:137:A:LEU:HD22	17	0.28
(1,122)	1:113:A:TYR:HD1	1:137:A:LEU:HD23	17	0.28
(1,122)	1:113:A:TYR:HD2	1:137:A:LEU:HD21	17	0.28
(1,122)	1:113:A:TYR:HD2	1:137:A:LEU:HD22	17	0.28
(1,122)	1:113:A:TYR:HD2	1:137:A:LEU:HD23	17	0.28
(1,122)	1:113:A:TYR:HD1	1:137:A:LEU:HD21	19	0.28
(1,122)	1:113:A:TYR:HD1	1:137:A:LEU:HD22	19	0.28
(1,122)	1:113:A:TYR:HD1	1:137:A:LEU:HD23	19	0.28
(1,122)	1:113:A:TYR:HD2	1:137:A:LEU:HD21	19	0.28
(1,122)	1:113:A:TYR:HD2	1:137:A:LEU:HD22	19	0.28
(1,122)	1:113:A:TYR:HD2	1:137:A:LEU:HD23	19	0.28
(1,1)	1:108:A:GLN:HA	1:109:A:LEU:HD21	11	0.28
(1,1)	1:108:A:GLN:HA	1:109:A:LEU:HD22	11	0.28
(1,1)	1:108:A:GLN:HA	1:109:A:LEU:HD23	11	0.28
(1,1)	1:108:A:GLN:HA	1:109:A:LEU:HD21	19	0.28
(1,1)	1:108:A:GLN:HA	1:109:A:LEU:HD22	19	0.28
(1,1)	1:108:A:GLN:HA	1:109:A:LEU:HD23	19	0.28
(1,2298)	1:156:C:VAL:HB	1:157:C:PRO:HD2	19	0.27
(1,2298)	1:156:C:VAL:HB	1:157:C:PRO:HD3	19	0.27
(1,2072)	1:156:B:VAL:HB	1:157:B:PRO:HD2	18	0.27
(1,2072)	1:156:B:VAL:HB	1:157:B:PRO:HD3	18	0.27
(1,2072)	1:156:B:VAL:HB	1:157:B:PRO:HD2	19	0.27
(1,2072)	1:156:B:VAL:HB	1:157:B:PRO:HD3	19	0.27
(1,2072)	1:156:B:VAL:HB	1:157:B:PRO:HD2	20	0.27
(1,2072)	1:156:B:VAL:HB	1:157:B:PRO:HD3	20	0.27
(1,1892)	1:161:A:LEU:HD11	1:162:A:GLY:HA2	14	0.27
(1,1892)	1:161:A:LEU:HD11	1:162:A:GLY:HA3	14	0.27
(1,1892)	1:161:A:LEU:HD12	1:162:A:GLY:HA2	14	0.27
(1,1892)	1:161:A:LEU:HD12	1:162:A:GLY:HA3	14	0.27
(1,1892)	1:161:A:LEU:HD13	1:162:A:GLY:HA2	14	0.27
(1,1892)	1:161:A:LEU:HD13	1:162:A:GLY:HA3	14	0.27
(1,1887)	1:156:A:VAL:HB	1:157:A:PRO:HD2	1	0.27
(1,1887)	1:156:A:VAL:HB	1:157:A:PRO:HD3	1	0.27
(1,1887)	1:156:A:VAL:HB	1:157:A:PRO:HD2	11	0.27
(1,1887)	1:156:A:VAL:HB	1:157:A:PRO:HD3	11	0.27
(1,1830)	1:102:A:VAL:HG11	1:111:A:ILE:HG12	3	0.27
(1,1830)	1:102:A:VAL:HG11	1:111:A:ILE:HG13	3	0.27
(1,1830)	1:102:A:VAL:HG12	1:111:A:ILE:HG12	3	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1830)	1:102:A:VAL:HG12	1:111:A:ILE:HG13	3	0.27
(1,1830)	1:102:A:VAL:HG13	1:111:A:ILE:HG12	3	0.27
(1,1830)	1:102:A:VAL:HG13	1:111:A:ILE:HG13	3	0.27
(1,1818)	1:95:B:SER:HB2	1:101:B:LEU:H	6	0.27
(1,1818)	1:95:B:SER:HB3	1:101:B:LEU:H	6	0.27
(1,1769)	1:178:B:PRO:HD3	1:179:B:ALA:H	7	0.27
(1,1768)	1:178:A:PRO:HD3	1:179:A:ALA:H	20	0.27
(1,1737)	1:194:A:LEU:HD21	1:195:A:TYR:H	15	0.27
(1,1737)	1:194:A:LEU:HD22	1:195:A:TYR:H	15	0.27
(1,1737)	1:194:A:LEU:HD23	1:195:A:TYR:H	15	0.27
(1,1522)	1:178:C:PRO:HG2	1:179:C:ALA:H	7	0.27
(1,1522)	1:178:C:PRO:HG3	1:179:C:ALA:H	7	0.27
(1,1522)	1:178:C:PRO:HG2	1:179:C:ALA:H	9	0.27
(1,1522)	1:178:C:PRO:HG3	1:179:C:ALA:H	9	0.27
(1,1521)	1:178:B:PRO:HG2	1:179:B:ALA:H	7	0.27
(1,1521)	1:178:B:PRO:HG3	1:179:B:ALA:H	7	0.27
(1,1521)	1:178:B:PRO:HG2	1:179:B:ALA:H	9	0.27
(1,1521)	1:178:B:PRO:HG3	1:179:B:ALA:H	9	0.27
(1,1520)	1:178:A:PRO:HG2	1:179:A:ALA:H	8	0.27
(1,1520)	1:178:A:PRO:HG3	1:179:A:ALA:H	8	0.27
(1,1364)	1:154:C:PRO:HA	1:155:C:ALA:H	10	0.27
(1,1363)	1:154:B:PRO:HA	1:155:B:ALA:H	10	0.27
(1,1362)	1:154:A:PRO:HA	1:155:A:ALA:H	10	0.27
(1,1073)	1:139:C:ARG:H	1:141:C:VAL:HB	5	0.27
(1,1072)	1:139:B:ARG:H	1:141:B:VAL:HB	5	0.27
(1,1030)	1:152:A:ALA:H	1:153:A:LYS:H	17	0.27
(1,965)	1:110:A:LEU:HD11	1:125:A:LYS:HB3	19	0.27
(1,965)	1:110:A:LEU:HD12	1:125:A:LYS:HB3	19	0.27
(1,965)	1:110:A:LEU:HD13	1:125:A:LYS:HB3	19	0.27
(1,958)	1:187:A:THR:HA	1:188:A:LEU:HD11	5	0.27
(1,958)	1:187:A:THR:HA	1:188:A:LEU:HD12	5	0.27
(1,958)	1:187:A:THR:HA	1:188:A:LEU:HD13	5	0.27
(1,958)	1:187:A:THR:HA	1:188:A:LEU:HD11	16	0.27
(1,958)	1:187:A:THR:HA	1:188:A:LEU:HD12	16	0.27
(1,958)	1:187:A:THR:HA	1:188:A:LEU:HD13	16	0.27
(1,889)	1:152:B:ALA:HA	1:157:B:PRO:HG2	19	0.27
(1,889)	1:152:B:ALA:HA	1:157:B:PRO:HG3	19	0.27
(1,842)	1:156:A:VAL:HB	1:157:A:PRO:HD2	7	0.27
(1,755)	1:189:C:CYS:H	1:192:C:VAL:HG11	16	0.27
(1,755)	1:189:C:CYS:H	1:192:C:VAL:HG12	16	0.27
(1,755)	1:189:C:CYS:H	1:192:C:VAL:HG13	16	0.27
(1,753)	1:189:A:CYS:H	1:192:A:VAL:HG11	10	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,753)	1:189:A:CYS:H	1:192:A:VAL:HG12	10	0.27
(1,753)	1:189:A:CYS:H	1:192:A:VAL:HG13	10	0.27
(1,728)	1:155:A:ALA:HB1	1:157:A:PRO:HD2	8	0.27
(1,728)	1:155:A:ALA:HB2	1:157:A:PRO:HD2	8	0.27
(1,728)	1:155:A:ALA:HB3	1:157:A:PRO:HD2	8	0.27
(1,435)	1:183:A:MET:HE1	1:186:A:SER:HA	6	0.27
(1,435)	1:183:A:MET:HE2	1:186:A:SER:HA	6	0.27
(1,435)	1:183:A:MET:HE3	1:186:A:SER:HA	6	0.27
(1,395)	1:109:A:LEU:HG	1:111:A:ILE:HD11	16	0.27
(1,395)	1:109:A:LEU:HG	1:111:A:ILE:HD12	16	0.27
(1,395)	1:109:A:LEU:HG	1:111:A:ILE:HD13	16	0.27
(1,301)	1:181:A:LEU:HD11	1:196:A:TYR:HE1	19	0.27
(1,301)	1:181:A:LEU:HD11	1:196:A:TYR:HE2	19	0.27
(1,301)	1:181:A:LEU:HD12	1:196:A:TYR:HE1	19	0.27
(1,301)	1:181:A:LEU:HD12	1:196:A:TYR:HE2	19	0.27
(1,301)	1:181:A:LEU:HD13	1:196:A:TYR:HE1	19	0.27
(1,301)	1:181:A:LEU:HD13	1:196:A:TYR:HE2	19	0.27
(1,249)	1:118:A:GLY:HA2	1:119:A:THR:HG21	5	0.27
(1,249)	1:118:A:GLY:HA2	1:119:A:THR:HG22	5	0.27
(1,249)	1:118:A:GLY:HA2	1:119:A:THR:HG23	5	0.27
(1,249)	1:118:A:GLY:HA2	1:119:A:THR:HG21	19	0.27
(1,249)	1:118:A:GLY:HA2	1:119:A:THR:HG22	19	0.27
(1,249)	1:118:A:GLY:HA2	1:119:A:THR:HG23	19	0.27
(1,228)	1:96:C:ILE:HD11	1:102:C:VAL:HG11	19	0.27
(1,228)	1:96:C:ILE:HD11	1:102:C:VAL:HG12	19	0.27
(1,228)	1:96:C:ILE:HD11	1:102:C:VAL:HG13	19	0.27
(1,228)	1:96:C:ILE:HD12	1:102:C:VAL:HG11	19	0.27
(1,228)	1:96:C:ILE:HD12	1:102:C:VAL:HG12	19	0.27
(1,228)	1:96:C:ILE:HD12	1:102:C:VAL:HG13	19	0.27
(1,228)	1:96:C:ILE:HD13	1:102:C:VAL:HG11	19	0.27
(1,228)	1:96:C:ILE:HD13	1:102:C:VAL:HG12	19	0.27
(1,228)	1:96:C:ILE:HD13	1:102:C:VAL:HG13	19	0.27
(1,228)	1:96:C:ILE:HD11	1:102:C:VAL:HG11	20	0.27
(1,228)	1:96:C:ILE:HD11	1:102:C:VAL:HG12	20	0.27
(1,228)	1:96:C:ILE:HD11	1:102:C:VAL:HG13	20	0.27
(1,228)	1:96:C:ILE:HD12	1:102:C:VAL:HG11	20	0.27
(1,228)	1:96:C:ILE:HD12	1:102:C:VAL:HG12	20	0.27
(1,228)	1:96:C:ILE:HD12	1:102:C:VAL:HG13	20	0.27
(1,228)	1:96:C:ILE:HD13	1:102:C:VAL:HG11	20	0.27
(1,228)	1:96:C:ILE:HD13	1:102:C:VAL:HG12	20	0.27
(1,228)	1:96:C:ILE:HD13	1:102:C:VAL:HG13	20	0.27
(1,227)	1:96:B:ILE:HD11	1:102:B:VAL:HG11	9	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,227)	1:96:B:ILE:HD11	1:102:B:VAL:HG12	9	0.27
(1,227)	1:96:B:ILE:HD11	1:102:B:VAL:HG13	9	0.27
(1,227)	1:96:B:ILE:HD12	1:102:B:VAL:HG11	9	0.27
(1,227)	1:96:B:ILE:HD12	1:102:B:VAL:HG12	9	0.27
(1,227)	1:96:B:ILE:HD12	1:102:B:VAL:HG13	9	0.27
(1,227)	1:96:B:ILE:HD13	1:102:B:VAL:HG11	9	0.27
(1,227)	1:96:B:ILE:HD13	1:102:B:VAL:HG12	9	0.27
(1,227)	1:96:B:ILE:HD13	1:102:B:VAL:HG13	9	0.27
(1,175)	1:179:A:ALA:HB1	1:181:A:LEU:HD21	12	0.27
(1,175)	1:179:A:ALA:HB1	1:181:A:LEU:HD22	12	0.27
(1,175)	1:179:A:ALA:HB1	1:181:A:LEU:HD23	12	0.27
(1,175)	1:179:A:ALA:HB2	1:181:A:LEU:HD21	12	0.27
(1,175)	1:179:A:ALA:HB2	1:181:A:LEU:HD22	12	0.27
(1,175)	1:179:A:ALA:HB2	1:181:A:LEU:HD23	12	0.27
(1,175)	1:179:A:ALA:HB3	1:181:A:LEU:HD21	12	0.27
(1,175)	1:179:A:ALA:HB3	1:181:A:LEU:HD22	12	0.27
(1,175)	1:179:A:ALA:HB3	1:181:A:LEU:HD23	12	0.27
(1,1)	1:108:A:GLN:HA	1:109:A:LEU:HD21	2	0.27
(1,1)	1:108:A:GLN:HA	1:109:A:LEU:HD22	2	0.27
(1,1)	1:108:A:GLN:HA	1:109:A:LEU:HD23	2	0.27
(1,2298)	1:156:C:VAL:HB	1:157:C:PRO:HD2	18	0.26
(1,2298)	1:156:C:VAL:HB	1:157:C:PRO:HD3	18	0.26
(1,2298)	1:156:C:VAL:HB	1:157:C:PRO:HD2	20	0.26
(1,2298)	1:156:C:VAL:HB	1:157:C:PRO:HD3	20	0.26
(1,2292)	1:154:C:PRO:HB2	1:167:C:ARG:H	13	0.26
(1,2292)	1:154:C:PRO:HB3	1:167:C:ARG:H	13	0.26
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD11	6	0.26
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD12	6	0.26
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD13	6	0.26
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD21	6	0.26
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD22	6	0.26
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD23	6	0.26
(1,1830)	1:102:A:VAL:HG11	1:111:A:ILE:HG12	11	0.26
(1,1830)	1:102:A:VAL:HG11	1:111:A:ILE:HG13	11	0.26
(1,1830)	1:102:A:VAL:HG12	1:111:A:ILE:HG12	11	0.26
(1,1830)	1:102:A:VAL:HG12	1:111:A:ILE:HG13	11	0.26
(1,1830)	1:102:A:VAL:HG13	1:111:A:ILE:HG12	11	0.26
(1,1830)	1:102:A:VAL:HG13	1:111:A:ILE:HG13	11	0.26
(1,1770)	1:178:C:PRO:HD3	1:179:C:ALA:H	5	0.26
(1,1770)	1:178:C:PRO:HD3	1:179:C:ALA:H	6	0.26
(1,1770)	1:178:C:PRO:HD3	1:179:C:ALA:H	8	0.26
(1,1770)	1:178:C:PRO:HD3	1:179:C:ALA:H	18	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1770)	1:178:C:PRO:HD3	1:179:C:ALA:H	20	0.26
(1,1769)	1:178:B:PRO:HD3	1:179:B:ALA:H	5	0.26
(1,1769)	1:178:B:PRO:HD3	1:179:B:ALA:H	6	0.26
(1,1769)	1:178:B:PRO:HD3	1:179:B:ALA:H	8	0.26
(1,1769)	1:178:B:PRO:HD3	1:179:B:ALA:H	18	0.26
(1,1769)	1:178:B:PRO:HD3	1:179:B:ALA:H	20	0.26
(1,1768)	1:178:A:PRO:HD3	1:179:A:ALA:H	14	0.26
(1,1737)	1:194:A:LEU:HD21	1:195:A:TYR:H	8	0.26
(1,1737)	1:194:A:LEU:HD22	1:195:A:TYR:H	8	0.26
(1,1737)	1:194:A:LEU:HD23	1:195:A:TYR:H	8	0.26
(1,1610)	1:118:A:GLY:H	1:192:A:VAL:HG21	10	0.26
(1,1610)	1:118:A:GLY:H	1:192:A:VAL:HG22	10	0.26
(1,1610)	1:118:A:GLY:H	1:192:A:VAL:HG23	10	0.26
(1,1551)	1:167:C:ARG:H	1:171:C:SER:HA	14	0.26
(1,1550)	1:167:B:ARG:H	1:171:B:SER:HA	14	0.26
(1,1549)	1:167:A:ARG:H	1:171:A:SER:HA	14	0.26
(1,1520)	1:178:A:PRO:HG2	1:179:A:ALA:H	20	0.26
(1,1520)	1:178:A:PRO:HG3	1:179:A:ALA:H	20	0.26
(1,1463)	1:180:C:PHE:H	1:181:C:LEU:HA	5	0.26
(1,1463)	1:180:C:PHE:H	1:181:C:LEU:HA	14	0.26
(1,1462)	1:180:B:PHE:H	1:181:B:LEU:HA	5	0.26
(1,1462)	1:180:B:PHE:H	1:181:B:LEU:HA	14	0.26
(1,1461)	1:180:A:PHE:H	1:181:A:LEU:HA	14	0.26
(1,1204)	1:149:A:SER:HB2	1:151:A:GLN:H	20	0.26
(1,1204)	1:149:A:SER:HB3	1:151:A:GLN:H	20	0.26
(1,1097)	1:157:C:PRO:HA	1:158:C:THR:H	6	0.26
(1,1097)	1:157:C:PRO:HA	1:158:C:THR:H	8	0.26
(1,1096)	1:157:B:PRO:HA	1:158:B:THR:H	6	0.26
(1,1096)	1:157:B:PRO:HA	1:158:B:THR:H	8	0.26
(1,1072)	1:139:B:ARG:H	1:141:B:VAL:HB	17	0.26
(1,1061)	1:178:C:PRO:HB3	1:179:C:ALA:H	3	0.26
(1,1060)	1:178:B:PRO:HB3	1:179:B:ALA:H	3	0.26
(1,1059)	1:178:A:PRO:HB3	1:179:A:ALA:H	3	0.26
(1,958)	1:187:A:THR:HA	1:188:A:LEU:HD11	14	0.26
(1,958)	1:187:A:THR:HA	1:188:A:LEU:HD12	14	0.26
(1,958)	1:187:A:THR:HA	1:188:A:LEU:HD13	14	0.26
(1,890)	1:152:C:ALA:HA	1:157:C:PRO:HG2	19	0.26
(1,890)	1:152:C:ALA:HA	1:157:C:PRO:HG3	19	0.26
(1,753)	1:189:A:CYS:H	1:192:A:VAL:HG11	2	0.26
(1,753)	1:189:A:CYS:H	1:192:A:VAL:HG12	2	0.26
(1,753)	1:189:A:CYS:H	1:192:A:VAL:HG13	2	0.26
(1,738)	1:175:B:GLY:HA2	1:179:B:ALA:HB1	4	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,738)	1:175:B:GLY:HA2	1:179:B:ALA:HB2	4	0.26
(1,738)	1:175:B:GLY:HA2	1:179:B:ALA:HB3	4	0.26
(1,738)	1:175:B:GLY:HA3	1:179:B:ALA:HB1	4	0.26
(1,738)	1:175:B:GLY:HA3	1:179:B:ALA:HB2	4	0.26
(1,738)	1:175:B:GLY:HA3	1:179:B:ALA:HB3	4	0.26
(1,737)	1:175:A:GLY:HA2	1:179:A:ALA:HB1	4	0.26
(1,737)	1:175:A:GLY:HA2	1:179:A:ALA:HB2	4	0.26
(1,737)	1:175:A:GLY:HA2	1:179:A:ALA:HB3	4	0.26
(1,737)	1:175:A:GLY:HA3	1:179:A:ALA:HB1	4	0.26
(1,737)	1:175:A:GLY:HA3	1:179:A:ALA:HB2	4	0.26
(1,737)	1:175:A:GLY:HA3	1:179:A:ALA:HB3	4	0.26
(1,728)	1:155:A:ALA:HB1	1:157:A:PRO:HD2	2	0.26
(1,728)	1:155:A:ALA:HB2	1:157:A:PRO:HD2	2	0.26
(1,728)	1:155:A:ALA:HB3	1:157:A:PRO:HD2	2	0.26
(1,728)	1:155:A:ALA:HB1	1:157:A:PRO:HD2	3	0.26
(1,728)	1:155:A:ALA:HB2	1:157:A:PRO:HD2	3	0.26
(1,728)	1:155:A:ALA:HB3	1:157:A:PRO:HD2	3	0.26
(1,635)	1:96:A:ILE:HG21	1:100:A:GLY:H	9	0.26
(1,635)	1:96:A:ILE:HG22	1:100:A:GLY:H	9	0.26
(1,635)	1:96:A:ILE:HG23	1:100:A:GLY:H	9	0.26
(1,395)	1:109:A:LEU:HG	1:111:A:ILE:HD11	15	0.26
(1,395)	1:109:A:LEU:HG	1:111:A:ILE:HD12	15	0.26
(1,395)	1:109:A:LEU:HG	1:111:A:ILE:HD13	15	0.26
(1,228)	1:96:C:ILE:HD11	1:102:C:VAL:HG11	7	0.26
(1,228)	1:96:C:ILE:HD11	1:102:C:VAL:HG12	7	0.26
(1,228)	1:96:C:ILE:HD11	1:102:C:VAL:HG13	7	0.26
(1,228)	1:96:C:ILE:HD12	1:102:C:VAL:HG11	7	0.26
(1,228)	1:96:C:ILE:HD12	1:102:C:VAL:HG12	7	0.26
(1,228)	1:96:C:ILE:HD12	1:102:C:VAL:HG13	7	0.26
(1,228)	1:96:C:ILE:HD13	1:102:C:VAL:HG11	7	0.26
(1,228)	1:96:C:ILE:HD13	1:102:C:VAL:HG12	7	0.26
(1,228)	1:96:C:ILE:HD13	1:102:C:VAL:HG13	7	0.26
(1,228)	1:96:C:ILE:HD11	1:102:C:VAL:HG11	17	0.26
(1,228)	1:96:C:ILE:HD11	1:102:C:VAL:HG12	17	0.26
(1,228)	1:96:C:ILE:HD11	1:102:C:VAL:HG13	17	0.26
(1,228)	1:96:C:ILE:HD12	1:102:C:VAL:HG11	17	0.26
(1,228)	1:96:C:ILE:HD12	1:102:C:VAL:HG12	17	0.26
(1,228)	1:96:C:ILE:HD12	1:102:C:VAL:HG13	17	0.26
(1,228)	1:96:C:ILE:HD13	1:102:C:VAL:HG11	17	0.26
(1,228)	1:96:C:ILE:HD13	1:102:C:VAL:HG12	17	0.26
(1,228)	1:96:C:ILE:HD13	1:102:C:VAL:HG13	17	0.26
(1,227)	1:96:B:ILE:HD11	1:102:B:VAL:HG11	7	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,227)	1:96:B:ILE:HD11	1:102:B:VAL:HG12	7	0.26
(1,227)	1:96:B:ILE:HD11	1:102:B:VAL:HG13	7	0.26
(1,227)	1:96:B:ILE:HD12	1:102:B:VAL:HG11	7	0.26
(1,227)	1:96:B:ILE:HD12	1:102:B:VAL:HG12	7	0.26
(1,227)	1:96:B:ILE:HD12	1:102:B:VAL:HG13	7	0.26
(1,227)	1:96:B:ILE:HD13	1:102:B:VAL:HG11	7	0.26
(1,227)	1:96:B:ILE:HD13	1:102:B:VAL:HG12	7	0.26
(1,227)	1:96:B:ILE:HD13	1:102:B:VAL:HG13	7	0.26
(1,227)	1:96:B:ILE:HD11	1:102:B:VAL:HG11	19	0.26
(1,227)	1:96:B:ILE:HD11	1:102:B:VAL:HG12	19	0.26
(1,227)	1:96:B:ILE:HD11	1:102:B:VAL:HG13	19	0.26
(1,227)	1:96:B:ILE:HD12	1:102:B:VAL:HG11	19	0.26
(1,227)	1:96:B:ILE:HD12	1:102:B:VAL:HG12	19	0.26
(1,227)	1:96:B:ILE:HD12	1:102:B:VAL:HG13	19	0.26
(1,227)	1:96:B:ILE:HD13	1:102:B:VAL:HG11	19	0.26
(1,227)	1:96:B:ILE:HD13	1:102:B:VAL:HG12	19	0.26
(1,227)	1:96:B:ILE:HD13	1:102:B:VAL:HG13	19	0.26
(1,226)	1:96:A:ILE:HD11	1:102:A:VAL:HG11	5	0.26
(1,226)	1:96:A:ILE:HD11	1:102:A:VAL:HG12	5	0.26
(1,226)	1:96:A:ILE:HD11	1:102:A:VAL:HG13	5	0.26
(1,226)	1:96:A:ILE:HD12	1:102:A:VAL:HG11	5	0.26
(1,226)	1:96:A:ILE:HD12	1:102:A:VAL:HG12	5	0.26
(1,226)	1:96:A:ILE:HD12	1:102:A:VAL:HG13	5	0.26
(1,226)	1:96:A:ILE:HD13	1:102:A:VAL:HG11	5	0.26
(1,226)	1:96:A:ILE:HD13	1:102:A:VAL:HG12	5	0.26
(1,226)	1:96:A:ILE:HD13	1:102:A:VAL:HG13	5	0.26
(1,205)	1:111:A:ILE:HD11	1:137:A:LEU:HD11	20	0.26
(1,205)	1:111:A:ILE:HD11	1:137:A:LEU:HD12	20	0.26
(1,205)	1:111:A:ILE:HD11	1:137:A:LEU:HD13	20	0.26
(1,205)	1:111:A:ILE:HD12	1:137:A:LEU:HD11	20	0.26
(1,205)	1:111:A:ILE:HD12	1:137:A:LEU:HD12	20	0.26
(1,205)	1:111:A:ILE:HD12	1:137:A:LEU:HD13	20	0.26
(1,205)	1:111:A:ILE:HD13	1:137:A:LEU:HD11	20	0.26
(1,205)	1:111:A:ILE:HD13	1:137:A:LEU:HD12	20	0.26
(1,205)	1:111:A:ILE:HD13	1:137:A:LEU:HD13	20	0.26
(1,175)	1:179:A:ALA:HB1	1:181:A:LEU:HD21	18	0.26
(1,175)	1:179:A:ALA:HB1	1:181:A:LEU:HD22	18	0.26
(1,175)	1:179:A:ALA:HB1	1:181:A:LEU:HD23	18	0.26
(1,175)	1:179:A:ALA:HB2	1:181:A:LEU:HD21	18	0.26
(1,175)	1:179:A:ALA:HB2	1:181:A:LEU:HD22	18	0.26
(1,175)	1:179:A:ALA:HB2	1:181:A:LEU:HD23	18	0.26
(1,175)	1:179:A:ALA:HB3	1:181:A:LEU:HD21	18	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,175)	1:179:A:ALA:HB3	1:181:A:LEU:HD22	18	0.26
(1,175)	1:179:A:ALA:HB3	1:181:A:LEU:HD23	18	0.26
(1,138)	1:192:A:VAL:HG21	1:135:B:GLU:HG2	18	0.26
(1,138)	1:192:A:VAL:HG21	1:135:B:GLU:HG3	18	0.26
(1,138)	1:192:A:VAL:HG22	1:135:B:GLU:HG2	18	0.26
(1,138)	1:192:A:VAL:HG22	1:135:B:GLU:HG3	18	0.26
(1,138)	1:192:A:VAL:HG23	1:135:B:GLU:HG2	18	0.26
(1,138)	1:192:A:VAL:HG23	1:135:B:GLU:HG3	18	0.26
(1,124)	1:96:A:ILE:H	1:101:A:LEU:HD21	1	0.26
(1,124)	1:96:A:ILE:H	1:101:A:LEU:HD22	1	0.26
(1,124)	1:96:A:ILE:H	1:101:A:LEU:HD23	1	0.26
(1,122)	1:113:A:TYR:HD1	1:137:A:LEU:HD21	2	0.26
(1,122)	1:113:A:TYR:HD1	1:137:A:LEU:HD22	2	0.26
(1,122)	1:113:A:TYR:HD1	1:137:A:LEU:HD23	2	0.26
(1,122)	1:113:A:TYR:HD2	1:137:A:LEU:HD21	2	0.26
(1,122)	1:113:A:TYR:HD2	1:137:A:LEU:HD22	2	0.26
(1,122)	1:113:A:TYR:HD2	1:137:A:LEU:HD23	2	0.26
(1,122)	1:113:A:TYR:HD1	1:137:A:LEU:HD21	10	0.26
(1,122)	1:113:A:TYR:HD1	1:137:A:LEU:HD22	10	0.26
(1,122)	1:113:A:TYR:HD1	1:137:A:LEU:HD23	10	0.26
(1,122)	1:113:A:TYR:HD2	1:137:A:LEU:HD21	10	0.26
(1,122)	1:113:A:TYR:HD2	1:137:A:LEU:HD22	10	0.26
(1,122)	1:113:A:TYR:HD2	1:137:A:LEU:HD23	10	0.26
(1,122)	1:113:A:TYR:HD1	1:137:A:LEU:HD21	11	0.26
(1,122)	1:113:A:TYR:HD1	1:137:A:LEU:HD22	11	0.26
(1,122)	1:113:A:TYR:HD1	1:137:A:LEU:HD23	11	0.26
(1,122)	1:113:A:TYR:HD2	1:137:A:LEU:HD21	11	0.26
(1,122)	1:113:A:TYR:HD2	1:137:A:LEU:HD22	11	0.26
(1,122)	1:113:A:TYR:HD2	1:137:A:LEU:HD23	11	0.26
(1,122)	1:113:A:TYR:HD1	1:137:A:LEU:HD21	18	0.26
(1,122)	1:113:A:TYR:HD1	1:137:A:LEU:HD22	18	0.26
(1,122)	1:113:A:TYR:HD1	1:137:A:LEU:HD23	18	0.26
(1,122)	1:113:A:TYR:HD2	1:137:A:LEU:HD21	18	0.26
(1,122)	1:113:A:TYR:HD2	1:137:A:LEU:HD22	18	0.26
(1,122)	1:113:A:TYR:HD2	1:137:A:LEU:HD23	18	0.26
(1,1)	1:108:A:GLN:HA	1:109:A:LEU:HD21	17	0.26
(1,1)	1:108:A:GLN:HA	1:109:A:LEU:HD22	17	0.26
(1,1)	1:108:A:GLN:HA	1:109:A:LEU:HD23	17	0.26
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD11	6	0.25
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD12	6	0.25
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD13	6	0.25
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD21	6	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD22	6	0.25
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD23	6	0.25
(1,2320)	1:172:C:ALA:HA	1:178:C:PRO:HD2	2	0.25
(1,2320)	1:172:C:ALA:HA	1:178:C:PRO:HD3	2	0.25
(1,2320)	1:172:C:ALA:HA	1:178:C:PRO:HD2	16	0.25
(1,2320)	1:172:C:ALA:HA	1:178:C:PRO:HD3	16	0.25
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG11	18	0.25
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG12	18	0.25
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG13	18	0.25
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG21	18	0.25
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG22	18	0.25
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG23	18	0.25
(1,2094)	1:172:B:ALA:HA	1:178:B:PRO:HD2	2	0.25
(1,2094)	1:172:B:ALA:HA	1:178:B:PRO:HD3	2	0.25
(1,2094)	1:172:B:ALA:HA	1:178:B:PRO:HD2	16	0.25
(1,2094)	1:172:B:ALA:HA	1:178:B:PRO:HD3	16	0.25
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG11	18	0.25
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG12	18	0.25
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG13	18	0.25
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG21	18	0.25
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG22	18	0.25
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG23	18	0.25
(1,2066)	1:154:B:PRO:HB2	1:167:B:ARG:H	13	0.25
(1,2066)	1:154:B:PRO:HB3	1:167:B:ARG:H	13	0.25
(1,1902)	1:172:A:ALA:HA	1:178:A:PRO:HD2	3	0.25
(1,1902)	1:172:A:ALA:HA	1:178:A:PRO:HD3	3	0.25
(1,1887)	1:156:A:VAL:HB	1:157:A:PRO:HD2	2	0.25
(1,1887)	1:156:A:VAL:HB	1:157:A:PRO:HD3	2	0.25
(1,1887)	1:156:A:VAL:HB	1:157:A:PRO:HD2	3	0.25
(1,1887)	1:156:A:VAL:HB	1:157:A:PRO:HD3	3	0.25
(1,1887)	1:156:A:VAL:HB	1:157:A:PRO:HD2	5	0.25
(1,1887)	1:156:A:VAL:HB	1:157:A:PRO:HD3	5	0.25
(1,1887)	1:156:A:VAL:HB	1:157:A:PRO:HD2	15	0.25
(1,1887)	1:156:A:VAL:HB	1:157:A:PRO:HD3	15	0.25
(1,1842)	1:121:A:CYS:HB2	1:189:A:CYS:H	1	0.25
(1,1842)	1:121:A:CYS:HB3	1:189:A:CYS:H	1	0.25
(1,1842)	1:121:A:CYS:HB2	1:189:A:CYS:H	10	0.25
(1,1842)	1:121:A:CYS:HB3	1:189:A:CYS:H	10	0.25
(1,1776)	1:125:C:LYS:H	1:126:C:ILE:HG21	4	0.25
(1,1776)	1:125:C:LYS:H	1:126:C:ILE:HG22	4	0.25
(1,1776)	1:125:C:LYS:H	1:126:C:ILE:HG23	4	0.25
(1,1775)	1:125:B:LYS:H	1:126:B:ILE:HG21	4	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1775)	1:125:B:LYS:H	1:126:B:ILE:HG22	4	0.25
(1,1775)	1:125:B:LYS:H	1:126:B:ILE:HG23	4	0.25
(1,1774)	1:125:A:LYS:H	1:126:A:ILE:HG21	3	0.25
(1,1774)	1:125:A:LYS:H	1:126:A:ILE:HG22	3	0.25
(1,1774)	1:125:A:LYS:H	1:126:A:ILE:HG23	3	0.25
(1,1770)	1:178:C:PRO:HD3	1:179:C:ALA:H	14	0.25
(1,1769)	1:178:B:PRO:HD3	1:179:B:ALA:H	14	0.25
(1,1768)	1:178:A:PRO:HD3	1:179:A:ALA:H	2	0.25
(1,1768)	1:178:A:PRO:HD3	1:179:A:ALA:H	5	0.25
(1,1768)	1:178:A:PRO:HD3	1:179:A:ALA:H	16	0.25
(1,1768)	1:178:A:PRO:HD3	1:179:A:ALA:H	17	0.25
(1,1768)	1:178:A:PRO:HD3	1:179:A:ALA:H	18	0.25
(1,1768)	1:178:A:PRO:HD3	1:179:A:ALA:H	19	0.25
(1,1737)	1:194:A:LEU:HD21	1:195:A:TYR:H	5	0.25
(1,1737)	1:194:A:LEU:HD22	1:195:A:TYR:H	5	0.25
(1,1737)	1:194:A:LEU:HD23	1:195:A:TYR:H	5	0.25
(1,1737)	1:194:A:LEU:HD21	1:195:A:TYR:H	12	0.25
(1,1737)	1:194:A:LEU:HD22	1:195:A:TYR:H	12	0.25
(1,1737)	1:194:A:LEU:HD23	1:195:A:TYR:H	12	0.25
(1,1737)	1:194:A:LEU:HD21	1:195:A:TYR:H	14	0.25
(1,1737)	1:194:A:LEU:HD22	1:195:A:TYR:H	14	0.25
(1,1737)	1:194:A:LEU:HD23	1:195:A:TYR:H	14	0.25
(1,1737)	1:194:A:LEU:HD21	1:195:A:TYR:H	17	0.25
(1,1737)	1:194:A:LEU:HD22	1:195:A:TYR:H	17	0.25
(1,1737)	1:194:A:LEU:HD23	1:195:A:TYR:H	17	0.25
(1,1737)	1:194:A:LEU:HD21	1:195:A:TYR:H	19	0.25
(1,1737)	1:194:A:LEU:HD22	1:195:A:TYR:H	19	0.25
(1,1737)	1:194:A:LEU:HD23	1:195:A:TYR:H	19	0.25
(1,1610)	1:118:A:GLY:H	1:192:A:VAL:HG21	1	0.25
(1,1610)	1:118:A:GLY:H	1:192:A:VAL:HG22	1	0.25
(1,1610)	1:118:A:GLY:H	1:192:A:VAL:HG23	1	0.25
(1,1522)	1:178:C:PRO:HG2	1:179:C:ALA:H	5	0.25
(1,1522)	1:178:C:PRO:HG3	1:179:C:ALA:H	5	0.25
(1,1522)	1:178:C:PRO:HG2	1:179:C:ALA:H	8	0.25
(1,1522)	1:178:C:PRO:HG3	1:179:C:ALA:H	8	0.25
(1,1522)	1:178:C:PRO:HG2	1:179:C:ALA:H	18	0.25
(1,1522)	1:178:C:PRO:HG3	1:179:C:ALA:H	18	0.25
(1,1522)	1:178:C:PRO:HG2	1:179:C:ALA:H	20	0.25
(1,1522)	1:178:C:PRO:HG3	1:179:C:ALA:H	20	0.25
(1,1521)	1:178:B:PRO:HG2	1:179:B:ALA:H	5	0.25
(1,1521)	1:178:B:PRO:HG3	1:179:B:ALA:H	5	0.25
(1,1521)	1:178:B:PRO:HG2	1:179:B:ALA:H	8	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1521)	1:178:B:PRO:HG3	1:179:B:ALA:H	8	0.25
(1,1521)	1:178:B:PRO:HG2	1:179:B:ALA:H	18	0.25
(1,1521)	1:178:B:PRO:HG3	1:179:B:ALA:H	18	0.25
(1,1521)	1:178:B:PRO:HG2	1:179:B:ALA:H	20	0.25
(1,1521)	1:178:B:PRO:HG3	1:179:B:ALA:H	20	0.25
(1,1520)	1:178:A:PRO:HG2	1:179:A:ALA:H	14	0.25
(1,1520)	1:178:A:PRO:HG3	1:179:A:ALA:H	14	0.25
(1,1463)	1:180:C:PHE:H	1:181:C:LEU:HA	7	0.25
(1,1463)	1:180:C:PHE:H	1:181:C:LEU:HA	13	0.25
(1,1462)	1:180:B:PHE:H	1:181:B:LEU:HA	13	0.25
(1,1461)	1:180:A:PHE:H	1:181:A:LEU:HA	7	0.25
(1,1362)	1:154:A:PRO:HA	1:155:A:ALA:H	18	0.25
(1,1205)	1:149:B:SER:HB2	1:151:B:GLN:H	20	0.25
(1,1205)	1:149:B:SER:HB3	1:151:B:GLN:H	20	0.25
(1,1095)	1:157:A:PRO:HA	1:158:A:THR:H	6	0.25
(1,1095)	1:157:A:PRO:HA	1:158:A:THR:H	8	0.25
(1,1073)	1:139:C:ARG:H	1:141:C:VAL:HB	17	0.25
(1,1071)	1:139:A:ARG:H	1:141:A:VAL:HB	10	0.25
(1,1032)	1:152:C:ALA:H	1:153:C:LYS:H	13	0.25
(1,1032)	1:152:C:ALA:H	1:153:C:LYS:H	17	0.25
(1,1031)	1:152:B:ALA:H	1:153:B:LYS:H	13	0.25
(1,1031)	1:152:B:ALA:H	1:153:B:LYS:H	17	0.25
(1,1030)	1:152:A:ALA:H	1:153:A:LYS:H	13	0.25
(1,965)	1:110:A:LEU:HD11	1:125:A:LYS:HB3	9	0.25
(1,965)	1:110:A:LEU:HD12	1:125:A:LYS:HB3	9	0.25
(1,965)	1:110:A:LEU:HD13	1:125:A:LYS:HB3	9	0.25
(1,890)	1:152:C:ALA:HA	1:157:C:PRO:HG2	13	0.25
(1,890)	1:152:C:ALA:HA	1:157:C:PRO:HG3	13	0.25
(1,889)	1:152:B:ALA:HA	1:157:B:PRO:HG2	13	0.25
(1,889)	1:152:B:ALA:HA	1:157:B:PRO:HG3	13	0.25
(1,755)	1:189:C:CYS:H	1:192:C:VAL:HG11	11	0.25
(1,755)	1:189:C:CYS:H	1:192:C:VAL:HG12	11	0.25
(1,755)	1:189:C:CYS:H	1:192:C:VAL:HG13	11	0.25
(1,755)	1:189:C:CYS:H	1:192:C:VAL:HG11	19	0.25
(1,755)	1:189:C:CYS:H	1:192:C:VAL:HG12	19	0.25
(1,755)	1:189:C:CYS:H	1:192:C:VAL:HG13	19	0.25
(1,754)	1:189:B:CYS:H	1:192:B:VAL:HG11	11	0.25
(1,754)	1:189:B:CYS:H	1:192:B:VAL:HG12	11	0.25
(1,754)	1:189:B:CYS:H	1:192:B:VAL:HG13	11	0.25
(1,754)	1:189:B:CYS:H	1:192:B:VAL:HG11	19	0.25
(1,754)	1:189:B:CYS:H	1:192:B:VAL:HG12	19	0.25
(1,754)	1:189:B:CYS:H	1:192:B:VAL:HG13	19	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,753)	1:189:A:CYS:H	1:192:A:VAL:HG11	3	0.25
(1,753)	1:189:A:CYS:H	1:192:A:VAL:HG12	3	0.25
(1,753)	1:189:A:CYS:H	1:192:A:VAL:HG13	3	0.25
(1,753)	1:189:A:CYS:H	1:192:A:VAL:HG11	15	0.25
(1,753)	1:189:A:CYS:H	1:192:A:VAL:HG12	15	0.25
(1,753)	1:189:A:CYS:H	1:192:A:VAL:HG13	15	0.25
(1,753)	1:189:A:CYS:H	1:192:A:VAL:HG11	17	0.25
(1,753)	1:189:A:CYS:H	1:192:A:VAL:HG12	17	0.25
(1,753)	1:189:A:CYS:H	1:192:A:VAL:HG13	17	0.25
(1,739)	1:175:C:GLY:HA2	1:179:C:ALA:HB1	4	0.25
(1,739)	1:175:C:GLY:HA2	1:179:C:ALA:HB2	4	0.25
(1,739)	1:175:C:GLY:HA2	1:179:C:ALA:HB3	4	0.25
(1,739)	1:175:C:GLY:HA3	1:179:C:ALA:HB1	4	0.25
(1,739)	1:175:C:GLY:HA3	1:179:C:ALA:HB2	4	0.25
(1,739)	1:175:C:GLY:HA3	1:179:C:ALA:HB3	4	0.25
(1,435)	1:183:A:MET:HE1	1:186:A:SER:HA	1	0.25
(1,435)	1:183:A:MET:HE2	1:186:A:SER:HA	1	0.25
(1,435)	1:183:A:MET:HE3	1:186:A:SER:HA	1	0.25
(1,435)	1:183:A:MET:HE1	1:186:A:SER:HA	9	0.25
(1,435)	1:183:A:MET:HE2	1:186:A:SER:HA	9	0.25
(1,435)	1:183:A:MET:HE3	1:186:A:SER:HA	9	0.25
(1,302)	1:161:A:LEU:HA	1:161:A:LEU:HD11	10	0.25
(1,302)	1:161:A:LEU:HA	1:161:A:LEU:HD12	10	0.25
(1,302)	1:161:A:LEU:HA	1:161:A:LEU:HD13	10	0.25
(1,301)	1:181:A:LEU:HD11	1:196:A:TYR:HE1	5	0.25
(1,301)	1:181:A:LEU:HD11	1:196:A:TYR:HE2	5	0.25
(1,301)	1:181:A:LEU:HD12	1:196:A:TYR:HE1	5	0.25
(1,301)	1:181:A:LEU:HD12	1:196:A:TYR:HE2	5	0.25
(1,301)	1:181:A:LEU:HD13	1:196:A:TYR:HE1	5	0.25
(1,301)	1:181:A:LEU:HD13	1:196:A:TYR:HE2	5	0.25
(1,301)	1:181:A:LEU:HD11	1:196:A:TYR:HE1	16	0.25
(1,301)	1:181:A:LEU:HD11	1:196:A:TYR:HE2	16	0.25
(1,301)	1:181:A:LEU:HD12	1:196:A:TYR:HE1	16	0.25
(1,301)	1:181:A:LEU:HD12	1:196:A:TYR:HE2	16	0.25
(1,301)	1:181:A:LEU:HD13	1:196:A:TYR:HE1	16	0.25
(1,301)	1:181:A:LEU:HD13	1:196:A:TYR:HE2	16	0.25
(1,251)	1:118:C:GLY:HA2	1:119:C:THR:HG21	4	0.25
(1,251)	1:118:C:GLY:HA2	1:119:C:THR:HG22	4	0.25
(1,251)	1:118:C:GLY:HA2	1:119:C:THR:HG23	4	0.25
(1,250)	1:118:B:GLY:HA2	1:119:B:THR:HG21	4	0.25
(1,250)	1:118:B:GLY:HA2	1:119:B:THR:HG22	4	0.25
(1,250)	1:118:B:GLY:HA2	1:119:B:THR:HG23	4	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,239)	1:102:A:VAL:HG21	1:137:A:LEU:HD21	8	0.25
(1,239)	1:102:A:VAL:HG21	1:137:A:LEU:HD22	8	0.25
(1,239)	1:102:A:VAL:HG21	1:137:A:LEU:HD23	8	0.25
(1,239)	1:102:A:VAL:HG22	1:137:A:LEU:HD21	8	0.25
(1,239)	1:102:A:VAL:HG22	1:137:A:LEU:HD22	8	0.25
(1,239)	1:102:A:VAL:HG22	1:137:A:LEU:HD23	8	0.25
(1,239)	1:102:A:VAL:HG23	1:137:A:LEU:HD21	8	0.25
(1,239)	1:102:A:VAL:HG23	1:137:A:LEU:HD22	8	0.25
(1,239)	1:102:A:VAL:HG23	1:137:A:LEU:HD23	8	0.25
(1,228)	1:96:C:ILE:HD11	1:102:C:VAL:HG11	5	0.25
(1,228)	1:96:C:ILE:HD11	1:102:C:VAL:HG12	5	0.25
(1,228)	1:96:C:ILE:HD11	1:102:C:VAL:HG13	5	0.25
(1,228)	1:96:C:ILE:HD12	1:102:C:VAL:HG11	5	0.25
(1,228)	1:96:C:ILE:HD12	1:102:C:VAL:HG12	5	0.25
(1,228)	1:96:C:ILE:HD12	1:102:C:VAL:HG13	5	0.25
(1,228)	1:96:C:ILE:HD13	1:102:C:VAL:HG11	5	0.25
(1,228)	1:96:C:ILE:HD13	1:102:C:VAL:HG12	5	0.25
(1,228)	1:96:C:ILE:HD13	1:102:C:VAL:HG13	5	0.25
(1,227)	1:96:B:ILE:HD11	1:102:B:VAL:HG11	17	0.25
(1,227)	1:96:B:ILE:HD11	1:102:B:VAL:HG12	17	0.25
(1,227)	1:96:B:ILE:HD11	1:102:B:VAL:HG13	17	0.25
(1,227)	1:96:B:ILE:HD12	1:102:B:VAL:HG11	17	0.25
(1,227)	1:96:B:ILE:HD12	1:102:B:VAL:HG12	17	0.25
(1,227)	1:96:B:ILE:HD12	1:102:B:VAL:HG13	17	0.25
(1,227)	1:96:B:ILE:HD13	1:102:B:VAL:HG11	17	0.25
(1,227)	1:96:B:ILE:HD13	1:102:B:VAL:HG12	17	0.25
(1,227)	1:96:B:ILE:HD13	1:102:B:VAL:HG13	17	0.25
(1,227)	1:96:B:ILE:HD11	1:102:B:VAL:HG11	20	0.25
(1,227)	1:96:B:ILE:HD11	1:102:B:VAL:HG12	20	0.25
(1,227)	1:96:B:ILE:HD11	1:102:B:VAL:HG13	20	0.25
(1,227)	1:96:B:ILE:HD12	1:102:B:VAL:HG11	20	0.25
(1,227)	1:96:B:ILE:HD12	1:102:B:VAL:HG12	20	0.25
(1,227)	1:96:B:ILE:HD12	1:102:B:VAL:HG13	20	0.25
(1,227)	1:96:B:ILE:HD13	1:102:B:VAL:HG11	20	0.25
(1,227)	1:96:B:ILE:HD13	1:102:B:VAL:HG12	20	0.25
(1,227)	1:96:B:ILE:HD13	1:102:B:VAL:HG13	20	0.25
(1,175)	1:179:A:ALA:HB1	1:181:A:LEU:HD21	16	0.25
(1,175)	1:179:A:ALA:HB1	1:181:A:LEU:HD22	16	0.25
(1,175)	1:179:A:ALA:HB1	1:181:A:LEU:HD23	16	0.25
(1,175)	1:179:A:ALA:HB2	1:181:A:LEU:HD21	16	0.25
(1,175)	1:179:A:ALA:HB2	1:181:A:LEU:HD22	16	0.25
(1,175)	1:179:A:ALA:HB2	1:181:A:LEU:HD23	16	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,175)	1:179:A:ALA:HB3	1:181:A:LEU:HD21	16	0.25
(1,175)	1:179:A:ALA:HB3	1:181:A:LEU:HD22	16	0.25
(1,175)	1:179:A:ALA:HB3	1:181:A:LEU:HD23	16	0.25
(1,175)	1:179:A:ALA:HB1	1:181:A:LEU:HD21	17	0.25
(1,175)	1:179:A:ALA:HB1	1:181:A:LEU:HD22	17	0.25
(1,175)	1:179:A:ALA:HB1	1:181:A:LEU:HD23	17	0.25
(1,175)	1:179:A:ALA:HB2	1:181:A:LEU:HD21	17	0.25
(1,175)	1:179:A:ALA:HB2	1:181:A:LEU:HD22	17	0.25
(1,175)	1:179:A:ALA:HB2	1:181:A:LEU:HD23	17	0.25
(1,175)	1:179:A:ALA:HB3	1:181:A:LEU:HD21	17	0.25
(1,175)	1:179:A:ALA:HB3	1:181:A:LEU:HD22	17	0.25
(1,175)	1:179:A:ALA:HB3	1:181:A:LEU:HD23	17	0.25
(1,122)	1:113:A:TYR:HD1	1:137:A:LEU:HD21	3	0.25
(1,122)	1:113:A:TYR:HD1	1:137:A:LEU:HD22	3	0.25
(1,122)	1:113:A:TYR:HD1	1:137:A:LEU:HD23	3	0.25
(1,122)	1:113:A:TYR:HD2	1:137:A:LEU:HD21	3	0.25
(1,122)	1:113:A:TYR:HD2	1:137:A:LEU:HD22	3	0.25
(1,122)	1:113:A:TYR:HD2	1:137:A:LEU:HD23	3	0.25
(1,2295)	1:155:C:ALA:HB1	1:157:C:PRO:HD2	13	0.24
(1,2295)	1:155:C:ALA:HB1	1:157:C:PRO:HD3	13	0.24
(1,2295)	1:155:C:ALA:HB2	1:157:C:PRO:HD2	13	0.24
(1,2295)	1:155:C:ALA:HB2	1:157:C:PRO:HD3	13	0.24
(1,2295)	1:155:C:ALA:HB3	1:157:C:PRO:HD2	13	0.24
(1,2295)	1:155:C:ALA:HB3	1:157:C:PRO:HD3	13	0.24
(1,2295)	1:155:C:ALA:HB1	1:157:C:PRO:HD2	19	0.24
(1,2295)	1:155:C:ALA:HB1	1:157:C:PRO:HD3	19	0.24
(1,2295)	1:155:C:ALA:HB2	1:157:C:PRO:HD2	19	0.24
(1,2295)	1:155:C:ALA:HB2	1:157:C:PRO:HD3	19	0.24
(1,2295)	1:155:C:ALA:HB3	1:157:C:PRO:HD2	19	0.24
(1,2295)	1:155:C:ALA:HB3	1:157:C:PRO:HD3	19	0.24
(1,2295)	1:155:C:ALA:HB1	1:157:C:PRO:HD2	20	0.24
(1,2295)	1:155:C:ALA:HB1	1:157:C:PRO:HD3	20	0.24
(1,2295)	1:155:C:ALA:HB2	1:157:C:PRO:HD2	20	0.24
(1,2295)	1:155:C:ALA:HB2	1:157:C:PRO:HD3	20	0.24
(1,2295)	1:155:C:ALA:HB3	1:157:C:PRO:HD2	20	0.24
(1,2295)	1:155:C:ALA:HB3	1:157:C:PRO:HD3	20	0.24
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG11	2	0.24
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG12	2	0.24
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG13	2	0.24
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG21	2	0.24
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG22	2	0.24
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG23	2	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2293)	1:155:C:ALA:H	1:156:C:VAL:HG11	14	0.24
(1,2293)	1:155:C:ALA:H	1:156:C:VAL:HG12	14	0.24
(1,2293)	1:155:C:ALA:H	1:156:C:VAL:HG13	14	0.24
(1,2293)	1:155:C:ALA:H	1:156:C:VAL:HG21	14	0.24
(1,2293)	1:155:C:ALA:H	1:156:C:VAL:HG22	14	0.24
(1,2293)	1:155:C:ALA:H	1:156:C:VAL:HG23	14	0.24
(1,2069)	1:155:B:ALA:HB1	1:157:B:PRO:HD2	13	0.24
(1,2069)	1:155:B:ALA:HB1	1:157:B:PRO:HD3	13	0.24
(1,2069)	1:155:B:ALA:HB2	1:157:B:PRO:HD2	13	0.24
(1,2069)	1:155:B:ALA:HB2	1:157:B:PRO:HD3	13	0.24
(1,2069)	1:155:B:ALA:HB3	1:157:B:PRO:HD2	13	0.24
(1,2069)	1:155:B:ALA:HB3	1:157:B:PRO:HD3	13	0.24
(1,2069)	1:155:B:ALA:HB1	1:157:B:PRO:HD2	19	0.24
(1,2069)	1:155:B:ALA:HB1	1:157:B:PRO:HD3	19	0.24
(1,2069)	1:155:B:ALA:HB2	1:157:B:PRO:HD2	19	0.24
(1,2069)	1:155:B:ALA:HB2	1:157:B:PRO:HD3	19	0.24
(1,2069)	1:155:B:ALA:HB3	1:157:B:PRO:HD2	19	0.24
(1,2069)	1:155:B:ALA:HB3	1:157:B:PRO:HD3	19	0.24
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG11	2	0.24
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG12	2	0.24
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG13	2	0.24
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG21	2	0.24
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG22	2	0.24
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG23	2	0.24
(1,2067)	1:155:B:ALA:H	1:156:B:VAL:HG11	14	0.24
(1,2067)	1:155:B:ALA:H	1:156:B:VAL:HG12	14	0.24
(1,2067)	1:155:B:ALA:H	1:156:B:VAL:HG13	14	0.24
(1,2067)	1:155:B:ALA:H	1:156:B:VAL:HG21	14	0.24
(1,2067)	1:155:B:ALA:H	1:156:B:VAL:HG22	14	0.24
(1,2067)	1:155:B:ALA:H	1:156:B:VAL:HG23	14	0.24
(1,2060)	1:151:B:GLN:HB2	1:152:B:ALA:HA	6	0.24
(1,2060)	1:151:B:GLN:HB3	1:152:B:ALA:HA	6	0.24
(1,1902)	1:172:A:ALA:HA	1:178:A:PRO:HD2	2	0.24
(1,1902)	1:172:A:ALA:HA	1:178:A:PRO:HD3	2	0.24
(1,1889)	1:156:A:VAL:HG11	1:157:A:PRO:HD2	5	0.24
(1,1889)	1:156:A:VAL:HG11	1:157:A:PRO:HD3	5	0.24
(1,1889)	1:156:A:VAL:HG12	1:157:A:PRO:HD2	5	0.24
(1,1889)	1:156:A:VAL:HG12	1:157:A:PRO:HD3	5	0.24
(1,1889)	1:156:A:VAL:HG13	1:157:A:PRO:HD2	5	0.24
(1,1889)	1:156:A:VAL:HG13	1:157:A:PRO:HD3	5	0.24
(1,1884)	1:154:A:PRO:HB2	1:167:A:ARG:H	13	0.24
(1,1884)	1:154:A:PRO:HB3	1:167:A:ARG:H	13	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1842)	1:121:A:CYS:HB2	1:189:A:CYS:H	7	0.24
(1,1842)	1:121:A:CYS:HB3	1:189:A:CYS:H	7	0.24
(1,1842)	1:121:A:CYS:HB2	1:189:A:CYS:H	9	0.24
(1,1842)	1:121:A:CYS:HB3	1:189:A:CYS:H	9	0.24
(1,1842)	1:121:A:CYS:HB2	1:189:A:CYS:H	18	0.24
(1,1842)	1:121:A:CYS:HB3	1:189:A:CYS:H	18	0.24
(1,1818)	1:95:B:SER:HB2	1:101:B:LEU:H	12	0.24
(1,1818)	1:95:B:SER:HB3	1:101:B:LEU:H	12	0.24
(1,1770)	1:178:C:PRO:HD3	1:179:C:ALA:H	2	0.24
(1,1770)	1:178:C:PRO:HD3	1:179:C:ALA:H	13	0.24
(1,1770)	1:178:C:PRO:HD3	1:179:C:ALA:H	15	0.24
(1,1770)	1:178:C:PRO:HD3	1:179:C:ALA:H	17	0.24
(1,1770)	1:178:C:PRO:HD3	1:179:C:ALA:H	19	0.24
(1,1769)	1:178:B:PRO:HD3	1:179:B:ALA:H	2	0.24
(1,1769)	1:178:B:PRO:HD3	1:179:B:ALA:H	13	0.24
(1,1769)	1:178:B:PRO:HD3	1:179:B:ALA:H	15	0.24
(1,1769)	1:178:B:PRO:HD3	1:179:B:ALA:H	16	0.24
(1,1769)	1:178:B:PRO:HD3	1:179:B:ALA:H	17	0.24
(1,1769)	1:178:B:PRO:HD3	1:179:B:ALA:H	19	0.24
(1,1768)	1:178:A:PRO:HD3	1:179:A:ALA:H	15	0.24
(1,1737)	1:194:A:LEU:HD21	1:195:A:TYR:H	1	0.24
(1,1737)	1:194:A:LEU:HD22	1:195:A:TYR:H	1	0.24
(1,1737)	1:194:A:LEU:HD23	1:195:A:TYR:H	1	0.24
(1,1737)	1:194:A:LEU:HD21	1:195:A:TYR:H	2	0.24
(1,1737)	1:194:A:LEU:HD22	1:195:A:TYR:H	2	0.24
(1,1737)	1:194:A:LEU:HD23	1:195:A:TYR:H	2	0.24
(1,1737)	1:194:A:LEU:HD21	1:195:A:TYR:H	3	0.24
(1,1737)	1:194:A:LEU:HD22	1:195:A:TYR:H	3	0.24
(1,1737)	1:194:A:LEU:HD23	1:195:A:TYR:H	3	0.24
(1,1737)	1:194:A:LEU:HD21	1:195:A:TYR:H	10	0.24
(1,1737)	1:194:A:LEU:HD22	1:195:A:TYR:H	10	0.24
(1,1737)	1:194:A:LEU:HD23	1:195:A:TYR:H	10	0.24
(1,1737)	1:194:A:LEU:HD21	1:195:A:TYR:H	11	0.24
(1,1737)	1:194:A:LEU:HD22	1:195:A:TYR:H	11	0.24
(1,1737)	1:194:A:LEU:HD23	1:195:A:TYR:H	11	0.24
(1,1737)	1:194:A:LEU:HD21	1:195:A:TYR:H	18	0.24
(1,1737)	1:194:A:LEU:HD22	1:195:A:TYR:H	18	0.24
(1,1737)	1:194:A:LEU:HD23	1:195:A:TYR:H	18	0.24
(1,1737)	1:194:A:LEU:HD21	1:195:A:TYR:H	20	0.24
(1,1737)	1:194:A:LEU:HD22	1:195:A:TYR:H	20	0.24
(1,1737)	1:194:A:LEU:HD23	1:195:A:TYR:H	20	0.24
(1,1548)	1:167:C:ARG:H	1:170:C:GLY:HA2	13	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1548)	1:167:C:ARG:H	1:170:C:GLY:HA3	13	0.24
(1,1547)	1:167:B:ARG:H	1:170:B:GLY:HA2	13	0.24
(1,1547)	1:167:B:ARG:H	1:170:B:GLY:HA3	13	0.24
(1,1546)	1:167:A:ARG:H	1:170:A:GLY:HA2	13	0.24
(1,1546)	1:167:A:ARG:H	1:170:A:GLY:HA3	13	0.24
(1,1534)	1:122:B:TYR:H	1:189:B:CYS:HB2	6	0.24
(1,1534)	1:122:B:TYR:H	1:189:B:CYS:HB3	6	0.24
(1,1534)	1:122:B:TYR:H	1:189:B:CYS:HB2	8	0.24
(1,1534)	1:122:B:TYR:H	1:189:B:CYS:HB3	8	0.24
(1,1522)	1:178:C:PRO:HG2	1:179:C:ALA:H	6	0.24
(1,1522)	1:178:C:PRO:HG3	1:179:C:ALA:H	6	0.24
(1,1522)	1:178:C:PRO:HG2	1:179:C:ALA:H	14	0.24
(1,1522)	1:178:C:PRO:HG3	1:179:C:ALA:H	14	0.24
(1,1521)	1:178:B:PRO:HG2	1:179:B:ALA:H	6	0.24
(1,1521)	1:178:B:PRO:HG3	1:179:B:ALA:H	6	0.24
(1,1521)	1:178:B:PRO:HG2	1:179:B:ALA:H	14	0.24
(1,1521)	1:178:B:PRO:HG3	1:179:B:ALA:H	14	0.24
(1,1520)	1:178:A:PRO:HG2	1:179:A:ALA:H	2	0.24
(1,1520)	1:178:A:PRO:HG3	1:179:A:ALA:H	2	0.24
(1,1520)	1:178:A:PRO:HG2	1:179:A:ALA:H	5	0.24
(1,1520)	1:178:A:PRO:HG3	1:179:A:ALA:H	5	0.24
(1,1520)	1:178:A:PRO:HG2	1:179:A:ALA:H	16	0.24
(1,1520)	1:178:A:PRO:HG3	1:179:A:ALA:H	16	0.24
(1,1520)	1:178:A:PRO:HG2	1:179:A:ALA:H	17	0.24
(1,1520)	1:178:A:PRO:HG3	1:179:A:ALA:H	17	0.24
(1,1520)	1:178:A:PRO:HG2	1:179:A:ALA:H	18	0.24
(1,1520)	1:178:A:PRO:HG3	1:179:A:ALA:H	18	0.24
(1,1520)	1:178:A:PRO:HG2	1:179:A:ALA:H	19	0.24
(1,1520)	1:178:A:PRO:HG3	1:179:A:ALA:H	19	0.24
(1,1507)	1:92:A:ALA:H	1:93:C:THR:HG21	8	0.24
(1,1507)	1:92:A:ALA:H	1:93:C:THR:HG22	8	0.24
(1,1507)	1:92:A:ALA:H	1:93:C:THR:HG23	8	0.24
(1,1506)	1:93:B:THR:HG21	1:92:C:ALA:H	8	0.24
(1,1506)	1:93:B:THR:HG22	1:92:C:ALA:H	8	0.24
(1,1506)	1:93:B:THR:HG23	1:92:C:ALA:H	8	0.24
(1,1462)	1:180:B:PHE:H	1:181:B:LEU:HA	7	0.24
(1,1462)	1:180:B:PHE:H	1:181:B:LEU:HA	16	0.24
(1,1461)	1:180:A:PHE:H	1:181:A:LEU:HA	13	0.24
(1,1430)	1:111:A:ILE:H	1:123:A:ILE:HG21	13	0.24
(1,1430)	1:111:A:ILE:H	1:123:A:ILE:HG22	13	0.24
(1,1430)	1:111:A:ILE:H	1:123:A:ILE:HG23	13	0.24
(1,1364)	1:154:C:PRO:HA	1:155:C:ALA:H	18	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1363)	1:154:B:PRO:HA	1:155:B:ALA:H	18	0.24
(1,1206)	1:149:C:SER:HB2	1:151:C:GLN:H	20	0.24
(1,1206)	1:149:C:SER:HB3	1:151:C:GLN:H	20	0.24
(1,1073)	1:139:C:ARG:H	1:141:C:VAL:HB	12	0.24
(1,1073)	1:139:C:ARG:H	1:141:C:VAL:HB	20	0.24
(1,1072)	1:139:B:ARG:H	1:141:B:VAL:HB	11	0.24
(1,1072)	1:139:B:ARG:H	1:141:B:VAL:HB	12	0.24
(1,1071)	1:139:A:ARG:H	1:141:A:VAL:HB	5	0.24
(1,1071)	1:139:A:ARG:H	1:141:A:VAL:HB	17	0.24
(1,1071)	1:139:A:ARG:H	1:141:A:VAL:HB	18	0.24
(1,1036)	1:188:A:LEU:HD21	1:134:B:LEU:H	2	0.24
(1,1036)	1:188:A:LEU:HD22	1:134:B:LEU:H	2	0.24
(1,1036)	1:188:A:LEU:HD23	1:134:B:LEU:H	2	0.24
(1,1036)	1:188:A:LEU:HD21	1:134:B:LEU:H	11	0.24
(1,1036)	1:188:A:LEU:HD22	1:134:B:LEU:H	11	0.24
(1,1036)	1:188:A:LEU:HD23	1:134:B:LEU:H	11	0.24
(1,958)	1:187:A:THR:HA	1:188:A:LEU:HD11	1	0.24
(1,958)	1:187:A:THR:HA	1:188:A:LEU:HD12	1	0.24
(1,958)	1:187:A:THR:HA	1:188:A:LEU:HD13	1	0.24
(1,958)	1:187:A:THR:HA	1:188:A:LEU:HD11	11	0.24
(1,958)	1:187:A:THR:HA	1:188:A:LEU:HD12	11	0.24
(1,958)	1:187:A:THR:HA	1:188:A:LEU:HD13	11	0.24
(1,842)	1:156:A:VAL:HB	1:157:A:PRO:HD2	16	0.24
(1,755)	1:189:C:CYS:H	1:192:C:VAL:HG11	1	0.24
(1,755)	1:189:C:CYS:H	1:192:C:VAL:HG12	1	0.24
(1,755)	1:189:C:CYS:H	1:192:C:VAL:HG13	1	0.24
(1,755)	1:189:C:CYS:H	1:192:C:VAL:HG11	4	0.24
(1,755)	1:189:C:CYS:H	1:192:C:VAL:HG12	4	0.24
(1,755)	1:189:C:CYS:H	1:192:C:VAL:HG13	4	0.24
(1,755)	1:189:C:CYS:H	1:192:C:VAL:HG11	9	0.24
(1,755)	1:189:C:CYS:H	1:192:C:VAL:HG12	9	0.24
(1,755)	1:189:C:CYS:H	1:192:C:VAL:HG13	9	0.24
(1,755)	1:189:C:CYS:H	1:192:C:VAL:HG11	12	0.24
(1,755)	1:189:C:CYS:H	1:192:C:VAL:HG12	12	0.24
(1,755)	1:189:C:CYS:H	1:192:C:VAL:HG13	12	0.24
(1,754)	1:189:B:CYS:H	1:192:B:VAL:HG11	1	0.24
(1,754)	1:189:B:CYS:H	1:192:B:VAL:HG12	1	0.24
(1,754)	1:189:B:CYS:H	1:192:B:VAL:HG13	1	0.24
(1,754)	1:189:B:CYS:H	1:192:B:VAL:HG11	9	0.24
(1,754)	1:189:B:CYS:H	1:192:B:VAL:HG12	9	0.24
(1,754)	1:189:B:CYS:H	1:192:B:VAL:HG13	9	0.24
(1,754)	1:189:B:CYS:H	1:192:B:VAL:HG11	12	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,754)	1:189:B:CYS:H	1:192:B:VAL:HG12	12	0.24
(1,754)	1:189:B:CYS:H	1:192:B:VAL:HG13	12	0.24
(1,749)	1:123:A:ILE:HG21	1:179:A:ALA:HB1	4	0.24
(1,749)	1:123:A:ILE:HG21	1:179:A:ALA:HB2	4	0.24
(1,749)	1:123:A:ILE:HG21	1:179:A:ALA:HB3	4	0.24
(1,749)	1:123:A:ILE:HG22	1:179:A:ALA:HB1	4	0.24
(1,749)	1:123:A:ILE:HG22	1:179:A:ALA:HB2	4	0.24
(1,749)	1:123:A:ILE:HG22	1:179:A:ALA:HB3	4	0.24
(1,749)	1:123:A:ILE:HG23	1:179:A:ALA:HB1	4	0.24
(1,749)	1:123:A:ILE:HG23	1:179:A:ALA:HB2	4	0.24
(1,749)	1:123:A:ILE:HG23	1:179:A:ALA:HB3	4	0.24
(1,635)	1:96:A:ILE:HG21	1:100:A:GLY:H	17	0.24
(1,635)	1:96:A:ILE:HG22	1:100:A:GLY:H	17	0.24
(1,635)	1:96:A:ILE:HG23	1:100:A:GLY:H	17	0.24
(1,395)	1:109:A:LEU:HG	1:111:A:ILE:HD11	1	0.24
(1,395)	1:109:A:LEU:HG	1:111:A:ILE:HD12	1	0.24
(1,395)	1:109:A:LEU:HG	1:111:A:ILE:HD13	1	0.24
(1,364)	1:126:A:ILE:HG21	1:131:A:ILE:HD11	18	0.24
(1,364)	1:126:A:ILE:HG21	1:131:A:ILE:HD12	18	0.24
(1,364)	1:126:A:ILE:HG21	1:131:A:ILE:HD13	18	0.24
(1,364)	1:126:A:ILE:HG22	1:131:A:ILE:HD11	18	0.24
(1,364)	1:126:A:ILE:HG22	1:131:A:ILE:HD12	18	0.24
(1,364)	1:126:A:ILE:HG22	1:131:A:ILE:HD13	18	0.24
(1,364)	1:126:A:ILE:HG23	1:131:A:ILE:HD11	18	0.24
(1,364)	1:126:A:ILE:HG23	1:131:A:ILE:HD12	18	0.24
(1,364)	1:126:A:ILE:HG23	1:131:A:ILE:HD13	18	0.24
(1,250)	1:118:B:GLY:HA2	1:119:B:THR:HG21	16	0.24
(1,250)	1:118:B:GLY:HA2	1:119:B:THR:HG22	16	0.24
(1,250)	1:118:B:GLY:HA2	1:119:B:THR:HG23	16	0.24
(1,249)	1:118:A:GLY:HA2	1:119:A:THR:HG21	4	0.24
(1,249)	1:118:A:GLY:HA2	1:119:A:THR:HG22	4	0.24
(1,249)	1:118:A:GLY:HA2	1:119:A:THR:HG23	4	0.24
(1,239)	1:102:A:VAL:HG21	1:137:A:LEU:HD21	6	0.24
(1,239)	1:102:A:VAL:HG21	1:137:A:LEU:HD22	6	0.24
(1,239)	1:102:A:VAL:HG21	1:137:A:LEU:HD23	6	0.24
(1,239)	1:102:A:VAL:HG22	1:137:A:LEU:HD21	6	0.24
(1,239)	1:102:A:VAL:HG22	1:137:A:LEU:HD22	6	0.24
(1,239)	1:102:A:VAL:HG22	1:137:A:LEU:HD23	6	0.24
(1,239)	1:102:A:VAL:HG23	1:137:A:LEU:HD21	6	0.24
(1,239)	1:102:A:VAL:HG23	1:137:A:LEU:HD22	6	0.24
(1,239)	1:102:A:VAL:HG23	1:137:A:LEU:HD23	6	0.24
(1,227)	1:96:B:ILE:HD11	1:102:B:VAL:HG11	5	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,227)	1:96:B:ILE:HD11	1:102:B:VAL:HG12	5	0.24
(1,227)	1:96:B:ILE:HD11	1:102:B:VAL:HG13	5	0.24
(1,227)	1:96:B:ILE:HD12	1:102:B:VAL:HG11	5	0.24
(1,227)	1:96:B:ILE:HD12	1:102:B:VAL:HG12	5	0.24
(1,227)	1:96:B:ILE:HD12	1:102:B:VAL:HG13	5	0.24
(1,227)	1:96:B:ILE:HD13	1:102:B:VAL:HG11	5	0.24
(1,227)	1:96:B:ILE:HD13	1:102:B:VAL:HG12	5	0.24
(1,227)	1:96:B:ILE:HD13	1:102:B:VAL:HG13	5	0.24
(1,226)	1:96:A:ILE:HD11	1:102:A:VAL:HG11	6	0.24
(1,226)	1:96:A:ILE:HD11	1:102:A:VAL:HG12	6	0.24
(1,226)	1:96:A:ILE:HD11	1:102:A:VAL:HG13	6	0.24
(1,226)	1:96:A:ILE:HD12	1:102:A:VAL:HG11	6	0.24
(1,226)	1:96:A:ILE:HD12	1:102:A:VAL:HG12	6	0.24
(1,226)	1:96:A:ILE:HD12	1:102:A:VAL:HG13	6	0.24
(1,226)	1:96:A:ILE:HD13	1:102:A:VAL:HG11	6	0.24
(1,226)	1:96:A:ILE:HD13	1:102:A:VAL:HG12	6	0.24
(1,226)	1:96:A:ILE:HD13	1:102:A:VAL:HG13	6	0.24
(1,124)	1:96:A:ILE:H	1:101:A:LEU:HD21	4	0.24
(1,124)	1:96:A:ILE:H	1:101:A:LEU:HD22	4	0.24
(1,124)	1:96:A:ILE:H	1:101:A:LEU:HD23	4	0.24
(1,56)	1:156:A:VAL:HG11	1:157:A:PRO:HD3	5	0.24
(1,56)	1:156:A:VAL:HG12	1:157:A:PRO:HD3	5	0.24
(1,56)	1:156:A:VAL:HG13	1:157:A:PRO:HD3	5	0.24
(1,2295)	1:155:C:ALA:HB1	1:157:C:PRO:HD2	11	0.23
(1,2295)	1:155:C:ALA:HB1	1:157:C:PRO:HD3	11	0.23
(1,2295)	1:155:C:ALA:HB2	1:157:C:PRO:HD2	11	0.23
(1,2295)	1:155:C:ALA:HB2	1:157:C:PRO:HD3	11	0.23
(1,2295)	1:155:C:ALA:HB3	1:157:C:PRO:HD2	11	0.23
(1,2295)	1:155:C:ALA:HB3	1:157:C:PRO:HD3	11	0.23
(1,2292)	1:154:C:PRO:HB2	1:167:C:ARG:H	14	0.23
(1,2292)	1:154:C:PRO:HB3	1:167:C:ARG:H	14	0.23
(1,2286)	1:151:C:GLN:HB2	1:152:C:ALA:HA	6	0.23
(1,2286)	1:151:C:GLN:HB3	1:152:C:ALA:HA	6	0.23
(1,2069)	1:155:B:ALA:HB1	1:157:B:PRO:HD2	11	0.23
(1,2069)	1:155:B:ALA:HB1	1:157:B:PRO:HD3	11	0.23
(1,2069)	1:155:B:ALA:HB2	1:157:B:PRO:HD2	11	0.23
(1,2069)	1:155:B:ALA:HB2	1:157:B:PRO:HD3	11	0.23
(1,2069)	1:155:B:ALA:HB3	1:157:B:PRO:HD2	11	0.23
(1,2069)	1:155:B:ALA:HB3	1:157:B:PRO:HD3	11	0.23
(1,2069)	1:155:B:ALA:HB1	1:157:B:PRO:HD2	20	0.23
(1,2069)	1:155:B:ALA:HB1	1:157:B:PRO:HD3	20	0.23
(1,2069)	1:155:B:ALA:HB2	1:157:B:PRO:HD2	20	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2069)	1:155:B:ALA:HB2	1:157:B:PRO:HD3	20	0.23
(1,2069)	1:155:B:ALA:HB3	1:157:B:PRO:HD2	20	0.23
(1,2069)	1:155:B:ALA:HB3	1:157:B:PRO:HD3	20	0.23
(1,1902)	1:172:A:ALA:HA	1:178:A:PRO:HD2	8	0.23
(1,1902)	1:172:A:ALA:HA	1:178:A:PRO:HD3	8	0.23
(1,1878)	1:151:A:GLN:HB2	1:152:A:ALA:HA	6	0.23
(1,1878)	1:151:A:GLN:HB3	1:152:A:ALA:HA	6	0.23
(1,1842)	1:121:A:CYS:HB2	1:189:A:CYS:H	2	0.23
(1,1842)	1:121:A:CYS:HB3	1:189:A:CYS:H	2	0.23
(1,1842)	1:121:A:CYS:HB2	1:189:A:CYS:H	11	0.23
(1,1842)	1:121:A:CYS:HB3	1:189:A:CYS:H	11	0.23
(1,1819)	1:95:C:SER:HB2	1:101:C:LEU:H	6	0.23
(1,1819)	1:95:C:SER:HB3	1:101:C:LEU:H	6	0.23
(1,1818)	1:95:B:SER:HB2	1:101:B:LEU:H	8	0.23
(1,1818)	1:95:B:SER:HB3	1:101:B:LEU:H	8	0.23
(1,1817)	1:95:A:SER:HB2	1:101:A:LEU:H	14	0.23
(1,1817)	1:95:A:SER:HB3	1:101:A:LEU:H	14	0.23
(1,1770)	1:178:C:PRO:HD3	1:179:C:ALA:H	1	0.23
(1,1770)	1:178:C:PRO:HD3	1:179:C:ALA:H	16	0.23
(1,1769)	1:178:B:PRO:HD3	1:179:B:ALA:H	1	0.23
(1,1768)	1:178:A:PRO:HD3	1:179:A:ALA:H	6	0.23
(1,1768)	1:178:A:PRO:HD3	1:179:A:ALA:H	13	0.23
(1,1737)	1:194:A:LEU:HD21	1:195:A:TYR:H	9	0.23
(1,1737)	1:194:A:LEU:HD22	1:195:A:TYR:H	9	0.23
(1,1737)	1:194:A:LEU:HD23	1:195:A:TYR:H	9	0.23
(1,1737)	1:194:A:LEU:HD21	1:195:A:TYR:H	16	0.23
(1,1737)	1:194:A:LEU:HD22	1:195:A:TYR:H	16	0.23
(1,1737)	1:194:A:LEU:HD23	1:195:A:TYR:H	16	0.23
(1,1546)	1:167:A:ARG:H	1:170:A:GLY:HA2	15	0.23
(1,1546)	1:167:A:ARG:H	1:170:A:GLY:HA3	15	0.23
(1,1546)	1:167:A:ARG:H	1:170:A:GLY:HA2	20	0.23
(1,1546)	1:167:A:ARG:H	1:170:A:GLY:HA3	20	0.23
(1,1535)	1:122:C:TYR:H	1:189:C:CYS:HB2	6	0.23
(1,1535)	1:122:C:TYR:H	1:189:C:CYS:HB3	6	0.23
(1,1526)	1:179:A:ALA:H	1:181:A:LEU:HD11	2	0.23
(1,1526)	1:179:A:ALA:H	1:181:A:LEU:HD12	2	0.23
(1,1526)	1:179:A:ALA:H	1:181:A:LEU:HD13	2	0.23
(1,1522)	1:178:C:PRO:HG2	1:179:C:ALA:H	15	0.23
(1,1522)	1:178:C:PRO:HG3	1:179:C:ALA:H	15	0.23
(1,1522)	1:178:C:PRO:HG2	1:179:C:ALA:H	19	0.23
(1,1522)	1:178:C:PRO:HG3	1:179:C:ALA:H	19	0.23
(1,1521)	1:178:B:PRO:HG2	1:179:B:ALA:H	13	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1521)	1:178:B:PRO:HG3	1:179:B:ALA:H	13	0.23
(1,1521)	1:178:B:PRO:HG2	1:179:B:ALA:H	15	0.23
(1,1521)	1:178:B:PRO:HG3	1:179:B:ALA:H	15	0.23
(1,1521)	1:178:B:PRO:HG2	1:179:B:ALA:H	17	0.23
(1,1521)	1:178:B:PRO:HG3	1:179:B:ALA:H	17	0.23
(1,1521)	1:178:B:PRO:HG2	1:179:B:ALA:H	19	0.23
(1,1521)	1:178:B:PRO:HG3	1:179:B:ALA:H	19	0.23
(1,1520)	1:178:A:PRO:HG2	1:179:A:ALA:H	15	0.23
(1,1520)	1:178:A:PRO:HG3	1:179:A:ALA:H	15	0.23
(1,1511)	1:137:A:LEU:H	1:137:A:LEU:HG	6	0.23
(1,1463)	1:180:C:PHE:H	1:181:C:LEU:HA	16	0.23
(1,1073)	1:139:C:ARG:H	1:141:C:VAL:HB	10	0.23
(1,1073)	1:139:C:ARG:H	1:141:C:VAL:HB	11	0.23
(1,1073)	1:139:C:ARG:H	1:141:C:VAL:HB	15	0.23
(1,1073)	1:139:C:ARG:H	1:141:C:VAL:HB	18	0.23
(1,1073)	1:139:C:ARG:H	1:141:C:VAL:HB	19	0.23
(1,1072)	1:139:B:ARG:H	1:141:B:VAL:HB	20	0.23
(1,1071)	1:139:A:ARG:H	1:141:A:VAL:HB	15	0.23
(1,1032)	1:152:C:ALA:H	1:153:C:LYS:H	19	0.23
(1,1031)	1:152:B:ALA:H	1:153:B:LYS:H	19	0.23
(1,1030)	1:152:A:ALA:H	1:153:A:LYS:H	19	0.23
(1,965)	1:110:A:LEU:HD11	1:125:A:LYS:HB3	5	0.23
(1,965)	1:110:A:LEU:HD12	1:125:A:LYS:HB3	5	0.23
(1,965)	1:110:A:LEU:HD13	1:125:A:LYS:HB3	5	0.23
(1,958)	1:187:A:THR:HA	1:188:A:LEU:HD11	13	0.23
(1,958)	1:187:A:THR:HA	1:188:A:LEU:HD12	13	0.23
(1,958)	1:187:A:THR:HA	1:188:A:LEU:HD13	13	0.23
(1,958)	1:187:A:THR:HA	1:188:A:LEU:HD11	19	0.23
(1,958)	1:187:A:THR:HA	1:188:A:LEU:HD12	19	0.23
(1,958)	1:187:A:THR:HA	1:188:A:LEU:HD13	19	0.23
(1,890)	1:152:C:ALA:HA	1:157:C:PRO:HG2	5	0.23
(1,890)	1:152:C:ALA:HA	1:157:C:PRO:HG3	5	0.23
(1,889)	1:152:B:ALA:HA	1:157:B:PRO:HG2	5	0.23
(1,889)	1:152:B:ALA:HA	1:157:B:PRO:HG3	5	0.23
(1,888)	1:152:A:ALA:HA	1:157:A:PRO:HG2	17	0.23
(1,888)	1:152:A:ALA:HA	1:157:A:PRO:HG3	17	0.23
(1,754)	1:189:B:CYS:H	1:192:B:VAL:HG11	4	0.23
(1,754)	1:189:B:CYS:H	1:192:B:VAL:HG12	4	0.23
(1,754)	1:189:B:CYS:H	1:192:B:VAL:HG13	4	0.23
(1,665)	1:113:A:TYR:HE1	1:197:A:ILE:HG21	14	0.23
(1,665)	1:113:A:TYR:HE1	1:197:A:ILE:HG22	14	0.23
(1,665)	1:113:A:TYR:HE1	1:197:A:ILE:HG23	14	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,665)	1:113:A:TYR:HE2	1:197:A:ILE:HG21	14	0.23
(1,665)	1:113:A:TYR:HE2	1:197:A:ILE:HG22	14	0.23
(1,665)	1:113:A:TYR:HE2	1:197:A:ILE:HG23	14	0.23
(1,635)	1:96:A:ILE:HG21	1:100:A:GLY:H	4	0.23
(1,635)	1:96:A:ILE:HG22	1:100:A:GLY:H	4	0.23
(1,635)	1:96:A:ILE:HG23	1:100:A:GLY:H	4	0.23
(1,395)	1:109:A:LEU:HG	1:111:A:ILE:HD11	4	0.23
(1,395)	1:109:A:LEU:HG	1:111:A:ILE:HD12	4	0.23
(1,395)	1:109:A:LEU:HG	1:111:A:ILE:HD13	4	0.23
(1,395)	1:109:A:LEU:HG	1:111:A:ILE:HD11	12	0.23
(1,395)	1:109:A:LEU:HG	1:111:A:ILE:HD12	12	0.23
(1,395)	1:109:A:LEU:HG	1:111:A:ILE:HD13	12	0.23
(1,365)	1:126:B:ILE:HG21	1:131:B:ILE:HD11	18	0.23
(1,365)	1:126:B:ILE:HG21	1:131:B:ILE:HD12	18	0.23
(1,365)	1:126:B:ILE:HG21	1:131:B:ILE:HD13	18	0.23
(1,365)	1:126:B:ILE:HG22	1:131:B:ILE:HD11	18	0.23
(1,365)	1:126:B:ILE:HG22	1:131:B:ILE:HD12	18	0.23
(1,365)	1:126:B:ILE:HG22	1:131:B:ILE:HD13	18	0.23
(1,365)	1:126:B:ILE:HG23	1:131:B:ILE:HD11	18	0.23
(1,365)	1:126:B:ILE:HG23	1:131:B:ILE:HD12	18	0.23
(1,365)	1:126:B:ILE:HG23	1:131:B:ILE:HD13	18	0.23
(1,251)	1:118:C:GLY:HA2	1:119:C:THR:HG21	16	0.23
(1,251)	1:118:C:GLY:HA2	1:119:C:THR:HG22	16	0.23
(1,251)	1:118:C:GLY:HA2	1:119:C:THR:HG23	16	0.23
(1,249)	1:118:A:GLY:HA2	1:119:A:THR:HG21	16	0.23
(1,249)	1:118:A:GLY:HA2	1:119:A:THR:HG22	16	0.23
(1,249)	1:118:A:GLY:HA2	1:119:A:THR:HG23	16	0.23
(1,226)	1:96:A:ILE:HD11	1:102:A:VAL:HG11	17	0.23
(1,226)	1:96:A:ILE:HD11	1:102:A:VAL:HG12	17	0.23
(1,226)	1:96:A:ILE:HD11	1:102:A:VAL:HG13	17	0.23
(1,226)	1:96:A:ILE:HD12	1:102:A:VAL:HG11	17	0.23
(1,226)	1:96:A:ILE:HD12	1:102:A:VAL:HG12	17	0.23
(1,226)	1:96:A:ILE:HD12	1:102:A:VAL:HG13	17	0.23
(1,226)	1:96:A:ILE:HD13	1:102:A:VAL:HG11	17	0.23
(1,226)	1:96:A:ILE:HD13	1:102:A:VAL:HG12	17	0.23
(1,226)	1:96:A:ILE:HD13	1:102:A:VAL:HG13	17	0.23
(1,226)	1:96:A:ILE:HD11	1:102:A:VAL:HG11	20	0.23
(1,226)	1:96:A:ILE:HD11	1:102:A:VAL:HG12	20	0.23
(1,226)	1:96:A:ILE:HD11	1:102:A:VAL:HG13	20	0.23
(1,226)	1:96:A:ILE:HD12	1:102:A:VAL:HG11	20	0.23
(1,226)	1:96:A:ILE:HD12	1:102:A:VAL:HG12	20	0.23
(1,226)	1:96:A:ILE:HD12	1:102:A:VAL:HG13	20	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,226)	1:96:A:ILE:HD13	1:102:A:VAL:HG11	20	0.23
(1,226)	1:96:A:ILE:HD13	1:102:A:VAL:HG12	20	0.23
(1,226)	1:96:A:ILE:HD13	1:102:A:VAL:HG13	20	0.23
(1,182)	1:137:A:LEU:HD11	1:141:A:VAL:HG11	4	0.23
(1,182)	1:137:A:LEU:HD11	1:141:A:VAL:HG12	4	0.23
(1,182)	1:137:A:LEU:HD11	1:141:A:VAL:HG13	4	0.23
(1,182)	1:137:A:LEU:HD12	1:141:A:VAL:HG11	4	0.23
(1,182)	1:137:A:LEU:HD12	1:141:A:VAL:HG12	4	0.23
(1,182)	1:137:A:LEU:HD12	1:141:A:VAL:HG13	4	0.23
(1,182)	1:137:A:LEU:HD13	1:141:A:VAL:HG11	4	0.23
(1,182)	1:137:A:LEU:HD13	1:141:A:VAL:HG12	4	0.23
(1,182)	1:137:A:LEU:HD13	1:141:A:VAL:HG13	4	0.23
(1,175)	1:179:A:ALA:HB1	1:181:A:LEU:HD21	5	0.23
(1,175)	1:179:A:ALA:HB1	1:181:A:LEU:HD22	5	0.23
(1,175)	1:179:A:ALA:HB1	1:181:A:LEU:HD23	5	0.23
(1,175)	1:179:A:ALA:HB2	1:181:A:LEU:HD21	5	0.23
(1,175)	1:179:A:ALA:HB2	1:181:A:LEU:HD22	5	0.23
(1,175)	1:179:A:ALA:HB2	1:181:A:LEU:HD23	5	0.23
(1,175)	1:179:A:ALA:HB3	1:181:A:LEU:HD21	5	0.23
(1,175)	1:179:A:ALA:HB3	1:181:A:LEU:HD22	5	0.23
(1,175)	1:179:A:ALA:HB3	1:181:A:LEU:HD23	5	0.23
(1,122)	1:113:A:TYR:HD1	1:137:A:LEU:HD21	4	0.23
(1,122)	1:113:A:TYR:HD1	1:137:A:LEU:HD22	4	0.23
(1,122)	1:113:A:TYR:HD1	1:137:A:LEU:HD23	4	0.23
(1,122)	1:113:A:TYR:HD2	1:137:A:LEU:HD21	4	0.23
(1,122)	1:113:A:TYR:HD2	1:137:A:LEU:HD22	4	0.23
(1,122)	1:113:A:TYR:HD2	1:137:A:LEU:HD23	4	0.23
(1,1)	1:108:A:GLN:HA	1:109:A:LEU:HD21	13	0.23
(1,1)	1:108:A:GLN:HA	1:109:A:LEU:HD22	13	0.23
(1,1)	1:108:A:GLN:HA	1:109:A:LEU:HD23	13	0.23
(1,2338)	1:179:C:ALA:HB1	1:181:C:LEU:HD11	12	0.22
(1,2338)	1:179:C:ALA:HB1	1:181:C:LEU:HD12	12	0.22
(1,2338)	1:179:C:ALA:HB1	1:181:C:LEU:HD13	12	0.22
(1,2338)	1:179:C:ALA:HB1	1:181:C:LEU:HD21	12	0.22
(1,2338)	1:179:C:ALA:HB1	1:181:C:LEU:HD22	12	0.22
(1,2338)	1:179:C:ALA:HB1	1:181:C:LEU:HD23	12	0.22
(1,2338)	1:179:C:ALA:HB2	1:181:C:LEU:HD11	12	0.22
(1,2338)	1:179:C:ALA:HB2	1:181:C:LEU:HD12	12	0.22
(1,2338)	1:179:C:ALA:HB2	1:181:C:LEU:HD13	12	0.22
(1,2338)	1:179:C:ALA:HB2	1:181:C:LEU:HD21	12	0.22
(1,2338)	1:179:C:ALA:HB2	1:181:C:LEU:HD22	12	0.22
(1,2338)	1:179:C:ALA:HB2	1:181:C:LEU:HD23	12	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2338)	1:179:C:ALA:HB3	1:181:C:LEU:HD11	12	0.22
(1,2338)	1:179:C:ALA:HB3	1:181:C:LEU:HD12	12	0.22
(1,2338)	1:179:C:ALA:HB3	1:181:C:LEU:HD13	12	0.22
(1,2338)	1:179:C:ALA:HB3	1:181:C:LEU:HD21	12	0.22
(1,2338)	1:179:C:ALA:HB3	1:181:C:LEU:HD22	12	0.22
(1,2338)	1:179:C:ALA:HB3	1:181:C:LEU:HD23	12	0.22
(1,2320)	1:172:C:ALA:HA	1:178:C:PRO:HD2	1	0.22
(1,2320)	1:172:C:ALA:HA	1:178:C:PRO:HD3	1	0.22
(1,2298)	1:156:C:VAL:HB	1:157:C:PRO:HD2	9	0.22
(1,2298)	1:156:C:VAL:HB	1:157:C:PRO:HD3	9	0.22
(1,2292)	1:154:C:PRO:HB2	1:167:C:ARG:H	19	0.22
(1,2292)	1:154:C:PRO:HB3	1:167:C:ARG:H	19	0.22
(1,2112)	1:179:B:ALA:HB1	1:181:B:LEU:HD11	12	0.22
(1,2112)	1:179:B:ALA:HB1	1:181:B:LEU:HD12	12	0.22
(1,2112)	1:179:B:ALA:HB1	1:181:B:LEU:HD13	12	0.22
(1,2112)	1:179:B:ALA:HB1	1:181:B:LEU:HD21	12	0.22
(1,2112)	1:179:B:ALA:HB1	1:181:B:LEU:HD22	12	0.22
(1,2112)	1:179:B:ALA:HB1	1:181:B:LEU:HD23	12	0.22
(1,2112)	1:179:B:ALA:HB2	1:181:B:LEU:HD11	12	0.22
(1,2112)	1:179:B:ALA:HB2	1:181:B:LEU:HD12	12	0.22
(1,2112)	1:179:B:ALA:HB2	1:181:B:LEU:HD13	12	0.22
(1,2112)	1:179:B:ALA:HB2	1:181:B:LEU:HD21	12	0.22
(1,2112)	1:179:B:ALA:HB2	1:181:B:LEU:HD22	12	0.22
(1,2112)	1:179:B:ALA:HB2	1:181:B:LEU:HD23	12	0.22
(1,2112)	1:179:B:ALA:HB3	1:181:B:LEU:HD11	12	0.22
(1,2112)	1:179:B:ALA:HB3	1:181:B:LEU:HD12	12	0.22
(1,2112)	1:179:B:ALA:HB3	1:181:B:LEU:HD13	12	0.22
(1,2112)	1:179:B:ALA:HB3	1:181:B:LEU:HD21	12	0.22
(1,2112)	1:179:B:ALA:HB3	1:181:B:LEU:HD22	12	0.22
(1,2112)	1:179:B:ALA:HB3	1:181:B:LEU:HD23	12	0.22
(1,2094)	1:172:B:ALA:HA	1:178:B:PRO:HD2	1	0.22
(1,2094)	1:172:B:ALA:HA	1:178:B:PRO:HD3	1	0.22
(1,2072)	1:156:B:VAL:HB	1:157:B:PRO:HD2	9	0.22
(1,2072)	1:156:B:VAL:HB	1:157:B:PRO:HD3	9	0.22
(1,2066)	1:154:B:PRO:HB2	1:167:B:ARG:H	14	0.22
(1,2066)	1:154:B:PRO:HB3	1:167:B:ARG:H	14	0.22
(1,2066)	1:154:B:PRO:HB2	1:167:B:ARG:H	19	0.22
(1,2066)	1:154:B:PRO:HB3	1:167:B:ARG:H	19	0.22
(1,1902)	1:172:A:ALA:HA	1:178:A:PRO:HD2	11	0.22
(1,1902)	1:172:A:ALA:HA	1:178:A:PRO:HD3	11	0.22
(1,1884)	1:154:A:PRO:HB2	1:167:A:ARG:H	7	0.22
(1,1884)	1:154:A:PRO:HB3	1:167:A:ARG:H	7	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1884)	1:154:A:PRO:HB2	1:167:A:ARG:H	19	0.22
(1,1884)	1:154:A:PRO:HB3	1:167:A:ARG:H	19	0.22
(1,1830)	1:102:A:VAL:HG11	1:111:A:ILE:HG12	4	0.22
(1,1830)	1:102:A:VAL:HG11	1:111:A:ILE:HG13	4	0.22
(1,1830)	1:102:A:VAL:HG12	1:111:A:ILE:HG12	4	0.22
(1,1830)	1:102:A:VAL:HG12	1:111:A:ILE:HG13	4	0.22
(1,1830)	1:102:A:VAL:HG13	1:111:A:ILE:HG12	4	0.22
(1,1830)	1:102:A:VAL:HG13	1:111:A:ILE:HG13	4	0.22
(1,1818)	1:95:B:SER:HB2	1:101:B:LEU:H	14	0.22
(1,1818)	1:95:B:SER:HB3	1:101:B:LEU:H	14	0.22
(1,1770)	1:178:C:PRO:HD3	1:179:C:ALA:H	11	0.22
(1,1769)	1:178:B:PRO:HD3	1:179:B:ALA:H	11	0.22
(1,1768)	1:178:A:PRO:HD3	1:179:A:ALA:H	1	0.22
(1,1614)	1:116:A:ALA:H	1:119:A:THR:HB	19	0.22
(1,1562)	1:145:A:GLN:HA	1:151:A:GLN:H	13	0.22
(1,1548)	1:167:C:ARG:H	1:170:C:GLY:HA2	15	0.22
(1,1548)	1:167:C:ARG:H	1:170:C:GLY:HA3	15	0.22
(1,1548)	1:167:C:ARG:H	1:170:C:GLY:HA2	19	0.22
(1,1548)	1:167:C:ARG:H	1:170:C:GLY:HA3	19	0.22
(1,1548)	1:167:C:ARG:H	1:170:C:GLY:HA2	20	0.22
(1,1548)	1:167:C:ARG:H	1:170:C:GLY:HA3	20	0.22
(1,1547)	1:167:B:ARG:H	1:170:B:GLY:HA2	15	0.22
(1,1547)	1:167:B:ARG:H	1:170:B:GLY:HA3	15	0.22
(1,1547)	1:167:B:ARG:H	1:170:B:GLY:HA2	19	0.22
(1,1547)	1:167:B:ARG:H	1:170:B:GLY:HA3	19	0.22
(1,1547)	1:167:B:ARG:H	1:170:B:GLY:HA2	20	0.22
(1,1547)	1:167:B:ARG:H	1:170:B:GLY:HA3	20	0.22
(1,1546)	1:167:A:ARG:H	1:170:A:GLY:HA2	19	0.22
(1,1546)	1:167:A:ARG:H	1:170:A:GLY:HA3	19	0.22
(1,1535)	1:122:C:TYR:H	1:189:C:CYS:HB2	8	0.22
(1,1535)	1:122:C:TYR:H	1:189:C:CYS:HB3	8	0.22
(1,1522)	1:178:C:PRO:HG2	1:179:C:ALA:H	2	0.22
(1,1522)	1:178:C:PRO:HG3	1:179:C:ALA:H	2	0.22
(1,1522)	1:178:C:PRO:HG2	1:179:C:ALA:H	13	0.22
(1,1522)	1:178:C:PRO:HG3	1:179:C:ALA:H	13	0.22
(1,1522)	1:178:C:PRO:HG2	1:179:C:ALA:H	16	0.22
(1,1522)	1:178:C:PRO:HG3	1:179:C:ALA:H	16	0.22
(1,1522)	1:178:C:PRO:HG2	1:179:C:ALA:H	17	0.22
(1,1522)	1:178:C:PRO:HG3	1:179:C:ALA:H	17	0.22
(1,1521)	1:178:B:PRO:HG2	1:179:B:ALA:H	2	0.22
(1,1521)	1:178:B:PRO:HG3	1:179:B:ALA:H	2	0.22
(1,1521)	1:178:B:PRO:HG2	1:179:B:ALA:H	16	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1521)	1:178:B:PRO:HG3	1:179:B:ALA:H	16	0.22
(1,1505)	1:93:A:THR:HG21	1:92:B:ALA:H	8	0.22
(1,1505)	1:93:A:THR:HG22	1:92:B:ALA:H	8	0.22
(1,1505)	1:93:A:THR:HG23	1:92:B:ALA:H	8	0.22
(1,1410)	1:152:C:ALA:HB1	1:153:C:LYS:H	16	0.22
(1,1410)	1:152:C:ALA:HB2	1:153:C:LYS:H	16	0.22
(1,1410)	1:152:C:ALA:HB3	1:153:C:LYS:H	16	0.22
(1,1409)	1:152:B:ALA:HB1	1:153:B:LYS:H	16	0.22
(1,1409)	1:152:B:ALA:HB2	1:153:B:LYS:H	16	0.22
(1,1409)	1:152:B:ALA:HB3	1:153:B:LYS:H	16	0.22
(1,1408)	1:152:A:ALA:HB1	1:153:A:LYS:H	16	0.22
(1,1408)	1:152:A:ALA:HB2	1:153:A:LYS:H	16	0.22
(1,1408)	1:152:A:ALA:HB3	1:153:A:LYS:H	16	0.22
(1,1247)	1:121:B:CYS:H	1:189:B:CYS:HB2	8	0.22
(1,1247)	1:121:B:CYS:H	1:189:B:CYS:HB3	8	0.22
(1,1073)	1:139:C:ARG:H	1:141:C:VAL:HB	1	0.22
(1,1073)	1:139:C:ARG:H	1:141:C:VAL:HB	8	0.22
(1,1073)	1:139:C:ARG:H	1:141:C:VAL:HB	9	0.22
(1,1072)	1:139:B:ARG:H	1:141:B:VAL:HB	1	0.22
(1,1072)	1:139:B:ARG:H	1:141:B:VAL:HB	15	0.22
(1,1072)	1:139:B:ARG:H	1:141:B:VAL:HB	18	0.22
(1,1072)	1:139:B:ARG:H	1:141:B:VAL:HB	19	0.22
(1,1071)	1:139:A:ARG:H	1:141:A:VAL:HB	2	0.22
(1,1047)	1:137:A:LEU:HG	1:138:A:THR:H	9	0.22
(1,958)	1:187:A:THR:HA	1:188:A:LEU:HD11	12	0.22
(1,958)	1:187:A:THR:HA	1:188:A:LEU:HD12	12	0.22
(1,958)	1:187:A:THR:HA	1:188:A:LEU:HD13	12	0.22
(1,928)	1:178:A:PRO:HG2	1:181:A:LEU:HD21	3	0.22
(1,928)	1:178:A:PRO:HG2	1:181:A:LEU:HD22	3	0.22
(1,928)	1:178:A:PRO:HG2	1:181:A:LEU:HD23	3	0.22
(1,928)	1:178:A:PRO:HG3	1:181:A:LEU:HD21	3	0.22
(1,928)	1:178:A:PRO:HG3	1:181:A:LEU:HD22	3	0.22
(1,928)	1:178:A:PRO:HG3	1:181:A:LEU:HD23	3	0.22
(1,928)	1:178:A:PRO:HG2	1:181:A:LEU:HD21	4	0.22
(1,928)	1:178:A:PRO:HG2	1:181:A:LEU:HD22	4	0.22
(1,928)	1:178:A:PRO:HG2	1:181:A:LEU:HD23	4	0.22
(1,928)	1:178:A:PRO:HG3	1:181:A:LEU:HD21	4	0.22
(1,928)	1:178:A:PRO:HG3	1:181:A:LEU:HD22	4	0.22
(1,928)	1:178:A:PRO:HG3	1:181:A:LEU:HD23	4	0.22
(1,928)	1:178:A:PRO:HG2	1:181:A:LEU:HD21	10	0.22
(1,928)	1:178:A:PRO:HG2	1:181:A:LEU:HD22	10	0.22
(1,928)	1:178:A:PRO:HG2	1:181:A:LEU:HD23	10	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,928)	1:178:A:PRO:HG3	1:181:A:LEU:HD21	10	0.22
(1,928)	1:178:A:PRO:HG3	1:181:A:LEU:HD22	10	0.22
(1,928)	1:178:A:PRO:HG3	1:181:A:LEU:HD23	10	0.22
(1,890)	1:152:C:ALA:HA	1:157:C:PRO:HG2	9	0.22
(1,890)	1:152:C:ALA:HA	1:157:C:PRO:HG3	9	0.22
(1,890)	1:152:C:ALA:HA	1:157:C:PRO:HG2	10	0.22
(1,890)	1:152:C:ALA:HA	1:157:C:PRO:HG3	10	0.22
(1,889)	1:152:B:ALA:HA	1:157:B:PRO:HG2	9	0.22
(1,889)	1:152:B:ALA:HA	1:157:B:PRO:HG3	9	0.22
(1,889)	1:152:B:ALA:HA	1:157:B:PRO:HG2	10	0.22
(1,889)	1:152:B:ALA:HA	1:157:B:PRO:HG3	10	0.22
(1,810)	1:176:A:GLY:H	1:177:A:ASP:HB3	3	0.22
(1,755)	1:189:C:CYS:H	1:192:C:VAL:HG11	7	0.22
(1,755)	1:189:C:CYS:H	1:192:C:VAL:HG12	7	0.22
(1,755)	1:189:C:CYS:H	1:192:C:VAL:HG13	7	0.22
(1,754)	1:189:B:CYS:H	1:192:B:VAL:HG11	10	0.22
(1,754)	1:189:B:CYS:H	1:192:B:VAL:HG12	10	0.22
(1,754)	1:189:B:CYS:H	1:192:B:VAL:HG13	10	0.22
(1,749)	1:123:A:ILE:HG21	1:179:A:ALA:HB1	7	0.22
(1,749)	1:123:A:ILE:HG21	1:179:A:ALA:HB2	7	0.22
(1,749)	1:123:A:ILE:HG21	1:179:A:ALA:HB3	7	0.22
(1,749)	1:123:A:ILE:HG22	1:179:A:ALA:HB1	7	0.22
(1,749)	1:123:A:ILE:HG22	1:179:A:ALA:HB2	7	0.22
(1,749)	1:123:A:ILE:HG22	1:179:A:ALA:HB3	7	0.22
(1,749)	1:123:A:ILE:HG23	1:179:A:ALA:HB1	7	0.22
(1,749)	1:123:A:ILE:HG23	1:179:A:ALA:HB2	7	0.22
(1,749)	1:123:A:ILE:HG23	1:179:A:ALA:HB3	7	0.22
(1,636)	1:96:B:ILE:HG21	1:100:B:GLY:H	9	0.22
(1,636)	1:96:B:ILE:HG22	1:100:B:GLY:H	9	0.22
(1,636)	1:96:B:ILE:HG23	1:100:B:GLY:H	9	0.22
(1,624)	1:96:B:ILE:HG21	1:138:B:THR:HB	8	0.22
(1,624)	1:96:B:ILE:HG22	1:138:B:THR:HB	8	0.22
(1,624)	1:96:B:ILE:HG23	1:138:B:THR:HB	8	0.22
(1,577)	1:178:A:PRO:HG2	1:194:A:LEU:HD21	6	0.22
(1,577)	1:178:A:PRO:HG2	1:194:A:LEU:HD22	6	0.22
(1,577)	1:178:A:PRO:HG2	1:194:A:LEU:HD23	6	0.22
(1,577)	1:178:A:PRO:HG3	1:194:A:LEU:HD21	6	0.22
(1,577)	1:178:A:PRO:HG3	1:194:A:LEU:HD22	6	0.22
(1,577)	1:178:A:PRO:HG3	1:194:A:LEU:HD23	6	0.22
(1,572)	1:121:A:CYS:H	1:194:A:LEU:HD21	8	0.22
(1,572)	1:121:A:CYS:H	1:194:A:LEU:HD22	8	0.22
(1,572)	1:121:A:CYS:H	1:194:A:LEU:HD23	8	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,539)	1:111:A:ILE:HG21	1:126:A:ILE:HG21	5	0.22
(1,539)	1:111:A:ILE:HG21	1:126:A:ILE:HG22	5	0.22
(1,539)	1:111:A:ILE:HG21	1:126:A:ILE:HG23	5	0.22
(1,539)	1:111:A:ILE:HG22	1:126:A:ILE:HG21	5	0.22
(1,539)	1:111:A:ILE:HG22	1:126:A:ILE:HG22	5	0.22
(1,539)	1:111:A:ILE:HG22	1:126:A:ILE:HG23	5	0.22
(1,539)	1:111:A:ILE:HG23	1:126:A:ILE:HG21	5	0.22
(1,539)	1:111:A:ILE:HG23	1:126:A:ILE:HG22	5	0.22
(1,539)	1:111:A:ILE:HG23	1:126:A:ILE:HG23	5	0.22
(1,437)	1:183:C:MET:HE1	1:186:C:SER:HA	1	0.22
(1,437)	1:183:C:MET:HE2	1:186:C:SER:HA	1	0.22
(1,437)	1:183:C:MET:HE3	1:186:C:SER:HA	1	0.22
(1,436)	1:183:B:MET:HE1	1:186:B:SER:HA	1	0.22
(1,436)	1:183:B:MET:HE2	1:186:B:SER:HA	1	0.22
(1,436)	1:183:B:MET:HE3	1:186:B:SER:HA	1	0.22
(1,435)	1:183:A:MET:HE1	1:186:A:SER:HA	16	0.22
(1,435)	1:183:A:MET:HE2	1:186:A:SER:HA	16	0.22
(1,435)	1:183:A:MET:HE3	1:186:A:SER:HA	16	0.22
(1,425)	1:89:A:VAL:HG11	1:183:A:MET:HE1	8	0.22
(1,425)	1:89:A:VAL:HG11	1:183:A:MET:HE2	8	0.22
(1,425)	1:89:A:VAL:HG11	1:183:A:MET:HE3	8	0.22
(1,425)	1:89:A:VAL:HG12	1:183:A:MET:HE1	8	0.22
(1,425)	1:89:A:VAL:HG12	1:183:A:MET:HE2	8	0.22
(1,425)	1:89:A:VAL:HG12	1:183:A:MET:HE3	8	0.22
(1,425)	1:89:A:VAL:HG13	1:183:A:MET:HE1	8	0.22
(1,425)	1:89:A:VAL:HG13	1:183:A:MET:HE2	8	0.22
(1,425)	1:89:A:VAL:HG13	1:183:A:MET:HE3	8	0.22
(1,366)	1:126:C:ILE:HG21	1:131:C:ILE:HD11	8	0.22
(1,366)	1:126:C:ILE:HG21	1:131:C:ILE:HD12	8	0.22
(1,366)	1:126:C:ILE:HG21	1:131:C:ILE:HD13	8	0.22
(1,366)	1:126:C:ILE:HG22	1:131:C:ILE:HD11	8	0.22
(1,366)	1:126:C:ILE:HG22	1:131:C:ILE:HD12	8	0.22
(1,366)	1:126:C:ILE:HG22	1:131:C:ILE:HD13	8	0.22
(1,366)	1:126:C:ILE:HG23	1:131:C:ILE:HD11	8	0.22
(1,366)	1:126:C:ILE:HG23	1:131:C:ILE:HD12	8	0.22
(1,366)	1:126:C:ILE:HG23	1:131:C:ILE:HD13	8	0.22
(1,366)	1:126:C:ILE:HG21	1:131:C:ILE:HD11	18	0.22
(1,366)	1:126:C:ILE:HG21	1:131:C:ILE:HD12	18	0.22
(1,366)	1:126:C:ILE:HG21	1:131:C:ILE:HD13	18	0.22
(1,366)	1:126:C:ILE:HG22	1:131:C:ILE:HD11	18	0.22
(1,366)	1:126:C:ILE:HG22	1:131:C:ILE:HD12	18	0.22
(1,366)	1:126:C:ILE:HG22	1:131:C:ILE:HD13	18	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,366)	1:126:C:ILE:HG23	1:131:C:ILE:HD11	18	0.22
(1,366)	1:126:C:ILE:HG23	1:131:C:ILE:HD12	18	0.22
(1,366)	1:126:C:ILE:HG23	1:131:C:ILE:HD13	18	0.22
(1,365)	1:126:B:ILE:HG21	1:131:B:ILE:HD11	8	0.22
(1,365)	1:126:B:ILE:HG21	1:131:B:ILE:HD12	8	0.22
(1,365)	1:126:B:ILE:HG21	1:131:B:ILE:HD13	8	0.22
(1,365)	1:126:B:ILE:HG22	1:131:B:ILE:HD11	8	0.22
(1,365)	1:126:B:ILE:HG22	1:131:B:ILE:HD12	8	0.22
(1,365)	1:126:B:ILE:HG22	1:131:B:ILE:HD13	8	0.22
(1,365)	1:126:B:ILE:HG23	1:131:B:ILE:HD11	8	0.22
(1,365)	1:126:B:ILE:HG23	1:131:B:ILE:HD12	8	0.22
(1,365)	1:126:B:ILE:HG23	1:131:B:ILE:HD13	8	0.22
(1,364)	1:126:A:ILE:HG21	1:131:A:ILE:HD11	17	0.22
(1,364)	1:126:A:ILE:HG21	1:131:A:ILE:HD12	17	0.22
(1,364)	1:126:A:ILE:HG21	1:131:A:ILE:HD13	17	0.22
(1,364)	1:126:A:ILE:HG22	1:131:A:ILE:HD11	17	0.22
(1,364)	1:126:A:ILE:HG22	1:131:A:ILE:HD12	17	0.22
(1,364)	1:126:A:ILE:HG22	1:131:A:ILE:HD13	17	0.22
(1,364)	1:126:A:ILE:HG23	1:131:A:ILE:HD11	17	0.22
(1,364)	1:126:A:ILE:HG23	1:131:A:ILE:HD12	17	0.22
(1,364)	1:126:A:ILE:HG23	1:131:A:ILE:HD13	17	0.22
(1,361)	1:183:A:MET:HG2	1:131:B:ILE:HD11	5	0.22
(1,361)	1:183:A:MET:HG2	1:131:B:ILE:HD12	5	0.22
(1,361)	1:183:A:MET:HG2	1:131:B:ILE:HD13	5	0.22
(1,361)	1:183:A:MET:HG3	1:131:B:ILE:HD11	5	0.22
(1,361)	1:183:A:MET:HG3	1:131:B:ILE:HD12	5	0.22
(1,361)	1:183:A:MET:HG3	1:131:B:ILE:HD13	5	0.22
(1,251)	1:118:C:GLY:HA2	1:119:C:THR:HG21	3	0.22
(1,251)	1:118:C:GLY:HA2	1:119:C:THR:HG22	3	0.22
(1,251)	1:118:C:GLY:HA2	1:119:C:THR:HG23	3	0.22
(1,250)	1:118:B:GLY:HA2	1:119:B:THR:HG21	3	0.22
(1,250)	1:118:B:GLY:HA2	1:119:B:THR:HG22	3	0.22
(1,250)	1:118:B:GLY:HA2	1:119:B:THR:HG23	3	0.22
(1,228)	1:96:C:ILE:HD11	1:102:C:VAL:HG11	6	0.22
(1,228)	1:96:C:ILE:HD11	1:102:C:VAL:HG12	6	0.22
(1,228)	1:96:C:ILE:HD11	1:102:C:VAL:HG13	6	0.22
(1,228)	1:96:C:ILE:HD12	1:102:C:VAL:HG11	6	0.22
(1,228)	1:96:C:ILE:HD12	1:102:C:VAL:HG12	6	0.22
(1,228)	1:96:C:ILE:HD12	1:102:C:VAL:HG13	6	0.22
(1,228)	1:96:C:ILE:HD13	1:102:C:VAL:HG11	6	0.22
(1,228)	1:96:C:ILE:HD13	1:102:C:VAL:HG12	6	0.22
(1,228)	1:96:C:ILE:HD13	1:102:C:VAL:HG13	6	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,227)	1:96:B:ILE:HD11	1:102:B:VAL:HG11	6	0.22
(1,227)	1:96:B:ILE:HD11	1:102:B:VAL:HG12	6	0.22
(1,227)	1:96:B:ILE:HD11	1:102:B:VAL:HG13	6	0.22
(1,227)	1:96:B:ILE:HD12	1:102:B:VAL:HG11	6	0.22
(1,227)	1:96:B:ILE:HD12	1:102:B:VAL:HG12	6	0.22
(1,227)	1:96:B:ILE:HD12	1:102:B:VAL:HG13	6	0.22
(1,227)	1:96:B:ILE:HD13	1:102:B:VAL:HG11	6	0.22
(1,227)	1:96:B:ILE:HD13	1:102:B:VAL:HG12	6	0.22
(1,227)	1:96:B:ILE:HD13	1:102:B:VAL:HG13	6	0.22
(1,122)	1:113:A:TYR:HD1	1:137:A:LEU:HD21	15	0.22
(1,122)	1:113:A:TYR:HD1	1:137:A:LEU:HD22	15	0.22
(1,122)	1:113:A:TYR:HD1	1:137:A:LEU:HD23	15	0.22
(1,122)	1:113:A:TYR:HD2	1:137:A:LEU:HD21	15	0.22
(1,122)	1:113:A:TYR:HD2	1:137:A:LEU:HD22	15	0.22
(1,122)	1:113:A:TYR:HD2	1:137:A:LEU:HD23	15	0.22
(1,1)	1:108:A:GLN:HA	1:109:A:LEU:HD21	5	0.22
(1,1)	1:108:A:GLN:HA	1:109:A:LEU:HD22	5	0.22
(1,1)	1:108:A:GLN:HA	1:109:A:LEU:HD23	5	0.22
(1,1)	1:108:A:GLN:HA	1:109:A:LEU:HD21	12	0.22
(1,1)	1:108:A:GLN:HA	1:109:A:LEU:HD22	12	0.22
(1,1)	1:108:A:GLN:HA	1:109:A:LEU:HD23	12	0.22
(1,1)	1:108:A:GLN:HA	1:109:A:LEU:HD21	14	0.22
(1,1)	1:108:A:GLN:HA	1:109:A:LEU:HD22	14	0.22
(1,1)	1:108:A:GLN:HA	1:109:A:LEU:HD23	14	0.22
(1,1)	1:108:A:GLN:HA	1:109:A:LEU:HD21	20	0.22
(1,1)	1:108:A:GLN:HA	1:109:A:LEU:HD22	20	0.22
(1,1)	1:108:A:GLN:HA	1:109:A:LEU:HD23	20	0.22
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD11	2	0.21
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD12	2	0.21
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD13	2	0.21
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD21	2	0.21
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD22	2	0.21
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD23	2	0.21
(1,2320)	1:172:C:ALA:HA	1:178:C:PRO:HD2	11	0.21
(1,2320)	1:172:C:ALA:HA	1:178:C:PRO:HD3	11	0.21
(1,2298)	1:156:C:VAL:HB	1:157:C:PRO:HD2	4	0.21
(1,2298)	1:156:C:VAL:HB	1:157:C:PRO:HD3	4	0.21
(1,2298)	1:156:C:VAL:HB	1:157:C:PRO:HD2	8	0.21
(1,2298)	1:156:C:VAL:HB	1:157:C:PRO:HD3	8	0.21
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG11	10	0.21
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG12	10	0.21
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG13	10	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG21	10	0.21
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG22	10	0.21
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG23	10	0.21
(1,2163)	1:89:C:VAL:HG11	1:183:C:MET:HE1	8	0.21
(1,2163)	1:89:C:VAL:HG11	1:183:C:MET:HE2	8	0.21
(1,2163)	1:89:C:VAL:HG11	1:183:C:MET:HE3	8	0.21
(1,2163)	1:89:C:VAL:HG12	1:183:C:MET:HE1	8	0.21
(1,2163)	1:89:C:VAL:HG12	1:183:C:MET:HE2	8	0.21
(1,2163)	1:89:C:VAL:HG12	1:183:C:MET:HE3	8	0.21
(1,2163)	1:89:C:VAL:HG13	1:183:C:MET:HE1	8	0.21
(1,2163)	1:89:C:VAL:HG13	1:183:C:MET:HE2	8	0.21
(1,2163)	1:89:C:VAL:HG13	1:183:C:MET:HE3	8	0.21
(1,2163)	1:89:C:VAL:HG21	1:183:C:MET:HE1	8	0.21
(1,2163)	1:89:C:VAL:HG21	1:183:C:MET:HE2	8	0.21
(1,2163)	1:89:C:VAL:HG21	1:183:C:MET:HE3	8	0.21
(1,2163)	1:89:C:VAL:HG22	1:183:C:MET:HE1	8	0.21
(1,2163)	1:89:C:VAL:HG22	1:183:C:MET:HE2	8	0.21
(1,2163)	1:89:C:VAL:HG22	1:183:C:MET:HE3	8	0.21
(1,2163)	1:89:C:VAL:HG23	1:183:C:MET:HE1	8	0.21
(1,2163)	1:89:C:VAL:HG23	1:183:C:MET:HE2	8	0.21
(1,2163)	1:89:C:VAL:HG23	1:183:C:MET:HE3	8	0.21
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD11	2	0.21
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD12	2	0.21
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD13	2	0.21
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD21	2	0.21
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD22	2	0.21
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD23	2	0.21
(1,2094)	1:172:B:ALA:HA	1:178:B:PRO:HD2	11	0.21
(1,2094)	1:172:B:ALA:HA	1:178:B:PRO:HD3	11	0.21
(1,2072)	1:156:B:VAL:HB	1:157:B:PRO:HD2	4	0.21
(1,2072)	1:156:B:VAL:HB	1:157:B:PRO:HD3	4	0.21
(1,2072)	1:156:B:VAL:HB	1:157:B:PRO:HD2	8	0.21
(1,2072)	1:156:B:VAL:HB	1:157:B:PRO:HD3	8	0.21
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG11	10	0.21
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG12	10	0.21
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG13	10	0.21
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG21	10	0.21
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG22	10	0.21
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG23	10	0.21
(1,1912)	1:178:A:PRO:HB2	1:194:A:LEU:HD21	8	0.21
(1,1912)	1:178:A:PRO:HB2	1:194:A:LEU:HD22	8	0.21
(1,1912)	1:178:A:PRO:HB2	1:194:A:LEU:HD23	8	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1912)	1:178:A:PRO:HB3	1:194:A:LEU:HD21	8	0.21
(1,1912)	1:178:A:PRO:HB3	1:194:A:LEU:HD22	8	0.21
(1,1912)	1:178:A:PRO:HB3	1:194:A:LEU:HD23	8	0.21
(1,1902)	1:172:A:ALA:HA	1:178:A:PRO:HD2	1	0.21
(1,1902)	1:172:A:ALA:HA	1:178:A:PRO:HD3	1	0.21
(1,1902)	1:172:A:ALA:HA	1:178:A:PRO:HD2	16	0.21
(1,1902)	1:172:A:ALA:HA	1:178:A:PRO:HD3	16	0.21
(1,1889)	1:156:A:VAL:HG11	1:157:A:PRO:HD2	4	0.21
(1,1889)	1:156:A:VAL:HG11	1:157:A:PRO:HD3	4	0.21
(1,1889)	1:156:A:VAL:HG12	1:157:A:PRO:HD2	4	0.21
(1,1889)	1:156:A:VAL:HG12	1:157:A:PRO:HD3	4	0.21
(1,1889)	1:156:A:VAL:HG13	1:157:A:PRO:HD2	4	0.21
(1,1889)	1:156:A:VAL:HG13	1:157:A:PRO:HD3	4	0.21
(1,1888)	1:156:A:VAL:HG11	1:157:A:PRO:HB2	12	0.21
(1,1888)	1:156:A:VAL:HG11	1:157:A:PRO:HB3	12	0.21
(1,1888)	1:156:A:VAL:HG12	1:157:A:PRO:HB2	12	0.21
(1,1888)	1:156:A:VAL:HG12	1:157:A:PRO:HB3	12	0.21
(1,1888)	1:156:A:VAL:HG13	1:157:A:PRO:HB2	12	0.21
(1,1888)	1:156:A:VAL:HG13	1:157:A:PRO:HB3	12	0.21
(1,1884)	1:154:A:PRO:HB2	1:167:A:ARG:H	14	0.21
(1,1884)	1:154:A:PRO:HB3	1:167:A:ARG:H	14	0.21
(1,1842)	1:121:A:CYS:HB2	1:189:A:CYS:H	15	0.21
(1,1842)	1:121:A:CYS:HB3	1:189:A:CYS:H	15	0.21
(1,1842)	1:121:A:CYS:HB2	1:189:A:CYS:H	20	0.21
(1,1842)	1:121:A:CYS:HB3	1:189:A:CYS:H	20	0.21
(1,1819)	1:95:C:SER:HB2	1:101:C:LEU:H	8	0.21
(1,1819)	1:95:C:SER:HB3	1:101:C:LEU:H	8	0.21
(1,1819)	1:95:C:SER:HB2	1:101:C:LEU:H	12	0.21
(1,1819)	1:95:C:SER:HB3	1:101:C:LEU:H	12	0.21
(1,1819)	1:95:C:SER:HB2	1:101:C:LEU:H	14	0.21
(1,1819)	1:95:C:SER:HB3	1:101:C:LEU:H	14	0.21
(1,1818)	1:95:B:SER:HB2	1:101:B:LEU:H	7	0.21
(1,1818)	1:95:B:SER:HB3	1:101:B:LEU:H	7	0.21
(1,1818)	1:95:B:SER:HB2	1:101:B:LEU:H	9	0.21
(1,1818)	1:95:B:SER:HB3	1:101:B:LEU:H	9	0.21
(1,1818)	1:95:B:SER:HB2	1:101:B:LEU:H	13	0.21
(1,1818)	1:95:B:SER:HB3	1:101:B:LEU:H	13	0.21
(1,1776)	1:125:C:LYS:H	1:126:C:ILE:HG21	3	0.21
(1,1776)	1:125:C:LYS:H	1:126:C:ILE:HG22	3	0.21
(1,1776)	1:125:C:LYS:H	1:126:C:ILE:HG23	3	0.21
(1,1775)	1:125:B:LYS:H	1:126:B:ILE:HG21	3	0.21
(1,1775)	1:125:B:LYS:H	1:126:B:ILE:HG22	3	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1775)	1:125:B:LYS:H	1:126:B:ILE:HG23	3	0.21
(1,1774)	1:125:A:LYS:H	1:126:A:ILE:HG21	9	0.21
(1,1774)	1:125:A:LYS:H	1:126:A:ILE:HG22	9	0.21
(1,1774)	1:125:A:LYS:H	1:126:A:ILE:HG23	9	0.21
(1,1614)	1:116:A:ALA:H	1:119:A:THR:HB	5	0.21
(1,1614)	1:116:A:ALA:H	1:119:A:THR:HB	10	0.21
(1,1610)	1:118:A:GLY:H	1:192:A:VAL:HG21	14	0.21
(1,1610)	1:118:A:GLY:H	1:192:A:VAL:HG22	14	0.21
(1,1610)	1:118:A:GLY:H	1:192:A:VAL:HG23	14	0.21
(1,1602)	1:89:A:VAL:HG21	1:91:A:THR:H	6	0.21
(1,1602)	1:89:A:VAL:HG22	1:91:A:THR:H	6	0.21
(1,1602)	1:89:A:VAL:HG23	1:91:A:THR:H	6	0.21
(1,1602)	1:89:A:VAL:HG21	1:91:A:THR:H	15	0.21
(1,1602)	1:89:A:VAL:HG22	1:91:A:THR:H	15	0.21
(1,1602)	1:89:A:VAL:HG23	1:91:A:THR:H	15	0.21
(1,1552)	1:156:A:VAL:HB	1:167:A:ARG:H	12	0.21
(1,1533)	1:122:A:TYR:H	1:189:A:CYS:HB2	19	0.21
(1,1533)	1:122:A:TYR:H	1:189:A:CYS:HB3	19	0.21
(1,1529)	1:91:C:THR:HG21	1:106:C:TYR:H	17	0.21
(1,1529)	1:91:C:THR:HG22	1:106:C:TYR:H	17	0.21
(1,1529)	1:91:C:THR:HG23	1:106:C:TYR:H	17	0.21
(1,1528)	1:91:B:THR:HG21	1:106:B:TYR:H	17	0.21
(1,1528)	1:91:B:THR:HG22	1:106:B:TYR:H	17	0.21
(1,1528)	1:91:B:THR:HG23	1:106:B:TYR:H	17	0.21
(1,1522)	1:178:C:PRO:HG2	1:179:C:ALA:H	1	0.21
(1,1522)	1:178:C:PRO:HG3	1:179:C:ALA:H	1	0.21
(1,1521)	1:178:B:PRO:HG2	1:179:B:ALA:H	1	0.21
(1,1521)	1:178:B:PRO:HG3	1:179:B:ALA:H	1	0.21
(1,1520)	1:178:A:PRO:HG2	1:179:A:ALA:H	1	0.21
(1,1520)	1:178:A:PRO:HG3	1:179:A:ALA:H	1	0.21
(1,1520)	1:178:A:PRO:HG2	1:179:A:ALA:H	6	0.21
(1,1520)	1:178:A:PRO:HG3	1:179:A:ALA:H	6	0.21
(1,1520)	1:178:A:PRO:HG2	1:179:A:ALA:H	13	0.21
(1,1520)	1:178:A:PRO:HG3	1:179:A:ALA:H	13	0.21
(1,1511)	1:137:A:LEU:H	1:137:A:LEU:HG	3	0.21
(1,1461)	1:180:A:PHE:H	1:181:A:LEU:HA	2	0.21
(1,1201)	1:196:A:TYR:H	1:196:A:TYR:HE1	3	0.21
(1,1201)	1:196:A:TYR:H	1:196:A:TYR:HE2	3	0.21
(1,1154)	1:156:A:VAL:HG11	1:158:A:THR:H	8	0.21
(1,1154)	1:156:A:VAL:HG12	1:158:A:THR:H	8	0.21
(1,1154)	1:156:A:VAL:HG13	1:158:A:THR:H	8	0.21
(1,1073)	1:139:C:ARG:H	1:141:C:VAL:HB	3	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1073)	1:139:C:ARG:H	1:141:C:VAL:HB	13	0.21
(1,1073)	1:139:C:ARG:H	1:141:C:VAL:HB	14	0.21
(1,1073)	1:139:C:ARG:H	1:141:C:VAL:HB	16	0.21
(1,1072)	1:139:B:ARG:H	1:141:B:VAL:HB	8	0.21
(1,1072)	1:139:B:ARG:H	1:141:B:VAL:HB	9	0.21
(1,1072)	1:139:B:ARG:H	1:141:B:VAL:HB	10	0.21
(1,1072)	1:139:B:ARG:H	1:141:B:VAL:HB	13	0.21
(1,1072)	1:139:B:ARG:H	1:141:B:VAL:HB	16	0.21
(1,1071)	1:139:A:ARG:H	1:141:A:VAL:HB	4	0.21
(1,1071)	1:139:A:ARG:H	1:141:A:VAL:HB	11	0.21
(1,1071)	1:139:A:ARG:H	1:141:A:VAL:HB	14	0.21
(1,1071)	1:139:A:ARG:H	1:141:A:VAL:HB	19	0.21
(1,1071)	1:139:A:ARG:H	1:141:A:VAL:HB	20	0.21
(1,1049)	1:137:C:LEU:HG	1:138:C:THR:H	1	0.21
(1,1049)	1:137:C:LEU:HG	1:138:C:THR:H	2	0.21
(1,1049)	1:137:C:LEU:HG	1:138:C:THR:H	9	0.21
(1,1049)	1:137:C:LEU:HG	1:138:C:THR:H	11	0.21
(1,1049)	1:137:C:LEU:HG	1:138:C:THR:H	12	0.21
(1,1049)	1:137:C:LEU:HG	1:138:C:THR:H	14	0.21
(1,1049)	1:137:C:LEU:HG	1:138:C:THR:H	19	0.21
(1,1048)	1:137:B:LEU:HG	1:138:B:THR:H	9	0.21
(1,1047)	1:137:A:LEU:HG	1:138:A:THR:H	11	0.21
(1,1047)	1:137:A:LEU:HG	1:138:A:THR:H	12	0.21
(1,1047)	1:137:A:LEU:HG	1:138:A:THR:H	14	0.21
(1,965)	1:110:A:LEU:HD11	1:125:A:LYS:HB3	7	0.21
(1,965)	1:110:A:LEU:HD12	1:125:A:LYS:HB3	7	0.21
(1,965)	1:110:A:LEU:HD13	1:125:A:LYS:HB3	7	0.21
(1,965)	1:110:A:LEU:HD11	1:125:A:LYS:HB3	16	0.21
(1,965)	1:110:A:LEU:HD12	1:125:A:LYS:HB3	16	0.21
(1,965)	1:110:A:LEU:HD13	1:125:A:LYS:HB3	16	0.21
(1,958)	1:187:A:THR:HA	1:188:A:LEU:HD11	4	0.21
(1,958)	1:187:A:THR:HA	1:188:A:LEU:HD12	4	0.21
(1,958)	1:187:A:THR:HA	1:188:A:LEU:HD13	4	0.21
(1,892)	1:165:B:GLU:HB2	1:167:B:ARG:HG2	20	0.21
(1,892)	1:165:B:GLU:HB2	1:167:B:ARG:HG3	20	0.21
(1,891)	1:165:A:GLU:HB2	1:167:A:ARG:HG2	20	0.21
(1,891)	1:165:A:GLU:HB2	1:167:A:ARG:HG3	20	0.21
(1,889)	1:152:B:ALA:HA	1:157:B:PRO:HG2	18	0.21
(1,889)	1:152:B:ALA:HA	1:157:B:PRO:HG3	18	0.21
(1,888)	1:152:A:ALA:HA	1:157:A:PRO:HG2	12	0.21
(1,888)	1:152:A:ALA:HA	1:157:A:PRO:HG3	12	0.21
(1,812)	1:176:C:GLY:H	1:177:C:ASP:HB3	3	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,811)	1:176:B:GLY:H	1:177:B:ASP:HB3	3	0.21
(1,755)	1:189:C:CYS:H	1:192:C:VAL:HG11	2	0.21
(1,755)	1:189:C:CYS:H	1:192:C:VAL:HG12	2	0.21
(1,755)	1:189:C:CYS:H	1:192:C:VAL:HG13	2	0.21
(1,755)	1:189:C:CYS:H	1:192:C:VAL:HG11	10	0.21
(1,755)	1:189:C:CYS:H	1:192:C:VAL:HG12	10	0.21
(1,755)	1:189:C:CYS:H	1:192:C:VAL:HG13	10	0.21
(1,755)	1:189:C:CYS:H	1:192:C:VAL:HG11	15	0.21
(1,755)	1:189:C:CYS:H	1:192:C:VAL:HG12	15	0.21
(1,755)	1:189:C:CYS:H	1:192:C:VAL:HG13	15	0.21
(1,754)	1:189:B:CYS:H	1:192:B:VAL:HG11	2	0.21
(1,754)	1:189:B:CYS:H	1:192:B:VAL:HG12	2	0.21
(1,754)	1:189:B:CYS:H	1:192:B:VAL:HG13	2	0.21
(1,754)	1:189:B:CYS:H	1:192:B:VAL:HG11	7	0.21
(1,754)	1:189:B:CYS:H	1:192:B:VAL:HG12	7	0.21
(1,754)	1:189:B:CYS:H	1:192:B:VAL:HG13	7	0.21
(1,754)	1:189:B:CYS:H	1:192:B:VAL:HG11	15	0.21
(1,754)	1:189:B:CYS:H	1:192:B:VAL:HG12	15	0.21
(1,754)	1:189:B:CYS:H	1:192:B:VAL:HG13	15	0.21
(1,749)	1:123:A:ILE:HG21	1:179:A:ALA:HB1	3	0.21
(1,749)	1:123:A:ILE:HG21	1:179:A:ALA:HB2	3	0.21
(1,749)	1:123:A:ILE:HG21	1:179:A:ALA:HB3	3	0.21
(1,749)	1:123:A:ILE:HG22	1:179:A:ALA:HB1	3	0.21
(1,749)	1:123:A:ILE:HG22	1:179:A:ALA:HB2	3	0.21
(1,749)	1:123:A:ILE:HG22	1:179:A:ALA:HB3	3	0.21
(1,749)	1:123:A:ILE:HG23	1:179:A:ALA:HB1	3	0.21
(1,749)	1:123:A:ILE:HG23	1:179:A:ALA:HB2	3	0.21
(1,749)	1:123:A:ILE:HG23	1:179:A:ALA:HB3	3	0.21
(1,749)	1:123:A:ILE:HG21	1:179:A:ALA:HB1	19	0.21
(1,749)	1:123:A:ILE:HG21	1:179:A:ALA:HB2	19	0.21
(1,749)	1:123:A:ILE:HG21	1:179:A:ALA:HB3	19	0.21
(1,749)	1:123:A:ILE:HG22	1:179:A:ALA:HB1	19	0.21
(1,749)	1:123:A:ILE:HG22	1:179:A:ALA:HB2	19	0.21
(1,749)	1:123:A:ILE:HG22	1:179:A:ALA:HB3	19	0.21
(1,749)	1:123:A:ILE:HG23	1:179:A:ALA:HB1	19	0.21
(1,749)	1:123:A:ILE:HG23	1:179:A:ALA:HB2	19	0.21
(1,749)	1:123:A:ILE:HG23	1:179:A:ALA:HB3	19	0.21
(1,712)	1:141:A:VAL:HG21	1:144:A:PHE:HD1	13	0.21
(1,712)	1:141:A:VAL:HG21	1:144:A:PHE:HD2	13	0.21
(1,712)	1:141:A:VAL:HG22	1:144:A:PHE:HD1	13	0.21
(1,712)	1:141:A:VAL:HG22	1:144:A:PHE:HD2	13	0.21
(1,712)	1:141:A:VAL:HG23	1:144:A:PHE:HD1	13	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,712)	1:141:A:VAL:HG23	1:144:A:PHE:HD2	13	0.21
(1,637)	1:96:C:ILE:HG21	1:100:C:GLY:H	9	0.21
(1,637)	1:96:C:ILE:HG22	1:100:C:GLY:H	9	0.21
(1,637)	1:96:C:ILE:HG23	1:100:C:GLY:H	9	0.21
(1,490)	1:88:C:LEU:H	1:89:C:VAL:HA	8	0.21
(1,489)	1:88:B:LEU:H	1:89:B:VAL:HA	8	0.21
(1,488)	1:88:A:LEU:H	1:89:A:VAL:HA	8	0.21
(1,451)	1:95:A:SER:HB2	1:101:A:LEU:HD21	9	0.21
(1,451)	1:95:A:SER:HB2	1:101:A:LEU:HD22	9	0.21
(1,451)	1:95:A:SER:HB2	1:101:A:LEU:HD23	9	0.21
(1,451)	1:95:A:SER:HB3	1:101:A:LEU:HD21	9	0.21
(1,451)	1:95:A:SER:HB3	1:101:A:LEU:HD22	9	0.21
(1,451)	1:95:A:SER:HB3	1:101:A:LEU:HD23	9	0.21
(1,435)	1:183:A:MET:HE1	1:186:A:SER:HA	5	0.21
(1,435)	1:183:A:MET:HE2	1:186:A:SER:HA	5	0.21
(1,435)	1:183:A:MET:HE3	1:186:A:SER:HA	5	0.21
(1,435)	1:183:A:MET:HE1	1:186:A:SER:HA	13	0.21
(1,435)	1:183:A:MET:HE2	1:186:A:SER:HA	13	0.21
(1,435)	1:183:A:MET:HE3	1:186:A:SER:HA	13	0.21
(1,435)	1:183:A:MET:HE1	1:186:A:SER:HA	20	0.21
(1,435)	1:183:A:MET:HE2	1:186:A:SER:HA	20	0.21
(1,435)	1:183:A:MET:HE3	1:186:A:SER:HA	20	0.21
(1,395)	1:109:A:LEU:HG	1:111:A:ILE:HD11	5	0.21
(1,395)	1:109:A:LEU:HG	1:111:A:ILE:HD12	5	0.21
(1,395)	1:109:A:LEU:HG	1:111:A:ILE:HD13	5	0.21
(1,364)	1:126:A:ILE:HG21	1:131:A:ILE:HD11	8	0.21
(1,364)	1:126:A:ILE:HG21	1:131:A:ILE:HD12	8	0.21
(1,364)	1:126:A:ILE:HG21	1:131:A:ILE:HD13	8	0.21
(1,364)	1:126:A:ILE:HG22	1:131:A:ILE:HD11	8	0.21
(1,364)	1:126:A:ILE:HG22	1:131:A:ILE:HD12	8	0.21
(1,364)	1:126:A:ILE:HG22	1:131:A:ILE:HD13	8	0.21
(1,364)	1:126:A:ILE:HG23	1:131:A:ILE:HD11	8	0.21
(1,364)	1:126:A:ILE:HG23	1:131:A:ILE:HD12	8	0.21
(1,364)	1:126:A:ILE:HG23	1:131:A:ILE:HD13	8	0.21
(1,249)	1:118:A:GLY:HA2	1:119:A:THR:HG21	3	0.21
(1,249)	1:118:A:GLY:HA2	1:119:A:THR:HG22	3	0.21
(1,249)	1:118:A:GLY:HA2	1:119:A:THR:HG23	3	0.21
(1,228)	1:96:C:ILE:HD11	1:102:C:VAL:HG11	16	0.21
(1,228)	1:96:C:ILE:HD11	1:102:C:VAL:HG12	16	0.21
(1,228)	1:96:C:ILE:HD11	1:102:C:VAL:HG13	16	0.21
(1,228)	1:96:C:ILE:HD12	1:102:C:VAL:HG11	16	0.21
(1,228)	1:96:C:ILE:HD12	1:102:C:VAL:HG12	16	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,228)	1:96:C:ILE:HD12	1:102:C:VAL:HG13	16	0.21
(1,228)	1:96:C:ILE:HD13	1:102:C:VAL:HG11	16	0.21
(1,228)	1:96:C:ILE:HD13	1:102:C:VAL:HG12	16	0.21
(1,228)	1:96:C:ILE:HD13	1:102:C:VAL:HG13	16	0.21
(1,227)	1:96:B:ILE:HD11	1:102:B:VAL:HG11	16	0.21
(1,227)	1:96:B:ILE:HD11	1:102:B:VAL:HG12	16	0.21
(1,227)	1:96:B:ILE:HD11	1:102:B:VAL:HG13	16	0.21
(1,227)	1:96:B:ILE:HD12	1:102:B:VAL:HG11	16	0.21
(1,227)	1:96:B:ILE:HD12	1:102:B:VAL:HG12	16	0.21
(1,227)	1:96:B:ILE:HD12	1:102:B:VAL:HG13	16	0.21
(1,227)	1:96:B:ILE:HD13	1:102:B:VAL:HG11	16	0.21
(1,227)	1:96:B:ILE:HD13	1:102:B:VAL:HG12	16	0.21
(1,227)	1:96:B:ILE:HD13	1:102:B:VAL:HG13	16	0.21
(1,226)	1:96:A:ILE:HD11	1:102:A:VAL:HG11	10	0.21
(1,226)	1:96:A:ILE:HD11	1:102:A:VAL:HG12	10	0.21
(1,226)	1:96:A:ILE:HD11	1:102:A:VAL:HG13	10	0.21
(1,226)	1:96:A:ILE:HD12	1:102:A:VAL:HG11	10	0.21
(1,226)	1:96:A:ILE:HD12	1:102:A:VAL:HG12	10	0.21
(1,226)	1:96:A:ILE:HD12	1:102:A:VAL:HG13	10	0.21
(1,226)	1:96:A:ILE:HD13	1:102:A:VAL:HG11	10	0.21
(1,226)	1:96:A:ILE:HD13	1:102:A:VAL:HG12	10	0.21
(1,226)	1:96:A:ILE:HD13	1:102:A:VAL:HG13	10	0.21
(1,226)	1:96:A:ILE:HD11	1:102:A:VAL:HG11	16	0.21
(1,226)	1:96:A:ILE:HD11	1:102:A:VAL:HG12	16	0.21
(1,226)	1:96:A:ILE:HD11	1:102:A:VAL:HG13	16	0.21
(1,226)	1:96:A:ILE:HD12	1:102:A:VAL:HG11	16	0.21
(1,226)	1:96:A:ILE:HD12	1:102:A:VAL:HG12	16	0.21
(1,226)	1:96:A:ILE:HD12	1:102:A:VAL:HG13	16	0.21
(1,226)	1:96:A:ILE:HD13	1:102:A:VAL:HG11	16	0.21
(1,226)	1:96:A:ILE:HD13	1:102:A:VAL:HG12	16	0.21
(1,226)	1:96:A:ILE:HD13	1:102:A:VAL:HG13	16	0.21
(1,175)	1:179:A:ALA:HB1	1:181:A:LEU:HD21	20	0.21
(1,175)	1:179:A:ALA:HB1	1:181:A:LEU:HD22	20	0.21
(1,175)	1:179:A:ALA:HB1	1:181:A:LEU:HD23	20	0.21
(1,175)	1:179:A:ALA:HB2	1:181:A:LEU:HD21	20	0.21
(1,175)	1:179:A:ALA:HB2	1:181:A:LEU:HD22	20	0.21
(1,175)	1:179:A:ALA:HB2	1:181:A:LEU:HD23	20	0.21
(1,175)	1:179:A:ALA:HB3	1:181:A:LEU:HD21	20	0.21
(1,175)	1:179:A:ALA:HB3	1:181:A:LEU:HD22	20	0.21
(1,175)	1:179:A:ALA:HB3	1:181:A:LEU:HD23	20	0.21
(1,56)	1:156:A:VAL:HG11	1:157:A:PRO:HD3	4	0.21
(1,56)	1:156:A:VAL:HG12	1:157:A:PRO:HD3	4	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,56)	1:156:A:VAL:HG13	1:157:A:PRO:HD3	4	0.21
(1,1)	1:108:A:GLN:HA	1:109:A:LEU:HD21	1	0.21
(1,1)	1:108:A:GLN:HA	1:109:A:LEU:HD22	1	0.21
(1,1)	1:108:A:GLN:HA	1:109:A:LEU:HD23	1	0.21
(1,1)	1:108:A:GLN:HA	1:109:A:LEU:HD21	16	0.21
(1,1)	1:108:A:GLN:HA	1:109:A:LEU:HD22	16	0.21
(1,1)	1:108:A:GLN:HA	1:109:A:LEU:HD23	16	0.21
(1,2298)	1:156:C:VAL:HB	1:157:C:PRO:HD2	1	0.2
(1,2298)	1:156:C:VAL:HB	1:157:C:PRO:HD3	1	0.2
(1,2298)	1:156:C:VAL:HB	1:157:C:PRO:HD2	6	0.2
(1,2298)	1:156:C:VAL:HB	1:157:C:PRO:HD3	6	0.2
(1,2295)	1:155:C:ALA:HB1	1:157:C:PRO:HD2	17	0.2
(1,2295)	1:155:C:ALA:HB1	1:157:C:PRO:HD3	17	0.2
(1,2295)	1:155:C:ALA:HB2	1:157:C:PRO:HD2	17	0.2
(1,2295)	1:155:C:ALA:HB2	1:157:C:PRO:HD3	17	0.2
(1,2295)	1:155:C:ALA:HB3	1:157:C:PRO:HD2	17	0.2
(1,2295)	1:155:C:ALA:HB3	1:157:C:PRO:HD3	17	0.2
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG11	3	0.2
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG12	3	0.2
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG13	3	0.2
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG21	3	0.2
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG22	3	0.2
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG23	3	0.2
(1,2072)	1:156:B:VAL:HB	1:157:B:PRO:HD2	1	0.2
(1,2072)	1:156:B:VAL:HB	1:157:B:PRO:HD3	1	0.2
(1,2072)	1:156:B:VAL:HB	1:157:B:PRO:HD2	6	0.2
(1,2072)	1:156:B:VAL:HB	1:157:B:PRO:HD3	6	0.2
(1,2069)	1:155:B:ALA:HB1	1:157:B:PRO:HD2	17	0.2
(1,2069)	1:155:B:ALA:HB1	1:157:B:PRO:HD3	17	0.2
(1,2069)	1:155:B:ALA:HB2	1:157:B:PRO:HD2	17	0.2
(1,2069)	1:155:B:ALA:HB2	1:157:B:PRO:HD3	17	0.2
(1,2069)	1:155:B:ALA:HB3	1:157:B:PRO:HD2	17	0.2
(1,2069)	1:155:B:ALA:HB3	1:157:B:PRO:HD3	17	0.2
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG11	3	0.2
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG12	3	0.2
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG13	3	0.2
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG21	3	0.2
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG22	3	0.2
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG23	3	0.2
(1,1889)	1:156:A:VAL:HG11	1:157:A:PRO:HD2	1	0.2
(1,1889)	1:156:A:VAL:HG11	1:157:A:PRO:HD3	1	0.2
(1,1889)	1:156:A:VAL:HG12	1:157:A:PRO:HD2	1	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1889)	1:156:A:VAL:HG12	1:157:A:PRO:HD3	1	0.2
(1,1889)	1:156:A:VAL:HG13	1:157:A:PRO:HD2	1	0.2
(1,1889)	1:156:A:VAL:HG13	1:157:A:PRO:HD3	1	0.2
(1,1889)	1:156:A:VAL:HG11	1:157:A:PRO:HD2	2	0.2
(1,1889)	1:156:A:VAL:HG11	1:157:A:PRO:HD3	2	0.2
(1,1889)	1:156:A:VAL:HG12	1:157:A:PRO:HD2	2	0.2
(1,1889)	1:156:A:VAL:HG12	1:157:A:PRO:HD3	2	0.2
(1,1889)	1:156:A:VAL:HG13	1:157:A:PRO:HD2	2	0.2
(1,1889)	1:156:A:VAL:HG13	1:157:A:PRO:HD3	2	0.2
(1,1889)	1:156:A:VAL:HG11	1:157:A:PRO:HD2	3	0.2
(1,1889)	1:156:A:VAL:HG11	1:157:A:PRO:HD3	3	0.2
(1,1889)	1:156:A:VAL:HG12	1:157:A:PRO:HD2	3	0.2
(1,1889)	1:156:A:VAL:HG12	1:157:A:PRO:HD3	3	0.2
(1,1889)	1:156:A:VAL:HG13	1:157:A:PRO:HD2	3	0.2
(1,1889)	1:156:A:VAL:HG13	1:157:A:PRO:HD3	3	0.2
(1,1889)	1:156:A:VAL:HG11	1:157:A:PRO:HD2	6	0.2
(1,1889)	1:156:A:VAL:HG11	1:157:A:PRO:HD3	6	0.2
(1,1889)	1:156:A:VAL:HG12	1:157:A:PRO:HD2	6	0.2
(1,1889)	1:156:A:VAL:HG12	1:157:A:PRO:HD3	6	0.2
(1,1889)	1:156:A:VAL:HG13	1:157:A:PRO:HD2	6	0.2
(1,1889)	1:156:A:VAL:HG13	1:157:A:PRO:HD3	6	0.2
(1,1889)	1:156:A:VAL:HG11	1:157:A:PRO:HD2	8	0.2
(1,1889)	1:156:A:VAL:HG11	1:157:A:PRO:HD3	8	0.2
(1,1889)	1:156:A:VAL:HG12	1:157:A:PRO:HD2	8	0.2
(1,1889)	1:156:A:VAL:HG12	1:157:A:PRO:HD3	8	0.2
(1,1889)	1:156:A:VAL:HG13	1:157:A:PRO:HD2	8	0.2
(1,1889)	1:156:A:VAL:HG13	1:157:A:PRO:HD3	8	0.2
(1,1889)	1:156:A:VAL:HG11	1:157:A:PRO:HD2	9	0.2
(1,1889)	1:156:A:VAL:HG11	1:157:A:PRO:HD3	9	0.2
(1,1889)	1:156:A:VAL:HG12	1:157:A:PRO:HD2	9	0.2
(1,1889)	1:156:A:VAL:HG12	1:157:A:PRO:HD3	9	0.2
(1,1889)	1:156:A:VAL:HG13	1:157:A:PRO:HD2	9	0.2
(1,1889)	1:156:A:VAL:HG13	1:157:A:PRO:HD3	9	0.2
(1,1889)	1:156:A:VAL:HG11	1:157:A:PRO:HD2	14	0.2
(1,1889)	1:156:A:VAL:HG11	1:157:A:PRO:HD3	14	0.2
(1,1889)	1:156:A:VAL:HG12	1:157:A:PRO:HD2	14	0.2
(1,1889)	1:156:A:VAL:HG12	1:157:A:PRO:HD3	14	0.2
(1,1889)	1:156:A:VAL:HG13	1:157:A:PRO:HD2	14	0.2
(1,1889)	1:156:A:VAL:HG13	1:157:A:PRO:HD3	14	0.2
(1,1889)	1:156:A:VAL:HG11	1:157:A:PRO:HD2	15	0.2
(1,1889)	1:156:A:VAL:HG11	1:157:A:PRO:HD3	15	0.2
(1,1889)	1:156:A:VAL:HG12	1:157:A:PRO:HD2	15	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1889)	1:156:A:VAL:HG12	1:157:A:PRO:HD3	15	0.2
(1,1889)	1:156:A:VAL:HG13	1:157:A:PRO:HD2	15	0.2
(1,1889)	1:156:A:VAL:HG13	1:157:A:PRO:HD3	15	0.2
(1,1842)	1:121:A:CYS:HB2	1:189:A:CYS:H	3	0.2
(1,1842)	1:121:A:CYS:HB3	1:189:A:CYS:H	3	0.2
(1,1842)	1:121:A:CYS:HB2	1:189:A:CYS:H	12	0.2
(1,1842)	1:121:A:CYS:HB3	1:189:A:CYS:H	12	0.2
(1,1835)	1:109:A:LEU:HB2	1:110:A:LEU:HD11	18	0.2
(1,1835)	1:109:A:LEU:HB2	1:110:A:LEU:HD12	18	0.2
(1,1835)	1:109:A:LEU:HB2	1:110:A:LEU:HD13	18	0.2
(1,1835)	1:109:A:LEU:HB3	1:110:A:LEU:HD11	18	0.2
(1,1835)	1:109:A:LEU:HB3	1:110:A:LEU:HD12	18	0.2
(1,1835)	1:109:A:LEU:HB3	1:110:A:LEU:HD13	18	0.2
(1,1830)	1:102:A:VAL:HG11	1:111:A:ILE:HG12	12	0.2
(1,1830)	1:102:A:VAL:HG11	1:111:A:ILE:HG13	12	0.2
(1,1830)	1:102:A:VAL:HG12	1:111:A:ILE:HG12	12	0.2
(1,1830)	1:102:A:VAL:HG12	1:111:A:ILE:HG13	12	0.2
(1,1830)	1:102:A:VAL:HG13	1:111:A:ILE:HG12	12	0.2
(1,1830)	1:102:A:VAL:HG13	1:111:A:ILE:HG13	12	0.2
(1,1818)	1:95:B:SER:HB2	1:101:B:LEU:H	19	0.2
(1,1818)	1:95:B:SER:HB3	1:101:B:LEU:H	19	0.2
(1,1768)	1:178:A:PRO:HD3	1:179:A:ALA:H	11	0.2
(1,1737)	1:194:A:LEU:HD21	1:195:A:TYR:H	7	0.2
(1,1737)	1:194:A:LEU:HD22	1:195:A:TYR:H	7	0.2
(1,1737)	1:194:A:LEU:HD23	1:195:A:TYR:H	7	0.2
(1,1687)	1:90:B:THR:H	1:91:B:THR:HB	9	0.2
(1,1686)	1:90:A:THR:H	1:91:A:THR:HB	9	0.2
(1,1614)	1:116:A:ALA:H	1:119:A:THR:HB	20	0.2
(1,1610)	1:118:A:GLY:H	1:192:A:VAL:HG21	2	0.2
(1,1610)	1:118:A:GLY:H	1:192:A:VAL:HG22	2	0.2
(1,1610)	1:118:A:GLY:H	1:192:A:VAL:HG23	2	0.2
(1,1610)	1:118:A:GLY:H	1:192:A:VAL:HG21	7	0.2
(1,1610)	1:118:A:GLY:H	1:192:A:VAL:HG22	7	0.2
(1,1610)	1:118:A:GLY:H	1:192:A:VAL:HG23	7	0.2
(1,1533)	1:122:A:TYR:H	1:189:A:CYS:HB2	4	0.2
(1,1533)	1:122:A:TYR:H	1:189:A:CYS:HB3	4	0.2
(1,1533)	1:122:A:TYR:H	1:189:A:CYS:HB2	9	0.2
(1,1533)	1:122:A:TYR:H	1:189:A:CYS:HB3	9	0.2
(1,1533)	1:122:A:TYR:H	1:189:A:CYS:HB2	17	0.2
(1,1533)	1:122:A:TYR:H	1:189:A:CYS:HB3	17	0.2
(1,1527)	1:91:A:THR:HG21	1:106:A:TYR:H	17	0.2
(1,1527)	1:91:A:THR:HG22	1:106:A:TYR:H	17	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1527)	1:91:A:THR:HG23	1:106:A:TYR:H	17	0.2
(1,1522)	1:178:C:PRO:HG2	1:179:C:ALA:H	11	0.2
(1,1522)	1:178:C:PRO:HG3	1:179:C:ALA:H	11	0.2
(1,1521)	1:178:B:PRO:HG2	1:179:B:ALA:H	11	0.2
(1,1521)	1:178:B:PRO:HG3	1:179:B:ALA:H	11	0.2
(1,1432)	1:111:C:ILE:H	1:123:C:ILE:HG21	4	0.2
(1,1432)	1:111:C:ILE:H	1:123:C:ILE:HG22	4	0.2
(1,1432)	1:111:C:ILE:H	1:123:C:ILE:HG23	4	0.2
(1,1408)	1:152:A:ALA:HB1	1:153:A:LYS:H	1	0.2
(1,1408)	1:152:A:ALA:HB2	1:153:A:LYS:H	1	0.2
(1,1408)	1:152:A:ALA:HB3	1:153:A:LYS:H	1	0.2
(1,1408)	1:152:A:ALA:HB1	1:153:A:LYS:H	8	0.2
(1,1408)	1:152:A:ALA:HB2	1:153:A:LYS:H	8	0.2
(1,1408)	1:152:A:ALA:HB3	1:153:A:LYS:H	8	0.2
(1,1276)	1:109:A:LEU:H	1:109:A:LEU:HG	19	0.2
(1,1248)	1:121:C:CYS:H	1:189:C:CYS:HB2	8	0.2
(1,1248)	1:121:C:CYS:H	1:189:C:CYS:HB3	8	0.2
(1,1246)	1:121:A:CYS:H	1:189:A:CYS:HB2	8	0.2
(1,1246)	1:121:A:CYS:H	1:189:A:CYS:HB3	8	0.2
(1,1201)	1:196:A:TYR:H	1:196:A:TYR:HE1	4	0.2
(1,1201)	1:196:A:TYR:H	1:196:A:TYR:HE2	4	0.2
(1,1201)	1:196:A:TYR:H	1:196:A:TYR:HE1	10	0.2
(1,1201)	1:196:A:TYR:H	1:196:A:TYR:HE2	10	0.2
(1,1161)	1:94:A:PHE:H	1:101:A:LEU:HD11	3	0.2
(1,1161)	1:94:A:PHE:H	1:101:A:LEU:HD12	3	0.2
(1,1161)	1:94:A:PHE:H	1:101:A:LEU:HD13	3	0.2
(1,1157)	1:167:C:ARG:HA	1:168:C:ASP:H	1	0.2
(1,1157)	1:167:C:ARG:HA	1:168:C:ASP:H	3	0.2
(1,1157)	1:167:C:ARG:HA	1:168:C:ASP:H	5	0.2
(1,1157)	1:167:C:ARG:HA	1:168:C:ASP:H	7	0.2
(1,1157)	1:167:C:ARG:HA	1:168:C:ASP:H	8	0.2
(1,1157)	1:167:C:ARG:HA	1:168:C:ASP:H	10	0.2
(1,1157)	1:167:C:ARG:HA	1:168:C:ASP:H	11	0.2
(1,1157)	1:167:C:ARG:HA	1:168:C:ASP:H	16	0.2
(1,1157)	1:167:C:ARG:HA	1:168:C:ASP:H	17	0.2
(1,1156)	1:167:B:ARG:HA	1:168:B:ASP:H	1	0.2
(1,1156)	1:167:B:ARG:HA	1:168:B:ASP:H	2	0.2
(1,1156)	1:167:B:ARG:HA	1:168:B:ASP:H	3	0.2
(1,1156)	1:167:B:ARG:HA	1:168:B:ASP:H	7	0.2
(1,1156)	1:167:B:ARG:HA	1:168:B:ASP:H	8	0.2
(1,1156)	1:167:B:ARG:HA	1:168:B:ASP:H	10	0.2
(1,1156)	1:167:B:ARG:HA	1:168:B:ASP:H	11	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1156)	1:167:B:ARG:HA	1:168:B:ASP:H	15	0.2
(1,1156)	1:167:B:ARG:HA	1:168:B:ASP:H	16	0.2
(1,1156)	1:167:B:ARG:HA	1:168:B:ASP:H	18	0.2
(1,1155)	1:167:A:ARG:HA	1:168:A:ASP:H	1	0.2
(1,1155)	1:167:A:ARG:HA	1:168:A:ASP:H	2	0.2
(1,1155)	1:167:A:ARG:HA	1:168:A:ASP:H	3	0.2
(1,1155)	1:167:A:ARG:HA	1:168:A:ASP:H	4	0.2
(1,1155)	1:167:A:ARG:HA	1:168:A:ASP:H	5	0.2
(1,1155)	1:167:A:ARG:HA	1:168:A:ASP:H	8	0.2
(1,1155)	1:167:A:ARG:HA	1:168:A:ASP:H	9	0.2
(1,1155)	1:167:A:ARG:HA	1:168:A:ASP:H	10	0.2
(1,1155)	1:167:A:ARG:HA	1:168:A:ASP:H	11	0.2
(1,1155)	1:167:A:ARG:HA	1:168:A:ASP:H	16	0.2
(1,1155)	1:167:A:ARG:HA	1:168:A:ASP:H	17	0.2
(1,1155)	1:167:A:ARG:HA	1:168:A:ASP:H	18	0.2
(1,1100)	1:167:C:ARG:H	1:167:C:ARG:HB2	20	0.2
(1,1099)	1:167:B:ARG:H	1:167:B:ARG:HB2	20	0.2
(1,1097)	1:157:C:PRO:HA	1:158:C:THR:H	5	0.2
(1,1097)	1:157:C:PRO:HA	1:158:C:THR:H	9	0.2
(1,1096)	1:157:B:PRO:HA	1:158:B:THR:H	5	0.2
(1,1096)	1:157:B:PRO:HA	1:158:B:THR:H	9	0.2
(1,1095)	1:157:A:PRO:HA	1:158:A:THR:H	9	0.2
(1,1073)	1:139:C:ARG:H	1:141:C:VAL:HB	4	0.2
(1,1072)	1:139:B:ARG:H	1:141:B:VAL:HB	3	0.2
(1,1072)	1:139:B:ARG:H	1:141:B:VAL:HB	4	0.2
(1,1072)	1:139:B:ARG:H	1:141:B:VAL:HB	14	0.2
(1,1049)	1:137:C:LEU:HG	1:138:C:THR:H	3	0.2
(1,1049)	1:137:C:LEU:HG	1:138:C:THR:H	5	0.2
(1,1049)	1:137:C:LEU:HG	1:138:C:THR:H	7	0.2
(1,1049)	1:137:C:LEU:HG	1:138:C:THR:H	10	0.2
(1,1049)	1:137:C:LEU:HG	1:138:C:THR:H	13	0.2
(1,1049)	1:137:C:LEU:HG	1:138:C:THR:H	15	0.2
(1,1049)	1:137:C:LEU:HG	1:138:C:THR:H	16	0.2
(1,1049)	1:137:C:LEU:HG	1:138:C:THR:H	17	0.2
(1,1049)	1:137:C:LEU:HG	1:138:C:THR:H	18	0.2
(1,1049)	1:137:C:LEU:HG	1:138:C:THR:H	20	0.2
(1,1048)	1:137:B:LEU:HG	1:138:B:THR:H	2	0.2
(1,1048)	1:137:B:LEU:HG	1:138:B:THR:H	7	0.2
(1,1048)	1:137:B:LEU:HG	1:138:B:THR:H	11	0.2
(1,1048)	1:137:B:LEU:HG	1:138:B:THR:H	12	0.2
(1,1048)	1:137:B:LEU:HG	1:138:B:THR:H	14	0.2
(1,1048)	1:137:B:LEU:HG	1:138:B:THR:H	16	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1048)	1:137:B:LEU:HG	1:138:B:THR:H	17	0.2
(1,1048)	1:137:B:LEU:HG	1:138:B:THR:H	18	0.2
(1,1047)	1:137:A:LEU:HG	1:138:A:THR:H	1	0.2
(1,1047)	1:137:A:LEU:HG	1:138:A:THR:H	2	0.2
(1,1047)	1:137:A:LEU:HG	1:138:A:THR:H	3	0.2
(1,1047)	1:137:A:LEU:HG	1:138:A:THR:H	13	0.2
(1,965)	1:110:A:LEU:HD11	1:125:A:LYS:HB3	15	0.2
(1,965)	1:110:A:LEU:HD12	1:125:A:LYS:HB3	15	0.2
(1,965)	1:110:A:LEU:HD13	1:125:A:LYS:HB3	15	0.2
(1,928)	1:178:A:PRO:HG2	1:181:A:LEU:HD21	15	0.2
(1,928)	1:178:A:PRO:HG2	1:181:A:LEU:HD22	15	0.2
(1,928)	1:178:A:PRO:HG2	1:181:A:LEU:HD23	15	0.2
(1,928)	1:178:A:PRO:HG3	1:181:A:LEU:HD21	15	0.2
(1,928)	1:178:A:PRO:HG3	1:181:A:LEU:HD22	15	0.2
(1,928)	1:178:A:PRO:HG3	1:181:A:LEU:HD23	15	0.2
(1,893)	1:165:C:GLU:HB2	1:167:C:ARG:HG2	20	0.2
(1,893)	1:165:C:GLU:HB2	1:167:C:ARG:HG3	20	0.2
(1,890)	1:152:C:ALA:HA	1:157:C:PRO:HG2	18	0.2
(1,890)	1:152:C:ALA:HA	1:157:C:PRO:HG3	18	0.2
(1,888)	1:152:A:ALA:HA	1:157:A:PRO:HG2	7	0.2
(1,888)	1:152:A:ALA:HA	1:157:A:PRO:HG3	7	0.2
(1,888)	1:152:A:ALA:HA	1:157:A:PRO:HG2	10	0.2
(1,888)	1:152:A:ALA:HA	1:157:A:PRO:HG3	10	0.2
(1,888)	1:152:A:ALA:HA	1:157:A:PRO:HG2	13	0.2
(1,888)	1:152:A:ALA:HA	1:157:A:PRO:HG3	13	0.2
(1,866)	1:153:C:LYS:HA	1:154:C:PRO:HD2	17	0.2
(1,865)	1:153:B:LYS:HA	1:154:B:PRO:HD2	17	0.2
(1,864)	1:153:A:LYS:HA	1:154:A:PRO:HD2	17	0.2
(1,783)	1:167:A:ARG:HD2	1:169:A:ALA:HB1	20	0.2
(1,783)	1:167:A:ARG:HD2	1:169:A:ALA:HB2	20	0.2
(1,783)	1:167:A:ARG:HD2	1:169:A:ALA:HB3	20	0.2
(1,783)	1:167:A:ARG:HD3	1:169:A:ALA:HB1	20	0.2
(1,783)	1:167:A:ARG:HD3	1:169:A:ALA:HB2	20	0.2
(1,783)	1:167:A:ARG:HD3	1:169:A:ALA:HB3	20	0.2
(1,755)	1:189:C:CYS:H	1:192:C:VAL:HG11	3	0.2
(1,755)	1:189:C:CYS:H	1:192:C:VAL:HG12	3	0.2
(1,755)	1:189:C:CYS:H	1:192:C:VAL:HG13	3	0.2
(1,755)	1:189:C:CYS:H	1:192:C:VAL:HG11	8	0.2
(1,755)	1:189:C:CYS:H	1:192:C:VAL:HG12	8	0.2
(1,755)	1:189:C:CYS:H	1:192:C:VAL:HG13	8	0.2
(1,754)	1:189:B:CYS:H	1:192:B:VAL:HG11	8	0.2
(1,754)	1:189:B:CYS:H	1:192:B:VAL:HG12	8	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,754)	1:189:B:CYS:H	1:192:B:VAL:HG13	8	0.2
(1,753)	1:189:A:CYS:H	1:192:A:VAL:HG11	13	0.2
(1,753)	1:189:A:CYS:H	1:192:A:VAL:HG12	13	0.2
(1,753)	1:189:A:CYS:H	1:192:A:VAL:HG13	13	0.2
(1,749)	1:123:A:ILE:HG21	1:179:A:ALA:HB1	10	0.2
(1,749)	1:123:A:ILE:HG21	1:179:A:ALA:HB2	10	0.2
(1,749)	1:123:A:ILE:HG21	1:179:A:ALA:HB3	10	0.2
(1,749)	1:123:A:ILE:HG22	1:179:A:ALA:HB1	10	0.2
(1,749)	1:123:A:ILE:HG22	1:179:A:ALA:HB2	10	0.2
(1,749)	1:123:A:ILE:HG22	1:179:A:ALA:HB3	10	0.2
(1,749)	1:123:A:ILE:HG23	1:179:A:ALA:HB1	10	0.2
(1,749)	1:123:A:ILE:HG23	1:179:A:ALA:HB2	10	0.2
(1,749)	1:123:A:ILE:HG23	1:179:A:ALA:HB3	10	0.2
(1,637)	1:96:C:ILE:HG21	1:100:C:GLY:H	7	0.2
(1,637)	1:96:C:ILE:HG22	1:100:C:GLY:H	7	0.2
(1,637)	1:96:C:ILE:HG23	1:100:C:GLY:H	7	0.2
(1,637)	1:96:C:ILE:HG21	1:100:C:GLY:H	17	0.2
(1,637)	1:96:C:ILE:HG22	1:100:C:GLY:H	17	0.2
(1,637)	1:96:C:ILE:HG23	1:100:C:GLY:H	17	0.2
(1,636)	1:96:B:ILE:HG21	1:100:B:GLY:H	7	0.2
(1,636)	1:96:B:ILE:HG22	1:100:B:GLY:H	7	0.2
(1,636)	1:96:B:ILE:HG23	1:100:B:GLY:H	7	0.2
(1,636)	1:96:B:ILE:HG21	1:100:B:GLY:H	17	0.2
(1,636)	1:96:B:ILE:HG22	1:100:B:GLY:H	17	0.2
(1,636)	1:96:B:ILE:HG23	1:100:B:GLY:H	17	0.2
(1,625)	1:96:C:ILE:HG21	1:138:C:THR:HB	8	0.2
(1,625)	1:96:C:ILE:HG22	1:138:C:THR:HB	8	0.2
(1,625)	1:96:C:ILE:HG23	1:138:C:THR:HB	8	0.2
(1,437)	1:183:C:MET:HE1	1:186:C:SER:HA	2	0.2
(1,437)	1:183:C:MET:HE2	1:186:C:SER:HA	2	0.2
(1,437)	1:183:C:MET:HE3	1:186:C:SER:HA	2	0.2
(1,437)	1:183:C:MET:HE1	1:186:C:SER:HA	9	0.2
(1,437)	1:183:C:MET:HE2	1:186:C:SER:HA	9	0.2
(1,437)	1:183:C:MET:HE3	1:186:C:SER:HA	9	0.2
(1,436)	1:183:B:MET:HE1	1:186:B:SER:HA	9	0.2
(1,436)	1:183:B:MET:HE2	1:186:B:SER:HA	9	0.2
(1,436)	1:183:B:MET:HE3	1:186:B:SER:HA	9	0.2
(1,435)	1:183:A:MET:HE1	1:186:A:SER:HA	3	0.2
(1,435)	1:183:A:MET:HE2	1:186:A:SER:HA	3	0.2
(1,435)	1:183:A:MET:HE3	1:186:A:SER:HA	3	0.2
(1,435)	1:183:A:MET:HE1	1:186:A:SER:HA	15	0.2
(1,435)	1:183:A:MET:HE2	1:186:A:SER:HA	15	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,435)	1:183:A:MET:HE3	1:186:A:SER:HA	15	0.2
(1,435)	1:183:A:MET:HE1	1:186:A:SER:HA	19	0.2
(1,435)	1:183:A:MET:HE2	1:186:A:SER:HA	19	0.2
(1,435)	1:183:A:MET:HE3	1:186:A:SER:HA	19	0.2
(1,395)	1:109:A:LEU:HG	1:111:A:ILE:HD11	9	0.2
(1,395)	1:109:A:LEU:HG	1:111:A:ILE:HD12	9	0.2
(1,395)	1:109:A:LEU:HG	1:111:A:ILE:HD13	9	0.2
(1,371)	1:96:A:ILE:HD11	1:102:A:VAL:HB	13	0.2
(1,371)	1:96:A:ILE:HD12	1:102:A:VAL:HB	13	0.2
(1,371)	1:96:A:ILE:HD13	1:102:A:VAL:HB	13	0.2
(1,365)	1:126:B:ILE:HG21	1:131:B:ILE:HD11	17	0.2
(1,365)	1:126:B:ILE:HG21	1:131:B:ILE:HD12	17	0.2
(1,365)	1:126:B:ILE:HG21	1:131:B:ILE:HD13	17	0.2
(1,365)	1:126:B:ILE:HG22	1:131:B:ILE:HD11	17	0.2
(1,365)	1:126:B:ILE:HG22	1:131:B:ILE:HD12	17	0.2
(1,365)	1:126:B:ILE:HG22	1:131:B:ILE:HD13	17	0.2
(1,365)	1:126:B:ILE:HG23	1:131:B:ILE:HD11	17	0.2
(1,365)	1:126:B:ILE:HG23	1:131:B:ILE:HD12	17	0.2
(1,365)	1:126:B:ILE:HG23	1:131:B:ILE:HD13	17	0.2
(1,228)	1:96:C:ILE:HD11	1:102:C:VAL:HG11	10	0.2
(1,228)	1:96:C:ILE:HD11	1:102:C:VAL:HG12	10	0.2
(1,228)	1:96:C:ILE:HD11	1:102:C:VAL:HG13	10	0.2
(1,228)	1:96:C:ILE:HD12	1:102:C:VAL:HG11	10	0.2
(1,228)	1:96:C:ILE:HD12	1:102:C:VAL:HG12	10	0.2
(1,228)	1:96:C:ILE:HD12	1:102:C:VAL:HG13	10	0.2
(1,228)	1:96:C:ILE:HD13	1:102:C:VAL:HG11	10	0.2
(1,228)	1:96:C:ILE:HD13	1:102:C:VAL:HG12	10	0.2
(1,228)	1:96:C:ILE:HD13	1:102:C:VAL:HG13	10	0.2
(1,227)	1:96:B:ILE:HD11	1:102:B:VAL:HG11	10	0.2
(1,227)	1:96:B:ILE:HD11	1:102:B:VAL:HG12	10	0.2
(1,227)	1:96:B:ILE:HD11	1:102:B:VAL:HG13	10	0.2
(1,227)	1:96:B:ILE:HD12	1:102:B:VAL:HG11	10	0.2
(1,227)	1:96:B:ILE:HD12	1:102:B:VAL:HG12	10	0.2
(1,227)	1:96:B:ILE:HD12	1:102:B:VAL:HG13	10	0.2
(1,227)	1:96:B:ILE:HD13	1:102:B:VAL:HG11	10	0.2
(1,227)	1:96:B:ILE:HD13	1:102:B:VAL:HG12	10	0.2
(1,227)	1:96:B:ILE:HD13	1:102:B:VAL:HG13	10	0.2
(1,219)	1:96:A:ILE:HG21	1:141:A:VAL:HG11	19	0.2
(1,219)	1:96:A:ILE:HG21	1:141:A:VAL:HG12	19	0.2
(1,219)	1:96:A:ILE:HG21	1:141:A:VAL:HG13	19	0.2
(1,219)	1:96:A:ILE:HG22	1:141:A:VAL:HG11	19	0.2
(1,219)	1:96:A:ILE:HG22	1:141:A:VAL:HG12	19	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,219)	1:96:A:ILE:HG22	1:141:A:VAL:HG13	19	0.2
(1,219)	1:96:A:ILE:HG23	1:141:A:VAL:HG11	19	0.2
(1,219)	1:96:A:ILE:HG23	1:141:A:VAL:HG12	19	0.2
(1,219)	1:96:A:ILE:HG23	1:141:A:VAL:HG13	19	0.2
(1,219)	1:96:A:ILE:HG21	1:141:A:VAL:HG11	20	0.2
(1,219)	1:96:A:ILE:HG21	1:141:A:VAL:HG12	20	0.2
(1,219)	1:96:A:ILE:HG21	1:141:A:VAL:HG13	20	0.2
(1,219)	1:96:A:ILE:HG22	1:141:A:VAL:HG11	20	0.2
(1,219)	1:96:A:ILE:HG22	1:141:A:VAL:HG12	20	0.2
(1,219)	1:96:A:ILE:HG22	1:141:A:VAL:HG13	20	0.2
(1,219)	1:96:A:ILE:HG23	1:141:A:VAL:HG11	20	0.2
(1,219)	1:96:A:ILE:HG23	1:141:A:VAL:HG12	20	0.2
(1,219)	1:96:A:ILE:HG23	1:141:A:VAL:HG13	20	0.2
(1,182)	1:137:A:LEU:HD11	1:141:A:VAL:HG11	3	0.2
(1,182)	1:137:A:LEU:HD11	1:141:A:VAL:HG12	3	0.2
(1,182)	1:137:A:LEU:HD11	1:141:A:VAL:HG13	3	0.2
(1,182)	1:137:A:LEU:HD12	1:141:A:VAL:HG11	3	0.2
(1,182)	1:137:A:LEU:HD12	1:141:A:VAL:HG12	3	0.2
(1,182)	1:137:A:LEU:HD12	1:141:A:VAL:HG13	3	0.2
(1,182)	1:137:A:LEU:HD13	1:141:A:VAL:HG11	3	0.2
(1,182)	1:137:A:LEU:HD13	1:141:A:VAL:HG12	3	0.2
(1,182)	1:137:A:LEU:HD13	1:141:A:VAL:HG13	3	0.2
(1,182)	1:137:A:LEU:HD11	1:141:A:VAL:HG11	12	0.2
(1,182)	1:137:A:LEU:HD11	1:141:A:VAL:HG12	12	0.2
(1,182)	1:137:A:LEU:HD11	1:141:A:VAL:HG13	12	0.2
(1,182)	1:137:A:LEU:HD12	1:141:A:VAL:HG11	12	0.2
(1,182)	1:137:A:LEU:HD12	1:141:A:VAL:HG12	12	0.2
(1,182)	1:137:A:LEU:HD12	1:141:A:VAL:HG13	12	0.2
(1,182)	1:137:A:LEU:HD13	1:141:A:VAL:HG11	12	0.2
(1,182)	1:137:A:LEU:HD13	1:141:A:VAL:HG12	12	0.2
(1,182)	1:137:A:LEU:HD13	1:141:A:VAL:HG13	12	0.2
(1,182)	1:137:A:LEU:HD11	1:141:A:VAL:HG11	17	0.2
(1,182)	1:137:A:LEU:HD11	1:141:A:VAL:HG12	17	0.2
(1,182)	1:137:A:LEU:HD11	1:141:A:VAL:HG13	17	0.2
(1,182)	1:137:A:LEU:HD12	1:141:A:VAL:HG11	17	0.2
(1,182)	1:137:A:LEU:HD12	1:141:A:VAL:HG12	17	0.2
(1,182)	1:137:A:LEU:HD12	1:141:A:VAL:HG13	17	0.2
(1,182)	1:137:A:LEU:HD13	1:141:A:VAL:HG11	17	0.2
(1,182)	1:137:A:LEU:HD13	1:141:A:VAL:HG12	17	0.2
(1,182)	1:137:A:LEU:HD13	1:141:A:VAL:HG13	17	0.2
(1,134)	1:110:A:LEU:HD11	1:111:A:ILE:HD11	8	0.2
(1,134)	1:110:A:LEU:HD11	1:111:A:ILE:HD12	8	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,134)	1:110:A:LEU:HD11	1:111:A:ILE:HD13	8	0.2
(1,134)	1:110:A:LEU:HD12	1:111:A:ILE:HD11	8	0.2
(1,134)	1:110:A:LEU:HD12	1:111:A:ILE:HD12	8	0.2
(1,134)	1:110:A:LEU:HD12	1:111:A:ILE:HD13	8	0.2
(1,134)	1:110:A:LEU:HD13	1:111:A:ILE:HD11	8	0.2
(1,134)	1:110:A:LEU:HD13	1:111:A:ILE:HD12	8	0.2
(1,134)	1:110:A:LEU:HD13	1:111:A:ILE:HD13	8	0.2
(1,124)	1:96:A:ILE:H	1:101:A:LEU:HD21	11	0.2
(1,124)	1:96:A:ILE:H	1:101:A:LEU:HD22	11	0.2
(1,124)	1:96:A:ILE:H	1:101:A:LEU:HD23	11	0.2
(1,124)	1:96:A:ILE:H	1:101:A:LEU:HD21	13	0.2
(1,124)	1:96:A:ILE:H	1:101:A:LEU:HD22	13	0.2
(1,124)	1:96:A:ILE:H	1:101:A:LEU:HD23	13	0.2
(1,56)	1:156:A:VAL:HG11	1:157:A:PRO:HD3	2	0.2
(1,56)	1:156:A:VAL:HG12	1:157:A:PRO:HD3	2	0.2
(1,56)	1:156:A:VAL:HG13	1:157:A:PRO:HD3	2	0.2
(1,56)	1:156:A:VAL:HG11	1:157:A:PRO:HD3	6	0.2
(1,56)	1:156:A:VAL:HG12	1:157:A:PRO:HD3	6	0.2
(1,56)	1:156:A:VAL:HG13	1:157:A:PRO:HD3	6	0.2
(1,56)	1:156:A:VAL:HG11	1:157:A:PRO:HD3	8	0.2
(1,56)	1:156:A:VAL:HG12	1:157:A:PRO:HD3	8	0.2
(1,56)	1:156:A:VAL:HG13	1:157:A:PRO:HD3	8	0.2
(1,56)	1:156:A:VAL:HG11	1:157:A:PRO:HD3	15	0.2
(1,56)	1:156:A:VAL:HG12	1:157:A:PRO:HD3	15	0.2
(1,56)	1:156:A:VAL:HG13	1:157:A:PRO:HD3	15	0.2
(1,1)	1:108:A:GLN:HA	1:109:A:LEU:HD21	3	0.2
(1,1)	1:108:A:GLN:HA	1:109:A:LEU:HD22	3	0.2
(1,1)	1:108:A:GLN:HA	1:109:A:LEU:HD23	3	0.2
(1,1)	1:108:A:GLN:HA	1:109:A:LEU:HD21	18	0.2
(1,1)	1:108:A:GLN:HA	1:109:A:LEU:HD22	18	0.2
(1,1)	1:108:A:GLN:HA	1:109:A:LEU:HD23	18	0.2
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD11	5	0.19
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD12	5	0.19
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD13	5	0.19
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD21	5	0.19
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD22	5	0.19
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD23	5	0.19
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD11	16	0.19
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD12	16	0.19
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD13	16	0.19
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD21	16	0.19
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD22	16	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD23	16	0.19
(1,2329)	1:178:C:PRO:HB2	1:179:C:ALA:H	4	0.19
(1,2329)	1:178:C:PRO:HB3	1:179:C:ALA:H	4	0.19
(1,2320)	1:172:C:ALA:HA	1:178:C:PRO:HD2	5	0.19
(1,2320)	1:172:C:ALA:HA	1:178:C:PRO:HD3	5	0.19
(1,2320)	1:172:C:ALA:HA	1:178:C:PRO:HD2	6	0.19
(1,2320)	1:172:C:ALA:HA	1:178:C:PRO:HD3	6	0.19
(1,2320)	1:172:C:ALA:HA	1:178:C:PRO:HD2	18	0.19
(1,2320)	1:172:C:ALA:HA	1:178:C:PRO:HD3	18	0.19
(1,2298)	1:156:C:VAL:HB	1:157:C:PRO:HD2	2	0.19
(1,2298)	1:156:C:VAL:HB	1:157:C:PRO:HD3	2	0.19
(1,2298)	1:156:C:VAL:HB	1:157:C:PRO:HD2	3	0.19
(1,2298)	1:156:C:VAL:HB	1:157:C:PRO:HD3	3	0.19
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD11	5	0.19
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD12	5	0.19
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD13	5	0.19
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD21	5	0.19
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD22	5	0.19
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD23	5	0.19
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD11	16	0.19
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD12	16	0.19
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD13	16	0.19
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD21	16	0.19
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD22	16	0.19
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD23	16	0.19
(1,2103)	1:178:B:PRO:HB2	1:179:B:ALA:H	4	0.19
(1,2103)	1:178:B:PRO:HB3	1:179:B:ALA:H	4	0.19
(1,2094)	1:172:B:ALA:HA	1:178:B:PRO:HD2	5	0.19
(1,2094)	1:172:B:ALA:HA	1:178:B:PRO:HD3	5	0.19
(1,2094)	1:172:B:ALA:HA	1:178:B:PRO:HD2	6	0.19
(1,2094)	1:172:B:ALA:HA	1:178:B:PRO:HD3	6	0.19
(1,2094)	1:172:B:ALA:HA	1:178:B:PRO:HD2	14	0.19
(1,2094)	1:172:B:ALA:HA	1:178:B:PRO:HD3	14	0.19
(1,2094)	1:172:B:ALA:HA	1:178:B:PRO:HD2	18	0.19
(1,2094)	1:172:B:ALA:HA	1:178:B:PRO:HD3	18	0.19
(1,2072)	1:156:B:VAL:HB	1:157:B:PRO:HD2	3	0.19
(1,2072)	1:156:B:VAL:HB	1:157:B:PRO:HD3	3	0.19
(1,1935)	1:89:B:VAL:HG11	1:183:B:MET:HE1	8	0.19
(1,1935)	1:89:B:VAL:HG11	1:183:B:MET:HE2	8	0.19
(1,1935)	1:89:B:VAL:HG11	1:183:B:MET:HE3	8	0.19
(1,1935)	1:89:B:VAL:HG12	1:183:B:MET:HE1	8	0.19
(1,1935)	1:89:B:VAL:HG12	1:183:B:MET:HE2	8	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1935)	1:89:B:VAL:HG12	1:183:B:MET:HE3	8	0.19
(1,1935)	1:89:B:VAL:HG13	1:183:B:MET:HE1	8	0.19
(1,1935)	1:89:B:VAL:HG13	1:183:B:MET:HE2	8	0.19
(1,1935)	1:89:B:VAL:HG13	1:183:B:MET:HE3	8	0.19
(1,1935)	1:89:B:VAL:HG21	1:183:B:MET:HE1	8	0.19
(1,1935)	1:89:B:VAL:HG21	1:183:B:MET:HE2	8	0.19
(1,1935)	1:89:B:VAL:HG21	1:183:B:MET:HE3	8	0.19
(1,1935)	1:89:B:VAL:HG22	1:183:B:MET:HE1	8	0.19
(1,1935)	1:89:B:VAL:HG22	1:183:B:MET:HE2	8	0.19
(1,1935)	1:89:B:VAL:HG22	1:183:B:MET:HE3	8	0.19
(1,1935)	1:89:B:VAL:HG23	1:183:B:MET:HE1	8	0.19
(1,1935)	1:89:B:VAL:HG23	1:183:B:MET:HE2	8	0.19
(1,1935)	1:89:B:VAL:HG23	1:183:B:MET:HE3	8	0.19
(1,1889)	1:156:A:VAL:HG11	1:157:A:PRO:HD2	10	0.19
(1,1889)	1:156:A:VAL:HG11	1:157:A:PRO:HD3	10	0.19
(1,1889)	1:156:A:VAL:HG12	1:157:A:PRO:HD2	10	0.19
(1,1889)	1:156:A:VAL:HG12	1:157:A:PRO:HD3	10	0.19
(1,1889)	1:156:A:VAL:HG13	1:157:A:PRO:HD2	10	0.19
(1,1889)	1:156:A:VAL:HG13	1:157:A:PRO:HD3	10	0.19
(1,1888)	1:156:A:VAL:HG11	1:157:A:PRO:HB2	11	0.19
(1,1888)	1:156:A:VAL:HG11	1:157:A:PRO:HB3	11	0.19
(1,1888)	1:156:A:VAL:HG12	1:157:A:PRO:HB2	11	0.19
(1,1888)	1:156:A:VAL:HG12	1:157:A:PRO:HB3	11	0.19
(1,1888)	1:156:A:VAL:HG13	1:157:A:PRO:HB2	11	0.19
(1,1888)	1:156:A:VAL:HG13	1:157:A:PRO:HB3	11	0.19
(1,1885)	1:155:A:ALA:HB1	1:157:A:PRO:HD2	13	0.19
(1,1885)	1:155:A:ALA:HB1	1:157:A:PRO:HD3	13	0.19
(1,1885)	1:155:A:ALA:HB2	1:157:A:PRO:HD2	13	0.19
(1,1885)	1:155:A:ALA:HB2	1:157:A:PRO:HD3	13	0.19
(1,1885)	1:155:A:ALA:HB3	1:157:A:PRO:HD2	13	0.19
(1,1885)	1:155:A:ALA:HB3	1:157:A:PRO:HD3	13	0.19
(1,1878)	1:151:A:GLN:HB2	1:152:A:ALA:HA	4	0.19
(1,1878)	1:151:A:GLN:HB3	1:152:A:ALA:HA	4	0.19
(1,1842)	1:121:A:CYS:HB2	1:189:A:CYS:H	5	0.19
(1,1842)	1:121:A:CYS:HB3	1:189:A:CYS:H	5	0.19
(1,1819)	1:95:C:SER:HB2	1:101:C:LEU:H	11	0.19
(1,1819)	1:95:C:SER:HB3	1:101:C:LEU:H	11	0.19
(1,1819)	1:95:C:SER:HB2	1:101:C:LEU:H	13	0.19
(1,1819)	1:95:C:SER:HB3	1:101:C:LEU:H	13	0.19
(1,1768)	1:178:A:PRO:HD3	1:179:A:ALA:H	12	0.19
(1,1692)	1:120:A:CYS:H	1:192:A:VAL:HG11	6	0.19
(1,1692)	1:120:A:CYS:H	1:192:A:VAL:HG12	6	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1692)	1:120:A:CYS:H	1:192:A:VAL:HG13	6	0.19
(1,1688)	1:90:C:THR:H	1:91:C:THR:HB	9	0.19
(1,1688)	1:90:C:THR:H	1:91:C:THR:HB	13	0.19
(1,1686)	1:90:A:THR:H	1:91:A:THR:HB	13	0.19
(1,1676)	1:94:A:PHE:H	1:102:A:VAL:HG11	18	0.19
(1,1676)	1:94:A:PHE:H	1:102:A:VAL:HG12	18	0.19
(1,1676)	1:94:A:PHE:H	1:102:A:VAL:HG13	18	0.19
(1,1614)	1:116:A:ALA:H	1:119:A:THR:HB	2	0.19
(1,1614)	1:116:A:ALA:H	1:119:A:THR:HB	12	0.19
(1,1614)	1:116:A:ALA:H	1:119:A:THR:HB	14	0.19
(1,1614)	1:116:A:ALA:H	1:119:A:THR:HB	17	0.19
(1,1602)	1:89:A:VAL:HG21	1:91:A:THR:H	14	0.19
(1,1602)	1:89:A:VAL:HG22	1:91:A:THR:H	14	0.19
(1,1602)	1:89:A:VAL:HG23	1:91:A:THR:H	14	0.19
(1,1555)	1:156:A:VAL:HG11	1:167:A:ARG:H	16	0.19
(1,1555)	1:156:A:VAL:HG12	1:167:A:ARG:H	16	0.19
(1,1555)	1:156:A:VAL:HG13	1:167:A:ARG:H	16	0.19
(1,1533)	1:122:A:TYR:H	1:189:A:CYS:HB2	7	0.19
(1,1533)	1:122:A:TYR:H	1:189:A:CYS:HB3	7	0.19
(1,1533)	1:122:A:TYR:H	1:189:A:CYS:HB2	8	0.19
(1,1533)	1:122:A:TYR:H	1:189:A:CYS:HB3	8	0.19
(1,1533)	1:122:A:TYR:H	1:189:A:CYS:HB2	10	0.19
(1,1533)	1:122:A:TYR:H	1:189:A:CYS:HB3	10	0.19
(1,1533)	1:122:A:TYR:H	1:189:A:CYS:HB2	15	0.19
(1,1533)	1:122:A:TYR:H	1:189:A:CYS:HB3	15	0.19
(1,1511)	1:137:A:LEU:H	1:137:A:LEU:HG	8	0.19
(1,1462)	1:180:B:PHE:H	1:181:B:LEU:HA	6	0.19
(1,1461)	1:180:A:PHE:H	1:181:A:LEU:HA	12	0.19
(1,1432)	1:111:C:ILE:H	1:123:C:ILE:HG21	13	0.19
(1,1432)	1:111:C:ILE:H	1:123:C:ILE:HG22	13	0.19
(1,1432)	1:111:C:ILE:H	1:123:C:ILE:HG23	13	0.19
(1,1431)	1:111:B:ILE:H	1:123:B:ILE:HG21	4	0.19
(1,1431)	1:111:B:ILE:H	1:123:B:ILE:HG22	4	0.19
(1,1431)	1:111:B:ILE:H	1:123:B:ILE:HG23	4	0.19
(1,1431)	1:111:B:ILE:H	1:123:B:ILE:HG21	13	0.19
(1,1431)	1:111:B:ILE:H	1:123:B:ILE:HG22	13	0.19
(1,1431)	1:111:B:ILE:H	1:123:B:ILE:HG23	13	0.19
(1,1410)	1:152:C:ALA:HB1	1:153:C:LYS:H	8	0.19
(1,1410)	1:152:C:ALA:HB2	1:153:C:LYS:H	8	0.19
(1,1410)	1:152:C:ALA:HB3	1:153:C:LYS:H	8	0.19
(1,1410)	1:152:C:ALA:HB1	1:153:C:LYS:H	11	0.19
(1,1410)	1:152:C:ALA:HB2	1:153:C:LYS:H	11	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1410)	1:152:C:ALA:HB3	1:153:C:LYS:H	11	0.19
(1,1409)	1:152:B:ALA:HB1	1:153:B:LYS:H	8	0.19
(1,1409)	1:152:B:ALA:HB2	1:153:B:LYS:H	8	0.19
(1,1409)	1:152:B:ALA:HB3	1:153:B:LYS:H	8	0.19
(1,1409)	1:152:B:ALA:HB1	1:153:B:LYS:H	11	0.19
(1,1409)	1:152:B:ALA:HB2	1:153:B:LYS:H	11	0.19
(1,1409)	1:152:B:ALA:HB3	1:153:B:LYS:H	11	0.19
(1,1157)	1:167:C:ARG:HA	1:168:C:ASP:H	2	0.19
(1,1157)	1:167:C:ARG:HA	1:168:C:ASP:H	4	0.19
(1,1157)	1:167:C:ARG:HA	1:168:C:ASP:H	6	0.19
(1,1157)	1:167:C:ARG:HA	1:168:C:ASP:H	9	0.19
(1,1157)	1:167:C:ARG:HA	1:168:C:ASP:H	12	0.19
(1,1157)	1:167:C:ARG:HA	1:168:C:ASP:H	13	0.19
(1,1157)	1:167:C:ARG:HA	1:168:C:ASP:H	15	0.19
(1,1157)	1:167:C:ARG:HA	1:168:C:ASP:H	18	0.19
(1,1157)	1:167:C:ARG:HA	1:168:C:ASP:H	19	0.19
(1,1157)	1:167:C:ARG:HA	1:168:C:ASP:H	20	0.19
(1,1156)	1:167:B:ARG:HA	1:168:B:ASP:H	4	0.19
(1,1156)	1:167:B:ARG:HA	1:168:B:ASP:H	5	0.19
(1,1156)	1:167:B:ARG:HA	1:168:B:ASP:H	6	0.19
(1,1156)	1:167:B:ARG:HA	1:168:B:ASP:H	9	0.19
(1,1156)	1:167:B:ARG:HA	1:168:B:ASP:H	12	0.19
(1,1156)	1:167:B:ARG:HA	1:168:B:ASP:H	13	0.19
(1,1156)	1:167:B:ARG:HA	1:168:B:ASP:H	17	0.19
(1,1156)	1:167:B:ARG:HA	1:168:B:ASP:H	19	0.19
(1,1156)	1:167:B:ARG:HA	1:168:B:ASP:H	20	0.19
(1,1155)	1:167:A:ARG:HA	1:168:A:ASP:H	6	0.19
(1,1155)	1:167:A:ARG:HA	1:168:A:ASP:H	7	0.19
(1,1155)	1:167:A:ARG:HA	1:168:A:ASP:H	12	0.19
(1,1155)	1:167:A:ARG:HA	1:168:A:ASP:H	13	0.19
(1,1155)	1:167:A:ARG:HA	1:168:A:ASP:H	15	0.19
(1,1155)	1:167:A:ARG:HA	1:168:A:ASP:H	19	0.19
(1,1155)	1:167:A:ARG:HA	1:168:A:ASP:H	20	0.19
(1,1098)	1:167:A:ARG:H	1:167:A:ARG:HB2	20	0.19
(1,1097)	1:157:C:PRO:HA	1:158:C:THR:H	1	0.19
(1,1096)	1:157:B:PRO:HA	1:158:B:THR:H	1	0.19
(1,1095)	1:157:A:PRO:HA	1:158:A:THR:H	5	0.19
(1,1073)	1:139:C:ARG:H	1:141:C:VAL:HB	2	0.19
(1,1073)	1:139:C:ARG:H	1:141:C:VAL:HB	6	0.19
(1,1072)	1:139:B:ARG:H	1:141:B:VAL:HB	2	0.19
(1,1072)	1:139:B:ARG:H	1:141:B:VAL:HB	6	0.19
(1,1072)	1:139:B:ARG:H	1:141:B:VAL:HB	7	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1071)	1:139:A:ARG:H	1:141:A:VAL:HB	9	0.19
(1,1071)	1:139:A:ARG:H	1:141:A:VAL:HB	16	0.19
(1,1049)	1:137:C:LEU:HG	1:138:C:THR:H	6	0.19
(1,1048)	1:137:B:LEU:HG	1:138:B:THR:H	1	0.19
(1,1048)	1:137:B:LEU:HG	1:138:B:THR:H	3	0.19
(1,1048)	1:137:B:LEU:HG	1:138:B:THR:H	5	0.19
(1,1048)	1:137:B:LEU:HG	1:138:B:THR:H	10	0.19
(1,1048)	1:137:B:LEU:HG	1:138:B:THR:H	13	0.19
(1,1048)	1:137:B:LEU:HG	1:138:B:THR:H	19	0.19
(1,1047)	1:137:A:LEU:HG	1:138:A:THR:H	5	0.19
(1,1047)	1:137:A:LEU:HG	1:138:A:THR:H	18	0.19
(1,958)	1:187:A:THR:HA	1:188:A:LEU:HD11	20	0.19
(1,958)	1:187:A:THR:HA	1:188:A:LEU:HD12	20	0.19
(1,958)	1:187:A:THR:HA	1:188:A:LEU:HD13	20	0.19
(1,928)	1:178:A:PRO:HG2	1:181:A:LEU:HD21	8	0.19
(1,928)	1:178:A:PRO:HG2	1:181:A:LEU:HD22	8	0.19
(1,928)	1:178:A:PRO:HG2	1:181:A:LEU:HD23	8	0.19
(1,928)	1:178:A:PRO:HG3	1:181:A:LEU:HD21	8	0.19
(1,928)	1:178:A:PRO:HG3	1:181:A:LEU:HD22	8	0.19
(1,928)	1:178:A:PRO:HG3	1:181:A:LEU:HD23	8	0.19
(1,928)	1:178:A:PRO:HG2	1:181:A:LEU:HD21	11	0.19
(1,928)	1:178:A:PRO:HG2	1:181:A:LEU:HD22	11	0.19
(1,928)	1:178:A:PRO:HG2	1:181:A:LEU:HD23	11	0.19
(1,928)	1:178:A:PRO:HG3	1:181:A:LEU:HD21	11	0.19
(1,928)	1:178:A:PRO:HG3	1:181:A:LEU:HD22	11	0.19
(1,928)	1:178:A:PRO:HG3	1:181:A:LEU:HD23	11	0.19
(1,928)	1:178:A:PRO:HG2	1:181:A:LEU:HD21	13	0.19
(1,928)	1:178:A:PRO:HG2	1:181:A:LEU:HD22	13	0.19
(1,928)	1:178:A:PRO:HG2	1:181:A:LEU:HD23	13	0.19
(1,928)	1:178:A:PRO:HG3	1:181:A:LEU:HD21	13	0.19
(1,928)	1:178:A:PRO:HG3	1:181:A:LEU:HD22	13	0.19
(1,928)	1:178:A:PRO:HG3	1:181:A:LEU:HD23	13	0.19
(1,893)	1:165:C:GLU:HB2	1:167:C:ARG:HG2	13	0.19
(1,893)	1:165:C:GLU:HB2	1:167:C:ARG:HG3	13	0.19
(1,891)	1:165:A:GLU:HB2	1:167:A:ARG:HG2	13	0.19
(1,891)	1:165:A:GLU:HB2	1:167:A:ARG:HG3	13	0.19
(1,890)	1:152:C:ALA:HA	1:157:C:PRO:HG2	8	0.19
(1,890)	1:152:C:ALA:HA	1:157:C:PRO:HG3	8	0.19
(1,888)	1:152:A:ALA:HA	1:157:A:PRO:HG2	18	0.19
(1,888)	1:152:A:ALA:HA	1:157:A:PRO:HG3	18	0.19
(1,866)	1:153:C:LYS:HA	1:154:C:PRO:HD2	5	0.19
(1,866)	1:153:C:LYS:HA	1:154:C:PRO:HD2	15	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,866)	1:153:C:LYS:HA	1:154:C:PRO:HD2	19	0.19
(1,866)	1:153:C:LYS:HA	1:154:C:PRO:HD2	20	0.19
(1,865)	1:153:B:LYS:HA	1:154:B:PRO:HD2	5	0.19
(1,865)	1:153:B:LYS:HA	1:154:B:PRO:HD2	15	0.19
(1,865)	1:153:B:LYS:HA	1:154:B:PRO:HD2	19	0.19
(1,865)	1:153:B:LYS:HA	1:154:B:PRO:HD2	20	0.19
(1,864)	1:153:A:LYS:HA	1:154:A:PRO:HD2	5	0.19
(1,864)	1:153:A:LYS:HA	1:154:A:PRO:HD2	15	0.19
(1,864)	1:153:A:LYS:HA	1:154:A:PRO:HD2	19	0.19
(1,864)	1:153:A:LYS:HA	1:154:A:PRO:HD2	20	0.19
(1,795)	1:150:A:LEU:HD11	1:153:A:LYS:HE2	3	0.19
(1,795)	1:150:A:LEU:HD11	1:153:A:LYS:HE3	3	0.19
(1,795)	1:150:A:LEU:HD12	1:153:A:LYS:HE2	3	0.19
(1,795)	1:150:A:LEU:HD12	1:153:A:LYS:HE3	3	0.19
(1,795)	1:150:A:LEU:HD13	1:153:A:LYS:HE2	3	0.19
(1,795)	1:150:A:LEU:HD13	1:153:A:LYS:HE3	3	0.19
(1,785)	1:167:C:ARG:HD2	1:169:C:ALA:HB1	14	0.19
(1,785)	1:167:C:ARG:HD2	1:169:C:ALA:HB2	14	0.19
(1,785)	1:167:C:ARG:HD2	1:169:C:ALA:HB3	14	0.19
(1,785)	1:167:C:ARG:HD3	1:169:C:ALA:HB1	14	0.19
(1,785)	1:167:C:ARG:HD3	1:169:C:ALA:HB2	14	0.19
(1,785)	1:167:C:ARG:HD3	1:169:C:ALA:HB3	14	0.19
(1,785)	1:167:C:ARG:HD2	1:169:C:ALA:HB1	20	0.19
(1,785)	1:167:C:ARG:HD2	1:169:C:ALA:HB2	20	0.19
(1,785)	1:167:C:ARG:HD2	1:169:C:ALA:HB3	20	0.19
(1,785)	1:167:C:ARG:HD3	1:169:C:ALA:HB1	20	0.19
(1,785)	1:167:C:ARG:HD3	1:169:C:ALA:HB2	20	0.19
(1,785)	1:167:C:ARG:HD3	1:169:C:ALA:HB3	20	0.19
(1,784)	1:167:B:ARG:HD2	1:169:B:ALA:HB1	14	0.19
(1,784)	1:167:B:ARG:HD2	1:169:B:ALA:HB2	14	0.19
(1,784)	1:167:B:ARG:HD2	1:169:B:ALA:HB3	14	0.19
(1,784)	1:167:B:ARG:HD3	1:169:B:ALA:HB1	14	0.19
(1,784)	1:167:B:ARG:HD3	1:169:B:ALA:HB2	14	0.19
(1,784)	1:167:B:ARG:HD3	1:169:B:ALA:HB3	14	0.19
(1,755)	1:189:C:CYS:H	1:192:C:VAL:HG11	18	0.19
(1,755)	1:189:C:CYS:H	1:192:C:VAL:HG12	18	0.19
(1,755)	1:189:C:CYS:H	1:192:C:VAL:HG13	18	0.19
(1,755)	1:189:C:CYS:H	1:192:C:VAL:HG11	20	0.19
(1,755)	1:189:C:CYS:H	1:192:C:VAL:HG12	20	0.19
(1,755)	1:189:C:CYS:H	1:192:C:VAL:HG13	20	0.19
(1,754)	1:189:B:CYS:H	1:192:B:VAL:HG11	3	0.19
(1,754)	1:189:B:CYS:H	1:192:B:VAL:HG12	3	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,754)	1:189:B:CYS:H	1:192:B:VAL:HG13	3	0.19
(1,754)	1:189:B:CYS:H	1:192:B:VAL:HG11	18	0.19
(1,754)	1:189:B:CYS:H	1:192:B:VAL:HG12	18	0.19
(1,754)	1:189:B:CYS:H	1:192:B:VAL:HG13	18	0.19
(1,749)	1:123:A:ILE:HG21	1:179:A:ALA:HB1	8	0.19
(1,749)	1:123:A:ILE:HG21	1:179:A:ALA:HB2	8	0.19
(1,749)	1:123:A:ILE:HG21	1:179:A:ALA:HB3	8	0.19
(1,749)	1:123:A:ILE:HG22	1:179:A:ALA:HB1	8	0.19
(1,749)	1:123:A:ILE:HG22	1:179:A:ALA:HB2	8	0.19
(1,749)	1:123:A:ILE:HG22	1:179:A:ALA:HB3	8	0.19
(1,749)	1:123:A:ILE:HG23	1:179:A:ALA:HB1	8	0.19
(1,749)	1:123:A:ILE:HG23	1:179:A:ALA:HB2	8	0.19
(1,749)	1:123:A:ILE:HG23	1:179:A:ALA:HB3	8	0.19
(1,749)	1:123:A:ILE:HG21	1:179:A:ALA:HB1	18	0.19
(1,749)	1:123:A:ILE:HG21	1:179:A:ALA:HB2	18	0.19
(1,749)	1:123:A:ILE:HG21	1:179:A:ALA:HB3	18	0.19
(1,749)	1:123:A:ILE:HG22	1:179:A:ALA:HB1	18	0.19
(1,749)	1:123:A:ILE:HG22	1:179:A:ALA:HB2	18	0.19
(1,749)	1:123:A:ILE:HG22	1:179:A:ALA:HB3	18	0.19
(1,749)	1:123:A:ILE:HG23	1:179:A:ALA:HB1	18	0.19
(1,749)	1:123:A:ILE:HG23	1:179:A:ALA:HB2	18	0.19
(1,749)	1:123:A:ILE:HG23	1:179:A:ALA:HB3	18	0.19
(1,659)	1:113:A:TYR:HD1	1:197:A:ILE:HG21	19	0.19
(1,659)	1:113:A:TYR:HD1	1:197:A:ILE:HG22	19	0.19
(1,659)	1:113:A:TYR:HD1	1:197:A:ILE:HG23	19	0.19
(1,659)	1:113:A:TYR:HD2	1:197:A:ILE:HG21	19	0.19
(1,659)	1:113:A:TYR:HD2	1:197:A:ILE:HG22	19	0.19
(1,659)	1:113:A:TYR:HD2	1:197:A:ILE:HG23	19	0.19
(1,636)	1:96:B:ILE:HG21	1:100:B:GLY:H	6	0.19
(1,636)	1:96:B:ILE:HG22	1:100:B:GLY:H	6	0.19
(1,636)	1:96:B:ILE:HG23	1:100:B:GLY:H	6	0.19
(1,635)	1:96:A:ILE:HG21	1:100:A:GLY:H	20	0.19
(1,635)	1:96:A:ILE:HG22	1:100:A:GLY:H	20	0.19
(1,635)	1:96:A:ILE:HG23	1:100:A:GLY:H	20	0.19
(1,573)	1:194:A:LEU:HD21	1:196:A:TYR:HE1	20	0.19
(1,573)	1:194:A:LEU:HD21	1:196:A:TYR:HE2	20	0.19
(1,573)	1:194:A:LEU:HD22	1:196:A:TYR:HE1	20	0.19
(1,573)	1:194:A:LEU:HD22	1:196:A:TYR:HE2	20	0.19
(1,573)	1:194:A:LEU:HD23	1:196:A:TYR:HE1	20	0.19
(1,573)	1:194:A:LEU:HD23	1:196:A:TYR:HE2	20	0.19
(1,539)	1:111:A:ILE:HG21	1:126:A:ILE:HG21	1	0.19
(1,539)	1:111:A:ILE:HG21	1:126:A:ILE:HG22	1	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,539)	1:111:A:ILE:HG21	1:126:A:ILE:HG23	1	0.19
(1,539)	1:111:A:ILE:HG22	1:126:A:ILE:HG21	1	0.19
(1,539)	1:111:A:ILE:HG22	1:126:A:ILE:HG22	1	0.19
(1,539)	1:111:A:ILE:HG22	1:126:A:ILE:HG23	1	0.19
(1,539)	1:111:A:ILE:HG23	1:126:A:ILE:HG21	1	0.19
(1,539)	1:111:A:ILE:HG23	1:126:A:ILE:HG22	1	0.19
(1,539)	1:111:A:ILE:HG23	1:126:A:ILE:HG23	1	0.19
(1,437)	1:183:C:MET:HE1	1:186:C:SER:HA	6	0.19
(1,437)	1:183:C:MET:HE2	1:186:C:SER:HA	6	0.19
(1,437)	1:183:C:MET:HE3	1:186:C:SER:HA	6	0.19
(1,437)	1:183:C:MET:HE1	1:186:C:SER:HA	15	0.19
(1,437)	1:183:C:MET:HE2	1:186:C:SER:HA	15	0.19
(1,437)	1:183:C:MET:HE3	1:186:C:SER:HA	15	0.19
(1,435)	1:183:A:MET:HE1	1:186:A:SER:HA	2	0.19
(1,435)	1:183:A:MET:HE2	1:186:A:SER:HA	2	0.19
(1,435)	1:183:A:MET:HE3	1:186:A:SER:HA	2	0.19
(1,435)	1:183:A:MET:HE1	1:186:A:SER:HA	10	0.19
(1,435)	1:183:A:MET:HE2	1:186:A:SER:HA	10	0.19
(1,435)	1:183:A:MET:HE3	1:186:A:SER:HA	10	0.19
(1,435)	1:183:A:MET:HE1	1:186:A:SER:HA	11	0.19
(1,435)	1:183:A:MET:HE2	1:186:A:SER:HA	11	0.19
(1,435)	1:183:A:MET:HE3	1:186:A:SER:HA	11	0.19
(1,371)	1:96:A:ILE:HD11	1:102:A:VAL:HB	11	0.19
(1,371)	1:96:A:ILE:HD12	1:102:A:VAL:HB	11	0.19
(1,371)	1:96:A:ILE:HD13	1:102:A:VAL:HB	11	0.19
(1,366)	1:126:C:ILE:HG21	1:131:C:ILE:HD11	17	0.19
(1,366)	1:126:C:ILE:HG21	1:131:C:ILE:HD12	17	0.19
(1,366)	1:126:C:ILE:HG21	1:131:C:ILE:HD13	17	0.19
(1,366)	1:126:C:ILE:HG22	1:131:C:ILE:HD11	17	0.19
(1,366)	1:126:C:ILE:HG22	1:131:C:ILE:HD12	17	0.19
(1,366)	1:126:C:ILE:HG22	1:131:C:ILE:HD13	17	0.19
(1,366)	1:126:C:ILE:HG23	1:131:C:ILE:HD11	17	0.19
(1,366)	1:126:C:ILE:HG23	1:131:C:ILE:HD12	17	0.19
(1,366)	1:126:C:ILE:HG23	1:131:C:ILE:HD13	17	0.19
(1,219)	1:96:A:ILE:HG21	1:141:A:VAL:HG11	3	0.19
(1,219)	1:96:A:ILE:HG21	1:141:A:VAL:HG12	3	0.19
(1,219)	1:96:A:ILE:HG21	1:141:A:VAL:HG13	3	0.19
(1,219)	1:96:A:ILE:HG22	1:141:A:VAL:HG11	3	0.19
(1,219)	1:96:A:ILE:HG22	1:141:A:VAL:HG12	3	0.19
(1,219)	1:96:A:ILE:HG22	1:141:A:VAL:HG13	3	0.19
(1,219)	1:96:A:ILE:HG23	1:141:A:VAL:HG11	3	0.19
(1,219)	1:96:A:ILE:HG23	1:141:A:VAL:HG12	3	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,219)	1:96:A:ILE:HG23	1:141:A:VAL:HG13	3	0.19
(1,219)	1:96:A:ILE:HG21	1:141:A:VAL:HG11	15	0.19
(1,219)	1:96:A:ILE:HG21	1:141:A:VAL:HG12	15	0.19
(1,219)	1:96:A:ILE:HG21	1:141:A:VAL:HG13	15	0.19
(1,219)	1:96:A:ILE:HG22	1:141:A:VAL:HG11	15	0.19
(1,219)	1:96:A:ILE:HG22	1:141:A:VAL:HG12	15	0.19
(1,219)	1:96:A:ILE:HG22	1:141:A:VAL:HG13	15	0.19
(1,219)	1:96:A:ILE:HG23	1:141:A:VAL:HG11	15	0.19
(1,219)	1:96:A:ILE:HG23	1:141:A:VAL:HG12	15	0.19
(1,219)	1:96:A:ILE:HG23	1:141:A:VAL:HG13	15	0.19
(1,182)	1:137:A:LEU:HD11	1:141:A:VAL:HG11	11	0.19
(1,182)	1:137:A:LEU:HD11	1:141:A:VAL:HG12	11	0.19
(1,182)	1:137:A:LEU:HD11	1:141:A:VAL:HG13	11	0.19
(1,182)	1:137:A:LEU:HD12	1:141:A:VAL:HG11	11	0.19
(1,182)	1:137:A:LEU:HD12	1:141:A:VAL:HG12	11	0.19
(1,182)	1:137:A:LEU:HD12	1:141:A:VAL:HG13	11	0.19
(1,182)	1:137:A:LEU:HD13	1:141:A:VAL:HG11	11	0.19
(1,182)	1:137:A:LEU:HD13	1:141:A:VAL:HG12	11	0.19
(1,182)	1:137:A:LEU:HD13	1:141:A:VAL:HG13	11	0.19
(1,56)	1:156:A:VAL:HG11	1:157:A:PRO:HD3	3	0.19
(1,56)	1:156:A:VAL:HG12	1:157:A:PRO:HD3	3	0.19
(1,56)	1:156:A:VAL:HG13	1:157:A:PRO:HD3	3	0.19
(1,1)	1:108:A:GLN:HA	1:109:A:LEU:HD21	8	0.19
(1,1)	1:108:A:GLN:HA	1:109:A:LEU:HD22	8	0.19
(1,1)	1:108:A:GLN:HA	1:109:A:LEU:HD23	8	0.19
(1,2320)	1:172:C:ALA:HA	1:178:C:PRO:HD2	7	0.18
(1,2320)	1:172:C:ALA:HA	1:178:C:PRO:HD3	7	0.18
(1,2320)	1:172:C:ALA:HA	1:178:C:PRO:HD2	9	0.18
(1,2320)	1:172:C:ALA:HA	1:178:C:PRO:HD3	9	0.18
(1,2320)	1:172:C:ALA:HA	1:178:C:PRO:HD2	14	0.18
(1,2320)	1:172:C:ALA:HA	1:178:C:PRO:HD3	14	0.18
(1,2298)	1:156:C:VAL:HB	1:157:C:PRO:HD2	5	0.18
(1,2298)	1:156:C:VAL:HB	1:157:C:PRO:HD3	5	0.18
(1,2298)	1:156:C:VAL:HB	1:157:C:PRO:HD2	15	0.18
(1,2298)	1:156:C:VAL:HB	1:157:C:PRO:HD3	15	0.18
(1,2295)	1:155:C:ALA:HB1	1:157:C:PRO:HD2	10	0.18
(1,2295)	1:155:C:ALA:HB1	1:157:C:PRO:HD3	10	0.18
(1,2295)	1:155:C:ALA:HB2	1:157:C:PRO:HD2	10	0.18
(1,2295)	1:155:C:ALA:HB2	1:157:C:PRO:HD3	10	0.18
(1,2295)	1:155:C:ALA:HB3	1:157:C:PRO:HD2	10	0.18
(1,2295)	1:155:C:ALA:HB3	1:157:C:PRO:HD3	10	0.18
(1,2295)	1:155:C:ALA:HB1	1:157:C:PRO:HD2	18	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2295)	1:155:C:ALA:HB1	1:157:C:PRO:HD3	18	0.18
(1,2295)	1:155:C:ALA:HB2	1:157:C:PRO:HD2	18	0.18
(1,2295)	1:155:C:ALA:HB2	1:157:C:PRO:HD3	18	0.18
(1,2295)	1:155:C:ALA:HB3	1:157:C:PRO:HD2	18	0.18
(1,2295)	1:155:C:ALA:HB3	1:157:C:PRO:HD3	18	0.18
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG11	1	0.18
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG12	1	0.18
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG13	1	0.18
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG21	1	0.18
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG22	1	0.18
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG23	1	0.18
(1,2286)	1:151:C:GLN:HB2	1:152:C:ALA:HA	4	0.18
(1,2286)	1:151:C:GLN:HB3	1:152:C:ALA:HA	4	0.18
(1,2112)	1:179:B:ALA:HB1	1:181:B:LEU:HD11	17	0.18
(1,2112)	1:179:B:ALA:HB1	1:181:B:LEU:HD12	17	0.18
(1,2112)	1:179:B:ALA:HB1	1:181:B:LEU:HD13	17	0.18
(1,2112)	1:179:B:ALA:HB1	1:181:B:LEU:HD21	17	0.18
(1,2112)	1:179:B:ALA:HB1	1:181:B:LEU:HD22	17	0.18
(1,2112)	1:179:B:ALA:HB1	1:181:B:LEU:HD23	17	0.18
(1,2112)	1:179:B:ALA:HB2	1:181:B:LEU:HD11	17	0.18
(1,2112)	1:179:B:ALA:HB2	1:181:B:LEU:HD12	17	0.18
(1,2112)	1:179:B:ALA:HB2	1:181:B:LEU:HD13	17	0.18
(1,2112)	1:179:B:ALA:HB2	1:181:B:LEU:HD21	17	0.18
(1,2112)	1:179:B:ALA:HB2	1:181:B:LEU:HD22	17	0.18
(1,2112)	1:179:B:ALA:HB2	1:181:B:LEU:HD23	17	0.18
(1,2112)	1:179:B:ALA:HB3	1:181:B:LEU:HD11	17	0.18
(1,2112)	1:179:B:ALA:HB3	1:181:B:LEU:HD12	17	0.18
(1,2112)	1:179:B:ALA:HB3	1:181:B:LEU:HD13	17	0.18
(1,2112)	1:179:B:ALA:HB3	1:181:B:LEU:HD21	17	0.18
(1,2112)	1:179:B:ALA:HB3	1:181:B:LEU:HD22	17	0.18
(1,2112)	1:179:B:ALA:HB3	1:181:B:LEU:HD23	17	0.18
(1,2094)	1:172:B:ALA:HA	1:178:B:PRO:HD2	7	0.18
(1,2094)	1:172:B:ALA:HA	1:178:B:PRO:HD3	7	0.18
(1,2094)	1:172:B:ALA:HA	1:178:B:PRO:HD2	9	0.18
(1,2094)	1:172:B:ALA:HA	1:178:B:PRO:HD3	9	0.18
(1,2094)	1:172:B:ALA:HA	1:178:B:PRO:HD2	17	0.18
(1,2094)	1:172:B:ALA:HA	1:178:B:PRO:HD3	17	0.18
(1,2072)	1:156:B:VAL:HB	1:157:B:PRO:HD2	2	0.18
(1,2072)	1:156:B:VAL:HB	1:157:B:PRO:HD3	2	0.18
(1,2072)	1:156:B:VAL:HB	1:157:B:PRO:HD2	5	0.18
(1,2072)	1:156:B:VAL:HB	1:157:B:PRO:HD3	5	0.18
(1,2072)	1:156:B:VAL:HB	1:157:B:PRO:HD2	15	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2072)	1:156:B:VAL:HB	1:157:B:PRO:HD3	15	0.18
(1,2069)	1:155:B:ALA:HB1	1:157:B:PRO:HD2	10	0.18
(1,2069)	1:155:B:ALA:HB1	1:157:B:PRO:HD3	10	0.18
(1,2069)	1:155:B:ALA:HB2	1:157:B:PRO:HD2	10	0.18
(1,2069)	1:155:B:ALA:HB2	1:157:B:PRO:HD3	10	0.18
(1,2069)	1:155:B:ALA:HB3	1:157:B:PRO:HD2	10	0.18
(1,2069)	1:155:B:ALA:HB3	1:157:B:PRO:HD3	10	0.18
(1,2069)	1:155:B:ALA:HB1	1:157:B:PRO:HD2	18	0.18
(1,2069)	1:155:B:ALA:HB1	1:157:B:PRO:HD3	18	0.18
(1,2069)	1:155:B:ALA:HB2	1:157:B:PRO:HD2	18	0.18
(1,2069)	1:155:B:ALA:HB2	1:157:B:PRO:HD3	18	0.18
(1,2069)	1:155:B:ALA:HB3	1:157:B:PRO:HD2	18	0.18
(1,2069)	1:155:B:ALA:HB3	1:157:B:PRO:HD3	18	0.18
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG11	1	0.18
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG12	1	0.18
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG13	1	0.18
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG21	1	0.18
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG22	1	0.18
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG23	1	0.18
(1,2060)	1:151:B:GLN:HB2	1:152:B:ALA:HA	4	0.18
(1,2060)	1:151:B:GLN:HB3	1:152:B:ALA:HA	4	0.18
(1,1911)	1:178:A:PRO:HB2	1:180:A:PHE:H	5	0.18
(1,1911)	1:178:A:PRO:HB3	1:180:A:PHE:H	5	0.18
(1,1910)	1:178:A:PRO:HB2	1:179:A:ALA:H	4	0.18
(1,1910)	1:178:A:PRO:HB3	1:179:A:ALA:H	4	0.18
(1,1902)	1:172:A:ALA:HA	1:178:A:PRO:HD2	6	0.18
(1,1902)	1:172:A:ALA:HA	1:178:A:PRO:HD3	6	0.18
(1,1889)	1:156:A:VAL:HG11	1:157:A:PRO:HD2	18	0.18
(1,1889)	1:156:A:VAL:HG11	1:157:A:PRO:HD3	18	0.18
(1,1889)	1:156:A:VAL:HG12	1:157:A:PRO:HD2	18	0.18
(1,1889)	1:156:A:VAL:HG12	1:157:A:PRO:HD3	18	0.18
(1,1889)	1:156:A:VAL:HG13	1:157:A:PRO:HD2	18	0.18
(1,1889)	1:156:A:VAL:HG13	1:157:A:PRO:HD3	18	0.18
(1,1885)	1:155:A:ALA:HB1	1:157:A:PRO:HD2	19	0.18
(1,1885)	1:155:A:ALA:HB1	1:157:A:PRO:HD3	19	0.18
(1,1885)	1:155:A:ALA:HB2	1:157:A:PRO:HD2	19	0.18
(1,1885)	1:155:A:ALA:HB2	1:157:A:PRO:HD3	19	0.18
(1,1885)	1:155:A:ALA:HB3	1:157:A:PRO:HD2	19	0.18
(1,1885)	1:155:A:ALA:HB3	1:157:A:PRO:HD3	19	0.18
(1,1867)	1:134:A:LEU:H	1:188:C:LEU:HD11	14	0.18
(1,1867)	1:134:A:LEU:H	1:188:C:LEU:HD12	14	0.18
(1,1867)	1:134:A:LEU:H	1:188:C:LEU:HD13	14	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1867)	1:134:A:LEU:H	1:188:C:LEU:HD21	14	0.18
(1,1867)	1:134:A:LEU:H	1:188:C:LEU:HD22	14	0.18
(1,1867)	1:134:A:LEU:H	1:188:C:LEU:HD23	14	0.18
(1,1842)	1:121:A:CYS:HB2	1:189:A:CYS:H	13	0.18
(1,1842)	1:121:A:CYS:HB3	1:189:A:CYS:H	13	0.18
(1,1842)	1:121:A:CYS:HB2	1:189:A:CYS:H	14	0.18
(1,1842)	1:121:A:CYS:HB3	1:189:A:CYS:H	14	0.18
(1,1819)	1:95:C:SER:HB2	1:101:C:LEU:H	7	0.18
(1,1819)	1:95:C:SER:HB3	1:101:C:LEU:H	7	0.18
(1,1818)	1:95:B:SER:HB2	1:101:B:LEU:H	11	0.18
(1,1818)	1:95:B:SER:HB3	1:101:B:LEU:H	11	0.18
(1,1775)	1:125:B:LYS:H	1:126:B:ILE:HG21	9	0.18
(1,1775)	1:125:B:LYS:H	1:126:B:ILE:HG22	9	0.18
(1,1775)	1:125:B:LYS:H	1:126:B:ILE:HG23	9	0.18
(1,1737)	1:194:A:LEU:HD21	1:195:A:TYR:H	4	0.18
(1,1737)	1:194:A:LEU:HD22	1:195:A:TYR:H	4	0.18
(1,1737)	1:194:A:LEU:HD23	1:195:A:TYR:H	4	0.18
(1,1687)	1:90:B:THR:H	1:91:B:THR:HB	10	0.18
(1,1687)	1:90:B:THR:H	1:91:B:THR:HB	13	0.18
(1,1621)	1:129:B:GLU:H	1:131:B:ILE:H	5	0.18
(1,1616)	1:116:C:ALA:H	1:119:C:THR:HB	10	0.18
(1,1615)	1:116:B:ALA:H	1:119:B:THR:HB	10	0.18
(1,1614)	1:116:A:ALA:H	1:119:A:THR:HB	7	0.18
(1,1614)	1:116:A:ALA:H	1:119:A:THR:HB	9	0.18
(1,1614)	1:116:A:ALA:H	1:119:A:THR:HB	13	0.18
(1,1614)	1:116:A:ALA:H	1:119:A:THR:HB	16	0.18
(1,1614)	1:116:A:ALA:H	1:119:A:THR:HB	18	0.18
(1,1610)	1:118:A:GLY:H	1:192:A:VAL:HG21	11	0.18
(1,1610)	1:118:A:GLY:H	1:192:A:VAL:HG22	11	0.18
(1,1610)	1:118:A:GLY:H	1:192:A:VAL:HG23	11	0.18
(1,1563)	1:145:B:GLN:HA	1:151:B:GLN:H	4	0.18
(1,1562)	1:145:A:GLN:HA	1:151:A:GLN:H	19	0.18
(1,1554)	1:156:C:VAL:HB	1:167:C:ARG:H	4	0.18
(1,1554)	1:156:C:VAL:HB	1:167:C:ARG:H	10	0.18
(1,1553)	1:156:B:VAL:HB	1:167:B:ARG:H	4	0.18
(1,1553)	1:156:B:VAL:HB	1:167:B:ARG:H	10	0.18
(1,1549)	1:167:A:ARG:H	1:171:A:SER:HA	12	0.18
(1,1548)	1:167:C:ARG:H	1:170:C:GLY:HA2	12	0.18
(1,1548)	1:167:C:ARG:H	1:170:C:GLY:HA3	12	0.18
(1,1547)	1:167:B:ARG:H	1:170:B:GLY:HA2	12	0.18
(1,1547)	1:167:B:ARG:H	1:170:B:GLY:HA3	12	0.18
(1,1546)	1:167:A:ARG:H	1:170:A:GLY:HA2	10	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1546)	1:167:A:ARG:H	1:170:A:GLY:HA3	10	0.18
(1,1546)	1:167:A:ARG:H	1:170:A:GLY:HA2	12	0.18
(1,1546)	1:167:A:ARG:H	1:170:A:GLY:HA3	12	0.18
(1,1520)	1:178:A:PRO:HG2	1:179:A:ALA:H	11	0.18
(1,1520)	1:178:A:PRO:HG3	1:179:A:ALA:H	11	0.18
(1,1511)	1:137:A:LEU:H	1:137:A:LEU:HG	12	0.18
(1,1511)	1:137:A:LEU:H	1:137:A:LEU:HG	19	0.18
(1,1511)	1:137:A:LEU:H	1:137:A:LEU:HG	20	0.18
(1,1463)	1:180:C:PHE:H	1:181:C:LEU:HA	2	0.18
(1,1463)	1:180:C:PHE:H	1:181:C:LEU:HA	6	0.18
(1,1463)	1:180:C:PHE:H	1:181:C:LEU:HA	12	0.18
(1,1462)	1:180:B:PHE:H	1:181:B:LEU:HA	2	0.18
(1,1462)	1:180:B:PHE:H	1:181:B:LEU:HA	12	0.18
(1,1461)	1:180:A:PHE:H	1:181:A:LEU:HA	6	0.18
(1,1431)	1:111:B:ILE:H	1:123:B:ILE:HG21	2	0.18
(1,1431)	1:111:B:ILE:H	1:123:B:ILE:HG22	2	0.18
(1,1431)	1:111:B:ILE:H	1:123:B:ILE:HG23	2	0.18
(1,1431)	1:111:B:ILE:H	1:123:B:ILE:HG21	3	0.18
(1,1431)	1:111:B:ILE:H	1:123:B:ILE:HG22	3	0.18
(1,1431)	1:111:B:ILE:H	1:123:B:ILE:HG23	3	0.18
(1,1410)	1:152:C:ALA:HB1	1:153:C:LYS:H	1	0.18
(1,1410)	1:152:C:ALA:HB2	1:153:C:LYS:H	1	0.18
(1,1410)	1:152:C:ALA:HB3	1:153:C:LYS:H	1	0.18
(1,1409)	1:152:B:ALA:HB1	1:153:B:LYS:H	1	0.18
(1,1409)	1:152:B:ALA:HB2	1:153:B:LYS:H	1	0.18
(1,1409)	1:152:B:ALA:HB3	1:153:B:LYS:H	1	0.18
(1,1409)	1:152:B:ALA:HB1	1:153:B:LYS:H	4	0.18
(1,1409)	1:152:B:ALA:HB2	1:153:B:LYS:H	4	0.18
(1,1409)	1:152:B:ALA:HB3	1:153:B:LYS:H	4	0.18
(1,1408)	1:152:A:ALA:HB1	1:153:A:LYS:H	3	0.18
(1,1408)	1:152:A:ALA:HB2	1:153:A:LYS:H	3	0.18
(1,1408)	1:152:A:ALA:HB3	1:153:A:LYS:H	3	0.18
(1,1408)	1:152:A:ALA:HB1	1:153:A:LYS:H	4	0.18
(1,1408)	1:152:A:ALA:HB2	1:153:A:LYS:H	4	0.18
(1,1408)	1:152:A:ALA:HB3	1:153:A:LYS:H	4	0.18
(1,1370)	1:154:C:PRO:HB3	1:155:C:ALA:H	7	0.18
(1,1369)	1:154:B:PRO:HB3	1:155:B:ALA:H	7	0.18
(1,1368)	1:154:A:PRO:HB3	1:155:A:ALA:H	7	0.18
(1,1276)	1:109:A:LEU:H	1:109:A:LEU:HG	16	0.18
(1,1099)	1:167:B:ARG:H	1:167:B:ARG:HB2	15	0.18
(1,1097)	1:157:C:PRO:HA	1:158:C:THR:H	2	0.18
(1,1097)	1:157:C:PRO:HA	1:158:C:THR:H	3	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1097)	1:157:C:PRO:HA	1:158:C:THR:H	11	0.18
(1,1097)	1:157:C:PRO:HA	1:158:C:THR:H	15	0.18
(1,1097)	1:157:C:PRO:HA	1:158:C:THR:H	16	0.18
(1,1096)	1:157:B:PRO:HA	1:158:B:THR:H	2	0.18
(1,1096)	1:157:B:PRO:HA	1:158:B:THR:H	3	0.18
(1,1096)	1:157:B:PRO:HA	1:158:B:THR:H	7	0.18
(1,1096)	1:157:B:PRO:HA	1:158:B:THR:H	15	0.18
(1,1096)	1:157:B:PRO:HA	1:158:B:THR:H	16	0.18
(1,1095)	1:157:A:PRO:HA	1:158:A:THR:H	1	0.18
(1,1095)	1:157:A:PRO:HA	1:158:A:THR:H	2	0.18
(1,1095)	1:157:A:PRO:HA	1:158:A:THR:H	15	0.18
(1,1073)	1:139:C:ARG:H	1:141:C:VAL:HB	7	0.18
(1,1049)	1:137:C:LEU:HG	1:138:C:THR:H	4	0.18
(1,1048)	1:137:B:LEU:HG	1:138:B:THR:H	6	0.18
(1,1048)	1:137:B:LEU:HG	1:138:B:THR:H	15	0.18
(1,1048)	1:137:B:LEU:HG	1:138:B:THR:H	20	0.18
(1,1047)	1:137:A:LEU:HG	1:138:A:THR:H	10	0.18
(1,1047)	1:137:A:LEU:HG	1:138:A:THR:H	17	0.18
(1,1047)	1:137:A:LEU:HG	1:138:A:THR:H	20	0.18
(1,1036)	1:188:A:LEU:HD21	1:134:B:LEU:H	13	0.18
(1,1036)	1:188:A:LEU:HD22	1:134:B:LEU:H	13	0.18
(1,1036)	1:188:A:LEU:HD23	1:134:B:LEU:H	13	0.18
(1,958)	1:187:A:THR:HA	1:188:A:LEU:HD11	3	0.18
(1,958)	1:187:A:THR:HA	1:188:A:LEU:HD12	3	0.18
(1,958)	1:187:A:THR:HA	1:188:A:LEU:HD13	3	0.18
(1,942)	1:101:A:LEU:HD11	1:188:A:LEU:HD21	14	0.18
(1,942)	1:101:A:LEU:HD11	1:188:A:LEU:HD22	14	0.18
(1,942)	1:101:A:LEU:HD11	1:188:A:LEU:HD23	14	0.18
(1,942)	1:101:A:LEU:HD12	1:188:A:LEU:HD21	14	0.18
(1,942)	1:101:A:LEU:HD12	1:188:A:LEU:HD22	14	0.18
(1,942)	1:101:A:LEU:HD12	1:188:A:LEU:HD23	14	0.18
(1,942)	1:101:A:LEU:HD13	1:188:A:LEU:HD21	14	0.18
(1,942)	1:101:A:LEU:HD13	1:188:A:LEU:HD22	14	0.18
(1,942)	1:101:A:LEU:HD13	1:188:A:LEU:HD23	14	0.18
(1,942)	1:101:A:LEU:HD11	1:188:A:LEU:HD21	19	0.18
(1,942)	1:101:A:LEU:HD11	1:188:A:LEU:HD22	19	0.18
(1,942)	1:101:A:LEU:HD11	1:188:A:LEU:HD23	19	0.18
(1,942)	1:101:A:LEU:HD12	1:188:A:LEU:HD21	19	0.18
(1,942)	1:101:A:LEU:HD12	1:188:A:LEU:HD22	19	0.18
(1,942)	1:101:A:LEU:HD12	1:188:A:LEU:HD23	19	0.18
(1,942)	1:101:A:LEU:HD13	1:188:A:LEU:HD21	19	0.18
(1,942)	1:101:A:LEU:HD13	1:188:A:LEU:HD22	19	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,942)	1:101:A:LEU:HD13	1:188:A:LEU:HD23	19	0.18
(1,928)	1:178:A:PRO:HG2	1:181:A:LEU:HD21	6	0.18
(1,928)	1:178:A:PRO:HG2	1:181:A:LEU:HD22	6	0.18
(1,928)	1:178:A:PRO:HG2	1:181:A:LEU:HD23	6	0.18
(1,928)	1:178:A:PRO:HG3	1:181:A:LEU:HD21	6	0.18
(1,928)	1:178:A:PRO:HG3	1:181:A:LEU:HD22	6	0.18
(1,928)	1:178:A:PRO:HG3	1:181:A:LEU:HD23	6	0.18
(1,928)	1:178:A:PRO:HG2	1:181:A:LEU:HD21	7	0.18
(1,928)	1:178:A:PRO:HG2	1:181:A:LEU:HD22	7	0.18
(1,928)	1:178:A:PRO:HG2	1:181:A:LEU:HD23	7	0.18
(1,928)	1:178:A:PRO:HG3	1:181:A:LEU:HD21	7	0.18
(1,928)	1:178:A:PRO:HG3	1:181:A:LEU:HD22	7	0.18
(1,928)	1:178:A:PRO:HG3	1:181:A:LEU:HD23	7	0.18
(1,892)	1:165:B:GLU:HB2	1:167:B:ARG:HG2	13	0.18
(1,892)	1:165:B:GLU:HB2	1:167:B:ARG:HG3	13	0.18
(1,891)	1:165:A:GLU:HB2	1:167:A:ARG:HG2	19	0.18
(1,891)	1:165:A:GLU:HB2	1:167:A:ARG:HG3	19	0.18
(1,889)	1:152:B:ALA:HA	1:157:B:PRO:HG2	4	0.18
(1,889)	1:152:B:ALA:HA	1:157:B:PRO:HG3	4	0.18
(1,889)	1:152:B:ALA:HA	1:157:B:PRO:HG2	8	0.18
(1,889)	1:152:B:ALA:HA	1:157:B:PRO:HG3	8	0.18
(1,888)	1:152:A:ALA:HA	1:157:A:PRO:HG2	5	0.18
(1,888)	1:152:A:ALA:HA	1:157:A:PRO:HG3	5	0.18
(1,866)	1:153:C:LYS:HA	1:154:C:PRO:HD2	1	0.18
(1,866)	1:153:C:LYS:HA	1:154:C:PRO:HD2	2	0.18
(1,866)	1:153:C:LYS:HA	1:154:C:PRO:HD2	3	0.18
(1,866)	1:153:C:LYS:HA	1:154:C:PRO:HD2	4	0.18
(1,866)	1:153:C:LYS:HA	1:154:C:PRO:HD2	6	0.18
(1,866)	1:153:C:LYS:HA	1:154:C:PRO:HD2	8	0.18
(1,866)	1:153:C:LYS:HA	1:154:C:PRO:HD2	10	0.18
(1,866)	1:153:C:LYS:HA	1:154:C:PRO:HD2	11	0.18
(1,866)	1:153:C:LYS:HA	1:154:C:PRO:HD2	12	0.18
(1,866)	1:153:C:LYS:HA	1:154:C:PRO:HD2	13	0.18
(1,866)	1:153:C:LYS:HA	1:154:C:PRO:HD2	18	0.18
(1,865)	1:153:B:LYS:HA	1:154:B:PRO:HD2	1	0.18
(1,865)	1:153:B:LYS:HA	1:154:B:PRO:HD2	2	0.18
(1,865)	1:153:B:LYS:HA	1:154:B:PRO:HD2	3	0.18
(1,865)	1:153:B:LYS:HA	1:154:B:PRO:HD2	4	0.18
(1,865)	1:153:B:LYS:HA	1:154:B:PRO:HD2	6	0.18
(1,865)	1:153:B:LYS:HA	1:154:B:PRO:HD2	8	0.18
(1,865)	1:153:B:LYS:HA	1:154:B:PRO:HD2	10	0.18
(1,865)	1:153:B:LYS:HA	1:154:B:PRO:HD2	11	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,865)	1:153:B:LYS:HA	1:154:B:PRO:HD2	12	0.18
(1,865)	1:153:B:LYS:HA	1:154:B:PRO:HD2	13	0.18
(1,865)	1:153:B:LYS:HA	1:154:B:PRO:HD2	18	0.18
(1,864)	1:153:A:LYS:HA	1:154:A:PRO:HD2	1	0.18
(1,864)	1:153:A:LYS:HA	1:154:A:PRO:HD2	2	0.18
(1,864)	1:153:A:LYS:HA	1:154:A:PRO:HD2	3	0.18
(1,864)	1:153:A:LYS:HA	1:154:A:PRO:HD2	4	0.18
(1,864)	1:153:A:LYS:HA	1:154:A:PRO:HD2	6	0.18
(1,864)	1:153:A:LYS:HA	1:154:A:PRO:HD2	8	0.18
(1,864)	1:153:A:LYS:HA	1:154:A:PRO:HD2	10	0.18
(1,864)	1:153:A:LYS:HA	1:154:A:PRO:HD2	11	0.18
(1,864)	1:153:A:LYS:HA	1:154:A:PRO:HD2	12	0.18
(1,864)	1:153:A:LYS:HA	1:154:A:PRO:HD2	13	0.18
(1,864)	1:153:A:LYS:HA	1:154:A:PRO:HD2	18	0.18
(1,812)	1:176:C:GLY:H	1:177:C:ASP:HB3	10	0.18
(1,784)	1:167:B:ARG:HD2	1:169:B:ALA:HB1	20	0.18
(1,784)	1:167:B:ARG:HD2	1:169:B:ALA:HB2	20	0.18
(1,784)	1:167:B:ARG:HD2	1:169:B:ALA:HB3	20	0.18
(1,784)	1:167:B:ARG:HD3	1:169:B:ALA:HB1	20	0.18
(1,784)	1:167:B:ARG:HD3	1:169:B:ALA:HB2	20	0.18
(1,784)	1:167:B:ARG:HD3	1:169:B:ALA:HB3	20	0.18
(1,769)	1:102:A:VAL:HG21	1:104:A:TYR:HE1	16	0.18
(1,769)	1:102:A:VAL:HG21	1:104:A:TYR:HE2	16	0.18
(1,769)	1:102:A:VAL:HG22	1:104:A:TYR:HE1	16	0.18
(1,769)	1:102:A:VAL:HG22	1:104:A:TYR:HE2	16	0.18
(1,769)	1:102:A:VAL:HG23	1:104:A:TYR:HE1	16	0.18
(1,769)	1:102:A:VAL:HG23	1:104:A:TYR:HE2	16	0.18
(1,754)	1:189:B:CYS:H	1:192:B:VAL:HG11	14	0.18
(1,754)	1:189:B:CYS:H	1:192:B:VAL:HG12	14	0.18
(1,754)	1:189:B:CYS:H	1:192:B:VAL:HG13	14	0.18
(1,754)	1:189:B:CYS:H	1:192:B:VAL:HG11	20	0.18
(1,754)	1:189:B:CYS:H	1:192:B:VAL:HG12	20	0.18
(1,754)	1:189:B:CYS:H	1:192:B:VAL:HG13	20	0.18
(1,665)	1:113:A:TYR:HE1	1:197:A:ILE:HG21	13	0.18
(1,665)	1:113:A:TYR:HE1	1:197:A:ILE:HG22	13	0.18
(1,665)	1:113:A:TYR:HE1	1:197:A:ILE:HG23	13	0.18
(1,665)	1:113:A:TYR:HE2	1:197:A:ILE:HG21	13	0.18
(1,665)	1:113:A:TYR:HE2	1:197:A:ILE:HG22	13	0.18
(1,665)	1:113:A:TYR:HE2	1:197:A:ILE:HG23	13	0.18
(1,655)	1:172:C:ALA:HB1	1:173:C:PRO:HD3	1	0.18
(1,655)	1:172:C:ALA:HB2	1:173:C:PRO:HD3	1	0.18
(1,655)	1:172:C:ALA:HB3	1:173:C:PRO:HD3	1	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,655)	1:172:C:ALA:HB1	1:173:C:PRO:HD3	3	0.18
(1,655)	1:172:C:ALA:HB2	1:173:C:PRO:HD3	3	0.18
(1,655)	1:172:C:ALA:HB3	1:173:C:PRO:HD3	3	0.18
(1,655)	1:172:C:ALA:HB1	1:173:C:PRO:HD3	5	0.18
(1,655)	1:172:C:ALA:HB2	1:173:C:PRO:HD3	5	0.18
(1,655)	1:172:C:ALA:HB3	1:173:C:PRO:HD3	5	0.18
(1,655)	1:172:C:ALA:HB1	1:173:C:PRO:HD3	6	0.18
(1,655)	1:172:C:ALA:HB2	1:173:C:PRO:HD3	6	0.18
(1,655)	1:172:C:ALA:HB3	1:173:C:PRO:HD3	6	0.18
(1,655)	1:172:C:ALA:HB1	1:173:C:PRO:HD3	7	0.18
(1,655)	1:172:C:ALA:HB2	1:173:C:PRO:HD3	7	0.18
(1,655)	1:172:C:ALA:HB3	1:173:C:PRO:HD3	7	0.18
(1,655)	1:172:C:ALA:HB1	1:173:C:PRO:HD3	10	0.18
(1,655)	1:172:C:ALA:HB2	1:173:C:PRO:HD3	10	0.18
(1,655)	1:172:C:ALA:HB3	1:173:C:PRO:HD3	10	0.18
(1,655)	1:172:C:ALA:HB1	1:173:C:PRO:HD3	11	0.18
(1,655)	1:172:C:ALA:HB2	1:173:C:PRO:HD3	11	0.18
(1,655)	1:172:C:ALA:HB3	1:173:C:PRO:HD3	11	0.18
(1,655)	1:172:C:ALA:HB1	1:173:C:PRO:HD3	13	0.18
(1,655)	1:172:C:ALA:HB2	1:173:C:PRO:HD3	13	0.18
(1,655)	1:172:C:ALA:HB3	1:173:C:PRO:HD3	13	0.18
(1,655)	1:172:C:ALA:HB1	1:173:C:PRO:HD3	16	0.18
(1,655)	1:172:C:ALA:HB2	1:173:C:PRO:HD3	16	0.18
(1,655)	1:172:C:ALA:HB3	1:173:C:PRO:HD3	16	0.18
(1,655)	1:172:C:ALA:HB1	1:173:C:PRO:HD3	17	0.18
(1,655)	1:172:C:ALA:HB2	1:173:C:PRO:HD3	17	0.18
(1,655)	1:172:C:ALA:HB3	1:173:C:PRO:HD3	17	0.18
(1,655)	1:172:C:ALA:HB1	1:173:C:PRO:HD3	18	0.18
(1,655)	1:172:C:ALA:HB2	1:173:C:PRO:HD3	18	0.18
(1,655)	1:172:C:ALA:HB3	1:173:C:PRO:HD3	18	0.18
(1,655)	1:172:C:ALA:HB1	1:173:C:PRO:HD3	19	0.18
(1,655)	1:172:C:ALA:HB2	1:173:C:PRO:HD3	19	0.18
(1,655)	1:172:C:ALA:HB3	1:173:C:PRO:HD3	19	0.18
(1,654)	1:172:B:ALA:HB1	1:173:B:PRO:HD3	1	0.18
(1,654)	1:172:B:ALA:HB2	1:173:B:PRO:HD3	1	0.18
(1,654)	1:172:B:ALA:HB3	1:173:B:PRO:HD3	1	0.18
(1,654)	1:172:B:ALA:HB1	1:173:B:PRO:HD3	3	0.18
(1,654)	1:172:B:ALA:HB2	1:173:B:PRO:HD3	3	0.18
(1,654)	1:172:B:ALA:HB3	1:173:B:PRO:HD3	3	0.18
(1,654)	1:172:B:ALA:HB1	1:173:B:PRO:HD3	5	0.18
(1,654)	1:172:B:ALA:HB2	1:173:B:PRO:HD3	5	0.18
(1,654)	1:172:B:ALA:HB3	1:173:B:PRO:HD3	5	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,654)	1:172:B:ALA:HB1	1:173:B:PRO:HD3	6	0.18
(1,654)	1:172:B:ALA:HB2	1:173:B:PRO:HD3	6	0.18
(1,654)	1:172:B:ALA:HB3	1:173:B:PRO:HD3	6	0.18
(1,654)	1:172:B:ALA:HB1	1:173:B:PRO:HD3	7	0.18
(1,654)	1:172:B:ALA:HB2	1:173:B:PRO:HD3	7	0.18
(1,654)	1:172:B:ALA:HB3	1:173:B:PRO:HD3	7	0.18
(1,654)	1:172:B:ALA:HB1	1:173:B:PRO:HD3	10	0.18
(1,654)	1:172:B:ALA:HB2	1:173:B:PRO:HD3	10	0.18
(1,654)	1:172:B:ALA:HB3	1:173:B:PRO:HD3	10	0.18
(1,654)	1:172:B:ALA:HB1	1:173:B:PRO:HD3	11	0.18
(1,654)	1:172:B:ALA:HB2	1:173:B:PRO:HD3	11	0.18
(1,654)	1:172:B:ALA:HB3	1:173:B:PRO:HD3	11	0.18
(1,654)	1:172:B:ALA:HB1	1:173:B:PRO:HD3	13	0.18
(1,654)	1:172:B:ALA:HB2	1:173:B:PRO:HD3	13	0.18
(1,654)	1:172:B:ALA:HB3	1:173:B:PRO:HD3	13	0.18
(1,654)	1:172:B:ALA:HB1	1:173:B:PRO:HD3	16	0.18
(1,654)	1:172:B:ALA:HB2	1:173:B:PRO:HD3	16	0.18
(1,654)	1:172:B:ALA:HB3	1:173:B:PRO:HD3	16	0.18
(1,654)	1:172:B:ALA:HB1	1:173:B:PRO:HD3	18	0.18
(1,654)	1:172:B:ALA:HB2	1:173:B:PRO:HD3	18	0.18
(1,654)	1:172:B:ALA:HB3	1:173:B:PRO:HD3	18	0.18
(1,653)	1:172:A:ALA:HB1	1:173:A:PRO:HD3	1	0.18
(1,653)	1:172:A:ALA:HB2	1:173:A:PRO:HD3	1	0.18
(1,653)	1:172:A:ALA:HB3	1:173:A:PRO:HD3	1	0.18
(1,653)	1:172:A:ALA:HB1	1:173:A:PRO:HD3	2	0.18
(1,653)	1:172:A:ALA:HB2	1:173:A:PRO:HD3	2	0.18
(1,653)	1:172:A:ALA:HB3	1:173:A:PRO:HD3	2	0.18
(1,653)	1:172:A:ALA:HB1	1:173:A:PRO:HD3	3	0.18
(1,653)	1:172:A:ALA:HB2	1:173:A:PRO:HD3	3	0.18
(1,653)	1:172:A:ALA:HB3	1:173:A:PRO:HD3	3	0.18
(1,653)	1:172:A:ALA:HB1	1:173:A:PRO:HD3	5	0.18
(1,653)	1:172:A:ALA:HB2	1:173:A:PRO:HD3	5	0.18
(1,653)	1:172:A:ALA:HB3	1:173:A:PRO:HD3	5	0.18
(1,653)	1:172:A:ALA:HB1	1:173:A:PRO:HD3	6	0.18
(1,653)	1:172:A:ALA:HB2	1:173:A:PRO:HD3	6	0.18
(1,653)	1:172:A:ALA:HB3	1:173:A:PRO:HD3	6	0.18
(1,653)	1:172:A:ALA:HB1	1:173:A:PRO:HD3	7	0.18
(1,653)	1:172:A:ALA:HB2	1:173:A:PRO:HD3	7	0.18
(1,653)	1:172:A:ALA:HB3	1:173:A:PRO:HD3	7	0.18
(1,653)	1:172:A:ALA:HB1	1:173:A:PRO:HD3	10	0.18
(1,653)	1:172:A:ALA:HB2	1:173:A:PRO:HD3	10	0.18
(1,653)	1:172:A:ALA:HB3	1:173:A:PRO:HD3	10	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,653)	1:172:A:ALA:HB1	1:173:A:PRO:HD3	11	0.18
(1,653)	1:172:A:ALA:HB2	1:173:A:PRO:HD3	11	0.18
(1,653)	1:172:A:ALA:HB3	1:173:A:PRO:HD3	11	0.18
(1,653)	1:172:A:ALA:HB1	1:173:A:PRO:HD3	13	0.18
(1,653)	1:172:A:ALA:HB2	1:173:A:PRO:HD3	13	0.18
(1,653)	1:172:A:ALA:HB3	1:173:A:PRO:HD3	13	0.18
(1,653)	1:172:A:ALA:HB1	1:173:A:PRO:HD3	16	0.18
(1,653)	1:172:A:ALA:HB2	1:173:A:PRO:HD3	16	0.18
(1,653)	1:172:A:ALA:HB3	1:173:A:PRO:HD3	16	0.18
(1,653)	1:172:A:ALA:HB1	1:173:A:PRO:HD3	17	0.18
(1,653)	1:172:A:ALA:HB2	1:173:A:PRO:HD3	17	0.18
(1,653)	1:172:A:ALA:HB3	1:173:A:PRO:HD3	17	0.18
(1,653)	1:172:A:ALA:HB1	1:173:A:PRO:HD3	18	0.18
(1,653)	1:172:A:ALA:HB2	1:173:A:PRO:HD3	18	0.18
(1,653)	1:172:A:ALA:HB3	1:173:A:PRO:HD3	18	0.18
(1,653)	1:172:A:ALA:HB1	1:173:A:PRO:HD3	19	0.18
(1,653)	1:172:A:ALA:HB2	1:173:A:PRO:HD3	19	0.18
(1,653)	1:172:A:ALA:HB3	1:173:A:PRO:HD3	19	0.18
(1,635)	1:96:A:ILE:HG21	1:100:A:GLY:H	5	0.18
(1,635)	1:96:A:ILE:HG22	1:100:A:GLY:H	5	0.18
(1,635)	1:96:A:ILE:HG23	1:100:A:GLY:H	5	0.18
(1,577)	1:178:A:PRO:HG2	1:194:A:LEU:HD21	19	0.18
(1,577)	1:178:A:PRO:HG2	1:194:A:LEU:HD22	19	0.18
(1,577)	1:178:A:PRO:HG2	1:194:A:LEU:HD23	19	0.18
(1,577)	1:178:A:PRO:HG3	1:194:A:LEU:HD21	19	0.18
(1,577)	1:178:A:PRO:HG3	1:194:A:LEU:HD22	19	0.18
(1,577)	1:178:A:PRO:HG3	1:194:A:LEU:HD23	19	0.18
(1,451)	1:95:A:SER:HB2	1:101:A:LEU:HD21	14	0.18
(1,451)	1:95:A:SER:HB2	1:101:A:LEU:HD22	14	0.18
(1,451)	1:95:A:SER:HB2	1:101:A:LEU:HD23	14	0.18
(1,451)	1:95:A:SER:HB3	1:101:A:LEU:HD21	14	0.18
(1,451)	1:95:A:SER:HB3	1:101:A:LEU:HD22	14	0.18
(1,451)	1:95:A:SER:HB3	1:101:A:LEU:HD23	14	0.18
(1,437)	1:183:C:MET:HE1	1:186:C:SER:HA	10	0.18
(1,437)	1:183:C:MET:HE2	1:186:C:SER:HA	10	0.18
(1,437)	1:183:C:MET:HE3	1:186:C:SER:HA	10	0.18
(1,436)	1:183:B:MET:HE1	1:186:B:SER:HA	2	0.18
(1,436)	1:183:B:MET:HE2	1:186:B:SER:HA	2	0.18
(1,436)	1:183:B:MET:HE3	1:186:B:SER:HA	2	0.18
(1,436)	1:183:B:MET:HE1	1:186:B:SER:HA	6	0.18
(1,436)	1:183:B:MET:HE2	1:186:B:SER:HA	6	0.18
(1,436)	1:183:B:MET:HE3	1:186:B:SER:HA	6	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,436)	1:183:B:MET:HE1	1:186:B:SER:HA	10	0.18
(1,436)	1:183:B:MET:HE2	1:186:B:SER:HA	10	0.18
(1,436)	1:183:B:MET:HE3	1:186:B:SER:HA	10	0.18
(1,435)	1:183:A:MET:HE1	1:186:A:SER:HA	12	0.18
(1,435)	1:183:A:MET:HE2	1:186:A:SER:HA	12	0.18
(1,435)	1:183:A:MET:HE3	1:186:A:SER:HA	12	0.18
(1,395)	1:109:A:LEU:HG	1:111:A:ILE:HD11	7	0.18
(1,395)	1:109:A:LEU:HG	1:111:A:ILE:HD12	7	0.18
(1,395)	1:109:A:LEU:HG	1:111:A:ILE:HD13	7	0.18
(1,302)	1:161:A:LEU:HA	1:161:A:LEU:HD11	14	0.18
(1,302)	1:161:A:LEU:HA	1:161:A:LEU:HD12	14	0.18
(1,302)	1:161:A:LEU:HA	1:161:A:LEU:HD13	14	0.18
(1,301)	1:181:A:LEU:HD11	1:196:A:TYR:HE1	13	0.18
(1,301)	1:181:A:LEU:HD11	1:196:A:TYR:HE2	13	0.18
(1,301)	1:181:A:LEU:HD12	1:196:A:TYR:HE1	13	0.18
(1,301)	1:181:A:LEU:HD12	1:196:A:TYR:HE2	13	0.18
(1,301)	1:181:A:LEU:HD13	1:196:A:TYR:HE1	13	0.18
(1,301)	1:181:A:LEU:HD13	1:196:A:TYR:HE2	13	0.18
(1,219)	1:96:A:ILE:HG21	1:141:A:VAL:HG11	12	0.18
(1,219)	1:96:A:ILE:HG21	1:141:A:VAL:HG12	12	0.18
(1,219)	1:96:A:ILE:HG21	1:141:A:VAL:HG13	12	0.18
(1,219)	1:96:A:ILE:HG22	1:141:A:VAL:HG11	12	0.18
(1,219)	1:96:A:ILE:HG22	1:141:A:VAL:HG12	12	0.18
(1,219)	1:96:A:ILE:HG22	1:141:A:VAL:HG13	12	0.18
(1,219)	1:96:A:ILE:HG23	1:141:A:VAL:HG11	12	0.18
(1,219)	1:96:A:ILE:HG23	1:141:A:VAL:HG12	12	0.18
(1,219)	1:96:A:ILE:HG23	1:141:A:VAL:HG13	12	0.18
(1,182)	1:137:A:LEU:HD11	1:141:A:VAL:HG11	13	0.18
(1,182)	1:137:A:LEU:HD11	1:141:A:VAL:HG12	13	0.18
(1,182)	1:137:A:LEU:HD11	1:141:A:VAL:HG13	13	0.18
(1,182)	1:137:A:LEU:HD12	1:141:A:VAL:HG11	13	0.18
(1,182)	1:137:A:LEU:HD12	1:141:A:VAL:HG12	13	0.18
(1,182)	1:137:A:LEU:HD12	1:141:A:VAL:HG13	13	0.18
(1,182)	1:137:A:LEU:HD13	1:141:A:VAL:HG11	13	0.18
(1,182)	1:137:A:LEU:HD13	1:141:A:VAL:HG12	13	0.18
(1,182)	1:137:A:LEU:HD13	1:141:A:VAL:HG13	13	0.18
(1,182)	1:137:A:LEU:HD11	1:141:A:VAL:HG11	18	0.18
(1,182)	1:137:A:LEU:HD11	1:141:A:VAL:HG12	18	0.18
(1,182)	1:137:A:LEU:HD11	1:141:A:VAL:HG13	18	0.18
(1,182)	1:137:A:LEU:HD12	1:141:A:VAL:HG11	18	0.18
(1,182)	1:137:A:LEU:HD12	1:141:A:VAL:HG12	18	0.18
(1,182)	1:137:A:LEU:HD12	1:141:A:VAL:HG13	18	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,182)	1:137:A:LEU:HD13	1:141:A:VAL:HG11	18	0.18
(1,182)	1:137:A:LEU:HD13	1:141:A:VAL:HG12	18	0.18
(1,182)	1:137:A:LEU:HD13	1:141:A:VAL:HG13	18	0.18
(1,175)	1:179:A:ALA:HB1	1:181:A:LEU:HD21	11	0.18
(1,175)	1:179:A:ALA:HB1	1:181:A:LEU:HD22	11	0.18
(1,175)	1:179:A:ALA:HB1	1:181:A:LEU:HD23	11	0.18
(1,175)	1:179:A:ALA:HB2	1:181:A:LEU:HD21	11	0.18
(1,175)	1:179:A:ALA:HB2	1:181:A:LEU:HD22	11	0.18
(1,175)	1:179:A:ALA:HB2	1:181:A:LEU:HD23	11	0.18
(1,175)	1:179:A:ALA:HB3	1:181:A:LEU:HD21	11	0.18
(1,175)	1:179:A:ALA:HB3	1:181:A:LEU:HD22	11	0.18
(1,175)	1:179:A:ALA:HB3	1:181:A:LEU:HD23	11	0.18
(1,175)	1:179:A:ALA:HB1	1:181:A:LEU:HD21	14	0.18
(1,175)	1:179:A:ALA:HB1	1:181:A:LEU:HD22	14	0.18
(1,175)	1:179:A:ALA:HB1	1:181:A:LEU:HD23	14	0.18
(1,175)	1:179:A:ALA:HB2	1:181:A:LEU:HD21	14	0.18
(1,175)	1:179:A:ALA:HB2	1:181:A:LEU:HD22	14	0.18
(1,175)	1:179:A:ALA:HB2	1:181:A:LEU:HD23	14	0.18
(1,175)	1:179:A:ALA:HB3	1:181:A:LEU:HD21	14	0.18
(1,175)	1:179:A:ALA:HB3	1:181:A:LEU:HD22	14	0.18
(1,175)	1:179:A:ALA:HB3	1:181:A:LEU:HD23	14	0.18
(1,175)	1:179:A:ALA:HB1	1:181:A:LEU:HD21	15	0.18
(1,175)	1:179:A:ALA:HB1	1:181:A:LEU:HD22	15	0.18
(1,175)	1:179:A:ALA:HB1	1:181:A:LEU:HD23	15	0.18
(1,175)	1:179:A:ALA:HB2	1:181:A:LEU:HD21	15	0.18
(1,175)	1:179:A:ALA:HB2	1:181:A:LEU:HD22	15	0.18
(1,175)	1:179:A:ALA:HB2	1:181:A:LEU:HD23	15	0.18
(1,175)	1:179:A:ALA:HB3	1:181:A:LEU:HD21	15	0.18
(1,175)	1:179:A:ALA:HB3	1:181:A:LEU:HD22	15	0.18
(1,175)	1:179:A:ALA:HB3	1:181:A:LEU:HD23	15	0.18
(1,154)	1:187:A:THR:HG21	1:188:A:LEU:HD21	2	0.18
(1,154)	1:187:A:THR:HG21	1:188:A:LEU:HD22	2	0.18
(1,154)	1:187:A:THR:HG21	1:188:A:LEU:HD23	2	0.18
(1,154)	1:187:A:THR:HG22	1:188:A:LEU:HD21	2	0.18
(1,154)	1:187:A:THR:HG22	1:188:A:LEU:HD22	2	0.18
(1,154)	1:187:A:THR:HG22	1:188:A:LEU:HD23	2	0.18
(1,154)	1:187:A:THR:HG23	1:188:A:LEU:HD21	2	0.18
(1,154)	1:187:A:THR:HG23	1:188:A:LEU:HD22	2	0.18
(1,154)	1:187:A:THR:HG23	1:188:A:LEU:HD23	2	0.18
(1,56)	1:156:A:VAL:HG11	1:157:A:PRO:HD3	1	0.18
(1,56)	1:156:A:VAL:HG12	1:157:A:PRO:HD3	1	0.18
(1,56)	1:156:A:VAL:HG13	1:157:A:PRO:HD3	1	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2345)	1:183:C:MET:HB2	1:183:C:MET:HE1	17	0.17
(1,2345)	1:183:C:MET:HB2	1:183:C:MET:HE2	17	0.17
(1,2345)	1:183:C:MET:HB2	1:183:C:MET:HE3	17	0.17
(1,2345)	1:183:C:MET:HB3	1:183:C:MET:HE1	17	0.17
(1,2345)	1:183:C:MET:HB3	1:183:C:MET:HE2	17	0.17
(1,2345)	1:183:C:MET:HB3	1:183:C:MET:HE3	17	0.17
(1,2338)	1:179:C:ALA:HB1	1:181:C:LEU:HD11	17	0.17
(1,2338)	1:179:C:ALA:HB1	1:181:C:LEU:HD12	17	0.17
(1,2338)	1:179:C:ALA:HB1	1:181:C:LEU:HD13	17	0.17
(1,2338)	1:179:C:ALA:HB1	1:181:C:LEU:HD21	17	0.17
(1,2338)	1:179:C:ALA:HB1	1:181:C:LEU:HD22	17	0.17
(1,2338)	1:179:C:ALA:HB1	1:181:C:LEU:HD23	17	0.17
(1,2338)	1:179:C:ALA:HB2	1:181:C:LEU:HD11	17	0.17
(1,2338)	1:179:C:ALA:HB2	1:181:C:LEU:HD12	17	0.17
(1,2338)	1:179:C:ALA:HB2	1:181:C:LEU:HD13	17	0.17
(1,2338)	1:179:C:ALA:HB2	1:181:C:LEU:HD21	17	0.17
(1,2338)	1:179:C:ALA:HB2	1:181:C:LEU:HD22	17	0.17
(1,2338)	1:179:C:ALA:HB2	1:181:C:LEU:HD23	17	0.17
(1,2338)	1:179:C:ALA:HB3	1:181:C:LEU:HD11	17	0.17
(1,2338)	1:179:C:ALA:HB3	1:181:C:LEU:HD12	17	0.17
(1,2338)	1:179:C:ALA:HB3	1:181:C:LEU:HD13	17	0.17
(1,2338)	1:179:C:ALA:HB3	1:181:C:LEU:HD21	17	0.17
(1,2338)	1:179:C:ALA:HB3	1:181:C:LEU:HD22	17	0.17
(1,2338)	1:179:C:ALA:HB3	1:181:C:LEU:HD23	17	0.17
(1,2329)	1:178:C:PRO:HB2	1:179:C:ALA:H	10	0.17
(1,2329)	1:178:C:PRO:HB3	1:179:C:ALA:H	10	0.17
(1,2320)	1:172:C:ALA:HA	1:178:C:PRO:HD2	13	0.17
(1,2320)	1:172:C:ALA:HA	1:178:C:PRO:HD3	13	0.17
(1,2320)	1:172:C:ALA:HA	1:178:C:PRO:HD2	15	0.17
(1,2320)	1:172:C:ALA:HA	1:178:C:PRO:HD3	15	0.17
(1,2320)	1:172:C:ALA:HA	1:178:C:PRO:HD2	17	0.17
(1,2320)	1:172:C:ALA:HA	1:178:C:PRO:HD3	17	0.17
(1,2295)	1:155:C:ALA:HB1	1:157:C:PRO:HD2	15	0.17
(1,2295)	1:155:C:ALA:HB1	1:157:C:PRO:HD3	15	0.17
(1,2295)	1:155:C:ALA:HB2	1:157:C:PRO:HD2	15	0.17
(1,2295)	1:155:C:ALA:HB2	1:157:C:PRO:HD3	15	0.17
(1,2295)	1:155:C:ALA:HB3	1:157:C:PRO:HD2	15	0.17
(1,2295)	1:155:C:ALA:HB3	1:157:C:PRO:HD3	15	0.17
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG11	9	0.17
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG12	9	0.17
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG13	9	0.17
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG21	9	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG22	9	0.17
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG23	9	0.17
(1,2119)	1:183:B:MET:HB2	1:183:B:MET:HE1	17	0.17
(1,2119)	1:183:B:MET:HB2	1:183:B:MET:HE2	17	0.17
(1,2119)	1:183:B:MET:HB2	1:183:B:MET:HE3	17	0.17
(1,2119)	1:183:B:MET:HB3	1:183:B:MET:HE1	17	0.17
(1,2119)	1:183:B:MET:HB3	1:183:B:MET:HE2	17	0.17
(1,2119)	1:183:B:MET:HB3	1:183:B:MET:HE3	17	0.17
(1,2103)	1:178:B:PRO:HB2	1:179:B:ALA:H	10	0.17
(1,2103)	1:178:B:PRO:HB3	1:179:B:ALA:H	10	0.17
(1,2096)	1:176:B:GLY:H	1:177:B:ASP:HB2	16	0.17
(1,2096)	1:176:B:GLY:H	1:177:B:ASP:HB3	16	0.17
(1,2094)	1:172:B:ALA:HA	1:178:B:PRO:HD2	13	0.17
(1,2094)	1:172:B:ALA:HA	1:178:B:PRO:HD3	13	0.17
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG11	9	0.17
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG12	9	0.17
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG13	9	0.17
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG21	9	0.17
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG22	9	0.17
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG23	9	0.17
(1,1918)	1:183:A:MET:HB2	1:183:A:MET:HE1	7	0.17
(1,1918)	1:183:A:MET:HB2	1:183:A:MET:HE2	7	0.17
(1,1918)	1:183:A:MET:HB2	1:183:A:MET:HE3	7	0.17
(1,1918)	1:183:A:MET:HB3	1:183:A:MET:HE1	7	0.17
(1,1918)	1:183:A:MET:HB3	1:183:A:MET:HE2	7	0.17
(1,1918)	1:183:A:MET:HB3	1:183:A:MET:HE3	7	0.17
(1,1918)	1:183:A:MET:HB2	1:183:A:MET:HE1	17	0.17
(1,1918)	1:183:A:MET:HB2	1:183:A:MET:HE2	17	0.17
(1,1918)	1:183:A:MET:HB2	1:183:A:MET:HE3	17	0.17
(1,1918)	1:183:A:MET:HB3	1:183:A:MET:HE1	17	0.17
(1,1918)	1:183:A:MET:HB3	1:183:A:MET:HE2	17	0.17
(1,1918)	1:183:A:MET:HB3	1:183:A:MET:HE3	17	0.17
(1,1911)	1:178:A:PRO:HB2	1:180:A:PHE:H	16	0.17
(1,1911)	1:178:A:PRO:HB3	1:180:A:PHE:H	16	0.17
(1,1910)	1:178:A:PRO:HB2	1:179:A:ALA:H	10	0.17
(1,1910)	1:178:A:PRO:HB3	1:179:A:ALA:H	10	0.17
(1,1903)	1:172:A:ALA:HB1	1:173:A:PRO:HD2	3	0.17
(1,1903)	1:172:A:ALA:HB1	1:173:A:PRO:HD3	3	0.17
(1,1903)	1:172:A:ALA:HB2	1:173:A:PRO:HD2	3	0.17
(1,1903)	1:172:A:ALA:HB2	1:173:A:PRO:HD3	3	0.17
(1,1903)	1:172:A:ALA:HB3	1:173:A:PRO:HD2	3	0.17
(1,1903)	1:172:A:ALA:HB3	1:173:A:PRO:HD3	3	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1903)	1:172:A:ALA:HB1	1:173:A:PRO:HD2	6	0.17
(1,1903)	1:172:A:ALA:HB1	1:173:A:PRO:HD3	6	0.17
(1,1903)	1:172:A:ALA:HB2	1:173:A:PRO:HD2	6	0.17
(1,1903)	1:172:A:ALA:HB2	1:173:A:PRO:HD3	6	0.17
(1,1903)	1:172:A:ALA:HB3	1:173:A:PRO:HD2	6	0.17
(1,1903)	1:172:A:ALA:HB3	1:173:A:PRO:HD3	6	0.17
(1,1902)	1:172:A:ALA:HA	1:178:A:PRO:HD2	14	0.17
(1,1902)	1:172:A:ALA:HA	1:178:A:PRO:HD3	14	0.17
(1,1889)	1:156:A:VAL:HG11	1:157:A:PRO:HD2	13	0.17
(1,1889)	1:156:A:VAL:HG11	1:157:A:PRO:HD3	13	0.17
(1,1889)	1:156:A:VAL:HG12	1:157:A:PRO:HD2	13	0.17
(1,1889)	1:156:A:VAL:HG12	1:157:A:PRO:HD3	13	0.17
(1,1889)	1:156:A:VAL:HG13	1:157:A:PRO:HD2	13	0.17
(1,1889)	1:156:A:VAL:HG13	1:157:A:PRO:HD3	13	0.17
(1,1889)	1:156:A:VAL:HG11	1:157:A:PRO:HD2	19	0.17
(1,1889)	1:156:A:VAL:HG11	1:157:A:PRO:HD3	19	0.17
(1,1889)	1:156:A:VAL:HG12	1:157:A:PRO:HD2	19	0.17
(1,1889)	1:156:A:VAL:HG12	1:157:A:PRO:HD3	19	0.17
(1,1889)	1:156:A:VAL:HG13	1:157:A:PRO:HD2	19	0.17
(1,1889)	1:156:A:VAL:HG13	1:157:A:PRO:HD3	19	0.17
(1,1889)	1:156:A:VAL:HG11	1:157:A:PRO:HD2	20	0.17
(1,1889)	1:156:A:VAL:HG11	1:157:A:PRO:HD3	20	0.17
(1,1889)	1:156:A:VAL:HG12	1:157:A:PRO:HD2	20	0.17
(1,1889)	1:156:A:VAL:HG12	1:157:A:PRO:HD3	20	0.17
(1,1889)	1:156:A:VAL:HG13	1:157:A:PRO:HD2	20	0.17
(1,1889)	1:156:A:VAL:HG13	1:157:A:PRO:HD3	20	0.17
(1,1885)	1:155:A:ALA:HB1	1:157:A:PRO:HD2	10	0.17
(1,1885)	1:155:A:ALA:HB1	1:157:A:PRO:HD3	10	0.17
(1,1885)	1:155:A:ALA:HB2	1:157:A:PRO:HD2	10	0.17
(1,1885)	1:155:A:ALA:HB2	1:157:A:PRO:HD3	10	0.17
(1,1885)	1:155:A:ALA:HB3	1:157:A:PRO:HD2	10	0.17
(1,1885)	1:155:A:ALA:HB3	1:157:A:PRO:HD3	10	0.17
(1,1885)	1:155:A:ALA:HB1	1:157:A:PRO:HD2	20	0.17
(1,1885)	1:155:A:ALA:HB1	1:157:A:PRO:HD3	20	0.17
(1,1885)	1:155:A:ALA:HB2	1:157:A:PRO:HD2	20	0.17
(1,1885)	1:155:A:ALA:HB2	1:157:A:PRO:HD3	20	0.17
(1,1885)	1:155:A:ALA:HB3	1:157:A:PRO:HD2	20	0.17
(1,1885)	1:155:A:ALA:HB3	1:157:A:PRO:HD3	20	0.17
(1,1842)	1:121:A:CYS:HB2	1:189:A:CYS:H	17	0.17
(1,1842)	1:121:A:CYS:HB3	1:189:A:CYS:H	17	0.17
(1,1835)	1:109:A:LEU:HB2	1:110:A:LEU:HD11	5	0.17
(1,1835)	1:109:A:LEU:HB2	1:110:A:LEU:HD12	5	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1835)	1:109:A:LEU:HB2	1:110:A:LEU:HD13	5	0.17
(1,1835)	1:109:A:LEU:HB3	1:110:A:LEU:HD11	5	0.17
(1,1835)	1:109:A:LEU:HB3	1:110:A:LEU:HD12	5	0.17
(1,1835)	1:109:A:LEU:HB3	1:110:A:LEU:HD13	5	0.17
(1,1835)	1:109:A:LEU:HB2	1:110:A:LEU:HD11	17	0.17
(1,1835)	1:109:A:LEU:HB2	1:110:A:LEU:HD12	17	0.17
(1,1835)	1:109:A:LEU:HB2	1:110:A:LEU:HD13	17	0.17
(1,1835)	1:109:A:LEU:HB3	1:110:A:LEU:HD11	17	0.17
(1,1835)	1:109:A:LEU:HB3	1:110:A:LEU:HD12	17	0.17
(1,1835)	1:109:A:LEU:HB3	1:110:A:LEU:HD13	17	0.17
(1,1819)	1:95:C:SER:HB2	1:101:C:LEU:H	1	0.17
(1,1819)	1:95:C:SER:HB3	1:101:C:LEU:H	1	0.17
(1,1819)	1:95:C:SER:HB2	1:101:C:LEU:H	4	0.17
(1,1819)	1:95:C:SER:HB3	1:101:C:LEU:H	4	0.17
(1,1817)	1:95:A:SER:HB2	1:101:A:LEU:H	7	0.17
(1,1817)	1:95:A:SER:HB3	1:101:A:LEU:H	7	0.17
(1,1776)	1:125:C:LYS:H	1:126:C:ILE:HG21	9	0.17
(1,1776)	1:125:C:LYS:H	1:126:C:ILE:HG22	9	0.17
(1,1776)	1:125:C:LYS:H	1:126:C:ILE:HG23	9	0.17
(1,1692)	1:120:A:CYS:H	1:192:A:VAL:HG11	18	0.17
(1,1692)	1:120:A:CYS:H	1:192:A:VAL:HG12	18	0.17
(1,1692)	1:120:A:CYS:H	1:192:A:VAL:HG13	18	0.17
(1,1688)	1:90:C:THR:H	1:91:C:THR:HB	10	0.17
(1,1686)	1:90:A:THR:H	1:91:A:THR:HB	8	0.17
(1,1620)	1:129:A:GLU:H	1:131:A:ILE:H	5	0.17
(1,1616)	1:116:C:ALA:H	1:119:C:THR:HB	2	0.17
(1,1616)	1:116:C:ALA:H	1:119:C:THR:HB	14	0.17
(1,1615)	1:116:B:ALA:H	1:119:B:THR:HB	8	0.17
(1,1615)	1:116:B:ALA:H	1:119:B:THR:HB	14	0.17
(1,1614)	1:116:A:ALA:H	1:119:A:THR:HB	8	0.17
(1,1614)	1:116:A:ALA:H	1:119:A:THR:HB	11	0.17
(1,1614)	1:116:A:ALA:H	1:119:A:THR:HB	15	0.17
(1,1564)	1:145:C:GLN:HA	1:151:C:GLN:H	4	0.17
(1,1562)	1:145:A:GLN:HA	1:151:A:GLN:H	4	0.17
(1,1562)	1:145:A:GLN:HA	1:151:A:GLN:H	9	0.17
(1,1562)	1:145:A:GLN:HA	1:151:A:GLN:H	11	0.17
(1,1554)	1:156:C:VAL:HB	1:167:C:ARG:H	14	0.17
(1,1551)	1:167:C:ARG:H	1:171:C:SER:HA	17	0.17
(1,1550)	1:167:B:ARG:H	1:171:B:SER:HA	17	0.17
(1,1549)	1:167:A:ARG:H	1:171:A:SER:HA	17	0.17
(1,1540)	1:136:B:ALA:HB1	1:140:B:LYS:H	17	0.17
(1,1540)	1:136:B:ALA:HB2	1:140:B:LYS:H	17	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1540)	1:136:B:ALA:HB3	1:140:B:LYS:H	17	0.17
(1,1534)	1:122:B:TYR:H	1:189:B:CYS:HB2	17	0.17
(1,1534)	1:122:B:TYR:H	1:189:B:CYS:HB3	17	0.17
(1,1533)	1:122:A:TYR:H	1:189:A:CYS:HB2	3	0.17
(1,1533)	1:122:A:TYR:H	1:189:A:CYS:HB3	3	0.17
(1,1533)	1:122:A:TYR:H	1:189:A:CYS:HB2	20	0.17
(1,1533)	1:122:A:TYR:H	1:189:A:CYS:HB3	20	0.17
(1,1511)	1:137:A:LEU:H	1:137:A:LEU:HG	16	0.17
(1,1460)	1:179:C:ALA:HA	1:180:C:PHE:H	4	0.17
(1,1459)	1:179:B:ALA:HA	1:180:B:PHE:H	4	0.17
(1,1459)	1:179:B:ALA:HA	1:180:B:PHE:H	10	0.17
(1,1458)	1:179:A:ALA:HA	1:180:A:PHE:H	4	0.17
(1,1458)	1:179:A:ALA:HA	1:180:A:PHE:H	10	0.17
(1,1432)	1:111:C:ILE:H	1:123:C:ILE:HG21	2	0.17
(1,1432)	1:111:C:ILE:H	1:123:C:ILE:HG22	2	0.17
(1,1432)	1:111:C:ILE:H	1:123:C:ILE:HG23	2	0.17
(1,1430)	1:111:A:ILE:H	1:123:A:ILE:HG21	2	0.17
(1,1430)	1:111:A:ILE:H	1:123:A:ILE:HG22	2	0.17
(1,1430)	1:111:A:ILE:H	1:123:A:ILE:HG23	2	0.17
(1,1410)	1:152:C:ALA:HB1	1:153:C:LYS:H	4	0.17
(1,1410)	1:152:C:ALA:HB2	1:153:C:LYS:H	4	0.17
(1,1410)	1:152:C:ALA:HB3	1:153:C:LYS:H	4	0.17
(1,1410)	1:152:C:ALA:HB1	1:153:C:LYS:H	6	0.17
(1,1410)	1:152:C:ALA:HB2	1:153:C:LYS:H	6	0.17
(1,1410)	1:152:C:ALA:HB3	1:153:C:LYS:H	6	0.17
(1,1409)	1:152:B:ALA:HB1	1:153:B:LYS:H	6	0.17
(1,1409)	1:152:B:ALA:HB2	1:153:B:LYS:H	6	0.17
(1,1409)	1:152:B:ALA:HB3	1:153:B:LYS:H	6	0.17
(1,1408)	1:152:A:ALA:HB1	1:153:A:LYS:H	6	0.17
(1,1408)	1:152:A:ALA:HB2	1:153:A:LYS:H	6	0.17
(1,1408)	1:152:A:ALA:HB3	1:153:A:LYS:H	6	0.17
(1,1408)	1:152:A:ALA:HB1	1:153:A:LYS:H	11	0.17
(1,1408)	1:152:A:ALA:HB2	1:153:A:LYS:H	11	0.17
(1,1408)	1:152:A:ALA:HB3	1:153:A:LYS:H	11	0.17
(1,1387)	1:141:A:VAL:HG21	1:142:A:HIS:H	13	0.17
(1,1387)	1:141:A:VAL:HG22	1:142:A:HIS:H	13	0.17
(1,1387)	1:141:A:VAL:HG23	1:142:A:HIS:H	13	0.17
(1,1278)	1:109:C:LEU:H	1:109:C:LEU:HG	19	0.17
(1,1277)	1:109:B:LEU:H	1:109:B:LEU:HG	19	0.17
(1,1154)	1:156:A:VAL:HG11	1:158:A:THR:H	6	0.17
(1,1154)	1:156:A:VAL:HG12	1:158:A:THR:H	6	0.17
(1,1154)	1:156:A:VAL:HG13	1:158:A:THR:H	6	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1100)	1:167:C:ARG:H	1:167:C:ARG:HB2	15	0.17
(1,1100)	1:167:C:ARG:H	1:167:C:ARG:HB2	19	0.17
(1,1099)	1:167:B:ARG:H	1:167:B:ARG:HB2	19	0.17
(1,1098)	1:167:A:ARG:H	1:167:A:ARG:HB2	15	0.17
(1,1098)	1:167:A:ARG:H	1:167:A:ARG:HB2	19	0.17
(1,1097)	1:157:C:PRO:HA	1:158:C:THR:H	7	0.17
(1,1097)	1:157:C:PRO:HA	1:158:C:THR:H	12	0.17
(1,1096)	1:157:B:PRO:HA	1:158:B:THR:H	11	0.17
(1,1096)	1:157:B:PRO:HA	1:158:B:THR:H	12	0.17
(1,1095)	1:157:A:PRO:HA	1:158:A:THR:H	3	0.17
(1,1095)	1:157:A:PRO:HA	1:158:A:THR:H	7	0.17
(1,1095)	1:157:A:PRO:HA	1:158:A:THR:H	11	0.17
(1,1095)	1:157:A:PRO:HA	1:158:A:THR:H	12	0.17
(1,1095)	1:157:A:PRO:HA	1:158:A:THR:H	16	0.17
(1,1071)	1:139:A:ARG:H	1:141:A:VAL:HB	1	0.17
(1,1071)	1:139:A:ARG:H	1:141:A:VAL:HB	7	0.17
(1,1049)	1:137:C:LEU:HG	1:138:C:THR:H	8	0.17
(1,1048)	1:137:B:LEU:HG	1:138:B:THR:H	4	0.17
(1,1047)	1:137:A:LEU:HG	1:138:A:THR:H	7	0.17
(1,1047)	1:137:A:LEU:HG	1:138:A:THR:H	8	0.17
(1,1047)	1:137:A:LEU:HG	1:138:A:THR:H	15	0.17
(1,1047)	1:137:A:LEU:HG	1:138:A:THR:H	16	0.17
(1,1047)	1:137:A:LEU:HG	1:138:A:THR:H	19	0.17
(1,1036)	1:188:A:LEU:HD21	1:134:B:LEU:H	4	0.17
(1,1036)	1:188:A:LEU:HD22	1:134:B:LEU:H	4	0.17
(1,1036)	1:188:A:LEU:HD23	1:134:B:LEU:H	4	0.17
(1,965)	1:110:A:LEU:HD11	1:125:A:LYS:HB3	10	0.17
(1,965)	1:110:A:LEU:HD12	1:125:A:LYS:HB3	10	0.17
(1,965)	1:110:A:LEU:HD13	1:125:A:LYS:HB3	10	0.17
(1,942)	1:101:A:LEU:HD11	1:188:A:LEU:HD21	3	0.17
(1,942)	1:101:A:LEU:HD11	1:188:A:LEU:HD22	3	0.17
(1,942)	1:101:A:LEU:HD11	1:188:A:LEU:HD23	3	0.17
(1,942)	1:101:A:LEU:HD12	1:188:A:LEU:HD21	3	0.17
(1,942)	1:101:A:LEU:HD12	1:188:A:LEU:HD22	3	0.17
(1,942)	1:101:A:LEU:HD12	1:188:A:LEU:HD23	3	0.17
(1,942)	1:101:A:LEU:HD13	1:188:A:LEU:HD21	3	0.17
(1,942)	1:101:A:LEU:HD13	1:188:A:LEU:HD22	3	0.17
(1,942)	1:101:A:LEU:HD13	1:188:A:LEU:HD23	3	0.17
(1,928)	1:178:A:PRO:HG2	1:181:A:LEU:HD21	14	0.17
(1,928)	1:178:A:PRO:HG2	1:181:A:LEU:HD22	14	0.17
(1,928)	1:178:A:PRO:HG2	1:181:A:LEU:HD23	14	0.17
(1,928)	1:178:A:PRO:HG3	1:181:A:LEU:HD21	14	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,928)	1:178:A:PRO:HG3	1:181:A:LEU:HD22	14	0.17
(1,928)	1:178:A:PRO:HG3	1:181:A:LEU:HD23	14	0.17
(1,928)	1:178:A:PRO:HG2	1:181:A:LEU:HD21	19	0.17
(1,928)	1:178:A:PRO:HG2	1:181:A:LEU:HD22	19	0.17
(1,928)	1:178:A:PRO:HG2	1:181:A:LEU:HD23	19	0.17
(1,928)	1:178:A:PRO:HG3	1:181:A:LEU:HD21	19	0.17
(1,928)	1:178:A:PRO:HG3	1:181:A:LEU:HD22	19	0.17
(1,928)	1:178:A:PRO:HG3	1:181:A:LEU:HD23	19	0.17
(1,893)	1:165:C:GLU:HB2	1:167:C:ARG:HG2	19	0.17
(1,893)	1:165:C:GLU:HB2	1:167:C:ARG:HG3	19	0.17
(1,892)	1:165:B:GLU:HB2	1:167:B:ARG:HG2	19	0.17
(1,892)	1:165:B:GLU:HB2	1:167:B:ARG:HG3	19	0.17
(1,890)	1:152:C:ALA:HA	1:157:C:PRO:HG2	4	0.17
(1,890)	1:152:C:ALA:HA	1:157:C:PRO:HG3	4	0.17
(1,815)	1:176:C:GLY:H	1:177:C:ASP:HB2	16	0.17
(1,814)	1:176:B:GLY:H	1:177:B:ASP:HB2	16	0.17
(1,813)	1:176:A:GLY:H	1:177:A:ASP:HB2	16	0.17
(1,811)	1:176:B:GLY:H	1:177:B:ASP:HB3	10	0.17
(1,810)	1:176:A:GLY:H	1:177:A:ASP:HB3	10	0.17
(1,792)	1:153:A:LYS:HE2	1:154:A:PRO:HG2	5	0.17
(1,792)	1:153:A:LYS:HE2	1:154:A:PRO:HG3	5	0.17
(1,792)	1:153:A:LYS:HE3	1:154:A:PRO:HG2	5	0.17
(1,792)	1:153:A:LYS:HE3	1:154:A:PRO:HG3	5	0.17
(1,783)	1:167:A:ARG:HD2	1:169:A:ALA:HB1	14	0.17
(1,783)	1:167:A:ARG:HD2	1:169:A:ALA:HB2	14	0.17
(1,783)	1:167:A:ARG:HD2	1:169:A:ALA:HB3	14	0.17
(1,783)	1:167:A:ARG:HD3	1:169:A:ALA:HB1	14	0.17
(1,783)	1:167:A:ARG:HD3	1:169:A:ALA:HB2	14	0.17
(1,783)	1:167:A:ARG:HD3	1:169:A:ALA:HB3	14	0.17
(1,755)	1:189:C:CYS:H	1:192:C:VAL:HG11	14	0.17
(1,755)	1:189:C:CYS:H	1:192:C:VAL:HG12	14	0.17
(1,755)	1:189:C:CYS:H	1:192:C:VAL:HG13	14	0.17
(1,712)	1:141:A:VAL:HG21	1:144:A:PHE:HD1	9	0.17
(1,712)	1:141:A:VAL:HG21	1:144:A:PHE:HD2	9	0.17
(1,712)	1:141:A:VAL:HG22	1:144:A:PHE:HD1	9	0.17
(1,712)	1:141:A:VAL:HG22	1:144:A:PHE:HD2	9	0.17
(1,712)	1:141:A:VAL:HG23	1:144:A:PHE:HD1	9	0.17
(1,712)	1:141:A:VAL:HG23	1:144:A:PHE:HD2	9	0.17
(1,655)	1:172:C:ALA:HB1	1:173:C:PRO:HD3	2	0.17
(1,655)	1:172:C:ALA:HB2	1:173:C:PRO:HD3	2	0.17
(1,655)	1:172:C:ALA:HB3	1:173:C:PRO:HD3	2	0.17
(1,655)	1:172:C:ALA:HB1	1:173:C:PRO:HD3	9	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,655)	1:172:C:ALA:HB2	1:173:C:PRO:HD3	9	0.17
(1,655)	1:172:C:ALA:HB3	1:173:C:PRO:HD3	9	0.17
(1,655)	1:172:C:ALA:HB1	1:173:C:PRO:HD3	12	0.17
(1,655)	1:172:C:ALA:HB2	1:173:C:PRO:HD3	12	0.17
(1,655)	1:172:C:ALA:HB3	1:173:C:PRO:HD3	12	0.17
(1,655)	1:172:C:ALA:HB1	1:173:C:PRO:HD3	14	0.17
(1,655)	1:172:C:ALA:HB2	1:173:C:PRO:HD3	14	0.17
(1,655)	1:172:C:ALA:HB3	1:173:C:PRO:HD3	14	0.17
(1,655)	1:172:C:ALA:HB1	1:173:C:PRO:HD3	15	0.17
(1,655)	1:172:C:ALA:HB2	1:173:C:PRO:HD3	15	0.17
(1,655)	1:172:C:ALA:HB3	1:173:C:PRO:HD3	15	0.17
(1,655)	1:172:C:ALA:HB1	1:173:C:PRO:HD3	20	0.17
(1,655)	1:172:C:ALA:HB2	1:173:C:PRO:HD3	20	0.17
(1,655)	1:172:C:ALA:HB3	1:173:C:PRO:HD3	20	0.17
(1,654)	1:172:B:ALA:HB1	1:173:B:PRO:HD3	2	0.17
(1,654)	1:172:B:ALA:HB2	1:173:B:PRO:HD3	2	0.17
(1,654)	1:172:B:ALA:HB3	1:173:B:PRO:HD3	2	0.17
(1,654)	1:172:B:ALA:HB1	1:173:B:PRO:HD3	9	0.17
(1,654)	1:172:B:ALA:HB2	1:173:B:PRO:HD3	9	0.17
(1,654)	1:172:B:ALA:HB3	1:173:B:PRO:HD3	9	0.17
(1,654)	1:172:B:ALA:HB1	1:173:B:PRO:HD3	12	0.17
(1,654)	1:172:B:ALA:HB2	1:173:B:PRO:HD3	12	0.17
(1,654)	1:172:B:ALA:HB3	1:173:B:PRO:HD3	12	0.17
(1,654)	1:172:B:ALA:HB1	1:173:B:PRO:HD3	14	0.17
(1,654)	1:172:B:ALA:HB2	1:173:B:PRO:HD3	14	0.17
(1,654)	1:172:B:ALA:HB3	1:173:B:PRO:HD3	14	0.17
(1,654)	1:172:B:ALA:HB1	1:173:B:PRO:HD3	15	0.17
(1,654)	1:172:B:ALA:HB2	1:173:B:PRO:HD3	15	0.17
(1,654)	1:172:B:ALA:HB3	1:173:B:PRO:HD3	15	0.17
(1,654)	1:172:B:ALA:HB1	1:173:B:PRO:HD3	17	0.17
(1,654)	1:172:B:ALA:HB2	1:173:B:PRO:HD3	17	0.17
(1,654)	1:172:B:ALA:HB3	1:173:B:PRO:HD3	17	0.17
(1,654)	1:172:B:ALA:HB1	1:173:B:PRO:HD3	19	0.17
(1,654)	1:172:B:ALA:HB2	1:173:B:PRO:HD3	19	0.17
(1,654)	1:172:B:ALA:HB3	1:173:B:PRO:HD3	19	0.17
(1,654)	1:172:B:ALA:HB1	1:173:B:PRO:HD3	20	0.17
(1,654)	1:172:B:ALA:HB2	1:173:B:PRO:HD3	20	0.17
(1,654)	1:172:B:ALA:HB3	1:173:B:PRO:HD3	20	0.17
(1,653)	1:172:A:ALA:HB1	1:173:A:PRO:HD3	8	0.17
(1,653)	1:172:A:ALA:HB2	1:173:A:PRO:HD3	8	0.17
(1,653)	1:172:A:ALA:HB3	1:173:A:PRO:HD3	8	0.17
(1,653)	1:172:A:ALA:HB1	1:173:A:PRO:HD3	9	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,653)	1:172:A:ALA:HB2	1:173:A:PRO:HD3	9	0.17
(1,653)	1:172:A:ALA:HB3	1:173:A:PRO:HD3	9	0.17
(1,653)	1:172:A:ALA:HB1	1:173:A:PRO:HD3	14	0.17
(1,653)	1:172:A:ALA:HB2	1:173:A:PRO:HD3	14	0.17
(1,653)	1:172:A:ALA:HB3	1:173:A:PRO:HD3	14	0.17
(1,653)	1:172:A:ALA:HB1	1:173:A:PRO:HD3	15	0.17
(1,653)	1:172:A:ALA:HB2	1:173:A:PRO:HD3	15	0.17
(1,653)	1:172:A:ALA:HB3	1:173:A:PRO:HD3	15	0.17
(1,653)	1:172:A:ALA:HB1	1:173:A:PRO:HD3	20	0.17
(1,653)	1:172:A:ALA:HB2	1:173:A:PRO:HD3	20	0.17
(1,653)	1:172:A:ALA:HB3	1:173:A:PRO:HD3	20	0.17
(1,635)	1:96:A:ILE:HG21	1:100:A:GLY:H	7	0.17
(1,635)	1:96:A:ILE:HG22	1:100:A:GLY:H	7	0.17
(1,635)	1:96:A:ILE:HG23	1:100:A:GLY:H	7	0.17
(1,575)	1:193:A:PRO:HA	1:194:A:LEU:HD21	13	0.17
(1,575)	1:193:A:PRO:HA	1:194:A:LEU:HD22	13	0.17
(1,575)	1:193:A:PRO:HA	1:194:A:LEU:HD23	13	0.17
(1,451)	1:95:A:SER:HB2	1:101:A:LEU:HD21	5	0.17
(1,451)	1:95:A:SER:HB2	1:101:A:LEU:HD22	5	0.17
(1,451)	1:95:A:SER:HB2	1:101:A:LEU:HD23	5	0.17
(1,451)	1:95:A:SER:HB3	1:101:A:LEU:HD21	5	0.17
(1,451)	1:95:A:SER:HB3	1:101:A:LEU:HD22	5	0.17
(1,451)	1:95:A:SER:HB3	1:101:A:LEU:HD23	5	0.17
(1,451)	1:95:A:SER:HB2	1:101:A:LEU:HD21	20	0.17
(1,451)	1:95:A:SER:HB2	1:101:A:LEU:HD22	20	0.17
(1,451)	1:95:A:SER:HB2	1:101:A:LEU:HD23	20	0.17
(1,451)	1:95:A:SER:HB3	1:101:A:LEU:HD21	20	0.17
(1,451)	1:95:A:SER:HB3	1:101:A:LEU:HD22	20	0.17
(1,451)	1:95:A:SER:HB3	1:101:A:LEU:HD23	20	0.17
(1,437)	1:183:C:MET:HE1	1:186:C:SER:HA	3	0.17
(1,437)	1:183:C:MET:HE2	1:186:C:SER:HA	3	0.17
(1,437)	1:183:C:MET:HE3	1:186:C:SER:HA	3	0.17
(1,437)	1:183:C:MET:HE1	1:186:C:SER:HA	5	0.17
(1,437)	1:183:C:MET:HE2	1:186:C:SER:HA	5	0.17
(1,437)	1:183:C:MET:HE3	1:186:C:SER:HA	5	0.17
(1,437)	1:183:C:MET:HE1	1:186:C:SER:HA	16	0.17
(1,437)	1:183:C:MET:HE2	1:186:C:SER:HA	16	0.17
(1,437)	1:183:C:MET:HE3	1:186:C:SER:HA	16	0.17
(1,437)	1:183:C:MET:HE1	1:186:C:SER:HA	20	0.17
(1,437)	1:183:C:MET:HE2	1:186:C:SER:HA	20	0.17
(1,437)	1:183:C:MET:HE3	1:186:C:SER:HA	20	0.17
(1,436)	1:183:B:MET:HE1	1:186:B:SER:HA	5	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,436)	1:183:B:MET:HE2	1:186:B:SER:HA	5	0.17
(1,436)	1:183:B:MET:HE3	1:186:B:SER:HA	5	0.17
(1,436)	1:183:B:MET:HE1	1:186:B:SER:HA	15	0.17
(1,436)	1:183:B:MET:HE2	1:186:B:SER:HA	15	0.17
(1,436)	1:183:B:MET:HE3	1:186:B:SER:HA	15	0.17
(1,436)	1:183:B:MET:HE1	1:186:B:SER:HA	16	0.17
(1,436)	1:183:B:MET:HE2	1:186:B:SER:HA	16	0.17
(1,436)	1:183:B:MET:HE3	1:186:B:SER:HA	16	0.17
(1,436)	1:183:B:MET:HE1	1:186:B:SER:HA	20	0.17
(1,436)	1:183:B:MET:HE2	1:186:B:SER:HA	20	0.17
(1,436)	1:183:B:MET:HE3	1:186:B:SER:HA	20	0.17
(1,435)	1:183:A:MET:HE1	1:186:A:SER:HA	14	0.17
(1,435)	1:183:A:MET:HE2	1:186:A:SER:HA	14	0.17
(1,435)	1:183:A:MET:HE3	1:186:A:SER:HA	14	0.17
(1,397)	1:109:C:LEU:HG	1:111:C:ILE:HD11	19	0.17
(1,397)	1:109:C:LEU:HG	1:111:C:ILE:HD12	19	0.17
(1,397)	1:109:C:LEU:HG	1:111:C:ILE:HD13	19	0.17
(1,396)	1:109:B:LEU:HG	1:111:B:ILE:HD11	19	0.17
(1,396)	1:109:B:LEU:HG	1:111:B:ILE:HD12	19	0.17
(1,396)	1:109:B:LEU:HG	1:111:B:ILE:HD13	19	0.17
(1,371)	1:96:A:ILE:HD11	1:102:A:VAL:HB	1	0.17
(1,371)	1:96:A:ILE:HD12	1:102:A:VAL:HB	1	0.17
(1,371)	1:96:A:ILE:HD13	1:102:A:VAL:HB	1	0.17
(1,363)	1:131:A:ILE:HD11	1:183:C:MET:HG2	5	0.17
(1,363)	1:131:A:ILE:HD11	1:183:C:MET:HG3	5	0.17
(1,363)	1:131:A:ILE:HD12	1:183:C:MET:HG2	5	0.17
(1,363)	1:131:A:ILE:HD12	1:183:C:MET:HG3	5	0.17
(1,363)	1:131:A:ILE:HD13	1:183:C:MET:HG2	5	0.17
(1,363)	1:131:A:ILE:HD13	1:183:C:MET:HG3	5	0.17
(1,228)	1:96:C:ILE:HD11	1:102:C:VAL:HG11	18	0.17
(1,228)	1:96:C:ILE:HD11	1:102:C:VAL:HG12	18	0.17
(1,228)	1:96:C:ILE:HD11	1:102:C:VAL:HG13	18	0.17
(1,228)	1:96:C:ILE:HD12	1:102:C:VAL:HG11	18	0.17
(1,228)	1:96:C:ILE:HD12	1:102:C:VAL:HG12	18	0.17
(1,228)	1:96:C:ILE:HD12	1:102:C:VAL:HG13	18	0.17
(1,228)	1:96:C:ILE:HD13	1:102:C:VAL:HG11	18	0.17
(1,228)	1:96:C:ILE:HD13	1:102:C:VAL:HG12	18	0.17
(1,228)	1:96:C:ILE:HD13	1:102:C:VAL:HG13	18	0.17
(1,227)	1:96:B:ILE:HD11	1:102:B:VAL:HG11	18	0.17
(1,227)	1:96:B:ILE:HD11	1:102:B:VAL:HG12	18	0.17
(1,227)	1:96:B:ILE:HD11	1:102:B:VAL:HG13	18	0.17
(1,227)	1:96:B:ILE:HD12	1:102:B:VAL:HG11	18	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,227)	1:96:B:ILE:HD12	1:102:B:VAL:HG12	18	0.17
(1,227)	1:96:B:ILE:HD12	1:102:B:VAL:HG13	18	0.17
(1,227)	1:96:B:ILE:HD13	1:102:B:VAL:HG11	18	0.17
(1,227)	1:96:B:ILE:HD13	1:102:B:VAL:HG12	18	0.17
(1,227)	1:96:B:ILE:HD13	1:102:B:VAL:HG13	18	0.17
(1,219)	1:96:A:ILE:HG21	1:141:A:VAL:HG11	7	0.17
(1,219)	1:96:A:ILE:HG21	1:141:A:VAL:HG12	7	0.17
(1,219)	1:96:A:ILE:HG21	1:141:A:VAL:HG13	7	0.17
(1,219)	1:96:A:ILE:HG22	1:141:A:VAL:HG11	7	0.17
(1,219)	1:96:A:ILE:HG22	1:141:A:VAL:HG12	7	0.17
(1,219)	1:96:A:ILE:HG22	1:141:A:VAL:HG13	7	0.17
(1,219)	1:96:A:ILE:HG23	1:141:A:VAL:HG11	7	0.17
(1,219)	1:96:A:ILE:HG23	1:141:A:VAL:HG12	7	0.17
(1,219)	1:96:A:ILE:HG23	1:141:A:VAL:HG13	7	0.17
(1,219)	1:96:A:ILE:HG21	1:141:A:VAL:HG11	13	0.17
(1,219)	1:96:A:ILE:HG21	1:141:A:VAL:HG12	13	0.17
(1,219)	1:96:A:ILE:HG21	1:141:A:VAL:HG13	13	0.17
(1,219)	1:96:A:ILE:HG22	1:141:A:VAL:HG11	13	0.17
(1,219)	1:96:A:ILE:HG22	1:141:A:VAL:HG12	13	0.17
(1,219)	1:96:A:ILE:HG22	1:141:A:VAL:HG13	13	0.17
(1,219)	1:96:A:ILE:HG23	1:141:A:VAL:HG11	13	0.17
(1,219)	1:96:A:ILE:HG23	1:141:A:VAL:HG12	13	0.17
(1,219)	1:96:A:ILE:HG23	1:141:A:VAL:HG13	13	0.17
(1,198)	1:109:A:LEU:H	1:110:A:LEU:HD21	6	0.17
(1,198)	1:109:A:LEU:H	1:110:A:LEU:HD22	6	0.17
(1,198)	1:109:A:LEU:H	1:110:A:LEU:HD23	6	0.17
(1,198)	1:109:A:LEU:H	1:110:A:LEU:HD21	7	0.17
(1,198)	1:109:A:LEU:H	1:110:A:LEU:HD22	7	0.17
(1,198)	1:109:A:LEU:H	1:110:A:LEU:HD23	7	0.17
(1,175)	1:179:A:ALA:HB1	1:181:A:LEU:HD21	1	0.17
(1,175)	1:179:A:ALA:HB1	1:181:A:LEU:HD22	1	0.17
(1,175)	1:179:A:ALA:HB1	1:181:A:LEU:HD23	1	0.17
(1,175)	1:179:A:ALA:HB2	1:181:A:LEU:HD21	1	0.17
(1,175)	1:179:A:ALA:HB2	1:181:A:LEU:HD22	1	0.17
(1,175)	1:179:A:ALA:HB2	1:181:A:LEU:HD23	1	0.17
(1,175)	1:179:A:ALA:HB3	1:181:A:LEU:HD21	1	0.17
(1,175)	1:179:A:ALA:HB3	1:181:A:LEU:HD22	1	0.17
(1,175)	1:179:A:ALA:HB3	1:181:A:LEU:HD23	1	0.17
(1,175)	1:179:A:ALA:HB1	1:181:A:LEU:HD21	9	0.17
(1,175)	1:179:A:ALA:HB1	1:181:A:LEU:HD22	9	0.17
(1,175)	1:179:A:ALA:HB1	1:181:A:LEU:HD23	9	0.17
(1,175)	1:179:A:ALA:HB2	1:181:A:LEU:HD21	9	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,175)	1:179:A:ALA:HB2	1:181:A:LEU:HD22	9	0.17
(1,175)	1:179:A:ALA:HB2	1:181:A:LEU:HD23	9	0.17
(1,175)	1:179:A:ALA:HB3	1:181:A:LEU:HD21	9	0.17
(1,175)	1:179:A:ALA:HB3	1:181:A:LEU:HD22	9	0.17
(1,175)	1:179:A:ALA:HB3	1:181:A:LEU:HD23	9	0.17
(1,175)	1:179:A:ALA:HB1	1:181:A:LEU:HD21	10	0.17
(1,175)	1:179:A:ALA:HB1	1:181:A:LEU:HD22	10	0.17
(1,175)	1:179:A:ALA:HB1	1:181:A:LEU:HD23	10	0.17
(1,175)	1:179:A:ALA:HB2	1:181:A:LEU:HD21	10	0.17
(1,175)	1:179:A:ALA:HB2	1:181:A:LEU:HD22	10	0.17
(1,175)	1:179:A:ALA:HB2	1:181:A:LEU:HD23	10	0.17
(1,175)	1:179:A:ALA:HB3	1:181:A:LEU:HD21	10	0.17
(1,175)	1:179:A:ALA:HB3	1:181:A:LEU:HD22	10	0.17
(1,175)	1:179:A:ALA:HB3	1:181:A:LEU:HD23	10	0.17
(1,157)	1:101:A:LEU:HD21	1:95:B:SER:HB2	3	0.17
(1,157)	1:101:A:LEU:HD21	1:95:B:SER:HB3	3	0.17
(1,157)	1:101:A:LEU:HD22	1:95:B:SER:HB2	3	0.17
(1,157)	1:101:A:LEU:HD22	1:95:B:SER:HB3	3	0.17
(1,157)	1:101:A:LEU:HD23	1:95:B:SER:HB2	3	0.17
(1,157)	1:101:A:LEU:HD23	1:95:B:SER:HB3	3	0.17
(1,124)	1:96:A:ILE:H	1:101:A:LEU:HD21	3	0.17
(1,124)	1:96:A:ILE:H	1:101:A:LEU:HD22	3	0.17
(1,124)	1:96:A:ILE:H	1:101:A:LEU:HD23	3	0.17
(1,2345)	1:183:C:MET:HB2	1:183:C:MET:HE1	7	0.16
(1,2345)	1:183:C:MET:HB2	1:183:C:MET:HE2	7	0.16
(1,2345)	1:183:C:MET:HB2	1:183:C:MET:HE3	7	0.16
(1,2345)	1:183:C:MET:HB3	1:183:C:MET:HE1	7	0.16
(1,2345)	1:183:C:MET:HB3	1:183:C:MET:HE2	7	0.16
(1,2345)	1:183:C:MET:HB3	1:183:C:MET:HE3	7	0.16
(1,2345)	1:183:C:MET:HB2	1:183:C:MET:HE1	8	0.16
(1,2345)	1:183:C:MET:HB2	1:183:C:MET:HE2	8	0.16
(1,2345)	1:183:C:MET:HB2	1:183:C:MET:HE3	8	0.16
(1,2345)	1:183:C:MET:HB3	1:183:C:MET:HE1	8	0.16
(1,2345)	1:183:C:MET:HB3	1:183:C:MET:HE2	8	0.16
(1,2345)	1:183:C:MET:HB3	1:183:C:MET:HE3	8	0.16
(1,2322)	1:176:C:GLY:H	1:177:C:ASP:HB2	16	0.16
(1,2322)	1:176:C:GLY:H	1:177:C:ASP:HB3	16	0.16
(1,2320)	1:172:C:ALA:HA	1:178:C:PRO:HD2	20	0.16
(1,2320)	1:172:C:ALA:HA	1:178:C:PRO:HD3	20	0.16
(1,2295)	1:155:C:ALA:HB1	1:157:C:PRO:HD2	7	0.16
(1,2295)	1:155:C:ALA:HB1	1:157:C:PRO:HD3	7	0.16
(1,2295)	1:155:C:ALA:HB2	1:157:C:PRO:HD2	7	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2295)	1:155:C:ALA:HB2	1:157:C:PRO:HD3	7	0.16
(1,2295)	1:155:C:ALA:HB3	1:157:C:PRO:HD2	7	0.16
(1,2295)	1:155:C:ALA:HB3	1:157:C:PRO:HD3	7	0.16
(1,2292)	1:154:C:PRO:HB2	1:167:C:ARG:H	17	0.16
(1,2292)	1:154:C:PRO:HB3	1:167:C:ARG:H	17	0.16
(1,2292)	1:154:C:PRO:HB2	1:167:C:ARG:H	20	0.16
(1,2292)	1:154:C:PRO:HB3	1:167:C:ARG:H	20	0.16
(1,2138)	1:188:B:LEU:HD11	1:134:C:LEU:H	10	0.16
(1,2138)	1:188:B:LEU:HD12	1:134:C:LEU:H	10	0.16
(1,2138)	1:188:B:LEU:HD13	1:134:C:LEU:H	10	0.16
(1,2138)	1:188:B:LEU:HD21	1:134:C:LEU:H	10	0.16
(1,2138)	1:188:B:LEU:HD22	1:134:C:LEU:H	10	0.16
(1,2138)	1:188:B:LEU:HD23	1:134:C:LEU:H	10	0.16
(1,2119)	1:183:B:MET:HB2	1:183:B:MET:HE1	7	0.16
(1,2119)	1:183:B:MET:HB2	1:183:B:MET:HE2	7	0.16
(1,2119)	1:183:B:MET:HB2	1:183:B:MET:HE3	7	0.16
(1,2119)	1:183:B:MET:HB3	1:183:B:MET:HE1	7	0.16
(1,2119)	1:183:B:MET:HB3	1:183:B:MET:HE2	7	0.16
(1,2119)	1:183:B:MET:HB3	1:183:B:MET:HE3	7	0.16
(1,2119)	1:183:B:MET:HB2	1:183:B:MET:HE1	8	0.16
(1,2119)	1:183:B:MET:HB2	1:183:B:MET:HE2	8	0.16
(1,2119)	1:183:B:MET:HB2	1:183:B:MET:HE3	8	0.16
(1,2119)	1:183:B:MET:HB3	1:183:B:MET:HE1	8	0.16
(1,2119)	1:183:B:MET:HB3	1:183:B:MET:HE2	8	0.16
(1,2119)	1:183:B:MET:HB3	1:183:B:MET:HE3	8	0.16
(1,2094)	1:172:B:ALA:HA	1:178:B:PRO:HD2	15	0.16
(1,2094)	1:172:B:ALA:HA	1:178:B:PRO:HD3	15	0.16
(1,2094)	1:172:B:ALA:HA	1:178:B:PRO:HD2	20	0.16
(1,2094)	1:172:B:ALA:HA	1:178:B:PRO:HD3	20	0.16
(1,2069)	1:155:B:ALA:HB1	1:157:B:PRO:HD2	7	0.16
(1,2069)	1:155:B:ALA:HB1	1:157:B:PRO:HD3	7	0.16
(1,2069)	1:155:B:ALA:HB2	1:157:B:PRO:HD2	7	0.16
(1,2069)	1:155:B:ALA:HB2	1:157:B:PRO:HD3	7	0.16
(1,2069)	1:155:B:ALA:HB3	1:157:B:PRO:HD2	7	0.16
(1,2069)	1:155:B:ALA:HB3	1:157:B:PRO:HD3	7	0.16
(1,2069)	1:155:B:ALA:HB1	1:157:B:PRO:HD2	15	0.16
(1,2069)	1:155:B:ALA:HB1	1:157:B:PRO:HD3	15	0.16
(1,2069)	1:155:B:ALA:HB2	1:157:B:PRO:HD2	15	0.16
(1,2069)	1:155:B:ALA:HB2	1:157:B:PRO:HD3	15	0.16
(1,2069)	1:155:B:ALA:HB3	1:157:B:PRO:HD2	15	0.16
(1,2069)	1:155:B:ALA:HB3	1:157:B:PRO:HD3	15	0.16
(1,2066)	1:154:B:PRO:HB2	1:167:B:ARG:H	20	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2066)	1:154:B:PRO:HB3	1:167:B:ARG:H	20	0.16
(1,2062)	1:153:B:LYS:H	1:154:B:PRO:HD2	14	0.16
(1,2062)	1:153:B:LYS:H	1:154:B:PRO:HD3	14	0.16
(1,2010)	1:121:B:CYS:HB2	1:189:B:CYS:H	1	0.16
(1,2010)	1:121:B:CYS:HB3	1:189:B:CYS:H	1	0.16
(1,2010)	1:121:B:CYS:HB2	1:189:B:CYS:H	15	0.16
(1,2010)	1:121:B:CYS:HB3	1:189:B:CYS:H	15	0.16
(1,1918)	1:183:A:MET:HB2	1:183:A:MET:HE1	8	0.16
(1,1918)	1:183:A:MET:HB2	1:183:A:MET:HE2	8	0.16
(1,1918)	1:183:A:MET:HB2	1:183:A:MET:HE3	8	0.16
(1,1918)	1:183:A:MET:HB3	1:183:A:MET:HE1	8	0.16
(1,1918)	1:183:A:MET:HB3	1:183:A:MET:HE2	8	0.16
(1,1918)	1:183:A:MET:HB3	1:183:A:MET:HE3	8	0.16
(1,1918)	1:183:A:MET:HB2	1:183:A:MET:HE1	18	0.16
(1,1918)	1:183:A:MET:HB2	1:183:A:MET:HE2	18	0.16
(1,1918)	1:183:A:MET:HB2	1:183:A:MET:HE3	18	0.16
(1,1918)	1:183:A:MET:HB3	1:183:A:MET:HE1	18	0.16
(1,1918)	1:183:A:MET:HB3	1:183:A:MET:HE2	18	0.16
(1,1918)	1:183:A:MET:HB3	1:183:A:MET:HE3	18	0.16
(1,1904)	1:176:A:GLY:H	1:177:A:ASP:HB2	6	0.16
(1,1904)	1:176:A:GLY:H	1:177:A:ASP:HB3	6	0.16
(1,1904)	1:176:A:GLY:H	1:177:A:ASP:HB2	16	0.16
(1,1904)	1:176:A:GLY:H	1:177:A:ASP:HB3	16	0.16
(1,1903)	1:172:A:ALA:HB1	1:173:A:PRO:HD2	5	0.16
(1,1903)	1:172:A:ALA:HB1	1:173:A:PRO:HD3	5	0.16
(1,1903)	1:172:A:ALA:HB2	1:173:A:PRO:HD2	5	0.16
(1,1903)	1:172:A:ALA:HB2	1:173:A:PRO:HD3	5	0.16
(1,1903)	1:172:A:ALA:HB3	1:173:A:PRO:HD2	5	0.16
(1,1903)	1:172:A:ALA:HB3	1:173:A:PRO:HD3	5	0.16
(1,1903)	1:172:A:ALA:HB1	1:173:A:PRO:HD2	7	0.16
(1,1903)	1:172:A:ALA:HB1	1:173:A:PRO:HD3	7	0.16
(1,1903)	1:172:A:ALA:HB2	1:173:A:PRO:HD2	7	0.16
(1,1903)	1:172:A:ALA:HB2	1:173:A:PRO:HD3	7	0.16
(1,1903)	1:172:A:ALA:HB3	1:173:A:PRO:HD2	7	0.16
(1,1903)	1:172:A:ALA:HB3	1:173:A:PRO:HD3	7	0.16
(1,1902)	1:172:A:ALA:HA	1:178:A:PRO:HD2	9	0.16
(1,1902)	1:172:A:ALA:HA	1:178:A:PRO:HD3	9	0.16
(1,1902)	1:172:A:ALA:HA	1:178:A:PRO:HD2	20	0.16
(1,1902)	1:172:A:ALA:HA	1:178:A:PRO:HD3	20	0.16
(1,1889)	1:156:A:VAL:HG11	1:157:A:PRO:HD2	17	0.16
(1,1889)	1:156:A:VAL:HG11	1:157:A:PRO:HD3	17	0.16
(1,1889)	1:156:A:VAL:HG12	1:157:A:PRO:HD2	17	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1889)	1:156:A:VAL:HG12	1:157:A:PRO:HD3	17	0.16
(1,1889)	1:156:A:VAL:HG13	1:157:A:PRO:HD2	17	0.16
(1,1889)	1:156:A:VAL:HG13	1:157:A:PRO:HD3	17	0.16
(1,1884)	1:154:A:PRO:HB2	1:167:A:ARG:H	20	0.16
(1,1884)	1:154:A:PRO:HB3	1:167:A:ARG:H	20	0.16
(1,1880)	1:153:A:LYS:H	1:154:A:PRO:HD2	14	0.16
(1,1880)	1:153:A:LYS:H	1:154:A:PRO:HD3	14	0.16
(1,1867)	1:134:A:LEU:H	1:188:C:LEU:HD11	10	0.16
(1,1867)	1:134:A:LEU:H	1:188:C:LEU:HD12	10	0.16
(1,1867)	1:134:A:LEU:H	1:188:C:LEU:HD13	10	0.16
(1,1867)	1:134:A:LEU:H	1:188:C:LEU:HD21	10	0.16
(1,1867)	1:134:A:LEU:H	1:188:C:LEU:HD22	10	0.16
(1,1867)	1:134:A:LEU:H	1:188:C:LEU:HD23	10	0.16
(1,1848)	1:124:A:MET:HB2	1:197:A:ILE:HD11	10	0.16
(1,1848)	1:124:A:MET:HB2	1:197:A:ILE:HD12	10	0.16
(1,1848)	1:124:A:MET:HB2	1:197:A:ILE:HD13	10	0.16
(1,1848)	1:124:A:MET:HB3	1:197:A:ILE:HD11	10	0.16
(1,1848)	1:124:A:MET:HB3	1:197:A:ILE:HD12	10	0.16
(1,1848)	1:124:A:MET:HB3	1:197:A:ILE:HD13	10	0.16
(1,1842)	1:121:A:CYS:HB2	1:189:A:CYS:H	19	0.16
(1,1842)	1:121:A:CYS:HB3	1:189:A:CYS:H	19	0.16
(1,1835)	1:109:A:LEU:HB2	1:110:A:LEU:HD11	14	0.16
(1,1835)	1:109:A:LEU:HB2	1:110:A:LEU:HD12	14	0.16
(1,1835)	1:109:A:LEU:HB2	1:110:A:LEU:HD13	14	0.16
(1,1835)	1:109:A:LEU:HB3	1:110:A:LEU:HD11	14	0.16
(1,1835)	1:109:A:LEU:HB3	1:110:A:LEU:HD12	14	0.16
(1,1835)	1:109:A:LEU:HB3	1:110:A:LEU:HD13	14	0.16
(1,1829)	1:96:A:ILE:HG12	1:102:A:VAL:HG21	4	0.16
(1,1829)	1:96:A:ILE:HG12	1:102:A:VAL:HG22	4	0.16
(1,1829)	1:96:A:ILE:HG12	1:102:A:VAL:HG23	4	0.16
(1,1829)	1:96:A:ILE:HG13	1:102:A:VAL:HG21	4	0.16
(1,1829)	1:96:A:ILE:HG13	1:102:A:VAL:HG22	4	0.16
(1,1829)	1:96:A:ILE:HG13	1:102:A:VAL:HG23	4	0.16
(1,1819)	1:95:C:SER:HB2	1:101:C:LEU:H	9	0.16
(1,1819)	1:95:C:SER:HB3	1:101:C:LEU:H	9	0.16
(1,1818)	1:95:B:SER:HB2	1:101:B:LEU:H	1	0.16
(1,1818)	1:95:B:SER:HB3	1:101:B:LEU:H	1	0.16
(1,1818)	1:95:B:SER:HB2	1:101:B:LEU:H	4	0.16
(1,1818)	1:95:B:SER:HB3	1:101:B:LEU:H	4	0.16
(1,1789)	1:96:C:ILE:HG21	1:101:C:LEU:H	18	0.16
(1,1789)	1:96:C:ILE:HG22	1:101:C:LEU:H	18	0.16
(1,1789)	1:96:C:ILE:HG23	1:101:C:LEU:H	18	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1787)	1:96:A:ILE:HG21	1:101:A:LEU:H	4	0.16
(1,1787)	1:96:A:ILE:HG22	1:101:A:LEU:H	4	0.16
(1,1787)	1:96:A:ILE:HG23	1:101:A:LEU:H	4	0.16
(1,1774)	1:125:A:LYS:H	1:126:A:ILE:HG21	1	0.16
(1,1774)	1:125:A:LYS:H	1:126:A:ILE:HG22	1	0.16
(1,1774)	1:125:A:LYS:H	1:126:A:ILE:HG23	1	0.16
(1,1770)	1:178:C:PRO:HD3	1:179:C:ALA:H	12	0.16
(1,1769)	1:178:B:PRO:HD3	1:179:B:ALA:H	12	0.16
(1,1692)	1:120:A:CYS:H	1:192:A:VAL:HG11	19	0.16
(1,1692)	1:120:A:CYS:H	1:192:A:VAL:HG12	19	0.16
(1,1692)	1:120:A:CYS:H	1:192:A:VAL:HG13	19	0.16
(1,1688)	1:90:C:THR:H	1:91:C:THR:HB	8	0.16
(1,1688)	1:90:C:THR:H	1:91:C:THR:HB	18	0.16
(1,1687)	1:90:B:THR:H	1:91:B:THR:HB	8	0.16
(1,1686)	1:90:A:THR:H	1:91:A:THR:HB	10	0.16
(1,1616)	1:116:C:ALA:H	1:119:C:THR:HB	7	0.16
(1,1616)	1:116:C:ALA:H	1:119:C:THR:HB	11	0.16
(1,1616)	1:116:C:ALA:H	1:119:C:THR:HB	12	0.16
(1,1616)	1:116:C:ALA:H	1:119:C:THR:HB	13	0.16
(1,1616)	1:116:C:ALA:H	1:119:C:THR:HB	17	0.16
(1,1616)	1:116:C:ALA:H	1:119:C:THR:HB	18	0.16
(1,1616)	1:116:C:ALA:H	1:119:C:THR:HB	19	0.16
(1,1616)	1:116:C:ALA:H	1:119:C:THR:HB	20	0.16
(1,1615)	1:116:B:ALA:H	1:119:B:THR:HB	2	0.16
(1,1615)	1:116:B:ALA:H	1:119:B:THR:HB	7	0.16
(1,1615)	1:116:B:ALA:H	1:119:B:THR:HB	11	0.16
(1,1615)	1:116:B:ALA:H	1:119:B:THR:HB	12	0.16
(1,1615)	1:116:B:ALA:H	1:119:B:THR:HB	13	0.16
(1,1615)	1:116:B:ALA:H	1:119:B:THR:HB	17	0.16
(1,1615)	1:116:B:ALA:H	1:119:B:THR:HB	18	0.16
(1,1615)	1:116:B:ALA:H	1:119:B:THR:HB	19	0.16
(1,1615)	1:116:B:ALA:H	1:119:B:THR:HB	20	0.16
(1,1610)	1:118:A:GLY:H	1:192:A:VAL:HG21	5	0.16
(1,1610)	1:118:A:GLY:H	1:192:A:VAL:HG22	5	0.16
(1,1610)	1:118:A:GLY:H	1:192:A:VAL:HG23	5	0.16
(1,1564)	1:145:C:GLN:HA	1:151:C:GLN:H	9	0.16
(1,1563)	1:145:B:GLN:HA	1:151:B:GLN:H	9	0.16
(1,1563)	1:145:B:GLN:HA	1:151:B:GLN:H	13	0.16
(1,1562)	1:145:A:GLN:HA	1:151:A:GLN:H	14	0.16
(1,1558)	1:155:C:ALA:HB1	1:167:C:ARG:H	4	0.16
(1,1558)	1:155:C:ALA:HB2	1:167:C:ARG:H	4	0.16
(1,1558)	1:155:C:ALA:HB3	1:167:C:ARG:H	4	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1556)	1:155:A:ALA:HB1	1:167:A:ARG:H	4	0.16
(1,1556)	1:155:A:ALA:HB2	1:167:A:ARG:H	4	0.16
(1,1556)	1:155:A:ALA:HB3	1:167:A:ARG:H	4	0.16
(1,1553)	1:156:B:VAL:HB	1:167:B:ARG:H	14	0.16
(1,1551)	1:167:C:ARG:H	1:171:C:SER:HA	4	0.16
(1,1550)	1:167:B:ARG:H	1:171:B:SER:HA	4	0.16
(1,1549)	1:167:A:ARG:H	1:171:A:SER:HA	4	0.16
(1,1549)	1:167:A:ARG:H	1:171:A:SER:HA	16	0.16
(1,1548)	1:167:C:ARG:H	1:170:C:GLY:HA2	3	0.16
(1,1548)	1:167:C:ARG:H	1:170:C:GLY:HA3	3	0.16
(1,1548)	1:167:C:ARG:H	1:170:C:GLY:HA2	10	0.16
(1,1548)	1:167:C:ARG:H	1:170:C:GLY:HA3	10	0.16
(1,1548)	1:167:C:ARG:H	1:170:C:GLY:HA2	17	0.16
(1,1548)	1:167:C:ARG:H	1:170:C:GLY:HA3	17	0.16
(1,1548)	1:167:C:ARG:H	1:170:C:GLY:HA2	18	0.16
(1,1548)	1:167:C:ARG:H	1:170:C:GLY:HA3	18	0.16
(1,1547)	1:167:B:ARG:H	1:170:B:GLY:HA2	10	0.16
(1,1547)	1:167:B:ARG:H	1:170:B:GLY:HA3	10	0.16
(1,1547)	1:167:B:ARG:H	1:170:B:GLY:HA2	17	0.16
(1,1547)	1:167:B:ARG:H	1:170:B:GLY:HA3	17	0.16
(1,1547)	1:167:B:ARG:H	1:170:B:GLY:HA2	18	0.16
(1,1547)	1:167:B:ARG:H	1:170:B:GLY:HA3	18	0.16
(1,1546)	1:167:A:ARG:H	1:170:A:GLY:HA2	17	0.16
(1,1546)	1:167:A:ARG:H	1:170:A:GLY:HA3	17	0.16
(1,1546)	1:167:A:ARG:H	1:170:A:GLY:HA2	18	0.16
(1,1546)	1:167:A:ARG:H	1:170:A:GLY:HA3	18	0.16
(1,1535)	1:122:C:TYR:H	1:189:C:CYS:HB2	17	0.16
(1,1535)	1:122:C:TYR:H	1:189:C:CYS:HB3	17	0.16
(1,1534)	1:122:B:TYR:H	1:189:B:CYS:HB2	18	0.16
(1,1534)	1:122:B:TYR:H	1:189:B:CYS:HB3	18	0.16
(1,1533)	1:122:A:TYR:H	1:189:A:CYS:HB2	1	0.16
(1,1533)	1:122:A:TYR:H	1:189:A:CYS:HB3	1	0.16
(1,1533)	1:122:A:TYR:H	1:189:A:CYS:HB2	2	0.16
(1,1533)	1:122:A:TYR:H	1:189:A:CYS:HB3	2	0.16
(1,1533)	1:122:A:TYR:H	1:189:A:CYS:HB2	14	0.16
(1,1533)	1:122:A:TYR:H	1:189:A:CYS:HB3	14	0.16
(1,1520)	1:178:A:PRO:HG2	1:179:A:ALA:H	12	0.16
(1,1520)	1:178:A:PRO:HG3	1:179:A:ALA:H	12	0.16
(1,1511)	1:137:A:LEU:H	1:137:A:LEU:HG	7	0.16
(1,1489)	1:131:A:ILE:HA	1:133:A:SER:H	17	0.16
(1,1463)	1:180:C:PHE:H	1:181:C:LEU:HA	9	0.16
(1,1461)	1:180:A:PHE:H	1:181:A:LEU:HA	9	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1460)	1:179:C:ALA:HA	1:180:C:PHE:H	3	0.16
(1,1460)	1:179:C:ALA:HA	1:180:C:PHE:H	10	0.16
(1,1459)	1:179:B:ALA:HA	1:180:B:PHE:H	3	0.16
(1,1458)	1:179:A:ALA:HA	1:180:A:PHE:H	3	0.16
(1,1432)	1:111:C:ILE:H	1:123:C:ILE:HG21	10	0.16
(1,1432)	1:111:C:ILE:H	1:123:C:ILE:HG22	10	0.16
(1,1432)	1:111:C:ILE:H	1:123:C:ILE:HG23	10	0.16
(1,1432)	1:111:C:ILE:H	1:123:C:ILE:HG21	20	0.16
(1,1432)	1:111:C:ILE:H	1:123:C:ILE:HG22	20	0.16
(1,1432)	1:111:C:ILE:H	1:123:C:ILE:HG23	20	0.16
(1,1431)	1:111:B:ILE:H	1:123:B:ILE:HG21	10	0.16
(1,1431)	1:111:B:ILE:H	1:123:B:ILE:HG22	10	0.16
(1,1431)	1:111:B:ILE:H	1:123:B:ILE:HG23	10	0.16
(1,1431)	1:111:B:ILE:H	1:123:B:ILE:HG21	20	0.16
(1,1431)	1:111:B:ILE:H	1:123:B:ILE:HG22	20	0.16
(1,1431)	1:111:B:ILE:H	1:123:B:ILE:HG23	20	0.16
(1,1430)	1:111:A:ILE:H	1:123:A:ILE:HG21	3	0.16
(1,1430)	1:111:A:ILE:H	1:123:A:ILE:HG22	3	0.16
(1,1430)	1:111:A:ILE:H	1:123:A:ILE:HG23	3	0.16
(1,1430)	1:111:A:ILE:H	1:123:A:ILE:HG21	4	0.16
(1,1430)	1:111:A:ILE:H	1:123:A:ILE:HG22	4	0.16
(1,1430)	1:111:A:ILE:H	1:123:A:ILE:HG23	4	0.16
(1,1276)	1:109:A:LEU:H	1:109:A:LEU:HG	12	0.16
(1,1203)	1:196:C:TYR:H	1:196:C:TYR:HE1	4	0.16
(1,1203)	1:196:C:TYR:H	1:196:C:TYR:HE2	4	0.16
(1,1202)	1:196:B:TYR:H	1:196:B:TYR:HE1	4	0.16
(1,1202)	1:196:B:TYR:H	1:196:B:TYR:HE2	4	0.16
(1,1201)	1:196:A:TYR:H	1:196:A:TYR:HE1	14	0.16
(1,1201)	1:196:A:TYR:H	1:196:A:TYR:HE2	14	0.16
(1,1100)	1:167:C:ARG:H	1:167:C:ARG:HB2	13	0.16
(1,1099)	1:167:B:ARG:H	1:167:B:ARG:HB2	13	0.16
(1,1098)	1:167:A:ARG:H	1:167:A:ARG:HB2	13	0.16
(1,1097)	1:157:C:PRO:HA	1:158:C:THR:H	20	0.16
(1,1071)	1:139:A:ARG:H	1:141:A:VAL:HB	12	0.16
(1,1047)	1:137:A:LEU:HG	1:138:A:THR:H	4	0.16
(1,1014)	1:104:B:TYR:H	1:112:B:ALA:H	18	0.16
(1,1013)	1:104:A:TYR:H	1:112:A:ALA:H	18	0.16
(1,965)	1:110:A:LEU:HD11	1:125:A:LYS:HB3	4	0.16
(1,965)	1:110:A:LEU:HD12	1:125:A:LYS:HB3	4	0.16
(1,965)	1:110:A:LEU:HD13	1:125:A:LYS:HB3	4	0.16
(1,965)	1:110:A:LEU:HD11	1:125:A:LYS:HB3	8	0.16
(1,965)	1:110:A:LEU:HD12	1:125:A:LYS:HB3	8	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,965)	1:110:A:LEU:HD13	1:125:A:LYS:HB3	8	0.16
(1,958)	1:187:A:THR:HA	1:188:A:LEU:HD11	17	0.16
(1,958)	1:187:A:THR:HA	1:188:A:LEU:HD12	17	0.16
(1,958)	1:187:A:THR:HA	1:188:A:LEU:HD13	17	0.16
(1,915)	1:140:A:LYS:HD2	1:141:A:VAL:HG11	4	0.16
(1,915)	1:140:A:LYS:HD2	1:141:A:VAL:HG12	4	0.16
(1,915)	1:140:A:LYS:HD2	1:141:A:VAL:HG13	4	0.16
(1,915)	1:140:A:LYS:HD3	1:141:A:VAL:HG11	4	0.16
(1,915)	1:140:A:LYS:HD3	1:141:A:VAL:HG12	4	0.16
(1,915)	1:140:A:LYS:HD3	1:141:A:VAL:HG13	4	0.16
(1,890)	1:152:C:ALA:HA	1:157:C:PRO:HG2	6	0.16
(1,890)	1:152:C:ALA:HA	1:157:C:PRO:HG3	6	0.16
(1,890)	1:152:C:ALA:HA	1:157:C:PRO:HG2	7	0.16
(1,890)	1:152:C:ALA:HA	1:157:C:PRO:HG3	7	0.16
(1,888)	1:152:A:ALA:HA	1:157:A:PRO:HG2	9	0.16
(1,888)	1:152:A:ALA:HA	1:157:A:PRO:HG3	9	0.16
(1,813)	1:176:A:GLY:H	1:177:A:ASP:HB2	7	0.16
(1,812)	1:176:C:GLY:H	1:177:C:ASP:HB3	4	0.16
(1,811)	1:176:B:GLY:H	1:177:B:ASP:HB3	4	0.16
(1,810)	1:176:A:GLY:H	1:177:A:ASP:HB3	4	0.16
(1,793)	1:153:B:LYS:HE2	1:154:B:PRO:HG2	5	0.16
(1,793)	1:153:B:LYS:HE2	1:154:B:PRO:HG3	5	0.16
(1,793)	1:153:B:LYS:HE3	1:154:B:PRO:HG2	5	0.16
(1,793)	1:153:B:LYS:HE3	1:154:B:PRO:HG3	5	0.16
(1,783)	1:167:A:ARG:HD2	1:169:A:ALA:HB1	15	0.16
(1,783)	1:167:A:ARG:HD2	1:169:A:ALA:HB2	15	0.16
(1,783)	1:167:A:ARG:HD2	1:169:A:ALA:HB3	15	0.16
(1,783)	1:167:A:ARG:HD3	1:169:A:ALA:HB1	15	0.16
(1,783)	1:167:A:ARG:HD3	1:169:A:ALA:HB2	15	0.16
(1,783)	1:167:A:ARG:HD3	1:169:A:ALA:HB3	15	0.16
(1,769)	1:102:A:VAL:HG21	1:104:A:TYR:HE1	8	0.16
(1,769)	1:102:A:VAL:HG21	1:104:A:TYR:HE2	8	0.16
(1,769)	1:102:A:VAL:HG22	1:104:A:TYR:HE1	8	0.16
(1,769)	1:102:A:VAL:HG22	1:104:A:TYR:HE2	8	0.16
(1,769)	1:102:A:VAL:HG23	1:104:A:TYR:HE1	8	0.16
(1,769)	1:102:A:VAL:HG23	1:104:A:TYR:HE2	8	0.16
(1,755)	1:189:C:CYS:H	1:192:C:VAL:HG11	17	0.16
(1,755)	1:189:C:CYS:H	1:192:C:VAL:HG12	17	0.16
(1,755)	1:189:C:CYS:H	1:192:C:VAL:HG13	17	0.16
(1,754)	1:189:B:CYS:H	1:192:B:VAL:HG11	17	0.16
(1,754)	1:189:B:CYS:H	1:192:B:VAL:HG12	17	0.16
(1,754)	1:189:B:CYS:H	1:192:B:VAL:HG13	17	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,749)	1:123:A:ILE:HG21	1:179:A:ALA:HB1	6	0.16
(1,749)	1:123:A:ILE:HG21	1:179:A:ALA:HB2	6	0.16
(1,749)	1:123:A:ILE:HG21	1:179:A:ALA:HB3	6	0.16
(1,749)	1:123:A:ILE:HG22	1:179:A:ALA:HB1	6	0.16
(1,749)	1:123:A:ILE:HG22	1:179:A:ALA:HB2	6	0.16
(1,749)	1:123:A:ILE:HG22	1:179:A:ALA:HB3	6	0.16
(1,749)	1:123:A:ILE:HG23	1:179:A:ALA:HB1	6	0.16
(1,749)	1:123:A:ILE:HG23	1:179:A:ALA:HB2	6	0.16
(1,749)	1:123:A:ILE:HG23	1:179:A:ALA:HB3	6	0.16
(1,739)	1:175:C:GLY:HA2	1:179:C:ALA:HB1	16	0.16
(1,739)	1:175:C:GLY:HA2	1:179:C:ALA:HB2	16	0.16
(1,739)	1:175:C:GLY:HA2	1:179:C:ALA:HB3	16	0.16
(1,739)	1:175:C:GLY:HA3	1:179:C:ALA:HB1	16	0.16
(1,739)	1:175:C:GLY:HA3	1:179:C:ALA:HB2	16	0.16
(1,739)	1:175:C:GLY:HA3	1:179:C:ALA:HB3	16	0.16
(1,712)	1:141:A:VAL:HG21	1:144:A:PHE:HD1	18	0.16
(1,712)	1:141:A:VAL:HG21	1:144:A:PHE:HD2	18	0.16
(1,712)	1:141:A:VAL:HG22	1:144:A:PHE:HD1	18	0.16
(1,712)	1:141:A:VAL:HG22	1:144:A:PHE:HD2	18	0.16
(1,712)	1:141:A:VAL:HG23	1:144:A:PHE:HD1	18	0.16
(1,712)	1:141:A:VAL:HG23	1:144:A:PHE:HD2	18	0.16
(1,655)	1:172:C:ALA:HB1	1:173:C:PRO:HD3	8	0.16
(1,655)	1:172:C:ALA:HB2	1:173:C:PRO:HD3	8	0.16
(1,655)	1:172:C:ALA:HB3	1:173:C:PRO:HD3	8	0.16
(1,654)	1:172:B:ALA:HB1	1:173:B:PRO:HD3	8	0.16
(1,654)	1:172:B:ALA:HB2	1:173:B:PRO:HD3	8	0.16
(1,654)	1:172:B:ALA:HB3	1:173:B:PRO:HD3	8	0.16
(1,653)	1:172:A:ALA:HB1	1:173:A:PRO:HD3	12	0.16
(1,653)	1:172:A:ALA:HB2	1:173:A:PRO:HD3	12	0.16
(1,653)	1:172:A:ALA:HB3	1:173:A:PRO:HD3	12	0.16
(1,637)	1:96:C:ILE:HG21	1:100:C:GLY:H	5	0.16
(1,637)	1:96:C:ILE:HG22	1:100:C:GLY:H	5	0.16
(1,637)	1:96:C:ILE:HG23	1:100:C:GLY:H	5	0.16
(1,637)	1:96:C:ILE:HG21	1:100:C:GLY:H	6	0.16
(1,637)	1:96:C:ILE:HG22	1:100:C:GLY:H	6	0.16
(1,637)	1:96:C:ILE:HG23	1:100:C:GLY:H	6	0.16
(1,637)	1:96:C:ILE:HG21	1:100:C:GLY:H	19	0.16
(1,637)	1:96:C:ILE:HG22	1:100:C:GLY:H	19	0.16
(1,637)	1:96:C:ILE:HG23	1:100:C:GLY:H	19	0.16
(1,637)	1:96:C:ILE:HG21	1:100:C:GLY:H	20	0.16
(1,637)	1:96:C:ILE:HG22	1:100:C:GLY:H	20	0.16
(1,637)	1:96:C:ILE:HG23	1:100:C:GLY:H	20	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,636)	1:96:B:ILE:HG21	1:100:B:GLY:H	5	0.16
(1,636)	1:96:B:ILE:HG22	1:100:B:GLY:H	5	0.16
(1,636)	1:96:B:ILE:HG23	1:100:B:GLY:H	5	0.16
(1,636)	1:96:B:ILE:HG21	1:100:B:GLY:H	19	0.16
(1,636)	1:96:B:ILE:HG22	1:100:B:GLY:H	19	0.16
(1,636)	1:96:B:ILE:HG23	1:100:B:GLY:H	19	0.16
(1,636)	1:96:B:ILE:HG21	1:100:B:GLY:H	20	0.16
(1,636)	1:96:B:ILE:HG22	1:100:B:GLY:H	20	0.16
(1,636)	1:96:B:ILE:HG23	1:100:B:GLY:H	20	0.16
(1,635)	1:96:A:ILE:HG21	1:100:A:GLY:H	6	0.16
(1,635)	1:96:A:ILE:HG22	1:100:A:GLY:H	6	0.16
(1,635)	1:96:A:ILE:HG23	1:100:A:GLY:H	6	0.16
(1,635)	1:96:A:ILE:HG21	1:100:A:GLY:H	14	0.16
(1,635)	1:96:A:ILE:HG22	1:100:A:GLY:H	14	0.16
(1,635)	1:96:A:ILE:HG23	1:100:A:GLY:H	14	0.16
(1,635)	1:96:A:ILE:HG21	1:100:A:GLY:H	19	0.16
(1,635)	1:96:A:ILE:HG22	1:100:A:GLY:H	19	0.16
(1,635)	1:96:A:ILE:HG23	1:100:A:GLY:H	19	0.16
(1,577)	1:178:A:PRO:HG2	1:194:A:LEU:HD21	3	0.16
(1,577)	1:178:A:PRO:HG2	1:194:A:LEU:HD22	3	0.16
(1,577)	1:178:A:PRO:HG2	1:194:A:LEU:HD23	3	0.16
(1,577)	1:178:A:PRO:HG3	1:194:A:LEU:HD21	3	0.16
(1,577)	1:178:A:PRO:HG3	1:194:A:LEU:HD22	3	0.16
(1,577)	1:178:A:PRO:HG3	1:194:A:LEU:HD23	3	0.16
(1,576)	1:189:A:CYS:HB2	1:194:A:LEU:HD21	19	0.16
(1,576)	1:189:A:CYS:HB2	1:194:A:LEU:HD22	19	0.16
(1,576)	1:189:A:CYS:HB2	1:194:A:LEU:HD23	19	0.16
(1,576)	1:189:A:CYS:HB3	1:194:A:LEU:HD21	19	0.16
(1,576)	1:189:A:CYS:HB3	1:194:A:LEU:HD22	19	0.16
(1,576)	1:189:A:CYS:HB3	1:194:A:LEU:HD23	19	0.16
(1,575)	1:193:A:PRO:HA	1:194:A:LEU:HD21	6	0.16
(1,575)	1:193:A:PRO:HA	1:194:A:LEU:HD22	6	0.16
(1,575)	1:193:A:PRO:HA	1:194:A:LEU:HD23	6	0.16
(1,539)	1:111:A:ILE:HG21	1:126:A:ILE:HG21	4	0.16
(1,539)	1:111:A:ILE:HG21	1:126:A:ILE:HG22	4	0.16
(1,539)	1:111:A:ILE:HG21	1:126:A:ILE:HG23	4	0.16
(1,539)	1:111:A:ILE:HG22	1:126:A:ILE:HG21	4	0.16
(1,539)	1:111:A:ILE:HG22	1:126:A:ILE:HG22	4	0.16
(1,539)	1:111:A:ILE:HG22	1:126:A:ILE:HG23	4	0.16
(1,539)	1:111:A:ILE:HG23	1:126:A:ILE:HG21	4	0.16
(1,539)	1:111:A:ILE:HG23	1:126:A:ILE:HG22	4	0.16
(1,539)	1:111:A:ILE:HG23	1:126:A:ILE:HG23	4	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,539)	1:111:A:ILE:HG21	1:126:A:ILE:HG21	12	0.16
(1,539)	1:111:A:ILE:HG21	1:126:A:ILE:HG22	12	0.16
(1,539)	1:111:A:ILE:HG21	1:126:A:ILE:HG23	12	0.16
(1,539)	1:111:A:ILE:HG22	1:126:A:ILE:HG21	12	0.16
(1,539)	1:111:A:ILE:HG22	1:126:A:ILE:HG22	12	0.16
(1,539)	1:111:A:ILE:HG22	1:126:A:ILE:HG23	12	0.16
(1,539)	1:111:A:ILE:HG23	1:126:A:ILE:HG21	12	0.16
(1,539)	1:111:A:ILE:HG23	1:126:A:ILE:HG22	12	0.16
(1,539)	1:111:A:ILE:HG23	1:126:A:ILE:HG23	12	0.16
(1,538)	1:111:C:ILE:HD11	1:131:C:ILE:HG21	9	0.16
(1,538)	1:111:C:ILE:HD11	1:131:C:ILE:HG22	9	0.16
(1,538)	1:111:C:ILE:HD11	1:131:C:ILE:HG23	9	0.16
(1,538)	1:111:C:ILE:HD12	1:131:C:ILE:HG21	9	0.16
(1,538)	1:111:C:ILE:HD12	1:131:C:ILE:HG22	9	0.16
(1,538)	1:111:C:ILE:HD12	1:131:C:ILE:HG23	9	0.16
(1,538)	1:111:C:ILE:HD13	1:131:C:ILE:HG21	9	0.16
(1,538)	1:111:C:ILE:HD13	1:131:C:ILE:HG22	9	0.16
(1,538)	1:111:C:ILE:HD13	1:131:C:ILE:HG23	9	0.16
(1,537)	1:111:B:ILE:HD11	1:131:B:ILE:HG21	9	0.16
(1,537)	1:111:B:ILE:HD11	1:131:B:ILE:HG22	9	0.16
(1,537)	1:111:B:ILE:HD11	1:131:B:ILE:HG23	9	0.16
(1,537)	1:111:B:ILE:HD12	1:131:B:ILE:HG21	9	0.16
(1,537)	1:111:B:ILE:HD12	1:131:B:ILE:HG22	9	0.16
(1,537)	1:111:B:ILE:HD12	1:131:B:ILE:HG23	9	0.16
(1,537)	1:111:B:ILE:HD13	1:131:B:ILE:HG21	9	0.16
(1,537)	1:111:B:ILE:HD13	1:131:B:ILE:HG22	9	0.16
(1,537)	1:111:B:ILE:HD13	1:131:B:ILE:HG23	9	0.16
(1,537)	1:111:B:ILE:HD11	1:131:B:ILE:HG21	16	0.16
(1,537)	1:111:B:ILE:HD11	1:131:B:ILE:HG22	16	0.16
(1,537)	1:111:B:ILE:HD11	1:131:B:ILE:HG23	16	0.16
(1,537)	1:111:B:ILE:HD12	1:131:B:ILE:HG21	16	0.16
(1,537)	1:111:B:ILE:HD12	1:131:B:ILE:HG22	16	0.16
(1,537)	1:111:B:ILE:HD12	1:131:B:ILE:HG23	16	0.16
(1,537)	1:111:B:ILE:HD13	1:131:B:ILE:HG21	16	0.16
(1,537)	1:111:B:ILE:HD13	1:131:B:ILE:HG22	16	0.16
(1,537)	1:111:B:ILE:HD13	1:131:B:ILE:HG23	16	0.16
(1,437)	1:183:C:MET:HE1	1:186:C:SER:HA	11	0.16
(1,437)	1:183:C:MET:HE2	1:186:C:SER:HA	11	0.16
(1,437)	1:183:C:MET:HE3	1:186:C:SER:HA	11	0.16
(1,437)	1:183:C:MET:HE1	1:186:C:SER:HA	13	0.16
(1,437)	1:183:C:MET:HE2	1:186:C:SER:HA	13	0.16
(1,437)	1:183:C:MET:HE3	1:186:C:SER:HA	13	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,437)	1:183:C:MET:HE1	1:186:C:SER:HA	14	0.16
(1,437)	1:183:C:MET:HE2	1:186:C:SER:HA	14	0.16
(1,437)	1:183:C:MET:HE3	1:186:C:SER:HA	14	0.16
(1,436)	1:183:B:MET:HE1	1:186:B:SER:HA	3	0.16
(1,436)	1:183:B:MET:HE2	1:186:B:SER:HA	3	0.16
(1,436)	1:183:B:MET:HE3	1:186:B:SER:HA	3	0.16
(1,436)	1:183:B:MET:HE1	1:186:B:SER:HA	13	0.16
(1,436)	1:183:B:MET:HE2	1:186:B:SER:HA	13	0.16
(1,436)	1:183:B:MET:HE3	1:186:B:SER:HA	13	0.16
(1,436)	1:183:B:MET:HE1	1:186:B:SER:HA	14	0.16
(1,436)	1:183:B:MET:HE2	1:186:B:SER:HA	14	0.16
(1,436)	1:183:B:MET:HE3	1:186:B:SER:HA	14	0.16
(1,425)	1:89:A:VAL:HG11	1:183:A:MET:HE1	17	0.16
(1,425)	1:89:A:VAL:HG11	1:183:A:MET:HE2	17	0.16
(1,425)	1:89:A:VAL:HG11	1:183:A:MET:HE3	17	0.16
(1,425)	1:89:A:VAL:HG12	1:183:A:MET:HE1	17	0.16
(1,425)	1:89:A:VAL:HG12	1:183:A:MET:HE2	17	0.16
(1,425)	1:89:A:VAL:HG12	1:183:A:MET:HE3	17	0.16
(1,425)	1:89:A:VAL:HG13	1:183:A:MET:HE1	17	0.16
(1,425)	1:89:A:VAL:HG13	1:183:A:MET:HE2	17	0.16
(1,425)	1:89:A:VAL:HG13	1:183:A:MET:HE3	17	0.16
(1,364)	1:126:A:ILE:HG21	1:131:A:ILE:HD11	10	0.16
(1,364)	1:126:A:ILE:HG21	1:131:A:ILE:HD12	10	0.16
(1,364)	1:126:A:ILE:HG21	1:131:A:ILE:HD13	10	0.16
(1,364)	1:126:A:ILE:HG22	1:131:A:ILE:HD11	10	0.16
(1,364)	1:126:A:ILE:HG22	1:131:A:ILE:HD12	10	0.16
(1,364)	1:126:A:ILE:HG22	1:131:A:ILE:HD13	10	0.16
(1,364)	1:126:A:ILE:HG23	1:131:A:ILE:HD11	10	0.16
(1,364)	1:126:A:ILE:HG23	1:131:A:ILE:HD12	10	0.16
(1,364)	1:126:A:ILE:HG23	1:131:A:ILE:HD13	10	0.16
(1,363)	1:131:A:ILE:HD11	1:183:C:MET:HG2	18	0.16
(1,363)	1:131:A:ILE:HD11	1:183:C:MET:HG3	18	0.16
(1,363)	1:131:A:ILE:HD12	1:183:C:MET:HG2	18	0.16
(1,363)	1:131:A:ILE:HD12	1:183:C:MET:HG3	18	0.16
(1,363)	1:131:A:ILE:HD13	1:183:C:MET:HG2	18	0.16
(1,363)	1:131:A:ILE:HD13	1:183:C:MET:HG3	18	0.16
(1,362)	1:183:B:MET:HG2	1:131:C:ILE:HD11	5	0.16
(1,362)	1:183:B:MET:HG2	1:131:C:ILE:HD12	5	0.16
(1,362)	1:183:B:MET:HG2	1:131:C:ILE:HD13	5	0.16
(1,362)	1:183:B:MET:HG3	1:131:C:ILE:HD11	5	0.16
(1,362)	1:183:B:MET:HG3	1:131:C:ILE:HD12	5	0.16
(1,362)	1:183:B:MET:HG3	1:131:C:ILE:HD13	5	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,361)	1:183:A:MET:HG2	1:131:B:ILE:HD11	18	0.16
(1,361)	1:183:A:MET:HG2	1:131:B:ILE:HD12	18	0.16
(1,361)	1:183:A:MET:HG2	1:131:B:ILE:HD13	18	0.16
(1,361)	1:183:A:MET:HG3	1:131:B:ILE:HD11	18	0.16
(1,361)	1:183:A:MET:HG3	1:131:B:ILE:HD12	18	0.16
(1,361)	1:183:A:MET:HG3	1:131:B:ILE:HD13	18	0.16
(1,219)	1:96:A:ILE:HG21	1:141:A:VAL:HG11	5	0.16
(1,219)	1:96:A:ILE:HG21	1:141:A:VAL:HG12	5	0.16
(1,219)	1:96:A:ILE:HG21	1:141:A:VAL:HG13	5	0.16
(1,219)	1:96:A:ILE:HG22	1:141:A:VAL:HG11	5	0.16
(1,219)	1:96:A:ILE:HG22	1:141:A:VAL:HG12	5	0.16
(1,219)	1:96:A:ILE:HG22	1:141:A:VAL:HG13	5	0.16
(1,219)	1:96:A:ILE:HG23	1:141:A:VAL:HG11	5	0.16
(1,219)	1:96:A:ILE:HG23	1:141:A:VAL:HG12	5	0.16
(1,219)	1:96:A:ILE:HG23	1:141:A:VAL:HG13	5	0.16
(1,219)	1:96:A:ILE:HG21	1:141:A:VAL:HG11	16	0.16
(1,219)	1:96:A:ILE:HG21	1:141:A:VAL:HG12	16	0.16
(1,219)	1:96:A:ILE:HG21	1:141:A:VAL:HG13	16	0.16
(1,219)	1:96:A:ILE:HG22	1:141:A:VAL:HG11	16	0.16
(1,219)	1:96:A:ILE:HG22	1:141:A:VAL:HG12	16	0.16
(1,219)	1:96:A:ILE:HG22	1:141:A:VAL:HG13	16	0.16
(1,219)	1:96:A:ILE:HG23	1:141:A:VAL:HG11	16	0.16
(1,219)	1:96:A:ILE:HG23	1:141:A:VAL:HG12	16	0.16
(1,219)	1:96:A:ILE:HG23	1:141:A:VAL:HG13	16	0.16
(1,198)	1:109:A:LEU:H	1:110:A:LEU:HD21	15	0.16
(1,198)	1:109:A:LEU:H	1:110:A:LEU:HD22	15	0.16
(1,198)	1:109:A:LEU:H	1:110:A:LEU:HD23	15	0.16
(1,182)	1:137:A:LEU:HD11	1:141:A:VAL:HG11	10	0.16
(1,182)	1:137:A:LEU:HD11	1:141:A:VAL:HG12	10	0.16
(1,182)	1:137:A:LEU:HD11	1:141:A:VAL:HG13	10	0.16
(1,182)	1:137:A:LEU:HD12	1:141:A:VAL:HG11	10	0.16
(1,182)	1:137:A:LEU:HD12	1:141:A:VAL:HG12	10	0.16
(1,182)	1:137:A:LEU:HD12	1:141:A:VAL:HG13	10	0.16
(1,182)	1:137:A:LEU:HD13	1:141:A:VAL:HG11	10	0.16
(1,182)	1:137:A:LEU:HD13	1:141:A:VAL:HG12	10	0.16
(1,182)	1:137:A:LEU:HD13	1:141:A:VAL:HG13	10	0.16
(1,175)	1:179:A:ALA:HB1	1:181:A:LEU:HD21	19	0.16
(1,175)	1:179:A:ALA:HB1	1:181:A:LEU:HD22	19	0.16
(1,175)	1:179:A:ALA:HB1	1:181:A:LEU:HD23	19	0.16
(1,175)	1:179:A:ALA:HB2	1:181:A:LEU:HD21	19	0.16
(1,175)	1:179:A:ALA:HB2	1:181:A:LEU:HD22	19	0.16
(1,175)	1:179:A:ALA:HB2	1:181:A:LEU:HD23	19	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,175)	1:179:A:ALA:HB3	1:181:A:LEU:HD21	19	0.16
(1,175)	1:179:A:ALA:HB3	1:181:A:LEU:HD22	19	0.16
(1,175)	1:179:A:ALA:HB3	1:181:A:LEU:HD23	19	0.16
(1,134)	1:110:A:LEU:HD11	1:111:A:ILE:HD11	10	0.16
(1,134)	1:110:A:LEU:HD11	1:111:A:ILE:HD12	10	0.16
(1,134)	1:110:A:LEU:HD11	1:111:A:ILE:HD13	10	0.16
(1,134)	1:110:A:LEU:HD12	1:111:A:ILE:HD11	10	0.16
(1,134)	1:110:A:LEU:HD12	1:111:A:ILE:HD12	10	0.16
(1,134)	1:110:A:LEU:HD12	1:111:A:ILE:HD13	10	0.16
(1,134)	1:110:A:LEU:HD13	1:111:A:ILE:HD11	10	0.16
(1,134)	1:110:A:LEU:HD13	1:111:A:ILE:HD12	10	0.16
(1,134)	1:110:A:LEU:HD13	1:111:A:ILE:HD13	10	0.16
(1,124)	1:96:A:ILE:H	1:101:A:LEU:HD21	14	0.16
(1,124)	1:96:A:ILE:H	1:101:A:LEU:HD22	14	0.16
(1,124)	1:96:A:ILE:H	1:101:A:LEU:HD23	14	0.16
(1,63)	1:110:A:LEU:HD11	1:123:A:ILE:HD11	13	0.16
(1,63)	1:110:A:LEU:HD11	1:123:A:ILE:HD12	13	0.16
(1,63)	1:110:A:LEU:HD11	1:123:A:ILE:HD13	13	0.16
(1,63)	1:110:A:LEU:HD12	1:123:A:ILE:HD11	13	0.16
(1,63)	1:110:A:LEU:HD12	1:123:A:ILE:HD12	13	0.16
(1,63)	1:110:A:LEU:HD12	1:123:A:ILE:HD13	13	0.16
(1,63)	1:110:A:LEU:HD13	1:123:A:ILE:HD11	13	0.16
(1,63)	1:110:A:LEU:HD13	1:123:A:ILE:HD12	13	0.16
(1,63)	1:110:A:LEU:HD13	1:123:A:ILE:HD13	13	0.16
(1,56)	1:156:A:VAL:HG11	1:157:A:PRO:HD3	9	0.16
(1,56)	1:156:A:VAL:HG12	1:157:A:PRO:HD3	9	0.16
(1,56)	1:156:A:VAL:HG13	1:157:A:PRO:HD3	9	0.16
(1,1)	1:108:A:GLN:HA	1:109:A:LEU:HD21	4	0.16
(1,1)	1:108:A:GLN:HA	1:109:A:LEU:HD22	4	0.16
(1,1)	1:108:A:GLN:HA	1:109:A:LEU:HD23	4	0.16
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD11	1	0.15
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD12	1	0.15
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD13	1	0.15
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD21	1	0.15
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD22	1	0.15
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD23	1	0.15
(1,2345)	1:183:C:MET:HB2	1:183:C:MET:HE1	18	0.15
(1,2345)	1:183:C:MET:HB2	1:183:C:MET:HE2	18	0.15
(1,2345)	1:183:C:MET:HB2	1:183:C:MET:HE3	18	0.15
(1,2345)	1:183:C:MET:HB3	1:183:C:MET:HE1	18	0.15
(1,2345)	1:183:C:MET:HB3	1:183:C:MET:HE2	18	0.15
(1,2345)	1:183:C:MET:HB3	1:183:C:MET:HE3	18	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2338)	1:179:C:ALA:HB1	1:181:C:LEU:HD11	10	0.15
(1,2338)	1:179:C:ALA:HB1	1:181:C:LEU:HD12	10	0.15
(1,2338)	1:179:C:ALA:HB1	1:181:C:LEU:HD13	10	0.15
(1,2338)	1:179:C:ALA:HB1	1:181:C:LEU:HD21	10	0.15
(1,2338)	1:179:C:ALA:HB1	1:181:C:LEU:HD22	10	0.15
(1,2338)	1:179:C:ALA:HB1	1:181:C:LEU:HD23	10	0.15
(1,2338)	1:179:C:ALA:HB2	1:181:C:LEU:HD11	10	0.15
(1,2338)	1:179:C:ALA:HB2	1:181:C:LEU:HD12	10	0.15
(1,2338)	1:179:C:ALA:HB2	1:181:C:LEU:HD13	10	0.15
(1,2338)	1:179:C:ALA:HB2	1:181:C:LEU:HD21	10	0.15
(1,2338)	1:179:C:ALA:HB2	1:181:C:LEU:HD22	10	0.15
(1,2338)	1:179:C:ALA:HB2	1:181:C:LEU:HD23	10	0.15
(1,2338)	1:179:C:ALA:HB3	1:181:C:LEU:HD11	10	0.15
(1,2338)	1:179:C:ALA:HB3	1:181:C:LEU:HD12	10	0.15
(1,2338)	1:179:C:ALA:HB3	1:181:C:LEU:HD13	10	0.15
(1,2338)	1:179:C:ALA:HB3	1:181:C:LEU:HD21	10	0.15
(1,2338)	1:179:C:ALA:HB3	1:181:C:LEU:HD22	10	0.15
(1,2338)	1:179:C:ALA:HB3	1:181:C:LEU:HD23	10	0.15
(1,2338)	1:179:C:ALA:HB1	1:181:C:LEU:HD11	20	0.15
(1,2338)	1:179:C:ALA:HB1	1:181:C:LEU:HD12	20	0.15
(1,2338)	1:179:C:ALA:HB1	1:181:C:LEU:HD13	20	0.15
(1,2338)	1:179:C:ALA:HB1	1:181:C:LEU:HD21	20	0.15
(1,2338)	1:179:C:ALA:HB1	1:181:C:LEU:HD22	20	0.15
(1,2338)	1:179:C:ALA:HB1	1:181:C:LEU:HD23	20	0.15
(1,2338)	1:179:C:ALA:HB2	1:181:C:LEU:HD11	20	0.15
(1,2338)	1:179:C:ALA:HB2	1:181:C:LEU:HD12	20	0.15
(1,2338)	1:179:C:ALA:HB2	1:181:C:LEU:HD13	20	0.15
(1,2338)	1:179:C:ALA:HB2	1:181:C:LEU:HD21	20	0.15
(1,2338)	1:179:C:ALA:HB2	1:181:C:LEU:HD22	20	0.15
(1,2338)	1:179:C:ALA:HB2	1:181:C:LEU:HD23	20	0.15
(1,2338)	1:179:C:ALA:HB3	1:181:C:LEU:HD11	20	0.15
(1,2338)	1:179:C:ALA:HB3	1:181:C:LEU:HD12	20	0.15
(1,2338)	1:179:C:ALA:HB3	1:181:C:LEU:HD13	20	0.15
(1,2338)	1:179:C:ALA:HB3	1:181:C:LEU:HD21	20	0.15
(1,2338)	1:179:C:ALA:HB3	1:181:C:LEU:HD22	20	0.15
(1,2338)	1:179:C:ALA:HB3	1:181:C:LEU:HD23	20	0.15
(1,2322)	1:176:C:GLY:H	1:177:C:ASP:HB2	3	0.15
(1,2322)	1:176:C:GLY:H	1:177:C:ASP:HB3	3	0.15
(1,2322)	1:176:C:GLY:H	1:177:C:ASP:HB2	5	0.15
(1,2322)	1:176:C:GLY:H	1:177:C:ASP:HB3	5	0.15
(1,2322)	1:176:C:GLY:H	1:177:C:ASP:HB2	6	0.15
(1,2322)	1:176:C:GLY:H	1:177:C:ASP:HB3	6	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2322)	1:176:C:GLY:H	1:177:C:ASP:HB2	7	0.15
(1,2322)	1:176:C:GLY:H	1:177:C:ASP:HB3	7	0.15
(1,2321)	1:172:C:ALA:HB1	1:173:C:PRO:HD2	3	0.15
(1,2321)	1:172:C:ALA:HB1	1:173:C:PRO:HD3	3	0.15
(1,2321)	1:172:C:ALA:HB2	1:173:C:PRO:HD2	3	0.15
(1,2321)	1:172:C:ALA:HB2	1:173:C:PRO:HD3	3	0.15
(1,2321)	1:172:C:ALA:HB3	1:173:C:PRO:HD2	3	0.15
(1,2321)	1:172:C:ALA:HB3	1:173:C:PRO:HD3	3	0.15
(1,2321)	1:172:C:ALA:HB1	1:173:C:PRO:HD2	5	0.15
(1,2321)	1:172:C:ALA:HB1	1:173:C:PRO:HD3	5	0.15
(1,2321)	1:172:C:ALA:HB2	1:173:C:PRO:HD2	5	0.15
(1,2321)	1:172:C:ALA:HB2	1:173:C:PRO:HD3	5	0.15
(1,2321)	1:172:C:ALA:HB3	1:173:C:PRO:HD2	5	0.15
(1,2321)	1:172:C:ALA:HB3	1:173:C:PRO:HD3	5	0.15
(1,2321)	1:172:C:ALA:HB1	1:173:C:PRO:HD2	6	0.15
(1,2321)	1:172:C:ALA:HB1	1:173:C:PRO:HD3	6	0.15
(1,2321)	1:172:C:ALA:HB2	1:173:C:PRO:HD2	6	0.15
(1,2321)	1:172:C:ALA:HB2	1:173:C:PRO:HD3	6	0.15
(1,2321)	1:172:C:ALA:HB3	1:173:C:PRO:HD2	6	0.15
(1,2321)	1:172:C:ALA:HB3	1:173:C:PRO:HD3	6	0.15
(1,2321)	1:172:C:ALA:HB1	1:173:C:PRO:HD2	7	0.15
(1,2321)	1:172:C:ALA:HB1	1:173:C:PRO:HD3	7	0.15
(1,2321)	1:172:C:ALA:HB2	1:173:C:PRO:HD2	7	0.15
(1,2321)	1:172:C:ALA:HB2	1:173:C:PRO:HD3	7	0.15
(1,2321)	1:172:C:ALA:HB3	1:173:C:PRO:HD2	7	0.15
(1,2321)	1:172:C:ALA:HB3	1:173:C:PRO:HD3	7	0.15
(1,2320)	1:172:C:ALA:HA	1:178:C:PRO:HD2	19	0.15
(1,2320)	1:172:C:ALA:HA	1:178:C:PRO:HD3	19	0.15
(1,2288)	1:153:C:LYS:H	1:154:C:PRO:HD2	7	0.15
(1,2288)	1:153:C:LYS:H	1:154:C:PRO:HD3	7	0.15
(1,2288)	1:153:C:LYS:H	1:154:C:PRO:HD2	14	0.15
(1,2288)	1:153:C:LYS:H	1:154:C:PRO:HD3	14	0.15
(1,2286)	1:151:C:GLN:HB2	1:152:C:ALA:HA	2	0.15
(1,2286)	1:151:C:GLN:HB3	1:152:C:ALA:HA	2	0.15
(1,2236)	1:121:C:CYS:HB2	1:189:C:CYS:H	1	0.15
(1,2236)	1:121:C:CYS:HB3	1:189:C:CYS:H	1	0.15
(1,2236)	1:121:C:CYS:HB2	1:189:C:CYS:H	3	0.15
(1,2236)	1:121:C:CYS:HB3	1:189:C:CYS:H	3	0.15
(1,2236)	1:121:C:CYS:HB2	1:189:C:CYS:H	15	0.15
(1,2236)	1:121:C:CYS:HB3	1:189:C:CYS:H	15	0.15
(1,2138)	1:188:B:LEU:HD11	1:134:C:LEU:H	14	0.15
(1,2138)	1:188:B:LEU:HD12	1:134:C:LEU:H	14	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2138)	1:188:B:LEU:HD13	1:134:C:LEU:H	14	0.15
(1,2138)	1:188:B:LEU:HD21	1:134:C:LEU:H	14	0.15
(1,2138)	1:188:B:LEU:HD22	1:134:C:LEU:H	14	0.15
(1,2138)	1:188:B:LEU:HD23	1:134:C:LEU:H	14	0.15
(1,2138)	1:188:B:LEU:HD11	1:134:C:LEU:H	15	0.15
(1,2138)	1:188:B:LEU:HD12	1:134:C:LEU:H	15	0.15
(1,2138)	1:188:B:LEU:HD13	1:134:C:LEU:H	15	0.15
(1,2138)	1:188:B:LEU:HD21	1:134:C:LEU:H	15	0.15
(1,2138)	1:188:B:LEU:HD22	1:134:C:LEU:H	15	0.15
(1,2138)	1:188:B:LEU:HD23	1:134:C:LEU:H	15	0.15
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD11	1	0.15
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD12	1	0.15
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD13	1	0.15
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD21	1	0.15
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD22	1	0.15
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD23	1	0.15
(1,2119)	1:183:B:MET:HB2	1:183:B:MET:HE1	18	0.15
(1,2119)	1:183:B:MET:HB2	1:183:B:MET:HE2	18	0.15
(1,2119)	1:183:B:MET:HB2	1:183:B:MET:HE3	18	0.15
(1,2119)	1:183:B:MET:HB3	1:183:B:MET:HE1	18	0.15
(1,2119)	1:183:B:MET:HB3	1:183:B:MET:HE2	18	0.15
(1,2119)	1:183:B:MET:HB3	1:183:B:MET:HE3	18	0.15
(1,2112)	1:179:B:ALA:HB1	1:181:B:LEU:HD11	10	0.15
(1,2112)	1:179:B:ALA:HB1	1:181:B:LEU:HD12	10	0.15
(1,2112)	1:179:B:ALA:HB1	1:181:B:LEU:HD13	10	0.15
(1,2112)	1:179:B:ALA:HB1	1:181:B:LEU:HD21	10	0.15
(1,2112)	1:179:B:ALA:HB1	1:181:B:LEU:HD22	10	0.15
(1,2112)	1:179:B:ALA:HB1	1:181:B:LEU:HD23	10	0.15
(1,2112)	1:179:B:ALA:HB2	1:181:B:LEU:HD11	10	0.15
(1,2112)	1:179:B:ALA:HB2	1:181:B:LEU:HD12	10	0.15
(1,2112)	1:179:B:ALA:HB2	1:181:B:LEU:HD13	10	0.15
(1,2112)	1:179:B:ALA:HB2	1:181:B:LEU:HD21	10	0.15
(1,2112)	1:179:B:ALA:HB2	1:181:B:LEU:HD22	10	0.15
(1,2112)	1:179:B:ALA:HB2	1:181:B:LEU:HD23	10	0.15
(1,2112)	1:179:B:ALA:HB3	1:181:B:LEU:HD11	10	0.15
(1,2112)	1:179:B:ALA:HB3	1:181:B:LEU:HD12	10	0.15
(1,2112)	1:179:B:ALA:HB3	1:181:B:LEU:HD13	10	0.15
(1,2112)	1:179:B:ALA:HB3	1:181:B:LEU:HD21	10	0.15
(1,2112)	1:179:B:ALA:HB3	1:181:B:LEU:HD22	10	0.15
(1,2112)	1:179:B:ALA:HB3	1:181:B:LEU:HD23	10	0.15
(1,2112)	1:179:B:ALA:HB1	1:181:B:LEU:HD11	20	0.15
(1,2112)	1:179:B:ALA:HB1	1:181:B:LEU:HD12	20	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2112)	1:179:B:ALA:HB1	1:181:B:LEU:HD13	20	0.15
(1,2112)	1:179:B:ALA:HB1	1:181:B:LEU:HD21	20	0.15
(1,2112)	1:179:B:ALA:HB1	1:181:B:LEU:HD22	20	0.15
(1,2112)	1:179:B:ALA:HB1	1:181:B:LEU:HD23	20	0.15
(1,2112)	1:179:B:ALA:HB2	1:181:B:LEU:HD11	20	0.15
(1,2112)	1:179:B:ALA:HB2	1:181:B:LEU:HD12	20	0.15
(1,2112)	1:179:B:ALA:HB2	1:181:B:LEU:HD13	20	0.15
(1,2112)	1:179:B:ALA:HB2	1:181:B:LEU:HD21	20	0.15
(1,2112)	1:179:B:ALA:HB2	1:181:B:LEU:HD22	20	0.15
(1,2112)	1:179:B:ALA:HB2	1:181:B:LEU:HD23	20	0.15
(1,2112)	1:179:B:ALA:HB3	1:181:B:LEU:HD11	20	0.15
(1,2112)	1:179:B:ALA:HB3	1:181:B:LEU:HD12	20	0.15
(1,2112)	1:179:B:ALA:HB3	1:181:B:LEU:HD13	20	0.15
(1,2112)	1:179:B:ALA:HB3	1:181:B:LEU:HD21	20	0.15
(1,2112)	1:179:B:ALA:HB3	1:181:B:LEU:HD22	20	0.15
(1,2112)	1:179:B:ALA:HB3	1:181:B:LEU:HD23	20	0.15
(1,2096)	1:176:B:GLY:H	1:177:B:ASP:HB2	3	0.15
(1,2096)	1:176:B:GLY:H	1:177:B:ASP:HB3	3	0.15
(1,2096)	1:176:B:GLY:H	1:177:B:ASP:HB2	5	0.15
(1,2096)	1:176:B:GLY:H	1:177:B:ASP:HB3	5	0.15
(1,2096)	1:176:B:GLY:H	1:177:B:ASP:HB2	6	0.15
(1,2096)	1:176:B:GLY:H	1:177:B:ASP:HB3	6	0.15
(1,2096)	1:176:B:GLY:H	1:177:B:ASP:HB2	7	0.15
(1,2096)	1:176:B:GLY:H	1:177:B:ASP:HB3	7	0.15
(1,2095)	1:172:B:ALA:HB1	1:173:B:PRO:HD2	3	0.15
(1,2095)	1:172:B:ALA:HB1	1:173:B:PRO:HD3	3	0.15
(1,2095)	1:172:B:ALA:HB2	1:173:B:PRO:HD2	3	0.15
(1,2095)	1:172:B:ALA:HB2	1:173:B:PRO:HD3	3	0.15
(1,2095)	1:172:B:ALA:HB3	1:173:B:PRO:HD2	3	0.15
(1,2095)	1:172:B:ALA:HB3	1:173:B:PRO:HD3	3	0.15
(1,2095)	1:172:B:ALA:HB1	1:173:B:PRO:HD2	6	0.15
(1,2095)	1:172:B:ALA:HB1	1:173:B:PRO:HD3	6	0.15
(1,2095)	1:172:B:ALA:HB2	1:173:B:PRO:HD2	6	0.15
(1,2095)	1:172:B:ALA:HB2	1:173:B:PRO:HD3	6	0.15
(1,2095)	1:172:B:ALA:HB3	1:173:B:PRO:HD2	6	0.15
(1,2095)	1:172:B:ALA:HB3	1:173:B:PRO:HD3	6	0.15
(1,2095)	1:172:B:ALA:HB1	1:173:B:PRO:HD2	7	0.15
(1,2095)	1:172:B:ALA:HB1	1:173:B:PRO:HD3	7	0.15
(1,2095)	1:172:B:ALA:HB2	1:173:B:PRO:HD2	7	0.15
(1,2095)	1:172:B:ALA:HB2	1:173:B:PRO:HD3	7	0.15
(1,2095)	1:172:B:ALA:HB3	1:173:B:PRO:HD2	7	0.15
(1,2095)	1:172:B:ALA:HB3	1:173:B:PRO:HD3	7	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2094)	1:172:B:ALA:HA	1:178:B:PRO:HD2	19	0.15
(1,2094)	1:172:B:ALA:HA	1:178:B:PRO:HD3	19	0.15
(1,2066)	1:154:B:PRO:HB2	1:167:B:ARG:H	17	0.15
(1,2066)	1:154:B:PRO:HB3	1:167:B:ARG:H	17	0.15
(1,2062)	1:153:B:LYS:H	1:154:B:PRO:HD2	7	0.15
(1,2062)	1:153:B:LYS:H	1:154:B:PRO:HD3	7	0.15
(1,2060)	1:151:B:GLN:HB2	1:152:B:ALA:HA	2	0.15
(1,2060)	1:151:B:GLN:HB3	1:152:B:ALA:HA	2	0.15
(1,2010)	1:121:B:CYS:HB2	1:189:B:CYS:H	3	0.15
(1,2010)	1:121:B:CYS:HB3	1:189:B:CYS:H	3	0.15
(1,2010)	1:121:B:CYS:HB2	1:189:B:CYS:H	7	0.15
(1,2010)	1:121:B:CYS:HB3	1:189:B:CYS:H	7	0.15
(1,2010)	1:121:B:CYS:HB2	1:189:B:CYS:H	9	0.15
(1,2010)	1:121:B:CYS:HB3	1:189:B:CYS:H	9	0.15
(1,2010)	1:121:B:CYS:HB2	1:189:B:CYS:H	10	0.15
(1,2010)	1:121:B:CYS:HB3	1:189:B:CYS:H	10	0.15
(1,2010)	1:121:B:CYS:HB2	1:189:B:CYS:H	18	0.15
(1,2010)	1:121:B:CYS:HB3	1:189:B:CYS:H	18	0.15
(1,1911)	1:178:A:PRO:HB2	1:180:A:PHE:H	2	0.15
(1,1911)	1:178:A:PRO:HB3	1:180:A:PHE:H	2	0.15
(1,1908)	1:177:A:ASP:HB2	1:180:A:PHE:H	19	0.15
(1,1908)	1:177:A:ASP:HB3	1:180:A:PHE:H	19	0.15
(1,1904)	1:176:A:GLY:H	1:177:A:ASP:HB2	3	0.15
(1,1904)	1:176:A:GLY:H	1:177:A:ASP:HB3	3	0.15
(1,1904)	1:176:A:GLY:H	1:177:A:ASP:HB2	5	0.15
(1,1904)	1:176:A:GLY:H	1:177:A:ASP:HB3	5	0.15
(1,1904)	1:176:A:GLY:H	1:177:A:ASP:HB2	11	0.15
(1,1904)	1:176:A:GLY:H	1:177:A:ASP:HB3	11	0.15
(1,1902)	1:172:A:ALA:HA	1:178:A:PRO:HD2	13	0.15
(1,1902)	1:172:A:ALA:HA	1:178:A:PRO:HD3	13	0.15
(1,1902)	1:172:A:ALA:HA	1:178:A:PRO:HD2	15	0.15
(1,1902)	1:172:A:ALA:HA	1:178:A:PRO:HD3	15	0.15
(1,1902)	1:172:A:ALA:HA	1:178:A:PRO:HD2	17	0.15
(1,1902)	1:172:A:ALA:HA	1:178:A:PRO:HD3	17	0.15
(1,1892)	1:161:A:LEU:HD11	1:162:A:GLY:HA2	8	0.15
(1,1892)	1:161:A:LEU:HD11	1:162:A:GLY:HA3	8	0.15
(1,1892)	1:161:A:LEU:HD12	1:162:A:GLY:HA2	8	0.15
(1,1892)	1:161:A:LEU:HD12	1:162:A:GLY:HA3	8	0.15
(1,1892)	1:161:A:LEU:HD13	1:162:A:GLY:HA2	8	0.15
(1,1892)	1:161:A:LEU:HD13	1:162:A:GLY:HA3	8	0.15
(1,1892)	1:161:A:LEU:HD11	1:162:A:GLY:HA2	15	0.15
(1,1892)	1:161:A:LEU:HD11	1:162:A:GLY:HA3	15	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1892)	1:161:A:LEU:HD12	1:162:A:GLY:HA2	15	0.15
(1,1892)	1:161:A:LEU:HD12	1:162:A:GLY:HA3	15	0.15
(1,1892)	1:161:A:LEU:HD13	1:162:A:GLY:HA2	15	0.15
(1,1892)	1:161:A:LEU:HD13	1:162:A:GLY:HA3	15	0.15
(1,1885)	1:155:A:ALA:HB1	1:157:A:PRO:HD2	7	0.15
(1,1885)	1:155:A:ALA:HB1	1:157:A:PRO:HD3	7	0.15
(1,1885)	1:155:A:ALA:HB2	1:157:A:PRO:HD2	7	0.15
(1,1885)	1:155:A:ALA:HB2	1:157:A:PRO:HD3	7	0.15
(1,1885)	1:155:A:ALA:HB3	1:157:A:PRO:HD2	7	0.15
(1,1885)	1:155:A:ALA:HB3	1:157:A:PRO:HD3	7	0.15
(1,1880)	1:153:A:LYS:H	1:154:A:PRO:HD2	7	0.15
(1,1880)	1:153:A:LYS:H	1:154:A:PRO:HD3	7	0.15
(1,1878)	1:151:A:GLN:HB2	1:152:A:ALA:HA	2	0.15
(1,1878)	1:151:A:GLN:HB3	1:152:A:ALA:HA	2	0.15
(1,1867)	1:134:A:LEU:H	1:188:C:LEU:HD11	15	0.15
(1,1867)	1:134:A:LEU:H	1:188:C:LEU:HD12	15	0.15
(1,1867)	1:134:A:LEU:H	1:188:C:LEU:HD13	15	0.15
(1,1867)	1:134:A:LEU:H	1:188:C:LEU:HD21	15	0.15
(1,1867)	1:134:A:LEU:H	1:188:C:LEU:HD22	15	0.15
(1,1867)	1:134:A:LEU:H	1:188:C:LEU:HD23	15	0.15
(1,1818)	1:95:B:SER:HB2	1:101:B:LEU:H	5	0.15
(1,1818)	1:95:B:SER:HB3	1:101:B:LEU:H	5	0.15
(1,1818)	1:95:B:SER:HB2	1:101:B:LEU:H	18	0.15
(1,1818)	1:95:B:SER:HB3	1:101:B:LEU:H	18	0.15
(1,1817)	1:95:A:SER:HB2	1:101:A:LEU:H	8	0.15
(1,1817)	1:95:A:SER:HB3	1:101:A:LEU:H	8	0.15
(1,1817)	1:95:A:SER:HB2	1:101:A:LEU:H	12	0.15
(1,1817)	1:95:A:SER:HB3	1:101:A:LEU:H	12	0.15
(1,1788)	1:96:B:ILE:HG21	1:101:B:LEU:H	18	0.15
(1,1788)	1:96:B:ILE:HG22	1:101:B:LEU:H	18	0.15
(1,1788)	1:96:B:ILE:HG23	1:101:B:LEU:H	18	0.15
(1,1774)	1:125:A:LYS:H	1:126:A:ILE:HG21	20	0.15
(1,1774)	1:125:A:LYS:H	1:126:A:ILE:HG22	20	0.15
(1,1774)	1:125:A:LYS:H	1:126:A:ILE:HG23	20	0.15
(1,1736)	1:194:C:LEU:HG	1:195:C:TYR:H	20	0.15
(1,1735)	1:194:B:LEU:HG	1:195:B:TYR:H	20	0.15
(1,1686)	1:90:A:THR:H	1:91:A:THR:HB	18	0.15
(1,1622)	1:129:C:GLU:H	1:131:C:ILE:H	5	0.15
(1,1616)	1:116:C:ALA:H	1:119:C:THR:HB	5	0.15
(1,1616)	1:116:C:ALA:H	1:119:C:THR:HB	6	0.15
(1,1616)	1:116:C:ALA:H	1:119:C:THR:HB	8	0.15
(1,1616)	1:116:C:ALA:H	1:119:C:THR:HB	9	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1615)	1:116:B:ALA:H	1:119:B:THR:HB	5	0.15
(1,1615)	1:116:B:ALA:H	1:119:B:THR:HB	6	0.15
(1,1614)	1:116:A:ALA:H	1:119:A:THR:HB	1	0.15
(1,1614)	1:116:A:ALA:H	1:119:A:THR:HB	6	0.15
(1,1610)	1:118:A:GLY:H	1:192:A:VAL:HG21	9	0.15
(1,1610)	1:118:A:GLY:H	1:192:A:VAL:HG22	9	0.15
(1,1610)	1:118:A:GLY:H	1:192:A:VAL:HG23	9	0.15
(1,1602)	1:89:A:VAL:HG21	1:91:A:THR:H	2	0.15
(1,1602)	1:89:A:VAL:HG22	1:91:A:THR:H	2	0.15
(1,1602)	1:89:A:VAL:HG23	1:91:A:THR:H	2	0.15
(1,1564)	1:145:C:GLN:HA	1:151:C:GLN:H	13	0.15
(1,1562)	1:145:A:GLN:HA	1:151:A:GLN:H	12	0.15
(1,1557)	1:155:B:ALA:HB1	1:167:B:ARG:H	4	0.15
(1,1557)	1:155:B:ALA:HB2	1:167:B:ARG:H	4	0.15
(1,1557)	1:155:B:ALA:HB3	1:167:B:ARG:H	4	0.15
(1,1550)	1:167:B:ARG:H	1:171:B:SER:HA	8	0.15
(1,1549)	1:167:A:ARG:H	1:171:A:SER:HA	8	0.15
(1,1548)	1:167:C:ARG:H	1:170:C:GLY:HA2	2	0.15
(1,1548)	1:167:C:ARG:H	1:170:C:GLY:HA3	2	0.15
(1,1547)	1:167:B:ARG:H	1:170:B:GLY:HA2	3	0.15
(1,1547)	1:167:B:ARG:H	1:170:B:GLY:HA3	3	0.15
(1,1546)	1:167:A:ARG:H	1:170:A:GLY:HA2	2	0.15
(1,1546)	1:167:A:ARG:H	1:170:A:GLY:HA3	2	0.15
(1,1546)	1:167:A:ARG:H	1:170:A:GLY:HA2	3	0.15
(1,1546)	1:167:A:ARG:H	1:170:A:GLY:HA3	3	0.15
(1,1535)	1:122:C:TYR:H	1:189:C:CYS:HB2	1	0.15
(1,1535)	1:122:C:TYR:H	1:189:C:CYS:HB3	1	0.15
(1,1535)	1:122:C:TYR:H	1:189:C:CYS:HB2	14	0.15
(1,1535)	1:122:C:TYR:H	1:189:C:CYS:HB3	14	0.15
(1,1535)	1:122:C:TYR:H	1:189:C:CYS:HB2	18	0.15
(1,1535)	1:122:C:TYR:H	1:189:C:CYS:HB3	18	0.15
(1,1535)	1:122:C:TYR:H	1:189:C:CYS:HB2	19	0.15
(1,1535)	1:122:C:TYR:H	1:189:C:CYS:HB3	19	0.15
(1,1535)	1:122:C:TYR:H	1:189:C:CYS:HB2	20	0.15
(1,1535)	1:122:C:TYR:H	1:189:C:CYS:HB3	20	0.15
(1,1534)	1:122:B:TYR:H	1:189:B:CYS:HB2	1	0.15
(1,1534)	1:122:B:TYR:H	1:189:B:CYS:HB3	1	0.15
(1,1534)	1:122:B:TYR:H	1:189:B:CYS:HB2	7	0.15
(1,1534)	1:122:B:TYR:H	1:189:B:CYS:HB3	7	0.15
(1,1534)	1:122:B:TYR:H	1:189:B:CYS:HB2	9	0.15
(1,1534)	1:122:B:TYR:H	1:189:B:CYS:HB3	9	0.15
(1,1534)	1:122:B:TYR:H	1:189:B:CYS:HB2	14	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1534)	1:122:B:TYR:H	1:189:B:CYS:HB3	14	0.15
(1,1534)	1:122:B:TYR:H	1:189:B:CYS:HB2	19	0.15
(1,1534)	1:122:B:TYR:H	1:189:B:CYS:HB3	19	0.15
(1,1534)	1:122:B:TYR:H	1:189:B:CYS:HB2	20	0.15
(1,1534)	1:122:B:TYR:H	1:189:B:CYS:HB3	20	0.15
(1,1533)	1:122:A:TYR:H	1:189:A:CYS:HB2	18	0.15
(1,1533)	1:122:A:TYR:H	1:189:A:CYS:HB3	18	0.15
(1,1512)	1:137:B:LEU:H	1:137:B:LEU:HG	8	0.15
(1,1511)	1:137:A:LEU:H	1:137:A:LEU:HG	15	0.15
(1,1504)	1:92:A:ALA:H	1:103:A:VAL:HG21	6	0.15
(1,1504)	1:92:A:ALA:H	1:103:A:VAL:HG22	6	0.15
(1,1504)	1:92:A:ALA:H	1:103:A:VAL:HG23	6	0.15
(1,1463)	1:180:C:PHE:H	1:181:C:LEU:HA	20	0.15
(1,1462)	1:180:B:PHE:H	1:181:B:LEU:HA	9	0.15
(1,1462)	1:180:B:PHE:H	1:181:B:LEU:HA	20	0.15
(1,1461)	1:180:A:PHE:H	1:181:A:LEU:HA	20	0.15
(1,1432)	1:111:C:ILE:H	1:123:C:ILE:HG21	3	0.15
(1,1432)	1:111:C:ILE:H	1:123:C:ILE:HG22	3	0.15
(1,1432)	1:111:C:ILE:H	1:123:C:ILE:HG23	3	0.15
(1,1410)	1:152:C:ALA:HB1	1:153:C:LYS:H	3	0.15
(1,1410)	1:152:C:ALA:HB2	1:153:C:LYS:H	3	0.15
(1,1410)	1:152:C:ALA:HB3	1:153:C:LYS:H	3	0.15
(1,1409)	1:152:B:ALA:HB1	1:153:B:LYS:H	3	0.15
(1,1409)	1:152:B:ALA:HB2	1:153:B:LYS:H	3	0.15
(1,1409)	1:152:B:ALA:HB3	1:153:B:LYS:H	3	0.15
(1,1408)	1:152:A:ALA:HB1	1:153:A:LYS:H	7	0.15
(1,1408)	1:152:A:ALA:HB2	1:153:A:LYS:H	7	0.15
(1,1408)	1:152:A:ALA:HB3	1:153:A:LYS:H	7	0.15
(1,1387)	1:141:A:VAL:HG21	1:142:A:HIS:H	9	0.15
(1,1387)	1:141:A:VAL:HG22	1:142:A:HIS:H	9	0.15
(1,1387)	1:141:A:VAL:HG23	1:142:A:HIS:H	9	0.15
(1,1374)	1:155:A:ALA:H	1:156:A:VAL:HG11	12	0.15
(1,1374)	1:155:A:ALA:H	1:156:A:VAL:HG12	12	0.15
(1,1374)	1:155:A:ALA:H	1:156:A:VAL:HG13	12	0.15
(1,1333)	1:171:B:SER:HA	1:172:B:ALA:H	14	0.15
(1,1332)	1:171:A:SER:HA	1:172:A:ALA:H	14	0.15
(1,1276)	1:109:A:LEU:H	1:109:A:LEU:HG	1	0.15
(1,1276)	1:109:A:LEU:H	1:109:A:LEU:HG	5	0.15
(1,1203)	1:196:C:TYR:H	1:196:C:TYR:HE1	3	0.15
(1,1203)	1:196:C:TYR:H	1:196:C:TYR:HE2	3	0.15
(1,1203)	1:196:C:TYR:H	1:196:C:TYR:HE1	14	0.15
(1,1203)	1:196:C:TYR:H	1:196:C:TYR:HE2	14	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1202)	1:196:B:TYR:H	1:196:B:TYR:HE1	3	0.15
(1,1202)	1:196:B:TYR:H	1:196:B:TYR:HE2	3	0.15
(1,1100)	1:167:C:ARG:H	1:167:C:ARG:HB2	12	0.15
(1,1099)	1:167:B:ARG:H	1:167:B:ARG:HB2	12	0.15
(1,1096)	1:157:B:PRO:HA	1:158:B:THR:H	20	0.15
(1,1095)	1:157:A:PRO:HA	1:158:A:THR:H	20	0.15
(1,1071)	1:139:A:ARG:H	1:141:A:VAL:HB	13	0.15
(1,1048)	1:137:B:LEU:HG	1:138:B:THR:H	8	0.15
(1,1047)	1:137:A:LEU:HG	1:138:A:THR:H	6	0.15
(1,1036)	1:188:A:LEU:HD21	1:134:B:LEU:H	5	0.15
(1,1036)	1:188:A:LEU:HD22	1:134:B:LEU:H	5	0.15
(1,1036)	1:188:A:LEU:HD23	1:134:B:LEU:H	5	0.15
(1,1015)	1:104:C:TYR:H	1:112:C:ALA:H	18	0.15
(1,965)	1:110:A:LEU:HD11	1:125:A:LYS:HB3	17	0.15
(1,965)	1:110:A:LEU:HD12	1:125:A:LYS:HB3	17	0.15
(1,965)	1:110:A:LEU:HD13	1:125:A:LYS:HB3	17	0.15
(1,965)	1:110:A:LEU:HD11	1:125:A:LYS:HB3	20	0.15
(1,965)	1:110:A:LEU:HD12	1:125:A:LYS:HB3	20	0.15
(1,965)	1:110:A:LEU:HD13	1:125:A:LYS:HB3	20	0.15
(1,892)	1:165:B:GLU:HB2	1:167:B:ARG:HG2	15	0.15
(1,892)	1:165:B:GLU:HB2	1:167:B:ARG:HG3	15	0.15
(1,889)	1:152:B:ALA:HA	1:157:B:PRO:HG2	1	0.15
(1,889)	1:152:B:ALA:HA	1:157:B:PRO:HG3	1	0.15
(1,889)	1:152:B:ALA:HA	1:157:B:PRO:HG2	6	0.15
(1,889)	1:152:B:ALA:HA	1:157:B:PRO:HG3	6	0.15
(1,889)	1:152:B:ALA:HA	1:157:B:PRO:HG2	7	0.15
(1,889)	1:152:B:ALA:HA	1:157:B:PRO:HG3	7	0.15
(1,888)	1:152:A:ALA:HA	1:157:A:PRO:HG2	8	0.15
(1,888)	1:152:A:ALA:HA	1:157:A:PRO:HG3	8	0.15
(1,848)	1:150:A:LEU:HD11	1:167:A:ARG:HG2	10	0.15
(1,848)	1:150:A:LEU:HD11	1:167:A:ARG:HG3	10	0.15
(1,848)	1:150:A:LEU:HD12	1:167:A:ARG:HG2	10	0.15
(1,848)	1:150:A:LEU:HD12	1:167:A:ARG:HG3	10	0.15
(1,848)	1:150:A:LEU:HD13	1:167:A:ARG:HG2	10	0.15
(1,848)	1:150:A:LEU:HD13	1:167:A:ARG:HG3	10	0.15
(1,815)	1:176:C:GLY:H	1:177:C:ASP:HB2	5	0.15
(1,814)	1:176:B:GLY:H	1:177:B:ASP:HB2	5	0.15
(1,794)	1:153:C:LYS:HE2	1:154:C:PRO:HG2	5	0.15
(1,794)	1:153:C:LYS:HE2	1:154:C:PRO:HG3	5	0.15
(1,794)	1:153:C:LYS:HE3	1:154:C:PRO:HG2	5	0.15
(1,794)	1:153:C:LYS:HE3	1:154:C:PRO:HG3	5	0.15
(1,793)	1:153:B:LYS:HE2	1:154:B:PRO:HG2	2	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,793)	1:153:B:LYS:HE2	1:154:B:PRO:HG3	2	0.15
(1,793)	1:153:B:LYS:HE3	1:154:B:PRO:HG2	2	0.15
(1,793)	1:153:B:LYS:HE3	1:154:B:PRO:HG3	2	0.15
(1,792)	1:153:A:LYS:HE2	1:154:A:PRO:HG2	2	0.15
(1,792)	1:153:A:LYS:HE2	1:154:A:PRO:HG3	2	0.15
(1,792)	1:153:A:LYS:HE3	1:154:A:PRO:HG2	2	0.15
(1,792)	1:153:A:LYS:HE3	1:154:A:PRO:HG3	2	0.15
(1,785)	1:167:C:ARG:HD2	1:169:C:ALA:HB1	15	0.15
(1,785)	1:167:C:ARG:HD2	1:169:C:ALA:HB2	15	0.15
(1,785)	1:167:C:ARG:HD2	1:169:C:ALA:HB3	15	0.15
(1,785)	1:167:C:ARG:HD3	1:169:C:ALA:HB1	15	0.15
(1,785)	1:167:C:ARG:HD3	1:169:C:ALA:HB2	15	0.15
(1,785)	1:167:C:ARG:HD3	1:169:C:ALA:HB3	15	0.15
(1,784)	1:167:B:ARG:HD2	1:169:B:ALA:HB1	15	0.15
(1,784)	1:167:B:ARG:HD2	1:169:B:ALA:HB2	15	0.15
(1,784)	1:167:B:ARG:HD2	1:169:B:ALA:HB3	15	0.15
(1,784)	1:167:B:ARG:HD3	1:169:B:ALA:HB1	15	0.15
(1,784)	1:167:B:ARG:HD3	1:169:B:ALA:HB2	15	0.15
(1,784)	1:167:B:ARG:HD3	1:169:B:ALA:HB3	15	0.15
(1,784)	1:167:B:ARG:HD2	1:169:B:ALA:HB1	19	0.15
(1,784)	1:167:B:ARG:HD2	1:169:B:ALA:HB2	19	0.15
(1,784)	1:167:B:ARG:HD2	1:169:B:ALA:HB3	19	0.15
(1,784)	1:167:B:ARG:HD3	1:169:B:ALA:HB1	19	0.15
(1,784)	1:167:B:ARG:HD3	1:169:B:ALA:HB2	19	0.15
(1,784)	1:167:B:ARG:HD3	1:169:B:ALA:HB3	19	0.15
(1,783)	1:167:A:ARG:HD2	1:169:A:ALA:HB1	19	0.15
(1,783)	1:167:A:ARG:HD2	1:169:A:ALA:HB2	19	0.15
(1,783)	1:167:A:ARG:HD2	1:169:A:ALA:HB3	19	0.15
(1,783)	1:167:A:ARG:HD3	1:169:A:ALA:HB1	19	0.15
(1,783)	1:167:A:ARG:HD3	1:169:A:ALA:HB2	19	0.15
(1,783)	1:167:A:ARG:HD3	1:169:A:ALA:HB3	19	0.15
(1,769)	1:102:A:VAL:HG21	1:104:A:TYR:HE1	15	0.15
(1,769)	1:102:A:VAL:HG21	1:104:A:TYR:HE2	15	0.15
(1,769)	1:102:A:VAL:HG22	1:104:A:TYR:HE1	15	0.15
(1,769)	1:102:A:VAL:HG22	1:104:A:TYR:HE2	15	0.15
(1,769)	1:102:A:VAL:HG23	1:104:A:TYR:HE1	15	0.15
(1,769)	1:102:A:VAL:HG23	1:104:A:TYR:HE2	15	0.15
(1,751)	1:123:C:ILE:HG21	1:179:C:ALA:HB1	4	0.15
(1,751)	1:123:C:ILE:HG21	1:179:C:ALA:HB2	4	0.15
(1,751)	1:123:C:ILE:HG21	1:179:C:ALA:HB3	4	0.15
(1,751)	1:123:C:ILE:HG22	1:179:C:ALA:HB1	4	0.15
(1,751)	1:123:C:ILE:HG22	1:179:C:ALA:HB2	4	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,751)	1:123:C:ILE:HG22	1:179:C:ALA:HB3	4	0.15
(1,751)	1:123:C:ILE:HG23	1:179:C:ALA:HB1	4	0.15
(1,751)	1:123:C:ILE:HG23	1:179:C:ALA:HB2	4	0.15
(1,751)	1:123:C:ILE:HG23	1:179:C:ALA:HB3	4	0.15
(1,751)	1:123:C:ILE:HG21	1:179:C:ALA:HB1	10	0.15
(1,751)	1:123:C:ILE:HG21	1:179:C:ALA:HB2	10	0.15
(1,751)	1:123:C:ILE:HG21	1:179:C:ALA:HB3	10	0.15
(1,751)	1:123:C:ILE:HG22	1:179:C:ALA:HB1	10	0.15
(1,751)	1:123:C:ILE:HG22	1:179:C:ALA:HB2	10	0.15
(1,751)	1:123:C:ILE:HG22	1:179:C:ALA:HB3	10	0.15
(1,751)	1:123:C:ILE:HG23	1:179:C:ALA:HB1	10	0.15
(1,751)	1:123:C:ILE:HG23	1:179:C:ALA:HB2	10	0.15
(1,751)	1:123:C:ILE:HG23	1:179:C:ALA:HB3	10	0.15
(1,750)	1:123:B:ILE:HG21	1:179:B:ALA:HB1	4	0.15
(1,750)	1:123:B:ILE:HG21	1:179:B:ALA:HB2	4	0.15
(1,750)	1:123:B:ILE:HG21	1:179:B:ALA:HB3	4	0.15
(1,750)	1:123:B:ILE:HG22	1:179:B:ALA:HB1	4	0.15
(1,750)	1:123:B:ILE:HG22	1:179:B:ALA:HB2	4	0.15
(1,750)	1:123:B:ILE:HG22	1:179:B:ALA:HB3	4	0.15
(1,750)	1:123:B:ILE:HG23	1:179:B:ALA:HB1	4	0.15
(1,750)	1:123:B:ILE:HG23	1:179:B:ALA:HB2	4	0.15
(1,750)	1:123:B:ILE:HG23	1:179:B:ALA:HB3	4	0.15
(1,737)	1:175:A:GLY:HA2	1:179:A:ALA:HB1	5	0.15
(1,737)	1:175:A:GLY:HA2	1:179:A:ALA:HB2	5	0.15
(1,737)	1:175:A:GLY:HA2	1:179:A:ALA:HB3	5	0.15
(1,737)	1:175:A:GLY:HA3	1:179:A:ALA:HB1	5	0.15
(1,737)	1:175:A:GLY:HA3	1:179:A:ALA:HB2	5	0.15
(1,737)	1:175:A:GLY:HA3	1:179:A:ALA:HB3	5	0.15
(1,737)	1:175:A:GLY:HA2	1:179:A:ALA:HB1	16	0.15
(1,737)	1:175:A:GLY:HA2	1:179:A:ALA:HB2	16	0.15
(1,737)	1:175:A:GLY:HA2	1:179:A:ALA:HB3	16	0.15
(1,737)	1:175:A:GLY:HA3	1:179:A:ALA:HB1	16	0.15
(1,737)	1:175:A:GLY:HA3	1:179:A:ALA:HB2	16	0.15
(1,737)	1:175:A:GLY:HA3	1:179:A:ALA:HB3	16	0.15
(1,665)	1:113:A:TYR:HE1	1:197:A:ILE:HG21	17	0.15
(1,665)	1:113:A:TYR:HE1	1:197:A:ILE:HG22	17	0.15
(1,665)	1:113:A:TYR:HE1	1:197:A:ILE:HG23	17	0.15
(1,665)	1:113:A:TYR:HE2	1:197:A:ILE:HG21	17	0.15
(1,665)	1:113:A:TYR:HE2	1:197:A:ILE:HG22	17	0.15
(1,665)	1:113:A:TYR:HE2	1:197:A:ILE:HG23	17	0.15
(1,637)	1:96:C:ILE:HG21	1:100:C:GLY:H	4	0.15
(1,637)	1:96:C:ILE:HG22	1:100:C:GLY:H	4	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,637)	1:96:C:ILE:HG23	1:100:C:GLY:H	4	0.15
(1,637)	1:96:C:ILE:HG21	1:100:C:GLY:H	14	0.15
(1,637)	1:96:C:ILE:HG22	1:100:C:GLY:H	14	0.15
(1,637)	1:96:C:ILE:HG23	1:100:C:GLY:H	14	0.15
(1,636)	1:96:B:ILE:HG21	1:100:B:GLY:H	4	0.15
(1,636)	1:96:B:ILE:HG22	1:100:B:GLY:H	4	0.15
(1,636)	1:96:B:ILE:HG23	1:100:B:GLY:H	4	0.15
(1,636)	1:96:B:ILE:HG21	1:100:B:GLY:H	14	0.15
(1,636)	1:96:B:ILE:HG22	1:100:B:GLY:H	14	0.15
(1,636)	1:96:B:ILE:HG23	1:100:B:GLY:H	14	0.15
(1,635)	1:96:A:ILE:HG21	1:100:A:GLY:H	13	0.15
(1,635)	1:96:A:ILE:HG22	1:100:A:GLY:H	13	0.15
(1,635)	1:96:A:ILE:HG23	1:100:A:GLY:H	13	0.15
(1,541)	1:111:C:ILE:HG21	1:126:C:ILE:HG21	7	0.15
(1,541)	1:111:C:ILE:HG21	1:126:C:ILE:HG22	7	0.15
(1,541)	1:111:C:ILE:HG21	1:126:C:ILE:HG23	7	0.15
(1,541)	1:111:C:ILE:HG22	1:126:C:ILE:HG21	7	0.15
(1,541)	1:111:C:ILE:HG22	1:126:C:ILE:HG22	7	0.15
(1,541)	1:111:C:ILE:HG22	1:126:C:ILE:HG23	7	0.15
(1,541)	1:111:C:ILE:HG23	1:126:C:ILE:HG21	7	0.15
(1,541)	1:111:C:ILE:HG23	1:126:C:ILE:HG22	7	0.15
(1,541)	1:111:C:ILE:HG23	1:126:C:ILE:HG23	7	0.15
(1,540)	1:111:B:ILE:HG21	1:126:B:ILE:HG21	7	0.15
(1,540)	1:111:B:ILE:HG21	1:126:B:ILE:HG22	7	0.15
(1,540)	1:111:B:ILE:HG21	1:126:B:ILE:HG23	7	0.15
(1,540)	1:111:B:ILE:HG22	1:126:B:ILE:HG21	7	0.15
(1,540)	1:111:B:ILE:HG22	1:126:B:ILE:HG22	7	0.15
(1,540)	1:111:B:ILE:HG22	1:126:B:ILE:HG23	7	0.15
(1,540)	1:111:B:ILE:HG23	1:126:B:ILE:HG21	7	0.15
(1,540)	1:111:B:ILE:HG23	1:126:B:ILE:HG22	7	0.15
(1,540)	1:111:B:ILE:HG23	1:126:B:ILE:HG23	7	0.15
(1,538)	1:111:C:ILE:HD11	1:131:C:ILE:HG21	16	0.15
(1,538)	1:111:C:ILE:HD11	1:131:C:ILE:HG22	16	0.15
(1,538)	1:111:C:ILE:HD11	1:131:C:ILE:HG23	16	0.15
(1,538)	1:111:C:ILE:HD12	1:131:C:ILE:HG21	16	0.15
(1,538)	1:111:C:ILE:HD12	1:131:C:ILE:HG22	16	0.15
(1,538)	1:111:C:ILE:HD12	1:131:C:ILE:HG23	16	0.15
(1,538)	1:111:C:ILE:HD13	1:131:C:ILE:HG21	16	0.15
(1,538)	1:111:C:ILE:HD13	1:131:C:ILE:HG22	16	0.15
(1,538)	1:111:C:ILE:HD13	1:131:C:ILE:HG23	16	0.15
(1,451)	1:95:A:SER:HB2	1:101:A:LEU:HD21	7	0.15
(1,451)	1:95:A:SER:HB2	1:101:A:LEU:HD22	7	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,451)	1:95:A:SER:HB2	1:101:A:LEU:HD23	7	0.15
(1,451)	1:95:A:SER:HB3	1:101:A:LEU:HD21	7	0.15
(1,451)	1:95:A:SER:HB3	1:101:A:LEU:HD22	7	0.15
(1,451)	1:95:A:SER:HB3	1:101:A:LEU:HD23	7	0.15
(1,437)	1:183:C:MET:HE1	1:186:C:SER:HA	12	0.15
(1,437)	1:183:C:MET:HE2	1:186:C:SER:HA	12	0.15
(1,437)	1:183:C:MET:HE3	1:186:C:SER:HA	12	0.15
(1,436)	1:183:B:MET:HE1	1:186:B:SER:HA	11	0.15
(1,436)	1:183:B:MET:HE2	1:186:B:SER:HA	11	0.15
(1,436)	1:183:B:MET:HE3	1:186:B:SER:HA	11	0.15
(1,436)	1:183:B:MET:HE1	1:186:B:SER:HA	12	0.15
(1,436)	1:183:B:MET:HE2	1:186:B:SER:HA	12	0.15
(1,436)	1:183:B:MET:HE3	1:186:B:SER:HA	12	0.15
(1,435)	1:183:A:MET:HE1	1:186:A:SER:HA	4	0.15
(1,435)	1:183:A:MET:HE2	1:186:A:SER:HA	4	0.15
(1,435)	1:183:A:MET:HE3	1:186:A:SER:HA	4	0.15
(1,397)	1:109:C:LEU:HG	1:111:C:ILE:HD11	3	0.15
(1,397)	1:109:C:LEU:HG	1:111:C:ILE:HD12	3	0.15
(1,397)	1:109:C:LEU:HG	1:111:C:ILE:HD13	3	0.15
(1,396)	1:109:B:LEU:HG	1:111:B:ILE:HD11	3	0.15
(1,396)	1:109:B:LEU:HG	1:111:B:ILE:HD12	3	0.15
(1,396)	1:109:B:LEU:HG	1:111:B:ILE:HD13	3	0.15
(1,396)	1:109:B:LEU:HG	1:111:B:ILE:HD11	10	0.15
(1,396)	1:109:B:LEU:HG	1:111:B:ILE:HD12	10	0.15
(1,396)	1:109:B:LEU:HG	1:111:B:ILE:HD13	10	0.15
(1,373)	1:96:C:ILE:HD11	1:102:C:VAL:HB	4	0.15
(1,373)	1:96:C:ILE:HD12	1:102:C:VAL:HB	4	0.15
(1,373)	1:96:C:ILE:HD13	1:102:C:VAL:HB	4	0.15
(1,365)	1:126:B:ILE:HG21	1:131:B:ILE:HD11	5	0.15
(1,365)	1:126:B:ILE:HG21	1:131:B:ILE:HD12	5	0.15
(1,365)	1:126:B:ILE:HG21	1:131:B:ILE:HD13	5	0.15
(1,365)	1:126:B:ILE:HG22	1:131:B:ILE:HD11	5	0.15
(1,365)	1:126:B:ILE:HG22	1:131:B:ILE:HD12	5	0.15
(1,365)	1:126:B:ILE:HG22	1:131:B:ILE:HD13	5	0.15
(1,365)	1:126:B:ILE:HG23	1:131:B:ILE:HD11	5	0.15
(1,365)	1:126:B:ILE:HG23	1:131:B:ILE:HD12	5	0.15
(1,365)	1:126:B:ILE:HG23	1:131:B:ILE:HD13	5	0.15
(1,365)	1:126:B:ILE:HG21	1:131:B:ILE:HD11	10	0.15
(1,365)	1:126:B:ILE:HG21	1:131:B:ILE:HD12	10	0.15
(1,365)	1:126:B:ILE:HG21	1:131:B:ILE:HD13	10	0.15
(1,365)	1:126:B:ILE:HG22	1:131:B:ILE:HD11	10	0.15
(1,365)	1:126:B:ILE:HG22	1:131:B:ILE:HD12	10	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,365)	1:126:B:ILE:HG22	1:131:B:ILE:HD13	10	0.15
(1,365)	1:126:B:ILE:HG23	1:131:B:ILE:HD11	10	0.15
(1,365)	1:126:B:ILE:HG23	1:131:B:ILE:HD12	10	0.15
(1,365)	1:126:B:ILE:HG23	1:131:B:ILE:HD13	10	0.15
(1,364)	1:126:A:ILE:HG21	1:131:A:ILE:HD11	5	0.15
(1,364)	1:126:A:ILE:HG21	1:131:A:ILE:HD12	5	0.15
(1,364)	1:126:A:ILE:HG21	1:131:A:ILE:HD13	5	0.15
(1,364)	1:126:A:ILE:HG22	1:131:A:ILE:HD11	5	0.15
(1,364)	1:126:A:ILE:HG22	1:131:A:ILE:HD12	5	0.15
(1,364)	1:126:A:ILE:HG22	1:131:A:ILE:HD13	5	0.15
(1,364)	1:126:A:ILE:HG23	1:131:A:ILE:HD11	5	0.15
(1,364)	1:126:A:ILE:HG23	1:131:A:ILE:HD12	5	0.15
(1,364)	1:126:A:ILE:HG23	1:131:A:ILE:HD13	5	0.15
(1,364)	1:126:A:ILE:HG21	1:131:A:ILE:HD11	7	0.15
(1,364)	1:126:A:ILE:HG21	1:131:A:ILE:HD12	7	0.15
(1,364)	1:126:A:ILE:HG21	1:131:A:ILE:HD13	7	0.15
(1,364)	1:126:A:ILE:HG22	1:131:A:ILE:HD11	7	0.15
(1,364)	1:126:A:ILE:HG22	1:131:A:ILE:HD12	7	0.15
(1,364)	1:126:A:ILE:HG22	1:131:A:ILE:HD13	7	0.15
(1,364)	1:126:A:ILE:HG23	1:131:A:ILE:HD11	7	0.15
(1,364)	1:126:A:ILE:HG23	1:131:A:ILE:HD12	7	0.15
(1,364)	1:126:A:ILE:HG23	1:131:A:ILE:HD13	7	0.15
(1,363)	1:131:A:ILE:HD11	1:183:C:MET:HG2	7	0.15
(1,363)	1:131:A:ILE:HD11	1:183:C:MET:HG3	7	0.15
(1,363)	1:131:A:ILE:HD12	1:183:C:MET:HG2	7	0.15
(1,363)	1:131:A:ILE:HD12	1:183:C:MET:HG3	7	0.15
(1,363)	1:131:A:ILE:HD13	1:183:C:MET:HG2	7	0.15
(1,363)	1:131:A:ILE:HD13	1:183:C:MET:HG3	7	0.15
(1,363)	1:131:A:ILE:HD11	1:183:C:MET:HG2	17	0.15
(1,363)	1:131:A:ILE:HD11	1:183:C:MET:HG3	17	0.15
(1,363)	1:131:A:ILE:HD12	1:183:C:MET:HG2	17	0.15
(1,363)	1:131:A:ILE:HD12	1:183:C:MET:HG3	17	0.15
(1,363)	1:131:A:ILE:HD13	1:183:C:MET:HG2	17	0.15
(1,363)	1:131:A:ILE:HD13	1:183:C:MET:HG3	17	0.15
(1,349)	1:123:A:ILE:HD11	1:196:A:TYR:HE1	14	0.15
(1,349)	1:123:A:ILE:HD11	1:196:A:TYR:HE2	14	0.15
(1,349)	1:123:A:ILE:HD12	1:196:A:TYR:HE1	14	0.15
(1,349)	1:123:A:ILE:HD12	1:196:A:TYR:HE2	14	0.15
(1,349)	1:123:A:ILE:HD13	1:196:A:TYR:HE1	14	0.15
(1,349)	1:123:A:ILE:HD13	1:196:A:TYR:HE2	14	0.15
(1,316)	1:112:A:ALA:HB1	1:123:A:ILE:HD11	18	0.15
(1,316)	1:112:A:ALA:HB1	1:123:A:ILE:HD12	18	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,316)	1:112:A:ALA:HB1	1:123:A:ILE:HD13	18	0.15
(1,316)	1:112:A:ALA:HB2	1:123:A:ILE:HD11	18	0.15
(1,316)	1:112:A:ALA:HB2	1:123:A:ILE:HD12	18	0.15
(1,316)	1:112:A:ALA:HB2	1:123:A:ILE:HD13	18	0.15
(1,316)	1:112:A:ALA:HB3	1:123:A:ILE:HD11	18	0.15
(1,316)	1:112:A:ALA:HB3	1:123:A:ILE:HD12	18	0.15
(1,316)	1:112:A:ALA:HB3	1:123:A:ILE:HD13	18	0.15
(1,301)	1:181:A:LEU:HD11	1:196:A:TYR:HE1	10	0.15
(1,301)	1:181:A:LEU:HD11	1:196:A:TYR:HE2	10	0.15
(1,301)	1:181:A:LEU:HD12	1:196:A:TYR:HE1	10	0.15
(1,301)	1:181:A:LEU:HD12	1:196:A:TYR:HE2	10	0.15
(1,301)	1:181:A:LEU:HD13	1:196:A:TYR:HE1	10	0.15
(1,301)	1:181:A:LEU:HD13	1:196:A:TYR:HE2	10	0.15
(1,239)	1:102:A:VAL:HG21	1:137:A:LEU:HD21	7	0.15
(1,239)	1:102:A:VAL:HG21	1:137:A:LEU:HD22	7	0.15
(1,239)	1:102:A:VAL:HG21	1:137:A:LEU:HD23	7	0.15
(1,239)	1:102:A:VAL:HG22	1:137:A:LEU:HD21	7	0.15
(1,239)	1:102:A:VAL:HG22	1:137:A:LEU:HD22	7	0.15
(1,239)	1:102:A:VAL:HG22	1:137:A:LEU:HD23	7	0.15
(1,239)	1:102:A:VAL:HG23	1:137:A:LEU:HD21	7	0.15
(1,239)	1:102:A:VAL:HG23	1:137:A:LEU:HD22	7	0.15
(1,239)	1:102:A:VAL:HG23	1:137:A:LEU:HD23	7	0.15
(1,216)	1:96:A:ILE:HG21	1:102:A:VAL:HG11	6	0.15
(1,216)	1:96:A:ILE:HG21	1:102:A:VAL:HG12	6	0.15
(1,216)	1:96:A:ILE:HG21	1:102:A:VAL:HG13	6	0.15
(1,216)	1:96:A:ILE:HG22	1:102:A:VAL:HG11	6	0.15
(1,216)	1:96:A:ILE:HG22	1:102:A:VAL:HG12	6	0.15
(1,216)	1:96:A:ILE:HG22	1:102:A:VAL:HG13	6	0.15
(1,216)	1:96:A:ILE:HG23	1:102:A:VAL:HG11	6	0.15
(1,216)	1:96:A:ILE:HG23	1:102:A:VAL:HG12	6	0.15
(1,216)	1:96:A:ILE:HG23	1:102:A:VAL:HG13	6	0.15
(1,182)	1:137:A:LEU:HD11	1:141:A:VAL:HG11	1	0.15
(1,182)	1:137:A:LEU:HD11	1:141:A:VAL:HG12	1	0.15
(1,182)	1:137:A:LEU:HD11	1:141:A:VAL:HG13	1	0.15
(1,182)	1:137:A:LEU:HD12	1:141:A:VAL:HG11	1	0.15
(1,182)	1:137:A:LEU:HD12	1:141:A:VAL:HG12	1	0.15
(1,182)	1:137:A:LEU:HD12	1:141:A:VAL:HG13	1	0.15
(1,182)	1:137:A:LEU:HD13	1:141:A:VAL:HG11	1	0.15
(1,182)	1:137:A:LEU:HD13	1:141:A:VAL:HG12	1	0.15
(1,182)	1:137:A:LEU:HD13	1:141:A:VAL:HG13	1	0.15
(1,182)	1:137:A:LEU:HD11	1:141:A:VAL:HG11	8	0.15
(1,182)	1:137:A:LEU:HD11	1:141:A:VAL:HG12	8	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,182)	1:137:A:LEU:HD11	1:141:A:VAL:HG13	8	0.15
(1,182)	1:137:A:LEU:HD12	1:141:A:VAL:HG11	8	0.15
(1,182)	1:137:A:LEU:HD12	1:141:A:VAL:HG12	8	0.15
(1,182)	1:137:A:LEU:HD12	1:141:A:VAL:HG13	8	0.15
(1,182)	1:137:A:LEU:HD13	1:141:A:VAL:HG11	8	0.15
(1,182)	1:137:A:LEU:HD13	1:141:A:VAL:HG12	8	0.15
(1,182)	1:137:A:LEU:HD13	1:141:A:VAL:HG13	8	0.15
(1,182)	1:137:A:LEU:HD11	1:141:A:VAL:HG11	15	0.15
(1,182)	1:137:A:LEU:HD11	1:141:A:VAL:HG12	15	0.15
(1,182)	1:137:A:LEU:HD11	1:141:A:VAL:HG13	15	0.15
(1,182)	1:137:A:LEU:HD12	1:141:A:VAL:HG11	15	0.15
(1,182)	1:137:A:LEU:HD12	1:141:A:VAL:HG12	15	0.15
(1,182)	1:137:A:LEU:HD12	1:141:A:VAL:HG13	15	0.15
(1,182)	1:137:A:LEU:HD13	1:141:A:VAL:HG11	15	0.15
(1,182)	1:137:A:LEU:HD13	1:141:A:VAL:HG12	15	0.15
(1,182)	1:137:A:LEU:HD13	1:141:A:VAL:HG13	15	0.15
(1,175)	1:179:A:ALA:HB1	1:181:A:LEU:HD21	8	0.15
(1,175)	1:179:A:ALA:HB1	1:181:A:LEU:HD22	8	0.15
(1,175)	1:179:A:ALA:HB1	1:181:A:LEU:HD23	8	0.15
(1,175)	1:179:A:ALA:HB2	1:181:A:LEU:HD21	8	0.15
(1,175)	1:179:A:ALA:HB2	1:181:A:LEU:HD22	8	0.15
(1,175)	1:179:A:ALA:HB2	1:181:A:LEU:HD23	8	0.15
(1,175)	1:179:A:ALA:HB3	1:181:A:LEU:HD21	8	0.15
(1,175)	1:179:A:ALA:HB3	1:181:A:LEU:HD22	8	0.15
(1,175)	1:179:A:ALA:HB3	1:181:A:LEU:HD23	8	0.15
(1,175)	1:179:A:ALA:HB1	1:181:A:LEU:HD21	13	0.15
(1,175)	1:179:A:ALA:HB1	1:181:A:LEU:HD22	13	0.15
(1,175)	1:179:A:ALA:HB1	1:181:A:LEU:HD23	13	0.15
(1,175)	1:179:A:ALA:HB2	1:181:A:LEU:HD21	13	0.15
(1,175)	1:179:A:ALA:HB2	1:181:A:LEU:HD22	13	0.15
(1,175)	1:179:A:ALA:HB2	1:181:A:LEU:HD23	13	0.15
(1,175)	1:179:A:ALA:HB3	1:181:A:LEU:HD21	13	0.15
(1,175)	1:179:A:ALA:HB3	1:181:A:LEU:HD22	13	0.15
(1,175)	1:179:A:ALA:HB3	1:181:A:LEU:HD23	13	0.15
(1,157)	1:101:A:LEU:HD21	1:95:B:SER:HB2	6	0.15
(1,157)	1:101:A:LEU:HD21	1:95:B:SER:HB3	6	0.15
(1,157)	1:101:A:LEU:HD22	1:95:B:SER:HB2	6	0.15
(1,157)	1:101:A:LEU:HD22	1:95:B:SER:HB3	6	0.15
(1,157)	1:101:A:LEU:HD23	1:95:B:SER:HB2	6	0.15
(1,157)	1:101:A:LEU:HD23	1:95:B:SER:HB3	6	0.15
(1,157)	1:101:A:LEU:HD21	1:95:B:SER:HB2	19	0.15
(1,157)	1:101:A:LEU:HD21	1:95:B:SER:HB3	19	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,157)	1:101:A:LEU:HD22	1:95:B:SER:HB2	19	0.15
(1,157)	1:101:A:LEU:HD22	1:95:B:SER:HB3	19	0.15
(1,157)	1:101:A:LEU:HD23	1:95:B:SER:HB2	19	0.15
(1,157)	1:101:A:LEU:HD23	1:95:B:SER:HB3	19	0.15
(1,154)	1:187:A:THR:HG21	1:188:A:LEU:HD21	1	0.15
(1,154)	1:187:A:THR:HG21	1:188:A:LEU:HD22	1	0.15
(1,154)	1:187:A:THR:HG21	1:188:A:LEU:HD23	1	0.15
(1,154)	1:187:A:THR:HG22	1:188:A:LEU:HD21	1	0.15
(1,154)	1:187:A:THR:HG22	1:188:A:LEU:HD22	1	0.15
(1,154)	1:187:A:THR:HG22	1:188:A:LEU:HD23	1	0.15
(1,154)	1:187:A:THR:HG23	1:188:A:LEU:HD21	1	0.15
(1,154)	1:187:A:THR:HG23	1:188:A:LEU:HD22	1	0.15
(1,154)	1:187:A:THR:HG23	1:188:A:LEU:HD23	1	0.15
(1,138)	1:192:A:VAL:HG21	1:135:B:GLU:HG2	14	0.15
(1,138)	1:192:A:VAL:HG21	1:135:B:GLU:HG3	14	0.15
(1,138)	1:192:A:VAL:HG22	1:135:B:GLU:HG2	14	0.15
(1,138)	1:192:A:VAL:HG22	1:135:B:GLU:HG3	14	0.15
(1,138)	1:192:A:VAL:HG23	1:135:B:GLU:HG2	14	0.15
(1,138)	1:192:A:VAL:HG23	1:135:B:GLU:HG3	14	0.15
(1,134)	1:110:A:LEU:HD11	1:111:A:ILE:HD11	2	0.15
(1,134)	1:110:A:LEU:HD11	1:111:A:ILE:HD12	2	0.15
(1,134)	1:110:A:LEU:HD11	1:111:A:ILE:HD13	2	0.15
(1,134)	1:110:A:LEU:HD12	1:111:A:ILE:HD11	2	0.15
(1,134)	1:110:A:LEU:HD12	1:111:A:ILE:HD12	2	0.15
(1,134)	1:110:A:LEU:HD12	1:111:A:ILE:HD13	2	0.15
(1,134)	1:110:A:LEU:HD13	1:111:A:ILE:HD11	2	0.15
(1,134)	1:110:A:LEU:HD13	1:111:A:ILE:HD12	2	0.15
(1,134)	1:110:A:LEU:HD13	1:111:A:ILE:HD13	2	0.15
(1,93)	1:155:A:ALA:HB1	1:157:A:PRO:HD3	12	0.15
(1,93)	1:155:A:ALA:HB2	1:157:A:PRO:HD3	12	0.15
(1,93)	1:155:A:ALA:HB3	1:157:A:PRO:HD3	12	0.15
(1,56)	1:156:A:VAL:HG11	1:157:A:PRO:HD3	10	0.15
(1,56)	1:156:A:VAL:HG12	1:157:A:PRO:HD3	10	0.15
(1,56)	1:156:A:VAL:HG13	1:157:A:PRO:HD3	10	0.15
(1,36)	1:102:A:VAL:HG21	1:112:A:ALA:H	4	0.15
(1,36)	1:102:A:VAL:HG22	1:112:A:ALA:H	4	0.15
(1,36)	1:102:A:VAL:HG23	1:112:A:ALA:H	4	0.15
(1,1)	1:108:A:GLN:HA	1:109:A:LEU:HD21	7	0.15
(1,1)	1:108:A:GLN:HA	1:109:A:LEU:HD22	7	0.15
(1,1)	1:108:A:GLN:HA	1:109:A:LEU:HD23	7	0.15
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD11	19	0.14
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD12	19	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD13	19	0.14
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD21	19	0.14
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD22	19	0.14
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD23	19	0.14
(1,2338)	1:179:C:ALA:HB1	1:181:C:LEU:HD11	14	0.14
(1,2338)	1:179:C:ALA:HB1	1:181:C:LEU:HD12	14	0.14
(1,2338)	1:179:C:ALA:HB1	1:181:C:LEU:HD13	14	0.14
(1,2338)	1:179:C:ALA:HB1	1:181:C:LEU:HD21	14	0.14
(1,2338)	1:179:C:ALA:HB1	1:181:C:LEU:HD22	14	0.14
(1,2338)	1:179:C:ALA:HB1	1:181:C:LEU:HD23	14	0.14
(1,2338)	1:179:C:ALA:HB2	1:181:C:LEU:HD11	14	0.14
(1,2338)	1:179:C:ALA:HB2	1:181:C:LEU:HD12	14	0.14
(1,2338)	1:179:C:ALA:HB2	1:181:C:LEU:HD13	14	0.14
(1,2338)	1:179:C:ALA:HB2	1:181:C:LEU:HD21	14	0.14
(1,2338)	1:179:C:ALA:HB2	1:181:C:LEU:HD22	14	0.14
(1,2338)	1:179:C:ALA:HB2	1:181:C:LEU:HD23	14	0.14
(1,2338)	1:179:C:ALA:HB3	1:181:C:LEU:HD11	14	0.14
(1,2338)	1:179:C:ALA:HB3	1:181:C:LEU:HD12	14	0.14
(1,2338)	1:179:C:ALA:HB3	1:181:C:LEU:HD13	14	0.14
(1,2338)	1:179:C:ALA:HB3	1:181:C:LEU:HD21	14	0.14
(1,2338)	1:179:C:ALA:HB3	1:181:C:LEU:HD22	14	0.14
(1,2338)	1:179:C:ALA:HB3	1:181:C:LEU:HD23	14	0.14
(1,2329)	1:178:C:PRO:HB2	1:179:C:ALA:H	3	0.14
(1,2329)	1:178:C:PRO:HB3	1:179:C:ALA:H	3	0.14
(1,2326)	1:177:C:ASP:HB2	1:180:C:PHE:H	19	0.14
(1,2326)	1:177:C:ASP:HB3	1:180:C:PHE:H	19	0.14
(1,2322)	1:176:C:GLY:H	1:177:C:ASP:HB2	2	0.14
(1,2322)	1:176:C:GLY:H	1:177:C:ASP:HB3	2	0.14
(1,2322)	1:176:C:GLY:H	1:177:C:ASP:HB2	4	0.14
(1,2322)	1:176:C:GLY:H	1:177:C:ASP:HB3	4	0.14
(1,2322)	1:176:C:GLY:H	1:177:C:ASP:HB2	10	0.14
(1,2322)	1:176:C:GLY:H	1:177:C:ASP:HB3	10	0.14
(1,2322)	1:176:C:GLY:H	1:177:C:ASP:HB2	11	0.14
(1,2322)	1:176:C:GLY:H	1:177:C:ASP:HB3	11	0.14
(1,2322)	1:176:C:GLY:H	1:177:C:ASP:HB2	14	0.14
(1,2322)	1:176:C:GLY:H	1:177:C:ASP:HB3	14	0.14
(1,2283)	1:150:C:LEU:HD11	1:167:C:ARG:HG2	19	0.14
(1,2283)	1:150:C:LEU:HD11	1:167:C:ARG:HG3	19	0.14
(1,2283)	1:150:C:LEU:HD12	1:167:C:ARG:HG2	19	0.14
(1,2283)	1:150:C:LEU:HD12	1:167:C:ARG:HG3	19	0.14
(1,2283)	1:150:C:LEU:HD13	1:167:C:ARG:HG2	19	0.14
(1,2283)	1:150:C:LEU:HD13	1:167:C:ARG:HG3	19	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2283)	1:150:C:LEU:HD21	1:167:C:ARG:HG2	19	0.14
(1,2283)	1:150:C:LEU:HD21	1:167:C:ARG:HG3	19	0.14
(1,2283)	1:150:C:LEU:HD22	1:167:C:ARG:HG2	19	0.14
(1,2283)	1:150:C:LEU:HD22	1:167:C:ARG:HG3	19	0.14
(1,2283)	1:150:C:LEU:HD23	1:167:C:ARG:HG2	19	0.14
(1,2283)	1:150:C:LEU:HD23	1:167:C:ARG:HG3	19	0.14
(1,2236)	1:121:C:CYS:HB2	1:189:C:CYS:H	10	0.14
(1,2236)	1:121:C:CYS:HB3	1:189:C:CYS:H	10	0.14
(1,2236)	1:121:C:CYS:HB2	1:189:C:CYS:H	14	0.14
(1,2236)	1:121:C:CYS:HB3	1:189:C:CYS:H	14	0.14
(1,2188)	1:102:C:VAL:HG11	1:112:C:ALA:H	4	0.14
(1,2188)	1:102:C:VAL:HG12	1:112:C:ALA:H	4	0.14
(1,2188)	1:102:C:VAL:HG13	1:112:C:ALA:H	4	0.14
(1,2188)	1:102:C:VAL:HG21	1:112:C:ALA:H	4	0.14
(1,2188)	1:102:C:VAL:HG22	1:112:C:ALA:H	4	0.14
(1,2188)	1:102:C:VAL:HG23	1:112:C:ALA:H	4	0.14
(1,2163)	1:89:C:VAL:HG11	1:183:C:MET:HE1	17	0.14
(1,2163)	1:89:C:VAL:HG11	1:183:C:MET:HE2	17	0.14
(1,2163)	1:89:C:VAL:HG11	1:183:C:MET:HE3	17	0.14
(1,2163)	1:89:C:VAL:HG12	1:183:C:MET:HE1	17	0.14
(1,2163)	1:89:C:VAL:HG12	1:183:C:MET:HE2	17	0.14
(1,2163)	1:89:C:VAL:HG12	1:183:C:MET:HE3	17	0.14
(1,2163)	1:89:C:VAL:HG13	1:183:C:MET:HE1	17	0.14
(1,2163)	1:89:C:VAL:HG13	1:183:C:MET:HE2	17	0.14
(1,2163)	1:89:C:VAL:HG13	1:183:C:MET:HE3	17	0.14
(1,2163)	1:89:C:VAL:HG21	1:183:C:MET:HE1	17	0.14
(1,2163)	1:89:C:VAL:HG21	1:183:C:MET:HE2	17	0.14
(1,2163)	1:89:C:VAL:HG21	1:183:C:MET:HE3	17	0.14
(1,2163)	1:89:C:VAL:HG22	1:183:C:MET:HE1	17	0.14
(1,2163)	1:89:C:VAL:HG22	1:183:C:MET:HE2	17	0.14
(1,2163)	1:89:C:VAL:HG22	1:183:C:MET:HE3	17	0.14
(1,2163)	1:89:C:VAL:HG23	1:183:C:MET:HE1	17	0.14
(1,2163)	1:89:C:VAL:HG23	1:183:C:MET:HE2	17	0.14
(1,2163)	1:89:C:VAL:HG23	1:183:C:MET:HE3	17	0.14
(1,2138)	1:188:B:LEU:HD11	1:134:C:LEU:H	9	0.14
(1,2138)	1:188:B:LEU:HD12	1:134:C:LEU:H	9	0.14
(1,2138)	1:188:B:LEU:HD13	1:134:C:LEU:H	9	0.14
(1,2138)	1:188:B:LEU:HD21	1:134:C:LEU:H	9	0.14
(1,2138)	1:188:B:LEU:HD22	1:134:C:LEU:H	9	0.14
(1,2138)	1:188:B:LEU:HD23	1:134:C:LEU:H	9	0.14
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD11	15	0.14
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD12	15	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD13	15	0.14
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD21	15	0.14
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD22	15	0.14
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD23	15	0.14
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD11	19	0.14
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD12	19	0.14
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD13	19	0.14
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD21	19	0.14
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD22	19	0.14
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD23	19	0.14
(1,2112)	1:179:B:ALA:HB1	1:181:B:LEU:HD11	14	0.14
(1,2112)	1:179:B:ALA:HB1	1:181:B:LEU:HD12	14	0.14
(1,2112)	1:179:B:ALA:HB1	1:181:B:LEU:HD13	14	0.14
(1,2112)	1:179:B:ALA:HB1	1:181:B:LEU:HD21	14	0.14
(1,2112)	1:179:B:ALA:HB1	1:181:B:LEU:HD22	14	0.14
(1,2112)	1:179:B:ALA:HB1	1:181:B:LEU:HD23	14	0.14
(1,2112)	1:179:B:ALA:HB2	1:181:B:LEU:HD11	14	0.14
(1,2112)	1:179:B:ALA:HB2	1:181:B:LEU:HD12	14	0.14
(1,2112)	1:179:B:ALA:HB2	1:181:B:LEU:HD13	14	0.14
(1,2112)	1:179:B:ALA:HB2	1:181:B:LEU:HD21	14	0.14
(1,2112)	1:179:B:ALA:HB2	1:181:B:LEU:HD22	14	0.14
(1,2112)	1:179:B:ALA:HB2	1:181:B:LEU:HD23	14	0.14
(1,2112)	1:179:B:ALA:HB3	1:181:B:LEU:HD11	14	0.14
(1,2112)	1:179:B:ALA:HB3	1:181:B:LEU:HD12	14	0.14
(1,2112)	1:179:B:ALA:HB3	1:181:B:LEU:HD13	14	0.14
(1,2112)	1:179:B:ALA:HB3	1:181:B:LEU:HD21	14	0.14
(1,2112)	1:179:B:ALA:HB3	1:181:B:LEU:HD22	14	0.14
(1,2112)	1:179:B:ALA:HB3	1:181:B:LEU:HD23	14	0.14
(1,2112)	1:179:B:ALA:HB1	1:181:B:LEU:HD11	15	0.14
(1,2112)	1:179:B:ALA:HB1	1:181:B:LEU:HD12	15	0.14
(1,2112)	1:179:B:ALA:HB1	1:181:B:LEU:HD13	15	0.14
(1,2112)	1:179:B:ALA:HB1	1:181:B:LEU:HD21	15	0.14
(1,2112)	1:179:B:ALA:HB1	1:181:B:LEU:HD22	15	0.14
(1,2112)	1:179:B:ALA:HB1	1:181:B:LEU:HD23	15	0.14
(1,2112)	1:179:B:ALA:HB2	1:181:B:LEU:HD11	15	0.14
(1,2112)	1:179:B:ALA:HB2	1:181:B:LEU:HD12	15	0.14
(1,2112)	1:179:B:ALA:HB2	1:181:B:LEU:HD13	15	0.14
(1,2112)	1:179:B:ALA:HB2	1:181:B:LEU:HD21	15	0.14
(1,2112)	1:179:B:ALA:HB2	1:181:B:LEU:HD22	15	0.14
(1,2112)	1:179:B:ALA:HB2	1:181:B:LEU:HD23	15	0.14
(1,2112)	1:179:B:ALA:HB3	1:181:B:LEU:HD11	15	0.14
(1,2112)	1:179:B:ALA:HB3	1:181:B:LEU:HD12	15	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2112)	1:179:B:ALA:HB3	1:181:B:LEU:HD13	15	0.14
(1,2112)	1:179:B:ALA:HB3	1:181:B:LEU:HD21	15	0.14
(1,2112)	1:179:B:ALA:HB3	1:181:B:LEU:HD22	15	0.14
(1,2112)	1:179:B:ALA:HB3	1:181:B:LEU:HD23	15	0.14
(1,2103)	1:178:B:PRO:HB2	1:179:B:ALA:H	3	0.14
(1,2103)	1:178:B:PRO:HB3	1:179:B:ALA:H	3	0.14
(1,2100)	1:177:B:ASP:HB2	1:180:B:PHE:H	19	0.14
(1,2100)	1:177:B:ASP:HB3	1:180:B:PHE:H	19	0.14
(1,2096)	1:176:B:GLY:H	1:177:B:ASP:HB2	2	0.14
(1,2096)	1:176:B:GLY:H	1:177:B:ASP:HB3	2	0.14
(1,2096)	1:176:B:GLY:H	1:177:B:ASP:HB2	4	0.14
(1,2096)	1:176:B:GLY:H	1:177:B:ASP:HB3	4	0.14
(1,2096)	1:176:B:GLY:H	1:177:B:ASP:HB2	10	0.14
(1,2096)	1:176:B:GLY:H	1:177:B:ASP:HB3	10	0.14
(1,2096)	1:176:B:GLY:H	1:177:B:ASP:HB2	11	0.14
(1,2096)	1:176:B:GLY:H	1:177:B:ASP:HB3	11	0.14
(1,2096)	1:176:B:GLY:H	1:177:B:ASP:HB2	14	0.14
(1,2096)	1:176:B:GLY:H	1:177:B:ASP:HB3	14	0.14
(1,2095)	1:172:B:ALA:HB1	1:173:B:PRO:HD2	5	0.14
(1,2095)	1:172:B:ALA:HB1	1:173:B:PRO:HD3	5	0.14
(1,2095)	1:172:B:ALA:HB2	1:173:B:PRO:HD2	5	0.14
(1,2095)	1:172:B:ALA:HB2	1:173:B:PRO:HD3	5	0.14
(1,2095)	1:172:B:ALA:HB3	1:173:B:PRO:HD2	5	0.14
(1,2095)	1:172:B:ALA:HB3	1:173:B:PRO:HD3	5	0.14
(1,2010)	1:121:B:CYS:HB2	1:189:B:CYS:H	14	0.14
(1,2010)	1:121:B:CYS:HB3	1:189:B:CYS:H	14	0.14
(1,2010)	1:121:B:CYS:HB2	1:189:B:CYS:H	17	0.14
(1,2010)	1:121:B:CYS:HB3	1:189:B:CYS:H	17	0.14
(1,1961)	1:102:B:VAL:HG11	1:112:B:ALA:H	4	0.14
(1,1961)	1:102:B:VAL:HG12	1:112:B:ALA:H	4	0.14
(1,1961)	1:102:B:VAL:HG13	1:112:B:ALA:H	4	0.14
(1,1961)	1:102:B:VAL:HG21	1:112:B:ALA:H	4	0.14
(1,1961)	1:102:B:VAL:HG22	1:112:B:ALA:H	4	0.14
(1,1961)	1:102:B:VAL:HG23	1:112:B:ALA:H	4	0.14
(1,1935)	1:89:B:VAL:HG11	1:183:B:MET:HE1	7	0.14
(1,1935)	1:89:B:VAL:HG11	1:183:B:MET:HE2	7	0.14
(1,1935)	1:89:B:VAL:HG11	1:183:B:MET:HE3	7	0.14
(1,1935)	1:89:B:VAL:HG12	1:183:B:MET:HE1	7	0.14
(1,1935)	1:89:B:VAL:HG12	1:183:B:MET:HE2	7	0.14
(1,1935)	1:89:B:VAL:HG12	1:183:B:MET:HE3	7	0.14
(1,1935)	1:89:B:VAL:HG13	1:183:B:MET:HE1	7	0.14
(1,1935)	1:89:B:VAL:HG13	1:183:B:MET:HE2	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1935)	1:89:B:VAL:HG13	1:183:B:MET:HE3	7	0.14
(1,1935)	1:89:B:VAL:HG21	1:183:B:MET:HE1	7	0.14
(1,1935)	1:89:B:VAL:HG21	1:183:B:MET:HE2	7	0.14
(1,1935)	1:89:B:VAL:HG21	1:183:B:MET:HE3	7	0.14
(1,1935)	1:89:B:VAL:HG22	1:183:B:MET:HE1	7	0.14
(1,1935)	1:89:B:VAL:HG22	1:183:B:MET:HE2	7	0.14
(1,1935)	1:89:B:VAL:HG22	1:183:B:MET:HE3	7	0.14
(1,1935)	1:89:B:VAL:HG23	1:183:B:MET:HE1	7	0.14
(1,1935)	1:89:B:VAL:HG23	1:183:B:MET:HE2	7	0.14
(1,1935)	1:89:B:VAL:HG23	1:183:B:MET:HE3	7	0.14
(1,1935)	1:89:B:VAL:HG11	1:183:B:MET:HE1	17	0.14
(1,1935)	1:89:B:VAL:HG11	1:183:B:MET:HE2	17	0.14
(1,1935)	1:89:B:VAL:HG11	1:183:B:MET:HE3	17	0.14
(1,1935)	1:89:B:VAL:HG12	1:183:B:MET:HE1	17	0.14
(1,1935)	1:89:B:VAL:HG12	1:183:B:MET:HE2	17	0.14
(1,1935)	1:89:B:VAL:HG12	1:183:B:MET:HE3	17	0.14
(1,1935)	1:89:B:VAL:HG13	1:183:B:MET:HE1	17	0.14
(1,1935)	1:89:B:VAL:HG13	1:183:B:MET:HE2	17	0.14
(1,1935)	1:89:B:VAL:HG13	1:183:B:MET:HE3	17	0.14
(1,1935)	1:89:B:VAL:HG21	1:183:B:MET:HE1	17	0.14
(1,1935)	1:89:B:VAL:HG21	1:183:B:MET:HE2	17	0.14
(1,1935)	1:89:B:VAL:HG21	1:183:B:MET:HE3	17	0.14
(1,1935)	1:89:B:VAL:HG22	1:183:B:MET:HE1	17	0.14
(1,1935)	1:89:B:VAL:HG22	1:183:B:MET:HE2	17	0.14
(1,1935)	1:89:B:VAL:HG22	1:183:B:MET:HE3	17	0.14
(1,1935)	1:89:B:VAL:HG23	1:183:B:MET:HE1	17	0.14
(1,1935)	1:89:B:VAL:HG23	1:183:B:MET:HE2	17	0.14
(1,1935)	1:89:B:VAL:HG23	1:183:B:MET:HE3	17	0.14
(1,1910)	1:178:A:PRO:HB2	1:179:A:ALA:H	3	0.14
(1,1910)	1:178:A:PRO:HB3	1:179:A:ALA:H	3	0.14
(1,1904)	1:176:A:GLY:H	1:177:A:ASP:HB2	4	0.14
(1,1904)	1:176:A:GLY:H	1:177:A:ASP:HB3	4	0.14
(1,1904)	1:176:A:GLY:H	1:177:A:ASP:HB2	7	0.14
(1,1904)	1:176:A:GLY:H	1:177:A:ASP:HB3	7	0.14
(1,1904)	1:176:A:GLY:H	1:177:A:ASP:HB2	10	0.14
(1,1904)	1:176:A:GLY:H	1:177:A:ASP:HB3	10	0.14
(1,1904)	1:176:A:GLY:H	1:177:A:ASP:HB2	13	0.14
(1,1904)	1:176:A:GLY:H	1:177:A:ASP:HB3	13	0.14
(1,1904)	1:176:A:GLY:H	1:177:A:ASP:HB2	14	0.14
(1,1904)	1:176:A:GLY:H	1:177:A:ASP:HB3	14	0.14
(1,1903)	1:172:A:ALA:HB1	1:173:A:PRO:HD2	1	0.14
(1,1903)	1:172:A:ALA:HB1	1:173:A:PRO:HD3	1	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1903)	1:172:A:ALA:HB2	1:173:A:PRO:HD2	1	0.14
(1,1903)	1:172:A:ALA:HB2	1:173:A:PRO:HD3	1	0.14
(1,1903)	1:172:A:ALA:HB3	1:173:A:PRO:HD2	1	0.14
(1,1903)	1:172:A:ALA:HB3	1:173:A:PRO:HD3	1	0.14
(1,1903)	1:172:A:ALA:HB1	1:173:A:PRO:HD2	10	0.14
(1,1903)	1:172:A:ALA:HB1	1:173:A:PRO:HD3	10	0.14
(1,1903)	1:172:A:ALA:HB2	1:173:A:PRO:HD2	10	0.14
(1,1903)	1:172:A:ALA:HB2	1:173:A:PRO:HD3	10	0.14
(1,1903)	1:172:A:ALA:HB3	1:173:A:PRO:HD2	10	0.14
(1,1903)	1:172:A:ALA:HB3	1:173:A:PRO:HD3	10	0.14
(1,1903)	1:172:A:ALA:HB1	1:173:A:PRO:HD2	13	0.14
(1,1903)	1:172:A:ALA:HB1	1:173:A:PRO:HD3	13	0.14
(1,1903)	1:172:A:ALA:HB2	1:173:A:PRO:HD2	13	0.14
(1,1903)	1:172:A:ALA:HB2	1:173:A:PRO:HD3	13	0.14
(1,1903)	1:172:A:ALA:HB3	1:173:A:PRO:HD2	13	0.14
(1,1903)	1:172:A:ALA:HB3	1:173:A:PRO:HD3	13	0.14
(1,1903)	1:172:A:ALA:HB1	1:173:A:PRO:HD2	18	0.14
(1,1903)	1:172:A:ALA:HB1	1:173:A:PRO:HD3	18	0.14
(1,1903)	1:172:A:ALA:HB2	1:173:A:PRO:HD2	18	0.14
(1,1903)	1:172:A:ALA:HB2	1:173:A:PRO:HD3	18	0.14
(1,1903)	1:172:A:ALA:HB3	1:173:A:PRO:HD2	18	0.14
(1,1903)	1:172:A:ALA:HB3	1:173:A:PRO:HD3	18	0.14
(1,1885)	1:155:A:ALA:HB1	1:157:A:PRO:HD2	18	0.14
(1,1885)	1:155:A:ALA:HB1	1:157:A:PRO:HD3	18	0.14
(1,1885)	1:155:A:ALA:HB2	1:157:A:PRO:HD2	18	0.14
(1,1885)	1:155:A:ALA:HB2	1:157:A:PRO:HD3	18	0.14
(1,1885)	1:155:A:ALA:HB3	1:157:A:PRO:HD2	18	0.14
(1,1885)	1:155:A:ALA:HB3	1:157:A:PRO:HD3	18	0.14
(1,1874)	1:143:A:ASN:HB2	1:144:A:PHE:HA	4	0.14
(1,1874)	1:143:A:ASN:HB3	1:144:A:PHE:HA	4	0.14
(1,1842)	1:121:A:CYS:HB2	1:189:A:CYS:H	4	0.14
(1,1842)	1:121:A:CYS:HB3	1:189:A:CYS:H	4	0.14
(1,1818)	1:95:B:SER:HB2	1:101:B:LEU:H	17	0.14
(1,1818)	1:95:B:SER:HB3	1:101:B:LEU:H	17	0.14
(1,1818)	1:95:B:SER:HB2	1:101:B:LEU:H	20	0.14
(1,1818)	1:95:B:SER:HB3	1:101:B:LEU:H	20	0.14
(1,1817)	1:95:A:SER:HB2	1:101:A:LEU:H	1	0.14
(1,1817)	1:95:A:SER:HB3	1:101:A:LEU:H	1	0.14
(1,1817)	1:95:A:SER:HB2	1:101:A:LEU:H	9	0.14
(1,1817)	1:95:A:SER:HB3	1:101:A:LEU:H	9	0.14
(1,1817)	1:95:A:SER:HB2	1:101:A:LEU:H	13	0.14
(1,1817)	1:95:A:SER:HB3	1:101:A:LEU:H	13	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1692)	1:120:A:CYS:H	1:192:A:VAL:HG11	1	0.14
(1,1692)	1:120:A:CYS:H	1:192:A:VAL:HG12	1	0.14
(1,1692)	1:120:A:CYS:H	1:192:A:VAL:HG13	1	0.14
(1,1692)	1:120:A:CYS:H	1:192:A:VAL:HG11	11	0.14
(1,1692)	1:120:A:CYS:H	1:192:A:VAL:HG12	11	0.14
(1,1692)	1:120:A:CYS:H	1:192:A:VAL:HG13	11	0.14
(1,1687)	1:90:B:THR:H	1:91:B:THR:HB	18	0.14
(1,1670)	1:101:A:LEU:HD11	1:102:A:VAL:H	3	0.14
(1,1670)	1:101:A:LEU:HD12	1:102:A:VAL:H	3	0.14
(1,1670)	1:101:A:LEU:HD13	1:102:A:VAL:H	3	0.14
(1,1620)	1:129:A:GLU:H	1:131:A:ILE:H	16	0.14
(1,1616)	1:116:C:ALA:H	1:119:C:THR:HB	3	0.14
(1,1616)	1:116:C:ALA:H	1:119:C:THR:HB	16	0.14
(1,1615)	1:116:B:ALA:H	1:119:B:THR:HB	3	0.14
(1,1615)	1:116:B:ALA:H	1:119:B:THR:HB	9	0.14
(1,1615)	1:116:B:ALA:H	1:119:B:THR:HB	16	0.14
(1,1564)	1:145:C:GLN:HA	1:151:C:GLN:H	11	0.14
(1,1564)	1:145:C:GLN:HA	1:151:C:GLN:H	19	0.14
(1,1563)	1:145:B:GLN:HA	1:151:B:GLN:H	11	0.14
(1,1563)	1:145:B:GLN:HA	1:151:B:GLN:H	19	0.14
(1,1562)	1:145:A:GLN:HA	1:151:A:GLN:H	16	0.14
(1,1562)	1:145:A:GLN:HA	1:151:A:GLN:H	18	0.14
(1,1552)	1:156:A:VAL:HB	1:167:A:ARG:H	14	0.14
(1,1551)	1:167:C:ARG:H	1:171:C:SER:HA	8	0.14
(1,1551)	1:167:C:ARG:H	1:171:C:SER:HA	20	0.14
(1,1549)	1:167:A:ARG:H	1:171:A:SER:HA	20	0.14
(1,1548)	1:167:C:ARG:H	1:170:C:GLY:HA2	4	0.14
(1,1548)	1:167:C:ARG:H	1:170:C:GLY:HA3	4	0.14
(1,1548)	1:167:C:ARG:H	1:170:C:GLY:HA2	5	0.14
(1,1548)	1:167:C:ARG:H	1:170:C:GLY:HA3	5	0.14
(1,1548)	1:167:C:ARG:H	1:170:C:GLY:HA2	6	0.14
(1,1548)	1:167:C:ARG:H	1:170:C:GLY:HA3	6	0.14
(1,1547)	1:167:B:ARG:H	1:170:B:GLY:HA2	2	0.14
(1,1547)	1:167:B:ARG:H	1:170:B:GLY:HA3	2	0.14
(1,1547)	1:167:B:ARG:H	1:170:B:GLY:HA2	4	0.14
(1,1547)	1:167:B:ARG:H	1:170:B:GLY:HA3	4	0.14
(1,1547)	1:167:B:ARG:H	1:170:B:GLY:HA2	5	0.14
(1,1547)	1:167:B:ARG:H	1:170:B:GLY:HA3	5	0.14
(1,1547)	1:167:B:ARG:H	1:170:B:GLY:HA2	6	0.14
(1,1547)	1:167:B:ARG:H	1:170:B:GLY:HA3	6	0.14
(1,1546)	1:167:A:ARG:H	1:170:A:GLY:HA2	8	0.14
(1,1546)	1:167:A:ARG:H	1:170:A:GLY:HA3	8	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1541)	1:136:C:ALA:HB1	1:140:C:LYS:H	4	0.14
(1,1541)	1:136:C:ALA:HB2	1:140:C:LYS:H	4	0.14
(1,1541)	1:136:C:ALA:HB3	1:140:C:LYS:H	4	0.14
(1,1539)	1:136:A:ALA:HB1	1:140:A:LYS:H	1	0.14
(1,1539)	1:136:A:ALA:HB2	1:140:A:LYS:H	1	0.14
(1,1539)	1:136:A:ALA:HB3	1:140:A:LYS:H	1	0.14
(1,1535)	1:122:C:TYR:H	1:189:C:CYS:HB2	4	0.14
(1,1535)	1:122:C:TYR:H	1:189:C:CYS:HB3	4	0.14
(1,1535)	1:122:C:TYR:H	1:189:C:CYS:HB2	9	0.14
(1,1535)	1:122:C:TYR:H	1:189:C:CYS:HB3	9	0.14
(1,1534)	1:122:B:TYR:H	1:189:B:CYS:HB2	4	0.14
(1,1534)	1:122:B:TYR:H	1:189:B:CYS:HB3	4	0.14
(1,1533)	1:122:A:TYR:H	1:189:A:CYS:HB2	12	0.14
(1,1533)	1:122:A:TYR:H	1:189:A:CYS:HB3	12	0.14
(1,1533)	1:122:A:TYR:H	1:189:A:CYS:HB2	16	0.14
(1,1533)	1:122:A:TYR:H	1:189:A:CYS:HB3	16	0.14
(1,1526)	1:179:A:ALA:H	1:181:A:LEU:HD11	3	0.14
(1,1526)	1:179:A:ALA:H	1:181:A:LEU:HD12	3	0.14
(1,1526)	1:179:A:ALA:H	1:181:A:LEU:HD13	3	0.14
(1,1504)	1:92:A:ALA:H	1:103:A:VAL:HG21	14	0.14
(1,1504)	1:92:A:ALA:H	1:103:A:VAL:HG22	14	0.14
(1,1504)	1:92:A:ALA:H	1:103:A:VAL:HG23	14	0.14
(1,1463)	1:180:C:PHE:H	1:181:C:LEU:HA	17	0.14
(1,1432)	1:111:C:ILE:H	1:123:C:ILE:HG21	1	0.14
(1,1432)	1:111:C:ILE:H	1:123:C:ILE:HG22	1	0.14
(1,1432)	1:111:C:ILE:H	1:123:C:ILE:HG23	1	0.14
(1,1432)	1:111:C:ILE:H	1:123:C:ILE:HG21	17	0.14
(1,1432)	1:111:C:ILE:H	1:123:C:ILE:HG22	17	0.14
(1,1432)	1:111:C:ILE:H	1:123:C:ILE:HG23	17	0.14
(1,1431)	1:111:B:ILE:H	1:123:B:ILE:HG21	1	0.14
(1,1431)	1:111:B:ILE:H	1:123:B:ILE:HG22	1	0.14
(1,1431)	1:111:B:ILE:H	1:123:B:ILE:HG23	1	0.14
(1,1431)	1:111:B:ILE:H	1:123:B:ILE:HG21	17	0.14
(1,1431)	1:111:B:ILE:H	1:123:B:ILE:HG22	17	0.14
(1,1431)	1:111:B:ILE:H	1:123:B:ILE:HG23	17	0.14
(1,1430)	1:111:A:ILE:H	1:123:A:ILE:HG21	7	0.14
(1,1430)	1:111:A:ILE:H	1:123:A:ILE:HG22	7	0.14
(1,1430)	1:111:A:ILE:H	1:123:A:ILE:HG23	7	0.14
(1,1430)	1:111:A:ILE:H	1:123:A:ILE:HG21	8	0.14
(1,1430)	1:111:A:ILE:H	1:123:A:ILE:HG22	8	0.14
(1,1430)	1:111:A:ILE:H	1:123:A:ILE:HG23	8	0.14
(1,1430)	1:111:A:ILE:H	1:123:A:ILE:HG21	17	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1430)	1:111:A:ILE:H	1:123:A:ILE:HG22	17	0.14
(1,1430)	1:111:A:ILE:H	1:123:A:ILE:HG23	17	0.14
(1,1430)	1:111:A:ILE:H	1:123:A:ILE:HG21	20	0.14
(1,1430)	1:111:A:ILE:H	1:123:A:ILE:HG22	20	0.14
(1,1430)	1:111:A:ILE:H	1:123:A:ILE:HG23	20	0.14
(1,1410)	1:152:C:ALA:HB1	1:153:C:LYS:H	5	0.14
(1,1410)	1:152:C:ALA:HB2	1:153:C:LYS:H	5	0.14
(1,1410)	1:152:C:ALA:HB3	1:153:C:LYS:H	5	0.14
(1,1410)	1:152:C:ALA:HB1	1:153:C:LYS:H	7	0.14
(1,1410)	1:152:C:ALA:HB2	1:153:C:LYS:H	7	0.14
(1,1410)	1:152:C:ALA:HB3	1:153:C:LYS:H	7	0.14
(1,1409)	1:152:B:ALA:HB1	1:153:B:LYS:H	5	0.14
(1,1409)	1:152:B:ALA:HB2	1:153:B:LYS:H	5	0.14
(1,1409)	1:152:B:ALA:HB3	1:153:B:LYS:H	5	0.14
(1,1409)	1:152:B:ALA:HB1	1:153:B:LYS:H	7	0.14
(1,1409)	1:152:B:ALA:HB2	1:153:B:LYS:H	7	0.14
(1,1409)	1:152:B:ALA:HB3	1:153:B:LYS:H	7	0.14
(1,1408)	1:152:A:ALA:HB1	1:153:A:LYS:H	5	0.14
(1,1408)	1:152:A:ALA:HB2	1:153:A:LYS:H	5	0.14
(1,1408)	1:152:A:ALA:HB3	1:153:A:LYS:H	5	0.14
(1,1350)	1:127:A:ALA:H	1:131:A:ILE:HG21	6	0.14
(1,1350)	1:127:A:ALA:H	1:131:A:ILE:HG22	6	0.14
(1,1350)	1:127:A:ALA:H	1:131:A:ILE:HG23	6	0.14
(1,1350)	1:127:A:ALA:H	1:131:A:ILE:HG21	7	0.14
(1,1350)	1:127:A:ALA:H	1:131:A:ILE:HG22	7	0.14
(1,1350)	1:127:A:ALA:H	1:131:A:ILE:HG23	7	0.14
(1,1350)	1:127:A:ALA:H	1:131:A:ILE:HG21	17	0.14
(1,1350)	1:127:A:ALA:H	1:131:A:ILE:HG22	17	0.14
(1,1350)	1:127:A:ALA:H	1:131:A:ILE:HG23	17	0.14
(1,1334)	1:171:C:SER:HA	1:172:C:ALA:H	14	0.14
(1,1276)	1:109:A:LEU:H	1:109:A:LEU:HG	9	0.14
(1,1276)	1:109:A:LEU:H	1:109:A:LEU:HG	18	0.14
(1,1276)	1:109:A:LEU:H	1:109:A:LEU:HG	20	0.14
(1,1237)	1:96:A:ILE:H	1:100:A:GLY:H	8	0.14
(1,1203)	1:196:C:TYR:H	1:196:C:TYR:HE1	10	0.14
(1,1203)	1:196:C:TYR:H	1:196:C:TYR:HE2	10	0.14
(1,1202)	1:196:B:TYR:H	1:196:B:TYR:HE1	10	0.14
(1,1202)	1:196:B:TYR:H	1:196:B:TYR:HE2	10	0.14
(1,1202)	1:196:B:TYR:H	1:196:B:TYR:HE1	14	0.14
(1,1202)	1:196:B:TYR:H	1:196:B:TYR:HE2	14	0.14
(1,1201)	1:196:A:TYR:H	1:196:A:TYR:HE1	12	0.14
(1,1201)	1:196:A:TYR:H	1:196:A:TYR:HE2	12	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1201)	1:196:A:TYR:H	1:196:A:TYR:HE1	15	0.14
(1,1201)	1:196:A:TYR:H	1:196:A:TYR:HE2	15	0.14
(1,1100)	1:167:C:ARG:H	1:167:C:ARG:HB2	5	0.14
(1,1100)	1:167:C:ARG:H	1:167:C:ARG:HB2	8	0.14
(1,1099)	1:167:B:ARG:H	1:167:B:ARG:HB2	5	0.14
(1,1099)	1:167:B:ARG:H	1:167:B:ARG:HB2	8	0.14
(1,1098)	1:167:A:ARG:H	1:167:A:ARG:HB2	4	0.14
(1,1098)	1:167:A:ARG:H	1:167:A:ARG:HB2	5	0.14
(1,1098)	1:167:A:ARG:H	1:167:A:ARG:HB2	8	0.14
(1,1098)	1:167:A:ARG:H	1:167:A:ARG:HB2	12	0.14
(1,1097)	1:157:C:PRO:HA	1:158:C:THR:H	4	0.14
(1,1096)	1:157:B:PRO:HA	1:158:B:THR:H	4	0.14
(1,1071)	1:139:A:ARG:H	1:141:A:VAL:HB	6	0.14
(1,1036)	1:188:A:LEU:HD21	1:134:B:LEU:H	16	0.14
(1,1036)	1:188:A:LEU:HD22	1:134:B:LEU:H	16	0.14
(1,1036)	1:188:A:LEU:HD23	1:134:B:LEU:H	16	0.14
(1,1036)	1:188:A:LEU:HD21	1:134:B:LEU:H	17	0.14
(1,1036)	1:188:A:LEU:HD22	1:134:B:LEU:H	17	0.14
(1,1036)	1:188:A:LEU:HD23	1:134:B:LEU:H	17	0.14
(1,1036)	1:188:A:LEU:HD21	1:134:B:LEU:H	19	0.14
(1,1036)	1:188:A:LEU:HD22	1:134:B:LEU:H	19	0.14
(1,1036)	1:188:A:LEU:HD23	1:134:B:LEU:H	19	0.14
(1,965)	1:110:A:LEU:HD11	1:125:A:LYS:HB3	6	0.14
(1,965)	1:110:A:LEU:HD12	1:125:A:LYS:HB3	6	0.14
(1,965)	1:110:A:LEU:HD13	1:125:A:LYS:HB3	6	0.14
(1,894)	1:165:A:GLU:HB3	1:169:A:ALA:HB1	12	0.14
(1,894)	1:165:A:GLU:HB3	1:169:A:ALA:HB2	12	0.14
(1,894)	1:165:A:GLU:HB3	1:169:A:ALA:HB3	12	0.14
(1,893)	1:165:C:GLU:HB2	1:167:C:ARG:HG2	15	0.14
(1,893)	1:165:C:GLU:HB2	1:167:C:ARG:HG3	15	0.14
(1,891)	1:165:A:GLU:HB2	1:167:A:ARG:HG2	12	0.14
(1,891)	1:165:A:GLU:HB2	1:167:A:ARG:HG3	12	0.14
(1,891)	1:165:A:GLU:HB2	1:167:A:ARG:HG2	15	0.14
(1,891)	1:165:A:GLU:HB2	1:167:A:ARG:HG3	15	0.14
(1,890)	1:152:C:ALA:HA	1:157:C:PRO:HG2	1	0.14
(1,890)	1:152:C:ALA:HA	1:157:C:PRO:HG3	1	0.14
(1,866)	1:153:C:LYS:HA	1:154:C:PRO:HD2	9	0.14
(1,866)	1:153:C:LYS:HA	1:154:C:PRO:HD2	16	0.14
(1,865)	1:153:B:LYS:HA	1:154:B:PRO:HD2	9	0.14
(1,865)	1:153:B:LYS:HA	1:154:B:PRO:HD2	16	0.14
(1,864)	1:153:A:LYS:HA	1:154:A:PRO:HD2	9	0.14
(1,864)	1:153:A:LYS:HA	1:154:A:PRO:HD2	16	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,848)	1:150:A:LEU:HD11	1:167:A:ARG:HG2	13	0.14
(1,848)	1:150:A:LEU:HD11	1:167:A:ARG:HG3	13	0.14
(1,848)	1:150:A:LEU:HD12	1:167:A:ARG:HG2	13	0.14
(1,848)	1:150:A:LEU:HD12	1:167:A:ARG:HG3	13	0.14
(1,848)	1:150:A:LEU:HD13	1:167:A:ARG:HG2	13	0.14
(1,848)	1:150:A:LEU:HD13	1:167:A:ARG:HG3	13	0.14
(1,848)	1:150:A:LEU:HD11	1:167:A:ARG:HG2	20	0.14
(1,848)	1:150:A:LEU:HD11	1:167:A:ARG:HG3	20	0.14
(1,848)	1:150:A:LEU:HD12	1:167:A:ARG:HG2	20	0.14
(1,848)	1:150:A:LEU:HD12	1:167:A:ARG:HG3	20	0.14
(1,848)	1:150:A:LEU:HD13	1:167:A:ARG:HG2	20	0.14
(1,848)	1:150:A:LEU:HD13	1:167:A:ARG:HG3	20	0.14
(1,815)	1:176:C:GLY:H	1:177:C:ASP:HB2	6	0.14
(1,815)	1:176:C:GLY:H	1:177:C:ASP:HB2	7	0.14
(1,814)	1:176:B:GLY:H	1:177:B:ASP:HB2	6	0.14
(1,814)	1:176:B:GLY:H	1:177:B:ASP:HB2	7	0.14
(1,813)	1:176:A:GLY:H	1:177:A:ASP:HB2	5	0.14
(1,794)	1:153:C:LYS:HE2	1:154:C:PRO:HG2	2	0.14
(1,794)	1:153:C:LYS:HE2	1:154:C:PRO:HG3	2	0.14
(1,794)	1:153:C:LYS:HE3	1:154:C:PRO:HG2	2	0.14
(1,794)	1:153:C:LYS:HE3	1:154:C:PRO:HG3	2	0.14
(1,785)	1:167:C:ARG:HD2	1:169:C:ALA:HB1	19	0.14
(1,785)	1:167:C:ARG:HD2	1:169:C:ALA:HB2	19	0.14
(1,785)	1:167:C:ARG:HD2	1:169:C:ALA:HB3	19	0.14
(1,785)	1:167:C:ARG:HD3	1:169:C:ALA:HB1	19	0.14
(1,785)	1:167:C:ARG:HD3	1:169:C:ALA:HB2	19	0.14
(1,785)	1:167:C:ARG:HD3	1:169:C:ALA:HB3	19	0.14
(1,769)	1:102:A:VAL:HG21	1:104:A:TYR:HE1	20	0.14
(1,769)	1:102:A:VAL:HG21	1:104:A:TYR:HE2	20	0.14
(1,769)	1:102:A:VAL:HG22	1:104:A:TYR:HE1	20	0.14
(1,769)	1:102:A:VAL:HG22	1:104:A:TYR:HE2	20	0.14
(1,769)	1:102:A:VAL:HG23	1:104:A:TYR:HE1	20	0.14
(1,769)	1:102:A:VAL:HG23	1:104:A:TYR:HE2	20	0.14
(1,755)	1:189:C:CYS:H	1:192:C:VAL:HG11	6	0.14
(1,755)	1:189:C:CYS:H	1:192:C:VAL:HG12	6	0.14
(1,755)	1:189:C:CYS:H	1:192:C:VAL:HG13	6	0.14
(1,750)	1:123:B:ILE:HG21	1:179:B:ALA:HB1	10	0.14
(1,750)	1:123:B:ILE:HG21	1:179:B:ALA:HB2	10	0.14
(1,750)	1:123:B:ILE:HG21	1:179:B:ALA:HB3	10	0.14
(1,750)	1:123:B:ILE:HG22	1:179:B:ALA:HB1	10	0.14
(1,750)	1:123:B:ILE:HG22	1:179:B:ALA:HB2	10	0.14
(1,750)	1:123:B:ILE:HG22	1:179:B:ALA:HB3	10	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,750)	1:123:B:ILE:HG23	1:179:B:ALA:HB1	10	0.14
(1,750)	1:123:B:ILE:HG23	1:179:B:ALA:HB2	10	0.14
(1,750)	1:123:B:ILE:HG23	1:179:B:ALA:HB3	10	0.14
(1,749)	1:123:A:ILE:HG21	1:179:A:ALA:HB1	14	0.14
(1,749)	1:123:A:ILE:HG21	1:179:A:ALA:HB2	14	0.14
(1,749)	1:123:A:ILE:HG21	1:179:A:ALA:HB3	14	0.14
(1,749)	1:123:A:ILE:HG22	1:179:A:ALA:HB1	14	0.14
(1,749)	1:123:A:ILE:HG22	1:179:A:ALA:HB2	14	0.14
(1,749)	1:123:A:ILE:HG22	1:179:A:ALA:HB3	14	0.14
(1,749)	1:123:A:ILE:HG23	1:179:A:ALA:HB1	14	0.14
(1,749)	1:123:A:ILE:HG23	1:179:A:ALA:HB2	14	0.14
(1,749)	1:123:A:ILE:HG23	1:179:A:ALA:HB3	14	0.14
(1,738)	1:175:B:GLY:HA2	1:179:B:ALA:HB1	16	0.14
(1,738)	1:175:B:GLY:HA2	1:179:B:ALA:HB2	16	0.14
(1,738)	1:175:B:GLY:HA2	1:179:B:ALA:HB3	16	0.14
(1,738)	1:175:B:GLY:HA3	1:179:B:ALA:HB1	16	0.14
(1,738)	1:175:B:GLY:HA3	1:179:B:ALA:HB2	16	0.14
(1,738)	1:175:B:GLY:HA3	1:179:B:ALA:HB3	16	0.14
(1,712)	1:141:A:VAL:HG21	1:144:A:PHE:HD1	15	0.14
(1,712)	1:141:A:VAL:HG21	1:144:A:PHE:HD2	15	0.14
(1,712)	1:141:A:VAL:HG22	1:144:A:PHE:HD1	15	0.14
(1,712)	1:141:A:VAL:HG22	1:144:A:PHE:HD2	15	0.14
(1,712)	1:141:A:VAL:HG23	1:144:A:PHE:HD1	15	0.14
(1,712)	1:141:A:VAL:HG23	1:144:A:PHE:HD2	15	0.14
(1,712)	1:141:A:VAL:HG21	1:144:A:PHE:HD1	19	0.14
(1,712)	1:141:A:VAL:HG21	1:144:A:PHE:HD2	19	0.14
(1,712)	1:141:A:VAL:HG22	1:144:A:PHE:HD1	19	0.14
(1,712)	1:141:A:VAL:HG22	1:144:A:PHE:HD2	19	0.14
(1,712)	1:141:A:VAL:HG23	1:144:A:PHE:HD1	19	0.14
(1,712)	1:141:A:VAL:HG23	1:144:A:PHE:HD2	19	0.14
(1,693)	1:123:A:ILE:H	1:124:A:MET:HE1	3	0.14
(1,693)	1:123:A:ILE:H	1:124:A:MET:HE2	3	0.14
(1,693)	1:123:A:ILE:H	1:124:A:MET:HE3	3	0.14
(1,635)	1:96:A:ILE:HG21	1:100:A:GLY:H	11	0.14
(1,635)	1:96:A:ILE:HG22	1:100:A:GLY:H	11	0.14
(1,635)	1:96:A:ILE:HG23	1:100:A:GLY:H	11	0.14
(1,541)	1:111:C:ILE:HG21	1:126:C:ILE:HG21	6	0.14
(1,541)	1:111:C:ILE:HG21	1:126:C:ILE:HG22	6	0.14
(1,541)	1:111:C:ILE:HG21	1:126:C:ILE:HG23	6	0.14
(1,541)	1:111:C:ILE:HG22	1:126:C:ILE:HG21	6	0.14
(1,541)	1:111:C:ILE:HG22	1:126:C:ILE:HG22	6	0.14
(1,541)	1:111:C:ILE:HG22	1:126:C:ILE:HG23	6	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,541)	1:111:C:ILE:HG23	1:126:C:ILE:HG21	6	0.14
(1,541)	1:111:C:ILE:HG23	1:126:C:ILE:HG22	6	0.14
(1,541)	1:111:C:ILE:HG23	1:126:C:ILE:HG23	6	0.14
(1,540)	1:111:B:ILE:HG21	1:126:B:ILE:HG21	6	0.14
(1,540)	1:111:B:ILE:HG21	1:126:B:ILE:HG22	6	0.14
(1,540)	1:111:B:ILE:HG21	1:126:B:ILE:HG23	6	0.14
(1,540)	1:111:B:ILE:HG22	1:126:B:ILE:HG21	6	0.14
(1,540)	1:111:B:ILE:HG22	1:126:B:ILE:HG22	6	0.14
(1,540)	1:111:B:ILE:HG22	1:126:B:ILE:HG23	6	0.14
(1,540)	1:111:B:ILE:HG23	1:126:B:ILE:HG21	6	0.14
(1,540)	1:111:B:ILE:HG23	1:126:B:ILE:HG22	6	0.14
(1,540)	1:111:B:ILE:HG23	1:126:B:ILE:HG23	6	0.14
(1,536)	1:111:A:ILE:HD11	1:131:A:ILE:HG21	9	0.14
(1,536)	1:111:A:ILE:HD11	1:131:A:ILE:HG22	9	0.14
(1,536)	1:111:A:ILE:HD11	1:131:A:ILE:HG23	9	0.14
(1,536)	1:111:A:ILE:HD12	1:131:A:ILE:HG21	9	0.14
(1,536)	1:111:A:ILE:HD12	1:131:A:ILE:HG22	9	0.14
(1,536)	1:111:A:ILE:HD12	1:131:A:ILE:HG23	9	0.14
(1,536)	1:111:A:ILE:HD13	1:131:A:ILE:HG21	9	0.14
(1,536)	1:111:A:ILE:HD13	1:131:A:ILE:HG22	9	0.14
(1,536)	1:111:A:ILE:HD13	1:131:A:ILE:HG23	9	0.14
(1,451)	1:95:A:SER:HB2	1:101:A:LEU:HD21	3	0.14
(1,451)	1:95:A:SER:HB2	1:101:A:LEU:HD22	3	0.14
(1,451)	1:95:A:SER:HB2	1:101:A:LEU:HD23	3	0.14
(1,451)	1:95:A:SER:HB3	1:101:A:LEU:HD21	3	0.14
(1,451)	1:95:A:SER:HB3	1:101:A:LEU:HD22	3	0.14
(1,451)	1:95:A:SER:HB3	1:101:A:LEU:HD23	3	0.14
(1,437)	1:183:C:MET:HE1	1:186:C:SER:HA	4	0.14
(1,437)	1:183:C:MET:HE2	1:186:C:SER:HA	4	0.14
(1,437)	1:183:C:MET:HE3	1:186:C:SER:HA	4	0.14
(1,437)	1:183:C:MET:HE1	1:186:C:SER:HA	19	0.14
(1,437)	1:183:C:MET:HE2	1:186:C:SER:HA	19	0.14
(1,437)	1:183:C:MET:HE3	1:186:C:SER:HA	19	0.14
(1,436)	1:183:B:MET:HE1	1:186:B:SER:HA	19	0.14
(1,436)	1:183:B:MET:HE2	1:186:B:SER:HA	19	0.14
(1,436)	1:183:B:MET:HE3	1:186:B:SER:HA	19	0.14
(1,425)	1:89:A:VAL:HG11	1:183:A:MET:HE1	7	0.14
(1,425)	1:89:A:VAL:HG11	1:183:A:MET:HE2	7	0.14
(1,425)	1:89:A:VAL:HG11	1:183:A:MET:HE3	7	0.14
(1,425)	1:89:A:VAL:HG12	1:183:A:MET:HE1	7	0.14
(1,425)	1:89:A:VAL:HG12	1:183:A:MET:HE2	7	0.14
(1,425)	1:89:A:VAL:HG12	1:183:A:MET:HE3	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,425)	1:89:A:VAL:HG13	1:183:A:MET:HE1	7	0.14
(1,425)	1:89:A:VAL:HG13	1:183:A:MET:HE2	7	0.14
(1,425)	1:89:A:VAL:HG13	1:183:A:MET:HE3	7	0.14
(1,366)	1:126:C:ILE:HG21	1:131:C:ILE:HD11	10	0.14
(1,366)	1:126:C:ILE:HG21	1:131:C:ILE:HD12	10	0.14
(1,366)	1:126:C:ILE:HG21	1:131:C:ILE:HD13	10	0.14
(1,366)	1:126:C:ILE:HG22	1:131:C:ILE:HD11	10	0.14
(1,366)	1:126:C:ILE:HG22	1:131:C:ILE:HD12	10	0.14
(1,366)	1:126:C:ILE:HG22	1:131:C:ILE:HD13	10	0.14
(1,366)	1:126:C:ILE:HG23	1:131:C:ILE:HD11	10	0.14
(1,366)	1:126:C:ILE:HG23	1:131:C:ILE:HD12	10	0.14
(1,366)	1:126:C:ILE:HG23	1:131:C:ILE:HD13	10	0.14
(1,363)	1:131:A:ILE:HD11	1:183:C:MET:HG2	8	0.14
(1,363)	1:131:A:ILE:HD11	1:183:C:MET:HG3	8	0.14
(1,363)	1:131:A:ILE:HD12	1:183:C:MET:HG2	8	0.14
(1,363)	1:131:A:ILE:HD12	1:183:C:MET:HG3	8	0.14
(1,363)	1:131:A:ILE:HD13	1:183:C:MET:HG2	8	0.14
(1,363)	1:131:A:ILE:HD13	1:183:C:MET:HG3	8	0.14
(1,361)	1:183:A:MET:HG2	1:131:B:ILE:HD11	16	0.14
(1,361)	1:183:A:MET:HG2	1:131:B:ILE:HD12	16	0.14
(1,361)	1:183:A:MET:HG2	1:131:B:ILE:HD13	16	0.14
(1,361)	1:183:A:MET:HG3	1:131:B:ILE:HD11	16	0.14
(1,361)	1:183:A:MET:HG3	1:131:B:ILE:HD12	16	0.14
(1,361)	1:183:A:MET:HG3	1:131:B:ILE:HD13	16	0.14
(1,219)	1:96:A:ILE:HG21	1:141:A:VAL:HG11	9	0.14
(1,219)	1:96:A:ILE:HG21	1:141:A:VAL:HG12	9	0.14
(1,219)	1:96:A:ILE:HG21	1:141:A:VAL:HG13	9	0.14
(1,219)	1:96:A:ILE:HG22	1:141:A:VAL:HG11	9	0.14
(1,219)	1:96:A:ILE:HG22	1:141:A:VAL:HG12	9	0.14
(1,219)	1:96:A:ILE:HG22	1:141:A:VAL:HG13	9	0.14
(1,219)	1:96:A:ILE:HG23	1:141:A:VAL:HG11	9	0.14
(1,219)	1:96:A:ILE:HG23	1:141:A:VAL:HG12	9	0.14
(1,219)	1:96:A:ILE:HG23	1:141:A:VAL:HG13	9	0.14
(1,182)	1:137:A:LEU:HD11	1:141:A:VAL:HG11	5	0.14
(1,182)	1:137:A:LEU:HD11	1:141:A:VAL:HG12	5	0.14
(1,182)	1:137:A:LEU:HD11	1:141:A:VAL:HG13	5	0.14
(1,182)	1:137:A:LEU:HD12	1:141:A:VAL:HG11	5	0.14
(1,182)	1:137:A:LEU:HD12	1:141:A:VAL:HG12	5	0.14
(1,182)	1:137:A:LEU:HD12	1:141:A:VAL:HG13	5	0.14
(1,182)	1:137:A:LEU:HD13	1:141:A:VAL:HG11	5	0.14
(1,182)	1:137:A:LEU:HD13	1:141:A:VAL:HG12	5	0.14
(1,182)	1:137:A:LEU:HD13	1:141:A:VAL:HG13	5	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,182)	1:137:A:LEU:HD11	1:141:A:VAL:HG11	14	0.14
(1,182)	1:137:A:LEU:HD11	1:141:A:VAL:HG12	14	0.14
(1,182)	1:137:A:LEU:HD11	1:141:A:VAL:HG13	14	0.14
(1,182)	1:137:A:LEU:HD12	1:141:A:VAL:HG11	14	0.14
(1,182)	1:137:A:LEU:HD12	1:141:A:VAL:HG12	14	0.14
(1,182)	1:137:A:LEU:HD12	1:141:A:VAL:HG13	14	0.14
(1,182)	1:137:A:LEU:HD13	1:141:A:VAL:HG11	14	0.14
(1,182)	1:137:A:LEU:HD13	1:141:A:VAL:HG12	14	0.14
(1,182)	1:137:A:LEU:HD13	1:141:A:VAL:HG13	14	0.14
(1,182)	1:137:A:LEU:HD11	1:141:A:VAL:HG11	20	0.14
(1,182)	1:137:A:LEU:HD11	1:141:A:VAL:HG12	20	0.14
(1,182)	1:137:A:LEU:HD11	1:141:A:VAL:HG13	20	0.14
(1,182)	1:137:A:LEU:HD12	1:141:A:VAL:HG11	20	0.14
(1,182)	1:137:A:LEU:HD12	1:141:A:VAL:HG12	20	0.14
(1,182)	1:137:A:LEU:HD12	1:141:A:VAL:HG13	20	0.14
(1,182)	1:137:A:LEU:HD13	1:141:A:VAL:HG11	20	0.14
(1,182)	1:137:A:LEU:HD13	1:141:A:VAL:HG12	20	0.14
(1,182)	1:137:A:LEU:HD13	1:141:A:VAL:HG13	20	0.14
(1,134)	1:110:A:LEU:HD11	1:111:A:ILE:HD11	17	0.14
(1,134)	1:110:A:LEU:HD11	1:111:A:ILE:HD12	17	0.14
(1,134)	1:110:A:LEU:HD11	1:111:A:ILE:HD13	17	0.14
(1,134)	1:110:A:LEU:HD12	1:111:A:ILE:HD11	17	0.14
(1,134)	1:110:A:LEU:HD12	1:111:A:ILE:HD12	17	0.14
(1,134)	1:110:A:LEU:HD12	1:111:A:ILE:HD13	17	0.14
(1,134)	1:110:A:LEU:HD13	1:111:A:ILE:HD11	17	0.14
(1,134)	1:110:A:LEU:HD13	1:111:A:ILE:HD12	17	0.14
(1,134)	1:110:A:LEU:HD13	1:111:A:ILE:HD13	17	0.14
(1,122)	1:113:A:TYR:HD1	1:137:A:LEU:HD21	20	0.14
(1,122)	1:113:A:TYR:HD1	1:137:A:LEU:HD22	20	0.14
(1,122)	1:113:A:TYR:HD1	1:137:A:LEU:HD23	20	0.14
(1,122)	1:113:A:TYR:HD2	1:137:A:LEU:HD21	20	0.14
(1,122)	1:113:A:TYR:HD2	1:137:A:LEU:HD22	20	0.14
(1,122)	1:113:A:TYR:HD2	1:137:A:LEU:HD23	20	0.14
(1,42)	1:188:A:LEU:HD11	1:106:B:TYR:HE1	2	0.14
(1,42)	1:188:A:LEU:HD11	1:106:B:TYR:HE2	2	0.14
(1,42)	1:188:A:LEU:HD12	1:106:B:TYR:HE1	2	0.14
(1,42)	1:188:A:LEU:HD12	1:106:B:TYR:HE2	2	0.14
(1,42)	1:188:A:LEU:HD13	1:106:B:TYR:HE1	2	0.14
(1,42)	1:188:A:LEU:HD13	1:106:B:TYR:HE2	2	0.14
(1,42)	1:188:A:LEU:HD11	1:106:B:TYR:HE1	8	0.14
(1,42)	1:188:A:LEU:HD11	1:106:B:TYR:HE2	8	0.14
(1,42)	1:188:A:LEU:HD12	1:106:B:TYR:HE1	8	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,42)	1:188:A:LEU:HD12	1:106:B:TYR:HE2	8	0.14
(1,42)	1:188:A:LEU:HD13	1:106:B:TYR:HE1	8	0.14
(1,42)	1:188:A:LEU:HD13	1:106:B:TYR:HE2	8	0.14
(1,42)	1:188:A:LEU:HD11	1:106:B:TYR:HE1	10	0.14
(1,42)	1:188:A:LEU:HD11	1:106:B:TYR:HE2	10	0.14
(1,42)	1:188:A:LEU:HD12	1:106:B:TYR:HE1	10	0.14
(1,42)	1:188:A:LEU:HD12	1:106:B:TYR:HE2	10	0.14
(1,42)	1:188:A:LEU:HD13	1:106:B:TYR:HE1	10	0.14
(1,42)	1:188:A:LEU:HD13	1:106:B:TYR:HE2	10	0.14
(1,36)	1:102:A:VAL:HG21	1:112:A:ALA:H	16	0.14
(1,36)	1:102:A:VAL:HG22	1:112:A:ALA:H	16	0.14
(1,36)	1:102:A:VAL:HG23	1:112:A:ALA:H	16	0.14
(1,1)	1:108:A:GLN:HA	1:109:A:LEU:HD21	9	0.14
(1,1)	1:108:A:GLN:HA	1:109:A:LEU:HD22	9	0.14
(1,1)	1:108:A:GLN:HA	1:109:A:LEU:HD23	9	0.14
(1,1)	1:108:A:GLN:HA	1:109:A:LEU:HD21	10	0.14
(1,1)	1:108:A:GLN:HA	1:109:A:LEU:HD22	10	0.14
(1,1)	1:108:A:GLN:HA	1:109:A:LEU:HD23	10	0.14
(1,1)	1:108:A:GLN:HA	1:109:A:LEU:HD21	15	0.14
(1,1)	1:108:A:GLN:HA	1:109:A:LEU:HD22	15	0.14
(1,1)	1:108:A:GLN:HA	1:109:A:LEU:HD23	15	0.14
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD11	12	0.13
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD12	12	0.13
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD13	12	0.13
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD21	12	0.13
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD22	12	0.13
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD23	12	0.13
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD11	15	0.13
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD12	15	0.13
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD13	15	0.13
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD21	15	0.13
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD22	15	0.13
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD23	15	0.13
(1,2338)	1:179:C:ALA:HB1	1:181:C:LEU:HD11	3	0.13
(1,2338)	1:179:C:ALA:HB1	1:181:C:LEU:HD12	3	0.13
(1,2338)	1:179:C:ALA:HB1	1:181:C:LEU:HD13	3	0.13
(1,2338)	1:179:C:ALA:HB1	1:181:C:LEU:HD21	3	0.13
(1,2338)	1:179:C:ALA:HB1	1:181:C:LEU:HD22	3	0.13
(1,2338)	1:179:C:ALA:HB1	1:181:C:LEU:HD23	3	0.13
(1,2338)	1:179:C:ALA:HB2	1:181:C:LEU:HD11	3	0.13
(1,2338)	1:179:C:ALA:HB2	1:181:C:LEU:HD12	3	0.13
(1,2338)	1:179:C:ALA:HB2	1:181:C:LEU:HD13	3	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2338)	1:179:C:ALA:HB2	1:181:C:LEU:HD21	3	0.13
(1,2338)	1:179:C:ALA:HB2	1:181:C:LEU:HD22	3	0.13
(1,2338)	1:179:C:ALA:HB2	1:181:C:LEU:HD23	3	0.13
(1,2338)	1:179:C:ALA:HB3	1:181:C:LEU:HD11	3	0.13
(1,2338)	1:179:C:ALA:HB3	1:181:C:LEU:HD12	3	0.13
(1,2338)	1:179:C:ALA:HB3	1:181:C:LEU:HD13	3	0.13
(1,2338)	1:179:C:ALA:HB3	1:181:C:LEU:HD21	3	0.13
(1,2338)	1:179:C:ALA:HB3	1:181:C:LEU:HD22	3	0.13
(1,2338)	1:179:C:ALA:HB3	1:181:C:LEU:HD23	3	0.13
(1,2338)	1:179:C:ALA:HB1	1:181:C:LEU:HD11	8	0.13
(1,2338)	1:179:C:ALA:HB1	1:181:C:LEU:HD12	8	0.13
(1,2338)	1:179:C:ALA:HB1	1:181:C:LEU:HD13	8	0.13
(1,2338)	1:179:C:ALA:HB1	1:181:C:LEU:HD21	8	0.13
(1,2338)	1:179:C:ALA:HB1	1:181:C:LEU:HD22	8	0.13
(1,2338)	1:179:C:ALA:HB1	1:181:C:LEU:HD23	8	0.13
(1,2338)	1:179:C:ALA:HB2	1:181:C:LEU:HD11	8	0.13
(1,2338)	1:179:C:ALA:HB2	1:181:C:LEU:HD12	8	0.13
(1,2338)	1:179:C:ALA:HB2	1:181:C:LEU:HD13	8	0.13
(1,2338)	1:179:C:ALA:HB2	1:181:C:LEU:HD21	8	0.13
(1,2338)	1:179:C:ALA:HB2	1:181:C:LEU:HD22	8	0.13
(1,2338)	1:179:C:ALA:HB2	1:181:C:LEU:HD23	8	0.13
(1,2338)	1:179:C:ALA:HB3	1:181:C:LEU:HD11	8	0.13
(1,2338)	1:179:C:ALA:HB3	1:181:C:LEU:HD12	8	0.13
(1,2338)	1:179:C:ALA:HB3	1:181:C:LEU:HD13	8	0.13
(1,2338)	1:179:C:ALA:HB3	1:181:C:LEU:HD21	8	0.13
(1,2338)	1:179:C:ALA:HB3	1:181:C:LEU:HD22	8	0.13
(1,2338)	1:179:C:ALA:HB3	1:181:C:LEU:HD23	8	0.13
(1,2338)	1:179:C:ALA:HB1	1:181:C:LEU:HD11	11	0.13
(1,2338)	1:179:C:ALA:HB1	1:181:C:LEU:HD12	11	0.13
(1,2338)	1:179:C:ALA:HB1	1:181:C:LEU:HD13	11	0.13
(1,2338)	1:179:C:ALA:HB1	1:181:C:LEU:HD21	11	0.13
(1,2338)	1:179:C:ALA:HB1	1:181:C:LEU:HD22	11	0.13
(1,2338)	1:179:C:ALA:HB1	1:181:C:LEU:HD23	11	0.13
(1,2338)	1:179:C:ALA:HB2	1:181:C:LEU:HD11	11	0.13
(1,2338)	1:179:C:ALA:HB2	1:181:C:LEU:HD12	11	0.13
(1,2338)	1:179:C:ALA:HB2	1:181:C:LEU:HD13	11	0.13
(1,2338)	1:179:C:ALA:HB2	1:181:C:LEU:HD21	11	0.13
(1,2338)	1:179:C:ALA:HB2	1:181:C:LEU:HD22	11	0.13
(1,2338)	1:179:C:ALA:HB2	1:181:C:LEU:HD23	11	0.13
(1,2338)	1:179:C:ALA:HB3	1:181:C:LEU:HD11	11	0.13
(1,2338)	1:179:C:ALA:HB3	1:181:C:LEU:HD12	11	0.13
(1,2338)	1:179:C:ALA:HB3	1:181:C:LEU:HD13	11	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2338)	1:179:C:ALA:HB3	1:181:C:LEU:HD21	11	0.13
(1,2338)	1:179:C:ALA:HB3	1:181:C:LEU:HD22	11	0.13
(1,2338)	1:179:C:ALA:HB3	1:181:C:LEU:HD23	11	0.13
(1,2338)	1:179:C:ALA:HB1	1:181:C:LEU:HD11	15	0.13
(1,2338)	1:179:C:ALA:HB1	1:181:C:LEU:HD12	15	0.13
(1,2338)	1:179:C:ALA:HB1	1:181:C:LEU:HD13	15	0.13
(1,2338)	1:179:C:ALA:HB1	1:181:C:LEU:HD21	15	0.13
(1,2338)	1:179:C:ALA:HB1	1:181:C:LEU:HD22	15	0.13
(1,2338)	1:179:C:ALA:HB1	1:181:C:LEU:HD23	15	0.13
(1,2338)	1:179:C:ALA:HB2	1:181:C:LEU:HD11	15	0.13
(1,2338)	1:179:C:ALA:HB2	1:181:C:LEU:HD12	15	0.13
(1,2338)	1:179:C:ALA:HB2	1:181:C:LEU:HD13	15	0.13
(1,2338)	1:179:C:ALA:HB2	1:181:C:LEU:HD21	15	0.13
(1,2338)	1:179:C:ALA:HB2	1:181:C:LEU:HD22	15	0.13
(1,2338)	1:179:C:ALA:HB2	1:181:C:LEU:HD23	15	0.13
(1,2338)	1:179:C:ALA:HB3	1:181:C:LEU:HD11	15	0.13
(1,2338)	1:179:C:ALA:HB3	1:181:C:LEU:HD12	15	0.13
(1,2338)	1:179:C:ALA:HB3	1:181:C:LEU:HD13	15	0.13
(1,2338)	1:179:C:ALA:HB3	1:181:C:LEU:HD21	15	0.13
(1,2338)	1:179:C:ALA:HB3	1:181:C:LEU:HD22	15	0.13
(1,2338)	1:179:C:ALA:HB3	1:181:C:LEU:HD23	15	0.13
(1,2322)	1:176:C:GLY:H	1:177:C:ASP:HB2	1	0.13
(1,2322)	1:176:C:GLY:H	1:177:C:ASP:HB3	1	0.13
(1,2322)	1:176:C:GLY:H	1:177:C:ASP:HB2	9	0.13
(1,2322)	1:176:C:GLY:H	1:177:C:ASP:HB3	9	0.13
(1,2322)	1:176:C:GLY:H	1:177:C:ASP:HB2	12	0.13
(1,2322)	1:176:C:GLY:H	1:177:C:ASP:HB3	12	0.13
(1,2322)	1:176:C:GLY:H	1:177:C:ASP:HB2	13	0.13
(1,2322)	1:176:C:GLY:H	1:177:C:ASP:HB3	13	0.13
(1,2322)	1:176:C:GLY:H	1:177:C:ASP:HB2	15	0.13
(1,2322)	1:176:C:GLY:H	1:177:C:ASP:HB3	15	0.13
(1,2322)	1:176:C:GLY:H	1:177:C:ASP:HB2	18	0.13
(1,2322)	1:176:C:GLY:H	1:177:C:ASP:HB3	18	0.13
(1,2321)	1:172:C:ALA:HB1	1:173:C:PRO:HD2	1	0.13
(1,2321)	1:172:C:ALA:HB1	1:173:C:PRO:HD3	1	0.13
(1,2321)	1:172:C:ALA:HB2	1:173:C:PRO:HD2	1	0.13
(1,2321)	1:172:C:ALA:HB2	1:173:C:PRO:HD3	1	0.13
(1,2321)	1:172:C:ALA:HB3	1:173:C:PRO:HD2	1	0.13
(1,2321)	1:172:C:ALA:HB3	1:173:C:PRO:HD3	1	0.13
(1,2321)	1:172:C:ALA:HB1	1:173:C:PRO:HD2	10	0.13
(1,2321)	1:172:C:ALA:HB1	1:173:C:PRO:HD3	10	0.13
(1,2321)	1:172:C:ALA:HB2	1:173:C:PRO:HD2	10	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2321)	1:172:C:ALA:HB2	1:173:C:PRO:HD3	10	0.13
(1,2321)	1:172:C:ALA:HB3	1:173:C:PRO:HD2	10	0.13
(1,2321)	1:172:C:ALA:HB3	1:173:C:PRO:HD3	10	0.13
(1,2321)	1:172:C:ALA:HB1	1:173:C:PRO:HD2	11	0.13
(1,2321)	1:172:C:ALA:HB1	1:173:C:PRO:HD3	11	0.13
(1,2321)	1:172:C:ALA:HB2	1:173:C:PRO:HD2	11	0.13
(1,2321)	1:172:C:ALA:HB2	1:173:C:PRO:HD3	11	0.13
(1,2321)	1:172:C:ALA:HB3	1:173:C:PRO:HD2	11	0.13
(1,2321)	1:172:C:ALA:HB3	1:173:C:PRO:HD3	11	0.13
(1,2321)	1:172:C:ALA:HB1	1:173:C:PRO:HD2	13	0.13
(1,2321)	1:172:C:ALA:HB1	1:173:C:PRO:HD3	13	0.13
(1,2321)	1:172:C:ALA:HB2	1:173:C:PRO:HD2	13	0.13
(1,2321)	1:172:C:ALA:HB2	1:173:C:PRO:HD3	13	0.13
(1,2321)	1:172:C:ALA:HB3	1:173:C:PRO:HD2	13	0.13
(1,2321)	1:172:C:ALA:HB3	1:173:C:PRO:HD3	13	0.13
(1,2321)	1:172:C:ALA:HB1	1:173:C:PRO:HD2	16	0.13
(1,2321)	1:172:C:ALA:HB1	1:173:C:PRO:HD3	16	0.13
(1,2321)	1:172:C:ALA:HB2	1:173:C:PRO:HD2	16	0.13
(1,2321)	1:172:C:ALA:HB2	1:173:C:PRO:HD3	16	0.13
(1,2321)	1:172:C:ALA:HB3	1:173:C:PRO:HD2	16	0.13
(1,2321)	1:172:C:ALA:HB3	1:173:C:PRO:HD3	16	0.13
(1,2321)	1:172:C:ALA:HB1	1:173:C:PRO:HD2	18	0.13
(1,2321)	1:172:C:ALA:HB1	1:173:C:PRO:HD3	18	0.13
(1,2321)	1:172:C:ALA:HB2	1:173:C:PRO:HD2	18	0.13
(1,2321)	1:172:C:ALA:HB2	1:173:C:PRO:HD3	18	0.13
(1,2321)	1:172:C:ALA:HB3	1:173:C:PRO:HD2	18	0.13
(1,2321)	1:172:C:ALA:HB3	1:173:C:PRO:HD3	18	0.13
(1,2295)	1:155:C:ALA:HB1	1:157:C:PRO:HD2	16	0.13
(1,2295)	1:155:C:ALA:HB1	1:157:C:PRO:HD3	16	0.13
(1,2295)	1:155:C:ALA:HB2	1:157:C:PRO:HD2	16	0.13
(1,2295)	1:155:C:ALA:HB2	1:157:C:PRO:HD3	16	0.13
(1,2295)	1:155:C:ALA:HB3	1:157:C:PRO:HD2	16	0.13
(1,2295)	1:155:C:ALA:HB3	1:157:C:PRO:HD3	16	0.13
(1,2283)	1:150:C:LEU:HD11	1:167:C:ARG:HG2	10	0.13
(1,2283)	1:150:C:LEU:HD11	1:167:C:ARG:HG3	10	0.13
(1,2283)	1:150:C:LEU:HD12	1:167:C:ARG:HG2	10	0.13
(1,2283)	1:150:C:LEU:HD12	1:167:C:ARG:HG3	10	0.13
(1,2283)	1:150:C:LEU:HD13	1:167:C:ARG:HG2	10	0.13
(1,2283)	1:150:C:LEU:HD13	1:167:C:ARG:HG3	10	0.13
(1,2283)	1:150:C:LEU:HD21	1:167:C:ARG:HG2	10	0.13
(1,2283)	1:150:C:LEU:HD21	1:167:C:ARG:HG3	10	0.13
(1,2283)	1:150:C:LEU:HD22	1:167:C:ARG:HG2	10	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2283)	1:150:C:LEU:HD22	1:167:C:ARG:HG3	10	0.13
(1,2283)	1:150:C:LEU:HD23	1:167:C:ARG:HG2	10	0.13
(1,2283)	1:150:C:LEU:HD23	1:167:C:ARG:HG3	10	0.13
(1,2283)	1:150:C:LEU:HD11	1:167:C:ARG:HG2	20	0.13
(1,2283)	1:150:C:LEU:HD11	1:167:C:ARG:HG3	20	0.13
(1,2283)	1:150:C:LEU:HD12	1:167:C:ARG:HG2	20	0.13
(1,2283)	1:150:C:LEU:HD12	1:167:C:ARG:HG3	20	0.13
(1,2283)	1:150:C:LEU:HD13	1:167:C:ARG:HG2	20	0.13
(1,2283)	1:150:C:LEU:HD13	1:167:C:ARG:HG3	20	0.13
(1,2283)	1:150:C:LEU:HD21	1:167:C:ARG:HG2	20	0.13
(1,2283)	1:150:C:LEU:HD21	1:167:C:ARG:HG3	20	0.13
(1,2283)	1:150:C:LEU:HD22	1:167:C:ARG:HG2	20	0.13
(1,2283)	1:150:C:LEU:HD22	1:167:C:ARG:HG3	20	0.13
(1,2283)	1:150:C:LEU:HD23	1:167:C:ARG:HG2	20	0.13
(1,2283)	1:150:C:LEU:HD23	1:167:C:ARG:HG3	20	0.13
(1,2236)	1:121:C:CYS:HB2	1:189:C:CYS:H	7	0.13
(1,2236)	1:121:C:CYS:HB3	1:189:C:CYS:H	7	0.13
(1,2236)	1:121:C:CYS:HB2	1:189:C:CYS:H	9	0.13
(1,2236)	1:121:C:CYS:HB3	1:189:C:CYS:H	9	0.13
(1,2236)	1:121:C:CYS:HB2	1:189:C:CYS:H	11	0.13
(1,2236)	1:121:C:CYS:HB3	1:189:C:CYS:H	11	0.13
(1,2236)	1:121:C:CYS:HB2	1:189:C:CYS:H	13	0.13
(1,2236)	1:121:C:CYS:HB3	1:189:C:CYS:H	13	0.13
(1,2236)	1:121:C:CYS:HB2	1:189:C:CYS:H	17	0.13
(1,2236)	1:121:C:CYS:HB3	1:189:C:CYS:H	17	0.13
(1,2236)	1:121:C:CYS:HB2	1:189:C:CYS:H	18	0.13
(1,2236)	1:121:C:CYS:HB3	1:189:C:CYS:H	18	0.13
(1,2163)	1:89:C:VAL:HG11	1:183:C:MET:HE1	7	0.13
(1,2163)	1:89:C:VAL:HG11	1:183:C:MET:HE2	7	0.13
(1,2163)	1:89:C:VAL:HG11	1:183:C:MET:HE3	7	0.13
(1,2163)	1:89:C:VAL:HG12	1:183:C:MET:HE1	7	0.13
(1,2163)	1:89:C:VAL:HG12	1:183:C:MET:HE2	7	0.13
(1,2163)	1:89:C:VAL:HG12	1:183:C:MET:HE3	7	0.13
(1,2163)	1:89:C:VAL:HG13	1:183:C:MET:HE1	7	0.13
(1,2163)	1:89:C:VAL:HG13	1:183:C:MET:HE2	7	0.13
(1,2163)	1:89:C:VAL:HG13	1:183:C:MET:HE3	7	0.13
(1,2163)	1:89:C:VAL:HG21	1:183:C:MET:HE1	7	0.13
(1,2163)	1:89:C:VAL:HG21	1:183:C:MET:HE2	7	0.13
(1,2163)	1:89:C:VAL:HG21	1:183:C:MET:HE3	7	0.13
(1,2163)	1:89:C:VAL:HG22	1:183:C:MET:HE1	7	0.13
(1,2163)	1:89:C:VAL:HG22	1:183:C:MET:HE2	7	0.13
(1,2163)	1:89:C:VAL:HG22	1:183:C:MET:HE3	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2163)	1:89:C:VAL:HG23	1:183:C:MET:HE1	7	0.13
(1,2163)	1:89:C:VAL:HG23	1:183:C:MET:HE2	7	0.13
(1,2163)	1:89:C:VAL:HG23	1:183:C:MET:HE3	7	0.13
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD11	12	0.13
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD12	12	0.13
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD13	12	0.13
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD21	12	0.13
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD22	12	0.13
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD23	12	0.13
(1,2112)	1:179:B:ALA:HB1	1:181:B:LEU:HD11	3	0.13
(1,2112)	1:179:B:ALA:HB1	1:181:B:LEU:HD12	3	0.13
(1,2112)	1:179:B:ALA:HB1	1:181:B:LEU:HD13	3	0.13
(1,2112)	1:179:B:ALA:HB1	1:181:B:LEU:HD21	3	0.13
(1,2112)	1:179:B:ALA:HB1	1:181:B:LEU:HD22	3	0.13
(1,2112)	1:179:B:ALA:HB1	1:181:B:LEU:HD23	3	0.13
(1,2112)	1:179:B:ALA:HB2	1:181:B:LEU:HD11	3	0.13
(1,2112)	1:179:B:ALA:HB2	1:181:B:LEU:HD12	3	0.13
(1,2112)	1:179:B:ALA:HB2	1:181:B:LEU:HD13	3	0.13
(1,2112)	1:179:B:ALA:HB2	1:181:B:LEU:HD21	3	0.13
(1,2112)	1:179:B:ALA:HB2	1:181:B:LEU:HD22	3	0.13
(1,2112)	1:179:B:ALA:HB2	1:181:B:LEU:HD23	3	0.13
(1,2112)	1:179:B:ALA:HB3	1:181:B:LEU:HD11	3	0.13
(1,2112)	1:179:B:ALA:HB3	1:181:B:LEU:HD12	3	0.13
(1,2112)	1:179:B:ALA:HB3	1:181:B:LEU:HD13	3	0.13
(1,2112)	1:179:B:ALA:HB3	1:181:B:LEU:HD21	3	0.13
(1,2112)	1:179:B:ALA:HB3	1:181:B:LEU:HD22	3	0.13
(1,2112)	1:179:B:ALA:HB3	1:181:B:LEU:HD23	3	0.13
(1,2112)	1:179:B:ALA:HB1	1:181:B:LEU:HD11	8	0.13
(1,2112)	1:179:B:ALA:HB1	1:181:B:LEU:HD12	8	0.13
(1,2112)	1:179:B:ALA:HB1	1:181:B:LEU:HD13	8	0.13
(1,2112)	1:179:B:ALA:HB1	1:181:B:LEU:HD21	8	0.13
(1,2112)	1:179:B:ALA:HB1	1:181:B:LEU:HD22	8	0.13
(1,2112)	1:179:B:ALA:HB1	1:181:B:LEU:HD23	8	0.13
(1,2112)	1:179:B:ALA:HB2	1:181:B:LEU:HD11	8	0.13
(1,2112)	1:179:B:ALA:HB2	1:181:B:LEU:HD12	8	0.13
(1,2112)	1:179:B:ALA:HB2	1:181:B:LEU:HD13	8	0.13
(1,2112)	1:179:B:ALA:HB2	1:181:B:LEU:HD21	8	0.13
(1,2112)	1:179:B:ALA:HB2	1:181:B:LEU:HD22	8	0.13
(1,2112)	1:179:B:ALA:HB2	1:181:B:LEU:HD23	8	0.13
(1,2112)	1:179:B:ALA:HB3	1:181:B:LEU:HD11	8	0.13
(1,2112)	1:179:B:ALA:HB3	1:181:B:LEU:HD12	8	0.13
(1,2112)	1:179:B:ALA:HB3	1:181:B:LEU:HD13	8	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2112)	1:179:B:ALA:HB3	1:181:B:LEU:HD21	8	0.13
(1,2112)	1:179:B:ALA:HB3	1:181:B:LEU:HD22	8	0.13
(1,2112)	1:179:B:ALA:HB3	1:181:B:LEU:HD23	8	0.13
(1,2112)	1:179:B:ALA:HB1	1:181:B:LEU:HD11	9	0.13
(1,2112)	1:179:B:ALA:HB1	1:181:B:LEU:HD12	9	0.13
(1,2112)	1:179:B:ALA:HB1	1:181:B:LEU:HD13	9	0.13
(1,2112)	1:179:B:ALA:HB1	1:181:B:LEU:HD21	9	0.13
(1,2112)	1:179:B:ALA:HB1	1:181:B:LEU:HD22	9	0.13
(1,2112)	1:179:B:ALA:HB1	1:181:B:LEU:HD23	9	0.13
(1,2112)	1:179:B:ALA:HB2	1:181:B:LEU:HD11	9	0.13
(1,2112)	1:179:B:ALA:HB2	1:181:B:LEU:HD12	9	0.13
(1,2112)	1:179:B:ALA:HB2	1:181:B:LEU:HD13	9	0.13
(1,2112)	1:179:B:ALA:HB2	1:181:B:LEU:HD21	9	0.13
(1,2112)	1:179:B:ALA:HB2	1:181:B:LEU:HD22	9	0.13
(1,2112)	1:179:B:ALA:HB2	1:181:B:LEU:HD23	9	0.13
(1,2112)	1:179:B:ALA:HB3	1:181:B:LEU:HD11	9	0.13
(1,2112)	1:179:B:ALA:HB3	1:181:B:LEU:HD12	9	0.13
(1,2112)	1:179:B:ALA:HB3	1:181:B:LEU:HD13	9	0.13
(1,2112)	1:179:B:ALA:HB3	1:181:B:LEU:HD21	9	0.13
(1,2112)	1:179:B:ALA:HB3	1:181:B:LEU:HD22	9	0.13
(1,2112)	1:179:B:ALA:HB3	1:181:B:LEU:HD23	9	0.13
(1,2112)	1:179:B:ALA:HB1	1:181:B:LEU:HD11	11	0.13
(1,2112)	1:179:B:ALA:HB1	1:181:B:LEU:HD12	11	0.13
(1,2112)	1:179:B:ALA:HB1	1:181:B:LEU:HD13	11	0.13
(1,2112)	1:179:B:ALA:HB1	1:181:B:LEU:HD21	11	0.13
(1,2112)	1:179:B:ALA:HB1	1:181:B:LEU:HD22	11	0.13
(1,2112)	1:179:B:ALA:HB1	1:181:B:LEU:HD23	11	0.13
(1,2112)	1:179:B:ALA:HB2	1:181:B:LEU:HD11	11	0.13
(1,2112)	1:179:B:ALA:HB2	1:181:B:LEU:HD12	11	0.13
(1,2112)	1:179:B:ALA:HB2	1:181:B:LEU:HD13	11	0.13
(1,2112)	1:179:B:ALA:HB2	1:181:B:LEU:HD21	11	0.13
(1,2112)	1:179:B:ALA:HB2	1:181:B:LEU:HD22	11	0.13
(1,2112)	1:179:B:ALA:HB2	1:181:B:LEU:HD23	11	0.13
(1,2112)	1:179:B:ALA:HB3	1:181:B:LEU:HD11	11	0.13
(1,2112)	1:179:B:ALA:HB3	1:181:B:LEU:HD12	11	0.13
(1,2112)	1:179:B:ALA:HB3	1:181:B:LEU:HD13	11	0.13
(1,2112)	1:179:B:ALA:HB3	1:181:B:LEU:HD21	11	0.13
(1,2112)	1:179:B:ALA:HB3	1:181:B:LEU:HD22	11	0.13
(1,2112)	1:179:B:ALA:HB3	1:181:B:LEU:HD23	11	0.13
(1,2096)	1:176:B:GLY:H	1:177:B:ASP:HB2	1	0.13
(1,2096)	1:176:B:GLY:H	1:177:B:ASP:HB3	1	0.13
(1,2096)	1:176:B:GLY:H	1:177:B:ASP:HB2	9	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2096)	1:176:B:GLY:H	1:177:B:ASP:HB3	9	0.13
(1,2096)	1:176:B:GLY:H	1:177:B:ASP:HB2	12	0.13
(1,2096)	1:176:B:GLY:H	1:177:B:ASP:HB3	12	0.13
(1,2096)	1:176:B:GLY:H	1:177:B:ASP:HB2	13	0.13
(1,2096)	1:176:B:GLY:H	1:177:B:ASP:HB3	13	0.13
(1,2096)	1:176:B:GLY:H	1:177:B:ASP:HB2	15	0.13
(1,2096)	1:176:B:GLY:H	1:177:B:ASP:HB3	15	0.13
(1,2096)	1:176:B:GLY:H	1:177:B:ASP:HB2	18	0.13
(1,2096)	1:176:B:GLY:H	1:177:B:ASP:HB3	18	0.13
(1,2095)	1:172:B:ALA:HB1	1:173:B:PRO:HD2	10	0.13
(1,2095)	1:172:B:ALA:HB1	1:173:B:PRO:HD3	10	0.13
(1,2095)	1:172:B:ALA:HB2	1:173:B:PRO:HD2	10	0.13
(1,2095)	1:172:B:ALA:HB2	1:173:B:PRO:HD3	10	0.13
(1,2095)	1:172:B:ALA:HB3	1:173:B:PRO:HD2	10	0.13
(1,2095)	1:172:B:ALA:HB3	1:173:B:PRO:HD3	10	0.13
(1,2095)	1:172:B:ALA:HB1	1:173:B:PRO:HD2	11	0.13
(1,2095)	1:172:B:ALA:HB1	1:173:B:PRO:HD3	11	0.13
(1,2095)	1:172:B:ALA:HB2	1:173:B:PRO:HD2	11	0.13
(1,2095)	1:172:B:ALA:HB2	1:173:B:PRO:HD3	11	0.13
(1,2095)	1:172:B:ALA:HB3	1:173:B:PRO:HD2	11	0.13
(1,2095)	1:172:B:ALA:HB3	1:173:B:PRO:HD3	11	0.13
(1,2095)	1:172:B:ALA:HB1	1:173:B:PRO:HD2	13	0.13
(1,2095)	1:172:B:ALA:HB1	1:173:B:PRO:HD3	13	0.13
(1,2095)	1:172:B:ALA:HB2	1:173:B:PRO:HD2	13	0.13
(1,2095)	1:172:B:ALA:HB2	1:173:B:PRO:HD3	13	0.13
(1,2095)	1:172:B:ALA:HB3	1:173:B:PRO:HD2	13	0.13
(1,2095)	1:172:B:ALA:HB3	1:173:B:PRO:HD3	13	0.13
(1,2095)	1:172:B:ALA:HB1	1:173:B:PRO:HD2	16	0.13
(1,2095)	1:172:B:ALA:HB1	1:173:B:PRO:HD3	16	0.13
(1,2095)	1:172:B:ALA:HB2	1:173:B:PRO:HD2	16	0.13
(1,2095)	1:172:B:ALA:HB2	1:173:B:PRO:HD3	16	0.13
(1,2095)	1:172:B:ALA:HB3	1:173:B:PRO:HD2	16	0.13
(1,2095)	1:172:B:ALA:HB3	1:173:B:PRO:HD3	16	0.13
(1,2069)	1:155:B:ALA:HB1	1:157:B:PRO:HD2	16	0.13
(1,2069)	1:155:B:ALA:HB1	1:157:B:PRO:HD3	16	0.13
(1,2069)	1:155:B:ALA:HB2	1:157:B:PRO:HD2	16	0.13
(1,2069)	1:155:B:ALA:HB2	1:157:B:PRO:HD3	16	0.13
(1,2069)	1:155:B:ALA:HB3	1:157:B:PRO:HD2	16	0.13
(1,2069)	1:155:B:ALA:HB3	1:157:B:PRO:HD3	16	0.13
(1,2057)	1:150:B:LEU:HD11	1:167:B:ARG:HG2	10	0.13
(1,2057)	1:150:B:LEU:HD11	1:167:B:ARG:HG3	10	0.13
(1,2057)	1:150:B:LEU:HD12	1:167:B:ARG:HG2	10	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2057)	1:150:B:LEU:HD12	1:167:B:ARG:HG3	10	0.13
(1,2057)	1:150:B:LEU:HD13	1:167:B:ARG:HG2	10	0.13
(1,2057)	1:150:B:LEU:HD13	1:167:B:ARG:HG3	10	0.13
(1,2057)	1:150:B:LEU:HD21	1:167:B:ARG:HG2	10	0.13
(1,2057)	1:150:B:LEU:HD21	1:167:B:ARG:HG3	10	0.13
(1,2057)	1:150:B:LEU:HD22	1:167:B:ARG:HG2	10	0.13
(1,2057)	1:150:B:LEU:HD22	1:167:B:ARG:HG3	10	0.13
(1,2057)	1:150:B:LEU:HD23	1:167:B:ARG:HG2	10	0.13
(1,2057)	1:150:B:LEU:HD23	1:167:B:ARG:HG3	10	0.13
(1,2057)	1:150:B:LEU:HD11	1:167:B:ARG:HG2	13	0.13
(1,2057)	1:150:B:LEU:HD11	1:167:B:ARG:HG3	13	0.13
(1,2057)	1:150:B:LEU:HD12	1:167:B:ARG:HG2	13	0.13
(1,2057)	1:150:B:LEU:HD12	1:167:B:ARG:HG3	13	0.13
(1,2057)	1:150:B:LEU:HD13	1:167:B:ARG:HG2	13	0.13
(1,2057)	1:150:B:LEU:HD13	1:167:B:ARG:HG3	13	0.13
(1,2057)	1:150:B:LEU:HD21	1:167:B:ARG:HG2	13	0.13
(1,2057)	1:150:B:LEU:HD21	1:167:B:ARG:HG3	13	0.13
(1,2057)	1:150:B:LEU:HD22	1:167:B:ARG:HG2	13	0.13
(1,2057)	1:150:B:LEU:HD22	1:167:B:ARG:HG3	13	0.13
(1,2057)	1:150:B:LEU:HD23	1:167:B:ARG:HG2	13	0.13
(1,2057)	1:150:B:LEU:HD23	1:167:B:ARG:HG3	13	0.13
(1,2057)	1:150:B:LEU:HD11	1:167:B:ARG:HG2	19	0.13
(1,2057)	1:150:B:LEU:HD11	1:167:B:ARG:HG3	19	0.13
(1,2057)	1:150:B:LEU:HD12	1:167:B:ARG:HG2	19	0.13
(1,2057)	1:150:B:LEU:HD12	1:167:B:ARG:HG3	19	0.13
(1,2057)	1:150:B:LEU:HD13	1:167:B:ARG:HG2	19	0.13
(1,2057)	1:150:B:LEU:HD13	1:167:B:ARG:HG3	19	0.13
(1,2057)	1:150:B:LEU:HD21	1:167:B:ARG:HG2	19	0.13
(1,2057)	1:150:B:LEU:HD21	1:167:B:ARG:HG3	19	0.13
(1,2057)	1:150:B:LEU:HD22	1:167:B:ARG:HG2	19	0.13
(1,2057)	1:150:B:LEU:HD22	1:167:B:ARG:HG3	19	0.13
(1,2057)	1:150:B:LEU:HD23	1:167:B:ARG:HG2	19	0.13
(1,2057)	1:150:B:LEU:HD23	1:167:B:ARG:HG3	19	0.13
(1,2010)	1:121:B:CYS:HB2	1:189:B:CYS:H	5	0.13
(1,2010)	1:121:B:CYS:HB3	1:189:B:CYS:H	5	0.13
(1,2010)	1:121:B:CYS:HB2	1:189:B:CYS:H	11	0.13
(1,2010)	1:121:B:CYS:HB3	1:189:B:CYS:H	11	0.13
(1,2005)	1:119:B:THR:H	1:192:B:VAL:HG11	3	0.13
(1,2005)	1:119:B:THR:H	1:192:B:VAL:HG12	3	0.13
(1,2005)	1:119:B:THR:H	1:192:B:VAL:HG13	3	0.13
(1,2005)	1:119:B:THR:H	1:192:B:VAL:HG21	3	0.13
(1,2005)	1:119:B:THR:H	1:192:B:VAL:HG22	3	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2005)	1:119:B:THR:H	1:192:B:VAL:HG23	3	0.13
(1,1911)	1:178:A:PRO:HB2	1:180:A:PHE:H	1	0.13
(1,1911)	1:178:A:PRO:HB3	1:180:A:PHE:H	1	0.13
(1,1904)	1:176:A:GLY:H	1:177:A:ASP:HB2	1	0.13
(1,1904)	1:176:A:GLY:H	1:177:A:ASP:HB3	1	0.13
(1,1904)	1:176:A:GLY:H	1:177:A:ASP:HB2	2	0.13
(1,1904)	1:176:A:GLY:H	1:177:A:ASP:HB3	2	0.13
(1,1904)	1:176:A:GLY:H	1:177:A:ASP:HB2	9	0.13
(1,1904)	1:176:A:GLY:H	1:177:A:ASP:HB3	9	0.13
(1,1904)	1:176:A:GLY:H	1:177:A:ASP:HB2	12	0.13
(1,1904)	1:176:A:GLY:H	1:177:A:ASP:HB3	12	0.13
(1,1904)	1:176:A:GLY:H	1:177:A:ASP:HB2	15	0.13
(1,1904)	1:176:A:GLY:H	1:177:A:ASP:HB3	15	0.13
(1,1904)	1:176:A:GLY:H	1:177:A:ASP:HB2	18	0.13
(1,1904)	1:176:A:GLY:H	1:177:A:ASP:HB3	18	0.13
(1,1904)	1:176:A:GLY:H	1:177:A:ASP:HB2	19	0.13
(1,1904)	1:176:A:GLY:H	1:177:A:ASP:HB3	19	0.13
(1,1903)	1:172:A:ALA:HB1	1:173:A:PRO:HD2	2	0.13
(1,1903)	1:172:A:ALA:HB1	1:173:A:PRO:HD3	2	0.13
(1,1903)	1:172:A:ALA:HB2	1:173:A:PRO:HD2	2	0.13
(1,1903)	1:172:A:ALA:HB2	1:173:A:PRO:HD3	2	0.13
(1,1903)	1:172:A:ALA:HB3	1:173:A:PRO:HD2	2	0.13
(1,1903)	1:172:A:ALA:HB3	1:173:A:PRO:HD3	2	0.13
(1,1903)	1:172:A:ALA:HB1	1:173:A:PRO:HD2	11	0.13
(1,1903)	1:172:A:ALA:HB1	1:173:A:PRO:HD3	11	0.13
(1,1903)	1:172:A:ALA:HB2	1:173:A:PRO:HD2	11	0.13
(1,1903)	1:172:A:ALA:HB2	1:173:A:PRO:HD3	11	0.13
(1,1903)	1:172:A:ALA:HB3	1:173:A:PRO:HD2	11	0.13
(1,1903)	1:172:A:ALA:HB3	1:173:A:PRO:HD3	11	0.13
(1,1903)	1:172:A:ALA:HB1	1:173:A:PRO:HD2	16	0.13
(1,1903)	1:172:A:ALA:HB1	1:173:A:PRO:HD3	16	0.13
(1,1903)	1:172:A:ALA:HB2	1:173:A:PRO:HD2	16	0.13
(1,1903)	1:172:A:ALA:HB2	1:173:A:PRO:HD3	16	0.13
(1,1903)	1:172:A:ALA:HB3	1:173:A:PRO:HD2	16	0.13
(1,1903)	1:172:A:ALA:HB3	1:173:A:PRO:HD3	16	0.13
(1,1903)	1:172:A:ALA:HB1	1:173:A:PRO:HD2	19	0.13
(1,1903)	1:172:A:ALA:HB1	1:173:A:PRO:HD3	19	0.13
(1,1903)	1:172:A:ALA:HB2	1:173:A:PRO:HD2	19	0.13
(1,1903)	1:172:A:ALA:HB2	1:173:A:PRO:HD3	19	0.13
(1,1903)	1:172:A:ALA:HB3	1:173:A:PRO:HD2	19	0.13
(1,1903)	1:172:A:ALA:HB3	1:173:A:PRO:HD3	19	0.13
(1,1902)	1:172:A:ALA:HA	1:178:A:PRO:HD2	19	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1902)	1:172:A:ALA:HA	1:178:A:PRO:HD3	19	0.13
(1,1885)	1:155:A:ALA:HB1	1:157:A:PRO:HD2	15	0.13
(1,1885)	1:155:A:ALA:HB1	1:157:A:PRO:HD3	15	0.13
(1,1885)	1:155:A:ALA:HB2	1:157:A:PRO:HD2	15	0.13
(1,1885)	1:155:A:ALA:HB2	1:157:A:PRO:HD3	15	0.13
(1,1885)	1:155:A:ALA:HB3	1:157:A:PRO:HD2	15	0.13
(1,1885)	1:155:A:ALA:HB3	1:157:A:PRO:HD3	15	0.13
(1,1885)	1:155:A:ALA:HB1	1:157:A:PRO:HD2	17	0.13
(1,1885)	1:155:A:ALA:HB1	1:157:A:PRO:HD3	17	0.13
(1,1885)	1:155:A:ALA:HB2	1:157:A:PRO:HD2	17	0.13
(1,1885)	1:155:A:ALA:HB2	1:157:A:PRO:HD3	17	0.13
(1,1885)	1:155:A:ALA:HB3	1:157:A:PRO:HD2	17	0.13
(1,1885)	1:155:A:ALA:HB3	1:157:A:PRO:HD3	17	0.13
(1,1842)	1:121:A:CYS:HB2	1:189:A:CYS:H	6	0.13
(1,1842)	1:121:A:CYS:HB3	1:189:A:CYS:H	6	0.13
(1,1819)	1:95:C:SER:HB2	1:101:C:LEU:H	17	0.13
(1,1819)	1:95:C:SER:HB3	1:101:C:LEU:H	17	0.13
(1,1818)	1:95:B:SER:HB2	1:101:B:LEU:H	10	0.13
(1,1818)	1:95:B:SER:HB3	1:101:B:LEU:H	10	0.13
(1,1817)	1:95:A:SER:HB2	1:101:A:LEU:H	11	0.13
(1,1817)	1:95:A:SER:HB3	1:101:A:LEU:H	11	0.13
(1,1817)	1:95:A:SER:HB2	1:101:A:LEU:H	17	0.13
(1,1817)	1:95:A:SER:HB3	1:101:A:LEU:H	17	0.13
(1,1801)	1:151:C:GLN:HA	1:152:C:ALA:H	3	0.13
(1,1801)	1:151:C:GLN:HA	1:152:C:ALA:H	8	0.13
(1,1801)	1:151:C:GLN:HA	1:152:C:ALA:H	16	0.13
(1,1800)	1:151:B:GLN:HA	1:152:B:ALA:H	3	0.13
(1,1800)	1:151:B:GLN:HA	1:152:B:ALA:H	8	0.13
(1,1800)	1:151:B:GLN:HA	1:152:B:ALA:H	16	0.13
(1,1799)	1:151:A:GLN:HA	1:152:A:ALA:H	3	0.13
(1,1799)	1:151:A:GLN:HA	1:152:A:ALA:H	8	0.13
(1,1799)	1:151:A:GLN:HA	1:152:A:ALA:H	16	0.13
(1,1787)	1:96:A:ILE:HG21	1:101:A:LEU:H	12	0.13
(1,1787)	1:96:A:ILE:HG22	1:101:A:LEU:H	12	0.13
(1,1787)	1:96:A:ILE:HG23	1:101:A:LEU:H	12	0.13
(1,1734)	1:194:A:LEU:HG	1:195:A:TYR:H	4	0.13
(1,1692)	1:120:A:CYS:H	1:192:A:VAL:HG11	7	0.13
(1,1692)	1:120:A:CYS:H	1:192:A:VAL:HG12	7	0.13
(1,1692)	1:120:A:CYS:H	1:192:A:VAL:HG13	7	0.13
(1,1692)	1:120:A:CYS:H	1:192:A:VAL:HG11	12	0.13
(1,1692)	1:120:A:CYS:H	1:192:A:VAL:HG12	12	0.13
(1,1692)	1:120:A:CYS:H	1:192:A:VAL:HG13	12	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1686)	1:90:A:THR:H	1:91:A:THR:HB	11	0.13
(1,1676)	1:94:A:PHE:H	1:102:A:VAL:HG11	8	0.13
(1,1676)	1:94:A:PHE:H	1:102:A:VAL:HG12	8	0.13
(1,1676)	1:94:A:PHE:H	1:102:A:VAL:HG13	8	0.13
(1,1622)	1:129:C:GLU:H	1:131:C:ILE:H	16	0.13
(1,1621)	1:129:B:GLU:H	1:131:B:ILE:H	16	0.13
(1,1616)	1:116:C:ALA:H	1:119:C:THR:HB	1	0.13
(1,1616)	1:116:C:ALA:H	1:119:C:THR:HB	15	0.13
(1,1615)	1:116:B:ALA:H	1:119:B:THR:HB	1	0.13
(1,1615)	1:116:B:ALA:H	1:119:B:THR:HB	15	0.13
(1,1614)	1:116:A:ALA:H	1:119:A:THR:HB	3	0.13
(1,1610)	1:118:A:GLY:H	1:192:A:VAL:HG21	15	0.13
(1,1610)	1:118:A:GLY:H	1:192:A:VAL:HG22	15	0.13
(1,1610)	1:118:A:GLY:H	1:192:A:VAL:HG23	15	0.13
(1,1602)	1:89:A:VAL:HG21	1:91:A:THR:H	16	0.13
(1,1602)	1:89:A:VAL:HG22	1:91:A:THR:H	16	0.13
(1,1602)	1:89:A:VAL:HG23	1:91:A:THR:H	16	0.13
(1,1574)	1:119:A:THR:H	1:192:A:VAL:HG11	3	0.13
(1,1574)	1:119:A:THR:H	1:192:A:VAL:HG12	3	0.13
(1,1574)	1:119:A:THR:H	1:192:A:VAL:HG13	3	0.13
(1,1564)	1:145:C:GLN:HA	1:151:C:GLN:H	14	0.13
(1,1563)	1:145:B:GLN:HA	1:151:B:GLN:H	12	0.13
(1,1563)	1:145:B:GLN:HA	1:151:B:GLN:H	14	0.13
(1,1562)	1:145:A:GLN:HA	1:151:A:GLN:H	6	0.13
(1,1562)	1:145:A:GLN:HA	1:151:A:GLN:H	7	0.13
(1,1562)	1:145:A:GLN:HA	1:151:A:GLN:H	15	0.13
(1,1562)	1:145:A:GLN:HA	1:151:A:GLN:H	20	0.13
(1,1554)	1:156:C:VAL:HB	1:167:C:ARG:H	6	0.13
(1,1553)	1:156:B:VAL:HB	1:167:B:ARG:H	6	0.13
(1,1551)	1:167:C:ARG:H	1:171:C:SER:HA	12	0.13
(1,1551)	1:167:C:ARG:H	1:171:C:SER:HA	19	0.13
(1,1550)	1:167:B:ARG:H	1:171:B:SER:HA	12	0.13
(1,1550)	1:167:B:ARG:H	1:171:B:SER:HA	20	0.13
(1,1548)	1:167:C:ARG:H	1:170:C:GLY:HA2	7	0.13
(1,1548)	1:167:C:ARG:H	1:170:C:GLY:HA3	7	0.13
(1,1548)	1:167:C:ARG:H	1:170:C:GLY:HA2	8	0.13
(1,1548)	1:167:C:ARG:H	1:170:C:GLY:HA3	8	0.13
(1,1548)	1:167:C:ARG:H	1:170:C:GLY:HA2	9	0.13
(1,1548)	1:167:C:ARG:H	1:170:C:GLY:HA3	9	0.13
(1,1547)	1:167:B:ARG:H	1:170:B:GLY:HA2	7	0.13
(1,1547)	1:167:B:ARG:H	1:170:B:GLY:HA3	7	0.13
(1,1547)	1:167:B:ARG:H	1:170:B:GLY:HA2	9	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1547)	1:167:B:ARG:H	1:170:B:GLY:HA3	9	0.13
(1,1546)	1:167:A:ARG:H	1:170:A:GLY:HA2	1	0.13
(1,1546)	1:167:A:ARG:H	1:170:A:GLY:HA3	1	0.13
(1,1546)	1:167:A:ARG:H	1:170:A:GLY:HA2	5	0.13
(1,1546)	1:167:A:ARG:H	1:170:A:GLY:HA3	5	0.13
(1,1546)	1:167:A:ARG:H	1:170:A:GLY:HA2	6	0.13
(1,1546)	1:167:A:ARG:H	1:170:A:GLY:HA3	6	0.13
(1,1546)	1:167:A:ARG:H	1:170:A:GLY:HA2	9	0.13
(1,1546)	1:167:A:ARG:H	1:170:A:GLY:HA3	9	0.13
(1,1540)	1:136:B:ALA:HB1	1:140:B:LYS:H	1	0.13
(1,1540)	1:136:B:ALA:HB2	1:140:B:LYS:H	1	0.13
(1,1540)	1:136:B:ALA:HB3	1:140:B:LYS:H	1	0.13
(1,1535)	1:122:C:TYR:H	1:189:C:CYS:HB2	7	0.13
(1,1535)	1:122:C:TYR:H	1:189:C:CYS:HB3	7	0.13
(1,1535)	1:122:C:TYR:H	1:189:C:CYS:HB2	11	0.13
(1,1535)	1:122:C:TYR:H	1:189:C:CYS:HB3	11	0.13
(1,1535)	1:122:C:TYR:H	1:189:C:CYS:HB2	16	0.13
(1,1535)	1:122:C:TYR:H	1:189:C:CYS:HB3	16	0.13
(1,1534)	1:122:B:TYR:H	1:189:B:CYS:HB2	3	0.13
(1,1534)	1:122:B:TYR:H	1:189:B:CYS:HB3	3	0.13
(1,1534)	1:122:B:TYR:H	1:189:B:CYS:HB2	15	0.13
(1,1534)	1:122:B:TYR:H	1:189:B:CYS:HB3	15	0.13
(1,1533)	1:122:A:TYR:H	1:189:A:CYS:HB2	5	0.13
(1,1533)	1:122:A:TYR:H	1:189:A:CYS:HB3	5	0.13
(1,1533)	1:122:A:TYR:H	1:189:A:CYS:HB2	11	0.13
(1,1533)	1:122:A:TYR:H	1:189:A:CYS:HB3	11	0.13
(1,1529)	1:91:C:THR:HG21	1:106:C:TYR:H	5	0.13
(1,1529)	1:91:C:THR:HG22	1:106:C:TYR:H	5	0.13
(1,1529)	1:91:C:THR:HG23	1:106:C:TYR:H	5	0.13
(1,1528)	1:91:B:THR:HG21	1:106:B:TYR:H	5	0.13
(1,1528)	1:91:B:THR:HG22	1:106:B:TYR:H	5	0.13
(1,1528)	1:91:B:THR:HG23	1:106:B:TYR:H	5	0.13
(1,1527)	1:91:A:THR:HG21	1:106:A:TYR:H	5	0.13
(1,1527)	1:91:A:THR:HG22	1:106:A:TYR:H	5	0.13
(1,1527)	1:91:A:THR:HG23	1:106:A:TYR:H	5	0.13
(1,1522)	1:178:C:PRO:HG2	1:179:C:ALA:H	12	0.13
(1,1522)	1:178:C:PRO:HG3	1:179:C:ALA:H	12	0.13
(1,1521)	1:178:B:PRO:HG2	1:179:B:ALA:H	12	0.13
(1,1521)	1:178:B:PRO:HG3	1:179:B:ALA:H	12	0.13
(1,1513)	1:137:C:LEU:H	1:137:C:LEU:HG	8	0.13
(1,1512)	1:137:B:LEU:H	1:137:B:LEU:HG	10	0.13
(1,1511)	1:137:A:LEU:H	1:137:A:LEU:HG	5	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1507)	1:92:A:ALA:H	1:93:C:THR:HG21	7	0.13
(1,1507)	1:92:A:ALA:H	1:93:C:THR:HG22	7	0.13
(1,1507)	1:92:A:ALA:H	1:93:C:THR:HG23	7	0.13
(1,1507)	1:92:A:ALA:H	1:93:C:THR:HG21	17	0.13
(1,1507)	1:92:A:ALA:H	1:93:C:THR:HG22	17	0.13
(1,1507)	1:92:A:ALA:H	1:93:C:THR:HG23	17	0.13
(1,1507)	1:92:A:ALA:H	1:93:C:THR:HG21	18	0.13
(1,1507)	1:92:A:ALA:H	1:93:C:THR:HG22	18	0.13
(1,1507)	1:92:A:ALA:H	1:93:C:THR:HG23	18	0.13
(1,1506)	1:93:B:THR:HG21	1:92:C:ALA:H	7	0.13
(1,1506)	1:93:B:THR:HG22	1:92:C:ALA:H	7	0.13
(1,1506)	1:93:B:THR:HG23	1:92:C:ALA:H	7	0.13
(1,1506)	1:93:B:THR:HG21	1:92:C:ALA:H	9	0.13
(1,1506)	1:93:B:THR:HG22	1:92:C:ALA:H	9	0.13
(1,1506)	1:93:B:THR:HG23	1:92:C:ALA:H	9	0.13
(1,1506)	1:93:B:THR:HG21	1:92:C:ALA:H	18	0.13
(1,1506)	1:93:B:THR:HG22	1:92:C:ALA:H	18	0.13
(1,1506)	1:93:B:THR:HG23	1:92:C:ALA:H	18	0.13
(1,1504)	1:92:A:ALA:H	1:103:A:VAL:HG21	9	0.13
(1,1504)	1:92:A:ALA:H	1:103:A:VAL:HG22	9	0.13
(1,1504)	1:92:A:ALA:H	1:103:A:VAL:HG23	9	0.13
(1,1489)	1:131:A:ILE:HA	1:133:A:SER:H	6	0.13
(1,1489)	1:131:A:ILE:HA	1:133:A:SER:H	8	0.13
(1,1462)	1:180:B:PHE:H	1:181:B:LEU:HA	17	0.13
(1,1461)	1:180:A:PHE:H	1:181:A:LEU:HA	17	0.13
(1,1408)	1:152:A:ALA:HB1	1:153:A:LYS:H	2	0.13
(1,1408)	1:152:A:ALA:HB2	1:153:A:LYS:H	2	0.13
(1,1408)	1:152:A:ALA:HB3	1:153:A:LYS:H	2	0.13
(1,1387)	1:141:A:VAL:HG21	1:142:A:HIS:H	2	0.13
(1,1387)	1:141:A:VAL:HG22	1:142:A:HIS:H	2	0.13
(1,1387)	1:141:A:VAL:HG23	1:142:A:HIS:H	2	0.13
(1,1387)	1:141:A:VAL:HG21	1:142:A:HIS:H	4	0.13
(1,1387)	1:141:A:VAL:HG22	1:142:A:HIS:H	4	0.13
(1,1387)	1:141:A:VAL:HG23	1:142:A:HIS:H	4	0.13
(1,1387)	1:141:A:VAL:HG21	1:142:A:HIS:H	7	0.13
(1,1387)	1:141:A:VAL:HG22	1:142:A:HIS:H	7	0.13
(1,1387)	1:141:A:VAL:HG23	1:142:A:HIS:H	7	0.13
(1,1350)	1:127:A:ALA:H	1:131:A:ILE:HG21	8	0.13
(1,1350)	1:127:A:ALA:H	1:131:A:ILE:HG22	8	0.13
(1,1350)	1:127:A:ALA:H	1:131:A:ILE:HG23	8	0.13
(1,1350)	1:127:A:ALA:H	1:131:A:ILE:HG21	18	0.13
(1,1350)	1:127:A:ALA:H	1:131:A:ILE:HG22	18	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1350)	1:127:A:ALA:H	1:131:A:ILE:HG23	18	0.13
(1,1204)	1:149:A:SER:HB2	1:151:A:GLN:H	1	0.13
(1,1204)	1:149:A:SER:HB3	1:151:A:GLN:H	1	0.13
(1,1204)	1:149:A:SER:HB2	1:151:A:GLN:H	15	0.13
(1,1204)	1:149:A:SER:HB3	1:151:A:GLN:H	15	0.13
(1,1202)	1:196:B:TYR:H	1:196:B:TYR:HE1	15	0.13
(1,1202)	1:196:B:TYR:H	1:196:B:TYR:HE2	15	0.13
(1,1201)	1:196:A:TYR:H	1:196:A:TYR:HE1	20	0.13
(1,1201)	1:196:A:TYR:H	1:196:A:TYR:HE2	20	0.13
(1,1100)	1:167:C:ARG:H	1:167:C:ARG:HB2	1	0.13
(1,1100)	1:167:C:ARG:H	1:167:C:ARG:HB2	2	0.13
(1,1100)	1:167:C:ARG:H	1:167:C:ARG:HB2	6	0.13
(1,1100)	1:167:C:ARG:H	1:167:C:ARG:HB2	7	0.13
(1,1100)	1:167:C:ARG:H	1:167:C:ARG:HB2	9	0.13
(1,1100)	1:167:C:ARG:H	1:167:C:ARG:HB2	10	0.13
(1,1100)	1:167:C:ARG:H	1:167:C:ARG:HB2	11	0.13
(1,1100)	1:167:C:ARG:H	1:167:C:ARG:HB2	16	0.13
(1,1100)	1:167:C:ARG:H	1:167:C:ARG:HB2	17	0.13
(1,1099)	1:167:B:ARG:H	1:167:B:ARG:HB2	1	0.13
(1,1099)	1:167:B:ARG:H	1:167:B:ARG:HB2	2	0.13
(1,1099)	1:167:B:ARG:H	1:167:B:ARG:HB2	3	0.13
(1,1099)	1:167:B:ARG:H	1:167:B:ARG:HB2	6	0.13
(1,1099)	1:167:B:ARG:H	1:167:B:ARG:HB2	7	0.13
(1,1099)	1:167:B:ARG:H	1:167:B:ARG:HB2	9	0.13
(1,1099)	1:167:B:ARG:H	1:167:B:ARG:HB2	10	0.13
(1,1099)	1:167:B:ARG:H	1:167:B:ARG:HB2	11	0.13
(1,1099)	1:167:B:ARG:H	1:167:B:ARG:HB2	16	0.13
(1,1099)	1:167:B:ARG:H	1:167:B:ARG:HB2	17	0.13
(1,1098)	1:167:A:ARG:H	1:167:A:ARG:HB2	1	0.13
(1,1098)	1:167:A:ARG:H	1:167:A:ARG:HB2	2	0.13
(1,1098)	1:167:A:ARG:H	1:167:A:ARG:HB2	3	0.13
(1,1098)	1:167:A:ARG:H	1:167:A:ARG:HB2	6	0.13
(1,1098)	1:167:A:ARG:H	1:167:A:ARG:HB2	7	0.13
(1,1098)	1:167:A:ARG:H	1:167:A:ARG:HB2	9	0.13
(1,1098)	1:167:A:ARG:H	1:167:A:ARG:HB2	10	0.13
(1,1098)	1:167:A:ARG:H	1:167:A:ARG:HB2	11	0.13
(1,1098)	1:167:A:ARG:H	1:167:A:ARG:HB2	16	0.13
(1,1098)	1:167:A:ARG:H	1:167:A:ARG:HB2	17	0.13
(1,1077)	1:173:A:PRO:HB3	1:174:A:SER:H	19	0.13
(1,1077)	1:173:A:PRO:HB3	1:174:A:SER:H	20	0.13
(1,1071)	1:139:A:ARG:H	1:141:A:VAL:HB	3	0.13
(1,1036)	1:188:A:LEU:HD21	1:134:B:LEU:H	1	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1036)	1:188:A:LEU:HD22	1:134:B:LEU:H	1	0.13
(1,1036)	1:188:A:LEU:HD23	1:134:B:LEU:H	1	0.13
(1,1036)	1:188:A:LEU:HD21	1:134:B:LEU:H	3	0.13
(1,1036)	1:188:A:LEU:HD22	1:134:B:LEU:H	3	0.13
(1,1036)	1:188:A:LEU:HD23	1:134:B:LEU:H	3	0.13
(1,1036)	1:188:A:LEU:HD21	1:134:B:LEU:H	12	0.13
(1,1036)	1:188:A:LEU:HD22	1:134:B:LEU:H	12	0.13
(1,1036)	1:188:A:LEU:HD23	1:134:B:LEU:H	12	0.13
(1,1036)	1:188:A:LEU:HD21	1:134:B:LEU:H	18	0.13
(1,1036)	1:188:A:LEU:HD22	1:134:B:LEU:H	18	0.13
(1,1036)	1:188:A:LEU:HD23	1:134:B:LEU:H	18	0.13
(1,965)	1:110:A:LEU:HD11	1:125:A:LYS:HB3	13	0.13
(1,965)	1:110:A:LEU:HD12	1:125:A:LYS:HB3	13	0.13
(1,965)	1:110:A:LEU:HD13	1:125:A:LYS:HB3	13	0.13
(1,958)	1:187:A:THR:HA	1:188:A:LEU:HD11	7	0.13
(1,958)	1:187:A:THR:HA	1:188:A:LEU:HD12	7	0.13
(1,958)	1:187:A:THR:HA	1:188:A:LEU:HD13	7	0.13
(1,948)	1:185:A:VAL:HG11	1:189:A:CYS:HB2	18	0.13
(1,948)	1:185:A:VAL:HG11	1:189:A:CYS:HB3	18	0.13
(1,948)	1:185:A:VAL:HG12	1:189:A:CYS:HB2	18	0.13
(1,948)	1:185:A:VAL:HG12	1:189:A:CYS:HB3	18	0.13
(1,948)	1:185:A:VAL:HG13	1:189:A:CYS:HB2	18	0.13
(1,948)	1:185:A:VAL:HG13	1:189:A:CYS:HB3	18	0.13
(1,891)	1:165:A:GLU:HB2	1:167:A:ARG:HG2	10	0.13
(1,891)	1:165:A:GLU:HB2	1:167:A:ARG:HG3	10	0.13
(1,890)	1:152:C:ALA:HA	1:157:C:PRO:HG2	3	0.13
(1,890)	1:152:C:ALA:HA	1:157:C:PRO:HG3	3	0.13
(1,889)	1:152:B:ALA:HA	1:157:B:PRO:HG2	3	0.13
(1,889)	1:152:B:ALA:HA	1:157:B:PRO:HG3	3	0.13
(1,888)	1:152:A:ALA:HA	1:157:A:PRO:HG2	3	0.13
(1,888)	1:152:A:ALA:HA	1:157:A:PRO:HG3	3	0.13
(1,848)	1:150:A:LEU:HD11	1:167:A:ARG:HG2	19	0.13
(1,848)	1:150:A:LEU:HD11	1:167:A:ARG:HG3	19	0.13
(1,848)	1:150:A:LEU:HD12	1:167:A:ARG:HG2	19	0.13
(1,848)	1:150:A:LEU:HD12	1:167:A:ARG:HG3	19	0.13
(1,848)	1:150:A:LEU:HD13	1:167:A:ARG:HG2	19	0.13
(1,848)	1:150:A:LEU:HD13	1:167:A:ARG:HG3	19	0.13
(1,844)	1:156:C:VAL:HB	1:157:C:PRO:HD2	7	0.13
(1,843)	1:156:B:VAL:HB	1:157:B:PRO:HD2	7	0.13
(1,813)	1:176:A:GLY:H	1:177:A:ASP:HB2	2	0.13
(1,813)	1:176:A:GLY:H	1:177:A:ASP:HB2	6	0.13
(1,813)	1:176:A:GLY:H	1:177:A:ASP:HB2	9	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,794)	1:153:C:LYS:HE2	1:154:C:PRO:HG2	20	0.13
(1,794)	1:153:C:LYS:HE2	1:154:C:PRO:HG3	20	0.13
(1,794)	1:153:C:LYS:HE3	1:154:C:PRO:HG2	20	0.13
(1,794)	1:153:C:LYS:HE3	1:154:C:PRO:HG3	20	0.13
(1,793)	1:153:B:LYS:HE2	1:154:B:PRO:HG2	20	0.13
(1,793)	1:153:B:LYS:HE2	1:154:B:PRO:HG3	20	0.13
(1,793)	1:153:B:LYS:HE3	1:154:B:PRO:HG2	20	0.13
(1,793)	1:153:B:LYS:HE3	1:154:B:PRO:HG3	20	0.13
(1,792)	1:153:A:LYS:HE2	1:154:A:PRO:HG2	20	0.13
(1,792)	1:153:A:LYS:HE2	1:154:A:PRO:HG3	20	0.13
(1,792)	1:153:A:LYS:HE3	1:154:A:PRO:HG2	20	0.13
(1,792)	1:153:A:LYS:HE3	1:154:A:PRO:HG3	20	0.13
(1,769)	1:102:A:VAL:HG21	1:104:A:TYR:HE1	6	0.13
(1,769)	1:102:A:VAL:HG21	1:104:A:TYR:HE2	6	0.13
(1,769)	1:102:A:VAL:HG22	1:104:A:TYR:HE1	6	0.13
(1,769)	1:102:A:VAL:HG22	1:104:A:TYR:HE2	6	0.13
(1,769)	1:102:A:VAL:HG23	1:104:A:TYR:HE1	6	0.13
(1,769)	1:102:A:VAL:HG23	1:104:A:TYR:HE2	6	0.13
(1,769)	1:102:A:VAL:HG21	1:104:A:TYR:HE1	9	0.13
(1,769)	1:102:A:VAL:HG21	1:104:A:TYR:HE2	9	0.13
(1,769)	1:102:A:VAL:HG22	1:104:A:TYR:HE1	9	0.13
(1,769)	1:102:A:VAL:HG22	1:104:A:TYR:HE2	9	0.13
(1,769)	1:102:A:VAL:HG23	1:104:A:TYR:HE1	9	0.13
(1,769)	1:102:A:VAL:HG23	1:104:A:TYR:HE2	9	0.13
(1,754)	1:189:B:CYS:H	1:192:B:VAL:HG11	6	0.13
(1,754)	1:189:B:CYS:H	1:192:B:VAL:HG12	6	0.13
(1,754)	1:189:B:CYS:H	1:192:B:VAL:HG13	6	0.13
(1,749)	1:123:A:ILE:HG21	1:179:A:ALA:HB1	1	0.13
(1,749)	1:123:A:ILE:HG21	1:179:A:ALA:HB2	1	0.13
(1,749)	1:123:A:ILE:HG21	1:179:A:ALA:HB3	1	0.13
(1,749)	1:123:A:ILE:HG22	1:179:A:ALA:HB1	1	0.13
(1,749)	1:123:A:ILE:HG22	1:179:A:ALA:HB2	1	0.13
(1,749)	1:123:A:ILE:HG22	1:179:A:ALA:HB3	1	0.13
(1,749)	1:123:A:ILE:HG23	1:179:A:ALA:HB1	1	0.13
(1,749)	1:123:A:ILE:HG23	1:179:A:ALA:HB2	1	0.13
(1,749)	1:123:A:ILE:HG23	1:179:A:ALA:HB3	1	0.13
(1,737)	1:175:A:GLY:HA2	1:179:A:ALA:HB1	18	0.13
(1,737)	1:175:A:GLY:HA2	1:179:A:ALA:HB2	18	0.13
(1,737)	1:175:A:GLY:HA2	1:179:A:ALA:HB3	18	0.13
(1,737)	1:175:A:GLY:HA3	1:179:A:ALA:HB1	18	0.13
(1,737)	1:175:A:GLY:HA3	1:179:A:ALA:HB2	18	0.13
(1,737)	1:175:A:GLY:HA3	1:179:A:ALA:HB3	18	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,695)	1:123:C:ILE:H	1:124:C:MET:HE1	3	0.13
(1,695)	1:123:C:ILE:H	1:124:C:MET:HE2	3	0.13
(1,695)	1:123:C:ILE:H	1:124:C:MET:HE3	3	0.13
(1,694)	1:123:B:ILE:H	1:124:B:MET:HE1	3	0.13
(1,694)	1:123:B:ILE:H	1:124:B:MET:HE2	3	0.13
(1,694)	1:123:B:ILE:H	1:124:B:MET:HE3	3	0.13
(1,665)	1:113:A:TYR:HE1	1:197:A:ILE:HG21	6	0.13
(1,665)	1:113:A:TYR:HE1	1:197:A:ILE:HG22	6	0.13
(1,665)	1:113:A:TYR:HE1	1:197:A:ILE:HG23	6	0.13
(1,665)	1:113:A:TYR:HE2	1:197:A:ILE:HG21	6	0.13
(1,665)	1:113:A:TYR:HE2	1:197:A:ILE:HG22	6	0.13
(1,665)	1:113:A:TYR:HE2	1:197:A:ILE:HG23	6	0.13
(1,650)	1:94:A:PHE:HE1	1:131:A:ILE:HG21	8	0.13
(1,650)	1:94:A:PHE:HE1	1:131:A:ILE:HG22	8	0.13
(1,650)	1:94:A:PHE:HE1	1:131:A:ILE:HG23	8	0.13
(1,650)	1:94:A:PHE:HE2	1:131:A:ILE:HG21	8	0.13
(1,650)	1:94:A:PHE:HE2	1:131:A:ILE:HG22	8	0.13
(1,650)	1:94:A:PHE:HE2	1:131:A:ILE:HG23	8	0.13
(1,636)	1:96:B:ILE:HG21	1:100:B:GLY:H	10	0.13
(1,636)	1:96:B:ILE:HG22	1:100:B:GLY:H	10	0.13
(1,636)	1:96:B:ILE:HG23	1:100:B:GLY:H	10	0.13
(1,635)	1:96:A:ILE:HG21	1:100:A:GLY:H	10	0.13
(1,635)	1:96:A:ILE:HG22	1:100:A:GLY:H	10	0.13
(1,635)	1:96:A:ILE:HG23	1:100:A:GLY:H	10	0.13
(1,624)	1:96:B:ILE:HG21	1:138:B:THR:HB	4	0.13
(1,624)	1:96:B:ILE:HG22	1:138:B:THR:HB	4	0.13
(1,624)	1:96:B:ILE:HG23	1:138:B:THR:HB	4	0.13
(1,577)	1:178:A:PRO:HG2	1:194:A:LEU:HD21	7	0.13
(1,577)	1:178:A:PRO:HG2	1:194:A:LEU:HD22	7	0.13
(1,577)	1:178:A:PRO:HG2	1:194:A:LEU:HD23	7	0.13
(1,577)	1:178:A:PRO:HG3	1:194:A:LEU:HD21	7	0.13
(1,577)	1:178:A:PRO:HG3	1:194:A:LEU:HD22	7	0.13
(1,577)	1:178:A:PRO:HG3	1:194:A:LEU:HD23	7	0.13
(1,572)	1:121:A:CYS:H	1:194:A:LEU:HD21	14	0.13
(1,572)	1:121:A:CYS:H	1:194:A:LEU:HD22	14	0.13
(1,572)	1:121:A:CYS:H	1:194:A:LEU:HD23	14	0.13
(1,572)	1:121:A:CYS:H	1:194:A:LEU:HD21	19	0.13
(1,572)	1:121:A:CYS:H	1:194:A:LEU:HD22	19	0.13
(1,572)	1:121:A:CYS:H	1:194:A:LEU:HD23	19	0.13
(1,568)	1:156:A:VAL:HB	1:161:A:LEU:HD11	10	0.13
(1,568)	1:156:A:VAL:HB	1:161:A:LEU:HD12	10	0.13
(1,568)	1:156:A:VAL:HB	1:161:A:LEU:HD13	10	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,538)	1:111:C:ILE:HD11	1:131:C:ILE:HG21	3	0.13
(1,538)	1:111:C:ILE:HD11	1:131:C:ILE:HG22	3	0.13
(1,538)	1:111:C:ILE:HD11	1:131:C:ILE:HG23	3	0.13
(1,538)	1:111:C:ILE:HD12	1:131:C:ILE:HG21	3	0.13
(1,538)	1:111:C:ILE:HD12	1:131:C:ILE:HG22	3	0.13
(1,538)	1:111:C:ILE:HD12	1:131:C:ILE:HG23	3	0.13
(1,538)	1:111:C:ILE:HD13	1:131:C:ILE:HG21	3	0.13
(1,538)	1:111:C:ILE:HD13	1:131:C:ILE:HG22	3	0.13
(1,538)	1:111:C:ILE:HD13	1:131:C:ILE:HG23	3	0.13
(1,436)	1:183:B:MET:HE1	1:186:B:SER:HA	4	0.13
(1,436)	1:183:B:MET:HE2	1:186:B:SER:HA	4	0.13
(1,436)	1:183:B:MET:HE3	1:186:B:SER:HA	4	0.13
(1,396)	1:109:B:LEU:HG	1:111:B:ILE:HD11	14	0.13
(1,396)	1:109:B:LEU:HG	1:111:B:ILE:HD12	14	0.13
(1,396)	1:109:B:LEU:HG	1:111:B:ILE:HD13	14	0.13
(1,372)	1:96:B:ILE:HD11	1:102:B:VAL:HB	4	0.13
(1,372)	1:96:B:ILE:HD12	1:102:B:VAL:HB	4	0.13
(1,372)	1:96:B:ILE:HD13	1:102:B:VAL:HB	4	0.13
(1,371)	1:96:A:ILE:HD11	1:102:A:VAL:HB	4	0.13
(1,371)	1:96:A:ILE:HD12	1:102:A:VAL:HB	4	0.13
(1,371)	1:96:A:ILE:HD13	1:102:A:VAL:HB	4	0.13
(1,371)	1:96:A:ILE:HD11	1:102:A:VAL:HB	12	0.13
(1,371)	1:96:A:ILE:HD12	1:102:A:VAL:HB	12	0.13
(1,371)	1:96:A:ILE:HD13	1:102:A:VAL:HB	12	0.13
(1,365)	1:126:B:ILE:HG21	1:131:B:ILE:HD11	7	0.13
(1,365)	1:126:B:ILE:HG21	1:131:B:ILE:HD12	7	0.13
(1,365)	1:126:B:ILE:HG21	1:131:B:ILE:HD13	7	0.13
(1,365)	1:126:B:ILE:HG22	1:131:B:ILE:HD11	7	0.13
(1,365)	1:126:B:ILE:HG22	1:131:B:ILE:HD12	7	0.13
(1,365)	1:126:B:ILE:HG22	1:131:B:ILE:HD13	7	0.13
(1,365)	1:126:B:ILE:HG23	1:131:B:ILE:HD11	7	0.13
(1,365)	1:126:B:ILE:HG23	1:131:B:ILE:HD12	7	0.13
(1,365)	1:126:B:ILE:HG23	1:131:B:ILE:HD13	7	0.13
(1,363)	1:131:A:ILE:HD11	1:183:C:MET:HG2	4	0.13
(1,363)	1:131:A:ILE:HD11	1:183:C:MET:HG3	4	0.13
(1,363)	1:131:A:ILE:HD12	1:183:C:MET:HG2	4	0.13
(1,363)	1:131:A:ILE:HD12	1:183:C:MET:HG3	4	0.13
(1,363)	1:131:A:ILE:HD13	1:183:C:MET:HG2	4	0.13
(1,363)	1:131:A:ILE:HD13	1:183:C:MET:HG3	4	0.13
(1,361)	1:183:A:MET:HG2	1:131:B:ILE:HD11	15	0.13
(1,361)	1:183:A:MET:HG2	1:131:B:ILE:HD12	15	0.13
(1,361)	1:183:A:MET:HG2	1:131:B:ILE:HD13	15	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,361)	1:183:A:MET:HG3	1:131:B:ILE:HD11	15	0.13
(1,361)	1:183:A:MET:HG3	1:131:B:ILE:HD12	15	0.13
(1,361)	1:183:A:MET:HG3	1:131:B:ILE:HD13	15	0.13
(1,349)	1:123:A:ILE:HD11	1:196:A:TYR:HE1	8	0.13
(1,349)	1:123:A:ILE:HD11	1:196:A:TYR:HE2	8	0.13
(1,349)	1:123:A:ILE:HD12	1:196:A:TYR:HE1	8	0.13
(1,349)	1:123:A:ILE:HD12	1:196:A:TYR:HE2	8	0.13
(1,349)	1:123:A:ILE:HD13	1:196:A:TYR:HE1	8	0.13
(1,349)	1:123:A:ILE:HD13	1:196:A:TYR:HE2	8	0.13
(1,349)	1:123:A:ILE:HD11	1:196:A:TYR:HE1	19	0.13
(1,349)	1:123:A:ILE:HD11	1:196:A:TYR:HE2	19	0.13
(1,349)	1:123:A:ILE:HD12	1:196:A:TYR:HE1	19	0.13
(1,349)	1:123:A:ILE:HD12	1:196:A:TYR:HE2	19	0.13
(1,349)	1:123:A:ILE:HD13	1:196:A:TYR:HE1	19	0.13
(1,349)	1:123:A:ILE:HD13	1:196:A:TYR:HE2	19	0.13
(1,283)	1:88:A:LEU:H	1:89:A:VAL:HG11	8	0.13
(1,283)	1:88:A:LEU:H	1:89:A:VAL:HG12	8	0.13
(1,283)	1:88:A:LEU:H	1:89:A:VAL:HG13	8	0.13
(1,239)	1:102:A:VAL:HG21	1:137:A:LEU:HD21	15	0.13
(1,239)	1:102:A:VAL:HG21	1:137:A:LEU:HD22	15	0.13
(1,239)	1:102:A:VAL:HG21	1:137:A:LEU:HD23	15	0.13
(1,239)	1:102:A:VAL:HG22	1:137:A:LEU:HD21	15	0.13
(1,239)	1:102:A:VAL:HG22	1:137:A:LEU:HD22	15	0.13
(1,239)	1:102:A:VAL:HG22	1:137:A:LEU:HD23	15	0.13
(1,239)	1:102:A:VAL:HG23	1:137:A:LEU:HD21	15	0.13
(1,239)	1:102:A:VAL:HG23	1:137:A:LEU:HD22	15	0.13
(1,239)	1:102:A:VAL:HG23	1:137:A:LEU:HD23	15	0.13
(1,219)	1:96:A:ILE:HG21	1:141:A:VAL:HG11	2	0.13
(1,219)	1:96:A:ILE:HG21	1:141:A:VAL:HG12	2	0.13
(1,219)	1:96:A:ILE:HG21	1:141:A:VAL:HG13	2	0.13
(1,219)	1:96:A:ILE:HG22	1:141:A:VAL:HG11	2	0.13
(1,219)	1:96:A:ILE:HG22	1:141:A:VAL:HG12	2	0.13
(1,219)	1:96:A:ILE:HG22	1:141:A:VAL:HG13	2	0.13
(1,219)	1:96:A:ILE:HG23	1:141:A:VAL:HG11	2	0.13
(1,219)	1:96:A:ILE:HG23	1:141:A:VAL:HG12	2	0.13
(1,219)	1:96:A:ILE:HG23	1:141:A:VAL:HG13	2	0.13
(1,218)	1:96:C:ILE:HG21	1:102:C:VAL:HG11	8	0.13
(1,218)	1:96:C:ILE:HG21	1:102:C:VAL:HG12	8	0.13
(1,218)	1:96:C:ILE:HG21	1:102:C:VAL:HG13	8	0.13
(1,218)	1:96:C:ILE:HG22	1:102:C:VAL:HG11	8	0.13
(1,218)	1:96:C:ILE:HG22	1:102:C:VAL:HG12	8	0.13
(1,218)	1:96:C:ILE:HG22	1:102:C:VAL:HG13	8	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,218)	1:96:C:ILE:HG23	1:102:C:VAL:HG11	8	0.13
(1,218)	1:96:C:ILE:HG23	1:102:C:VAL:HG12	8	0.13
(1,218)	1:96:C:ILE:HG23	1:102:C:VAL:HG13	8	0.13
(1,217)	1:96:B:ILE:HG21	1:102:B:VAL:HG11	8	0.13
(1,217)	1:96:B:ILE:HG21	1:102:B:VAL:HG12	8	0.13
(1,217)	1:96:B:ILE:HG21	1:102:B:VAL:HG13	8	0.13
(1,217)	1:96:B:ILE:HG22	1:102:B:VAL:HG11	8	0.13
(1,217)	1:96:B:ILE:HG22	1:102:B:VAL:HG12	8	0.13
(1,217)	1:96:B:ILE:HG22	1:102:B:VAL:HG13	8	0.13
(1,217)	1:96:B:ILE:HG23	1:102:B:VAL:HG11	8	0.13
(1,217)	1:96:B:ILE:HG23	1:102:B:VAL:HG12	8	0.13
(1,217)	1:96:B:ILE:HG23	1:102:B:VAL:HG13	8	0.13
(1,198)	1:109:A:LEU:H	1:110:A:LEU:HD21	8	0.13
(1,198)	1:109:A:LEU:H	1:110:A:LEU:HD22	8	0.13
(1,198)	1:109:A:LEU:H	1:110:A:LEU:HD23	8	0.13
(1,182)	1:137:A:LEU:HD11	1:141:A:VAL:HG11	2	0.13
(1,182)	1:137:A:LEU:HD11	1:141:A:VAL:HG12	2	0.13
(1,182)	1:137:A:LEU:HD11	1:141:A:VAL:HG13	2	0.13
(1,182)	1:137:A:LEU:HD12	1:141:A:VAL:HG11	2	0.13
(1,182)	1:137:A:LEU:HD12	1:141:A:VAL:HG12	2	0.13
(1,182)	1:137:A:LEU:HD12	1:141:A:VAL:HG13	2	0.13
(1,182)	1:137:A:LEU:HD13	1:141:A:VAL:HG11	2	0.13
(1,182)	1:137:A:LEU:HD13	1:141:A:VAL:HG12	2	0.13
(1,182)	1:137:A:LEU:HD13	1:141:A:VAL:HG13	2	0.13
(1,182)	1:137:A:LEU:HD11	1:141:A:VAL:HG11	19	0.13
(1,182)	1:137:A:LEU:HD11	1:141:A:VAL:HG12	19	0.13
(1,182)	1:137:A:LEU:HD11	1:141:A:VAL:HG13	19	0.13
(1,182)	1:137:A:LEU:HD12	1:141:A:VAL:HG11	19	0.13
(1,182)	1:137:A:LEU:HD12	1:141:A:VAL:HG12	19	0.13
(1,182)	1:137:A:LEU:HD12	1:141:A:VAL:HG13	19	0.13
(1,182)	1:137:A:LEU:HD13	1:141:A:VAL:HG11	19	0.13
(1,182)	1:137:A:LEU:HD13	1:141:A:VAL:HG12	19	0.13
(1,182)	1:137:A:LEU:HD13	1:141:A:VAL:HG13	19	0.13
(1,175)	1:179:A:ALA:HB1	1:181:A:LEU:HD21	6	0.13
(1,175)	1:179:A:ALA:HB1	1:181:A:LEU:HD22	6	0.13
(1,175)	1:179:A:ALA:HB1	1:181:A:LEU:HD23	6	0.13
(1,175)	1:179:A:ALA:HB2	1:181:A:LEU:HD21	6	0.13
(1,175)	1:179:A:ALA:HB2	1:181:A:LEU:HD22	6	0.13
(1,175)	1:179:A:ALA:HB2	1:181:A:LEU:HD23	6	0.13
(1,175)	1:179:A:ALA:HB3	1:181:A:LEU:HD21	6	0.13
(1,175)	1:179:A:ALA:HB3	1:181:A:LEU:HD22	6	0.13
(1,175)	1:179:A:ALA:HB3	1:181:A:LEU:HD23	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,55)	1:156:A:VAL:HG11	1:157:A:PRO:HD2	5	0.13
(1,55)	1:156:A:VAL:HG12	1:157:A:PRO:HD2	5	0.13
(1,55)	1:156:A:VAL:HG13	1:157:A:PRO:HD2	5	0.13
(1,51)	1:185:A:VAL:HB	1:188:A:LEU:HD11	7	0.13
(1,51)	1:185:A:VAL:HB	1:188:A:LEU:HD12	7	0.13
(1,51)	1:185:A:VAL:HB	1:188:A:LEU:HD13	7	0.13
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD11	11	0.12
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD12	11	0.12
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD13	11	0.12
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD21	11	0.12
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD22	11	0.12
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD23	11	0.12
(1,2339)	1:180:C:PHE:H	1:181:C:LEU:HB2	11	0.12
(1,2339)	1:180:C:PHE:H	1:181:C:LEU:HB3	11	0.12
(1,2339)	1:180:C:PHE:H	1:181:C:LEU:HB2	12	0.12
(1,2339)	1:180:C:PHE:H	1:181:C:LEU:HB3	12	0.12
(1,2338)	1:179:C:ALA:HB1	1:181:C:LEU:HD11	1	0.12
(1,2338)	1:179:C:ALA:HB1	1:181:C:LEU:HD12	1	0.12
(1,2338)	1:179:C:ALA:HB1	1:181:C:LEU:HD13	1	0.12
(1,2338)	1:179:C:ALA:HB1	1:181:C:LEU:HD21	1	0.12
(1,2338)	1:179:C:ALA:HB1	1:181:C:LEU:HD22	1	0.12
(1,2338)	1:179:C:ALA:HB1	1:181:C:LEU:HD23	1	0.12
(1,2338)	1:179:C:ALA:HB2	1:181:C:LEU:HD11	1	0.12
(1,2338)	1:179:C:ALA:HB2	1:181:C:LEU:HD12	1	0.12
(1,2338)	1:179:C:ALA:HB2	1:181:C:LEU:HD13	1	0.12
(1,2338)	1:179:C:ALA:HB2	1:181:C:LEU:HD21	1	0.12
(1,2338)	1:179:C:ALA:HB2	1:181:C:LEU:HD22	1	0.12
(1,2338)	1:179:C:ALA:HB2	1:181:C:LEU:HD23	1	0.12
(1,2338)	1:179:C:ALA:HB3	1:181:C:LEU:HD11	1	0.12
(1,2338)	1:179:C:ALA:HB3	1:181:C:LEU:HD12	1	0.12
(1,2338)	1:179:C:ALA:HB3	1:181:C:LEU:HD13	1	0.12
(1,2338)	1:179:C:ALA:HB3	1:181:C:LEU:HD21	1	0.12
(1,2338)	1:179:C:ALA:HB3	1:181:C:LEU:HD22	1	0.12
(1,2338)	1:179:C:ALA:HB3	1:181:C:LEU:HD23	1	0.12
(1,2338)	1:179:C:ALA:HB1	1:181:C:LEU:HD11	9	0.12
(1,2338)	1:179:C:ALA:HB1	1:181:C:LEU:HD12	9	0.12
(1,2338)	1:179:C:ALA:HB1	1:181:C:LEU:HD13	9	0.12
(1,2338)	1:179:C:ALA:HB1	1:181:C:LEU:HD21	9	0.12
(1,2338)	1:179:C:ALA:HB1	1:181:C:LEU:HD22	9	0.12
(1,2338)	1:179:C:ALA:HB1	1:181:C:LEU:HD23	9	0.12
(1,2338)	1:179:C:ALA:HB2	1:181:C:LEU:HD11	9	0.12
(1,2338)	1:179:C:ALA:HB2	1:181:C:LEU:HD12	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2338)	1:179:C:ALA:HB2	1:181:C:LEU:HD13	9	0.12
(1,2338)	1:179:C:ALA:HB2	1:181:C:LEU:HD21	9	0.12
(1,2338)	1:179:C:ALA:HB2	1:181:C:LEU:HD22	9	0.12
(1,2338)	1:179:C:ALA:HB2	1:181:C:LEU:HD23	9	0.12
(1,2338)	1:179:C:ALA:HB3	1:181:C:LEU:HD11	9	0.12
(1,2338)	1:179:C:ALA:HB3	1:181:C:LEU:HD12	9	0.12
(1,2338)	1:179:C:ALA:HB3	1:181:C:LEU:HD13	9	0.12
(1,2338)	1:179:C:ALA:HB3	1:181:C:LEU:HD21	9	0.12
(1,2338)	1:179:C:ALA:HB3	1:181:C:LEU:HD22	9	0.12
(1,2338)	1:179:C:ALA:HB3	1:181:C:LEU:HD23	9	0.12
(1,2322)	1:176:C:GLY:H	1:177:C:ASP:HB2	8	0.12
(1,2322)	1:176:C:GLY:H	1:177:C:ASP:HB3	8	0.12
(1,2322)	1:176:C:GLY:H	1:177:C:ASP:HB2	19	0.12
(1,2322)	1:176:C:GLY:H	1:177:C:ASP:HB3	19	0.12
(1,2322)	1:176:C:GLY:H	1:177:C:ASP:HB2	20	0.12
(1,2322)	1:176:C:GLY:H	1:177:C:ASP:HB3	20	0.12
(1,2321)	1:172:C:ALA:HB1	1:173:C:PRO:HD2	2	0.12
(1,2321)	1:172:C:ALA:HB1	1:173:C:PRO:HD3	2	0.12
(1,2321)	1:172:C:ALA:HB2	1:173:C:PRO:HD2	2	0.12
(1,2321)	1:172:C:ALA:HB2	1:173:C:PRO:HD3	2	0.12
(1,2321)	1:172:C:ALA:HB3	1:173:C:PRO:HD2	2	0.12
(1,2321)	1:172:C:ALA:HB3	1:173:C:PRO:HD3	2	0.12
(1,2321)	1:172:C:ALA:HB1	1:173:C:PRO:HD2	12	0.12
(1,2321)	1:172:C:ALA:HB1	1:173:C:PRO:HD3	12	0.12
(1,2321)	1:172:C:ALA:HB2	1:173:C:PRO:HD2	12	0.12
(1,2321)	1:172:C:ALA:HB2	1:173:C:PRO:HD3	12	0.12
(1,2321)	1:172:C:ALA:HB3	1:173:C:PRO:HD2	12	0.12
(1,2321)	1:172:C:ALA:HB3	1:173:C:PRO:HD3	12	0.12
(1,2321)	1:172:C:ALA:HB1	1:173:C:PRO:HD2	15	0.12
(1,2321)	1:172:C:ALA:HB1	1:173:C:PRO:HD3	15	0.12
(1,2321)	1:172:C:ALA:HB2	1:173:C:PRO:HD2	15	0.12
(1,2321)	1:172:C:ALA:HB2	1:173:C:PRO:HD3	15	0.12
(1,2321)	1:172:C:ALA:HB3	1:173:C:PRO:HD2	15	0.12
(1,2321)	1:172:C:ALA:HB3	1:173:C:PRO:HD3	15	0.12
(1,2321)	1:172:C:ALA:HB1	1:173:C:PRO:HD2	17	0.12
(1,2321)	1:172:C:ALA:HB1	1:173:C:PRO:HD3	17	0.12
(1,2321)	1:172:C:ALA:HB2	1:173:C:PRO:HD2	17	0.12
(1,2321)	1:172:C:ALA:HB2	1:173:C:PRO:HD3	17	0.12
(1,2321)	1:172:C:ALA:HB3	1:173:C:PRO:HD2	17	0.12
(1,2321)	1:172:C:ALA:HB3	1:173:C:PRO:HD3	17	0.12
(1,2321)	1:172:C:ALA:HB1	1:173:C:PRO:HD2	19	0.12
(1,2321)	1:172:C:ALA:HB1	1:173:C:PRO:HD3	19	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2321)	1:172:C:ALA:HB2	1:173:C:PRO:HD2	19	0.12
(1,2321)	1:172:C:ALA:HB2	1:173:C:PRO:HD3	19	0.12
(1,2321)	1:172:C:ALA:HB3	1:173:C:PRO:HD2	19	0.12
(1,2321)	1:172:C:ALA:HB3	1:173:C:PRO:HD3	19	0.12
(1,2295)	1:155:C:ALA:HB1	1:157:C:PRO:HD2	9	0.12
(1,2295)	1:155:C:ALA:HB1	1:157:C:PRO:HD3	9	0.12
(1,2295)	1:155:C:ALA:HB2	1:157:C:PRO:HD2	9	0.12
(1,2295)	1:155:C:ALA:HB2	1:157:C:PRO:HD3	9	0.12
(1,2295)	1:155:C:ALA:HB3	1:157:C:PRO:HD2	9	0.12
(1,2295)	1:155:C:ALA:HB3	1:157:C:PRO:HD3	9	0.12
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG11	4	0.12
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG12	4	0.12
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG13	4	0.12
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG21	4	0.12
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG22	4	0.12
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG23	4	0.12
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG11	5	0.12
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG12	5	0.12
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG13	5	0.12
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG21	5	0.12
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG22	5	0.12
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG23	5	0.12
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG11	6	0.12
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG12	6	0.12
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG13	6	0.12
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG21	6	0.12
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG22	6	0.12
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG23	6	0.12
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG11	8	0.12
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG12	8	0.12
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG13	8	0.12
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG21	8	0.12
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG22	8	0.12
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG23	8	0.12
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG11	11	0.12
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG12	11	0.12
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG13	11	0.12
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG21	11	0.12
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG22	11	0.12
(1,2294)	1:155:C:ALA:HA	1:156:C:VAL:HG23	11	0.12
(1,2286)	1:151:C:GLN:HB2	1:152:C:ALA:HA	11	0.12
(1,2286)	1:151:C:GLN:HB3	1:152:C:ALA:HA	11	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2283)	1:150:C:LEU:HD11	1:167:C:ARG:HG2	13	0.12
(1,2283)	1:150:C:LEU:HD11	1:167:C:ARG:HG3	13	0.12
(1,2283)	1:150:C:LEU:HD12	1:167:C:ARG:HG2	13	0.12
(1,2283)	1:150:C:LEU:HD12	1:167:C:ARG:HG3	13	0.12
(1,2283)	1:150:C:LEU:HD13	1:167:C:ARG:HG2	13	0.12
(1,2283)	1:150:C:LEU:HD13	1:167:C:ARG:HG3	13	0.12
(1,2283)	1:150:C:LEU:HD21	1:167:C:ARG:HG2	13	0.12
(1,2283)	1:150:C:LEU:HD21	1:167:C:ARG:HG3	13	0.12
(1,2283)	1:150:C:LEU:HD22	1:167:C:ARG:HG2	13	0.12
(1,2283)	1:150:C:LEU:HD22	1:167:C:ARG:HG3	13	0.12
(1,2283)	1:150:C:LEU:HD23	1:167:C:ARG:HG2	13	0.12
(1,2283)	1:150:C:LEU:HD23	1:167:C:ARG:HG3	13	0.12
(1,2236)	1:121:C:CYS:HB2	1:189:C:CYS:H	2	0.12
(1,2236)	1:121:C:CYS:HB3	1:189:C:CYS:H	2	0.12
(1,2236)	1:121:C:CYS:HB2	1:189:C:CYS:H	4	0.12
(1,2236)	1:121:C:CYS:HB3	1:189:C:CYS:H	4	0.12
(1,2236)	1:121:C:CYS:HB2	1:189:C:CYS:H	5	0.12
(1,2236)	1:121:C:CYS:HB3	1:189:C:CYS:H	5	0.12
(1,2231)	1:119:C:THR:H	1:192:C:VAL:HG11	3	0.12
(1,2231)	1:119:C:THR:H	1:192:C:VAL:HG12	3	0.12
(1,2231)	1:119:C:THR:H	1:192:C:VAL:HG13	3	0.12
(1,2231)	1:119:C:THR:H	1:192:C:VAL:HG21	3	0.12
(1,2231)	1:119:C:THR:H	1:192:C:VAL:HG22	3	0.12
(1,2231)	1:119:C:THR:H	1:192:C:VAL:HG23	3	0.12
(1,2155)	1:88:C:LEU:H	1:89:C:VAL:HG11	8	0.12
(1,2155)	1:88:C:LEU:H	1:89:C:VAL:HG12	8	0.12
(1,2155)	1:88:C:LEU:H	1:89:C:VAL:HG13	8	0.12
(1,2155)	1:88:C:LEU:H	1:89:C:VAL:HG21	8	0.12
(1,2155)	1:88:C:LEU:H	1:89:C:VAL:HG22	8	0.12
(1,2155)	1:88:C:LEU:H	1:89:C:VAL:HG23	8	0.12
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD11	4	0.12
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD12	4	0.12
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD13	4	0.12
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD21	4	0.12
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD22	4	0.12
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD23	4	0.12
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD11	9	0.12
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD12	9	0.12
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD13	9	0.12
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD21	9	0.12
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD22	9	0.12
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD23	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD11	11	0.12
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD12	11	0.12
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD13	11	0.12
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD21	11	0.12
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD22	11	0.12
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD23	11	0.12
(1,2113)	1:180:B:PHE:H	1:181:B:LEU:HB2	11	0.12
(1,2113)	1:180:B:PHE:H	1:181:B:LEU:HB3	11	0.12
(1,2113)	1:180:B:PHE:H	1:181:B:LEU:HB2	12	0.12
(1,2113)	1:180:B:PHE:H	1:181:B:LEU:HB3	12	0.12
(1,2112)	1:179:B:ALA:HB1	1:181:B:LEU:HD11	1	0.12
(1,2112)	1:179:B:ALA:HB1	1:181:B:LEU:HD12	1	0.12
(1,2112)	1:179:B:ALA:HB1	1:181:B:LEU:HD13	1	0.12
(1,2112)	1:179:B:ALA:HB1	1:181:B:LEU:HD21	1	0.12
(1,2112)	1:179:B:ALA:HB1	1:181:B:LEU:HD22	1	0.12
(1,2112)	1:179:B:ALA:HB1	1:181:B:LEU:HD23	1	0.12
(1,2112)	1:179:B:ALA:HB2	1:181:B:LEU:HD11	1	0.12
(1,2112)	1:179:B:ALA:HB2	1:181:B:LEU:HD12	1	0.12
(1,2112)	1:179:B:ALA:HB2	1:181:B:LEU:HD13	1	0.12
(1,2112)	1:179:B:ALA:HB2	1:181:B:LEU:HD21	1	0.12
(1,2112)	1:179:B:ALA:HB2	1:181:B:LEU:HD22	1	0.12
(1,2112)	1:179:B:ALA:HB2	1:181:B:LEU:HD23	1	0.12
(1,2112)	1:179:B:ALA:HB3	1:181:B:LEU:HD11	1	0.12
(1,2112)	1:179:B:ALA:HB3	1:181:B:LEU:HD12	1	0.12
(1,2112)	1:179:B:ALA:HB3	1:181:B:LEU:HD13	1	0.12
(1,2112)	1:179:B:ALA:HB3	1:181:B:LEU:HD21	1	0.12
(1,2112)	1:179:B:ALA:HB3	1:181:B:LEU:HD22	1	0.12
(1,2112)	1:179:B:ALA:HB3	1:181:B:LEU:HD23	1	0.12
(1,2096)	1:176:B:GLY:H	1:177:B:ASP:HB2	8	0.12
(1,2096)	1:176:B:GLY:H	1:177:B:ASP:HB3	8	0.12
(1,2096)	1:176:B:GLY:H	1:177:B:ASP:HB2	19	0.12
(1,2096)	1:176:B:GLY:H	1:177:B:ASP:HB3	19	0.12
(1,2096)	1:176:B:GLY:H	1:177:B:ASP:HB2	20	0.12
(1,2096)	1:176:B:GLY:H	1:177:B:ASP:HB3	20	0.12
(1,2095)	1:172:B:ALA:HB1	1:173:B:PRO:HD2	1	0.12
(1,2095)	1:172:B:ALA:HB1	1:173:B:PRO:HD3	1	0.12
(1,2095)	1:172:B:ALA:HB2	1:173:B:PRO:HD2	1	0.12
(1,2095)	1:172:B:ALA:HB2	1:173:B:PRO:HD3	1	0.12
(1,2095)	1:172:B:ALA:HB3	1:173:B:PRO:HD2	1	0.12
(1,2095)	1:172:B:ALA:HB3	1:173:B:PRO:HD3	1	0.12
(1,2095)	1:172:B:ALA:HB1	1:173:B:PRO:HD2	2	0.12
(1,2095)	1:172:B:ALA:HB1	1:173:B:PRO:HD3	2	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2095)	1:172:B:ALA:HB2	1:173:B:PRO:HD2	2	0.12
(1,2095)	1:172:B:ALA:HB2	1:173:B:PRO:HD3	2	0.12
(1,2095)	1:172:B:ALA:HB3	1:173:B:PRO:HD2	2	0.12
(1,2095)	1:172:B:ALA:HB3	1:173:B:PRO:HD3	2	0.12
(1,2095)	1:172:B:ALA:HB1	1:173:B:PRO:HD2	12	0.12
(1,2095)	1:172:B:ALA:HB1	1:173:B:PRO:HD3	12	0.12
(1,2095)	1:172:B:ALA:HB2	1:173:B:PRO:HD2	12	0.12
(1,2095)	1:172:B:ALA:HB2	1:173:B:PRO:HD3	12	0.12
(1,2095)	1:172:B:ALA:HB3	1:173:B:PRO:HD2	12	0.12
(1,2095)	1:172:B:ALA:HB3	1:173:B:PRO:HD3	12	0.12
(1,2095)	1:172:B:ALA:HB1	1:173:B:PRO:HD2	15	0.12
(1,2095)	1:172:B:ALA:HB1	1:173:B:PRO:HD3	15	0.12
(1,2095)	1:172:B:ALA:HB2	1:173:B:PRO:HD2	15	0.12
(1,2095)	1:172:B:ALA:HB2	1:173:B:PRO:HD3	15	0.12
(1,2095)	1:172:B:ALA:HB3	1:173:B:PRO:HD2	15	0.12
(1,2095)	1:172:B:ALA:HB3	1:173:B:PRO:HD3	15	0.12
(1,2095)	1:172:B:ALA:HB1	1:173:B:PRO:HD2	17	0.12
(1,2095)	1:172:B:ALA:HB1	1:173:B:PRO:HD3	17	0.12
(1,2095)	1:172:B:ALA:HB2	1:173:B:PRO:HD2	17	0.12
(1,2095)	1:172:B:ALA:HB2	1:173:B:PRO:HD3	17	0.12
(1,2095)	1:172:B:ALA:HB3	1:173:B:PRO:HD2	17	0.12
(1,2095)	1:172:B:ALA:HB3	1:173:B:PRO:HD3	17	0.12
(1,2095)	1:172:B:ALA:HB1	1:173:B:PRO:HD2	18	0.12
(1,2095)	1:172:B:ALA:HB1	1:173:B:PRO:HD3	18	0.12
(1,2095)	1:172:B:ALA:HB2	1:173:B:PRO:HD2	18	0.12
(1,2095)	1:172:B:ALA:HB2	1:173:B:PRO:HD3	18	0.12
(1,2095)	1:172:B:ALA:HB3	1:173:B:PRO:HD2	18	0.12
(1,2095)	1:172:B:ALA:HB3	1:173:B:PRO:HD3	18	0.12
(1,2069)	1:155:B:ALA:HB1	1:157:B:PRO:HD2	9	0.12
(1,2069)	1:155:B:ALA:HB1	1:157:B:PRO:HD3	9	0.12
(1,2069)	1:155:B:ALA:HB2	1:157:B:PRO:HD2	9	0.12
(1,2069)	1:155:B:ALA:HB2	1:157:B:PRO:HD3	9	0.12
(1,2069)	1:155:B:ALA:HB3	1:157:B:PRO:HD2	9	0.12
(1,2069)	1:155:B:ALA:HB3	1:157:B:PRO:HD3	9	0.12
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG11	4	0.12
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG12	4	0.12
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG13	4	0.12
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG21	4	0.12
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG22	4	0.12
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG23	4	0.12
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG11	5	0.12
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG12	5	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG13	5	0.12
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG21	5	0.12
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG22	5	0.12
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG23	5	0.12
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG11	6	0.12
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG12	6	0.12
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG13	6	0.12
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG21	6	0.12
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG22	6	0.12
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG23	6	0.12
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG11	8	0.12
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG12	8	0.12
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG13	8	0.12
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG21	8	0.12
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG22	8	0.12
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG23	8	0.12
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG11	11	0.12
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG12	11	0.12
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG13	11	0.12
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG21	11	0.12
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG22	11	0.12
(1,2068)	1:155:B:ALA:HA	1:156:B:VAL:HG23	11	0.12
(1,2060)	1:151:B:GLN:HB2	1:152:B:ALA:HA	11	0.12
(1,2060)	1:151:B:GLN:HB3	1:152:B:ALA:HA	11	0.12
(1,2057)	1:150:B:LEU:HD11	1:167:B:ARG:HG2	20	0.12
(1,2057)	1:150:B:LEU:HD11	1:167:B:ARG:HG3	20	0.12
(1,2057)	1:150:B:LEU:HD12	1:167:B:ARG:HG2	20	0.12
(1,2057)	1:150:B:LEU:HD12	1:167:B:ARG:HG3	20	0.12
(1,2057)	1:150:B:LEU:HD13	1:167:B:ARG:HG2	20	0.12
(1,2057)	1:150:B:LEU:HD13	1:167:B:ARG:HG3	20	0.12
(1,2057)	1:150:B:LEU:HD21	1:167:B:ARG:HG2	20	0.12
(1,2057)	1:150:B:LEU:HD21	1:167:B:ARG:HG3	20	0.12
(1,2057)	1:150:B:LEU:HD22	1:167:B:ARG:HG2	20	0.12
(1,2057)	1:150:B:LEU:HD22	1:167:B:ARG:HG3	20	0.12
(1,2057)	1:150:B:LEU:HD23	1:167:B:ARG:HG2	20	0.12
(1,2057)	1:150:B:LEU:HD23	1:167:B:ARG:HG3	20	0.12
(1,2010)	1:121:B:CYS:HB2	1:189:B:CYS:H	2	0.12
(1,2010)	1:121:B:CYS:HB3	1:189:B:CYS:H	2	0.12
(1,2010)	1:121:B:CYS:HB2	1:189:B:CYS:H	4	0.12
(1,2010)	1:121:B:CYS:HB3	1:189:B:CYS:H	4	0.12
(1,2010)	1:121:B:CYS:HB2	1:189:B:CYS:H	8	0.12
(1,2010)	1:121:B:CYS:HB3	1:189:B:CYS:H	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2010)	1:121:B:CYS:HB2	1:189:B:CYS:H	20	0.12
(1,2010)	1:121:B:CYS:HB3	1:189:B:CYS:H	20	0.12
(1,1927)	1:88:B:LEU:H	1:89:B:VAL:HG11	8	0.12
(1,1927)	1:88:B:LEU:H	1:89:B:VAL:HG12	8	0.12
(1,1927)	1:88:B:LEU:H	1:89:B:VAL:HG13	8	0.12
(1,1927)	1:88:B:LEU:H	1:89:B:VAL:HG21	8	0.12
(1,1927)	1:88:B:LEU:H	1:89:B:VAL:HG22	8	0.12
(1,1927)	1:88:B:LEU:H	1:89:B:VAL:HG23	8	0.12
(1,1912)	1:178:A:PRO:HB2	1:194:A:LEU:HD21	14	0.12
(1,1912)	1:178:A:PRO:HB2	1:194:A:LEU:HD22	14	0.12
(1,1912)	1:178:A:PRO:HB2	1:194:A:LEU:HD23	14	0.12
(1,1912)	1:178:A:PRO:HB3	1:194:A:LEU:HD21	14	0.12
(1,1912)	1:178:A:PRO:HB3	1:194:A:LEU:HD22	14	0.12
(1,1912)	1:178:A:PRO:HB3	1:194:A:LEU:HD23	14	0.12
(1,1911)	1:178:A:PRO:HB2	1:180:A:PHE:H	18	0.12
(1,1911)	1:178:A:PRO:HB3	1:180:A:PHE:H	18	0.12
(1,1904)	1:176:A:GLY:H	1:177:A:ASP:HB2	8	0.12
(1,1904)	1:176:A:GLY:H	1:177:A:ASP:HB3	8	0.12
(1,1904)	1:176:A:GLY:H	1:177:A:ASP:HB2	17	0.12
(1,1904)	1:176:A:GLY:H	1:177:A:ASP:HB3	17	0.12
(1,1904)	1:176:A:GLY:H	1:177:A:ASP:HB2	20	0.12
(1,1904)	1:176:A:GLY:H	1:177:A:ASP:HB3	20	0.12
(1,1903)	1:172:A:ALA:HB1	1:173:A:PRO:HD2	9	0.12
(1,1903)	1:172:A:ALA:HB1	1:173:A:PRO:HD3	9	0.12
(1,1903)	1:172:A:ALA:HB2	1:173:A:PRO:HD2	9	0.12
(1,1903)	1:172:A:ALA:HB2	1:173:A:PRO:HD3	9	0.12
(1,1903)	1:172:A:ALA:HB3	1:173:A:PRO:HD2	9	0.12
(1,1903)	1:172:A:ALA:HB3	1:173:A:PRO:HD3	9	0.12
(1,1903)	1:172:A:ALA:HB1	1:173:A:PRO:HD2	17	0.12
(1,1903)	1:172:A:ALA:HB1	1:173:A:PRO:HD3	17	0.12
(1,1903)	1:172:A:ALA:HB2	1:173:A:PRO:HD2	17	0.12
(1,1903)	1:172:A:ALA:HB2	1:173:A:PRO:HD3	17	0.12
(1,1903)	1:172:A:ALA:HB3	1:173:A:PRO:HD2	17	0.12
(1,1903)	1:172:A:ALA:HB3	1:173:A:PRO:HD3	17	0.12
(1,1902)	1:172:A:ALA:HA	1:178:A:PRO:HD2	18	0.12
(1,1902)	1:172:A:ALA:HA	1:178:A:PRO:HD3	18	0.12
(1,1885)	1:155:A:ALA:HB1	1:157:A:PRO:HD2	16	0.12
(1,1885)	1:155:A:ALA:HB1	1:157:A:PRO:HD3	16	0.12
(1,1885)	1:155:A:ALA:HB2	1:157:A:PRO:HD2	16	0.12
(1,1885)	1:155:A:ALA:HB2	1:157:A:PRO:HD3	16	0.12
(1,1885)	1:155:A:ALA:HB3	1:157:A:PRO:HD2	16	0.12
(1,1885)	1:155:A:ALA:HB3	1:157:A:PRO:HD3	16	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1884)	1:154:A:PRO:HB2	1:167:A:ARG:H	17	0.12
(1,1884)	1:154:A:PRO:HB3	1:167:A:ARG:H	17	0.12
(1,1867)	1:134:A:LEU:H	1:188:C:LEU:HD11	9	0.12
(1,1867)	1:134:A:LEU:H	1:188:C:LEU:HD12	9	0.12
(1,1867)	1:134:A:LEU:H	1:188:C:LEU:HD13	9	0.12
(1,1867)	1:134:A:LEU:H	1:188:C:LEU:HD21	9	0.12
(1,1867)	1:134:A:LEU:H	1:188:C:LEU:HD22	9	0.12
(1,1867)	1:134:A:LEU:H	1:188:C:LEU:HD23	9	0.12
(1,1848)	1:124:A:MET:HB2	1:197:A:ILE:HD11	14	0.12
(1,1848)	1:124:A:MET:HB2	1:197:A:ILE:HD12	14	0.12
(1,1848)	1:124:A:MET:HB2	1:197:A:ILE:HD13	14	0.12
(1,1848)	1:124:A:MET:HB3	1:197:A:ILE:HD11	14	0.12
(1,1848)	1:124:A:MET:HB3	1:197:A:ILE:HD12	14	0.12
(1,1848)	1:124:A:MET:HB3	1:197:A:ILE:HD13	14	0.12
(1,1842)	1:121:A:CYS:HB2	1:189:A:CYS:H	8	0.12
(1,1842)	1:121:A:CYS:HB3	1:189:A:CYS:H	8	0.12
(1,1835)	1:109:A:LEU:HB2	1:110:A:LEU:HD11	2	0.12
(1,1835)	1:109:A:LEU:HB2	1:110:A:LEU:HD12	2	0.12
(1,1835)	1:109:A:LEU:HB2	1:110:A:LEU:HD13	2	0.12
(1,1835)	1:109:A:LEU:HB3	1:110:A:LEU:HD11	2	0.12
(1,1835)	1:109:A:LEU:HB3	1:110:A:LEU:HD12	2	0.12
(1,1835)	1:109:A:LEU:HB3	1:110:A:LEU:HD13	2	0.12
(1,1832)	1:108:A:GLN:H	1:108:A:GLN:HG2	14	0.12
(1,1832)	1:108:A:GLN:H	1:108:A:GLN:HG3	14	0.12
(1,1819)	1:95:C:SER:HB2	1:101:C:LEU:H	5	0.12
(1,1819)	1:95:C:SER:HB3	1:101:C:LEU:H	5	0.12
(1,1819)	1:95:C:SER:HB2	1:101:C:LEU:H	19	0.12
(1,1819)	1:95:C:SER:HB3	1:101:C:LEU:H	19	0.12
(1,1818)	1:95:B:SER:HB2	1:101:B:LEU:H	16	0.12
(1,1818)	1:95:B:SER:HB3	1:101:B:LEU:H	16	0.12
(1,1801)	1:151:C:GLN:HA	1:152:C:ALA:H	20	0.12
(1,1799)	1:151:A:GLN:HA	1:152:A:ALA:H	20	0.12
(1,1788)	1:96:B:ILE:HG21	1:101:B:LEU:H	4	0.12
(1,1788)	1:96:B:ILE:HG22	1:101:B:LEU:H	4	0.12
(1,1788)	1:96:B:ILE:HG23	1:101:B:LEU:H	4	0.12
(1,1774)	1:125:A:LYS:H	1:126:A:ILE:HG21	16	0.12
(1,1774)	1:125:A:LYS:H	1:126:A:ILE:HG22	16	0.12
(1,1774)	1:125:A:LYS:H	1:126:A:ILE:HG23	16	0.12
(1,1744)	1:184:A:ALA:HB1	1:188:A:LEU:H	14	0.12
(1,1744)	1:184:A:ALA:HB2	1:188:A:LEU:H	14	0.12
(1,1744)	1:184:A:ALA:HB3	1:188:A:LEU:H	14	0.12
(1,1692)	1:120:A:CYS:H	1:192:A:VAL:HG11	14	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1692)	1:120:A:CYS:H	1:192:A:VAL:HG12	14	0.12
(1,1692)	1:120:A:CYS:H	1:192:A:VAL:HG13	14	0.12
(1,1692)	1:120:A:CYS:H	1:192:A:VAL:HG11	15	0.12
(1,1692)	1:120:A:CYS:H	1:192:A:VAL:HG12	15	0.12
(1,1692)	1:120:A:CYS:H	1:192:A:VAL:HG13	15	0.12
(1,1692)	1:120:A:CYS:H	1:192:A:VAL:HG11	17	0.12
(1,1692)	1:120:A:CYS:H	1:192:A:VAL:HG12	17	0.12
(1,1692)	1:120:A:CYS:H	1:192:A:VAL:HG13	17	0.12
(1,1687)	1:90:B:THR:H	1:91:B:THR:HB	7	0.12
(1,1610)	1:118:A:GLY:H	1:192:A:VAL:HG21	18	0.12
(1,1610)	1:118:A:GLY:H	1:192:A:VAL:HG22	18	0.12
(1,1610)	1:118:A:GLY:H	1:192:A:VAL:HG23	18	0.12
(1,1564)	1:145:C:GLN:HA	1:151:C:GLN:H	6	0.12
(1,1564)	1:145:C:GLN:HA	1:151:C:GLN:H	12	0.12
(1,1563)	1:145:B:GLN:HA	1:151:B:GLN:H	6	0.12
(1,1562)	1:145:A:GLN:HA	1:151:A:GLN:H	3	0.12
(1,1556)	1:155:A:ALA:HB1	1:167:A:ARG:H	16	0.12
(1,1556)	1:155:A:ALA:HB2	1:167:A:ARG:H	16	0.12
(1,1556)	1:155:A:ALA:HB3	1:167:A:ARG:H	16	0.12
(1,1554)	1:156:C:VAL:HB	1:167:C:ARG:H	19	0.12
(1,1554)	1:156:C:VAL:HB	1:167:C:ARG:H	20	0.12
(1,1553)	1:156:B:VAL:HB	1:167:B:ARG:H	20	0.12
(1,1551)	1:167:C:ARG:H	1:171:C:SER:HA	10	0.12
(1,1550)	1:167:B:ARG:H	1:171:B:SER:HA	10	0.12
(1,1550)	1:167:B:ARG:H	1:171:B:SER:HA	19	0.12
(1,1549)	1:167:A:ARG:H	1:171:A:SER:HA	10	0.12
(1,1549)	1:167:A:ARG:H	1:171:A:SER:HA	19	0.12
(1,1548)	1:167:C:ARG:H	1:170:C:GLY:HA2	1	0.12
(1,1548)	1:167:C:ARG:H	1:170:C:GLY:HA3	1	0.12
(1,1548)	1:167:C:ARG:H	1:170:C:GLY:HA2	11	0.12
(1,1548)	1:167:C:ARG:H	1:170:C:GLY:HA3	11	0.12
(1,1547)	1:167:B:ARG:H	1:170:B:GLY:HA2	1	0.12
(1,1547)	1:167:B:ARG:H	1:170:B:GLY:HA3	1	0.12
(1,1547)	1:167:B:ARG:H	1:170:B:GLY:HA2	8	0.12
(1,1547)	1:167:B:ARG:H	1:170:B:GLY:HA3	8	0.12
(1,1547)	1:167:B:ARG:H	1:170:B:GLY:HA2	11	0.12
(1,1547)	1:167:B:ARG:H	1:170:B:GLY:HA3	11	0.12
(1,1546)	1:167:A:ARG:H	1:170:A:GLY:HA2	4	0.12
(1,1546)	1:167:A:ARG:H	1:170:A:GLY:HA3	4	0.12
(1,1546)	1:167:A:ARG:H	1:170:A:GLY:HA2	16	0.12
(1,1546)	1:167:A:ARG:H	1:170:A:GLY:HA3	16	0.12
(1,1540)	1:136:B:ALA:HB1	1:140:B:LYS:H	4	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1540)	1:136:B:ALA:HB2	1:140:B:LYS:H	4	0.12
(1,1540)	1:136:B:ALA:HB3	1:140:B:LYS:H	4	0.12
(1,1535)	1:122:C:TYR:H	1:189:C:CYS:HB2	3	0.12
(1,1535)	1:122:C:TYR:H	1:189:C:CYS:HB3	3	0.12
(1,1534)	1:122:B:TYR:H	1:189:B:CYS:HB2	16	0.12
(1,1534)	1:122:B:TYR:H	1:189:B:CYS:HB3	16	0.12
(1,1533)	1:122:A:TYR:H	1:189:A:CYS:HB2	13	0.12
(1,1533)	1:122:A:TYR:H	1:189:A:CYS:HB3	13	0.12
(1,1513)	1:137:C:LEU:H	1:137:C:LEU:HG	10	0.12
(1,1512)	1:137:B:LEU:H	1:137:B:LEU:HG	6	0.12
(1,1511)	1:137:A:LEU:H	1:137:A:LEU:HG	10	0.12
(1,1507)	1:92:A:ALA:H	1:93:C:THR:HG21	9	0.12
(1,1507)	1:92:A:ALA:H	1:93:C:THR:HG22	9	0.12
(1,1507)	1:92:A:ALA:H	1:93:C:THR:HG23	9	0.12
(1,1505)	1:93:A:THR:HG21	1:92:B:ALA:H	3	0.12
(1,1505)	1:93:A:THR:HG22	1:92:B:ALA:H	3	0.12
(1,1505)	1:93:A:THR:HG23	1:92:B:ALA:H	3	0.12
(1,1504)	1:92:A:ALA:H	1:103:A:VAL:HG21	11	0.12
(1,1504)	1:92:A:ALA:H	1:103:A:VAL:HG22	11	0.12
(1,1504)	1:92:A:ALA:H	1:103:A:VAL:HG23	11	0.12
(1,1504)	1:92:A:ALA:H	1:103:A:VAL:HG21	12	0.12
(1,1504)	1:92:A:ALA:H	1:103:A:VAL:HG22	12	0.12
(1,1504)	1:92:A:ALA:H	1:103:A:VAL:HG23	12	0.12
(1,1491)	1:131:C:ILE:HA	1:133:C:SER:H	8	0.12
(1,1463)	1:180:C:PHE:H	1:181:C:LEU:HA	1	0.12
(1,1463)	1:180:C:PHE:H	1:181:C:LEU:HA	8	0.12
(1,1462)	1:180:B:PHE:H	1:181:B:LEU:HA	1	0.12
(1,1462)	1:180:B:PHE:H	1:181:B:LEU:HA	8	0.12
(1,1432)	1:111:C:ILE:H	1:123:C:ILE:HG21	7	0.12
(1,1432)	1:111:C:ILE:H	1:123:C:ILE:HG22	7	0.12
(1,1432)	1:111:C:ILE:H	1:123:C:ILE:HG23	7	0.12
(1,1432)	1:111:C:ILE:H	1:123:C:ILE:HG21	11	0.12
(1,1432)	1:111:C:ILE:H	1:123:C:ILE:HG22	11	0.12
(1,1432)	1:111:C:ILE:H	1:123:C:ILE:HG23	11	0.12
(1,1432)	1:111:C:ILE:H	1:123:C:ILE:HG21	15	0.12
(1,1432)	1:111:C:ILE:H	1:123:C:ILE:HG22	15	0.12
(1,1432)	1:111:C:ILE:H	1:123:C:ILE:HG23	15	0.12
(1,1431)	1:111:B:ILE:H	1:123:B:ILE:HG21	7	0.12
(1,1431)	1:111:B:ILE:H	1:123:B:ILE:HG22	7	0.12
(1,1431)	1:111:B:ILE:H	1:123:B:ILE:HG23	7	0.12
(1,1431)	1:111:B:ILE:H	1:123:B:ILE:HG21	15	0.12
(1,1431)	1:111:B:ILE:H	1:123:B:ILE:HG22	15	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1431)	1:111:B:ILE:H	1:123:B:ILE:HG23	15	0.12
(1,1410)	1:152:C:ALA:HB1	1:153:C:LYS:H	2	0.12
(1,1410)	1:152:C:ALA:HB2	1:153:C:LYS:H	2	0.12
(1,1410)	1:152:C:ALA:HB3	1:153:C:LYS:H	2	0.12
(1,1410)	1:152:C:ALA:HB1	1:153:C:LYS:H	9	0.12
(1,1410)	1:152:C:ALA:HB2	1:153:C:LYS:H	9	0.12
(1,1410)	1:152:C:ALA:HB3	1:153:C:LYS:H	9	0.12
(1,1409)	1:152:B:ALA:HB1	1:153:B:LYS:H	2	0.12
(1,1409)	1:152:B:ALA:HB2	1:153:B:LYS:H	2	0.12
(1,1409)	1:152:B:ALA:HB3	1:153:B:LYS:H	2	0.12
(1,1409)	1:152:B:ALA:HB1	1:153:B:LYS:H	9	0.12
(1,1409)	1:152:B:ALA:HB2	1:153:B:LYS:H	9	0.12
(1,1409)	1:152:B:ALA:HB3	1:153:B:LYS:H	9	0.12
(1,1408)	1:152:A:ALA:HB1	1:153:A:LYS:H	9	0.12
(1,1408)	1:152:A:ALA:HB2	1:153:A:LYS:H	9	0.12
(1,1408)	1:152:A:ALA:HB3	1:153:A:LYS:H	9	0.12
(1,1396)	1:152:A:ALA:HA	1:153:A:LYS:H	14	0.12
(1,1387)	1:141:A:VAL:HG21	1:142:A:HIS:H	3	0.12
(1,1387)	1:141:A:VAL:HG22	1:142:A:HIS:H	3	0.12
(1,1387)	1:141:A:VAL:HG23	1:142:A:HIS:H	3	0.12
(1,1387)	1:141:A:VAL:HG21	1:142:A:HIS:H	6	0.12
(1,1387)	1:141:A:VAL:HG22	1:142:A:HIS:H	6	0.12
(1,1387)	1:141:A:VAL:HG23	1:142:A:HIS:H	6	0.12
(1,1387)	1:141:A:VAL:HG21	1:142:A:HIS:H	8	0.12
(1,1387)	1:141:A:VAL:HG22	1:142:A:HIS:H	8	0.12
(1,1387)	1:141:A:VAL:HG23	1:142:A:HIS:H	8	0.12
(1,1387)	1:141:A:VAL:HG21	1:142:A:HIS:H	11	0.12
(1,1387)	1:141:A:VAL:HG22	1:142:A:HIS:H	11	0.12
(1,1387)	1:141:A:VAL:HG23	1:142:A:HIS:H	11	0.12
(1,1387)	1:141:A:VAL:HG21	1:142:A:HIS:H	12	0.12
(1,1387)	1:141:A:VAL:HG22	1:142:A:HIS:H	12	0.12
(1,1387)	1:141:A:VAL:HG23	1:142:A:HIS:H	12	0.12
(1,1387)	1:141:A:VAL:HG21	1:142:A:HIS:H	18	0.12
(1,1387)	1:141:A:VAL:HG22	1:142:A:HIS:H	18	0.12
(1,1387)	1:141:A:VAL:HG23	1:142:A:HIS:H	18	0.12
(1,1352)	1:127:C:ALA:H	1:131:C:ILE:HG21	6	0.12
(1,1352)	1:127:C:ALA:H	1:131:C:ILE:HG22	6	0.12
(1,1352)	1:127:C:ALA:H	1:131:C:ILE:HG23	6	0.12
(1,1294)	1:103:A:VAL:HB	1:112:A:ALA:H	10	0.12
(1,1276)	1:109:A:LEU:H	1:109:A:LEU:HG	3	0.12
(1,1276)	1:109:A:LEU:H	1:109:A:LEU:HG	4	0.12
(1,1276)	1:109:A:LEU:H	1:109:A:LEU:HG	13	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1276)	1:109:A:LEU:H	1:109:A:LEU:HG	14	0.12
(1,1276)	1:109:A:LEU:H	1:109:A:LEU:HG	15	0.12
(1,1203)	1:196:C:TYR:H	1:196:C:TYR:HE1	15	0.12
(1,1203)	1:196:C:TYR:H	1:196:C:TYR:HE2	15	0.12
(1,1201)	1:196:A:TYR:H	1:196:A:TYR:HE1	13	0.12
(1,1201)	1:196:A:TYR:H	1:196:A:TYR:HE2	13	0.12
(1,1201)	1:196:A:TYR:H	1:196:A:TYR:HE1	17	0.12
(1,1201)	1:196:A:TYR:H	1:196:A:TYR:HE2	17	0.12
(1,1100)	1:167:C:ARG:H	1:167:C:ARG:HB2	3	0.12
(1,1100)	1:167:C:ARG:H	1:167:C:ARG:HB2	4	0.12
(1,1100)	1:167:C:ARG:H	1:167:C:ARG:HB2	18	0.12
(1,1099)	1:167:B:ARG:H	1:167:B:ARG:HB2	4	0.12
(1,1099)	1:167:B:ARG:H	1:167:B:ARG:HB2	18	0.12
(1,1098)	1:167:A:ARG:H	1:167:A:ARG:HB2	18	0.12
(1,1095)	1:157:A:PRO:HA	1:158:A:THR:H	4	0.12
(1,1079)	1:173:C:PRO:HB3	1:174:C:SER:H	3	0.12
(1,1079)	1:173:C:PRO:HB3	1:174:C:SER:H	18	0.12
(1,1079)	1:173:C:PRO:HB3	1:174:C:SER:H	19	0.12
(1,1079)	1:173:C:PRO:HB3	1:174:C:SER:H	20	0.12
(1,1078)	1:173:B:PRO:HB3	1:174:B:SER:H	3	0.12
(1,1078)	1:173:B:PRO:HB3	1:174:B:SER:H	18	0.12
(1,1078)	1:173:B:PRO:HB3	1:174:B:SER:H	19	0.12
(1,1078)	1:173:B:PRO:HB3	1:174:B:SER:H	20	0.12
(1,1077)	1:173:A:PRO:HB3	1:174:A:SER:H	18	0.12
(1,1036)	1:188:A:LEU:HD21	1:134:B:LEU:H	8	0.12
(1,1036)	1:188:A:LEU:HD22	1:134:B:LEU:H	8	0.12
(1,1036)	1:188:A:LEU:HD23	1:134:B:LEU:H	8	0.12
(1,965)	1:110:A:LEU:HD11	1:125:A:LYS:HB3	11	0.12
(1,965)	1:110:A:LEU:HD12	1:125:A:LYS:HB3	11	0.12
(1,965)	1:110:A:LEU:HD13	1:125:A:LYS:HB3	11	0.12
(1,958)	1:187:A:THR:HA	1:188:A:LEU:HD11	18	0.12
(1,958)	1:187:A:THR:HA	1:188:A:LEU:HD12	18	0.12
(1,958)	1:187:A:THR:HA	1:188:A:LEU:HD13	18	0.12
(1,896)	1:165:C:GLU:HB3	1:169:C:ALA:HB1	12	0.12
(1,896)	1:165:C:GLU:HB3	1:169:C:ALA:HB2	12	0.12
(1,896)	1:165:C:GLU:HB3	1:169:C:ALA:HB3	12	0.12
(1,895)	1:165:B:GLU:HB3	1:169:B:ALA:HB1	12	0.12
(1,895)	1:165:B:GLU:HB3	1:169:B:ALA:HB2	12	0.12
(1,895)	1:165:B:GLU:HB3	1:169:B:ALA:HB3	12	0.12
(1,893)	1:165:C:GLU:HB2	1:167:C:ARG:HG2	12	0.12
(1,893)	1:165:C:GLU:HB2	1:167:C:ARG:HG3	12	0.12
(1,893)	1:165:C:GLU:HB2	1:167:C:ARG:HG2	18	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,893)	1:165:C:GLU:HB2	1:167:C:ARG:HG3	18	0.12
(1,892)	1:165:B:GLU:HB2	1:167:B:ARG:HG2	10	0.12
(1,892)	1:165:B:GLU:HB2	1:167:B:ARG:HG3	10	0.12
(1,892)	1:165:B:GLU:HB2	1:167:B:ARG:HG2	12	0.12
(1,892)	1:165:B:GLU:HB2	1:167:B:ARG:HG3	12	0.12
(1,891)	1:165:A:GLU:HB2	1:167:A:ARG:HG2	18	0.12
(1,891)	1:165:A:GLU:HB2	1:167:A:ARG:HG3	18	0.12
(1,890)	1:152:C:ALA:HA	1:157:C:PRO:HG2	12	0.12
(1,890)	1:152:C:ALA:HA	1:157:C:PRO:HG3	12	0.12
(1,889)	1:152:B:ALA:HA	1:157:B:PRO:HG2	12	0.12
(1,889)	1:152:B:ALA:HA	1:157:B:PRO:HG3	12	0.12
(1,888)	1:152:A:ALA:HA	1:157:A:PRO:HG2	11	0.12
(1,888)	1:152:A:ALA:HA	1:157:A:PRO:HG3	11	0.12
(1,815)	1:176:C:GLY:H	1:177:C:ASP:HB2	2	0.12
(1,815)	1:176:C:GLY:H	1:177:C:ASP:HB2	9	0.12
(1,815)	1:176:C:GLY:H	1:177:C:ASP:HB2	11	0.12
(1,815)	1:176:C:GLY:H	1:177:C:ASP:HB2	14	0.12
(1,814)	1:176:B:GLY:H	1:177:B:ASP:HB2	2	0.12
(1,814)	1:176:B:GLY:H	1:177:B:ASP:HB2	9	0.12
(1,814)	1:176:B:GLY:H	1:177:B:ASP:HB2	11	0.12
(1,814)	1:176:B:GLY:H	1:177:B:ASP:HB2	14	0.12
(1,813)	1:176:A:GLY:H	1:177:A:ASP:HB2	8	0.12
(1,813)	1:176:A:GLY:H	1:177:A:ASP:HB2	14	0.12
(1,795)	1:150:A:LEU:HD11	1:153:A:LYS:HE2	13	0.12
(1,795)	1:150:A:LEU:HD11	1:153:A:LYS:HE3	13	0.12
(1,795)	1:150:A:LEU:HD12	1:153:A:LYS:HE2	13	0.12
(1,795)	1:150:A:LEU:HD12	1:153:A:LYS:HE3	13	0.12
(1,795)	1:150:A:LEU:HD13	1:153:A:LYS:HE2	13	0.12
(1,795)	1:150:A:LEU:HD13	1:153:A:LYS:HE3	13	0.12
(1,772)	1:102:A:VAL:HG21	1:113:A:TYR:HD1	14	0.12
(1,772)	1:102:A:VAL:HG21	1:113:A:TYR:HD2	14	0.12
(1,772)	1:102:A:VAL:HG22	1:113:A:TYR:HD1	14	0.12
(1,772)	1:102:A:VAL:HG22	1:113:A:TYR:HD2	14	0.12
(1,772)	1:102:A:VAL:HG23	1:113:A:TYR:HD1	14	0.12
(1,772)	1:102:A:VAL:HG23	1:113:A:TYR:HD2	14	0.12
(1,769)	1:102:A:VAL:HG21	1:104:A:TYR:HE1	2	0.12
(1,769)	1:102:A:VAL:HG21	1:104:A:TYR:HE2	2	0.12
(1,769)	1:102:A:VAL:HG22	1:104:A:TYR:HE1	2	0.12
(1,769)	1:102:A:VAL:HG22	1:104:A:TYR:HE2	2	0.12
(1,769)	1:102:A:VAL:HG23	1:104:A:TYR:HE1	2	0.12
(1,769)	1:102:A:VAL:HG23	1:104:A:TYR:HE2	2	0.12
(1,755)	1:189:C:CYS:H	1:192:C:VAL:HG11	13	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,755)	1:189:C:CYS:H	1:192:C:VAL:HG12	13	0.12
(1,755)	1:189:C:CYS:H	1:192:C:VAL:HG13	13	0.12
(1,754)	1:189:B:CYS:H	1:192:B:VAL:HG11	13	0.12
(1,754)	1:189:B:CYS:H	1:192:B:VAL:HG12	13	0.12
(1,754)	1:189:B:CYS:H	1:192:B:VAL:HG13	13	0.12
(1,739)	1:175:C:GLY:HA2	1:179:C:ALA:HB1	5	0.12
(1,739)	1:175:C:GLY:HA2	1:179:C:ALA:HB2	5	0.12
(1,739)	1:175:C:GLY:HA2	1:179:C:ALA:HB3	5	0.12
(1,739)	1:175:C:GLY:HA3	1:179:C:ALA:HB1	5	0.12
(1,739)	1:175:C:GLY:HA3	1:179:C:ALA:HB2	5	0.12
(1,739)	1:175:C:GLY:HA3	1:179:C:ALA:HB3	5	0.12
(1,739)	1:175:C:GLY:HA2	1:179:C:ALA:HB1	18	0.12
(1,739)	1:175:C:GLY:HA2	1:179:C:ALA:HB2	18	0.12
(1,739)	1:175:C:GLY:HA2	1:179:C:ALA:HB3	18	0.12
(1,739)	1:175:C:GLY:HA3	1:179:C:ALA:HB1	18	0.12
(1,739)	1:175:C:GLY:HA3	1:179:C:ALA:HB2	18	0.12
(1,739)	1:175:C:GLY:HA3	1:179:C:ALA:HB3	18	0.12
(1,738)	1:175:B:GLY:HA2	1:179:B:ALA:HB1	5	0.12
(1,738)	1:175:B:GLY:HA2	1:179:B:ALA:HB2	5	0.12
(1,738)	1:175:B:GLY:HA2	1:179:B:ALA:HB3	5	0.12
(1,738)	1:175:B:GLY:HA3	1:179:B:ALA:HB1	5	0.12
(1,738)	1:175:B:GLY:HA3	1:179:B:ALA:HB2	5	0.12
(1,738)	1:175:B:GLY:HA3	1:179:B:ALA:HB3	5	0.12
(1,738)	1:175:B:GLY:HA2	1:179:B:ALA:HB1	18	0.12
(1,738)	1:175:B:GLY:HA2	1:179:B:ALA:HB2	18	0.12
(1,738)	1:175:B:GLY:HA2	1:179:B:ALA:HB3	18	0.12
(1,738)	1:175:B:GLY:HA3	1:179:B:ALA:HB1	18	0.12
(1,738)	1:175:B:GLY:HA3	1:179:B:ALA:HB2	18	0.12
(1,738)	1:175:B:GLY:HA3	1:179:B:ALA:HB3	18	0.12
(1,737)	1:175:A:GLY:HA2	1:179:A:ALA:HB1	20	0.12
(1,737)	1:175:A:GLY:HA2	1:179:A:ALA:HB2	20	0.12
(1,737)	1:175:A:GLY:HA2	1:179:A:ALA:HB3	20	0.12
(1,737)	1:175:A:GLY:HA3	1:179:A:ALA:HB1	20	0.12
(1,737)	1:175:A:GLY:HA3	1:179:A:ALA:HB2	20	0.12
(1,737)	1:175:A:GLY:HA3	1:179:A:ALA:HB3	20	0.12
(1,665)	1:113:A:TYR:HE1	1:197:A:ILE:HG21	2	0.12
(1,665)	1:113:A:TYR:HE1	1:197:A:ILE:HG22	2	0.12
(1,665)	1:113:A:TYR:HE1	1:197:A:ILE:HG23	2	0.12
(1,665)	1:113:A:TYR:HE2	1:197:A:ILE:HG21	2	0.12
(1,665)	1:113:A:TYR:HE2	1:197:A:ILE:HG22	2	0.12
(1,665)	1:113:A:TYR:HE2	1:197:A:ILE:HG23	2	0.12
(1,665)	1:113:A:TYR:HE1	1:197:A:ILE:HG21	11	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,665)	1:113:A:TYR:HE1	1:197:A:ILE:HG22	11	0.12
(1,665)	1:113:A:TYR:HE1	1:197:A:ILE:HG23	11	0.12
(1,665)	1:113:A:TYR:HE2	1:197:A:ILE:HG21	11	0.12
(1,665)	1:113:A:TYR:HE2	1:197:A:ILE:HG22	11	0.12
(1,665)	1:113:A:TYR:HE2	1:197:A:ILE:HG23	11	0.12
(1,665)	1:113:A:TYR:HE1	1:197:A:ILE:HG21	12	0.12
(1,665)	1:113:A:TYR:HE1	1:197:A:ILE:HG22	12	0.12
(1,665)	1:113:A:TYR:HE1	1:197:A:ILE:HG23	12	0.12
(1,665)	1:113:A:TYR:HE2	1:197:A:ILE:HG21	12	0.12
(1,665)	1:113:A:TYR:HE2	1:197:A:ILE:HG22	12	0.12
(1,665)	1:113:A:TYR:HE2	1:197:A:ILE:HG23	12	0.12
(1,665)	1:113:A:TYR:HE1	1:197:A:ILE:HG21	20	0.12
(1,665)	1:113:A:TYR:HE1	1:197:A:ILE:HG22	20	0.12
(1,665)	1:113:A:TYR:HE1	1:197:A:ILE:HG23	20	0.12
(1,665)	1:113:A:TYR:HE2	1:197:A:ILE:HG21	20	0.12
(1,665)	1:113:A:TYR:HE2	1:197:A:ILE:HG22	20	0.12
(1,665)	1:113:A:TYR:HE2	1:197:A:ILE:HG23	20	0.12
(1,650)	1:94:A:PHE:HE1	1:131:A:ILE:HG21	6	0.12
(1,650)	1:94:A:PHE:HE1	1:131:A:ILE:HG22	6	0.12
(1,650)	1:94:A:PHE:HE1	1:131:A:ILE:HG23	6	0.12
(1,650)	1:94:A:PHE:HE2	1:131:A:ILE:HG21	6	0.12
(1,650)	1:94:A:PHE:HE2	1:131:A:ILE:HG22	6	0.12
(1,650)	1:94:A:PHE:HE2	1:131:A:ILE:HG23	6	0.12
(1,637)	1:96:C:ILE:HG21	1:100:C:GLY:H	10	0.12
(1,637)	1:96:C:ILE:HG22	1:100:C:GLY:H	10	0.12
(1,637)	1:96:C:ILE:HG23	1:100:C:GLY:H	10	0.12
(1,637)	1:96:C:ILE:HG21	1:100:C:GLY:H	13	0.12
(1,637)	1:96:C:ILE:HG22	1:100:C:GLY:H	13	0.12
(1,637)	1:96:C:ILE:HG23	1:100:C:GLY:H	13	0.12
(1,636)	1:96:B:ILE:HG21	1:100:B:GLY:H	13	0.12
(1,636)	1:96:B:ILE:HG22	1:100:B:GLY:H	13	0.12
(1,636)	1:96:B:ILE:HG23	1:100:B:GLY:H	13	0.12
(1,635)	1:96:A:ILE:HG21	1:100:A:GLY:H	12	0.12
(1,635)	1:96:A:ILE:HG22	1:100:A:GLY:H	12	0.12
(1,635)	1:96:A:ILE:HG23	1:100:A:GLY:H	12	0.12
(1,577)	1:178:A:PRO:HG2	1:194:A:LEU:HD21	18	0.12
(1,577)	1:178:A:PRO:HG2	1:194:A:LEU:HD22	18	0.12
(1,577)	1:178:A:PRO:HG2	1:194:A:LEU:HD23	18	0.12
(1,577)	1:178:A:PRO:HG3	1:194:A:LEU:HD21	18	0.12
(1,577)	1:178:A:PRO:HG3	1:194:A:LEU:HD22	18	0.12
(1,577)	1:178:A:PRO:HG3	1:194:A:LEU:HD23	18	0.12
(1,576)	1:189:A:CYS:HB2	1:194:A:LEU:HD21	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,576)	1:189:A:CYS:HB2	1:194:A:LEU:HD22	8	0.12
(1,576)	1:189:A:CYS:HB2	1:194:A:LEU:HD23	8	0.12
(1,576)	1:189:A:CYS:HB3	1:194:A:LEU:HD21	8	0.12
(1,576)	1:189:A:CYS:HB3	1:194:A:LEU:HD22	8	0.12
(1,576)	1:189:A:CYS:HB3	1:194:A:LEU:HD23	8	0.12
(1,556)	1:110:A:LEU:HD21	1:111:A:ILE:H	15	0.12
(1,556)	1:110:A:LEU:HD22	1:111:A:ILE:H	15	0.12
(1,556)	1:110:A:LEU:HD23	1:111:A:ILE:H	15	0.12
(1,539)	1:111:A:ILE:HG21	1:126:A:ILE:HG21	3	0.12
(1,539)	1:111:A:ILE:HG21	1:126:A:ILE:HG22	3	0.12
(1,539)	1:111:A:ILE:HG21	1:126:A:ILE:HG23	3	0.12
(1,539)	1:111:A:ILE:HG22	1:126:A:ILE:HG21	3	0.12
(1,539)	1:111:A:ILE:HG22	1:126:A:ILE:HG22	3	0.12
(1,539)	1:111:A:ILE:HG22	1:126:A:ILE:HG23	3	0.12
(1,539)	1:111:A:ILE:HG23	1:126:A:ILE:HG21	3	0.12
(1,539)	1:111:A:ILE:HG23	1:126:A:ILE:HG22	3	0.12
(1,539)	1:111:A:ILE:HG23	1:126:A:ILE:HG23	3	0.12
(1,539)	1:111:A:ILE:HG21	1:126:A:ILE:HG21	9	0.12
(1,539)	1:111:A:ILE:HG21	1:126:A:ILE:HG22	9	0.12
(1,539)	1:111:A:ILE:HG21	1:126:A:ILE:HG23	9	0.12
(1,539)	1:111:A:ILE:HG22	1:126:A:ILE:HG21	9	0.12
(1,539)	1:111:A:ILE:HG22	1:126:A:ILE:HG22	9	0.12
(1,539)	1:111:A:ILE:HG22	1:126:A:ILE:HG23	9	0.12
(1,539)	1:111:A:ILE:HG23	1:126:A:ILE:HG21	9	0.12
(1,539)	1:111:A:ILE:HG23	1:126:A:ILE:HG22	9	0.12
(1,539)	1:111:A:ILE:HG23	1:126:A:ILE:HG23	9	0.12
(1,538)	1:111:C:ILE:HD11	1:131:C:ILE:HG21	4	0.12
(1,538)	1:111:C:ILE:HD11	1:131:C:ILE:HG22	4	0.12
(1,538)	1:111:C:ILE:HD11	1:131:C:ILE:HG23	4	0.12
(1,538)	1:111:C:ILE:HD12	1:131:C:ILE:HG21	4	0.12
(1,538)	1:111:C:ILE:HD12	1:131:C:ILE:HG22	4	0.12
(1,538)	1:111:C:ILE:HD12	1:131:C:ILE:HG23	4	0.12
(1,538)	1:111:C:ILE:HD13	1:131:C:ILE:HG21	4	0.12
(1,538)	1:111:C:ILE:HD13	1:131:C:ILE:HG22	4	0.12
(1,538)	1:111:C:ILE:HD13	1:131:C:ILE:HG23	4	0.12
(1,537)	1:111:B:ILE:HD11	1:131:B:ILE:HG21	3	0.12
(1,537)	1:111:B:ILE:HD11	1:131:B:ILE:HG22	3	0.12
(1,537)	1:111:B:ILE:HD11	1:131:B:ILE:HG23	3	0.12
(1,537)	1:111:B:ILE:HD12	1:131:B:ILE:HG21	3	0.12
(1,537)	1:111:B:ILE:HD12	1:131:B:ILE:HG22	3	0.12
(1,537)	1:111:B:ILE:HD12	1:131:B:ILE:HG23	3	0.12
(1,537)	1:111:B:ILE:HD13	1:131:B:ILE:HG21	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,537)	1:111:B:ILE:HD13	1:131:B:ILE:HG22	3	0.12
(1,537)	1:111:B:ILE:HD13	1:131:B:ILE:HG23	3	0.12
(1,397)	1:109:C:LEU:HG	1:111:C:ILE:HD11	10	0.12
(1,397)	1:109:C:LEU:HG	1:111:C:ILE:HD12	10	0.12
(1,397)	1:109:C:LEU:HG	1:111:C:ILE:HD13	10	0.12
(1,396)	1:109:B:LEU:HG	1:111:B:ILE:HD11	13	0.12
(1,396)	1:109:B:LEU:HG	1:111:B:ILE:HD12	13	0.12
(1,396)	1:109:B:LEU:HG	1:111:B:ILE:HD13	13	0.12
(1,396)	1:109:B:LEU:HG	1:111:B:ILE:HD11	15	0.12
(1,396)	1:109:B:LEU:HG	1:111:B:ILE:HD12	15	0.12
(1,396)	1:109:B:LEU:HG	1:111:B:ILE:HD13	15	0.12
(1,396)	1:109:B:LEU:HG	1:111:B:ILE:HD11	20	0.12
(1,396)	1:109:B:LEU:HG	1:111:B:ILE:HD12	20	0.12
(1,396)	1:109:B:LEU:HG	1:111:B:ILE:HD13	20	0.12
(1,373)	1:96:C:ILE:HD11	1:102:C:VAL:HB	11	0.12
(1,373)	1:96:C:ILE:HD12	1:102:C:VAL:HB	11	0.12
(1,373)	1:96:C:ILE:HD13	1:102:C:VAL:HB	11	0.12
(1,372)	1:96:B:ILE:HD11	1:102:B:VAL:HB	11	0.12
(1,372)	1:96:B:ILE:HD12	1:102:B:VAL:HB	11	0.12
(1,372)	1:96:B:ILE:HD13	1:102:B:VAL:HB	11	0.12
(1,371)	1:96:A:ILE:HD11	1:102:A:VAL:HB	14	0.12
(1,371)	1:96:A:ILE:HD12	1:102:A:VAL:HB	14	0.12
(1,371)	1:96:A:ILE:HD13	1:102:A:VAL:HB	14	0.12
(1,362)	1:183:B:MET:HG2	1:131:C:ILE:HD11	4	0.12
(1,362)	1:183:B:MET:HG2	1:131:C:ILE:HD12	4	0.12
(1,362)	1:183:B:MET:HG2	1:131:C:ILE:HD13	4	0.12
(1,362)	1:183:B:MET:HG3	1:131:C:ILE:HD11	4	0.12
(1,362)	1:183:B:MET:HG3	1:131:C:ILE:HD12	4	0.12
(1,362)	1:183:B:MET:HG3	1:131:C:ILE:HD13	4	0.12
(1,362)	1:183:B:MET:HG2	1:131:C:ILE:HD11	18	0.12
(1,362)	1:183:B:MET:HG2	1:131:C:ILE:HD12	18	0.12
(1,362)	1:183:B:MET:HG2	1:131:C:ILE:HD13	18	0.12
(1,362)	1:183:B:MET:HG3	1:131:C:ILE:HD11	18	0.12
(1,362)	1:183:B:MET:HG3	1:131:C:ILE:HD12	18	0.12
(1,362)	1:183:B:MET:HG3	1:131:C:ILE:HD13	18	0.12
(1,361)	1:183:A:MET:HG2	1:131:B:ILE:HD11	3	0.12
(1,361)	1:183:A:MET:HG2	1:131:B:ILE:HD12	3	0.12
(1,361)	1:183:A:MET:HG2	1:131:B:ILE:HD13	3	0.12
(1,361)	1:183:A:MET:HG3	1:131:B:ILE:HD11	3	0.12
(1,361)	1:183:A:MET:HG3	1:131:B:ILE:HD12	3	0.12
(1,361)	1:183:A:MET:HG3	1:131:B:ILE:HD13	3	0.12
(1,361)	1:183:A:MET:HG2	1:131:B:ILE:HD11	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,361)	1:183:A:MET:HG2	1:131:B:ILE:HD12	8	0.12
(1,361)	1:183:A:MET:HG2	1:131:B:ILE:HD13	8	0.12
(1,361)	1:183:A:MET:HG3	1:131:B:ILE:HD11	8	0.12
(1,361)	1:183:A:MET:HG3	1:131:B:ILE:HD12	8	0.12
(1,361)	1:183:A:MET:HG3	1:131:B:ILE:HD13	8	0.12
(1,361)	1:183:A:MET:HG2	1:131:B:ILE:HD11	10	0.12
(1,361)	1:183:A:MET:HG2	1:131:B:ILE:HD12	10	0.12
(1,361)	1:183:A:MET:HG2	1:131:B:ILE:HD13	10	0.12
(1,361)	1:183:A:MET:HG3	1:131:B:ILE:HD11	10	0.12
(1,361)	1:183:A:MET:HG3	1:131:B:ILE:HD12	10	0.12
(1,361)	1:183:A:MET:HG3	1:131:B:ILE:HD13	10	0.12
(1,351)	1:123:C:ILE:HD11	1:196:C:TYR:HE1	19	0.12
(1,351)	1:123:C:ILE:HD11	1:196:C:TYR:HE2	19	0.12
(1,351)	1:123:C:ILE:HD12	1:196:C:TYR:HE1	19	0.12
(1,351)	1:123:C:ILE:HD12	1:196:C:TYR:HE2	19	0.12
(1,351)	1:123:C:ILE:HD13	1:196:C:TYR:HE1	19	0.12
(1,351)	1:123:C:ILE:HD13	1:196:C:TYR:HE2	19	0.12
(1,350)	1:123:B:ILE:HD11	1:196:B:TYR:HE1	13	0.12
(1,350)	1:123:B:ILE:HD11	1:196:B:TYR:HE2	13	0.12
(1,350)	1:123:B:ILE:HD12	1:196:B:TYR:HE1	13	0.12
(1,350)	1:123:B:ILE:HD12	1:196:B:TYR:HE2	13	0.12
(1,350)	1:123:B:ILE:HD13	1:196:B:TYR:HE1	13	0.12
(1,350)	1:123:B:ILE:HD13	1:196:B:TYR:HE2	13	0.12
(1,349)	1:123:A:ILE:HD11	1:196:A:TYR:HE1	18	0.12
(1,349)	1:123:A:ILE:HD11	1:196:A:TYR:HE2	18	0.12
(1,349)	1:123:A:ILE:HD12	1:196:A:TYR:HE1	18	0.12
(1,349)	1:123:A:ILE:HD12	1:196:A:TYR:HE2	18	0.12
(1,349)	1:123:A:ILE:HD13	1:196:A:TYR:HE1	18	0.12
(1,349)	1:123:A:ILE:HD13	1:196:A:TYR:HE2	18	0.12
(1,301)	1:181:A:LEU:HD11	1:196:A:TYR:HE1	4	0.12
(1,301)	1:181:A:LEU:HD11	1:196:A:TYR:HE2	4	0.12
(1,301)	1:181:A:LEU:HD12	1:196:A:TYR:HE1	4	0.12
(1,301)	1:181:A:LEU:HD12	1:196:A:TYR:HE2	4	0.12
(1,301)	1:181:A:LEU:HD13	1:196:A:TYR:HE1	4	0.12
(1,301)	1:181:A:LEU:HD13	1:196:A:TYR:HE2	4	0.12
(1,280)	1:123:A:ILE:HD11	1:189:A:CYS:HB2	7	0.12
(1,280)	1:123:A:ILE:HD11	1:189:A:CYS:HB3	7	0.12
(1,280)	1:123:A:ILE:HD12	1:189:A:CYS:HB2	7	0.12
(1,280)	1:123:A:ILE:HD12	1:189:A:CYS:HB3	7	0.12
(1,280)	1:123:A:ILE:HD13	1:189:A:CYS:HB2	7	0.12
(1,280)	1:123:A:ILE:HD13	1:189:A:CYS:HB3	7	0.12
(1,280)	1:123:A:ILE:HD11	1:189:A:CYS:HB2	11	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,280)	1:123:A:ILE:HD11	1:189:A:CYS:HB3	11	0.12
(1,280)	1:123:A:ILE:HD12	1:189:A:CYS:HB2	11	0.12
(1,280)	1:123:A:ILE:HD12	1:189:A:CYS:HB3	11	0.12
(1,280)	1:123:A:ILE:HD13	1:189:A:CYS:HB2	11	0.12
(1,280)	1:123:A:ILE:HD13	1:189:A:CYS:HB3	11	0.12
(1,226)	1:96:A:ILE:HD11	1:102:A:VAL:HG11	18	0.12
(1,226)	1:96:A:ILE:HD11	1:102:A:VAL:HG12	18	0.12
(1,226)	1:96:A:ILE:HD11	1:102:A:VAL:HG13	18	0.12
(1,226)	1:96:A:ILE:HD12	1:102:A:VAL:HG11	18	0.12
(1,226)	1:96:A:ILE:HD12	1:102:A:VAL:HG12	18	0.12
(1,226)	1:96:A:ILE:HD12	1:102:A:VAL:HG13	18	0.12
(1,226)	1:96:A:ILE:HD13	1:102:A:VAL:HG11	18	0.12
(1,226)	1:96:A:ILE:HD13	1:102:A:VAL:HG12	18	0.12
(1,226)	1:96:A:ILE:HD13	1:102:A:VAL:HG13	18	0.12
(1,198)	1:109:A:LEU:H	1:110:A:LEU:HD21	10	0.12
(1,198)	1:109:A:LEU:H	1:110:A:LEU:HD22	10	0.12
(1,198)	1:109:A:LEU:H	1:110:A:LEU:HD23	10	0.12
(1,182)	1:137:A:LEU:HD11	1:141:A:VAL:HG11	6	0.12
(1,182)	1:137:A:LEU:HD11	1:141:A:VAL:HG12	6	0.12
(1,182)	1:137:A:LEU:HD11	1:141:A:VAL:HG13	6	0.12
(1,182)	1:137:A:LEU:HD12	1:141:A:VAL:HG11	6	0.12
(1,182)	1:137:A:LEU:HD12	1:141:A:VAL:HG12	6	0.12
(1,182)	1:137:A:LEU:HD12	1:141:A:VAL:HG13	6	0.12
(1,182)	1:137:A:LEU:HD13	1:141:A:VAL:HG11	6	0.12
(1,182)	1:137:A:LEU:HD13	1:141:A:VAL:HG12	6	0.12
(1,182)	1:137:A:LEU:HD13	1:141:A:VAL:HG13	6	0.12
(1,182)	1:137:A:LEU:HD11	1:141:A:VAL:HG11	9	0.12
(1,182)	1:137:A:LEU:HD11	1:141:A:VAL:HG12	9	0.12
(1,182)	1:137:A:LEU:HD11	1:141:A:VAL:HG13	9	0.12
(1,182)	1:137:A:LEU:HD12	1:141:A:VAL:HG11	9	0.12
(1,182)	1:137:A:LEU:HD12	1:141:A:VAL:HG12	9	0.12
(1,182)	1:137:A:LEU:HD12	1:141:A:VAL:HG13	9	0.12
(1,182)	1:137:A:LEU:HD13	1:141:A:VAL:HG11	9	0.12
(1,182)	1:137:A:LEU:HD13	1:141:A:VAL:HG12	9	0.12
(1,182)	1:137:A:LEU:HD13	1:141:A:VAL:HG13	9	0.12
(1,175)	1:179:A:ALA:HB1	1:181:A:LEU:HD21	3	0.12
(1,175)	1:179:A:ALA:HB1	1:181:A:LEU:HD22	3	0.12
(1,175)	1:179:A:ALA:HB1	1:181:A:LEU:HD23	3	0.12
(1,175)	1:179:A:ALA:HB2	1:181:A:LEU:HD21	3	0.12
(1,175)	1:179:A:ALA:HB2	1:181:A:LEU:HD22	3	0.12
(1,175)	1:179:A:ALA:HB2	1:181:A:LEU:HD23	3	0.12
(1,175)	1:179:A:ALA:HB3	1:181:A:LEU:HD21	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,175)	1:179:A:ALA:HB3	1:181:A:LEU:HD22	3	0.12
(1,175)	1:179:A:ALA:HB3	1:181:A:LEU:HD23	3	0.12
(1,157)	1:101:A:LEU:HD21	1:95:B:SER:HB2	5	0.12
(1,157)	1:101:A:LEU:HD21	1:95:B:SER:HB3	5	0.12
(1,157)	1:101:A:LEU:HD22	1:95:B:SER:HB2	5	0.12
(1,157)	1:101:A:LEU:HD22	1:95:B:SER:HB3	5	0.12
(1,157)	1:101:A:LEU:HD23	1:95:B:SER:HB2	5	0.12
(1,157)	1:101:A:LEU:HD23	1:95:B:SER:HB3	5	0.12
(1,157)	1:101:A:LEU:HD21	1:95:B:SER:HB2	18	0.12
(1,157)	1:101:A:LEU:HD21	1:95:B:SER:HB3	18	0.12
(1,157)	1:101:A:LEU:HD22	1:95:B:SER:HB2	18	0.12
(1,157)	1:101:A:LEU:HD22	1:95:B:SER:HB3	18	0.12
(1,157)	1:101:A:LEU:HD23	1:95:B:SER:HB2	18	0.12
(1,157)	1:101:A:LEU:HD23	1:95:B:SER:HB3	18	0.12
(1,154)	1:187:A:THR:HG21	1:188:A:LEU:HD21	5	0.12
(1,154)	1:187:A:THR:HG21	1:188:A:LEU:HD22	5	0.12
(1,154)	1:187:A:THR:HG21	1:188:A:LEU:HD23	5	0.12
(1,154)	1:187:A:THR:HG22	1:188:A:LEU:HD21	5	0.12
(1,154)	1:187:A:THR:HG22	1:188:A:LEU:HD22	5	0.12
(1,154)	1:187:A:THR:HG22	1:188:A:LEU:HD23	5	0.12
(1,154)	1:187:A:THR:HG23	1:188:A:LEU:HD21	5	0.12
(1,154)	1:187:A:THR:HG23	1:188:A:LEU:HD22	5	0.12
(1,154)	1:187:A:THR:HG23	1:188:A:LEU:HD23	5	0.12
(1,134)	1:110:A:LEU:HD11	1:111:A:ILE:HD11	11	0.12
(1,134)	1:110:A:LEU:HD11	1:111:A:ILE:HD12	11	0.12
(1,134)	1:110:A:LEU:HD11	1:111:A:ILE:HD13	11	0.12
(1,134)	1:110:A:LEU:HD12	1:111:A:ILE:HD11	11	0.12
(1,134)	1:110:A:LEU:HD12	1:111:A:ILE:HD12	11	0.12
(1,134)	1:110:A:LEU:HD12	1:111:A:ILE:HD13	11	0.12
(1,134)	1:110:A:LEU:HD13	1:111:A:ILE:HD11	11	0.12
(1,134)	1:110:A:LEU:HD13	1:111:A:ILE:HD12	11	0.12
(1,134)	1:110:A:LEU:HD13	1:111:A:ILE:HD13	11	0.12
(1,55)	1:156:A:VAL:HG11	1:157:A:PRO:HD2	13	0.12
(1,55)	1:156:A:VAL:HG12	1:157:A:PRO:HD2	13	0.12
(1,55)	1:156:A:VAL:HG13	1:157:A:PRO:HD2	13	0.12
(1,55)	1:156:A:VAL:HG11	1:157:A:PRO:HD2	19	0.12
(1,55)	1:156:A:VAL:HG12	1:157:A:PRO:HD2	19	0.12
(1,55)	1:156:A:VAL:HG13	1:157:A:PRO:HD2	19	0.12
(1,55)	1:156:A:VAL:HG11	1:157:A:PRO:HD2	20	0.12
(1,55)	1:156:A:VAL:HG12	1:157:A:PRO:HD2	20	0.12
(1,55)	1:156:A:VAL:HG13	1:157:A:PRO:HD2	20	0.12
(1,51)	1:185:A:VAL:HB	1:188:A:LEU:HD11	18	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,51)	1:185:A:VAL:HB	1:188:A:LEU:HD12	18	0.12
(1,51)	1:185:A:VAL:HB	1:188:A:LEU:HD13	18	0.12
(1,42)	1:188:A:LEU:HD11	1:106:B:TYR:HE1	6	0.12
(1,42)	1:188:A:LEU:HD11	1:106:B:TYR:HE2	6	0.12
(1,42)	1:188:A:LEU:HD12	1:106:B:TYR:HE1	6	0.12
(1,42)	1:188:A:LEU:HD12	1:106:B:TYR:HE2	6	0.12
(1,42)	1:188:A:LEU:HD13	1:106:B:TYR:HE1	6	0.12
(1,42)	1:188:A:LEU:HD13	1:106:B:TYR:HE2	6	0.12
(1,42)	1:188:A:LEU:HD11	1:106:B:TYR:HE1	9	0.12
(1,42)	1:188:A:LEU:HD11	1:106:B:TYR:HE2	9	0.12
(1,42)	1:188:A:LEU:HD12	1:106:B:TYR:HE1	9	0.12
(1,42)	1:188:A:LEU:HD12	1:106:B:TYR:HE2	9	0.12
(1,42)	1:188:A:LEU:HD13	1:106:B:TYR:HE1	9	0.12
(1,42)	1:188:A:LEU:HD13	1:106:B:TYR:HE2	9	0.12
(1,42)	1:188:A:LEU:HD11	1:106:B:TYR:HE1	14	0.12
(1,42)	1:188:A:LEU:HD11	1:106:B:TYR:HE2	14	0.12
(1,42)	1:188:A:LEU:HD12	1:106:B:TYR:HE1	14	0.12
(1,42)	1:188:A:LEU:HD12	1:106:B:TYR:HE2	14	0.12
(1,42)	1:188:A:LEU:HD13	1:106:B:TYR:HE1	14	0.12
(1,42)	1:188:A:LEU:HD13	1:106:B:TYR:HE2	14	0.12
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD11	9	0.11
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD12	9	0.11
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD13	9	0.11
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD21	9	0.11
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD22	9	0.11
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD23	9	0.11
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD11	10	0.11
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD12	10	0.11
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD13	10	0.11
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD21	10	0.11
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD22	10	0.11
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD23	10	0.11
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD11	20	0.11
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD12	20	0.11
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD13	20	0.11
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD21	20	0.11
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD22	20	0.11
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD23	20	0.11
(1,2322)	1:176:C:GLY:H	1:177:C:ASP:HB2	17	0.11
(1,2322)	1:176:C:GLY:H	1:177:C:ASP:HB3	17	0.11
(1,2321)	1:172:C:ALA:HB1	1:173:C:PRO:HD2	9	0.11
(1,2321)	1:172:C:ALA:HB1	1:173:C:PRO:HD3	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2321)	1:172:C:ALA:HB2	1:173:C:PRO:HD2	9	0.11
(1,2321)	1:172:C:ALA:HB2	1:173:C:PRO:HD3	9	0.11
(1,2321)	1:172:C:ALA:HB3	1:173:C:PRO:HD2	9	0.11
(1,2321)	1:172:C:ALA:HB3	1:173:C:PRO:HD3	9	0.11
(1,2321)	1:172:C:ALA:HB1	1:173:C:PRO:HD2	20	0.11
(1,2321)	1:172:C:ALA:HB1	1:173:C:PRO:HD3	20	0.11
(1,2321)	1:172:C:ALA:HB2	1:173:C:PRO:HD2	20	0.11
(1,2321)	1:172:C:ALA:HB2	1:173:C:PRO:HD3	20	0.11
(1,2321)	1:172:C:ALA:HB3	1:173:C:PRO:HD2	20	0.11
(1,2321)	1:172:C:ALA:HB3	1:173:C:PRO:HD3	20	0.11
(1,2295)	1:155:C:ALA:HB1	1:157:C:PRO:HD2	4	0.11
(1,2295)	1:155:C:ALA:HB1	1:157:C:PRO:HD3	4	0.11
(1,2295)	1:155:C:ALA:HB2	1:157:C:PRO:HD2	4	0.11
(1,2295)	1:155:C:ALA:HB2	1:157:C:PRO:HD3	4	0.11
(1,2295)	1:155:C:ALA:HB3	1:157:C:PRO:HD2	4	0.11
(1,2295)	1:155:C:ALA:HB3	1:157:C:PRO:HD3	4	0.11
(1,2241)	1:124:C:MET:HB2	1:197:C:ILE:HD11	10	0.11
(1,2241)	1:124:C:MET:HB2	1:197:C:ILE:HD12	10	0.11
(1,2241)	1:124:C:MET:HB2	1:197:C:ILE:HD13	10	0.11
(1,2241)	1:124:C:MET:HB3	1:197:C:ILE:HD11	10	0.11
(1,2241)	1:124:C:MET:HB3	1:197:C:ILE:HD12	10	0.11
(1,2241)	1:124:C:MET:HB3	1:197:C:ILE:HD13	10	0.11
(1,2236)	1:121:C:CYS:HB2	1:189:C:CYS:H	6	0.11
(1,2236)	1:121:C:CYS:HB3	1:189:C:CYS:H	6	0.11
(1,2236)	1:121:C:CYS:HB2	1:189:C:CYS:H	8	0.11
(1,2236)	1:121:C:CYS:HB3	1:189:C:CYS:H	8	0.11
(1,2236)	1:121:C:CYS:HB2	1:189:C:CYS:H	12	0.11
(1,2236)	1:121:C:CYS:HB3	1:189:C:CYS:H	12	0.11
(1,2236)	1:121:C:CYS:HB2	1:189:C:CYS:H	20	0.11
(1,2236)	1:121:C:CYS:HB3	1:189:C:CYS:H	20	0.11
(1,2160)	1:89:C:VAL:HG11	1:91:C:THR:H	15	0.11
(1,2160)	1:89:C:VAL:HG12	1:91:C:THR:H	15	0.11
(1,2160)	1:89:C:VAL:HG13	1:91:C:THR:H	15	0.11
(1,2160)	1:89:C:VAL:HG21	1:91:C:THR:H	15	0.11
(1,2160)	1:89:C:VAL:HG22	1:91:C:THR:H	15	0.11
(1,2160)	1:89:C:VAL:HG23	1:91:C:THR:H	15	0.11
(1,2137)	1:188:B:LEU:HD11	1:106:C:TYR:HE1	6	0.11
(1,2137)	1:188:B:LEU:HD11	1:106:C:TYR:HE2	6	0.11
(1,2137)	1:188:B:LEU:HD12	1:106:C:TYR:HE1	6	0.11
(1,2137)	1:188:B:LEU:HD12	1:106:C:TYR:HE2	6	0.11
(1,2137)	1:188:B:LEU:HD13	1:106:C:TYR:HE1	6	0.11
(1,2137)	1:188:B:LEU:HD13	1:106:C:TYR:HE2	6	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2137)	1:188:B:LEU:HD21	1:106:C:TYR:HE1	6	0.11
(1,2137)	1:188:B:LEU:HD21	1:106:C:TYR:HE2	6	0.11
(1,2137)	1:188:B:LEU:HD22	1:106:C:TYR:HE1	6	0.11
(1,2137)	1:188:B:LEU:HD22	1:106:C:TYR:HE2	6	0.11
(1,2137)	1:188:B:LEU:HD23	1:106:C:TYR:HE1	6	0.11
(1,2137)	1:188:B:LEU:HD23	1:106:C:TYR:HE2	6	0.11
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD11	3	0.11
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD12	3	0.11
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD13	3	0.11
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD21	3	0.11
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD22	3	0.11
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD23	3	0.11
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD11	20	0.11
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD12	20	0.11
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD13	20	0.11
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD21	20	0.11
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD22	20	0.11
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD23	20	0.11
(1,2096)	1:176:B:GLY:H	1:177:B:ASP:HB2	17	0.11
(1,2096)	1:176:B:GLY:H	1:177:B:ASP:HB3	17	0.11
(1,2095)	1:172:B:ALA:HB1	1:173:B:PRO:HD2	9	0.11
(1,2095)	1:172:B:ALA:HB1	1:173:B:PRO:HD3	9	0.11
(1,2095)	1:172:B:ALA:HB2	1:173:B:PRO:HD2	9	0.11
(1,2095)	1:172:B:ALA:HB2	1:173:B:PRO:HD3	9	0.11
(1,2095)	1:172:B:ALA:HB3	1:173:B:PRO:HD2	9	0.11
(1,2095)	1:172:B:ALA:HB3	1:173:B:PRO:HD3	9	0.11
(1,2095)	1:172:B:ALA:HB1	1:173:B:PRO:HD2	19	0.11
(1,2095)	1:172:B:ALA:HB1	1:173:B:PRO:HD3	19	0.11
(1,2095)	1:172:B:ALA:HB2	1:173:B:PRO:HD2	19	0.11
(1,2095)	1:172:B:ALA:HB2	1:173:B:PRO:HD3	19	0.11
(1,2095)	1:172:B:ALA:HB3	1:173:B:PRO:HD2	19	0.11
(1,2095)	1:172:B:ALA:HB3	1:173:B:PRO:HD3	19	0.11
(1,2095)	1:172:B:ALA:HB1	1:173:B:PRO:HD2	20	0.11
(1,2095)	1:172:B:ALA:HB1	1:173:B:PRO:HD3	20	0.11
(1,2095)	1:172:B:ALA:HB2	1:173:B:PRO:HD2	20	0.11
(1,2095)	1:172:B:ALA:HB2	1:173:B:PRO:HD3	20	0.11
(1,2095)	1:172:B:ALA:HB3	1:173:B:PRO:HD2	20	0.11
(1,2095)	1:172:B:ALA:HB3	1:173:B:PRO:HD3	20	0.11
(1,2069)	1:155:B:ALA:HB1	1:157:B:PRO:HD2	1	0.11
(1,2069)	1:155:B:ALA:HB1	1:157:B:PRO:HD3	1	0.11
(1,2069)	1:155:B:ALA:HB2	1:157:B:PRO:HD2	1	0.11
(1,2069)	1:155:B:ALA:HB2	1:157:B:PRO:HD3	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2069)	1:155:B:ALA:HB3	1:157:B:PRO:HD2	1	0.11
(1,2069)	1:155:B:ALA:HB3	1:157:B:PRO:HD3	1	0.11
(1,2069)	1:155:B:ALA:HB1	1:157:B:PRO:HD2	4	0.11
(1,2069)	1:155:B:ALA:HB1	1:157:B:PRO:HD3	4	0.11
(1,2069)	1:155:B:ALA:HB2	1:157:B:PRO:HD2	4	0.11
(1,2069)	1:155:B:ALA:HB2	1:157:B:PRO:HD3	4	0.11
(1,2069)	1:155:B:ALA:HB3	1:157:B:PRO:HD2	4	0.11
(1,2069)	1:155:B:ALA:HB3	1:157:B:PRO:HD3	4	0.11
(1,2015)	1:124:B:MET:HB2	1:197:B:ILE:HD11	10	0.11
(1,2015)	1:124:B:MET:HB2	1:197:B:ILE:HD12	10	0.11
(1,2015)	1:124:B:MET:HB2	1:197:B:ILE:HD13	10	0.11
(1,2015)	1:124:B:MET:HB3	1:197:B:ILE:HD11	10	0.11
(1,2015)	1:124:B:MET:HB3	1:197:B:ILE:HD12	10	0.11
(1,2015)	1:124:B:MET:HB3	1:197:B:ILE:HD13	10	0.11
(1,2010)	1:121:B:CYS:HB2	1:189:B:CYS:H	6	0.11
(1,2010)	1:121:B:CYS:HB3	1:189:B:CYS:H	6	0.11
(1,2010)	1:121:B:CYS:HB2	1:189:B:CYS:H	12	0.11
(1,2010)	1:121:B:CYS:HB3	1:189:B:CYS:H	12	0.11
(1,2010)	1:121:B:CYS:HB2	1:189:B:CYS:H	13	0.11
(1,2010)	1:121:B:CYS:HB3	1:189:B:CYS:H	13	0.11
(1,1916)	1:180:A:PHE:H	1:181:A:LEU:HB2	11	0.11
(1,1916)	1:180:A:PHE:H	1:181:A:LEU:HB3	11	0.11
(1,1916)	1:180:A:PHE:H	1:181:A:LEU:HB2	12	0.11
(1,1916)	1:180:A:PHE:H	1:181:A:LEU:HB3	12	0.11
(1,1903)	1:172:A:ALA:HB1	1:173:A:PRO:HD2	14	0.11
(1,1903)	1:172:A:ALA:HB1	1:173:A:PRO:HD3	14	0.11
(1,1903)	1:172:A:ALA:HB2	1:173:A:PRO:HD2	14	0.11
(1,1903)	1:172:A:ALA:HB2	1:173:A:PRO:HD3	14	0.11
(1,1903)	1:172:A:ALA:HB3	1:173:A:PRO:HD2	14	0.11
(1,1903)	1:172:A:ALA:HB3	1:173:A:PRO:HD3	14	0.11
(1,1903)	1:172:A:ALA:HB1	1:173:A:PRO:HD2	15	0.11
(1,1903)	1:172:A:ALA:HB1	1:173:A:PRO:HD3	15	0.11
(1,1903)	1:172:A:ALA:HB2	1:173:A:PRO:HD2	15	0.11
(1,1903)	1:172:A:ALA:HB2	1:173:A:PRO:HD3	15	0.11
(1,1903)	1:172:A:ALA:HB3	1:173:A:PRO:HD2	15	0.11
(1,1903)	1:172:A:ALA:HB3	1:173:A:PRO:HD3	15	0.11
(1,1902)	1:172:A:ALA:HA	1:178:A:PRO:HD2	7	0.11
(1,1902)	1:172:A:ALA:HA	1:178:A:PRO:HD3	7	0.11
(1,1892)	1:161:A:LEU:HD11	1:162:A:GLY:HA2	12	0.11
(1,1892)	1:161:A:LEU:HD11	1:162:A:GLY:HA3	12	0.11
(1,1892)	1:161:A:LEU:HD12	1:162:A:GLY:HA2	12	0.11
(1,1892)	1:161:A:LEU:HD12	1:162:A:GLY:HA3	12	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1892)	1:161:A:LEU:HD13	1:162:A:GLY:HA2	12	0.11
(1,1892)	1:161:A:LEU:HD13	1:162:A:GLY:HA3	12	0.11
(1,1872)	1:140:A:LYS:HG2	1:146:A:MET:HE1	4	0.11
(1,1872)	1:140:A:LYS:HG2	1:146:A:MET:HE2	4	0.11
(1,1872)	1:140:A:LYS:HG2	1:146:A:MET:HE3	4	0.11
(1,1872)	1:140:A:LYS:HG3	1:146:A:MET:HE1	4	0.11
(1,1872)	1:140:A:LYS:HG3	1:146:A:MET:HE2	4	0.11
(1,1872)	1:140:A:LYS:HG3	1:146:A:MET:HE3	4	0.11
(1,1847)	1:124:A:MET:HB2	1:197:A:ILE:HG12	13	0.11
(1,1847)	1:124:A:MET:HB2	1:197:A:ILE:HG13	13	0.11
(1,1847)	1:124:A:MET:HB3	1:197:A:ILE:HG12	13	0.11
(1,1847)	1:124:A:MET:HB3	1:197:A:ILE:HG13	13	0.11
(1,1832)	1:108:A:GLN:H	1:108:A:GLN:HG2	4	0.11
(1,1832)	1:108:A:GLN:H	1:108:A:GLN:HG3	4	0.11
(1,1831)	1:106:A:TYR:HE1	1:188:C:LEU:HD11	6	0.11
(1,1831)	1:106:A:TYR:HE1	1:188:C:LEU:HD12	6	0.11
(1,1831)	1:106:A:TYR:HE1	1:188:C:LEU:HD13	6	0.11
(1,1831)	1:106:A:TYR:HE1	1:188:C:LEU:HD21	6	0.11
(1,1831)	1:106:A:TYR:HE1	1:188:C:LEU:HD22	6	0.11
(1,1831)	1:106:A:TYR:HE1	1:188:C:LEU:HD23	6	0.11
(1,1831)	1:106:A:TYR:HE2	1:188:C:LEU:HD11	6	0.11
(1,1831)	1:106:A:TYR:HE2	1:188:C:LEU:HD12	6	0.11
(1,1831)	1:106:A:TYR:HE2	1:188:C:LEU:HD13	6	0.11
(1,1831)	1:106:A:TYR:HE2	1:188:C:LEU:HD21	6	0.11
(1,1831)	1:106:A:TYR:HE2	1:188:C:LEU:HD22	6	0.11
(1,1831)	1:106:A:TYR:HE2	1:188:C:LEU:HD23	6	0.11
(1,1831)	1:106:A:TYR:HE1	1:188:C:LEU:HD11	8	0.11
(1,1831)	1:106:A:TYR:HE1	1:188:C:LEU:HD12	8	0.11
(1,1831)	1:106:A:TYR:HE1	1:188:C:LEU:HD13	8	0.11
(1,1831)	1:106:A:TYR:HE1	1:188:C:LEU:HD21	8	0.11
(1,1831)	1:106:A:TYR:HE1	1:188:C:LEU:HD22	8	0.11
(1,1831)	1:106:A:TYR:HE1	1:188:C:LEU:HD23	8	0.11
(1,1831)	1:106:A:TYR:HE2	1:188:C:LEU:HD11	8	0.11
(1,1831)	1:106:A:TYR:HE2	1:188:C:LEU:HD12	8	0.11
(1,1831)	1:106:A:TYR:HE2	1:188:C:LEU:HD13	8	0.11
(1,1831)	1:106:A:TYR:HE2	1:188:C:LEU:HD21	8	0.11
(1,1831)	1:106:A:TYR:HE2	1:188:C:LEU:HD22	8	0.11
(1,1831)	1:106:A:TYR:HE2	1:188:C:LEU:HD23	8	0.11
(1,1819)	1:95:C:SER:HB2	1:101:C:LEU:H	10	0.11
(1,1819)	1:95:C:SER:HB3	1:101:C:LEU:H	10	0.11
(1,1819)	1:95:C:SER:HB2	1:101:C:LEU:H	16	0.11
(1,1819)	1:95:C:SER:HB3	1:101:C:LEU:H	16	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1819)	1:95:C:SER:HB2	1:101:C:LEU:H	18	0.11
(1,1819)	1:95:C:SER:HB3	1:101:C:LEU:H	18	0.11
(1,1819)	1:95:C:SER:HB2	1:101:C:LEU:H	20	0.11
(1,1819)	1:95:C:SER:HB3	1:101:C:LEU:H	20	0.11
(1,1818)	1:95:B:SER:HB2	1:101:B:LEU:H	2	0.11
(1,1818)	1:95:B:SER:HB3	1:101:B:LEU:H	2	0.11
(1,1817)	1:95:A:SER:HB2	1:101:A:LEU:H	4	0.11
(1,1817)	1:95:A:SER:HB3	1:101:A:LEU:H	4	0.11
(1,1817)	1:95:A:SER:HB2	1:101:A:LEU:H	6	0.11
(1,1817)	1:95:A:SER:HB3	1:101:A:LEU:H	6	0.11
(1,1817)	1:95:A:SER:HB2	1:101:A:LEU:H	19	0.11
(1,1817)	1:95:A:SER:HB3	1:101:A:LEU:H	19	0.11
(1,1800)	1:151:B:GLN:HA	1:152:B:ALA:H	20	0.11
(1,1790)	1:101:A:LEU:H	1:101:A:LEU:HD21	3	0.11
(1,1790)	1:101:A:LEU:H	1:101:A:LEU:HD22	3	0.11
(1,1790)	1:101:A:LEU:H	1:101:A:LEU:HD23	3	0.11
(1,1789)	1:96:C:ILE:HG21	1:101:C:LEU:H	4	0.11
(1,1789)	1:96:C:ILE:HG22	1:101:C:LEU:H	4	0.11
(1,1789)	1:96:C:ILE:HG23	1:101:C:LEU:H	4	0.11
(1,1774)	1:125:A:LYS:H	1:126:A:ILE:HG21	12	0.11
(1,1774)	1:125:A:LYS:H	1:126:A:ILE:HG22	12	0.11
(1,1774)	1:125:A:LYS:H	1:126:A:ILE:HG23	12	0.11
(1,1734)	1:194:A:LEU:HG	1:195:A:TYR:H	6	0.11
(1,1688)	1:90:C:THR:H	1:91:C:THR:HB	3	0.11
(1,1688)	1:90:C:THR:H	1:91:C:THR:HB	5	0.11
(1,1688)	1:90:C:THR:H	1:91:C:THR:HB	7	0.11
(1,1688)	1:90:C:THR:H	1:91:C:THR:HB	11	0.11
(1,1687)	1:90:B:THR:H	1:91:B:THR:HB	3	0.11
(1,1687)	1:90:B:THR:H	1:91:B:THR:HB	5	0.11
(1,1686)	1:90:A:THR:H	1:91:A:THR:HB	3	0.11
(1,1686)	1:90:A:THR:H	1:91:A:THR:HB	4	0.11
(1,1686)	1:90:A:THR:H	1:91:A:THR:HB	5	0.11
(1,1686)	1:90:A:THR:H	1:91:A:THR:HB	7	0.11
(1,1670)	1:101:A:LEU:HD11	1:102:A:VAL:H	13	0.11
(1,1670)	1:101:A:LEU:HD12	1:102:A:VAL:H	13	0.11
(1,1670)	1:101:A:LEU:HD13	1:102:A:VAL:H	13	0.11
(1,1620)	1:129:A:GLU:H	1:131:A:ILE:H	19	0.11
(1,1616)	1:116:C:ALA:H	1:119:C:THR:HB	4	0.11
(1,1615)	1:116:B:ALA:H	1:119:B:THR:HB	4	0.11
(1,1614)	1:116:A:ALA:H	1:119:A:THR:HB	4	0.11
(1,1610)	1:118:A:GLY:H	1:192:A:VAL:HG21	13	0.11
(1,1610)	1:118:A:GLY:H	1:192:A:VAL:HG22	13	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1610)	1:118:A:GLY:H	1:192:A:VAL:HG23	13	0.11
(1,1610)	1:118:A:GLY:H	1:192:A:VAL:HG21	19	0.11
(1,1610)	1:118:A:GLY:H	1:192:A:VAL:HG22	19	0.11
(1,1610)	1:118:A:GLY:H	1:192:A:VAL:HG23	19	0.11
(1,1610)	1:118:A:GLY:H	1:192:A:VAL:HG21	20	0.11
(1,1610)	1:118:A:GLY:H	1:192:A:VAL:HG22	20	0.11
(1,1610)	1:118:A:GLY:H	1:192:A:VAL:HG23	20	0.11
(1,1574)	1:119:A:THR:H	1:192:A:VAL:HG11	16	0.11
(1,1574)	1:119:A:THR:H	1:192:A:VAL:HG12	16	0.11
(1,1574)	1:119:A:THR:H	1:192:A:VAL:HG13	16	0.11
(1,1564)	1:145:C:GLN:HA	1:151:C:GLN:H	2	0.11
(1,1564)	1:145:C:GLN:HA	1:151:C:GLN:H	15	0.11
(1,1563)	1:145:B:GLN:HA	1:151:B:GLN:H	15	0.11
(1,1563)	1:145:B:GLN:HA	1:151:B:GLN:H	16	0.11
(1,1563)	1:145:B:GLN:HA	1:151:B:GLN:H	18	0.11
(1,1563)	1:145:B:GLN:HA	1:151:B:GLN:H	20	0.11
(1,1562)	1:145:A:GLN:HA	1:151:A:GLN:H	5	0.11
(1,1556)	1:155:A:ALA:HB1	1:167:A:ARG:H	3	0.11
(1,1556)	1:155:A:ALA:HB2	1:167:A:ARG:H	3	0.11
(1,1556)	1:155:A:ALA:HB3	1:167:A:ARG:H	3	0.11
(1,1554)	1:156:C:VAL:HB	1:167:C:ARG:H	8	0.11
(1,1554)	1:156:C:VAL:HB	1:167:C:ARG:H	13	0.11
(1,1553)	1:156:B:VAL:HB	1:167:B:ARG:H	8	0.11
(1,1553)	1:156:B:VAL:HB	1:167:B:ARG:H	13	0.11
(1,1553)	1:156:B:VAL:HB	1:167:B:ARG:H	19	0.11
(1,1552)	1:156:A:VAL:HB	1:167:A:ARG:H	11	0.11
(1,1551)	1:167:C:ARG:H	1:171:C:SER:HA	18	0.11
(1,1550)	1:167:B:ARG:H	1:171:B:SER:HA	18	0.11
(1,1549)	1:167:A:ARG:H	1:171:A:SER:HA	11	0.11
(1,1549)	1:167:A:ARG:H	1:171:A:SER:HA	18	0.11
(1,1548)	1:167:C:ARG:H	1:170:C:GLY:HA2	16	0.11
(1,1548)	1:167:C:ARG:H	1:170:C:GLY:HA3	16	0.11
(1,1547)	1:167:B:ARG:H	1:170:B:GLY:HA2	16	0.11
(1,1547)	1:167:B:ARG:H	1:170:B:GLY:HA3	16	0.11
(1,1546)	1:167:A:ARG:H	1:170:A:GLY:HA2	7	0.11
(1,1546)	1:167:A:ARG:H	1:170:A:GLY:HA3	7	0.11
(1,1546)	1:167:A:ARG:H	1:170:A:GLY:HA2	11	0.11
(1,1546)	1:167:A:ARG:H	1:170:A:GLY:HA3	11	0.11
(1,1541)	1:136:C:ALA:HB1	1:140:C:LYS:H	1	0.11
(1,1541)	1:136:C:ALA:HB2	1:140:C:LYS:H	1	0.11
(1,1541)	1:136:C:ALA:HB3	1:140:C:LYS:H	1	0.11
(1,1539)	1:136:A:ALA:HB1	1:140:A:LYS:H	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1539)	1:136:A:ALA:HB2	1:140:A:LYS:H	4	0.11
(1,1539)	1:136:A:ALA:HB3	1:140:A:LYS:H	4	0.11
(1,1535)	1:122:C:TYR:H	1:189:C:CYS:HB2	15	0.11
(1,1535)	1:122:C:TYR:H	1:189:C:CYS:HB3	15	0.11
(1,1534)	1:122:B:TYR:H	1:189:B:CYS:HB2	2	0.11
(1,1534)	1:122:B:TYR:H	1:189:B:CYS:HB3	2	0.11
(1,1534)	1:122:B:TYR:H	1:189:B:CYS:HB2	11	0.11
(1,1534)	1:122:B:TYR:H	1:189:B:CYS:HB3	11	0.11
(1,1512)	1:137:B:LEU:H	1:137:B:LEU:HG	3	0.11
(1,1512)	1:137:B:LEU:H	1:137:B:LEU:HG	15	0.11
(1,1512)	1:137:B:LEU:H	1:137:B:LEU:HG	19	0.11
(1,1512)	1:137:B:LEU:H	1:137:B:LEU:HG	20	0.11
(1,1511)	1:137:A:LEU:H	1:137:A:LEU:HG	1	0.11
(1,1511)	1:137:A:LEU:H	1:137:A:LEU:HG	9	0.11
(1,1506)	1:93:B:THR:HG21	1:92:C:ALA:H	17	0.11
(1,1506)	1:93:B:THR:HG22	1:92:C:ALA:H	17	0.11
(1,1506)	1:93:B:THR:HG23	1:92:C:ALA:H	17	0.11
(1,1504)	1:92:A:ALA:H	1:103:A:VAL:HG21	17	0.11
(1,1504)	1:92:A:ALA:H	1:103:A:VAL:HG22	17	0.11
(1,1504)	1:92:A:ALA:H	1:103:A:VAL:HG23	17	0.11
(1,1504)	1:92:A:ALA:H	1:103:A:VAL:HG21	19	0.11
(1,1504)	1:92:A:ALA:H	1:103:A:VAL:HG22	19	0.11
(1,1504)	1:92:A:ALA:H	1:103:A:VAL:HG23	19	0.11
(1,1491)	1:131:C:ILE:HA	1:133:C:SER:H	17	0.11
(1,1489)	1:131:A:ILE:HA	1:133:A:SER:H	7	0.11
(1,1471)	1:181:A:LEU:H	1:181:A:LEU:HD11	1	0.11
(1,1471)	1:181:A:LEU:H	1:181:A:LEU:HD12	1	0.11
(1,1471)	1:181:A:LEU:H	1:181:A:LEU:HD13	1	0.11
(1,1461)	1:180:A:PHE:H	1:181:A:LEU:HA	1	0.11
(1,1461)	1:180:A:PHE:H	1:181:A:LEU:HA	8	0.11
(1,1431)	1:111:B:ILE:H	1:123:B:ILE:HG21	11	0.11
(1,1431)	1:111:B:ILE:H	1:123:B:ILE:HG22	11	0.11
(1,1431)	1:111:B:ILE:H	1:123:B:ILE:HG23	11	0.11
(1,1430)	1:111:A:ILE:H	1:123:A:ILE:HG21	1	0.11
(1,1430)	1:111:A:ILE:H	1:123:A:ILE:HG22	1	0.11
(1,1430)	1:111:A:ILE:H	1:123:A:ILE:HG23	1	0.11
(1,1430)	1:111:A:ILE:H	1:123:A:ILE:HG21	6	0.11
(1,1430)	1:111:A:ILE:H	1:123:A:ILE:HG22	6	0.11
(1,1430)	1:111:A:ILE:H	1:123:A:ILE:HG23	6	0.11
(1,1430)	1:111:A:ILE:H	1:123:A:ILE:HG21	10	0.11
(1,1430)	1:111:A:ILE:H	1:123:A:ILE:HG22	10	0.11
(1,1430)	1:111:A:ILE:H	1:123:A:ILE:HG23	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1430)	1:111:A:ILE:H	1:123:A:ILE:HG21	11	0.11
(1,1430)	1:111:A:ILE:H	1:123:A:ILE:HG22	11	0.11
(1,1430)	1:111:A:ILE:H	1:123:A:ILE:HG23	11	0.11
(1,1430)	1:111:A:ILE:H	1:123:A:ILE:HG21	19	0.11
(1,1430)	1:111:A:ILE:H	1:123:A:ILE:HG22	19	0.11
(1,1430)	1:111:A:ILE:H	1:123:A:ILE:HG23	19	0.11
(1,1398)	1:152:C:ALA:HA	1:153:C:LYS:H	14	0.11
(1,1397)	1:152:B:ALA:HA	1:153:B:LYS:H	14	0.11
(1,1387)	1:141:A:VAL:HG21	1:142:A:HIS:H	10	0.11
(1,1387)	1:141:A:VAL:HG22	1:142:A:HIS:H	10	0.11
(1,1387)	1:141:A:VAL:HG23	1:142:A:HIS:H	10	0.11
(1,1387)	1:141:A:VAL:HG21	1:142:A:HIS:H	15	0.11
(1,1387)	1:141:A:VAL:HG22	1:142:A:HIS:H	15	0.11
(1,1387)	1:141:A:VAL:HG23	1:142:A:HIS:H	15	0.11
(1,1387)	1:141:A:VAL:HG21	1:142:A:HIS:H	19	0.11
(1,1387)	1:141:A:VAL:HG22	1:142:A:HIS:H	19	0.11
(1,1387)	1:141:A:VAL:HG23	1:142:A:HIS:H	19	0.11
(1,1351)	1:127:B:ALA:H	1:131:B:ILE:HG21	6	0.11
(1,1351)	1:127:B:ALA:H	1:131:B:ILE:HG22	6	0.11
(1,1351)	1:127:B:ALA:H	1:131:B:ILE:HG23	6	0.11
(1,1350)	1:127:A:ALA:H	1:131:A:ILE:HG21	10	0.11
(1,1350)	1:127:A:ALA:H	1:131:A:ILE:HG22	10	0.11
(1,1350)	1:127:A:ALA:H	1:131:A:ILE:HG23	10	0.11
(1,1276)	1:109:A:LEU:H	1:109:A:LEU:HG	2	0.11
(1,1276)	1:109:A:LEU:H	1:109:A:LEU:HG	8	0.11
(1,1276)	1:109:A:LEU:H	1:109:A:LEU:HG	11	0.11
(1,1276)	1:109:A:LEU:H	1:109:A:LEU:HG	17	0.11
(1,1237)	1:96:A:ILE:H	1:100:A:GLY:H	18	0.11
(1,1225)	1:101:A:LEU:H	1:114:A:LYS:H	12	0.11
(1,1206)	1:149:C:SER:HB2	1:151:C:GLN:H	15	0.11
(1,1206)	1:149:C:SER:HB3	1:151:C:GLN:H	15	0.11
(1,1205)	1:149:B:SER:HB2	1:151:B:GLN:H	15	0.11
(1,1205)	1:149:B:SER:HB3	1:151:B:GLN:H	15	0.11
(1,1201)	1:196:A:TYR:H	1:196:A:TYR:HE1	2	0.11
(1,1201)	1:196:A:TYR:H	1:196:A:TYR:HE2	2	0.11
(1,1161)	1:94:A:PHE:H	1:101:A:LEU:HD11	8	0.11
(1,1161)	1:94:A:PHE:H	1:101:A:LEU:HD12	8	0.11
(1,1161)	1:94:A:PHE:H	1:101:A:LEU:HD13	8	0.11
(1,1123)	1:87:B:HIS:H	1:88:B:LEU:H	8	0.11
(1,1122)	1:87:A:HIS:H	1:88:A:LEU:H	8	0.11
(1,1079)	1:173:C:PRO:HB3	1:174:C:SER:H	13	0.11
(1,1079)	1:173:C:PRO:HB3	1:174:C:SER:H	15	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1078)	1:173:B:PRO:HB3	1:174:B:SER:H	13	0.11
(1,1078)	1:173:B:PRO:HB3	1:174:B:SER:H	15	0.11
(1,1077)	1:173:A:PRO:HB3	1:174:A:SER:H	3	0.11
(1,1077)	1:173:A:PRO:HB3	1:174:A:SER:H	15	0.11
(1,1040)	1:137:A:LEU:HD11	1:140:A:LYS:H	11	0.11
(1,1040)	1:137:A:LEU:HD12	1:140:A:LYS:H	11	0.11
(1,1040)	1:137:A:LEU:HD13	1:140:A:LYS:H	11	0.11
(1,1040)	1:137:A:LEU:HD11	1:140:A:LYS:H	14	0.11
(1,1040)	1:137:A:LEU:HD12	1:140:A:LYS:H	14	0.11
(1,1040)	1:137:A:LEU:HD13	1:140:A:LYS:H	14	0.11
(1,1036)	1:188:A:LEU:HD21	1:134:B:LEU:H	7	0.11
(1,1036)	1:188:A:LEU:HD22	1:134:B:LEU:H	7	0.11
(1,1036)	1:188:A:LEU:HD23	1:134:B:LEU:H	7	0.11
(1,948)	1:185:A:VAL:HG11	1:189:A:CYS:HB2	7	0.11
(1,948)	1:185:A:VAL:HG11	1:189:A:CYS:HB3	7	0.11
(1,948)	1:185:A:VAL:HG12	1:189:A:CYS:HB2	7	0.11
(1,948)	1:185:A:VAL:HG12	1:189:A:CYS:HB3	7	0.11
(1,948)	1:185:A:VAL:HG13	1:189:A:CYS:HB2	7	0.11
(1,948)	1:185:A:VAL:HG13	1:189:A:CYS:HB3	7	0.11
(1,911)	1:140:C:LYS:HD2	1:197:C:ILE:HG21	17	0.11
(1,911)	1:140:C:LYS:HD2	1:197:C:ILE:HG22	17	0.11
(1,911)	1:140:C:LYS:HD2	1:197:C:ILE:HG23	17	0.11
(1,911)	1:140:C:LYS:HD3	1:197:C:ILE:HG21	17	0.11
(1,911)	1:140:C:LYS:HD3	1:197:C:ILE:HG22	17	0.11
(1,911)	1:140:C:LYS:HD3	1:197:C:ILE:HG23	17	0.11
(1,910)	1:140:B:LYS:HD2	1:197:B:ILE:HG21	17	0.11
(1,910)	1:140:B:LYS:HD2	1:197:B:ILE:HG22	17	0.11
(1,910)	1:140:B:LYS:HD2	1:197:B:ILE:HG23	17	0.11
(1,910)	1:140:B:LYS:HD3	1:197:B:ILE:HG21	17	0.11
(1,910)	1:140:B:LYS:HD3	1:197:B:ILE:HG22	17	0.11
(1,910)	1:140:B:LYS:HD3	1:197:B:ILE:HG23	17	0.11
(1,896)	1:165:C:GLU:HB3	1:169:C:ALA:HB1	13	0.11
(1,896)	1:165:C:GLU:HB3	1:169:C:ALA:HB2	13	0.11
(1,896)	1:165:C:GLU:HB3	1:169:C:ALA:HB3	13	0.11
(1,895)	1:165:B:GLU:HB3	1:169:B:ALA:HB1	3	0.11
(1,895)	1:165:B:GLU:HB3	1:169:B:ALA:HB2	3	0.11
(1,895)	1:165:B:GLU:HB3	1:169:B:ALA:HB3	3	0.11
(1,895)	1:165:B:GLU:HB3	1:169:B:ALA:HB1	13	0.11
(1,895)	1:165:B:GLU:HB3	1:169:B:ALA:HB2	13	0.11
(1,895)	1:165:B:GLU:HB3	1:169:B:ALA:HB3	13	0.11
(1,893)	1:165:C:GLU:HB2	1:167:C:ARG:HG2	10	0.11
(1,893)	1:165:C:GLU:HB2	1:167:C:ARG:HG3	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,892)	1:165:B:GLU:HB2	1:167:B:ARG:HG2	18	0.11
(1,892)	1:165:B:GLU:HB2	1:167:B:ARG:HG3	18	0.11
(1,891)	1:165:A:GLU:HB2	1:167:A:ARG:HG2	11	0.11
(1,891)	1:165:A:GLU:HB2	1:167:A:ARG:HG3	11	0.11
(1,888)	1:152:A:ALA:HA	1:157:A:PRO:HG2	15	0.11
(1,888)	1:152:A:ALA:HA	1:157:A:PRO:HG3	15	0.11
(1,844)	1:156:C:VAL:HB	1:157:C:PRO:HD2	16	0.11
(1,843)	1:156:B:VAL:HB	1:157:B:PRO:HD2	16	0.11
(1,828)	1:102:A:VAL:HB	1:113:A:TYR:HA	2	0.11
(1,815)	1:176:C:GLY:H	1:177:C:ASP:HB2	8	0.11
(1,815)	1:176:C:GLY:H	1:177:C:ASP:HB2	18	0.11
(1,814)	1:176:B:GLY:H	1:177:B:ASP:HB2	8	0.11
(1,814)	1:176:B:GLY:H	1:177:B:ASP:HB2	18	0.11
(1,813)	1:176:A:GLY:H	1:177:A:ASP:HB2	11	0.11
(1,795)	1:150:A:LEU:HD11	1:153:A:LYS:HE2	19	0.11
(1,795)	1:150:A:LEU:HD11	1:153:A:LYS:HE3	19	0.11
(1,795)	1:150:A:LEU:HD12	1:153:A:LYS:HE2	19	0.11
(1,795)	1:150:A:LEU:HD12	1:153:A:LYS:HE3	19	0.11
(1,795)	1:150:A:LEU:HD13	1:153:A:LYS:HE2	19	0.11
(1,795)	1:150:A:LEU:HD13	1:153:A:LYS:HE3	19	0.11
(1,785)	1:167:C:ARG:HD2	1:169:C:ALA:HB1	13	0.11
(1,785)	1:167:C:ARG:HD2	1:169:C:ALA:HB2	13	0.11
(1,785)	1:167:C:ARG:HD2	1:169:C:ALA:HB3	13	0.11
(1,785)	1:167:C:ARG:HD3	1:169:C:ALA:HB1	13	0.11
(1,785)	1:167:C:ARG:HD3	1:169:C:ALA:HB2	13	0.11
(1,785)	1:167:C:ARG:HD3	1:169:C:ALA:HB3	13	0.11
(1,784)	1:167:B:ARG:HD2	1:169:B:ALA:HB1	12	0.11
(1,784)	1:167:B:ARG:HD2	1:169:B:ALA:HB2	12	0.11
(1,784)	1:167:B:ARG:HD2	1:169:B:ALA:HB3	12	0.11
(1,784)	1:167:B:ARG:HD3	1:169:B:ALA:HB1	12	0.11
(1,784)	1:167:B:ARG:HD3	1:169:B:ALA:HB2	12	0.11
(1,784)	1:167:B:ARG:HD3	1:169:B:ALA:HB3	12	0.11
(1,784)	1:167:B:ARG:HD2	1:169:B:ALA:HB1	13	0.11
(1,784)	1:167:B:ARG:HD2	1:169:B:ALA:HB2	13	0.11
(1,784)	1:167:B:ARG:HD2	1:169:B:ALA:HB3	13	0.11
(1,784)	1:167:B:ARG:HD3	1:169:B:ALA:HB1	13	0.11
(1,784)	1:167:B:ARG:HD3	1:169:B:ALA:HB2	13	0.11
(1,784)	1:167:B:ARG:HD3	1:169:B:ALA:HB3	13	0.11
(1,784)	1:167:B:ARG:HD2	1:169:B:ALA:HB1	17	0.11
(1,784)	1:167:B:ARG:HD2	1:169:B:ALA:HB2	17	0.11
(1,784)	1:167:B:ARG:HD2	1:169:B:ALA:HB3	17	0.11
(1,784)	1:167:B:ARG:HD3	1:169:B:ALA:HB1	17	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,784)	1:167:B:ARG:HD3	1:169:B:ALA:HB2	17	0.11
(1,784)	1:167:B:ARG:HD3	1:169:B:ALA:HB3	17	0.11
(1,783)	1:167:A:ARG:HD2	1:169:A:ALA:HB1	13	0.11
(1,783)	1:167:A:ARG:HD2	1:169:A:ALA:HB2	13	0.11
(1,783)	1:167:A:ARG:HD2	1:169:A:ALA:HB3	13	0.11
(1,783)	1:167:A:ARG:HD3	1:169:A:ALA:HB1	13	0.11
(1,783)	1:167:A:ARG:HD3	1:169:A:ALA:HB2	13	0.11
(1,783)	1:167:A:ARG:HD3	1:169:A:ALA:HB3	13	0.11
(1,783)	1:167:A:ARG:HD2	1:169:A:ALA:HB1	17	0.11
(1,783)	1:167:A:ARG:HD2	1:169:A:ALA:HB2	17	0.11
(1,783)	1:167:A:ARG:HD2	1:169:A:ALA:HB3	17	0.11
(1,783)	1:167:A:ARG:HD3	1:169:A:ALA:HB1	17	0.11
(1,783)	1:167:A:ARG:HD3	1:169:A:ALA:HB2	17	0.11
(1,783)	1:167:A:ARG:HD3	1:169:A:ALA:HB3	17	0.11
(1,751)	1:123:C:ILE:HG21	1:179:C:ALA:HB1	3	0.11
(1,751)	1:123:C:ILE:HG21	1:179:C:ALA:HB2	3	0.11
(1,751)	1:123:C:ILE:HG21	1:179:C:ALA:HB3	3	0.11
(1,751)	1:123:C:ILE:HG22	1:179:C:ALA:HB1	3	0.11
(1,751)	1:123:C:ILE:HG22	1:179:C:ALA:HB2	3	0.11
(1,751)	1:123:C:ILE:HG22	1:179:C:ALA:HB3	3	0.11
(1,751)	1:123:C:ILE:HG23	1:179:C:ALA:HB1	3	0.11
(1,751)	1:123:C:ILE:HG23	1:179:C:ALA:HB2	3	0.11
(1,751)	1:123:C:ILE:HG23	1:179:C:ALA:HB3	3	0.11
(1,751)	1:123:C:ILE:HG21	1:179:C:ALA:HB1	8	0.11
(1,751)	1:123:C:ILE:HG21	1:179:C:ALA:HB2	8	0.11
(1,751)	1:123:C:ILE:HG21	1:179:C:ALA:HB3	8	0.11
(1,751)	1:123:C:ILE:HG22	1:179:C:ALA:HB1	8	0.11
(1,751)	1:123:C:ILE:HG22	1:179:C:ALA:HB2	8	0.11
(1,751)	1:123:C:ILE:HG22	1:179:C:ALA:HB3	8	0.11
(1,751)	1:123:C:ILE:HG23	1:179:C:ALA:HB1	8	0.11
(1,751)	1:123:C:ILE:HG23	1:179:C:ALA:HB2	8	0.11
(1,751)	1:123:C:ILE:HG23	1:179:C:ALA:HB3	8	0.11
(1,750)	1:123:B:ILE:HG21	1:179:B:ALA:HB1	3	0.11
(1,750)	1:123:B:ILE:HG21	1:179:B:ALA:HB2	3	0.11
(1,750)	1:123:B:ILE:HG21	1:179:B:ALA:HB3	3	0.11
(1,750)	1:123:B:ILE:HG22	1:179:B:ALA:HB1	3	0.11
(1,750)	1:123:B:ILE:HG22	1:179:B:ALA:HB2	3	0.11
(1,750)	1:123:B:ILE:HG22	1:179:B:ALA:HB3	3	0.11
(1,750)	1:123:B:ILE:HG23	1:179:B:ALA:HB1	3	0.11
(1,750)	1:123:B:ILE:HG23	1:179:B:ALA:HB2	3	0.11
(1,750)	1:123:B:ILE:HG23	1:179:B:ALA:HB3	3	0.11
(1,749)	1:123:A:ILE:HG21	1:179:A:ALA:HB1	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,749)	1:123:A:ILE:HG21	1:179:A:ALA:HB2	9	0.11
(1,749)	1:123:A:ILE:HG21	1:179:A:ALA:HB3	9	0.11
(1,749)	1:123:A:ILE:HG22	1:179:A:ALA:HB1	9	0.11
(1,749)	1:123:A:ILE:HG22	1:179:A:ALA:HB2	9	0.11
(1,749)	1:123:A:ILE:HG22	1:179:A:ALA:HB3	9	0.11
(1,749)	1:123:A:ILE:HG23	1:179:A:ALA:HB1	9	0.11
(1,749)	1:123:A:ILE:HG23	1:179:A:ALA:HB2	9	0.11
(1,749)	1:123:A:ILE:HG23	1:179:A:ALA:HB3	9	0.11
(1,749)	1:123:A:ILE:HG21	1:179:A:ALA:HB1	16	0.11
(1,749)	1:123:A:ILE:HG21	1:179:A:ALA:HB2	16	0.11
(1,749)	1:123:A:ILE:HG21	1:179:A:ALA:HB3	16	0.11
(1,749)	1:123:A:ILE:HG22	1:179:A:ALA:HB1	16	0.11
(1,749)	1:123:A:ILE:HG22	1:179:A:ALA:HB2	16	0.11
(1,749)	1:123:A:ILE:HG22	1:179:A:ALA:HB3	16	0.11
(1,749)	1:123:A:ILE:HG23	1:179:A:ALA:HB1	16	0.11
(1,749)	1:123:A:ILE:HG23	1:179:A:ALA:HB2	16	0.11
(1,749)	1:123:A:ILE:HG23	1:179:A:ALA:HB3	16	0.11
(1,749)	1:123:A:ILE:HG21	1:179:A:ALA:HB1	17	0.11
(1,749)	1:123:A:ILE:HG21	1:179:A:ALA:HB2	17	0.11
(1,749)	1:123:A:ILE:HG21	1:179:A:ALA:HB3	17	0.11
(1,749)	1:123:A:ILE:HG22	1:179:A:ALA:HB1	17	0.11
(1,749)	1:123:A:ILE:HG22	1:179:A:ALA:HB2	17	0.11
(1,749)	1:123:A:ILE:HG22	1:179:A:ALA:HB3	17	0.11
(1,749)	1:123:A:ILE:HG23	1:179:A:ALA:HB1	17	0.11
(1,749)	1:123:A:ILE:HG23	1:179:A:ALA:HB2	17	0.11
(1,749)	1:123:A:ILE:HG23	1:179:A:ALA:HB3	17	0.11
(1,739)	1:175:C:GLY:HA2	1:179:C:ALA:HB1	13	0.11
(1,739)	1:175:C:GLY:HA2	1:179:C:ALA:HB2	13	0.11
(1,739)	1:175:C:GLY:HA2	1:179:C:ALA:HB3	13	0.11
(1,739)	1:175:C:GLY:HA3	1:179:C:ALA:HB1	13	0.11
(1,739)	1:175:C:GLY:HA3	1:179:C:ALA:HB2	13	0.11
(1,739)	1:175:C:GLY:HA3	1:179:C:ALA:HB3	13	0.11
(1,738)	1:175:B:GLY:HA2	1:179:B:ALA:HB1	13	0.11
(1,738)	1:175:B:GLY:HA2	1:179:B:ALA:HB2	13	0.11
(1,738)	1:175:B:GLY:HA2	1:179:B:ALA:HB3	13	0.11
(1,738)	1:175:B:GLY:HA3	1:179:B:ALA:HB1	13	0.11
(1,738)	1:175:B:GLY:HA3	1:179:B:ALA:HB2	13	0.11
(1,738)	1:175:B:GLY:HA3	1:179:B:ALA:HB3	13	0.11
(1,712)	1:141:A:VAL:HG21	1:144:A:PHE:HD1	2	0.11
(1,712)	1:141:A:VAL:HG21	1:144:A:PHE:HD2	2	0.11
(1,712)	1:141:A:VAL:HG22	1:144:A:PHE:HD1	2	0.11
(1,712)	1:141:A:VAL:HG22	1:144:A:PHE:HD2	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,712)	1:141:A:VAL:HG23	1:144:A:PHE:HD1	2	0.11
(1,712)	1:141:A:VAL:HG23	1:144:A:PHE:HD2	2	0.11
(1,712)	1:141:A:VAL:HG21	1:144:A:PHE:HD1	12	0.11
(1,712)	1:141:A:VAL:HG21	1:144:A:PHE:HD2	12	0.11
(1,712)	1:141:A:VAL:HG22	1:144:A:PHE:HD1	12	0.11
(1,712)	1:141:A:VAL:HG22	1:144:A:PHE:HD2	12	0.11
(1,712)	1:141:A:VAL:HG23	1:144:A:PHE:HD1	12	0.11
(1,712)	1:141:A:VAL:HG23	1:144:A:PHE:HD2	12	0.11
(1,712)	1:141:A:VAL:HG21	1:144:A:PHE:HD1	20	0.11
(1,712)	1:141:A:VAL:HG21	1:144:A:PHE:HD2	20	0.11
(1,712)	1:141:A:VAL:HG22	1:144:A:PHE:HD1	20	0.11
(1,712)	1:141:A:VAL:HG22	1:144:A:PHE:HD2	20	0.11
(1,712)	1:141:A:VAL:HG23	1:144:A:PHE:HD1	20	0.11
(1,712)	1:141:A:VAL:HG23	1:144:A:PHE:HD2	20	0.11
(1,695)	1:123:C:ILE:H	1:124:C:MET:HE1	20	0.11
(1,695)	1:123:C:ILE:H	1:124:C:MET:HE2	20	0.11
(1,695)	1:123:C:ILE:H	1:124:C:MET:HE3	20	0.11
(1,694)	1:123:B:ILE:H	1:124:B:MET:HE1	20	0.11
(1,694)	1:123:B:ILE:H	1:124:B:MET:HE2	20	0.11
(1,694)	1:123:B:ILE:H	1:124:B:MET:HE3	20	0.11
(1,693)	1:123:A:ILE:H	1:124:A:MET:HE1	20	0.11
(1,693)	1:123:A:ILE:H	1:124:A:MET:HE2	20	0.11
(1,693)	1:123:A:ILE:H	1:124:A:MET:HE3	20	0.11
(1,665)	1:113:A:TYR:HE1	1:197:A:ILE:HG21	5	0.11
(1,665)	1:113:A:TYR:HE1	1:197:A:ILE:HG22	5	0.11
(1,665)	1:113:A:TYR:HE1	1:197:A:ILE:HG23	5	0.11
(1,665)	1:113:A:TYR:HE2	1:197:A:ILE:HG21	5	0.11
(1,665)	1:113:A:TYR:HE2	1:197:A:ILE:HG22	5	0.11
(1,665)	1:113:A:TYR:HE2	1:197:A:ILE:HG23	5	0.11
(1,665)	1:113:A:TYR:HE1	1:197:A:ILE:HG21	10	0.11
(1,665)	1:113:A:TYR:HE1	1:197:A:ILE:HG22	10	0.11
(1,665)	1:113:A:TYR:HE1	1:197:A:ILE:HG23	10	0.11
(1,665)	1:113:A:TYR:HE2	1:197:A:ILE:HG21	10	0.11
(1,665)	1:113:A:TYR:HE2	1:197:A:ILE:HG22	10	0.11
(1,665)	1:113:A:TYR:HE2	1:197:A:ILE:HG23	10	0.11
(1,665)	1:113:A:TYR:HE1	1:197:A:ILE:HG21	16	0.11
(1,665)	1:113:A:TYR:HE1	1:197:A:ILE:HG22	16	0.11
(1,665)	1:113:A:TYR:HE1	1:197:A:ILE:HG23	16	0.11
(1,665)	1:113:A:TYR:HE2	1:197:A:ILE:HG21	16	0.11
(1,665)	1:113:A:TYR:HE2	1:197:A:ILE:HG22	16	0.11
(1,665)	1:113:A:TYR:HE2	1:197:A:ILE:HG23	16	0.11
(1,658)	1:169:C:ALA:HA	1:172:C:ALA:HB1	14	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,658)	1:169:C:ALA:HA	1:172:C:ALA:HB2	14	0.11
(1,658)	1:169:C:ALA:HA	1:172:C:ALA:HB3	14	0.11
(1,657)	1:169:B:ALA:HA	1:172:B:ALA:HB1	14	0.11
(1,657)	1:169:B:ALA:HA	1:172:B:ALA:HB2	14	0.11
(1,657)	1:169:B:ALA:HA	1:172:B:ALA:HB3	14	0.11
(1,652)	1:94:C:PHE:HE1	1:131:C:ILE:HG21	8	0.11
(1,652)	1:94:C:PHE:HE1	1:131:C:ILE:HG22	8	0.11
(1,652)	1:94:C:PHE:HE1	1:131:C:ILE:HG23	8	0.11
(1,652)	1:94:C:PHE:HE2	1:131:C:ILE:HG21	8	0.11
(1,652)	1:94:C:PHE:HE2	1:131:C:ILE:HG22	8	0.11
(1,652)	1:94:C:PHE:HE2	1:131:C:ILE:HG23	8	0.11
(1,625)	1:96:C:ILE:HG21	1:138:C:THR:HB	4	0.11
(1,625)	1:96:C:ILE:HG22	1:138:C:THR:HB	4	0.11
(1,625)	1:96:C:ILE:HG23	1:138:C:THR:HB	4	0.11
(1,623)	1:96:A:ILE:HG21	1:138:A:THR:HB	4	0.11
(1,623)	1:96:A:ILE:HG22	1:138:A:THR:HB	4	0.11
(1,623)	1:96:A:ILE:HG23	1:138:A:THR:HB	4	0.11
(1,573)	1:194:A:LEU:HD21	1:196:A:TYR:HE1	4	0.11
(1,573)	1:194:A:LEU:HD21	1:196:A:TYR:HE2	4	0.11
(1,573)	1:194:A:LEU:HD22	1:196:A:TYR:HE1	4	0.11
(1,573)	1:194:A:LEU:HD22	1:196:A:TYR:HE2	4	0.11
(1,573)	1:194:A:LEU:HD23	1:196:A:TYR:HE1	4	0.11
(1,573)	1:194:A:LEU:HD23	1:196:A:TYR:HE2	4	0.11
(1,573)	1:194:A:LEU:HD21	1:196:A:TYR:HE1	17	0.11
(1,573)	1:194:A:LEU:HD21	1:196:A:TYR:HE2	17	0.11
(1,573)	1:194:A:LEU:HD22	1:196:A:TYR:HE1	17	0.11
(1,573)	1:194:A:LEU:HD22	1:196:A:TYR:HE2	17	0.11
(1,573)	1:194:A:LEU:HD23	1:196:A:TYR:HE1	17	0.11
(1,573)	1:194:A:LEU:HD23	1:196:A:TYR:HE2	17	0.11
(1,568)	1:156:A:VAL:HB	1:161:A:LEU:HD11	19	0.11
(1,568)	1:156:A:VAL:HB	1:161:A:LEU:HD12	19	0.11
(1,568)	1:156:A:VAL:HB	1:161:A:LEU:HD13	19	0.11
(1,539)	1:111:A:ILE:HG21	1:126:A:ILE:HG21	15	0.11
(1,539)	1:111:A:ILE:HG21	1:126:A:ILE:HG22	15	0.11
(1,539)	1:111:A:ILE:HG21	1:126:A:ILE:HG23	15	0.11
(1,539)	1:111:A:ILE:HG22	1:126:A:ILE:HG21	15	0.11
(1,539)	1:111:A:ILE:HG22	1:126:A:ILE:HG22	15	0.11
(1,539)	1:111:A:ILE:HG22	1:126:A:ILE:HG23	15	0.11
(1,539)	1:111:A:ILE:HG23	1:126:A:ILE:HG21	15	0.11
(1,539)	1:111:A:ILE:HG23	1:126:A:ILE:HG22	15	0.11
(1,539)	1:111:A:ILE:HG23	1:126:A:ILE:HG23	15	0.11
(1,536)	1:111:A:ILE:HD11	1:131:A:ILE:HG21	16	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,536)	1:111:A:ILE:HD11	1:131:A:ILE:HG22	16	0.11
(1,536)	1:111:A:ILE:HD11	1:131:A:ILE:HG23	16	0.11
(1,536)	1:111:A:ILE:HD12	1:131:A:ILE:HG21	16	0.11
(1,536)	1:111:A:ILE:HD12	1:131:A:ILE:HG22	16	0.11
(1,536)	1:111:A:ILE:HD12	1:131:A:ILE:HG23	16	0.11
(1,536)	1:111:A:ILE:HD13	1:131:A:ILE:HG21	16	0.11
(1,536)	1:111:A:ILE:HD13	1:131:A:ILE:HG22	16	0.11
(1,536)	1:111:A:ILE:HD13	1:131:A:ILE:HG23	16	0.11
(1,512)	1:102:A:VAL:HG11	1:103:A:VAL:H	12	0.11
(1,512)	1:102:A:VAL:HG12	1:103:A:VAL:H	12	0.11
(1,512)	1:102:A:VAL:HG13	1:103:A:VAL:H	12	0.11
(1,487)	1:158:C:THR:HA	1:161:C:LEU:HB2	14	0.11
(1,487)	1:158:C:THR:HA	1:161:C:LEU:HB3	14	0.11
(1,486)	1:158:B:THR:HA	1:161:B:LEU:HB2	14	0.11
(1,486)	1:158:B:THR:HA	1:161:B:LEU:HB3	14	0.11
(1,485)	1:158:A:THR:HA	1:161:A:LEU:HB2	10	0.11
(1,485)	1:158:A:THR:HA	1:161:A:LEU:HB3	10	0.11
(1,452)	1:101:A:LEU:HD11	1:95:B:SER:HB2	2	0.11
(1,452)	1:101:A:LEU:HD11	1:95:B:SER:HB3	2	0.11
(1,452)	1:101:A:LEU:HD12	1:95:B:SER:HB2	2	0.11
(1,452)	1:101:A:LEU:HD12	1:95:B:SER:HB3	2	0.11
(1,452)	1:101:A:LEU:HD13	1:95:B:SER:HB2	2	0.11
(1,452)	1:101:A:LEU:HD13	1:95:B:SER:HB3	2	0.11
(1,425)	1:89:A:VAL:HG11	1:183:A:MET:HE1	6	0.11
(1,425)	1:89:A:VAL:HG11	1:183:A:MET:HE2	6	0.11
(1,425)	1:89:A:VAL:HG11	1:183:A:MET:HE3	6	0.11
(1,425)	1:89:A:VAL:HG12	1:183:A:MET:HE1	6	0.11
(1,425)	1:89:A:VAL:HG12	1:183:A:MET:HE2	6	0.11
(1,425)	1:89:A:VAL:HG12	1:183:A:MET:HE3	6	0.11
(1,425)	1:89:A:VAL:HG13	1:183:A:MET:HE1	6	0.11
(1,425)	1:89:A:VAL:HG13	1:183:A:MET:HE2	6	0.11
(1,425)	1:89:A:VAL:HG13	1:183:A:MET:HE3	6	0.11
(1,397)	1:109:C:LEU:HG	1:111:C:ILE:HD11	13	0.11
(1,397)	1:109:C:LEU:HG	1:111:C:ILE:HD12	13	0.11
(1,397)	1:109:C:LEU:HG	1:111:C:ILE:HD13	13	0.11
(1,397)	1:109:C:LEU:HG	1:111:C:ILE:HD11	14	0.11
(1,397)	1:109:C:LEU:HG	1:111:C:ILE:HD12	14	0.11
(1,397)	1:109:C:LEU:HG	1:111:C:ILE:HD13	14	0.11
(1,397)	1:109:C:LEU:HG	1:111:C:ILE:HD11	20	0.11
(1,397)	1:109:C:LEU:HG	1:111:C:ILE:HD12	20	0.11
(1,397)	1:109:C:LEU:HG	1:111:C:ILE:HD13	20	0.11
(1,396)	1:109:B:LEU:HG	1:111:B:ILE:HD11	11	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,396)	1:109:B:LEU:HG	1:111:B:ILE:HD12	11	0.11
(1,396)	1:109:B:LEU:HG	1:111:B:ILE:HD13	11	0.11
(1,373)	1:96:C:ILE:HD11	1:102:C:VAL:HB	13	0.11
(1,373)	1:96:C:ILE:HD12	1:102:C:VAL:HB	13	0.11
(1,373)	1:96:C:ILE:HD13	1:102:C:VAL:HB	13	0.11
(1,372)	1:96:B:ILE:HD11	1:102:B:VAL:HB	13	0.11
(1,372)	1:96:B:ILE:HD12	1:102:B:VAL:HB	13	0.11
(1,372)	1:96:B:ILE:HD13	1:102:B:VAL:HB	13	0.11
(1,366)	1:126:C:ILE:HG21	1:131:C:ILE:HD11	7	0.11
(1,366)	1:126:C:ILE:HG21	1:131:C:ILE:HD12	7	0.11
(1,366)	1:126:C:ILE:HG21	1:131:C:ILE:HD13	7	0.11
(1,366)	1:126:C:ILE:HG22	1:131:C:ILE:HD11	7	0.11
(1,366)	1:126:C:ILE:HG22	1:131:C:ILE:HD12	7	0.11
(1,366)	1:126:C:ILE:HG22	1:131:C:ILE:HD13	7	0.11
(1,366)	1:126:C:ILE:HG23	1:131:C:ILE:HD11	7	0.11
(1,366)	1:126:C:ILE:HG23	1:131:C:ILE:HD12	7	0.11
(1,366)	1:126:C:ILE:HG23	1:131:C:ILE:HD13	7	0.11
(1,363)	1:131:A:ILE:HD11	1:183:C:MET:HG2	13	0.11
(1,363)	1:131:A:ILE:HD11	1:183:C:MET:HG3	13	0.11
(1,363)	1:131:A:ILE:HD12	1:183:C:MET:HG2	13	0.11
(1,363)	1:131:A:ILE:HD12	1:183:C:MET:HG3	13	0.11
(1,363)	1:131:A:ILE:HD13	1:183:C:MET:HG2	13	0.11
(1,363)	1:131:A:ILE:HD13	1:183:C:MET:HG3	13	0.11
(1,362)	1:183:B:MET:HG2	1:131:C:ILE:HD11	3	0.11
(1,362)	1:183:B:MET:HG2	1:131:C:ILE:HD12	3	0.11
(1,362)	1:183:B:MET:HG2	1:131:C:ILE:HD13	3	0.11
(1,362)	1:183:B:MET:HG3	1:131:C:ILE:HD11	3	0.11
(1,362)	1:183:B:MET:HG3	1:131:C:ILE:HD12	3	0.11
(1,362)	1:183:B:MET:HG3	1:131:C:ILE:HD13	3	0.11
(1,361)	1:183:A:MET:HG2	1:131:B:ILE:HD11	4	0.11
(1,361)	1:183:A:MET:HG2	1:131:B:ILE:HD12	4	0.11
(1,361)	1:183:A:MET:HG2	1:131:B:ILE:HD13	4	0.11
(1,361)	1:183:A:MET:HG3	1:131:B:ILE:HD11	4	0.11
(1,361)	1:183:A:MET:HG3	1:131:B:ILE:HD12	4	0.11
(1,361)	1:183:A:MET:HG3	1:131:B:ILE:HD13	4	0.11
(1,361)	1:183:A:MET:HG2	1:131:B:ILE:HD11	7	0.11
(1,361)	1:183:A:MET:HG2	1:131:B:ILE:HD12	7	0.11
(1,361)	1:183:A:MET:HG2	1:131:B:ILE:HD13	7	0.11
(1,361)	1:183:A:MET:HG3	1:131:B:ILE:HD11	7	0.11
(1,361)	1:183:A:MET:HG3	1:131:B:ILE:HD12	7	0.11
(1,361)	1:183:A:MET:HG3	1:131:B:ILE:HD13	7	0.11
(1,361)	1:183:A:MET:HG2	1:131:B:ILE:HD11	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,361)	1:183:A:MET:HG2	1:131:B:ILE:HD12	9	0.11
(1,361)	1:183:A:MET:HG2	1:131:B:ILE:HD13	9	0.11
(1,361)	1:183:A:MET:HG3	1:131:B:ILE:HD11	9	0.11
(1,361)	1:183:A:MET:HG3	1:131:B:ILE:HD12	9	0.11
(1,361)	1:183:A:MET:HG3	1:131:B:ILE:HD13	9	0.11
(1,361)	1:183:A:MET:HG2	1:131:B:ILE:HD11	12	0.11
(1,361)	1:183:A:MET:HG2	1:131:B:ILE:HD12	12	0.11
(1,361)	1:183:A:MET:HG2	1:131:B:ILE:HD13	12	0.11
(1,361)	1:183:A:MET:HG3	1:131:B:ILE:HD11	12	0.11
(1,361)	1:183:A:MET:HG3	1:131:B:ILE:HD12	12	0.11
(1,361)	1:183:A:MET:HG3	1:131:B:ILE:HD13	12	0.11
(1,361)	1:183:A:MET:HG2	1:131:B:ILE:HD11	17	0.11
(1,361)	1:183:A:MET:HG2	1:131:B:ILE:HD12	17	0.11
(1,361)	1:183:A:MET:HG2	1:131:B:ILE:HD13	17	0.11
(1,361)	1:183:A:MET:HG3	1:131:B:ILE:HD11	17	0.11
(1,361)	1:183:A:MET:HG3	1:131:B:ILE:HD12	17	0.11
(1,361)	1:183:A:MET:HG3	1:131:B:ILE:HD13	17	0.11
(1,361)	1:183:A:MET:HG2	1:131:B:ILE:HD11	19	0.11
(1,361)	1:183:A:MET:HG2	1:131:B:ILE:HD12	19	0.11
(1,361)	1:183:A:MET:HG2	1:131:B:ILE:HD13	19	0.11
(1,361)	1:183:A:MET:HG3	1:131:B:ILE:HD11	19	0.11
(1,361)	1:183:A:MET:HG3	1:131:B:ILE:HD12	19	0.11
(1,361)	1:183:A:MET:HG3	1:131:B:ILE:HD13	19	0.11
(1,351)	1:123:C:ILE:HD11	1:196:C:TYR:HE1	8	0.11
(1,351)	1:123:C:ILE:HD11	1:196:C:TYR:HE2	8	0.11
(1,351)	1:123:C:ILE:HD12	1:196:C:TYR:HE1	8	0.11
(1,351)	1:123:C:ILE:HD12	1:196:C:TYR:HE2	8	0.11
(1,351)	1:123:C:ILE:HD13	1:196:C:TYR:HE1	8	0.11
(1,351)	1:123:C:ILE:HD13	1:196:C:TYR:HE2	8	0.11
(1,351)	1:123:C:ILE:HD11	1:196:C:TYR:HE1	13	0.11
(1,351)	1:123:C:ILE:HD11	1:196:C:TYR:HE2	13	0.11
(1,351)	1:123:C:ILE:HD12	1:196:C:TYR:HE1	13	0.11
(1,351)	1:123:C:ILE:HD12	1:196:C:TYR:HE2	13	0.11
(1,351)	1:123:C:ILE:HD13	1:196:C:TYR:HE1	13	0.11
(1,351)	1:123:C:ILE:HD13	1:196:C:TYR:HE2	13	0.11
(1,351)	1:123:C:ILE:HD11	1:196:C:TYR:HE1	14	0.11
(1,351)	1:123:C:ILE:HD11	1:196:C:TYR:HE2	14	0.11
(1,351)	1:123:C:ILE:HD12	1:196:C:TYR:HE1	14	0.11
(1,351)	1:123:C:ILE:HD12	1:196:C:TYR:HE2	14	0.11
(1,351)	1:123:C:ILE:HD13	1:196:C:TYR:HE1	14	0.11
(1,351)	1:123:C:ILE:HD13	1:196:C:TYR:HE2	14	0.11
(1,350)	1:123:B:ILE:HD11	1:196:B:TYR:HE1	8	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,350)	1:123:B:ILE:HD11	1:196:B:TYR:HE2	8	0.11
(1,350)	1:123:B:ILE:HD12	1:196:B:TYR:HE1	8	0.11
(1,350)	1:123:B:ILE:HD12	1:196:B:TYR:HE2	8	0.11
(1,350)	1:123:B:ILE:HD13	1:196:B:TYR:HE1	8	0.11
(1,350)	1:123:B:ILE:HD13	1:196:B:TYR:HE2	8	0.11
(1,350)	1:123:B:ILE:HD11	1:196:B:TYR:HE1	14	0.11
(1,350)	1:123:B:ILE:HD11	1:196:B:TYR:HE2	14	0.11
(1,350)	1:123:B:ILE:HD12	1:196:B:TYR:HE1	14	0.11
(1,350)	1:123:B:ILE:HD12	1:196:B:TYR:HE2	14	0.11
(1,350)	1:123:B:ILE:HD13	1:196:B:TYR:HE1	14	0.11
(1,350)	1:123:B:ILE:HD13	1:196:B:TYR:HE2	14	0.11
(1,350)	1:123:B:ILE:HD11	1:196:B:TYR:HE1	19	0.11
(1,350)	1:123:B:ILE:HD11	1:196:B:TYR:HE2	19	0.11
(1,350)	1:123:B:ILE:HD12	1:196:B:TYR:HE1	19	0.11
(1,350)	1:123:B:ILE:HD12	1:196:B:TYR:HE2	19	0.11
(1,350)	1:123:B:ILE:HD13	1:196:B:TYR:HE1	19	0.11
(1,350)	1:123:B:ILE:HD13	1:196:B:TYR:HE2	19	0.11
(1,280)	1:123:A:ILE:HD11	1:189:A:CYS:HB2	1	0.11
(1,280)	1:123:A:ILE:HD11	1:189:A:CYS:HB3	1	0.11
(1,280)	1:123:A:ILE:HD12	1:189:A:CYS:HB2	1	0.11
(1,280)	1:123:A:ILE:HD12	1:189:A:CYS:HB3	1	0.11
(1,280)	1:123:A:ILE:HD13	1:189:A:CYS:HB2	1	0.11
(1,280)	1:123:A:ILE:HD13	1:189:A:CYS:HB3	1	0.11
(1,280)	1:123:A:ILE:HD11	1:189:A:CYS:HB2	6	0.11
(1,280)	1:123:A:ILE:HD11	1:189:A:CYS:HB3	6	0.11
(1,280)	1:123:A:ILE:HD12	1:189:A:CYS:HB2	6	0.11
(1,280)	1:123:A:ILE:HD12	1:189:A:CYS:HB3	6	0.11
(1,280)	1:123:A:ILE:HD13	1:189:A:CYS:HB2	6	0.11
(1,280)	1:123:A:ILE:HD13	1:189:A:CYS:HB3	6	0.11
(1,280)	1:123:A:ILE:HD11	1:189:A:CYS:HB2	12	0.11
(1,280)	1:123:A:ILE:HD11	1:189:A:CYS:HB3	12	0.11
(1,280)	1:123:A:ILE:HD12	1:189:A:CYS:HB2	12	0.11
(1,280)	1:123:A:ILE:HD12	1:189:A:CYS:HB3	12	0.11
(1,280)	1:123:A:ILE:HD13	1:189:A:CYS:HB2	12	0.11
(1,280)	1:123:A:ILE:HD13	1:189:A:CYS:HB3	12	0.11
(1,257)	1:111:C:ILE:H	1:124:C:MET:HE1	3	0.11
(1,257)	1:111:C:ILE:H	1:124:C:MET:HE2	3	0.11
(1,257)	1:111:C:ILE:H	1:124:C:MET:HE3	3	0.11
(1,256)	1:111:B:ILE:H	1:124:B:MET:HE1	3	0.11
(1,256)	1:111:B:ILE:H	1:124:B:MET:HE2	3	0.11
(1,256)	1:111:B:ILE:H	1:124:B:MET:HE3	3	0.11
(1,256)	1:111:B:ILE:H	1:124:B:MET:HE1	20	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,256)	1:111:B:ILE:H	1:124:B:MET:HE2	20	0.11
(1,256)	1:111:B:ILE:H	1:124:B:MET:HE3	20	0.11
(1,255)	1:111:A:ILE:H	1:124:A:MET:HE1	3	0.11
(1,255)	1:111:A:ILE:H	1:124:A:MET:HE2	3	0.11
(1,255)	1:111:A:ILE:H	1:124:A:MET:HE3	3	0.11
(1,239)	1:102:A:VAL:HG21	1:137:A:LEU:HD21	20	0.11
(1,239)	1:102:A:VAL:HG21	1:137:A:LEU:HD22	20	0.11
(1,239)	1:102:A:VAL:HG21	1:137:A:LEU:HD23	20	0.11
(1,239)	1:102:A:VAL:HG22	1:137:A:LEU:HD21	20	0.11
(1,239)	1:102:A:VAL:HG22	1:137:A:LEU:HD22	20	0.11
(1,239)	1:102:A:VAL:HG22	1:137:A:LEU:HD23	20	0.11
(1,239)	1:102:A:VAL:HG23	1:137:A:LEU:HD21	20	0.11
(1,239)	1:102:A:VAL:HG23	1:137:A:LEU:HD22	20	0.11
(1,239)	1:102:A:VAL:HG23	1:137:A:LEU:HD23	20	0.11
(1,216)	1:96:A:ILE:HG21	1:102:A:VAL:HG11	18	0.11
(1,216)	1:96:A:ILE:HG21	1:102:A:VAL:HG12	18	0.11
(1,216)	1:96:A:ILE:HG21	1:102:A:VAL:HG13	18	0.11
(1,216)	1:96:A:ILE:HG22	1:102:A:VAL:HG11	18	0.11
(1,216)	1:96:A:ILE:HG22	1:102:A:VAL:HG12	18	0.11
(1,216)	1:96:A:ILE:HG22	1:102:A:VAL:HG13	18	0.11
(1,216)	1:96:A:ILE:HG23	1:102:A:VAL:HG11	18	0.11
(1,216)	1:96:A:ILE:HG23	1:102:A:VAL:HG12	18	0.11
(1,216)	1:96:A:ILE:HG23	1:102:A:VAL:HG13	18	0.11
(1,182)	1:137:A:LEU:HD11	1:141:A:VAL:HG11	16	0.11
(1,182)	1:137:A:LEU:HD11	1:141:A:VAL:HG12	16	0.11
(1,182)	1:137:A:LEU:HD11	1:141:A:VAL:HG13	16	0.11
(1,182)	1:137:A:LEU:HD12	1:141:A:VAL:HG11	16	0.11
(1,182)	1:137:A:LEU:HD12	1:141:A:VAL:HG12	16	0.11
(1,182)	1:137:A:LEU:HD12	1:141:A:VAL:HG13	16	0.11
(1,182)	1:137:A:LEU:HD13	1:141:A:VAL:HG11	16	0.11
(1,182)	1:137:A:LEU:HD13	1:141:A:VAL:HG12	16	0.11
(1,182)	1:137:A:LEU:HD13	1:141:A:VAL:HG13	16	0.11
(1,157)	1:101:A:LEU:HD21	1:95:B:SER:HB2	7	0.11
(1,157)	1:101:A:LEU:HD21	1:95:B:SER:HB3	7	0.11
(1,157)	1:101:A:LEU:HD22	1:95:B:SER:HB2	7	0.11
(1,157)	1:101:A:LEU:HD22	1:95:B:SER:HB3	7	0.11
(1,157)	1:101:A:LEU:HD23	1:95:B:SER:HB2	7	0.11
(1,157)	1:101:A:LEU:HD23	1:95:B:SER:HB3	7	0.11
(1,156)	1:187:C:THR:HG21	1:188:C:LEU:HD21	2	0.11
(1,156)	1:187:C:THR:HG21	1:188:C:LEU:HD22	2	0.11
(1,156)	1:187:C:THR:HG21	1:188:C:LEU:HD23	2	0.11
(1,156)	1:187:C:THR:HG22	1:188:C:LEU:HD21	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,156)	1:187:C:THR:HG22	1:188:C:LEU:HD22	2	0.11
(1,156)	1:187:C:THR:HG22	1:188:C:LEU:HD23	2	0.11
(1,156)	1:187:C:THR:HG23	1:188:C:LEU:HD21	2	0.11
(1,156)	1:187:C:THR:HG23	1:188:C:LEU:HD22	2	0.11
(1,156)	1:187:C:THR:HG23	1:188:C:LEU:HD23	2	0.11
(1,154)	1:187:A:THR:HG21	1:188:A:LEU:HD21	4	0.11
(1,154)	1:187:A:THR:HG21	1:188:A:LEU:HD22	4	0.11
(1,154)	1:187:A:THR:HG21	1:188:A:LEU:HD23	4	0.11
(1,154)	1:187:A:THR:HG22	1:188:A:LEU:HD21	4	0.11
(1,154)	1:187:A:THR:HG22	1:188:A:LEU:HD22	4	0.11
(1,154)	1:187:A:THR:HG22	1:188:A:LEU:HD23	4	0.11
(1,154)	1:187:A:THR:HG23	1:188:A:LEU:HD21	4	0.11
(1,154)	1:187:A:THR:HG23	1:188:A:LEU:HD22	4	0.11
(1,154)	1:187:A:THR:HG23	1:188:A:LEU:HD23	4	0.11
(1,154)	1:187:A:THR:HG21	1:188:A:LEU:HD21	12	0.11
(1,154)	1:187:A:THR:HG21	1:188:A:LEU:HD22	12	0.11
(1,154)	1:187:A:THR:HG21	1:188:A:LEU:HD23	12	0.11
(1,154)	1:187:A:THR:HG22	1:188:A:LEU:HD21	12	0.11
(1,154)	1:187:A:THR:HG22	1:188:A:LEU:HD22	12	0.11
(1,154)	1:187:A:THR:HG22	1:188:A:LEU:HD23	12	0.11
(1,154)	1:187:A:THR:HG23	1:188:A:LEU:HD21	12	0.11
(1,154)	1:187:A:THR:HG23	1:188:A:LEU:HD22	12	0.11
(1,154)	1:187:A:THR:HG23	1:188:A:LEU:HD23	12	0.11
(1,134)	1:110:A:LEU:HD11	1:111:A:ILE:HD11	13	0.11
(1,134)	1:110:A:LEU:HD11	1:111:A:ILE:HD12	13	0.11
(1,134)	1:110:A:LEU:HD11	1:111:A:ILE:HD13	13	0.11
(1,134)	1:110:A:LEU:HD12	1:111:A:ILE:HD11	13	0.11
(1,134)	1:110:A:LEU:HD12	1:111:A:ILE:HD12	13	0.11
(1,134)	1:110:A:LEU:HD12	1:111:A:ILE:HD13	13	0.11
(1,134)	1:110:A:LEU:HD13	1:111:A:ILE:HD11	13	0.11
(1,134)	1:110:A:LEU:HD13	1:111:A:ILE:HD12	13	0.11
(1,134)	1:110:A:LEU:HD13	1:111:A:ILE:HD13	13	0.11
(1,134)	1:110:A:LEU:HD11	1:111:A:ILE:HD11	18	0.11
(1,134)	1:110:A:LEU:HD11	1:111:A:ILE:HD12	18	0.11
(1,134)	1:110:A:LEU:HD11	1:111:A:ILE:HD13	18	0.11
(1,134)	1:110:A:LEU:HD12	1:111:A:ILE:HD11	18	0.11
(1,134)	1:110:A:LEU:HD12	1:111:A:ILE:HD12	18	0.11
(1,134)	1:110:A:LEU:HD12	1:111:A:ILE:HD13	18	0.11
(1,134)	1:110:A:LEU:HD13	1:111:A:ILE:HD11	18	0.11
(1,134)	1:110:A:LEU:HD13	1:111:A:ILE:HD12	18	0.11
(1,134)	1:110:A:LEU:HD13	1:111:A:ILE:HD13	18	0.11
(1,63)	1:110:A:LEU:HD11	1:123:A:ILE:HD11	8	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,63)	1:110:A:LEU:HD11	1:123:A:ILE:HD12	8	0.11
(1,63)	1:110:A:LEU:HD11	1:123:A:ILE:HD13	8	0.11
(1,63)	1:110:A:LEU:HD12	1:123:A:ILE:HD11	8	0.11
(1,63)	1:110:A:LEU:HD12	1:123:A:ILE:HD12	8	0.11
(1,63)	1:110:A:LEU:HD12	1:123:A:ILE:HD13	8	0.11
(1,63)	1:110:A:LEU:HD13	1:123:A:ILE:HD11	8	0.11
(1,63)	1:110:A:LEU:HD13	1:123:A:ILE:HD12	8	0.11
(1,63)	1:110:A:LEU:HD13	1:123:A:ILE:HD13	8	0.11
(1,56)	1:156:A:VAL:HG11	1:157:A:PRO:HD3	12	0.11
(1,56)	1:156:A:VAL:HG12	1:157:A:PRO:HD3	12	0.11
(1,56)	1:156:A:VAL:HG13	1:157:A:PRO:HD3	12	0.11
(1,56)	1:156:A:VAL:HG11	1:157:A:PRO:HD3	13	0.11
(1,56)	1:156:A:VAL:HG12	1:157:A:PRO:HD3	13	0.11
(1,56)	1:156:A:VAL:HG13	1:157:A:PRO:HD3	13	0.11
(1,56)	1:156:A:VAL:HG11	1:157:A:PRO:HD3	18	0.11
(1,56)	1:156:A:VAL:HG12	1:157:A:PRO:HD3	18	0.11
(1,56)	1:156:A:VAL:HG13	1:157:A:PRO:HD3	18	0.11
(1,55)	1:156:A:VAL:HG11	1:157:A:PRO:HD2	1	0.11
(1,55)	1:156:A:VAL:HG12	1:157:A:PRO:HD2	1	0.11
(1,55)	1:156:A:VAL:HG13	1:157:A:PRO:HD2	1	0.11
(1,55)	1:156:A:VAL:HG11	1:157:A:PRO:HD2	9	0.11
(1,55)	1:156:A:VAL:HG12	1:157:A:PRO:HD2	9	0.11
(1,55)	1:156:A:VAL:HG13	1:157:A:PRO:HD2	9	0.11
(1,55)	1:156:A:VAL:HG11	1:157:A:PRO:HD2	10	0.11
(1,55)	1:156:A:VAL:HG12	1:157:A:PRO:HD2	10	0.11
(1,55)	1:156:A:VAL:HG13	1:157:A:PRO:HD2	10	0.11
(1,55)	1:156:A:VAL:HG11	1:157:A:PRO:HD2	17	0.11
(1,55)	1:156:A:VAL:HG12	1:157:A:PRO:HD2	17	0.11
(1,55)	1:156:A:VAL:HG13	1:157:A:PRO:HD2	17	0.11
(1,55)	1:156:A:VAL:HG11	1:157:A:PRO:HD2	18	0.11
(1,55)	1:156:A:VAL:HG12	1:157:A:PRO:HD2	18	0.11
(1,55)	1:156:A:VAL:HG13	1:157:A:PRO:HD2	18	0.11
(1,51)	1:185:A:VAL:HB	1:188:A:LEU:HD11	8	0.11
(1,51)	1:185:A:VAL:HB	1:188:A:LEU:HD12	8	0.11
(1,51)	1:185:A:VAL:HB	1:188:A:LEU:HD13	8	0.11
(1,51)	1:185:A:VAL:HB	1:188:A:LEU:HD11	17	0.11
(1,51)	1:185:A:VAL:HB	1:188:A:LEU:HD12	17	0.11
(1,51)	1:185:A:VAL:HB	1:188:A:LEU:HD13	17	0.11
(1,36)	1:102:A:VAL:HG21	1:112:A:ALA:H	15	0.11
(1,36)	1:102:A:VAL:HG22	1:112:A:ALA:H	15	0.11
(1,36)	1:102:A:VAL:HG23	1:112:A:ALA:H	15	0.11
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD11	4	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD12	4	0.1
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD13	4	0.1
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD21	4	0.1
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD22	4	0.1
(1,2358)	1:187:C:THR:HA	1:188:C:LEU:HD23	4	0.1
(1,2300)	1:156:C:VAL:HG11	1:157:C:PRO:HB2	7	0.1
(1,2300)	1:156:C:VAL:HG11	1:157:C:PRO:HB3	7	0.1
(1,2300)	1:156:C:VAL:HG12	1:157:C:PRO:HB2	7	0.1
(1,2300)	1:156:C:VAL:HG12	1:157:C:PRO:HB3	7	0.1
(1,2300)	1:156:C:VAL:HG13	1:157:C:PRO:HB2	7	0.1
(1,2300)	1:156:C:VAL:HG13	1:157:C:PRO:HB3	7	0.1
(1,2300)	1:156:C:VAL:HG21	1:157:C:PRO:HB2	7	0.1
(1,2300)	1:156:C:VAL:HG21	1:157:C:PRO:HB3	7	0.1
(1,2300)	1:156:C:VAL:HG22	1:157:C:PRO:HB2	7	0.1
(1,2300)	1:156:C:VAL:HG22	1:157:C:PRO:HB3	7	0.1
(1,2300)	1:156:C:VAL:HG23	1:157:C:PRO:HB2	7	0.1
(1,2300)	1:156:C:VAL:HG23	1:157:C:PRO:HB3	7	0.1
(1,2295)	1:155:C:ALA:HB1	1:157:C:PRO:HD2	1	0.1
(1,2295)	1:155:C:ALA:HB1	1:157:C:PRO:HD3	1	0.1
(1,2295)	1:155:C:ALA:HB2	1:157:C:PRO:HD2	1	0.1
(1,2295)	1:155:C:ALA:HB2	1:157:C:PRO:HD3	1	0.1
(1,2295)	1:155:C:ALA:HB3	1:157:C:PRO:HD2	1	0.1
(1,2295)	1:155:C:ALA:HB3	1:157:C:PRO:HD3	1	0.1
(1,2292)	1:154:C:PRO:HB2	1:167:C:ARG:H	10	0.1
(1,2292)	1:154:C:PRO:HB3	1:167:C:ARG:H	10	0.1
(1,2280)	1:143:C:ASN:HB2	1:144:C:PHE:HA	4	0.1
(1,2280)	1:143:C:ASN:HB3	1:144:C:PHE:HA	4	0.1
(1,2163)	1:89:C:VAL:HG11	1:183:C:MET:HE1	18	0.1
(1,2163)	1:89:C:VAL:HG11	1:183:C:MET:HE2	18	0.1
(1,2163)	1:89:C:VAL:HG11	1:183:C:MET:HE3	18	0.1
(1,2163)	1:89:C:VAL:HG12	1:183:C:MET:HE1	18	0.1
(1,2163)	1:89:C:VAL:HG12	1:183:C:MET:HE2	18	0.1
(1,2163)	1:89:C:VAL:HG12	1:183:C:MET:HE3	18	0.1
(1,2163)	1:89:C:VAL:HG13	1:183:C:MET:HE1	18	0.1
(1,2163)	1:89:C:VAL:HG13	1:183:C:MET:HE2	18	0.1
(1,2163)	1:89:C:VAL:HG13	1:183:C:MET:HE3	18	0.1
(1,2163)	1:89:C:VAL:HG21	1:183:C:MET:HE1	18	0.1
(1,2163)	1:89:C:VAL:HG21	1:183:C:MET:HE2	18	0.1
(1,2163)	1:89:C:VAL:HG21	1:183:C:MET:HE3	18	0.1
(1,2163)	1:89:C:VAL:HG22	1:183:C:MET:HE1	18	0.1
(1,2163)	1:89:C:VAL:HG22	1:183:C:MET:HE2	18	0.1
(1,2163)	1:89:C:VAL:HG22	1:183:C:MET:HE3	18	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2163)	1:89:C:VAL:HG23	1:183:C:MET:HE1	18	0.1
(1,2163)	1:89:C:VAL:HG23	1:183:C:MET:HE2	18	0.1
(1,2163)	1:89:C:VAL:HG23	1:183:C:MET:HE3	18	0.1
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD11	10	0.1
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD12	10	0.1
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD13	10	0.1
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD21	10	0.1
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD22	10	0.1
(1,2132)	1:187:B:THR:HA	1:188:B:LEU:HD23	10	0.1
(1,2074)	1:156:B:VAL:HG11	1:157:B:PRO:HB2	7	0.1
(1,2074)	1:156:B:VAL:HG11	1:157:B:PRO:HB3	7	0.1
(1,2074)	1:156:B:VAL:HG12	1:157:B:PRO:HB2	7	0.1
(1,2074)	1:156:B:VAL:HG12	1:157:B:PRO:HB3	7	0.1
(1,2074)	1:156:B:VAL:HG13	1:157:B:PRO:HB2	7	0.1
(1,2074)	1:156:B:VAL:HG13	1:157:B:PRO:HB3	7	0.1
(1,2074)	1:156:B:VAL:HG21	1:157:B:PRO:HB2	7	0.1
(1,2074)	1:156:B:VAL:HG21	1:157:B:PRO:HB3	7	0.1
(1,2074)	1:156:B:VAL:HG22	1:157:B:PRO:HB2	7	0.1
(1,2074)	1:156:B:VAL:HG22	1:157:B:PRO:HB3	7	0.1
(1,2074)	1:156:B:VAL:HG23	1:157:B:PRO:HB2	7	0.1
(1,2074)	1:156:B:VAL:HG23	1:157:B:PRO:HB3	7	0.1
(1,1935)	1:89:B:VAL:HG11	1:183:B:MET:HE1	18	0.1
(1,1935)	1:89:B:VAL:HG11	1:183:B:MET:HE2	18	0.1
(1,1935)	1:89:B:VAL:HG11	1:183:B:MET:HE3	18	0.1
(1,1935)	1:89:B:VAL:HG12	1:183:B:MET:HE1	18	0.1
(1,1935)	1:89:B:VAL:HG12	1:183:B:MET:HE2	18	0.1
(1,1935)	1:89:B:VAL:HG12	1:183:B:MET:HE3	18	0.1
(1,1935)	1:89:B:VAL:HG13	1:183:B:MET:HE1	18	0.1
(1,1935)	1:89:B:VAL:HG13	1:183:B:MET:HE2	18	0.1
(1,1935)	1:89:B:VAL:HG13	1:183:B:MET:HE3	18	0.1
(1,1935)	1:89:B:VAL:HG21	1:183:B:MET:HE1	18	0.1
(1,1935)	1:89:B:VAL:HG21	1:183:B:MET:HE2	18	0.1
(1,1935)	1:89:B:VAL:HG21	1:183:B:MET:HE3	18	0.1
(1,1935)	1:89:B:VAL:HG22	1:183:B:MET:HE1	18	0.1
(1,1935)	1:89:B:VAL:HG22	1:183:B:MET:HE2	18	0.1
(1,1935)	1:89:B:VAL:HG22	1:183:B:MET:HE3	18	0.1
(1,1935)	1:89:B:VAL:HG23	1:183:B:MET:HE1	18	0.1
(1,1935)	1:89:B:VAL:HG23	1:183:B:MET:HE2	18	0.1
(1,1935)	1:89:B:VAL:HG23	1:183:B:MET:HE3	18	0.1
(1,1903)	1:172:A:ALA:HB1	1:173:A:PRO:HD2	20	0.1
(1,1903)	1:172:A:ALA:HB1	1:173:A:PRO:HD3	20	0.1
(1,1903)	1:172:A:ALA:HB2	1:173:A:PRO:HD2	20	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1903)	1:172:A:ALA:HB2	1:173:A:PRO:HD3	20	0.1
(1,1903)	1:172:A:ALA:HB3	1:173:A:PRO:HD2	20	0.1
(1,1903)	1:172:A:ALA:HB3	1:173:A:PRO:HD3	20	0.1
(1,1902)	1:172:A:ALA:HA	1:178:A:PRO:HD2	12	0.1
(1,1902)	1:172:A:ALA:HA	1:178:A:PRO:HD3	12	0.1
(1,1884)	1:154:A:PRO:HB2	1:167:A:ARG:H	10	0.1
(1,1884)	1:154:A:PRO:HB3	1:167:A:ARG:H	10	0.1
(1,1848)	1:124:A:MET:HB2	1:197:A:ILE:HD11	2	0.1
(1,1848)	1:124:A:MET:HB2	1:197:A:ILE:HD12	2	0.1
(1,1848)	1:124:A:MET:HB2	1:197:A:ILE:HD13	2	0.1
(1,1848)	1:124:A:MET:HB3	1:197:A:ILE:HD11	2	0.1
(1,1848)	1:124:A:MET:HB3	1:197:A:ILE:HD12	2	0.1
(1,1848)	1:124:A:MET:HB3	1:197:A:ILE:HD13	2	0.1
(1,1817)	1:95:A:SER:HB2	1:101:A:LEU:H	20	0.1
(1,1817)	1:95:A:SER:HB3	1:101:A:LEU:H	20	0.1
(1,1787)	1:96:A:ILE:HG21	1:101:A:LEU:H	1	0.1
(1,1787)	1:96:A:ILE:HG22	1:101:A:LEU:H	1	0.1
(1,1787)	1:96:A:ILE:HG23	1:101:A:LEU:H	1	0.1
(1,1687)	1:90:B:THR:H	1:91:B:THR:HB	11	0.1
(1,1621)	1:129:B:GLU:H	1:131:B:ILE:H	19	0.1
(1,1574)	1:119:A:THR:H	1:192:A:VAL:HG11	4	0.1
(1,1574)	1:119:A:THR:H	1:192:A:VAL:HG12	4	0.1
(1,1574)	1:119:A:THR:H	1:192:A:VAL:HG13	4	0.1
(1,1564)	1:145:C:GLN:HA	1:151:C:GLN:H	7	0.1
(1,1564)	1:145:C:GLN:HA	1:151:C:GLN:H	18	0.1
(1,1564)	1:145:C:GLN:HA	1:151:C:GLN:H	20	0.1
(1,1563)	1:145:B:GLN:HA	1:151:B:GLN:H	7	0.1
(1,1552)	1:156:A:VAL:HB	1:167:A:ARG:H	8	0.1
(1,1551)	1:167:C:ARG:H	1:171:C:SER:HA	3	0.1
(1,1541)	1:136:C:ALA:HB1	1:140:C:LYS:H	17	0.1
(1,1541)	1:136:C:ALA:HB2	1:140:C:LYS:H	17	0.1
(1,1541)	1:136:C:ALA:HB3	1:140:C:LYS:H	17	0.1
(1,1535)	1:122:C:TYR:H	1:189:C:CYS:HB2	2	0.1
(1,1535)	1:122:C:TYR:H	1:189:C:CYS:HB3	2	0.1
(1,1535)	1:122:C:TYR:H	1:189:C:CYS:HB2	12	0.1
(1,1535)	1:122:C:TYR:H	1:189:C:CYS:HB3	12	0.1
(1,1526)	1:179:A:ALA:H	1:181:A:LEU:HD11	4	0.1
(1,1526)	1:179:A:ALA:H	1:181:A:LEU:HD12	4	0.1
(1,1526)	1:179:A:ALA:H	1:181:A:LEU:HD13	4	0.1
(1,1511)	1:137:A:LEU:H	1:137:A:LEU:HG	13	0.1
(1,1511)	1:137:A:LEU:H	1:137:A:LEU:HG	18	0.1
(1,1507)	1:92:A:ALA:H	1:93:C:THR:HG21	20	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1507)	1:92:A:ALA:H	1:93:C:THR:HG22	20	0.1
(1,1507)	1:92:A:ALA:H	1:93:C:THR:HG23	20	0.1
(1,1505)	1:93:A:THR:HG21	1:92:B:ALA:H	18	0.1
(1,1505)	1:93:A:THR:HG22	1:92:B:ALA:H	18	0.1
(1,1505)	1:93:A:THR:HG23	1:92:B:ALA:H	18	0.1
(1,1491)	1:131:C:ILE:HA	1:133:C:SER:H	6	0.1
(1,1490)	1:131:B:ILE:HA	1:133:B:SER:H	17	0.1
(1,1471)	1:181:A:LEU:H	1:181:A:LEU:HD11	20	0.1
(1,1471)	1:181:A:LEU:H	1:181:A:LEU:HD12	20	0.1
(1,1471)	1:181:A:LEU:H	1:181:A:LEU:HD13	20	0.1
(1,1439)	1:155:A:ALA:HB1	1:156:A:VAL:H	14	0.1
(1,1439)	1:155:A:ALA:HB2	1:156:A:VAL:H	14	0.1
(1,1439)	1:155:A:ALA:HB3	1:156:A:VAL:H	14	0.1
(1,1432)	1:111:C:ILE:H	1:123:C:ILE:HG21	6	0.1
(1,1432)	1:111:C:ILE:H	1:123:C:ILE:HG22	6	0.1
(1,1432)	1:111:C:ILE:H	1:123:C:ILE:HG23	6	0.1
(1,1432)	1:111:C:ILE:H	1:123:C:ILE:HG21	8	0.1
(1,1432)	1:111:C:ILE:H	1:123:C:ILE:HG22	8	0.1
(1,1432)	1:111:C:ILE:H	1:123:C:ILE:HG23	8	0.1
(1,1432)	1:111:C:ILE:H	1:123:C:ILE:HG21	9	0.1
(1,1432)	1:111:C:ILE:H	1:123:C:ILE:HG22	9	0.1
(1,1432)	1:111:C:ILE:H	1:123:C:ILE:HG23	9	0.1
(1,1431)	1:111:B:ILE:H	1:123:B:ILE:HG21	6	0.1
(1,1431)	1:111:B:ILE:H	1:123:B:ILE:HG22	6	0.1
(1,1431)	1:111:B:ILE:H	1:123:B:ILE:HG23	6	0.1
(1,1431)	1:111:B:ILE:H	1:123:B:ILE:HG21	9	0.1
(1,1431)	1:111:B:ILE:H	1:123:B:ILE:HG22	9	0.1
(1,1431)	1:111:B:ILE:H	1:123:B:ILE:HG23	9	0.1
(1,1431)	1:111:B:ILE:H	1:123:B:ILE:HG21	14	0.1
(1,1431)	1:111:B:ILE:H	1:123:B:ILE:HG22	14	0.1
(1,1431)	1:111:B:ILE:H	1:123:B:ILE:HG23	14	0.1
(1,1387)	1:141:A:VAL:HG21	1:142:A:HIS:H	14	0.1
(1,1387)	1:141:A:VAL:HG22	1:142:A:HIS:H	14	0.1
(1,1387)	1:141:A:VAL:HG23	1:142:A:HIS:H	14	0.1
(1,1387)	1:141:A:VAL:HG21	1:142:A:HIS:H	17	0.1
(1,1387)	1:141:A:VAL:HG22	1:142:A:HIS:H	17	0.1
(1,1387)	1:141:A:VAL:HG23	1:142:A:HIS:H	17	0.1
(1,1202)	1:196:B:TYR:H	1:196:B:TYR:HE1	13	0.1
(1,1202)	1:196:B:TYR:H	1:196:B:TYR:HE2	13	0.1
(1,1202)	1:196:B:TYR:H	1:196:B:TYR:HE1	20	0.1
(1,1202)	1:196:B:TYR:H	1:196:B:TYR:HE2	20	0.1
(1,1201)	1:196:A:TYR:H	1:196:A:TYR:HE1	9	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1201)	1:196:A:TYR:H	1:196:A:TYR:HE2	9	0.1
(1,1161)	1:94:A:PHE:H	1:101:A:LEU:HD11	9	0.1
(1,1161)	1:94:A:PHE:H	1:101:A:LEU:HD12	9	0.1
(1,1161)	1:94:A:PHE:H	1:101:A:LEU:HD13	9	0.1
(1,1161)	1:94:A:PHE:H	1:101:A:LEU:HD11	14	0.1
(1,1161)	1:94:A:PHE:H	1:101:A:LEU:HD12	14	0.1
(1,1161)	1:94:A:PHE:H	1:101:A:LEU:HD13	14	0.1
(1,1155)	1:167:A:ARG:HA	1:168:A:ASP:H	14	0.1
(1,1127)	1:153:C:LYS:H	1:154:C:PRO:HD2	14	0.1
(1,1126)	1:153:B:LYS:H	1:154:B:PRO:HD2	14	0.1
(1,1125)	1:153:A:LYS:H	1:154:A:PRO:HD2	7	0.1
(1,1125)	1:153:A:LYS:H	1:154:A:PRO:HD2	14	0.1
(1,1124)	1:87:C:HIS:H	1:88:C:LEU:H	8	0.1
(1,1079)	1:173:C:PRO:HB3	1:174:C:SER:H	17	0.1
(1,1077)	1:173:A:PRO:HB3	1:174:A:SER:H	13	0.1
(1,1077)	1:173:A:PRO:HB3	1:174:A:SER:H	17	0.1
(1,1071)	1:139:A:ARG:H	1:141:A:VAL:HB	8	0.1
(1,1040)	1:137:A:LEU:HD11	1:140:A:LYS:H	2	0.1
(1,1040)	1:137:A:LEU:HD12	1:140:A:LYS:H	2	0.1
(1,1040)	1:137:A:LEU:HD13	1:140:A:LYS:H	2	0.1
(1,978)	1:196:C:TYR:H	1:197:C:ILE:HG21	10	0.1
(1,978)	1:196:C:TYR:H	1:197:C:ILE:HG22	10	0.1
(1,978)	1:196:C:TYR:H	1:197:C:ILE:HG23	10	0.1
(1,977)	1:196:B:TYR:H	1:197:B:ILE:HG21	10	0.1
(1,977)	1:196:B:TYR:H	1:197:B:ILE:HG22	10	0.1
(1,977)	1:196:B:TYR:H	1:197:B:ILE:HG23	10	0.1
(1,976)	1:196:A:TYR:H	1:197:A:ILE:HG21	10	0.1
(1,976)	1:196:A:TYR:H	1:197:A:ILE:HG22	10	0.1
(1,976)	1:196:A:TYR:H	1:197:A:ILE:HG23	10	0.1
(1,976)	1:196:A:TYR:H	1:197:A:ILE:HG21	12	0.1
(1,976)	1:196:A:TYR:H	1:197:A:ILE:HG22	12	0.1
(1,976)	1:196:A:TYR:H	1:197:A:ILE:HG23	12	0.1
(1,976)	1:196:A:TYR:H	1:197:A:ILE:HG21	14	0.1
(1,976)	1:196:A:TYR:H	1:197:A:ILE:HG22	14	0.1
(1,976)	1:196:A:TYR:H	1:197:A:ILE:HG23	14	0.1
(1,976)	1:196:A:TYR:H	1:197:A:ILE:HG21	17	0.1
(1,976)	1:196:A:TYR:H	1:197:A:ILE:HG22	17	0.1
(1,976)	1:196:A:TYR:H	1:197:A:ILE:HG23	17	0.1
(1,965)	1:110:A:LEU:HD11	1:125:A:LYS:HB3	3	0.1
(1,965)	1:110:A:LEU:HD12	1:125:A:LYS:HB3	3	0.1
(1,965)	1:110:A:LEU:HD13	1:125:A:LYS:HB3	3	0.1
(1,943)	1:109:A:LEU:HB2	1:110:A:LEU:HD11	14	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,943)	1:109:A:LEU:HB2	1:110:A:LEU:HD12	14	0.1
(1,943)	1:109:A:LEU:HB2	1:110:A:LEU:HD13	14	0.1
(1,910)	1:140:B:LYS:HD2	1:197:B:ILE:HG21	4	0.1
(1,910)	1:140:B:LYS:HD2	1:197:B:ILE:HG22	4	0.1
(1,910)	1:140:B:LYS:HD2	1:197:B:ILE:HG23	4	0.1
(1,910)	1:140:B:LYS:HD3	1:197:B:ILE:HG21	4	0.1
(1,910)	1:140:B:LYS:HD3	1:197:B:ILE:HG22	4	0.1
(1,910)	1:140:B:LYS:HD3	1:197:B:ILE:HG23	4	0.1
(1,896)	1:165:C:GLU:HB3	1:169:C:ALA:HB1	2	0.1
(1,896)	1:165:C:GLU:HB3	1:169:C:ALA:HB2	2	0.1
(1,896)	1:165:C:GLU:HB3	1:169:C:ALA:HB3	2	0.1
(1,896)	1:165:C:GLU:HB3	1:169:C:ALA:HB1	6	0.1
(1,896)	1:165:C:GLU:HB3	1:169:C:ALA:HB2	6	0.1
(1,896)	1:165:C:GLU:HB3	1:169:C:ALA:HB3	6	0.1
(1,896)	1:165:C:GLU:HB3	1:169:C:ALA:HB1	16	0.1
(1,896)	1:165:C:GLU:HB3	1:169:C:ALA:HB2	16	0.1
(1,896)	1:165:C:GLU:HB3	1:169:C:ALA:HB3	16	0.1
(1,895)	1:165:B:GLU:HB3	1:169:B:ALA:HB1	2	0.1
(1,895)	1:165:B:GLU:HB3	1:169:B:ALA:HB2	2	0.1
(1,895)	1:165:B:GLU:HB3	1:169:B:ALA:HB3	2	0.1
(1,895)	1:165:B:GLU:HB3	1:169:B:ALA:HB1	6	0.1
(1,895)	1:165:B:GLU:HB3	1:169:B:ALA:HB2	6	0.1
(1,895)	1:165:B:GLU:HB3	1:169:B:ALA:HB3	6	0.1
(1,895)	1:165:B:GLU:HB3	1:169:B:ALA:HB1	16	0.1
(1,895)	1:165:B:GLU:HB3	1:169:B:ALA:HB2	16	0.1
(1,895)	1:165:B:GLU:HB3	1:169:B:ALA:HB3	16	0.1
(1,894)	1:165:A:GLU:HB3	1:169:A:ALA:HB1	6	0.1
(1,894)	1:165:A:GLU:HB3	1:169:A:ALA:HB2	6	0.1
(1,894)	1:165:A:GLU:HB3	1:169:A:ALA:HB3	6	0.1
(1,893)	1:165:C:GLU:HB2	1:167:C:ARG:HG2	6	0.1
(1,893)	1:165:C:GLU:HB2	1:167:C:ARG:HG3	6	0.1
(1,892)	1:165:B:GLU:HB2	1:167:B:ARG:HG2	6	0.1
(1,892)	1:165:B:GLU:HB2	1:167:B:ARG:HG3	6	0.1
(1,891)	1:165:A:GLU:HB2	1:167:A:ARG:HG2	2	0.1
(1,891)	1:165:A:GLU:HB2	1:167:A:ARG:HG3	2	0.1
(1,890)	1:152:C:ALA:HA	1:157:C:PRO:HG2	15	0.1
(1,890)	1:152:C:ALA:HA	1:157:C:PRO:HG3	15	0.1
(1,889)	1:152:B:ALA:HA	1:157:B:PRO:HG2	15	0.1
(1,889)	1:152:B:ALA:HA	1:157:B:PRO:HG3	15	0.1
(1,888)	1:152:A:ALA:HA	1:157:A:PRO:HG2	4	0.1
(1,888)	1:152:A:ALA:HA	1:157:A:PRO:HG3	4	0.1
(1,815)	1:176:C:GLY:H	1:177:C:ASP:HB2	1	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,813)	1:176:A:GLY:H	1:177:A:ASP:HB2	18	0.1
(1,792)	1:153:A:LYS:HE2	1:154:A:PRO:HG2	10	0.1
(1,792)	1:153:A:LYS:HE2	1:154:A:PRO:HG3	10	0.1
(1,792)	1:153:A:LYS:HE3	1:154:A:PRO:HG2	10	0.1
(1,792)	1:153:A:LYS:HE3	1:154:A:PRO:HG3	10	0.1
(1,792)	1:153:A:LYS:HE2	1:154:A:PRO:HG2	17	0.1
(1,792)	1:153:A:LYS:HE2	1:154:A:PRO:HG3	17	0.1
(1,792)	1:153:A:LYS:HE3	1:154:A:PRO:HG2	17	0.1
(1,792)	1:153:A:LYS:HE3	1:154:A:PRO:HG3	17	0.1
(1,785)	1:167:C:ARG:HD2	1:169:C:ALA:HB1	10	0.1
(1,785)	1:167:C:ARG:HD2	1:169:C:ALA:HB2	10	0.1
(1,785)	1:167:C:ARG:HD2	1:169:C:ALA:HB3	10	0.1
(1,785)	1:167:C:ARG:HD3	1:169:C:ALA:HB1	10	0.1
(1,785)	1:167:C:ARG:HD3	1:169:C:ALA:HB2	10	0.1
(1,785)	1:167:C:ARG:HD3	1:169:C:ALA:HB3	10	0.1
(1,785)	1:167:C:ARG:HD2	1:169:C:ALA:HB1	12	0.1
(1,785)	1:167:C:ARG:HD2	1:169:C:ALA:HB2	12	0.1
(1,785)	1:167:C:ARG:HD2	1:169:C:ALA:HB3	12	0.1
(1,785)	1:167:C:ARG:HD3	1:169:C:ALA:HB1	12	0.1
(1,785)	1:167:C:ARG:HD3	1:169:C:ALA:HB2	12	0.1
(1,785)	1:167:C:ARG:HD3	1:169:C:ALA:HB3	12	0.1
(1,785)	1:167:C:ARG:HD2	1:169:C:ALA:HB1	17	0.1
(1,785)	1:167:C:ARG:HD2	1:169:C:ALA:HB2	17	0.1
(1,785)	1:167:C:ARG:HD2	1:169:C:ALA:HB3	17	0.1
(1,785)	1:167:C:ARG:HD3	1:169:C:ALA:HB1	17	0.1
(1,785)	1:167:C:ARG:HD3	1:169:C:ALA:HB2	17	0.1
(1,785)	1:167:C:ARG:HD3	1:169:C:ALA:HB3	17	0.1
(1,784)	1:167:B:ARG:HD2	1:169:B:ALA:HB1	10	0.1
(1,784)	1:167:B:ARG:HD2	1:169:B:ALA:HB2	10	0.1
(1,784)	1:167:B:ARG:HD2	1:169:B:ALA:HB3	10	0.1
(1,784)	1:167:B:ARG:HD3	1:169:B:ALA:HB1	10	0.1
(1,784)	1:167:B:ARG:HD3	1:169:B:ALA:HB2	10	0.1
(1,784)	1:167:B:ARG:HD3	1:169:B:ALA:HB3	10	0.1
(1,783)	1:167:A:ARG:HD2	1:169:A:ALA:HB1	5	0.1
(1,783)	1:167:A:ARG:HD2	1:169:A:ALA:HB2	5	0.1
(1,783)	1:167:A:ARG:HD2	1:169:A:ALA:HB3	5	0.1
(1,783)	1:167:A:ARG:HD3	1:169:A:ALA:HB1	5	0.1
(1,783)	1:167:A:ARG:HD3	1:169:A:ALA:HB2	5	0.1
(1,783)	1:167:A:ARG:HD3	1:169:A:ALA:HB3	5	0.1
(1,750)	1:123:B:ILE:HG21	1:179:B:ALA:HB1	8	0.1
(1,750)	1:123:B:ILE:HG21	1:179:B:ALA:HB2	8	0.1
(1,750)	1:123:B:ILE:HG21	1:179:B:ALA:HB3	8	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,750)	1:123:B:ILE:HG22	1:179:B:ALA:HB1	8	0.1
(1,750)	1:123:B:ILE:HG22	1:179:B:ALA:HB2	8	0.1
(1,750)	1:123:B:ILE:HG22	1:179:B:ALA:HB3	8	0.1
(1,750)	1:123:B:ILE:HG23	1:179:B:ALA:HB1	8	0.1
(1,750)	1:123:B:ILE:HG23	1:179:B:ALA:HB2	8	0.1
(1,750)	1:123:B:ILE:HG23	1:179:B:ALA:HB3	8	0.1
(1,749)	1:123:A:ILE:HG21	1:179:A:ALA:HB1	13	0.1
(1,749)	1:123:A:ILE:HG21	1:179:A:ALA:HB2	13	0.1
(1,749)	1:123:A:ILE:HG21	1:179:A:ALA:HB3	13	0.1
(1,749)	1:123:A:ILE:HG22	1:179:A:ALA:HB1	13	0.1
(1,749)	1:123:A:ILE:HG22	1:179:A:ALA:HB2	13	0.1
(1,749)	1:123:A:ILE:HG22	1:179:A:ALA:HB3	13	0.1
(1,749)	1:123:A:ILE:HG23	1:179:A:ALA:HB1	13	0.1
(1,749)	1:123:A:ILE:HG23	1:179:A:ALA:HB2	13	0.1
(1,749)	1:123:A:ILE:HG23	1:179:A:ALA:HB3	13	0.1
(1,739)	1:175:C:GLY:HA2	1:179:C:ALA:HB1	19	0.1
(1,739)	1:175:C:GLY:HA2	1:179:C:ALA:HB2	19	0.1
(1,739)	1:175:C:GLY:HA2	1:179:C:ALA:HB3	19	0.1
(1,739)	1:175:C:GLY:HA3	1:179:C:ALA:HB1	19	0.1
(1,739)	1:175:C:GLY:HA3	1:179:C:ALA:HB2	19	0.1
(1,739)	1:175:C:GLY:HA3	1:179:C:ALA:HB3	19	0.1
(1,712)	1:141:A:VAL:HG21	1:144:A:PHE:HD1	11	0.1
(1,712)	1:141:A:VAL:HG21	1:144:A:PHE:HD2	11	0.1
(1,712)	1:141:A:VAL:HG22	1:144:A:PHE:HD1	11	0.1
(1,712)	1:141:A:VAL:HG22	1:144:A:PHE:HD2	11	0.1
(1,712)	1:141:A:VAL:HG23	1:144:A:PHE:HD1	11	0.1
(1,712)	1:141:A:VAL:HG23	1:144:A:PHE:HD2	11	0.1
(1,712)	1:141:A:VAL:HG21	1:144:A:PHE:HD1	17	0.1
(1,712)	1:141:A:VAL:HG21	1:144:A:PHE:HD2	17	0.1
(1,712)	1:141:A:VAL:HG22	1:144:A:PHE:HD1	17	0.1
(1,712)	1:141:A:VAL:HG22	1:144:A:PHE:HD2	17	0.1
(1,712)	1:141:A:VAL:HG23	1:144:A:PHE:HD1	17	0.1
(1,712)	1:141:A:VAL:HG23	1:144:A:PHE:HD2	17	0.1
(1,656)	1:169:A:ALA:HA	1:172:A:ALA:HB1	14	0.1
(1,656)	1:169:A:ALA:HA	1:172:A:ALA:HB2	14	0.1
(1,656)	1:169:A:ALA:HA	1:172:A:ALA:HB3	14	0.1
(1,651)	1:94:B:PHE:HE1	1:131:B:ILE:HG21	6	0.1
(1,651)	1:94:B:PHE:HE1	1:131:B:ILE:HG22	6	0.1
(1,651)	1:94:B:PHE:HE1	1:131:B:ILE:HG23	6	0.1
(1,651)	1:94:B:PHE:HE2	1:131:B:ILE:HG21	6	0.1
(1,651)	1:94:B:PHE:HE2	1:131:B:ILE:HG22	6	0.1
(1,651)	1:94:B:PHE:HE2	1:131:B:ILE:HG23	6	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,651)	1:94:B:PHE:HE1	1:131:B:ILE:HG21	8	0.1
(1,651)	1:94:B:PHE:HE1	1:131:B:ILE:HG22	8	0.1
(1,651)	1:94:B:PHE:HE1	1:131:B:ILE:HG23	8	0.1
(1,651)	1:94:B:PHE:HE2	1:131:B:ILE:HG21	8	0.1
(1,651)	1:94:B:PHE:HE2	1:131:B:ILE:HG22	8	0.1
(1,651)	1:94:B:PHE:HE2	1:131:B:ILE:HG23	8	0.1
(1,637)	1:96:C:ILE:HG21	1:100:C:GLY:H	11	0.1
(1,637)	1:96:C:ILE:HG22	1:100:C:GLY:H	11	0.1
(1,637)	1:96:C:ILE:HG23	1:100:C:GLY:H	11	0.1
(1,636)	1:96:B:ILE:HG21	1:100:B:GLY:H	11	0.1
(1,636)	1:96:B:ILE:HG22	1:100:B:GLY:H	11	0.1
(1,636)	1:96:B:ILE:HG23	1:100:B:GLY:H	11	0.1
(1,636)	1:96:B:ILE:HG21	1:100:B:GLY:H	16	0.1
(1,636)	1:96:B:ILE:HG22	1:100:B:GLY:H	16	0.1
(1,636)	1:96:B:ILE:HG23	1:100:B:GLY:H	16	0.1
(1,614)	1:122:A:TYR:H	1:197:A:ILE:HD11	11	0.1
(1,614)	1:122:A:TYR:H	1:197:A:ILE:HD12	11	0.1
(1,614)	1:122:A:TYR:H	1:197:A:ILE:HD13	11	0.1
(1,572)	1:121:A:CYS:H	1:194:A:LEU:HD21	18	0.1
(1,572)	1:121:A:CYS:H	1:194:A:LEU:HD22	18	0.1
(1,572)	1:121:A:CYS:H	1:194:A:LEU:HD23	18	0.1
(1,538)	1:111:C:ILE:HD11	1:131:C:ILE:HG21	12	0.1
(1,538)	1:111:C:ILE:HD11	1:131:C:ILE:HG22	12	0.1
(1,538)	1:111:C:ILE:HD11	1:131:C:ILE:HG23	12	0.1
(1,538)	1:111:C:ILE:HD12	1:131:C:ILE:HG21	12	0.1
(1,538)	1:111:C:ILE:HD12	1:131:C:ILE:HG22	12	0.1
(1,538)	1:111:C:ILE:HD12	1:131:C:ILE:HG23	12	0.1
(1,538)	1:111:C:ILE:HD13	1:131:C:ILE:HG21	12	0.1
(1,538)	1:111:C:ILE:HD13	1:131:C:ILE:HG22	12	0.1
(1,538)	1:111:C:ILE:HD13	1:131:C:ILE:HG23	12	0.1
(1,512)	1:102:A:VAL:HG11	1:103:A:VAL:H	1	0.1
(1,512)	1:102:A:VAL:HG12	1:103:A:VAL:H	1	0.1
(1,512)	1:102:A:VAL:HG13	1:103:A:VAL:H	1	0.1
(1,429)	1:89:A:VAL:HA	1:183:A:MET:HE1	3	0.1
(1,429)	1:89:A:VAL:HA	1:183:A:MET:HE2	3	0.1
(1,429)	1:89:A:VAL:HA	1:183:A:MET:HE3	3	0.1
(1,425)	1:89:A:VAL:HG11	1:183:A:MET:HE1	18	0.1
(1,425)	1:89:A:VAL:HG11	1:183:A:MET:HE2	18	0.1
(1,425)	1:89:A:VAL:HG11	1:183:A:MET:HE3	18	0.1
(1,425)	1:89:A:VAL:HG12	1:183:A:MET:HE1	18	0.1
(1,425)	1:89:A:VAL:HG12	1:183:A:MET:HE2	18	0.1
(1,425)	1:89:A:VAL:HG12	1:183:A:MET:HE3	18	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,425)	1:89:A:VAL:HG13	1:183:A:MET:HE1	18	0.1
(1,425)	1:89:A:VAL:HG13	1:183:A:MET:HE2	18	0.1
(1,425)	1:89:A:VAL:HG13	1:183:A:MET:HE3	18	0.1
(1,396)	1:109:B:LEU:HG	1:111:B:ILE:HD11	2	0.1
(1,396)	1:109:B:LEU:HG	1:111:B:ILE:HD12	2	0.1
(1,396)	1:109:B:LEU:HG	1:111:B:ILE:HD13	2	0.1
(1,373)	1:96:C:ILE:HD11	1:102:C:VAL:HB	14	0.1
(1,373)	1:96:C:ILE:HD12	1:102:C:VAL:HB	14	0.1
(1,373)	1:96:C:ILE:HD13	1:102:C:VAL:HB	14	0.1
(1,365)	1:126:B:ILE:HG21	1:131:B:ILE:HD11	11	0.1
(1,365)	1:126:B:ILE:HG21	1:131:B:ILE:HD12	11	0.1
(1,365)	1:126:B:ILE:HG21	1:131:B:ILE:HD13	11	0.1
(1,365)	1:126:B:ILE:HG22	1:131:B:ILE:HD11	11	0.1
(1,365)	1:126:B:ILE:HG22	1:131:B:ILE:HD12	11	0.1
(1,365)	1:126:B:ILE:HG22	1:131:B:ILE:HD13	11	0.1
(1,365)	1:126:B:ILE:HG23	1:131:B:ILE:HD11	11	0.1
(1,365)	1:126:B:ILE:HG23	1:131:B:ILE:HD12	11	0.1
(1,365)	1:126:B:ILE:HG23	1:131:B:ILE:HD13	11	0.1
(1,362)	1:183:B:MET:HG2	1:131:C:ILE:HD11	8	0.1
(1,362)	1:183:B:MET:HG2	1:131:C:ILE:HD12	8	0.1
(1,362)	1:183:B:MET:HG2	1:131:C:ILE:HD13	8	0.1
(1,362)	1:183:B:MET:HG3	1:131:C:ILE:HD11	8	0.1
(1,362)	1:183:B:MET:HG3	1:131:C:ILE:HD12	8	0.1
(1,362)	1:183:B:MET:HG3	1:131:C:ILE:HD13	8	0.1
(1,301)	1:181:A:LEU:HD11	1:196:A:TYR:HE1	3	0.1
(1,301)	1:181:A:LEU:HD11	1:196:A:TYR:HE2	3	0.1
(1,301)	1:181:A:LEU:HD12	1:196:A:TYR:HE1	3	0.1
(1,301)	1:181:A:LEU:HD12	1:196:A:TYR:HE2	3	0.1
(1,301)	1:181:A:LEU:HD13	1:196:A:TYR:HE1	3	0.1
(1,301)	1:181:A:LEU:HD13	1:196:A:TYR:HE2	3	0.1
(1,257)	1:111:C:ILE:H	1:124:C:MET:HE1	20	0.1
(1,257)	1:111:C:ILE:H	1:124:C:MET:HE2	20	0.1
(1,257)	1:111:C:ILE:H	1:124:C:MET:HE3	20	0.1
(1,175)	1:179:A:ALA:HB1	1:181:A:LEU:HD21	4	0.1
(1,175)	1:179:A:ALA:HB1	1:181:A:LEU:HD22	4	0.1
(1,175)	1:179:A:ALA:HB1	1:181:A:LEU:HD23	4	0.1
(1,175)	1:179:A:ALA:HB2	1:181:A:LEU:HD21	4	0.1
(1,175)	1:179:A:ALA:HB2	1:181:A:LEU:HD22	4	0.1
(1,175)	1:179:A:ALA:HB2	1:181:A:LEU:HD23	4	0.1
(1,175)	1:179:A:ALA:HB3	1:181:A:LEU:HD21	4	0.1
(1,175)	1:179:A:ALA:HB3	1:181:A:LEU:HD22	4	0.1
(1,175)	1:179:A:ALA:HB3	1:181:A:LEU:HD23	4	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,157)	1:101:A:LEU:HD21	1:95:B:SER:HB2	8	0.1
(1,157)	1:101:A:LEU:HD21	1:95:B:SER:HB3	8	0.1
(1,157)	1:101:A:LEU:HD22	1:95:B:SER:HB2	8	0.1
(1,157)	1:101:A:LEU:HD22	1:95:B:SER:HB3	8	0.1
(1,157)	1:101:A:LEU:HD23	1:95:B:SER:HB2	8	0.1
(1,157)	1:101:A:LEU:HD23	1:95:B:SER:HB3	8	0.1
(1,157)	1:101:A:LEU:HD21	1:95:B:SER:HB2	20	0.1
(1,157)	1:101:A:LEU:HD21	1:95:B:SER:HB3	20	0.1
(1,157)	1:101:A:LEU:HD22	1:95:B:SER:HB2	20	0.1
(1,157)	1:101:A:LEU:HD22	1:95:B:SER:HB3	20	0.1
(1,157)	1:101:A:LEU:HD23	1:95:B:SER:HB2	20	0.1
(1,157)	1:101:A:LEU:HD23	1:95:B:SER:HB3	20	0.1
(1,56)	1:156:A:VAL:HG11	1:157:A:PRO:HD3	19	0.1
(1,56)	1:156:A:VAL:HG12	1:157:A:PRO:HD3	19	0.1
(1,56)	1:156:A:VAL:HG13	1:157:A:PRO:HD3	19	0.1
(1,56)	1:156:A:VAL:HG11	1:157:A:PRO:HD3	20	0.1
(1,56)	1:156:A:VAL:HG12	1:157:A:PRO:HD3	20	0.1
(1,56)	1:156:A:VAL:HG13	1:157:A:PRO:HD3	20	0.1
(1,55)	1:156:A:VAL:HG11	1:157:A:PRO:HD2	3	0.1
(1,55)	1:156:A:VAL:HG12	1:157:A:PRO:HD2	3	0.1
(1,55)	1:156:A:VAL:HG13	1:157:A:PRO:HD2	3	0.1

10 Dihedral-angle violation analysis

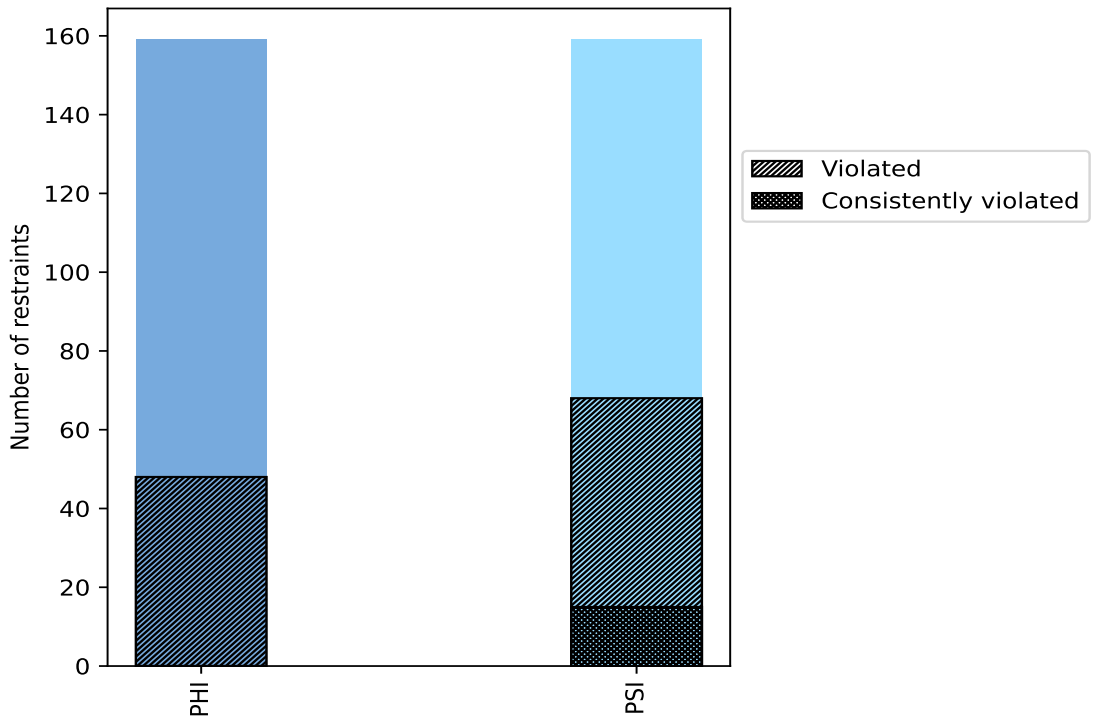
10.1 Summary of dihedral-angle violations

The following table provides the summary of dihedral-angle violations in different dihedral-angle types. Violations less than 1° are not included in the calculation.

Angle type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
PHI	159	50.0	48	30.2	15.1	0	0.0	0.0
PSI	159	50.0	68	42.8	21.4	15	9.4	4.7
Total	318	100.0	116	36.5	36.5	15	4.7	4.7

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

10.1.1 Bar chart : Distribution of dihedral-angles and violations



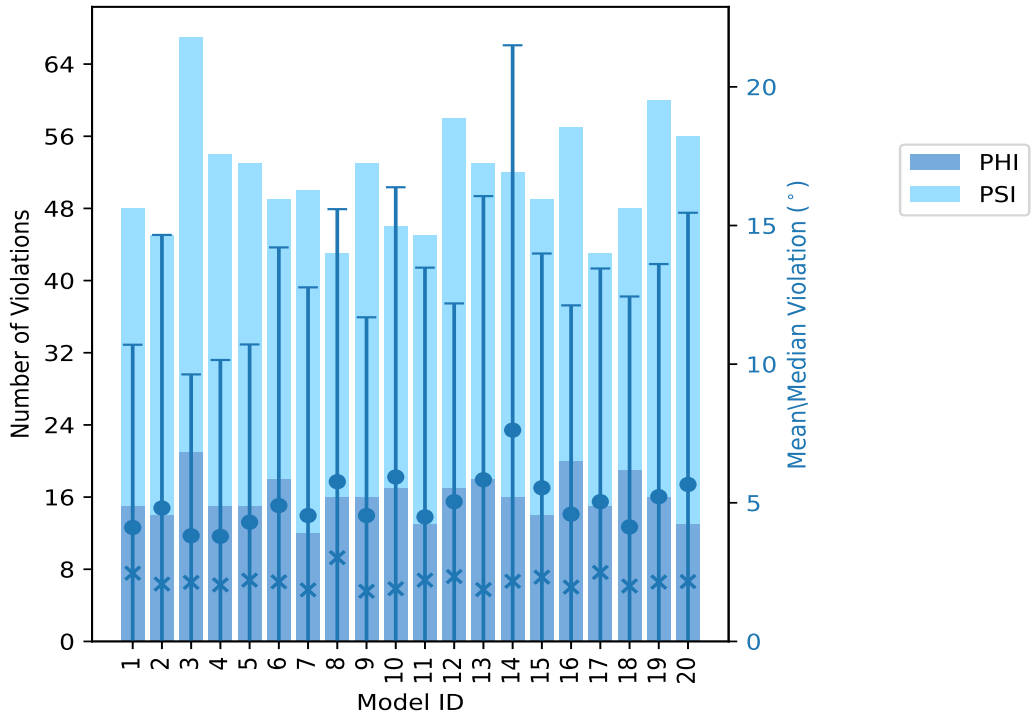
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	15	33	48	4.11	29.99	6.59	2.46
2	14	31	45	4.81	42.15	9.85	2.07
3	21	46	67	3.81	29.43	5.82	2.13
4	15	39	54	3.79	30.13	6.36	2.04
5	15	38	53	4.3	30.25	6.41	2.21
6	18	31	49	4.9	40.89	9.31	2.15
7	12	38	50	4.54	36.64	8.23	1.86
8	16	27	43	5.76	41.68	9.83	3.02
9	16	37	53	4.54	26.81	7.15	1.81
10	17	29	46	5.93	38.72	10.45	1.9
11	13	32	45	4.49	39.12	8.99	2.21
12	17	41	58	5.04	28.95	7.15	2.34
13	18	35	53	5.83	40.48	10.23	1.87
14	16	36	52	7.62	48.12	13.88	2.17
15	14	35	49	5.54	28.42	8.45	2.32
16	20	37	57	4.59	29.14	7.53	1.96
17	15	28	43	5.04	35.0	8.41	2.49
18	19	29	48	4.13	36.61	8.31	2.0
19	16	44	60	5.22	31.68	8.39	2.14
20	13	43	56	5.66	37.09	9.8	2.16

10.2.1 Bar graph : Dihedral violation statistics for each model



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

10.3 Dihedral-angle violation statistics for the ensemble

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

Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count[1]	%
5	11	16	1	5.0
6	6	12	2	10.0
9	3	12	3	15.0
2	2	4	4	20.0
6	6	12	5	25.0
1	5	6	6	30.0
1	0	1	7	35.0
3	1	4	8	40.0
1	1	2	9	45.0
3	0	3	10	50.0
2	1	3	11	55.0

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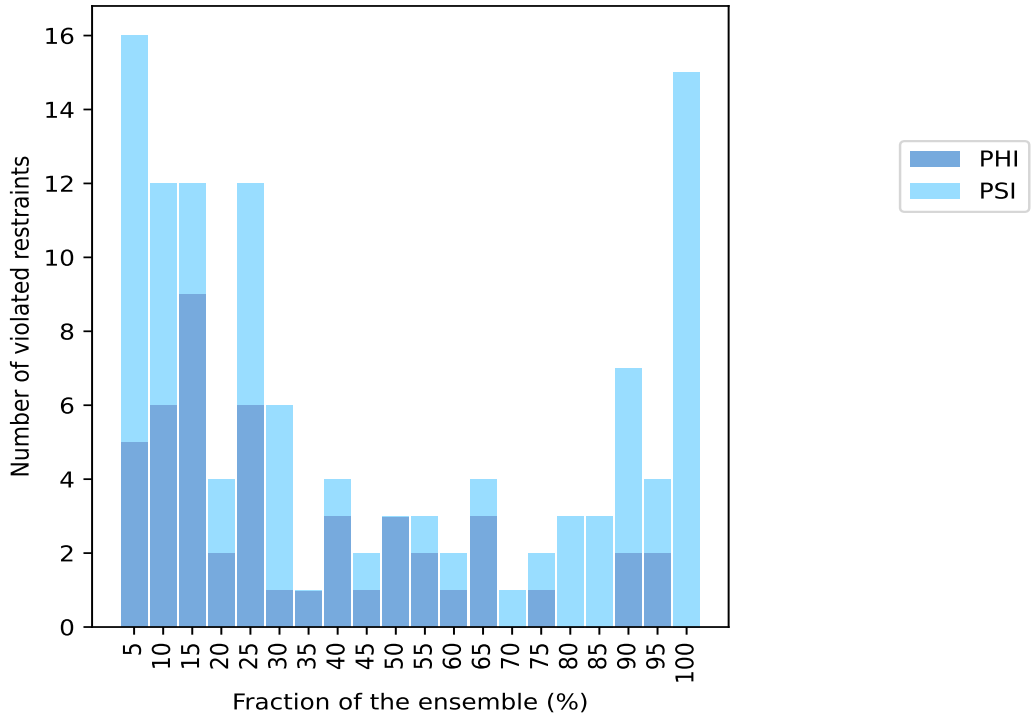
Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count[1]	%
1	1	2	12	60.0
3	1	4	13	65.0
0	1	1	14	70.0
1	1	2	15	75.0
0	3	3	16	80.0
0	3	3	17	85.0
2	5	7	18	90.0
2	2	4	19	95.0
0	15	15	20	100.0

[1] Number of models with violations

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

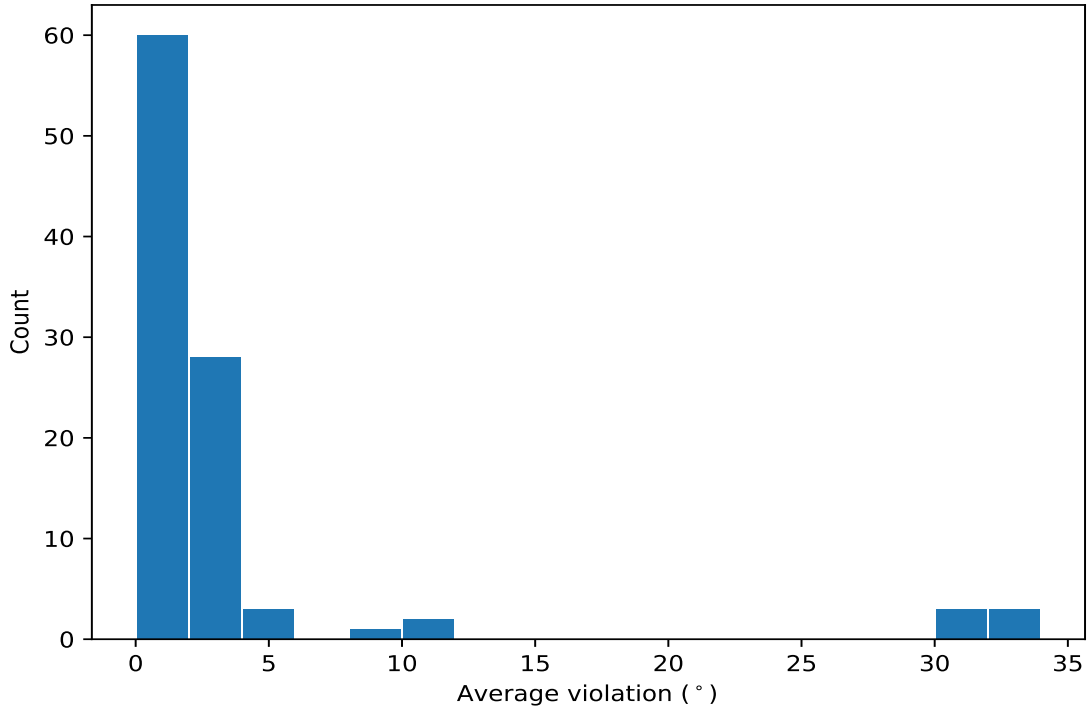


10.4 Most violated dihedral-angle restraints in the ensemble

10.4.1 Histogram : Distribution of mean dihedral-angle violations

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

in the ensemble



10.4.2 Table: Most violated dihedral-angle restraints

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,158)	1:127:B:ALA:N	1:127:B:ALA:CA	1:127:B:ALA:C	1:128:B:PRO:N	20	33.83	5.38	32.62
(1,264)	1:127:C:ALA:N	1:127:C:ALA:CA	1:127:C:ALA:C	1:128:C:PRO:N	20	33.72	5.51	32.76
(1,52)	1:127:A:ALA:N	1:127:A:ALA:CA	1:127:A:ALA:C	1:128:A:PRO:N	20	33.68	5.62	32.17
(1,68)	1:139:A:ARG:N	1:139:A:ARG:CA	1:139:A:ARG:C	1:140:A:LYS:N	20	4.6	0.79	4.4
(1,174)	1:139:B:ARG:N	1:139:B:ARG:CA	1:139:B:ARG:C	1:140:B:LYS:N	20	3.35	0.3	3.32
(1,280)	1:139:C:ARG:N	1:139:C:ARG:CA	1:139:C:ARG:C	1:140:C:LYS:N	20	3.32	0.29	3.29
(1,170)	1:137:B:LEU:N	1:137:B:LEU:CA	1:137:B:LEU:C	1:138:B:THR:N	20	3.02	0.48	2.92
(1,276)	1:137:C:LEU:N	1:137:C:LEU:CA	1:137:C:LEU:C	1:138:C:THR:N	20	2.77	0.39	2.68
(1,150)	1:123:B:ILE:N	1:123:B:ILE:CA	1:123:B:ILE:C	1:124:B:MET:N	20	2.64	0.46	2.58
(1,250)	1:118:C:GLY:N	1:118:C:GLY:CA	1:118:C:GLY:C	1:119:C:THR:N	20	2.63	0.64	2.44
(1,144)	1:118:B:GLY:N	1:118:B:GLY:CA	1:118:B:GLY:C	1:119:B:THR:N	20	2.62	0.67	2.52
(1,256)	1:123:C:ILE:N	1:123:C:ILE:CA	1:123:C:ILE:C	1:124:C:MET:N	20	2.58	0.48	2.56
(1,44)	1:123:A:ILE:N	1:123:A:ILE:CA	1:123:A:ILE:C	1:124:A:MET:N	20	2.21	0.5	2.18
(1,38)	1:118:A:GLY:N	1:118:A:GLY:CA	1:118:A:GLY:C	1:119:A:THR:N	20	2.12	0.94	1.8
(1,182)	1:143:B:ASN:N	1:143:B:ASN:CA	1:143:B:ASN:C	1:144:B:PHE:N	20	1.88	0.55	1.78
(1,64)	1:137:A:LEU:N	1:137:A:LEU:CA	1:137:A:LEU:C	1:138:A:THR:N	19	2.66	0.65	2.69
(1,35)	1:115:A:PRO:C	1:116:A:ALA:N	1:116:A:ALA:CA	1:116:A:ALA:C	19	2.37	0.72	2.33
(1,69)	1:139:A:ARG:C	1:140:A:LYS:N	1:140:A:LYS:CA	1:140:A:LYS:C	19	2.05	0.76	1.95
(1,288)	1:143:C:ASN:N	1:143:C:ASN:CA	1:143:C:ASN:C	1:144:C:PHE:N	19	1.67	0.44	1.54
(1,226)	1:100:C:GLY:N	1:100:C:GLY:CA	1:100:C:GLY:C	1:101:C:LEU:N	18	11.24	7.43	9.96

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,120)	1:100:B:GLY:N	1:100:B:GLY:CA	1:100:B:GLY:C	1:101:B:LEU:N	18	11.08	7.39	9.25
(1,14)	1:100:A:GLY:N	1:100:A:GLY:CA	1:100:A:GLY:C	1:101:A:LEU:N	18	8.74	7.21	5.5
(1,102)	1:194:A:LEU:N	1:194:A:LEU:CA	1:194:A:LEU:C	1:195:A:TYR:N	18	2.89	0.65	2.94
(1,247)	1:115:C:PRO:C	1:116:C:ALA:N	1:116:C:ALA:CA	1:116:C:ALA:C	18	2.11	0.76	1.92
(1,141)	1:115:B:PRO:C	1:116:B:ALA:N	1:116:B:ALA:CA	1:116:B:ALA:C	18	1.99	0.7	1.88
(1,86)	1:184:A:ALA:N	1:184:A:ALA:CA	1:184:A:ALA:C	1:185:A:VAL:N	18	1.83	0.41	1.82
(1,308)	1:189:C:CYS:N	1:189:C:CYS:CA	1:189:C:CYS:C	1:190:C:GLY:N	17	2.78	0.33	2.83
(1,202)	1:189:B:CYS:N	1:189:B:CYS:CA	1:189:B:CYS:C	1:190:B:GLY:N	17	2.74	0.31	2.76
(1,76)	1:143:A:ASN:N	1:143:A:ASN:CA	1:143:A:ASN:C	1:144:A:PHE:N	17	1.62	0.45	1.5
(1,96)	1:189:A:CYS:N	1:189:A:CYS:CA	1:189:A:CYS:C	1:190:A:GLY:N	16	2.85	0.61	2.92
(1,160)	1:129:B:GLU:N	1:129:B:GLU:CA	1:129:B:GLU:C	1:130:B:SER:N	16	1.41	0.25	1.38
(1,266)	1:129:C:GLU:N	1:129:C:GLU:CA	1:129:C:GLU:C	1:130:C:SER:N	16	1.34	0.18	1.34
(1,167)	1:135:B:GLU:C	1:136:B:ALA:N	1:136:B:ALA:CA	1:136:B:ALA:C	15	1.78	0.59	1.71
(1,54)	1:129:A:GLU:N	1:129:A:GLU:CA	1:129:A:GLU:C	1:130:A:SER:N	15	1.44	0.15	1.4
(1,92)	1:187:A:THR:N	1:187:A:THR:CA	1:187:A:THR:C	1:188:A:LEU:N	14	2.39	0.83	2.28
(1,259)	1:124:C:MET:C	1:125:C:LYS:N	1:125:C:LYS:CA	1:125:C:LYS:C	13	3.0	0.96	3.17
(1,153)	1:124:B:MET:C	1:125:B:LYS:N	1:125:B:LYS:CA	1:125:B:LYS:C	13	2.93	1.01	3.03
(1,103)	1:194:A:LEU:C	1:195:A:TYR:N	1:195:A:TYR:CA	1:195:A:TYR:C	13	2.11	0.59	2.04
(1,298)	1:184:C:ALA:N	1:184:C:ALA:CA	1:184:C:ALA:C	1:185:C:VAL:N	13	1.47	0.32	1.47
(1,243)	1:112:C:ALA:C	1:113:C:TYR:N	1:113:C:TYR:CA	1:113:C:TYR:C	12	1.57	0.44	1.49
(1,192)	1:184:B:ALA:N	1:184:B:ALA:CA	1:184:B:ALA:C	1:185:B:VAL:N	12	1.48	0.29	1.44
(1,58)	1:133:A:SER:N	1:133:A:SER:CA	1:133:A:SER:C	1:134:A:LEU:N	11	2.36	0.89	2.14
(1,137)	1:112:B:ALA:C	1:113:B:TYR:N	1:113:B:TYR:CA	1:113:B:TYR:C	11	1.57	0.38	1.51
(1,149)	1:122:B:TYR:C	1:123:B:ILE:N	1:123:B:ILE:CA	1:123:B:ILE:C	11	1.5	0.32	1.48
(1,33)	1:113:A:TYR:C	1:114:A:LYS:N	1:114:A:LYS:CA	1:114:A:LYS:C	10	2.13	1.05	1.88
(1,255)	1:122:C:TYR:C	1:123:C:ILE:N	1:123:C:ILE:CA	1:123:C:ILE:C	10	1.41	0.29	1.36
(1,91)	1:186:A:SER:C	1:187:A:THR:N	1:187:A:THR:CA	1:187:A:THR:C	10	1.33	0.35	1.16
(1,270)	1:133:C:SER:N	1:133:C:SER:CA	1:133:C:SER:C	1:134:C:LEU:N	9	1.87	0.7	1.4
(1,189)	1:182:B:GLY:C	1:183:B:MET:N	1:183:B:MET:CA	1:183:B:MET:C	9	1.38	0.3	1.31
(1,164)	1:133:B:SER:N	1:133:B:SER:CA	1:133:B:SER:C	1:134:B:LEU:N	8	2.37	0.83	2.37
(1,47)	1:124:A:MET:C	1:125:A:LYS:N	1:125:A:LYS:CA	1:125:A:LYS:C	8	1.83	0.52	1.76
(1,83)	1:182:A:GLY:C	1:183:A:MET:N	1:183:A:MET:CA	1:183:A:MET:C	8	1.74	0.43	1.78
(1,295)	1:182:C:GLY:C	1:183:C:MET:N	1:183:C:MET:CA	1:183:C:MET:C	8	1.4	0.33	1.32
(1,43)	1:122:A:TYR:C	1:123:A:ILE:N	1:123:A:ILE:CA	1:123:A:ILE:C	7	1.61	0.53	1.58
(1,186)	1:168:B:ASP:N	1:168:B:ASP:CA	1:168:B:ASP:C	1:169:B:ALA:N	6	31.93	8.67	29.61
(1,292)	1:168:C:ASP:N	1:168:C:ASP:CA	1:168:C:ASP:C	1:169:C:ALA:N	6	31.91	8.73	29.52
(1,80)	1:168:A:ASP:N	1:168:A:ASP:CA	1:168:A:ASP:C	1:169:A:ALA:N	6	31.66	9.2	29.7
(1,2)	1:91:A:THR:N	1:91:A:THR:CA	1:91:A:THR:C	1:92:A:ALA:N	6	1.91	0.68	1.81
(1,198)	1:187:B:THR:N	1:187:B:THR:CA	1:187:B:THR:C	1:188:B:LEU:N	6	1.75	0.48	1.76
(1,175)	1:139:B:ARG:C	1:140:B:LYS:N	1:140:B:LYS:CA	1:140:B:LYS:C	6	1.23	0.2	1.2
(1,40)	1:121:A:CYS:N	1:121:A:CYS:CA	1:121:A:CYS:C	1:122:A:TYR:N	5	2.35	1.18	1.96
(1,159)	1:128:B:PRO:C	1:129:B:GLU:N	1:129:B:GLU:CA	1:129:B:GLU:C	5	1.93	0.56	1.6
(1,24)	1:109:A:LEU:N	1:109:A:LEU:CA	1:109:A:LEU:C	1:110:A:LEU:N	5	1.9	0.69	1.52
(1,31)	1:112:A:ALA:C	1:113:A:TYR:N	1:113:A:TYR:CA	1:113:A:TYR:C	5	1.76	0.71	1.5
(1,304)	1:187:C:THR:N	1:187:C:THR:CA	1:187:C:THR:C	1:188:C:LEU:N	5	1.75	0.38	1.92
(1,265)	1:128:C:PRO:C	1:129:C:GLU:N	1:129:C:GLU:CA	1:129:C:GLU:C	5	1.6	0.66	1.46
(1,214)	1:91:C:THR:N	1:91:C:THR:CA	1:91:C:THR:C	1:92:C:ALA:N	5	1.53	0.44	1.38
(1,41)	1:121:A:CYS:C	1:122:A:TYR:N	1:122:A:TYR:CA	1:122:A:TYR:C	5	1.46	0.54	1.34
(1,200)	1:188:B:LEU:N	1:188:B:LEU:CA	1:188:B:LEU:C	1:189:B:CYS:N	5	1.33	0.3	1.19
(1,281)	1:139:C:ARG:C	1:140:C:LYS:N	1:140:C:LYS:CA	1:140:C:LYS:C	5	1.29	0.12	1.36
(1,314)	1:194:C:LEU:N	1:194:C:LEU:CA	1:194:C:LEU:C	1:195:C:TYR:N	5	1.29	0.18	1.23

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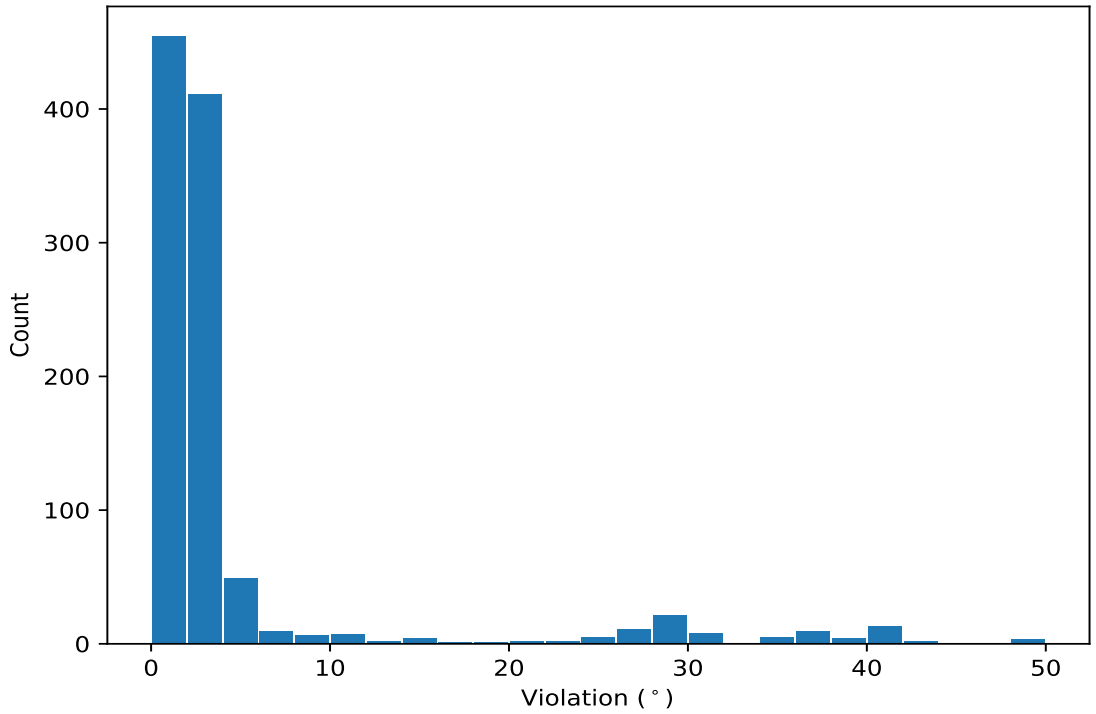
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,197)	1:186:B:SER:C	1:187:B:THR:N	1:187:B:THR:CA	1:187:B:THR:C	5	1.19	0.12	1.16
(1,3)	1:91:A:THR:C	1:92:A:ALA:N	1:92:A:ALA:CA	1:92:A:ALA:C	4	5.28	1.03	5.04
(1,109)	1:91:B:THR:C	1:92:B:ALA:N	1:92:B:ALA:CA	1:92:B:ALA:C	4	3.59	2.66	2.66
(1,108)	1:91:B:THR:N	1:91:B:THR:CA	1:91:B:THR:C	1:92:B:ALA:N	4	1.49	0.18	1.54
(1,208)	1:194:B:LEU:N	1:194:B:LEU:CA	1:194:B:LEU:C	1:195:B:TYR:N	4	1.35	0.18	1.34
(1,15)	1:100:A:GLY:C	1:101:A:LEU:N	1:101:A:LEU:CA	1:101:A:LEU:C	3	2.17	0.73	2.25
(1,53)	1:128:A:PRO:C	1:129:A:GLU:N	1:129:A:GLU:CA	1:129:A:GLU:C	3	1.92	0.5	1.83
(1,252)	1:121:C:CYS:N	1:121:C:CYS:CA	1:121:C:CYS:C	1:122:C:TYR:N	3	1.88	0.3	1.74
(1,146)	1:121:B:CYS:N	1:121:B:CYS:CA	1:121:B:CYS:C	1:122:B:TYR:N	3	1.76	0.29	1.74
(1,13)	1:99:A:THR:C	1:100:A:GLY:N	1:100:A:GLY:CA	1:100:A:GLY:C	3	1.46	0.26	1.55
(1,253)	1:121:C:CYS:C	1:122:C:TYR:N	1:122:C:TYR:CA	1:122:C:TYR:C	3	1.37	0.25	1.49
(1,147)	1:121:B:CYS:C	1:122:B:TYR:N	1:122:B:TYR:CA	1:122:B:TYR:C	3	1.35	0.14	1.36
(1,306)	1:188:C:LEU:N	1:188:C:LEU:CA	1:188:C:LEU:C	1:189:C:CYS:N	3	1.28	0.29	1.16
(1,139)	1:113:B:TYR:C	1:114:B:LYS:N	1:114:B:LYS:CA	1:114:B:LYS:C	3	1.23	0.2	1.1
(1,303)	1:186:C:SER:C	1:187:C:THR:N	1:187:C:THR:CA	1:187:C:THR:C	3	1.21	0.2	1.09
(1,245)	1:113:C:TYR:C	1:114:C:LYS:N	1:114:C:LYS:CA	1:114:C:LYS:C	3	1.17	0.16	1.06
(1,225)	1:99:C:THR:C	1:100:C:GLY:N	1:100:C:GLY:CA	1:100:C:GLY:C	3	1.14	0.17	1.02
(1,215)	1:91:C:THR:C	1:92:C:ALA:N	1:92:C:ALA:CA	1:92:C:ALA:C	2	4.95	1.61	4.95
(1,4)	1:92:A:ALA:N	1:92:A:ALA:CA	1:92:A:ALA:C	1:93:A:THR:N	2	1.62	0.25	1.62
(1,260)	1:125:C:LYS:N	1:125:C:LYS:CA	1:125:C:LYS:C	1:126:C:ILE:N	2	1.46	0.19	1.46
(1,273)	1:135:C:GLU:C	1:136:C:ALA:N	1:136:C:ALA:CA	1:136:C:ALA:C	2	1.39	0.08	1.39
(1,48)	1:125:A:LYS:N	1:125:A:LYS:CA	1:125:A:LYS:C	1:126:A:ILE:N	2	1.36	0.16	1.36
(1,154)	1:125:B:LYS:N	1:125:B:LYS:CA	1:125:B:LYS:C	1:126:B:ILE:N	2	1.32	0.22	1.32
(1,119)	1:99:B:THR:C	1:100:B:GLY:N	1:100:B:GLY:CA	1:100:B:GLY:C	2	1.28	0.24	1.28
(1,220)	1:94:C:PHE:N	1:94:C:PHE:CA	1:94:C:PHE:C	1:95:C:SER:N	2	1.2	0.12	1.2
(1,93)	1:187:A:THR:C	1:188:A:LEU:N	1:188:A:LEU:CA	1:188:A:LEU:C	2	1.16	0.05	1.16
(1,20)	1:103:A:VAL:N	1:103:A:VAL:CA	1:103:A:VAL:C	1:104:A:TYR:N	2	1.14	0.03	1.14
(1,51)	1:126:A:ILE:C	1:127:A:ALA:N	1:127:A:ALA:CA	1:127:A:ALA:C	2	1.14	0.01	1.14
(1,157)	1:126:B:ILE:C	1:127:B:ALA:N	1:127:B:ALA:CA	1:127:B:ALA:C	2	1.1	0.03	1.1

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

10.5 All violated dihedral-angle restraints (i)

10.5.1 Histogram : Distribution of violations (i)

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



10.5.2 Table: All violated dihedral-angle restraints

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,292)	1:168:C:ASP:N	1:168:C:ASP:CA	1:168:C:ASP:C	1:169:C:ALA:N	14	48.12
(1,80)	1:168:A:ASP:N	1:168:A:ASP:CA	1:168:A:ASP:C	1:169:A:ALA:N	14	48.09
(1,186)	1:168:B:ASP:N	1:168:B:ASP:CA	1:168:B:ASP:C	1:169:B:ALA:N	14	48.08
(1,158)	1:127:B:ALA:N	1:127:B:ALA:CA	1:127:B:ALA:C	1:128:B:PRO:N	2	42.15
(1,52)	1:127:A:ALA:N	1:127:A:ALA:CA	1:127:A:ALA:C	1:128:A:PRO:N	14	42.12
(1,52)	1:127:A:ALA:N	1:127:A:ALA:CA	1:127:A:ALA:C	1:128:A:PRO:N	8	41.68
(1,158)	1:127:B:ALA:N	1:127:B:ALA:CA	1:127:B:ALA:C	1:128:B:PRO:N	14	41.66
(1,264)	1:127:C:ALA:N	1:127:C:ALA:CA	1:127:C:ALA:C	1:128:C:PRO:N	14	41.63
(1,264)	1:127:C:ALA:N	1:127:C:ALA:CA	1:127:C:ALA:C	1:128:C:PRO:N	2	41.4
(1,264)	1:127:C:ALA:N	1:127:C:ALA:CA	1:127:C:ALA:C	1:128:C:PRO:N	8	41.11
(1,158)	1:127:B:ALA:N	1:127:B:ALA:CA	1:127:B:ALA:C	1:128:B:PRO:N	6	40.89
(1,158)	1:127:B:ALA:N	1:127:B:ALA:CA	1:127:B:ALA:C	1:128:B:PRO:N	8	40.84
(1,52)	1:127:A:ALA:N	1:127:A:ALA:CA	1:127:A:ALA:C	1:128:A:PRO:N	2	40.74
(1,52)	1:127:A:ALA:N	1:127:A:ALA:CA	1:127:A:ALA:C	1:128:A:PRO:N	6	40.58
(1,52)	1:127:A:ALA:N	1:127:A:ALA:CA	1:127:A:ALA:C	1:128:A:PRO:N	13	40.48
(1,158)	1:127:B:ALA:N	1:127:B:ALA:CA	1:127:B:ALA:C	1:128:B:PRO:N	13	40.21
(1,264)	1:127:C:ALA:N	1:127:C:ALA:CA	1:127:C:ALA:C	1:128:C:PRO:N	13	40.1
(1,264)	1:127:C:ALA:N	1:127:C:ALA:CA	1:127:C:ALA:C	1:128:C:PRO:N	6	40.07
(1,52)	1:127:A:ALA:N	1:127:A:ALA:CA	1:127:A:ALA:C	1:128:A:PRO:N	11	39.12
(1,264)	1:127:C:ALA:N	1:127:C:ALA:CA	1:127:C:ALA:C	1:128:C:PRO:N	10	38.72
(1,52)	1:127:A:ALA:N	1:127:A:ALA:CA	1:127:A:ALA:C	1:128:A:PRO:N	10	38.08

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,158)	1:127:B:ALA:N	1:127:B:ALA:CA	1:127:B:ALA:C	1:128:B:PRO:N	10	38.01
(1,264)	1:127:C:ALA:N	1:127:C:ALA:CA	1:127:C:ALA:C	1:128:C:PRO:N	11	37.87
(1,80)	1:168:A:ASP:N	1:168:A:ASP:CA	1:168:A:ASP:C	1:169:A:ALA:N	20	37.09
(1,158)	1:127:B:ALA:N	1:127:B:ALA:CA	1:127:B:ALA:C	1:128:B:PRO:N	11	37.01
(1,292)	1:168:C:ASP:N	1:168:C:ASP:CA	1:168:C:ASP:C	1:169:C:ALA:N	20	36.72
(1,158)	1:127:B:ALA:N	1:127:B:ALA:CA	1:127:B:ALA:C	1:128:B:PRO:N	7	36.64
(1,264)	1:127:C:ALA:N	1:127:C:ALA:CA	1:127:C:ALA:C	1:128:C:PRO:N	18	36.61
(1,186)	1:168:B:ASP:N	1:168:B:ASP:CA	1:168:B:ASP:C	1:169:B:ALA:N	20	36.54
(1,264)	1:127:C:ALA:N	1:127:C:ALA:CA	1:127:C:ALA:C	1:128:C:PRO:N	7	36.41
(1,52)	1:127:A:ALA:N	1:127:A:ALA:CA	1:127:A:ALA:C	1:128:A:PRO:N	18	36.11
(1,158)	1:127:B:ALA:N	1:127:B:ALA:CA	1:127:B:ALA:C	1:128:B:PRO:N	18	35.98
(1,52)	1:127:A:ALA:N	1:127:A:ALA:CA	1:127:A:ALA:C	1:128:A:PRO:N	7	35.84
(1,264)	1:127:C:ALA:N	1:127:C:ALA:CA	1:127:C:ALA:C	1:128:C:PRO:N	17	35.0
(1,158)	1:127:B:ALA:N	1:127:B:ALA:CA	1:127:B:ALA:C	1:128:B:PRO:N	17	34.35
(1,52)	1:127:A:ALA:N	1:127:A:ALA:CA	1:127:A:ALA:C	1:128:A:PRO:N	17	34.1
(1,186)	1:168:B:ASP:N	1:168:B:ASP:CA	1:168:B:ASP:C	1:169:B:ALA:N	19	31.68
(1,292)	1:168:C:ASP:N	1:168:C:ASP:CA	1:168:C:ASP:C	1:169:C:ALA:N	19	31.34
(1,80)	1:168:A:ASP:N	1:168:A:ASP:CA	1:168:A:ASP:C	1:169:A:ALA:N	19	31.3
(1,158)	1:127:B:ALA:N	1:127:B:ALA:CA	1:127:B:ALA:C	1:128:B:PRO:N	20	30.88
(1,264)	1:127:C:ALA:N	1:127:C:ALA:CA	1:127:C:ALA:C	1:128:C:PRO:N	20	30.51
(1,52)	1:127:A:ALA:N	1:127:A:ALA:CA	1:127:A:ALA:C	1:128:A:PRO:N	5	30.25
(1,158)	1:127:B:ALA:N	1:127:B:ALA:CA	1:127:B:ALA:C	1:128:B:PRO:N	4	30.13
(1,52)	1:127:A:ALA:N	1:127:A:ALA:CA	1:127:A:ALA:C	1:128:A:PRO:N	20	30.04
(1,158)	1:127:B:ALA:N	1:127:B:ALA:CA	1:127:B:ALA:C	1:128:B:PRO:N	1	29.99
(1,264)	1:127:C:ALA:N	1:127:C:ALA:CA	1:127:C:ALA:C	1:128:C:PRO:N	4	29.85
(1,264)	1:127:C:ALA:N	1:127:C:ALA:CA	1:127:C:ALA:C	1:128:C:PRO:N	1	29.65
(1,158)	1:127:B:ALA:N	1:127:B:ALA:CA	1:127:B:ALA:C	1:128:B:PRO:N	3	29.43
(1,52)	1:127:A:ALA:N	1:127:A:ALA:CA	1:127:A:ALA:C	1:128:A:PRO:N	16	29.14
(1,264)	1:127:C:ALA:N	1:127:C:ALA:CA	1:127:C:ALA:C	1:128:C:PRO:N	3	29.09
(1,52)	1:127:A:ALA:N	1:127:A:ALA:CA	1:127:A:ALA:C	1:128:A:PRO:N	19	29.06
(1,158)	1:127:B:ALA:N	1:127:B:ALA:CA	1:127:B:ALA:C	1:128:B:PRO:N	5	29.02
(1,52)	1:127:A:ALA:N	1:127:A:ALA:CA	1:127:A:ALA:C	1:128:A:PRO:N	4	29.02
(1,158)	1:127:B:ALA:N	1:127:B:ALA:CA	1:127:B:ALA:C	1:128:B:PRO:N	12	28.95
(1,52)	1:127:A:ALA:N	1:127:A:ALA:CA	1:127:A:ALA:C	1:128:A:PRO:N	3	28.85
(1,264)	1:127:C:ALA:N	1:127:C:ALA:CA	1:127:C:ALA:C	1:128:C:PRO:N	5	28.68
(1,264)	1:127:C:ALA:N	1:127:C:ALA:CA	1:127:C:ALA:C	1:128:C:PRO:N	12	28.66
(1,158)	1:127:B:ALA:N	1:127:B:ALA:CA	1:127:B:ALA:C	1:128:B:PRO:N	16	28.51
(1,158)	1:127:B:ALA:N	1:127:B:ALA:CA	1:127:B:ALA:C	1:128:B:PRO:N	15	28.42
(1,52)	1:127:A:ALA:N	1:127:A:ALA:CA	1:127:A:ALA:C	1:128:A:PRO:N	1	28.42
(1,158)	1:127:B:ALA:N	1:127:B:ALA:CA	1:127:B:ALA:C	1:128:B:PRO:N	19	28.37
(1,264)	1:127:C:ALA:N	1:127:C:ALA:CA	1:127:C:ALA:C	1:128:C:PRO:N	15	28.15
(1,264)	1:127:C:ALA:N	1:127:C:ALA:CA	1:127:C:ALA:C	1:128:C:PRO:N	19	28.13
(1,80)	1:168:A:ASP:N	1:168:A:ASP:CA	1:168:A:ASP:C	1:169:A:ALA:N	15	28.1
(1,264)	1:127:C:ALA:N	1:127:C:ALA:CA	1:127:C:ALA:C	1:128:C:PRO:N	16	28.08
(1,52)	1:127:A:ALA:N	1:127:A:ALA:CA	1:127:A:ALA:C	1:128:A:PRO:N	15	27.78
(1,292)	1:168:C:ASP:N	1:168:C:ASP:CA	1:168:C:ASP:C	1:169:C:ALA:N	15	27.7
(1,186)	1:168:B:ASP:N	1:168:B:ASP:CA	1:168:B:ASP:C	1:169:B:ALA:N	15	27.54
(1,52)	1:127:A:ALA:N	1:127:A:ALA:CA	1:127:A:ALA:C	1:128:A:PRO:N	12	27.16
(1,292)	1:168:C:ASP:N	1:168:C:ASP:CA	1:168:C:ASP:C	1:169:C:ALA:N	13	27.08
(1,186)	1:168:B:ASP:N	1:168:B:ASP:CA	1:168:B:ASP:C	1:169:B:ALA:N	13	26.99
(1,226)	1:100:C:GLY:N	1:100:C:GLY:CA	1:100:C:GLY:C	1:101:C:LEU:N	10	26.86

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,80)	1:168:A:ASP:N	1:168:A:ASP:CA	1:168:A:ASP:C	1:169:A:ALA:N	13	26.84
(1,120)	1:100:B:GLY:N	1:100:B:GLY:CA	1:100:B:GLY:C	1:101:B:LEU:N	9	26.81
(1,120)	1:100:B:GLY:N	1:100:B:GLY:CA	1:100:B:GLY:C	1:101:B:LEU:N	10	26.34
(1,226)	1:100:C:GLY:N	1:100:C:GLY:CA	1:100:C:GLY:C	1:101:C:LEU:N	9	26.16
(1,14)	1:100:A:GLY:N	1:100:A:GLY:CA	1:100:A:GLY:C	1:101:A:LEU:N	10	25.28
(1,158)	1:127:B:ALA:N	1:127:B:ALA:CA	1:127:B:ALA:C	1:128:B:PRO:N	9	25.08
(1,52)	1:127:A:ALA:N	1:127:A:ALA:CA	1:127:A:ALA:C	1:128:A:PRO:N	9	24.94
(1,264)	1:127:C:ALA:N	1:127:C:ALA:CA	1:127:C:ALA:C	1:128:C:PRO:N	9	24.69
(1,226)	1:100:C:GLY:N	1:100:C:GLY:CA	1:100:C:GLY:C	1:101:C:LEU:N	16	24.6
(1,120)	1:100:B:GLY:N	1:100:B:GLY:CA	1:100:B:GLY:C	1:101:B:LEU:N	16	23.84
(1,14)	1:100:A:GLY:N	1:100:A:GLY:CA	1:100:A:GLY:C	1:101:A:LEU:N	16	23.78
(1,186)	1:168:B:ASP:N	1:168:B:ASP:CA	1:168:B:ASP:C	1:169:B:ALA:N	12	20.73
(1,292)	1:168:C:ASP:N	1:168:C:ASP:CA	1:168:C:ASP:C	1:169:C:ALA:N	12	20.51
(1,80)	1:168:A:ASP:N	1:168:A:ASP:CA	1:168:A:ASP:C	1:169:A:ALA:N	12	18.54
(1,14)	1:100:A:GLY:N	1:100:A:GLY:CA	1:100:A:GLY:C	1:101:A:LEU:N	9	17.67
(1,14)	1:100:A:GLY:N	1:100:A:GLY:CA	1:100:A:GLY:C	1:101:A:LEU:N	14	15.86
(1,120)	1:100:B:GLY:N	1:100:B:GLY:CA	1:100:B:GLY:C	1:101:B:LEU:N	14	14.75
(1,226)	1:100:C:GLY:N	1:100:C:GLY:CA	1:100:C:GLY:C	1:101:C:LEU:N	14	14.44
(1,226)	1:100:C:GLY:N	1:100:C:GLY:CA	1:100:C:GLY:C	1:101:C:LEU:N	12	14.27
(1,14)	1:100:A:GLY:N	1:100:A:GLY:CA	1:100:A:GLY:C	1:101:A:LEU:N	12	13.82
(1,120)	1:100:B:GLY:N	1:100:B:GLY:CA	1:100:B:GLY:C	1:101:B:LEU:N	12	13.66
(1,120)	1:100:B:GLY:N	1:100:B:GLY:CA	1:100:B:GLY:C	1:101:B:LEU:N	17	11.95
(1,120)	1:100:B:GLY:N	1:100:B:GLY:CA	1:100:B:GLY:C	1:101:B:LEU:N	3	11.87
(1,226)	1:100:C:GLY:N	1:100:C:GLY:CA	1:100:C:GLY:C	1:101:C:LEU:N	6	11.58
(1,226)	1:100:C:GLY:N	1:100:C:GLY:CA	1:100:C:GLY:C	1:101:C:LEU:N	3	11.57
(1,226)	1:100:C:GLY:N	1:100:C:GLY:CA	1:100:C:GLY:C	1:101:C:LEU:N	17	11.54
(1,120)	1:100:B:GLY:N	1:100:B:GLY:CA	1:100:B:GLY:C	1:101:B:LEU:N	6	10.53
(1,226)	1:100:C:GLY:N	1:100:C:GLY:CA	1:100:C:GLY:C	1:101:C:LEU:N	7	10.32
(1,120)	1:100:B:GLY:N	1:100:B:GLY:CA	1:100:B:GLY:C	1:101:B:LEU:N	7	9.89
(1,226)	1:100:C:GLY:N	1:100:C:GLY:CA	1:100:C:GLY:C	1:101:C:LEU:N	5	9.61
(1,14)	1:100:A:GLY:N	1:100:A:GLY:CA	1:100:A:GLY:C	1:101:A:LEU:N	17	9.59
(1,226)	1:100:C:GLY:N	1:100:C:GLY:CA	1:100:C:GLY:C	1:101:C:LEU:N	19	8.86
(1,120)	1:100:B:GLY:N	1:100:B:GLY:CA	1:100:B:GLY:C	1:101:B:LEU:N	19	8.62
(1,120)	1:100:B:GLY:N	1:100:B:GLY:CA	1:100:B:GLY:C	1:101:B:LEU:N	5	8.45
(1,109)	1:91:B:THR:C	1:92:B:ALA:N	1:92:B:ALA:CA	1:92:B:ALA:C	5	7.97
(1,14)	1:100:A:GLY:N	1:100:A:GLY:CA	1:100:A:GLY:C	1:101:A:LEU:N	3	7.66
(1,3)	1:91:A:THR:C	1:92:A:ALA:N	1:92:A:ALA:CA	1:92:A:ALA:C	5	6.9
(1,68)	1:139:A:ARG:N	1:139:A:ARG:CA	1:139:A:ARG:C	1:140:A:LYS:N	8	6.87
(1,14)	1:100:A:GLY:N	1:100:A:GLY:CA	1:100:A:GLY:C	1:101:A:LEU:N	15	6.61
(1,120)	1:100:B:GLY:N	1:100:B:GLY:CA	1:100:B:GLY:C	1:101:B:LEU:N	8	6.6
(1,215)	1:91:C:THR:C	1:92:C:ALA:N	1:92:C:ALA:CA	1:92:C:ALA:C	5	6.56
(1,226)	1:100:C:GLY:N	1:100:C:GLY:CA	1:100:C:GLY:C	1:101:C:LEU:N	8	6.26
(1,120)	1:100:B:GLY:N	1:100:B:GLY:CA	1:100:B:GLY:C	1:101:B:LEU:N	20	6.02
(1,14)	1:100:A:GLY:N	1:100:A:GLY:CA	1:100:A:GLY:C	1:101:A:LEU:N	1	5.82
(1,68)	1:139:A:ARG:N	1:139:A:ARG:CA	1:139:A:ARG:C	1:140:A:LYS:N	6	5.81
(1,226)	1:100:C:GLY:N	1:100:C:GLY:CA	1:100:C:GLY:C	1:101:C:LEU:N	13	5.67
(1,120)	1:100:B:GLY:N	1:100:B:GLY:CA	1:100:B:GLY:C	1:101:B:LEU:N	2	5.66
(1,226)	1:100:C:GLY:N	1:100:C:GLY:CA	1:100:C:GLY:C	1:101:C:LEU:N	20	5.54
(1,68)	1:139:A:ARG:N	1:139:A:ARG:CA	1:139:A:ARG:C	1:140:A:LYS:N	1	5.45
(1,68)	1:139:A:ARG:N	1:139:A:ARG:CA	1:139:A:ARG:C	1:140:A:LYS:N	3	5.42
(1,3)	1:91:A:THR:C	1:92:A:ALA:N	1:92:A:ALA:CA	1:92:A:ALA:C	10	5.34

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,120)	1:100:B:GLY:N	1:100:B:GLY:CA	1:100:B:GLY:C	1:101:B:LEU:N	13	5.33
(1,14)	1:100:A:GLY:N	1:100:A:GLY:CA	1:100:A:GLY:C	1:101:A:LEU:N	8	5.18
(1,226)	1:100:C:GLY:N	1:100:C:GLY:CA	1:100:C:GLY:C	1:101:C:LEU:N	15	5.13
(1,226)	1:100:C:GLY:N	1:100:C:GLY:CA	1:100:C:GLY:C	1:101:C:LEU:N	2	5.03
(1,68)	1:139:A:ARG:N	1:139:A:ARG:CA	1:139:A:ARG:C	1:140:A:LYS:N	12	5.01
(1,33)	1:113:A:TYR:C	1:114:A:LYS:N	1:114:A:LYS:CA	1:114:A:LYS:C	3	4.96
(1,144)	1:118:B:GLY:N	1:118:B:GLY:CA	1:118:B:GLY:C	1:119:B:THR:N	8	4.95
(1,14)	1:100:A:GLY:N	1:100:A:GLY:CA	1:100:A:GLY:C	1:101:A:LEU:N	5	4.86
(1,14)	1:100:A:GLY:N	1:100:A:GLY:CA	1:100:A:GLY:C	1:101:A:LEU:N	7	4.84
(1,250)	1:118:C:GLY:N	1:118:C:GLY:CA	1:118:C:GLY:C	1:119:C:THR:N	8	4.82
(1,69)	1:139:A:ARG:C	1:140:A:LYS:N	1:140:A:LYS:CA	1:140:A:LYS:C	8	4.78
(1,3)	1:91:A:THR:C	1:92:A:ALA:N	1:92:A:ALA:CA	1:92:A:ALA:C	13	4.75
(1,35)	1:115:A:PRO:C	1:116:A:ALA:N	1:116:A:ALA:CA	1:116:A:ALA:C	8	4.67
(1,68)	1:139:A:ARG:N	1:139:A:ARG:CA	1:139:A:ARG:C	1:140:A:LYS:N	20	4.66
(1,68)	1:139:A:ARG:N	1:139:A:ARG:CA	1:139:A:ARG:C	1:140:A:LYS:N	4	4.64
(1,38)	1:118:A:GLY:N	1:118:A:GLY:CA	1:118:A:GLY:C	1:119:A:THR:N	8	4.64
(1,153)	1:124:B:MET:C	1:125:B:LYS:N	1:125:B:LYS:CA	1:125:B:LYS:C	4	4.62
(1,68)	1:139:A:ARG:N	1:139:A:ARG:CA	1:139:A:ARG:C	1:140:A:LYS:N	15	4.62
(1,68)	1:139:A:ARG:N	1:139:A:ARG:CA	1:139:A:ARG:C	1:140:A:LYS:N	19	4.62
(1,247)	1:115:C:PRO:C	1:116:C:ALA:N	1:116:C:ALA:CA	1:116:C:ALA:C	8	4.55
(1,92)	1:187:A:THR:N	1:187:A:THR:CA	1:187:A:THR:C	1:188:A:LEU:N	5	4.54
(1,259)	1:124:C:MET:C	1:125:C:LYS:N	1:125:C:LYS:CA	1:125:C:LYS:C	4	4.51
(1,68)	1:139:A:ARG:N	1:139:A:ARG:CA	1:139:A:ARG:C	1:140:A:LYS:N	7	4.46
(1,68)	1:139:A:ARG:N	1:139:A:ARG:CA	1:139:A:ARG:C	1:140:A:LYS:N	2	4.35
(1,68)	1:139:A:ARG:N	1:139:A:ARG:CA	1:139:A:ARG:C	1:140:A:LYS:N	16	4.35
(1,170)	1:137:B:LEU:N	1:137:B:LEU:CA	1:137:B:LEU:C	1:138:B:THR:N	8	4.3
(1,141)	1:115:B:PRO:C	1:116:B:ALA:N	1:116:B:ALA:CA	1:116:B:ALA:C	8	4.3
(1,68)	1:139:A:ARG:N	1:139:A:ARG:CA	1:139:A:ARG:C	1:140:A:LYS:N	17	4.29
(1,68)	1:139:A:ARG:N	1:139:A:ARG:CA	1:139:A:ARG:C	1:140:A:LYS:N	5	4.28
(1,68)	1:139:A:ARG:N	1:139:A:ARG:CA	1:139:A:ARG:C	1:140:A:LYS:N	13	4.24
(1,64)	1:137:A:LEU:N	1:137:A:LEU:CA	1:137:A:LEU:C	1:138:A:THR:N	4	4.22
(1,170)	1:137:B:LEU:N	1:137:B:LEU:CA	1:137:B:LEU:C	1:138:B:THR:N	4	4.21
(1,40)	1:121:A:CYS:N	1:121:A:CYS:CA	1:121:A:CYS:C	1:122:A:TYR:N	7	4.17
(1,259)	1:124:C:MET:C	1:125:C:LYS:N	1:125:C:LYS:CA	1:125:C:LYS:C	15	4.16
(1,68)	1:139:A:ARG:N	1:139:A:ARG:CA	1:139:A:ARG:C	1:140:A:LYS:N	11	4.16
(1,3)	1:91:A:THR:C	1:92:A:ALA:N	1:92:A:ALA:CA	1:92:A:ALA:C	3	4.13
(1,259)	1:124:C:MET:C	1:125:C:LYS:N	1:125:C:LYS:CA	1:125:C:LYS:C	9	4.12
(1,102)	1:194:A:LEU:N	1:194:A:LEU:CA	1:194:A:LEU:C	1:195:A:TYR:N	7	4.11
(1,120)	1:100:B:GLY:N	1:100:B:GLY:CA	1:100:B:GLY:C	1:101:B:LEU:N	15	4.09
(1,153)	1:124:B:MET:C	1:125:B:LYS:N	1:125:B:LYS:CA	1:125:B:LYS:C	15	4.02
(1,38)	1:118:A:GLY:N	1:118:A:GLY:CA	1:118:A:GLY:C	1:119:A:THR:N	3	4.01
(1,280)	1:139:C:ARG:N	1:139:C:ARG:CA	1:139:C:ARG:C	1:140:C:LYS:N	2	3.98
(1,174)	1:139:B:ARG:N	1:139:B:ARG:CA	1:139:B:ARG:C	1:140:B:LYS:N	2	3.98
(1,68)	1:139:A:ARG:N	1:139:A:ARG:CA	1:139:A:ARG:C	1:140:A:LYS:N	9	3.91
(1,276)	1:137:C:LEU:N	1:137:C:LEU:CA	1:137:C:LEU:C	1:138:C:THR:N	4	3.9
(1,174)	1:139:B:ARG:N	1:139:B:ARG:CA	1:139:B:ARG:C	1:140:B:LYS:N	6	3.9
(1,102)	1:194:A:LEU:N	1:194:A:LEU:CA	1:194:A:LEU:C	1:195:A:TYR:N	16	3.9
(1,58)	1:133:A:SER:N	1:133:A:SER:CA	1:133:A:SER:C	1:134:A:LEU:N	12	3.88
(1,96)	1:189:A:CYS:N	1:189:A:CYS:CA	1:189:A:CYS:C	1:190:A:GLY:N	19	3.82
(1,153)	1:124:B:MET:C	1:125:B:LYS:N	1:125:B:LYS:CA	1:125:B:LYS:C	9	3.81
(1,14)	1:100:A:GLY:N	1:100:A:GLY:CA	1:100:A:GLY:C	1:101:A:LEU:N	2	3.81

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,276)	1:137:C:LEU:N	1:137:C:LEU:CA	1:137:C:LEU:C	1:138:C:THR:N	8	3.79
(1,153)	1:124:B:MET:C	1:125:B:LYS:N	1:125:B:LYS:CA	1:125:B:LYS:C	19	3.79
(1,96)	1:189:A:CYS:N	1:189:A:CYS:CA	1:189:A:CYS:C	1:190:A:GLY:N	16	3.75
(1,68)	1:139:A:ARG:N	1:139:A:ARG:CA	1:139:A:ARG:C	1:140:A:LYS:N	18	3.74
(1,259)	1:124:C:MET:C	1:125:C:LYS:N	1:125:C:LYS:CA	1:125:C:LYS:C	19	3.73
(1,280)	1:139:C:ARG:N	1:139:C:ARG:CA	1:139:C:ARG:C	1:140:C:LYS:N	7	3.72
(1,14)	1:100:A:GLY:N	1:100:A:GLY:CA	1:100:A:GLY:C	1:101:A:LEU:N	13	3.71
(1,280)	1:139:C:ARG:N	1:139:C:ARG:CA	1:139:C:ARG:C	1:140:C:LYS:N	6	3.7
(1,174)	1:139:B:ARG:N	1:139:B:ARG:CA	1:139:B:ARG:C	1:140:B:LYS:N	7	3.7
(1,144)	1:118:B:GLY:N	1:118:B:GLY:CA	1:118:B:GLY:C	1:119:B:THR:N	3	3.7
(1,250)	1:118:C:GLY:N	1:118:C:GLY:CA	1:118:C:GLY:C	1:119:C:THR:N	3	3.69
(1,14)	1:100:A:GLY:N	1:100:A:GLY:CA	1:100:A:GLY:C	1:101:A:LEU:N	6	3.66
(1,174)	1:139:B:ARG:N	1:139:B:ARG:CA	1:139:B:ARG:C	1:140:B:LYS:N	8	3.65
(1,153)	1:124:B:MET:C	1:125:B:LYS:N	1:125:B:LYS:CA	1:125:B:LYS:C	1	3.64
(1,280)	1:139:C:ARG:N	1:139:C:ARG:CA	1:139:C:ARG:C	1:140:C:LYS:N	17	3.63
(1,280)	1:139:C:ARG:N	1:139:C:ARG:CA	1:139:C:ARG:C	1:140:C:LYS:N	8	3.61
(1,68)	1:139:A:ARG:N	1:139:A:ARG:CA	1:139:A:ARG:C	1:140:A:LYS:N	14	3.6
(1,58)	1:133:A:SER:N	1:133:A:SER:CA	1:133:A:SER:C	1:134:A:LEU:N	20	3.6
(1,174)	1:139:B:ARG:N	1:139:B:ARG:CA	1:139:B:ARG:C	1:140:B:LYS:N	17	3.58
(1,102)	1:194:A:LEU:N	1:194:A:LEU:CA	1:194:A:LEU:C	1:195:A:TYR:N	4	3.54
(1,256)	1:123:C:ILE:N	1:123:C:ILE:CA	1:123:C:ILE:C	1:124:C:MET:N	19	3.52
(1,174)	1:139:B:ARG:N	1:139:B:ARG:CA	1:139:B:ARG:C	1:140:B:LYS:N	3	3.47
(1,150)	1:123:B:ILE:N	1:123:B:ILE:CA	1:123:B:ILE:C	1:124:B:MET:N	15	3.47
(1,150)	1:123:B:ILE:N	1:123:B:ILE:CA	1:123:B:ILE:C	1:124:B:MET:N	19	3.47
(1,96)	1:189:A:CYS:N	1:189:A:CYS:CA	1:189:A:CYS:C	1:190:A:GLY:N	13	3.47
(1,280)	1:139:C:ARG:N	1:139:C:ARG:CA	1:139:C:ARG:C	1:140:C:LYS:N	1	3.46
(1,174)	1:139:B:ARG:N	1:139:B:ARG:CA	1:139:B:ARG:C	1:140:B:LYS:N	11	3.46
(1,174)	1:139:B:ARG:N	1:139:B:ARG:CA	1:139:B:ARG:C	1:140:B:LYS:N	20	3.45
(1,170)	1:137:B:LEU:N	1:137:B:LEU:CA	1:137:B:LEU:C	1:138:B:THR:N	13	3.45
(1,259)	1:124:C:MET:C	1:125:C:LYS:N	1:125:C:LYS:CA	1:125:C:LYS:C	1	3.44
(1,68)	1:139:A:ARG:N	1:139:A:ARG:CA	1:139:A:ARG:C	1:140:A:LYS:N	10	3.44
(1,280)	1:139:C:ARG:N	1:139:C:ARG:CA	1:139:C:ARG:C	1:140:C:LYS:N	4	3.43
(1,280)	1:139:C:ARG:N	1:139:C:ARG:CA	1:139:C:ARG:C	1:140:C:LYS:N	11	3.42
(1,174)	1:139:B:ARG:N	1:139:B:ARG:CA	1:139:B:ARG:C	1:140:B:LYS:N	4	3.4
(1,96)	1:189:A:CYS:N	1:189:A:CYS:CA	1:189:A:CYS:C	1:190:A:GLY:N	4	3.39
(1,109)	1:91:B:THR:C	1:92:B:ALA:N	1:92:B:ALA:CA	1:92:B:ALA:C	10	3.38
(1,308)	1:189:C:CYS:N	1:189:C:CYS:CA	1:189:C:CYS:C	1:190:C:GLY:N	13	3.37
(1,102)	1:194:A:LEU:N	1:194:A:LEU:CA	1:194:A:LEU:C	1:195:A:TYR:N	9	3.37
(1,92)	1:187:A:THR:N	1:187:A:THR:CA	1:187:A:THR:C	1:188:A:LEU:N	16	3.37
(1,202)	1:189:B:CYS:N	1:189:B:CYS:CA	1:189:B:CYS:C	1:190:B:GLY:N	13	3.36
(1,215)	1:91:C:THR:C	1:92:C:ALA:N	1:92:C:ALA:CA	1:92:C:ALA:C	10	3.34
(1,164)	1:133:B:SER:N	1:133:B:SER:CA	1:133:B:SER:C	1:134:B:LEU:N	20	3.34
(1,226)	1:100:C:GLY:N	1:100:C:GLY:CA	1:100:C:GLY:C	1:101:C:LEU:N	1	3.33
(1,174)	1:139:B:ARG:N	1:139:B:ARG:CA	1:139:B:ARG:C	1:140:B:LYS:N	19	3.33
(1,164)	1:133:B:SER:N	1:133:B:SER:CA	1:133:B:SER:C	1:134:B:LEU:N	12	3.33
(1,102)	1:194:A:LEU:N	1:194:A:LEU:CA	1:194:A:LEU:C	1:195:A:TYR:N	5	3.33
(1,280)	1:139:C:ARG:N	1:139:C:ARG:CA	1:139:C:ARG:C	1:140:C:LYS:N	12	3.32
(1,64)	1:137:A:LEU:N	1:137:A:LEU:CA	1:137:A:LEU:C	1:138:A:THR:N	17	3.32
(1,96)	1:189:A:CYS:N	1:189:A:CYS:CA	1:189:A:CYS:C	1:190:A:GLY:N	7	3.31
(1,174)	1:139:B:ARG:N	1:139:B:ARG:CA	1:139:B:ARG:C	1:140:B:LYS:N	1	3.3
(1,280)	1:139:C:ARG:N	1:139:C:ARG:CA	1:139:C:ARG:C	1:140:C:LYS:N	3	3.29

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,280)	1:139:C:ARG:N	1:139:C:ARG:CA	1:139:C:ARG:C	1:140:C:LYS:N	20	3.29
(1,153)	1:124:B:MET:C	1:125:B:LYS:N	1:125:B:LYS:CA	1:125:B:LYS:C	12	3.29
(1,102)	1:194:A:LEU:N	1:194:A:LEU:CA	1:194:A:LEU:C	1:195:A:TYR:N	15	3.29
(1,96)	1:189:A:CYS:N	1:189:A:CYS:CA	1:189:A:CYS:C	1:190:A:GLY:N	5	3.29
(1,174)	1:139:B:ARG:N	1:139:B:ARG:CA	1:139:B:ARG:C	1:140:B:LYS:N	12	3.28
(1,64)	1:137:A:LEU:N	1:137:A:LEU:CA	1:137:A:LEU:C	1:138:A:THR:N	10	3.28
(1,247)	1:115:C:PRO:C	1:116:C:ALA:N	1:116:C:ALA:CA	1:116:C:ALA:C	14	3.27
(1,280)	1:139:C:ARG:N	1:139:C:ARG:CA	1:139:C:ARG:C	1:140:C:LYS:N	15	3.26
(1,102)	1:194:A:LEU:N	1:194:A:LEU:CA	1:194:A:LEU:C	1:195:A:TYR:N	2	3.26
(1,40)	1:121:A:CYS:N	1:121:A:CYS:CA	1:121:A:CYS:C	1:122:A:TYR:N	19	3.26
(1,174)	1:139:B:ARG:N	1:139:B:ARG:CA	1:139:B:ARG:C	1:140:B:LYS:N	15	3.24
(1,202)	1:189:B:CYS:N	1:189:B:CYS:CA	1:189:B:CYS:C	1:190:B:GLY:N	16	3.22
(1,35)	1:115:A:PRO:C	1:116:A:ALA:N	1:116:A:ALA:CA	1:116:A:ALA:C	20	3.22
(1,308)	1:189:C:CYS:N	1:189:C:CYS:CA	1:189:C:CYS:C	1:190:C:GLY:N	16	3.21
(1,174)	1:139:B:ARG:N	1:139:B:ARG:CA	1:139:B:ARG:C	1:140:B:LYS:N	13	3.21
(1,170)	1:137:B:LEU:N	1:137:B:LEU:CA	1:137:B:LEU:C	1:138:B:THR:N	5	3.2
(1,150)	1:123:B:ILE:N	1:123:B:ILE:CA	1:123:B:ILE:C	1:124:B:MET:N	20	3.2
(1,120)	1:100:B:GLY:N	1:100:B:GLY:CA	1:100:B:GLY:C	1:101:B:LEU:N	1	3.2
(1,308)	1:189:C:CYS:N	1:189:C:CYS:CA	1:189:C:CYS:C	1:190:C:GLY:N	19	3.19
(1,182)	1:143:B:ASN:N	1:143:B:ASN:CA	1:143:B:ASN:C	1:144:B:PHE:N	1	3.19
(1,164)	1:133:B:SER:N	1:133:B:SER:CA	1:133:B:SER:C	1:134:B:LEU:N	3	3.19
(1,38)	1:118:A:GLY:N	1:118:A:GLY:CA	1:118:A:GLY:C	1:119:A:THR:N	6	3.19
(1,270)	1:133:C:SER:N	1:133:C:SER:CA	1:133:C:SER:C	1:134:C:LEU:N	20	3.18
(1,259)	1:124:C:MET:C	1:125:C:LYS:N	1:125:C:LYS:CA	1:125:C:LYS:C	12	3.18
(1,170)	1:137:B:LEU:N	1:137:B:LEU:CA	1:137:B:LEU:C	1:138:B:THR:N	20	3.18
(1,64)	1:137:A:LEU:N	1:137:A:LEU:CA	1:137:A:LEU:C	1:138:A:THR:N	7	3.18
(1,259)	1:124:C:MET:C	1:125:C:LYS:N	1:125:C:LYS:CA	1:125:C:LYS:C	3	3.17
(1,38)	1:118:A:GLY:N	1:118:A:GLY:CA	1:118:A:GLY:C	1:119:A:THR:N	4	3.17
(1,102)	1:194:A:LEU:N	1:194:A:LEU:CA	1:194:A:LEU:C	1:195:A:TYR:N	11	3.16
(1,256)	1:123:C:ILE:N	1:123:C:ILE:CA	1:123:C:ILE:C	1:124:C:MET:N	13	3.15
(1,256)	1:123:C:ILE:N	1:123:C:ILE:CA	1:123:C:ILE:C	1:124:C:MET:N	15	3.15
(1,174)	1:139:B:ARG:N	1:139:B:ARG:CA	1:139:B:ARG:C	1:140:B:LYS:N	9	3.15
(1,58)	1:133:A:SER:N	1:133:A:SER:CA	1:133:A:SER:C	1:134:A:LEU:N	3	3.15
(1,256)	1:123:C:ILE:N	1:123:C:ILE:CA	1:123:C:ILE:C	1:124:C:MET:N	8	3.13
(1,170)	1:137:B:LEU:N	1:137:B:LEU:CA	1:137:B:LEU:C	1:138:B:THR:N	15	3.13
(1,280)	1:139:C:ARG:N	1:139:C:ARG:CA	1:139:C:ARG:C	1:140:C:LYS:N	19	3.12
(1,170)	1:137:B:LEU:N	1:137:B:LEU:CA	1:137:B:LEU:C	1:138:B:THR:N	3	3.12
(1,31)	1:112:A:ALA:C	1:113:A:TYR:N	1:113:A:TYR:CA	1:113:A:TYR:C	9	3.12
(1,280)	1:139:C:ARG:N	1:139:C:ARG:CA	1:139:C:ARG:C	1:140:C:LYS:N	9	3.11
(1,280)	1:139:C:ARG:N	1:139:C:ARG:CA	1:139:C:ARG:C	1:140:C:LYS:N	16	3.1
(1,250)	1:118:C:GLY:N	1:118:C:GLY:CA	1:118:C:GLY:C	1:119:C:THR:N	4	3.1
(1,174)	1:139:B:ARG:N	1:139:B:ARG:CA	1:139:B:ARG:C	1:140:B:LYS:N	16	3.1
(1,2)	1:91:A:THR:N	1:91:A:THR:CA	1:91:A:THR:C	1:92:A:ALA:N	6	3.1
(1,280)	1:139:C:ARG:N	1:139:C:ARG:CA	1:139:C:ARG:C	1:140:C:LYS:N	13	3.09
(1,170)	1:137:B:LEU:N	1:137:B:LEU:CA	1:137:B:LEU:C	1:138:B:THR:N	6	3.08
(1,102)	1:194:A:LEU:N	1:194:A:LEU:CA	1:194:A:LEU:C	1:195:A:TYR:N	8	3.08
(1,280)	1:139:C:ARG:N	1:139:C:ARG:CA	1:139:C:ARG:C	1:140:C:LYS:N	14	3.07
(1,256)	1:123:C:ILE:N	1:123:C:ILE:CA	1:123:C:ILE:C	1:124:C:MET:N	20	3.07
(1,103)	1:194:A:LEU:C	1:195:A:TYR:N	1:195:A:TYR:CA	1:195:A:TYR:C	12	3.07
(1,47)	1:124:A:MET:C	1:125:A:LYS:N	1:125:A:LYS:CA	1:125:A:LYS:C	4	3.07
(1,24)	1:109:A:LEU:N	1:109:A:LEU:CA	1:109:A:LEU:C	1:110:A:LEU:N	2	3.07

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,96)	1:189:A:CYS:N	1:189:A:CYS:CA	1:189:A:CYS:C	1:190:A:GLY:N	20	3.06
(1,202)	1:189:B:CYS:N	1:189:B:CYS:CA	1:189:B:CYS:C	1:190:B:GLY:N	8	3.05
(1,174)	1:139:B:ARG:N	1:139:B:ARG:CA	1:139:B:ARG:C	1:140:B:LYS:N	14	3.05
(1,150)	1:123:B:ILE:N	1:123:B:ILE:CA	1:123:B:ILE:C	1:124:B:MET:N	9	3.05
(1,96)	1:189:A:CYS:N	1:189:A:CYS:CA	1:189:A:CYS:C	1:190:A:GLY:N	11	3.05
(1,64)	1:137:A:LEU:N	1:137:A:LEU:CA	1:137:A:LEU:C	1:138:A:THR:N	15	3.05
(1,280)	1:139:C:ARG:N	1:139:C:ARG:CA	1:139:C:ARG:C	1:140:C:LYS:N	18	3.04
(1,153)	1:124:B:MET:C	1:125:B:LYS:N	1:125:B:LYS:CA	1:125:B:LYS:C	3	3.03
(1,69)	1:139:A:ARG:C	1:140:A:LYS:N	1:140:A:LYS:CA	1:140:A:LYS:C	6	3.03
(1,15)	1:100:A:GLY:C	1:101:A:LEU:N	1:101:A:LEU:CA	1:101:A:LEU:C	3	3.03
(1,308)	1:189:C:CYS:N	1:189:C:CYS:CA	1:189:C:CYS:C	1:190:C:GLY:N	4	3.02
(1,182)	1:143:B:ASN:N	1:143:B:ASN:CA	1:143:B:ASN:C	1:144:B:PHE:N	8	3.02
(1,159)	1:128:B:PRO:C	1:129:B:GLU:N	1:129:B:GLU:CA	1:129:B:GLU:C	17	3.02
(1,150)	1:123:B:ILE:N	1:123:B:ILE:CA	1:123:B:ILE:C	1:124:B:MET:N	13	3.02
(1,250)	1:118:C:GLY:N	1:118:C:GLY:CA	1:118:C:GLY:C	1:119:C:THR:N	1	3.01
(1,150)	1:123:B:ILE:N	1:123:B:ILE:CA	1:123:B:ILE:C	1:124:B:MET:N	8	3.01
(1,174)	1:139:B:ARG:N	1:139:B:ARG:CA	1:139:B:ARG:C	1:140:B:LYS:N	5	3.0
(1,170)	1:137:B:LEU:N	1:137:B:LEU:CA	1:137:B:LEU:C	1:138:B:THR:N	1	2.99
(1,256)	1:123:C:ILE:N	1:123:C:ILE:CA	1:123:C:ILE:C	1:124:C:MET:N	3	2.98
(1,174)	1:139:B:ARG:N	1:139:B:ARG:CA	1:139:B:ARG:C	1:140:B:LYS:N	18	2.98
(1,167)	1:135:B:GLU:C	1:136:B:ALA:N	1:136:B:ALA:CA	1:136:B:ALA:C	4	2.98
(1,144)	1:118:B:GLY:N	1:118:B:GLY:CA	1:118:B:GLY:C	1:119:B:THR:N	1	2.97
(1,103)	1:194:A:LEU:C	1:195:A:TYR:N	1:195:A:TYR:CA	1:195:A:TYR:C	15	2.97
(1,276)	1:137:C:LEU:N	1:137:C:LEU:CA	1:137:C:LEU:C	1:138:C:THR:N	6	2.96
(1,141)	1:115:B:PRO:C	1:116:B:ALA:N	1:116:B:ALA:CA	1:116:B:ALA:C	14	2.96
(1,170)	1:137:B:LEU:N	1:137:B:LEU:CA	1:137:B:LEU:C	1:138:B:THR:N	12	2.94
(1,308)	1:189:C:CYS:N	1:189:C:CYS:CA	1:189:C:CYS:C	1:190:C:GLY:N	6	2.92
(1,308)	1:189:C:CYS:N	1:189:C:CYS:CA	1:189:C:CYS:C	1:190:C:GLY:N	8	2.92
(1,58)	1:133:A:SER:N	1:133:A:SER:CA	1:133:A:SER:C	1:134:A:LEU:N	7	2.92
(1,170)	1:137:B:LEU:N	1:137:B:LEU:CA	1:137:B:LEU:C	1:138:B:THR:N	11	2.91
(1,64)	1:137:A:LEU:N	1:137:A:LEU:CA	1:137:A:LEU:C	1:138:A:THR:N	16	2.91
(1,308)	1:189:C:CYS:N	1:189:C:CYS:CA	1:189:C:CYS:C	1:190:C:GLY:N	12	2.9
(1,280)	1:139:C:ARG:N	1:139:C:ARG:CA	1:139:C:ARG:C	1:140:C:LYS:N	5	2.9
(1,202)	1:189:B:CYS:N	1:189:B:CYS:CA	1:189:B:CYS:C	1:190:B:GLY:N	6	2.9
(1,44)	1:123:A:ILE:N	1:123:A:ILE:CA	1:123:A:ILE:C	1:124:A:MET:N	18	2.9
(1,150)	1:123:B:ILE:N	1:123:B:ILE:CA	1:123:B:ILE:C	1:124:B:MET:N	18	2.89
(1,64)	1:137:A:LEU:N	1:137:A:LEU:CA	1:137:A:LEU:C	1:138:A:THR:N	18	2.89
(1,144)	1:118:B:GLY:N	1:118:B:GLY:CA	1:118:B:GLY:C	1:119:B:THR:N	4	2.88
(1,276)	1:137:C:LEU:N	1:137:C:LEU:CA	1:137:C:LEU:C	1:138:C:THR:N	7	2.87
(1,265)	1:128:C:PRO:C	1:129:C:GLU:N	1:129:C:GLU:CA	1:129:C:GLU:C	17	2.87
(1,92)	1:187:A:THR:N	1:187:A:THR:CA	1:187:A:THR:C	1:188:A:LEU:N	12	2.87
(1,280)	1:139:C:ARG:N	1:139:C:ARG:CA	1:139:C:ARG:C	1:140:C:LYS:N	10	2.86
(1,202)	1:189:B:CYS:N	1:189:B:CYS:CA	1:189:B:CYS:C	1:190:B:GLY:N	1	2.86
(1,170)	1:137:B:LEU:N	1:137:B:LEU:CA	1:137:B:LEU:C	1:138:B:THR:N	19	2.86
(1,44)	1:123:A:ILE:N	1:123:A:ILE:CA	1:123:A:ILE:C	1:124:A:MET:N	19	2.86
(1,276)	1:137:C:LEU:N	1:137:C:LEU:CA	1:137:C:LEU:C	1:138:C:THR:N	13	2.85
(1,256)	1:123:C:ILE:N	1:123:C:ILE:CA	1:123:C:ILE:C	1:124:C:MET:N	9	2.85
(1,64)	1:137:A:LEU:N	1:137:A:LEU:CA	1:137:A:LEU:C	1:138:A:THR:N	2	2.85
(1,308)	1:189:C:CYS:N	1:189:C:CYS:CA	1:189:C:CYS:C	1:190:C:GLY:N	1	2.84
(1,202)	1:189:B:CYS:N	1:189:B:CYS:CA	1:189:B:CYS:C	1:190:B:GLY:N	12	2.84
(1,202)	1:189:B:CYS:N	1:189:B:CYS:CA	1:189:B:CYS:C	1:190:B:GLY:N	19	2.84

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,308)	1:189:C:CYS:N	1:189:C:CYS:CA	1:189:C:CYS:C	1:190:C:GLY:N	9	2.83
(1,256)	1:123:C:ILE:N	1:123:C:ILE:CA	1:123:C:ILE:C	1:124:C:MET:N	18	2.83
(1,202)	1:189:B:CYS:N	1:189:B:CYS:CA	1:189:B:CYS:C	1:190:B:GLY:N	20	2.83
(1,150)	1:123:B:ILE:N	1:123:B:ILE:CA	1:123:B:ILE:C	1:124:B:MET:N	3	2.83
(1,44)	1:123:A:ILE:N	1:123:A:ILE:CA	1:123:A:ILE:C	1:124:A:MET:N	3	2.82
(1,276)	1:137:C:LEU:N	1:137:C:LEU:CA	1:137:C:LEU:C	1:138:C:THR:N	16	2.81
(1,276)	1:137:C:LEU:N	1:137:C:LEU:CA	1:137:C:LEU:C	1:138:C:THR:N	17	2.81
(1,170)	1:137:B:LEU:N	1:137:B:LEU:CA	1:137:B:LEU:C	1:138:B:THR:N	18	2.81
(1,167)	1:135:B:GLU:C	1:136:B:ALA:N	1:136:B:ALA:CA	1:136:B:ALA:C	8	2.8
(1,102)	1:194:A:LEU:N	1:194:A:LEU:CA	1:194:A:LEU:C	1:195:A:TYR:N	18	2.8
(1,44)	1:123:A:ILE:N	1:123:A:ILE:CA	1:123:A:ILE:C	1:124:A:MET:N	15	2.8
(1,288)	1:143:C:ASN:N	1:143:C:ASN:CA	1:143:C:ASN:C	1:144:C:PHE:N	1	2.79
(1,250)	1:118:C:GLY:N	1:118:C:GLY:CA	1:118:C:GLY:C	1:119:C:THR:N	6	2.79
(1,96)	1:189:A:CYS:N	1:189:A:CYS:CA	1:189:A:CYS:C	1:190:A:GLY:N	1	2.79
(1,35)	1:115:A:PRO:C	1:116:A:ALA:N	1:116:A:ALA:CA	1:116:A:ALA:C	12	2.79
(1,276)	1:137:C:LEU:N	1:137:C:LEU:CA	1:137:C:LEU:C	1:138:C:THR:N	5	2.78
(1,276)	1:137:C:LEU:N	1:137:C:LEU:CA	1:137:C:LEU:C	1:138:C:THR:N	15	2.78
(1,202)	1:189:B:CYS:N	1:189:B:CYS:CA	1:189:B:CYS:C	1:190:B:GLY:N	4	2.76
(1,170)	1:137:B:LEU:N	1:137:B:LEU:CA	1:137:B:LEU:C	1:138:B:THR:N	14	2.76
(1,170)	1:137:B:LEU:N	1:137:B:LEU:CA	1:137:B:LEU:C	1:138:B:THR:N	16	2.76
(1,92)	1:187:A:THR:N	1:187:A:THR:CA	1:187:A:THR:C	1:188:A:LEU:N	1	2.76
(1,308)	1:189:C:CYS:N	1:189:C:CYS:CA	1:189:C:CYS:C	1:190:C:GLY:N	7	2.75
(1,174)	1:139:B:ARG:N	1:139:B:ARG:CA	1:139:B:ARG:C	1:140:B:LYS:N	10	2.75
(1,102)	1:194:A:LEU:N	1:194:A:LEU:CA	1:194:A:LEU:C	1:195:A:TYR:N	3	2.75
(1,64)	1:137:A:LEU:N	1:137:A:LEU:CA	1:137:A:LEU:C	1:138:A:THR:N	8	2.75
(1,308)	1:189:C:CYS:N	1:189:C:CYS:CA	1:189:C:CYS:C	1:190:C:GLY:N	20	2.74
(1,202)	1:189:B:CYS:N	1:189:B:CYS:CA	1:189:B:CYS:C	1:190:B:GLY:N	5	2.74
(1,202)	1:189:B:CYS:N	1:189:B:CYS:CA	1:189:B:CYS:C	1:190:B:GLY:N	9	2.73
(1,144)	1:118:B:GLY:N	1:118:B:GLY:CA	1:118:B:GLY:C	1:119:B:THR:N	6	2.73
(1,92)	1:187:A:THR:N	1:187:A:THR:CA	1:187:A:THR:C	1:188:A:LEU:N	3	2.73
(1,308)	1:189:C:CYS:N	1:189:C:CYS:CA	1:189:C:CYS:C	1:190:C:GLY:N	5	2.72
(1,276)	1:137:C:LEU:N	1:137:C:LEU:CA	1:137:C:LEU:C	1:138:C:THR:N	11	2.72
(1,250)	1:118:C:GLY:N	1:118:C:GLY:CA	1:118:C:GLY:C	1:119:C:THR:N	11	2.72
(1,202)	1:189:B:CYS:N	1:189:B:CYS:CA	1:189:B:CYS:C	1:190:B:GLY:N	7	2.72
(1,144)	1:118:B:GLY:N	1:118:B:GLY:CA	1:118:B:GLY:C	1:119:B:THR:N	9	2.72
(1,35)	1:115:A:PRO:C	1:116:A:ALA:N	1:116:A:ALA:CA	1:116:A:ALA:C	2	2.72
(1,35)	1:115:A:PRO:C	1:116:A:ALA:N	1:116:A:ALA:CA	1:116:A:ALA:C	19	2.71
(1,170)	1:137:B:LEU:N	1:137:B:LEU:CA	1:137:B:LEU:C	1:138:B:THR:N	7	2.7
(1,33)	1:113:A:TYR:C	1:114:A:LYS:N	1:114:A:LYS:CA	1:114:A:LYS:C	14	2.7
(1,64)	1:137:A:LEU:N	1:137:A:LEU:CA	1:137:A:LEU:C	1:138:A:THR:N	19	2.69
(1,150)	1:123:B:ILE:N	1:123:B:ILE:CA	1:123:B:ILE:C	1:124:B:MET:N	14	2.68
(1,259)	1:124:C:MET:C	1:125:C:LYS:N	1:125:C:LYS:CA	1:125:C:LYS:C	20	2.67
(1,243)	1:112:C:ALA:C	1:113:C:TYR:N	1:113:C:TYR:CA	1:113:C:TYR:C	9	2.67
(1,256)	1:123:C:ILE:N	1:123:C:ILE:CA	1:123:C:ILE:C	1:124:C:MET:N	17	2.66
(1,250)	1:118:C:GLY:N	1:118:C:GLY:CA	1:118:C:GLY:C	1:119:C:THR:N	9	2.66
(1,64)	1:137:A:LEU:N	1:137:A:LEU:CA	1:137:A:LEU:C	1:138:A:THR:N	6	2.66
(1,144)	1:118:B:GLY:N	1:118:B:GLY:CA	1:118:B:GLY:C	1:119:B:THR:N	12	2.65
(1,270)	1:133:C:SER:N	1:133:C:SER:CA	1:133:C:SER:C	1:134:C:LEU:N	12	2.64
(1,150)	1:123:B:ILE:N	1:123:B:ILE:CA	1:123:B:ILE:C	1:124:B:MET:N	4	2.64
(1,144)	1:118:B:GLY:N	1:118:B:GLY:CA	1:118:B:GLY:C	1:119:B:THR:N	15	2.64
(1,276)	1:137:C:LEU:N	1:137:C:LEU:CA	1:137:C:LEU:C	1:138:C:THR:N	3	2.63

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,256)	1:123:C:ILE:N	1:123:C:ILE:CA	1:123:C:ILE:C	1:124:C:MET:N	14	2.63
(1,144)	1:118:B:GLY:N	1:118:B:GLY:CA	1:118:B:GLY:C	1:119:B:THR:N	14	2.63
(1,44)	1:123:A:ILE:N	1:123:A:ILE:CA	1:123:A:ILE:C	1:124:A:MET:N	8	2.63
(1,288)	1:143:C:ASN:N	1:143:C:ASN:CA	1:143:C:ASN:C	1:144:C:PHE:N	8	2.62
(1,170)	1:137:B:LEU:N	1:137:B:LEU:CA	1:137:B:LEU:C	1:138:B:THR:N	17	2.62
(1,76)	1:143:A:ASN:N	1:143:A:ASN:CA	1:143:A:ASN:C	1:144:A:PHE:N	1	2.62
(1,35)	1:115:A:PRO:C	1:116:A:ALA:N	1:116:A:ALA:CA	1:116:A:ALA:C	17	2.62
(1,276)	1:137:C:LEU:N	1:137:C:LEU:CA	1:137:C:LEU:C	1:138:C:THR:N	18	2.61
(1,103)	1:194:A:LEU:C	1:195:A:TYR:N	1:195:A:TYR:CA	1:195:A:TYR:C	3	2.61
(1,250)	1:118:C:GLY:N	1:118:C:GLY:CA	1:118:C:GLY:C	1:119:C:THR:N	15	2.6
(1,144)	1:118:B:GLY:N	1:118:B:GLY:CA	1:118:B:GLY:C	1:119:B:THR:N	11	2.59
(1,44)	1:123:A:ILE:N	1:123:A:ILE:CA	1:123:A:ILE:C	1:124:A:MET:N	13	2.59
(1,44)	1:123:A:ILE:N	1:123:A:ILE:CA	1:123:A:ILE:C	1:124:A:MET:N	16	2.59
(1,53)	1:128:A:PRO:C	1:129:A:GLU:N	1:129:A:GLU:CA	1:129:A:GLU:C	17	2.58
(1,103)	1:194:A:LEU:C	1:195:A:TYR:N	1:195:A:TYR:CA	1:195:A:TYR:C	14	2.57
(1,96)	1:189:A:CYS:N	1:189:A:CYS:CA	1:189:A:CYS:C	1:190:A:GLY:N	17	2.57
(1,64)	1:137:A:LEU:N	1:137:A:LEU:CA	1:137:A:LEU:C	1:138:A:THR:N	5	2.57
(1,182)	1:143:B:ASN:N	1:143:B:ASN:CA	1:143:B:ASN:C	1:144:B:PHE:N	11	2.56
(1,153)	1:124:B:MET:C	1:125:B:LYS:N	1:125:B:LYS:CA	1:125:B:LYS:C	20	2.56
(1,35)	1:115:A:PRO:C	1:116:A:ALA:N	1:116:A:ALA:CA	1:116:A:ALA:C	14	2.56
(1,308)	1:189:C:CYS:N	1:189:C:CYS:CA	1:189:C:CYS:C	1:190:C:GLY:N	11	2.55
(1,276)	1:137:C:LEU:N	1:137:C:LEU:CA	1:137:C:LEU:C	1:138:C:THR:N	20	2.55
(1,170)	1:137:B:LEU:N	1:137:B:LEU:CA	1:137:B:LEU:C	1:138:B:THR:N	2	2.55
(1,44)	1:123:A:ILE:N	1:123:A:ILE:CA	1:123:A:ILE:C	1:124:A:MET:N	17	2.55
(1,250)	1:118:C:GLY:N	1:118:C:GLY:CA	1:118:C:GLY:C	1:119:C:THR:N	17	2.53
(1,150)	1:123:B:ILE:N	1:123:B:ILE:CA	1:123:B:ILE:C	1:124:B:MET:N	17	2.53
(1,92)	1:187:A:THR:N	1:187:A:THR:CA	1:187:A:THR:C	1:188:A:LEU:N	19	2.53
(1,12)	1:96:A:ILE:N	1:96:A:ILE:CA	1:96:A:ILE:C	1:97:A:GLY:N	3	2.53
(1,276)	1:137:C:LEU:N	1:137:C:LEU:CA	1:137:C:LEU:C	1:138:C:THR:N	10	2.52
(1,103)	1:194:A:LEU:C	1:195:A:TYR:N	1:195:A:TYR:CA	1:195:A:TYR:C	10	2.52
(1,64)	1:137:A:LEU:N	1:137:A:LEU:CA	1:137:A:LEU:C	1:138:A:THR:N	13	2.52
(1,167)	1:135:B:GLU:C	1:136:B:ALA:N	1:136:B:ALA:CA	1:136:B:ALA:C	3	2.51
(1,41)	1:121:A:CYS:C	1:122:A:TYR:N	1:122:A:TYR:CA	1:122:A:TYR:C	12	2.51
(1,276)	1:137:C:LEU:N	1:137:C:LEU:CA	1:137:C:LEU:C	1:138:C:THR:N	1	2.5
(1,276)	1:137:C:LEU:N	1:137:C:LEU:CA	1:137:C:LEU:C	1:138:C:THR:N	9	2.5
(1,256)	1:123:C:ILE:N	1:123:C:ILE:CA	1:123:C:ILE:C	1:124:C:MET:N	7	2.5
(1,38)	1:118:A:GLY:N	1:118:A:GLY:CA	1:118:A:GLY:C	1:119:A:THR:N	1	2.5
(1,308)	1:189:C:CYS:N	1:189:C:CYS:CA	1:189:C:CYS:C	1:190:C:GLY:N	17	2.49
(1,276)	1:137:C:LEU:N	1:137:C:LEU:CA	1:137:C:LEU:C	1:138:C:THR:N	12	2.49
(1,202)	1:189:B:CYS:N	1:189:B:CYS:CA	1:189:B:CYS:C	1:190:B:GLY:N	17	2.49
(1,170)	1:137:B:LEU:N	1:137:B:LEU:CA	1:137:B:LEU:C	1:138:B:THR:N	10	2.49
(1,96)	1:189:A:CYS:N	1:189:A:CYS:CA	1:189:A:CYS:C	1:190:A:GLY:N	12	2.49
(1,86)	1:184:A:ALA:N	1:184:A:ALA:CA	1:184:A:ALA:C	1:185:A:VAL:N	2	2.49
(1,276)	1:137:C:LEU:N	1:137:C:LEU:CA	1:137:C:LEU:C	1:138:C:THR:N	2	2.48
(1,198)	1:187:B:THR:N	1:187:B:THR:CA	1:187:B:THR:C	1:188:B:LEU:N	5	2.48
(1,250)	1:118:C:GLY:N	1:118:C:GLY:CA	1:118:C:GLY:C	1:119:C:THR:N	14	2.47
(1,164)	1:133:B:SER:N	1:133:B:SER:CA	1:133:B:SER:C	1:134:B:LEU:N	1	2.47
(1,83)	1:182:A:GLY:C	1:183:A:MET:N	1:183:A:MET:CA	1:183:A:MET:C	19	2.47
(1,35)	1:115:A:PRO:C	1:116:A:ALA:N	1:116:A:ALA:CA	1:116:A:ALA:C	5	2.47
(1,247)	1:115:C:PRO:C	1:116:C:ALA:N	1:116:C:ALA:CA	1:116:C:ALA:C	20	2.46
(1,202)	1:189:B:CYS:N	1:189:B:CYS:CA	1:189:B:CYS:C	1:190:B:GLY:N	11	2.46

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,150)	1:123:B:ILE:N	1:123:B:ILE:CA	1:123:B:ILE:C	1:124:B:MET:N	6	2.46
(1,144)	1:118:B:GLY:N	1:118:B:GLY:CA	1:118:B:GLY:C	1:119:B:THR:N	13	2.46
(1,102)	1:194:A:LEU:N	1:194:A:LEU:CA	1:194:A:LEU:C	1:195:A:TYR:N	1	2.46
(1,276)	1:137:C:LEU:N	1:137:C:LEU:CA	1:137:C:LEU:C	1:138:C:THR:N	14	2.45
(1,58)	1:133:A:SER:N	1:133:A:SER:CA	1:133:A:SER:C	1:134:A:LEU:N	5	2.45
(1,259)	1:124:C:MET:C	1:125:C:LYS:N	1:125:C:LYS:CA	1:125:C:LYS:C	18	2.44
(1,76)	1:143:A:ASN:N	1:143:A:ASN:CA	1:143:A:ASN:C	1:144:A:PHE:N	8	2.44
(1,170)	1:137:B:LEU:N	1:137:B:LEU:CA	1:137:B:LEU:C	1:138:B:THR:N	9	2.43
(1,102)	1:194:A:LEU:N	1:194:A:LEU:CA	1:194:A:LEU:C	1:195:A:TYR:N	10	2.43
(1,102)	1:194:A:LEU:N	1:194:A:LEU:CA	1:194:A:LEU:C	1:195:A:TYR:N	19	2.43
(1,276)	1:137:C:LEU:N	1:137:C:LEU:CA	1:137:C:LEU:C	1:138:C:THR:N	19	2.42
(1,137)	1:112:B:ALA:C	1:113:B:TYR:N	1:113:B:TYR:CA	1:113:B:TYR:C	9	2.42
(1,43)	1:122:A:TYR:C	1:123:A:ILE:N	1:123:A:ILE:CA	1:123:A:ILE:C	4	2.42
(1,259)	1:124:C:MET:C	1:125:C:LYS:N	1:125:C:LYS:CA	1:125:C:LYS:C	5	2.41
(1,44)	1:123:A:ILE:N	1:123:A:ILE:CA	1:123:A:ILE:C	1:124:A:MET:N	11	2.41
(1,250)	1:118:C:GLY:N	1:118:C:GLY:CA	1:118:C:GLY:C	1:119:C:THR:N	12	2.4
(1,247)	1:115:C:PRO:C	1:116:C:ALA:N	1:116:C:ALA:CA	1:116:C:ALA:C	11	2.4
(1,150)	1:123:B:ILE:N	1:123:B:ILE:CA	1:123:B:ILE:C	1:124:B:MET:N	7	2.4
(1,86)	1:184:A:ALA:N	1:184:A:ALA:CA	1:184:A:ALA:C	1:185:A:VAL:N	5	2.4
(1,182)	1:143:B:ASN:N	1:143:B:ASN:CA	1:143:B:ASN:C	1:144:B:PHE:N	3	2.39
(1,96)	1:189:A:CYS:N	1:189:A:CYS:CA	1:189:A:CYS:C	1:190:A:GLY:N	6	2.39
(1,308)	1:189:C:CYS:N	1:189:C:CYS:CA	1:189:C:CYS:C	1:190:C:GLY:N	14	2.38
(1,153)	1:124:B:MET:C	1:125:B:LYS:N	1:125:B:LYS:CA	1:125:B:LYS:C	5	2.38
(1,308)	1:189:C:CYS:N	1:189:C:CYS:CA	1:189:C:CYS:C	1:190:C:GLY:N	18	2.37
(1,202)	1:189:B:CYS:N	1:189:B:CYS:CA	1:189:B:CYS:C	1:190:B:GLY:N	18	2.37
(1,144)	1:118:B:GLY:N	1:118:B:GLY:CA	1:118:B:GLY:C	1:119:B:THR:N	7	2.37
(1,150)	1:123:B:ILE:N	1:123:B:ILE:CA	1:123:B:ILE:C	1:124:B:MET:N	2	2.36
(1,144)	1:118:B:GLY:N	1:118:B:GLY:CA	1:118:B:GLY:C	1:119:B:THR:N	16	2.36
(1,35)	1:115:A:PRO:C	1:116:A:ALA:N	1:116:A:ALA:CA	1:116:A:ALA:C	10	2.36
(1,150)	1:123:B:ILE:N	1:123:B:ILE:CA	1:123:B:ILE:C	1:124:B:MET:N	12	2.35
(1,144)	1:118:B:GLY:N	1:118:B:GLY:CA	1:118:B:GLY:C	1:119:B:THR:N	17	2.34
(1,69)	1:139:A:ARG:C	1:140:A:LYS:N	1:140:A:LYS:CA	1:140:A:LYS:C	3	2.34
(1,256)	1:123:C:ILE:N	1:123:C:ILE:CA	1:123:C:ILE:C	1:124:C:MET:N	1	2.33
(1,256)	1:123:C:ILE:N	1:123:C:ILE:CA	1:123:C:ILE:C	1:124:C:MET:N	4	2.33
(1,250)	1:118:C:GLY:N	1:118:C:GLY:CA	1:118:C:GLY:C	1:119:C:THR:N	10	2.33
(1,35)	1:115:A:PRO:C	1:116:A:ALA:N	1:116:A:ALA:CA	1:116:A:ALA:C	7	2.33
(1,270)	1:133:C:SER:N	1:133:C:SER:CA	1:133:C:SER:C	1:134:C:LEU:N	1	2.32
(1,102)	1:194:A:LEU:N	1:194:A:LEU:CA	1:194:A:LEU:C	1:195:A:TYR:N	12	2.32
(1,92)	1:187:A:THR:N	1:187:A:THR:CA	1:187:A:THR:C	1:188:A:LEU:N	15	2.32
(1,86)	1:184:A:ALA:N	1:184:A:ALA:CA	1:184:A:ALA:C	1:185:A:VAL:N	17	2.32
(1,150)	1:123:B:ILE:N	1:123:B:ILE:CA	1:123:B:ILE:C	1:124:B:MET:N	1	2.31
(1,38)	1:118:A:GLY:N	1:118:A:GLY:CA	1:118:A:GLY:C	1:119:A:THR:N	16	2.31
(1,252)	1:121:C:CYS:N	1:121:C:CYS:CA	1:121:C:CYS:C	1:122:C:TYR:N	19	2.3
(1,247)	1:115:C:PRO:C	1:116:C:ALA:N	1:116:C:ALA:CA	1:116:C:ALA:C	2	2.3
(1,247)	1:115:C:PRO:C	1:116:C:ALA:N	1:116:C:ALA:CA	1:116:C:ALA:C	12	2.3
(1,43)	1:122:A:TYR:C	1:123:A:ILE:N	1:123:A:ILE:CA	1:123:A:ILE:C	6	2.3
(1,24)	1:109:A:LEU:N	1:109:A:LEU:CA	1:109:A:LEU:C	1:110:A:LEU:N	11	2.3
(1,259)	1:124:C:MET:C	1:125:C:LYS:N	1:125:C:LYS:CA	1:125:C:LYS:C	16	2.29
(1,250)	1:118:C:GLY:N	1:118:C:GLY:CA	1:118:C:GLY:C	1:119:C:THR:N	13	2.29
(1,96)	1:189:A:CYS:N	1:189:A:CYS:CA	1:189:A:CYS:C	1:190:A:GLY:N	3	2.29
(1,2)	1:91:A:THR:N	1:91:A:THR:CA	1:91:A:THR:C	1:92:A:ALA:N	18	2.29

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,250)	1:118:C:GLY:N	1:118:C:GLY:CA	1:118:C:GLY:C	1:119:C:THR:N	7	2.28
(1,144)	1:118:B:GLY:N	1:118:B:GLY:CA	1:118:B:GLY:C	1:119:B:THR:N	10	2.28
(1,86)	1:184:A:ALA:N	1:184:A:ALA:CA	1:184:A:ALA:C	1:185:A:VAL:N	19	2.28
(1,69)	1:139:A:ARG:C	1:140:A:LYS:N	1:140:A:LYS:CA	1:140:A:LYS:C	2	2.28
(1,64)	1:137:A:LEU:N	1:137:A:LEU:CA	1:137:A:LEU:C	1:138:A:THR:N	11	2.28
(1,270)	1:133:C:SER:N	1:133:C:SER:CA	1:133:C:SER:C	1:134:C:LEU:N	3	2.27
(1,164)	1:133:B:SER:N	1:133:B:SER:CA	1:133:B:SER:C	1:134:B:LEU:N	4	2.27
(1,35)	1:115:A:PRO:C	1:116:A:ALA:N	1:116:A:ALA:CA	1:116:A:ALA:C	11	2.27
(1,153)	1:124:B:MET:C	1:125:B:LYS:N	1:125:B:LYS:CA	1:125:B:LYS:C	18	2.26
(1,256)	1:123:C:ILE:N	1:123:C:ILE:CA	1:123:C:ILE:C	1:124:C:MET:N	16	2.25
(1,250)	1:118:C:GLY:N	1:118:C:GLY:CA	1:118:C:GLY:C	1:119:C:THR:N	16	2.25
(1,247)	1:115:C:PRO:C	1:116:C:ALA:N	1:116:C:ALA:CA	1:116:C:ALA:C	18	2.25
(1,202)	1:189:B:CYS:N	1:189:B:CYS:CA	1:189:B:CYS:C	1:190:B:GLY:N	14	2.25
(1,141)	1:115:B:PRO:C	1:116:B:ALA:N	1:116:B:ALA:CA	1:116:B:ALA:C	20	2.25
(1,92)	1:187:A:THR:N	1:187:A:THR:CA	1:187:A:THR:C	1:188:A:LEU:N	10	2.25
(1,76)	1:143:A:ASN:N	1:143:A:ASN:CA	1:143:A:ASN:C	1:144:A:PHE:N	11	2.25
(1,15)	1:100:A:GLY:C	1:101:A:LEU:N	1:101:A:LEU:CA	1:101:A:LEU:C	12	2.25
(1,91)	1:186:A:SER:C	1:187:A:THR:N	1:187:A:THR:CA	1:187:A:THR:C	6	2.24
(1,64)	1:137:A:LEU:N	1:137:A:LEU:CA	1:137:A:LEU:C	1:138:A:THR:N	14	2.24
(1,38)	1:118:A:GLY:N	1:118:A:GLY:CA	1:118:A:GLY:C	1:119:A:THR:N	11	2.24
(1,64)	1:137:A:LEU:N	1:137:A:LEU:CA	1:137:A:LEU:C	1:138:A:THR:N	1	2.23
(1,69)	1:139:A:ARG:C	1:140:A:LYS:N	1:140:A:LYS:CA	1:140:A:LYS:C	1	2.22
(1,288)	1:143:C:ASN:N	1:143:C:ASN:CA	1:143:C:ASN:C	1:144:C:PHE:N	11	2.21
(1,83)	1:182:A:GLY:C	1:183:A:MET:N	1:183:A:MET:CA	1:183:A:MET:C	5	2.21
(1,153)	1:124:B:MET:C	1:125:B:LYS:N	1:125:B:LYS:CA	1:125:B:LYS:C	16	2.2
(1,141)	1:115:B:PRO:C	1:116:B:ALA:N	1:116:B:ALA:CA	1:116:B:ALA:C	2	2.2
(1,44)	1:123:A:ILE:N	1:123:A:ILE:CA	1:123:A:ILE:C	1:124:A:MET:N	5	2.19
(1,256)	1:123:C:ILE:N	1:123:C:ILE:CA	1:123:C:ILE:C	1:124:C:MET:N	2	2.18
(1,150)	1:123:B:ILE:N	1:123:B:ILE:CA	1:123:B:ILE:C	1:124:B:MET:N	16	2.18
(1,103)	1:194:A:LEU:C	1:195:A:TYR:N	1:195:A:TYR:CA	1:195:A:TYR:C	17	2.18
(1,44)	1:123:A:ILE:N	1:123:A:ILE:CA	1:123:A:ILE:C	1:124:A:MET:N	20	2.18
(1,33)	1:113:A:TYR:C	1:114:A:LYS:N	1:114:A:LYS:CA	1:114:A:LYS:C	12	2.18
(1,250)	1:118:C:GLY:N	1:118:C:GLY:CA	1:118:C:GLY:C	1:119:C:THR:N	5	2.17
(1,141)	1:115:B:PRO:C	1:116:B:ALA:N	1:116:B:ALA:CA	1:116:B:ALA:C	18	2.17
(1,64)	1:137:A:LEU:N	1:137:A:LEU:CA	1:137:A:LEU:C	1:138:A:THR:N	20	2.17
(1,33)	1:113:A:TYR:C	1:114:A:LYS:N	1:114:A:LYS:CA	1:114:A:LYS:C	1	2.17
(1,298)	1:184:C:ALA:N	1:184:C:ALA:CA	1:184:C:ALA:C	1:185:C:VAL:N	19	2.16
(1,86)	1:184:A:ALA:N	1:184:A:ALA:CA	1:184:A:ALA:C	1:185:A:VAL:N	6	2.16
(1,2)	1:91:A:THR:N	1:91:A:THR:CA	1:91:A:THR:C	1:92:A:ALA:N	15	2.16
(1,256)	1:123:C:ILE:N	1:123:C:ILE:CA	1:123:C:ILE:C	1:124:C:MET:N	6	2.15
(1,141)	1:115:B:PRO:C	1:116:B:ALA:N	1:116:B:ALA:CA	1:116:B:ALA:C	11	2.15
(1,69)	1:139:A:ARG:C	1:140:A:LYS:N	1:140:A:LYS:CA	1:140:A:LYS:C	13	2.15
(1,256)	1:123:C:ILE:N	1:123:C:ILE:CA	1:123:C:ILE:C	1:124:C:MET:N	12	2.14
(1,250)	1:118:C:GLY:N	1:118:C:GLY:CA	1:118:C:GLY:C	1:119:C:THR:N	2	2.14
(1,250)	1:118:C:GLY:N	1:118:C:GLY:CA	1:118:C:GLY:C	1:119:C:THR:N	20	2.14
(1,86)	1:184:A:ALA:N	1:184:A:ALA:CA	1:184:A:ALA:C	1:185:A:VAL:N	16	2.14
(1,58)	1:133:A:SER:N	1:133:A:SER:CA	1:133:A:SER:C	1:134:A:LEU:N	4	2.14
(1,256)	1:123:C:ILE:N	1:123:C:ILE:CA	1:123:C:ILE:C	1:124:C:MET:N	11	2.13
(1,202)	1:189:B:CYS:N	1:189:B:CYS:CA	1:189:B:CYS:C	1:190:B:GLY:N	3	2.13
(1,146)	1:121:B:CYS:N	1:121:B:CYS:CA	1:121:B:CYS:C	1:122:B:TYR:N	19	2.13
(1,102)	1:194:A:LEU:N	1:194:A:LEU:CA	1:194:A:LEU:C	1:195:A:TYR:N	20	2.13

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Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,182)	1:143:B:ASN:N	1:143:B:ASN:CA	1:143:B:ASN:C	1:144:B:PHE:N	18	2.12
(1,44)	1:123:A:ILE:N	1:123:A:ILE:CA	1:123:A:ILE:C	1:124:A:MET:N	6	2.12
(1,14)	1:100:A:GLY:N	1:100:A:GLY:CA	1:100:A:GLY:C	1:101:A:LEU:N	20	2.12
(1,250)	1:118:C:GLY:N	1:118:C:GLY:CA	1:118:C:GLY:C	1:119:C:THR:N	18	2.11
(1,250)	1:118:C:GLY:N	1:118:C:GLY:CA	1:118:C:GLY:C	1:119:C:THR:N	19	2.11
(1,214)	1:91:C:THR:N	1:91:C:THR:CA	1:91:C:THR:C	1:92:C:ALA:N	6	2.11
(1,192)	1:184:B:ALA:N	1:184:B:ALA:CA	1:184:B:ALA:C	1:185:B:VAL:N	19	2.11
(1,295)	1:182:C:GLY:C	1:183:C:MET:N	1:183:C:MET:CA	1:183:C:MET:C	19	2.1
(1,182)	1:143:B:ASN:N	1:143:B:ASN:CA	1:143:B:ASN:C	1:144:B:PHE:N	5	2.1
(1,167)	1:135:B:GLU:C	1:136:B:ALA:N	1:136:B:ALA:CA	1:136:B:ALA:C	13	2.1
(1,150)	1:123:B:ILE:N	1:123:B:ILE:CA	1:123:B:ILE:C	1:124:B:MET:N	11	2.1
(1,96)	1:189:A:CYS:N	1:189:A:CYS:CA	1:189:A:CYS:C	1:190:A:GLY:N	18	2.1
(1,38)	1:118:A:GLY:N	1:118:A:GLY:CA	1:118:A:GLY:C	1:119:A:THR:N	14	2.1
(1,149)	1:122:B:TYR:C	1:123:B:ILE:N	1:123:B:ILE:CA	1:123:B:ILE:C	6	2.09
(1,144)	1:118:B:GLY:N	1:118:B:GLY:CA	1:118:B:GLY:C	1:119:B:THR:N	20	2.09
(1,141)	1:115:B:PRO:C	1:116:B:ALA:N	1:116:B:ALA:CA	1:116:B:ALA:C	10	2.09
(1,92)	1:187:A:THR:N	1:187:A:THR:CA	1:187:A:THR:C	1:188:A:LEU:N	4	2.09
(1,304)	1:187:C:THR:N	1:187:C:THR:CA	1:187:C:THR:C	1:188:C:LEU:N	3	2.08
(1,86)	1:184:A:ALA:N	1:184:A:ALA:CA	1:184:A:ALA:C	1:185:A:VAL:N	7	2.08
(1,35)	1:115:A:PRO:C	1:116:A:ALA:N	1:116:A:ALA:CA	1:116:A:ALA:C	16	2.08
(1,243)	1:112:C:ALA:C	1:113:C:TYR:N	1:113:C:TYR:CA	1:113:C:TYR:C	4	2.07
(1,144)	1:118:B:GLY:N	1:118:B:GLY:CA	1:118:B:GLY:C	1:119:B:THR:N	2	2.07
(1,96)	1:189:A:CYS:N	1:189:A:CYS:CA	1:189:A:CYS:C	1:190:A:GLY:N	9	2.07
(1,69)	1:139:A:ARG:C	1:140:A:LYS:N	1:140:A:LYS:CA	1:140:A:LYS:C	20	2.07
(1,198)	1:187:B:THR:N	1:187:B:THR:CA	1:187:B:THR:C	1:188:B:LEU:N	16	2.06
(1,160)	1:129:B:GLU:N	1:129:B:GLU:CA	1:129:B:GLU:C	1:130:B:SER:N	5	2.06
(1,150)	1:123:B:ILE:N	1:123:B:ILE:CA	1:123:B:ILE:C	1:124:B:MET:N	5	2.06
(1,141)	1:115:B:PRO:C	1:116:B:ALA:N	1:116:B:ALA:CA	1:116:B:ALA:C	12	2.06
(1,255)	1:122:C:TYR:C	1:123:C:ILE:N	1:123:C:ILE:CA	1:123:C:ILE:C	6	2.05
(1,256)	1:123:C:ILE:N	1:123:C:ILE:CA	1:123:C:ILE:C	1:124:C:MET:N	5	2.04
(1,103)	1:194:A:LEU:C	1:195:A:TYR:N	1:195:A:TYR:CA	1:195:A:TYR:C	20	2.04
(1,69)	1:139:A:ARG:C	1:140:A:LYS:N	1:140:A:LYS:CA	1:140:A:LYS:C	11	2.04
(1,247)	1:115:C:PRO:C	1:116:C:ALA:N	1:116:C:ALA:CA	1:116:C:ALA:C	1	2.03
(1,189)	1:182:B:GLY:C	1:183:B:MET:N	1:183:B:MET:CA	1:183:B:MET:C	19	2.03
(1,144)	1:118:B:GLY:N	1:118:B:GLY:CA	1:118:B:GLY:C	1:119:B:THR:N	5	2.03
(1,308)	1:189:C:CYS:N	1:189:C:CYS:CA	1:189:C:CYS:C	1:190:C:GLY:N	3	2.02
(1,137)	1:112:B:ALA:C	1:113:B:TYR:N	1:113:B:TYR:CA	1:113:B:TYR:C	4	2.02
(1,35)	1:115:A:PRO:C	1:116:A:ALA:N	1:116:A:ALA:CA	1:116:A:ALA:C	1	2.02
(1,167)	1:135:B:GLU:C	1:136:B:ALA:N	1:136:B:ALA:CA	1:136:B:ALA:C	1	2.01
(1,144)	1:118:B:GLY:N	1:118:B:GLY:CA	1:118:B:GLY:C	1:119:B:THR:N	19	2.01
(1,103)	1:194:A:LEU:C	1:195:A:TYR:N	1:195:A:TYR:CA	1:195:A:TYR:C	1	2.01
(1,44)	1:123:A:ILE:N	1:123:A:ILE:CA	1:123:A:ILE:C	1:124:A:MET:N	2	2.01
(1,35)	1:115:A:PRO:C	1:116:A:ALA:N	1:116:A:ALA:CA	1:116:A:ALA:C	18	2.01
(1,44)	1:123:A:ILE:N	1:123:A:ILE:CA	1:123:A:ILE:C	1:124:A:MET:N	14	2.0
(1,214)	1:91:C:THR:N	1:91:C:THR:CA	1:91:C:THR:C	1:92:C:ALA:N	18	1.99
(1,198)	1:187:B:THR:N	1:187:B:THR:CA	1:187:B:THR:C	1:188:B:LEU:N	3	1.99
(1,102)	1:194:A:LEU:N	1:194:A:LEU:CA	1:194:A:LEU:C	1:195:A:TYR:N	17	1.99
(1,35)	1:115:A:PRO:C	1:116:A:ALA:N	1:116:A:ALA:CA	1:116:A:ALA:C	9	1.99
(1,33)	1:113:A:TYR:C	1:114:A:LYS:N	1:114:A:LYS:CA	1:114:A:LYS:C	8	1.99
(1,304)	1:187:C:THR:N	1:187:C:THR:CA	1:187:C:THR:C	1:188:C:LEU:N	12	1.98
(1,288)	1:143:C:ASN:N	1:143:C:ASN:CA	1:143:C:ASN:C	1:144:C:PHE:N	3	1.97

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,149)	1:122:B:TYR:C	1:123:B:ILE:N	1:123:B:ILE:CA	1:123:B:ILE:C	4	1.97
(1,69)	1:139:A:ARG:C	1:140:A:LYS:N	1:140:A:LYS:CA	1:140:A:LYS:C	12	1.97
(1,58)	1:133:A:SER:N	1:133:A:SER:CA	1:133:A:SER:C	1:134:A:LEU:N	18	1.97
(1,38)	1:118:A:GLY:N	1:118:A:GLY:CA	1:118:A:GLY:C	1:119:A:THR:N	9	1.97
(1,192)	1:184:B:ALA:N	1:184:B:ALA:CA	1:184:B:ALA:C	1:185:B:VAL:N	16	1.96
(1,40)	1:121:A:CYS:N	1:121:A:CYS:CA	1:121:A:CYS:C	1:122:A:TYR:N	18	1.96
(1,164)	1:133:B:SER:N	1:133:B:SER:CA	1:133:B:SER:C	1:134:B:LEU:N	5	1.95
(1,144)	1:118:B:GLY:N	1:118:B:GLY:CA	1:118:B:GLY:C	1:119:B:THR:N	18	1.95
(1,69)	1:139:A:ARG:C	1:140:A:LYS:N	1:140:A:LYS:CA	1:140:A:LYS:C	7	1.95
(1,247)	1:115:C:PRO:C	1:116:C:ALA:N	1:116:C:ALA:CA	1:116:C:ALA:C	10	1.94
(1,266)	1:129:C:GLU:N	1:129:C:GLU:CA	1:129:C:GLU:C	1:130:C:SER:N	5	1.93
(1,224)	1:96:C:ILE:N	1:96:C:ILE:CA	1:96:C:ILE:C	1:97:C:GLY:N	3	1.93
(1,141)	1:115:B:PRO:C	1:116:B:ALA:N	1:116:B:ALA:CA	1:116:B:ALA:C	17	1.93
(1,109)	1:91:B:THR:C	1:92:B:ALA:N	1:92:B:ALA:CA	1:92:B:ALA:C	20	1.93
(1,304)	1:187:C:THR:N	1:187:C:THR:CA	1:187:C:THR:C	1:188:C:LEU:N	5	1.92
(1,182)	1:143:B:ASN:N	1:143:B:ASN:CA	1:143:B:ASN:C	1:144:B:PHE:N	16	1.92
(1,120)	1:100:B:GLY:N	1:100:B:GLY:CA	1:100:B:GLY:C	1:101:B:LEU:N	11	1.91
(1,86)	1:184:A:ALA:N	1:184:A:ALA:CA	1:184:A:ALA:C	1:185:A:VAL:N	20	1.91
(1,76)	1:143:A:ASN:N	1:143:A:ASN:CA	1:143:A:ASN:C	1:144:A:PHE:N	3	1.91
(1,58)	1:133:A:SER:N	1:133:A:SER:CA	1:133:A:SER:C	1:134:A:LEU:N	19	1.91
(1,47)	1:124:A:MET:C	1:125:A:LYS:N	1:125:A:LYS:CA	1:125:A:LYS:C	15	1.91
(1,243)	1:112:C:ALA:C	1:113:C:TYR:N	1:113:C:TYR:CA	1:113:C:TYR:C	11	1.9
(1,247)	1:115:C:PRO:C	1:116:C:ALA:N	1:116:C:ALA:CA	1:116:C:ALA:C	17	1.89
(1,159)	1:128:B:PRO:C	1:129:B:GLU:N	1:129:B:GLU:CA	1:129:B:GLU:C	16	1.89
(1,69)	1:139:A:ARG:C	1:140:A:LYS:N	1:140:A:LYS:CA	1:140:A:LYS:C	16	1.89
(1,92)	1:187:A:THR:N	1:187:A:THR:CA	1:187:A:THR:C	1:188:A:LEU:N	11	1.88
(1,92)	1:187:A:THR:N	1:187:A:THR:CA	1:187:A:THR:C	1:188:A:LEU:N	20	1.87
(1,86)	1:184:A:ALA:N	1:184:A:ALA:CA	1:184:A:ALA:C	1:185:A:VAL:N	3	1.87
(1,4)	1:92:A:ALA:N	1:92:A:ALA:CA	1:92:A:ALA:C	1:93:A:THR:N	13	1.87
(1,76)	1:143:A:ASN:N	1:143:A:ASN:CA	1:143:A:ASN:C	1:144:A:PHE:N	13	1.86
(1,182)	1:143:B:ASN:N	1:143:B:ASN:CA	1:143:B:ASN:C	1:144:B:PHE:N	10	1.85
(1,182)	1:143:B:ASN:N	1:143:B:ASN:CA	1:143:B:ASN:C	1:144:B:PHE:N	15	1.85
(1,167)	1:135:B:GLU:C	1:136:B:ALA:N	1:136:B:ALA:CA	1:136:B:ALA:C	20	1.85
(1,38)	1:118:A:GLY:N	1:118:A:GLY:CA	1:118:A:GLY:C	1:119:A:THR:N	13	1.85
(1,288)	1:143:C:ASN:N	1:143:C:ASN:CA	1:143:C:ASN:C	1:144:C:PHE:N	18	1.84
(1,103)	1:194:A:LEU:C	1:195:A:TYR:N	1:195:A:TYR:CA	1:195:A:TYR:C	4	1.84
(1,83)	1:182:A:GLY:C	1:183:A:MET:N	1:183:A:MET:CA	1:183:A:MET:C	13	1.84
(1,44)	1:123:A:ILE:N	1:123:A:ILE:CA	1:123:A:ILE:C	1:124:A:MET:N	4	1.84
(1,298)	1:184:C:ALA:N	1:184:C:ALA:CA	1:184:C:ALA:C	1:185:C:VAL:N	16	1.83
(1,96)	1:189:A:CYS:N	1:189:A:CYS:CA	1:189:A:CYS:C	1:190:A:GLY:N	8	1.83
(1,53)	1:128:A:PRO:C	1:129:A:GLU:N	1:129:A:GLU:CA	1:129:A:GLU:C	16	1.83
(1,47)	1:124:A:MET:C	1:125:A:LYS:N	1:125:A:LYS:CA	1:125:A:LYS:C	1	1.83
(1,35)	1:115:A:PRO:C	1:116:A:ALA:N	1:116:A:ALA:CA	1:116:A:ALA:C	13	1.83
(1,141)	1:115:B:PRO:C	1:116:B:ALA:N	1:116:B:ALA:CA	1:116:B:ALA:C	19	1.82
(1,199)	1:187:B:THR:C	1:188:B:LEU:N	1:188:B:LEU:CA	1:188:B:LEU:C	6	1.81
(1,44)	1:123:A:ILE:N	1:123:A:ILE:CA	1:123:A:ILE:C	1:124:A:MET:N	9	1.81
(1,200)	1:188:B:LEU:N	1:188:B:LEU:CA	1:188:B:LEU:C	1:189:B:CYS:N	3	1.8
(1,83)	1:182:A:GLY:C	1:183:A:MET:N	1:183:A:MET:CA	1:183:A:MET:C	16	1.8
(1,54)	1:129:A:GLU:N	1:129:A:GLU:CA	1:129:A:GLU:C	1:130:A:SER:N	5	1.8
(1,305)	1:187:C:THR:C	1:188:C:LEU:N	1:188:C:LEU:CA	1:188:C:LEU:C	6	1.79
(1,247)	1:115:C:PRO:C	1:116:C:ALA:N	1:116:C:ALA:CA	1:116:C:ALA:C	19	1.79

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,182)	1:143:B:ASN:N	1:143:B:ASN:CA	1:143:B:ASN:C	1:144:B:PHE:N	14	1.79
(1,167)	1:135:B:GLU:C	1:136:B:ALA:N	1:136:B:ALA:CA	1:136:B:ALA:C	5	1.79
(1,69)	1:139:A:ARG:C	1:140:A:LYS:N	1:140:A:LYS:CA	1:140:A:LYS:C	15	1.79
(1,61)	1:135:A:GLU:C	1:136:A:ALA:N	1:136:A:ALA:CA	1:136:A:ALA:C	8	1.79
(1,182)	1:143:B:ASN:N	1:143:B:ASN:CA	1:143:B:ASN:C	1:144:B:PHE:N	7	1.78
(1,58)	1:133:A:SER:N	1:133:A:SER:CA	1:133:A:SER:C	1:134:A:LEU:N	1	1.78
(1,47)	1:124:A:MET:C	1:125:A:LYS:N	1:125:A:LYS:CA	1:125:A:LYS:C	19	1.78
(1,304)	1:187:C:THR:N	1:187:C:THR:CA	1:187:C:THR:C	1:188:C:LEU:N	16	1.77
(1,86)	1:184:A:ALA:N	1:184:A:ALA:CA	1:184:A:ALA:C	1:185:A:VAL:N	9	1.77
(1,247)	1:115:C:PRO:C	1:116:C:ALA:N	1:116:C:ALA:CA	1:116:C:ALA:C	7	1.76
(1,183)	1:155:B:ALA:C	1:156:B:VAL:N	1:156:B:VAL:CA	1:156:B:VAL:C	10	1.76
(1,137)	1:112:B:ALA:C	1:113:B:TYR:N	1:113:B:TYR:CA	1:113:B:TYR:C	3	1.76
(1,33)	1:113:A:TYR:C	1:114:A:LYS:N	1:114:A:LYS:CA	1:114:A:LYS:C	4	1.76
(1,298)	1:184:C:ALA:N	1:184:C:ALA:CA	1:184:C:ALA:C	1:185:C:VAL:N	14	1.75
(1,83)	1:182:A:GLY:C	1:183:A:MET:N	1:183:A:MET:CA	1:183:A:MET:C	18	1.75
(1,252)	1:121:C:CYS:N	1:121:C:CYS:CA	1:121:C:CYS:C	1:122:C:TYR:N	7	1.74
(1,182)	1:143:B:ASN:N	1:143:B:ASN:CA	1:143:B:ASN:C	1:144:B:PHE:N	20	1.74
(1,146)	1:121:B:CYS:N	1:121:B:CYS:CA	1:121:B:CYS:C	1:122:B:TYR:N	7	1.74
(1,38)	1:118:A:GLY:N	1:118:A:GLY:CA	1:118:A:GLY:C	1:119:A:THR:N	17	1.74
(1,38)	1:118:A:GLY:N	1:118:A:GLY:CA	1:118:A:GLY:C	1:119:A:THR:N	19	1.74
(1,247)	1:115:C:PRO:C	1:116:C:ALA:N	1:116:C:ALA:CA	1:116:C:ALA:C	5	1.73
(1,160)	1:129:B:GLU:N	1:129:B:GLU:CA	1:129:B:GLU:C	1:130:B:SER:N	19	1.73
(1,141)	1:115:B:PRO:C	1:116:B:ALA:N	1:116:B:ALA:CA	1:116:B:ALA:C	1	1.73
(1,47)	1:124:A:MET:C	1:125:A:LYS:N	1:125:A:LYS:CA	1:125:A:LYS:C	9	1.73
(1,13)	1:99:A:THR:C	1:100:A:GLY:N	1:100:A:GLY:CA	1:100:A:GLY:C	3	1.73
(1,247)	1:115:C:PRO:C	1:116:C:ALA:N	1:116:C:ALA:CA	1:116:C:ALA:C	13	1.72
(1,182)	1:143:B:ASN:N	1:143:B:ASN:CA	1:143:B:ASN:C	1:144:B:PHE:N	19	1.72
(1,167)	1:135:B:GLU:C	1:136:B:ALA:N	1:136:B:ALA:CA	1:136:B:ALA:C	12	1.71
(1,150)	1:123:B:ILE:N	1:123:B:ILE:CA	1:123:B:ILE:C	1:124:B:MET:N	10	1.71
(1,149)	1:122:B:TYR:C	1:123:B:ILE:N	1:123:B:ILE:CA	1:123:B:ILE:C	15	1.71
(1,137)	1:112:B:ALA:C	1:113:B:TYR:N	1:113:B:TYR:CA	1:113:B:TYR:C	11	1.71
(1,86)	1:184:A:ALA:N	1:184:A:ALA:CA	1:184:A:ALA:C	1:185:A:VAL:N	10	1.71
(1,69)	1:139:A:ARG:C	1:140:A:LYS:N	1:140:A:LYS:CA	1:140:A:LYS:C	17	1.71
(1,64)	1:137:A:LEU:N	1:137:A:LEU:CA	1:137:A:LEU:C	1:138:A:THR:N	9	1.71
(1,35)	1:115:A:PRO:C	1:116:A:ALA:N	1:116:A:ALA:CA	1:116:A:ALA:C	15	1.71
(1,33)	1:113:A:TYR:C	1:114:A:LYS:N	1:114:A:LYS:CA	1:114:A:LYS:C	11	1.71
(1,8)	1:94:A:PHE:N	1:94:A:PHE:CA	1:94:A:PHE:C	1:95:A:SER:N	19	1.71
(1,92)	1:187:A:THR:N	1:187:A:THR:CA	1:187:A:THR:C	1:188:A:LEU:N	9	1.7
(1,69)	1:139:A:ARG:C	1:140:A:LYS:N	1:140:A:LYS:CA	1:140:A:LYS:C	4	1.7
(1,44)	1:123:A:ILE:N	1:123:A:ILE:CA	1:123:A:ILE:C	1:124:A:MET:N	7	1.7
(1,76)	1:143:A:ASN:N	1:143:A:ASN:CA	1:143:A:ASN:C	1:144:A:PHE:N	6	1.69
(1,54)	1:129:A:GLU:N	1:129:A:GLU:CA	1:129:A:GLU:C	1:130:A:SER:N	19	1.69
(1,47)	1:124:A:MET:C	1:125:A:LYS:N	1:125:A:LYS:CA	1:125:A:LYS:C	3	1.69
(1,31)	1:112:A:ALA:C	1:113:A:TYR:N	1:113:A:TYR:CA	1:113:A:TYR:C	2	1.69
(1,306)	1:188:C:LEU:N	1:188:C:LEU:CA	1:188:C:LEU:C	1:189:C:CYS:N	3	1.68
(1,108)	1:91:B:THR:N	1:91:B:THR:CA	1:91:B:THR:C	1:92:B:ALA:N	15	1.68
(1,16)	1:101:A:LEU:N	1:101:A:LEU:CA	1:101:A:LEU:C	1:102:A:VAL:N	4	1.68
(1,288)	1:143:C:ASN:N	1:143:C:ASN:CA	1:143:C:ASN:C	1:144:C:PHE:N	7	1.67
(1,288)	1:143:C:ASN:N	1:143:C:ASN:CA	1:143:C:ASN:C	1:144:C:PHE:N	14	1.67
(1,255)	1:122:C:TYR:C	1:123:C:ILE:N	1:123:C:ILE:CA	1:123:C:ILE:C	15	1.67
(1,141)	1:115:B:PRO:C	1:116:B:ALA:N	1:116:B:ALA:CA	1:116:B:ALA:C	7	1.67

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,86)	1:184:A:ALA:N	1:184:A:ALA:CA	1:184:A:ALA:C	1:185:A:VAL:N	12	1.67
(1,43)	1:122:A:TYR:C	1:123:A:ILE:N	1:123:A:ILE:CA	1:123:A:ILE:C	13	1.67
(1,14)	1:100:A:GLY:N	1:100:A:GLY:CA	1:100:A:GLY:C	1:101:A:LEU:N	19	1.67
(1,298)	1:184:C:ALA:N	1:184:C:ALA:CA	1:184:C:ALA:C	1:185:C:VAL:N	5	1.65
(1,295)	1:182:C:GLY:C	1:183:C:MET:N	1:183:C:MET:CA	1:183:C:MET:C	13	1.65
(1,260)	1:125:C:LYS:N	1:125:C:LYS:CA	1:125:C:LYS:C	1:126:C:ILE:N	4	1.65
(1,86)	1:184:A:ALA:N	1:184:A:ALA:CA	1:184:A:ALA:C	1:185:A:VAL:N	13	1.65
(1,226)	1:100:C:GLY:N	1:100:C:GLY:CA	1:100:C:GLY:C	1:101:C:LEU:N	11	1.64
(1,103)	1:194:A:LEU:C	1:195:A:TYR:N	1:195:A:TYR:CA	1:195:A:TYR:C	9	1.64
(1,243)	1:112:C:ALA:C	1:113:C:TYR:N	1:113:C:TYR:CA	1:113:C:TYR:C	10	1.63
(1,182)	1:143:B:ASN:N	1:143:B:ASN:CA	1:143:B:ASN:C	1:144:B:PHE:N	6	1.63
(1,160)	1:129:B:GLU:N	1:129:B:GLU:CA	1:129:B:GLU:C	1:130:B:SER:N	20	1.63
(1,189)	1:182:B:GLY:C	1:183:B:MET:N	1:183:B:MET:CA	1:183:B:MET:C	13	1.62
(1,167)	1:135:B:GLU:C	1:136:B:ALA:N	1:136:B:ALA:CA	1:136:B:ALA:C	16	1.62
(1,149)	1:122:B:TYR:C	1:123:B:ILE:N	1:123:B:ILE:CA	1:123:B:ILE:C	3	1.62
(1,102)	1:194:A:LEU:N	1:194:A:LEU:CA	1:194:A:LEU:C	1:195:A:TYR:N	14	1.62
(1,76)	1:143:A:ASN:N	1:143:A:ASN:CA	1:143:A:ASN:C	1:144:A:PHE:N	14	1.62
(1,298)	1:184:C:ALA:N	1:184:C:ALA:CA	1:184:C:ALA:C	1:185:C:VAL:N	7	1.61
(1,252)	1:121:C:CYS:N	1:121:C:CYS:CA	1:121:C:CYS:C	1:122:C:TYR:N	9	1.61
(1,255)	1:122:C:TYR:C	1:123:C:ILE:N	1:123:C:ILE:CA	1:123:C:ILE:C	4	1.6
(1,253)	1:121:C:CYS:C	1:122:C:TYR:N	1:122:C:TYR:CA	1:122:C:TYR:C	18	1.6
(1,159)	1:128:B:PRO:C	1:129:B:GLU:N	1:129:B:GLU:CA	1:129:B:GLU:C	18	1.6
(1,141)	1:115:B:PRO:C	1:116:B:ALA:N	1:116:B:ALA:CA	1:116:B:ALA:C	9	1.6
(1,137)	1:112:B:ALA:C	1:113:B:TYR:N	1:113:B:TYR:CA	1:113:B:TYR:C	10	1.6
(1,76)	1:143:A:ASN:N	1:143:A:ASN:CA	1:143:A:ASN:C	1:144:A:PHE:N	18	1.6
(1,288)	1:143:C:ASN:N	1:143:C:ASN:CA	1:143:C:ASN:C	1:144:C:PHE:N	15	1.59
(1,108)	1:91:B:THR:N	1:91:B:THR:CA	1:91:B:THR:C	1:92:B:ALA:N	18	1.59
(1,288)	1:143:C:ASN:N	1:143:C:ASN:CA	1:143:C:ASN:C	1:144:C:PHE:N	5	1.58
(1,243)	1:112:C:ALA:C	1:113:C:TYR:N	1:113:C:TYR:CA	1:113:C:TYR:C	3	1.58
(1,208)	1:194:B:LEU:N	1:194:B:LEU:CA	1:194:B:LEU:C	1:195:B:TYR:N	15	1.58
(1,192)	1:184:B:ALA:N	1:184:B:ALA:CA	1:184:B:ALA:C	1:185:B:VAL:N	5	1.58
(1,182)	1:143:B:ASN:N	1:143:B:ASN:CA	1:143:B:ASN:C	1:144:B:PHE:N	13	1.58
(1,159)	1:128:B:PRO:C	1:129:B:GLU:N	1:129:B:GLU:CA	1:129:B:GLU:C	10	1.58
(1,54)	1:129:A:GLU:N	1:129:A:GLU:CA	1:129:A:GLU:C	1:130:A:SER:N	13	1.58
(1,43)	1:122:A:TYR:C	1:123:A:ILE:N	1:123:A:ILE:CA	1:123:A:ILE:C	9	1.58
(1,256)	1:123:C:ILE:N	1:123:C:ILE:CA	1:123:C:ILE:C	1:124:C:MET:N	10	1.57
(1,192)	1:184:B:ALA:N	1:184:B:ALA:CA	1:184:B:ALA:C	1:185:B:VAL:N	3	1.57
(1,159)	1:128:B:PRO:C	1:129:B:GLU:N	1:129:B:GLU:CA	1:129:B:GLU:C	5	1.57
(1,298)	1:184:C:ALA:N	1:184:C:ALA:CA	1:184:C:ALA:C	1:185:C:VAL:N	17	1.56
(1,289)	1:155:C:ALA:C	1:156:C:VAL:N	1:156:C:VAL:CA	1:156:C:VAL:C	10	1.56
(1,200)	1:188:B:LEU:N	1:188:B:LEU:CA	1:188:B:LEU:C	1:189:B:CYS:N	6	1.56
(1,141)	1:115:B:PRO:C	1:116:B:ALA:N	1:116:B:ALA:CA	1:116:B:ALA:C	6	1.56
(1,314)	1:194:C:LEU:N	1:194:C:LEU:CA	1:194:C:LEU:C	1:195:C:TYR:N	15	1.55
(1,141)	1:115:B:PRO:C	1:116:B:ALA:N	1:116:B:ALA:CA	1:116:B:ALA:C	5	1.55
(1,91)	1:186:A:SER:C	1:187:A:THR:N	1:187:A:THR:CA	1:187:A:THR:C	8	1.55
(1,13)	1:99:A:THR:C	1:100:A:GLY:N	1:100:A:GLY:CA	1:100:A:GLY:C	13	1.55
(1,295)	1:182:C:GLY:C	1:183:C:MET:N	1:183:C:MET:CA	1:183:C:MET:C	16	1.54
(1,288)	1:143:C:ASN:N	1:143:C:ASN:CA	1:143:C:ASN:C	1:144:C:PHE:N	16	1.54
(1,288)	1:143:C:ASN:N	1:143:C:ASN:CA	1:143:C:ASN:C	1:144:C:PHE:N	19	1.54
(1,243)	1:112:C:ALA:C	1:113:C:TYR:N	1:113:C:TYR:CA	1:113:C:TYR:C	19	1.54
(1,192)	1:184:B:ALA:N	1:184:B:ALA:CA	1:184:B:ALA:C	1:185:B:VAL:N	17	1.54

Continued on next page...

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,154)	1:125:B:LYS:N	1:125:B:LYS:CA	1:125:B:LYS:C	1:126:B:ILE:N	4	1.54
(1,54)	1:129:A:GLU:N	1:129:A:GLU:CA	1:129:A:GLU:C	1:130:A:SER:N	2	1.54
(1,44)	1:123:A:ILE:N	1:123:A:ILE:CA	1:123:A:ILE:C	1:124:A:MET:N	1	1.54
(1,288)	1:143:C:ASN:N	1:143:C:ASN:CA	1:143:C:ASN:C	1:144:C:PHE:N	6	1.53
(1,141)	1:115:B:PRO:C	1:116:B:ALA:N	1:116:B:ALA:CA	1:116:B:ALA:C	13	1.53
(1,38)	1:118:A:GLY:N	1:118:A:GLY:CA	1:118:A:GLY:C	1:119:A:THR:N	18	1.53
(1,198)	1:187:B:THR:N	1:187:B:THR:CA	1:187:B:THR:C	1:188:B:LEU:N	19	1.52
(1,167)	1:135:B:GLU:C	1:136:B:ALA:N	1:136:B:ALA:CA	1:136:B:ALA:C	19	1.52
(1,139)	1:113:B:TYR:C	1:114:B:LYS:N	1:114:B:LYS:CA	1:114:B:LYS:C	3	1.52
(1,119)	1:99:B:THR:C	1:100:B:GLY:N	1:100:B:GLY:CA	1:100:B:GLY:C	13	1.52
(1,54)	1:129:A:GLU:N	1:129:A:GLU:CA	1:129:A:GLU:C	1:130:A:SER:N	1	1.52
(1,24)	1:109:A:LEU:N	1:109:A:LEU:CA	1:109:A:LEU:C	1:110:A:LEU:N	12	1.52
(1,247)	1:115:C:PRO:C	1:116:C:ALA:N	1:116:C:ALA:CA	1:116:C:ALA:C	6	1.51
(1,160)	1:129:B:GLU:N	1:129:B:GLU:CA	1:129:B:GLU:C	1:130:B:SER:N	2	1.51
(1,147)	1:121:B:CYS:C	1:122:B:TYR:N	1:122:B:TYR:CA	1:122:B:TYR:C	15	1.51
(1,137)	1:112:B:ALA:C	1:113:B:TYR:N	1:113:B:TYR:CA	1:113:B:TYR:C	19	1.51
(1,48)	1:125:A:LYS:N	1:125:A:LYS:CA	1:125:A:LYS:C	1:126:A:ILE:N	4	1.51
(1,288)	1:143:C:ASN:N	1:143:C:ASN:CA	1:143:C:ASN:C	1:144:C:PHE:N	13	1.5
(1,247)	1:115:C:PRO:C	1:116:C:ALA:N	1:116:C:ALA:CA	1:116:C:ALA:C	9	1.5
(1,182)	1:143:B:ASN:N	1:143:B:ASN:CA	1:143:B:ASN:C	1:144:B:PHE:N	2	1.5
(1,160)	1:129:B:GLU:N	1:129:B:GLU:CA	1:129:B:GLU:C	1:130:B:SER:N	7	1.5
(1,149)	1:122:B:TYR:C	1:123:B:ILE:N	1:123:B:ILE:CA	1:123:B:ILE:C	19	1.5
(1,114)	1:94:B:PHE:N	1:94:B:PHE:CA	1:94:B:PHE:C	1:95:B:SER:N	19	1.5
(1,108)	1:91:B:THR:N	1:91:B:THR:CA	1:91:B:THR:C	1:92:B:ALA:N	6	1.5
(1,76)	1:143:A:ASN:N	1:143:A:ASN:CA	1:143:A:ASN:C	1:144:A:PHE:N	5	1.5
(1,38)	1:118:A:GLY:N	1:118:A:GLY:CA	1:118:A:GLY:C	1:119:A:THR:N	15	1.5
(1,31)	1:112:A:ALA:C	1:113:A:TYR:N	1:113:A:TYR:CA	1:113:A:TYR:C	7	1.5
(1,303)	1:186:C:SER:C	1:187:C:THR:N	1:187:C:THR:CA	1:187:C:THR:C	2	1.49
(1,253)	1:121:C:CYS:C	1:122:C:TYR:N	1:122:C:TYR:CA	1:122:C:TYR:C	15	1.49
(1,175)	1:139:B:ARG:C	1:140:B:LYS:N	1:140:B:LYS:CA	1:140:B:LYS:C	2	1.49
(1,137)	1:112:B:ALA:C	1:113:B:TYR:N	1:113:B:TYR:CA	1:113:B:TYR:C	20	1.49
(1,118)	1:96:B:ILE:N	1:96:B:ILE:CA	1:96:B:ILE:C	1:97:B:GLY:N	3	1.49
(1,91)	1:186:A:SER:C	1:187:A:THR:N	1:187:A:THR:CA	1:187:A:THR:C	9	1.49
(1,38)	1:118:A:GLY:N	1:118:A:GLY:CA	1:118:A:GLY:C	1:119:A:THR:N	12	1.49
(1,265)	1:128:C:PRO:C	1:129:C:GLU:N	1:129:C:GLU:CA	1:129:C:GLU:C	16	1.48
(1,189)	1:182:B:GLY:C	1:183:B:MET:N	1:183:B:MET:CA	1:183:B:MET:C	14	1.48
(1,149)	1:122:B:TYR:C	1:123:B:ILE:N	1:123:B:ILE:CA	1:123:B:ILE:C	16	1.48
(1,103)	1:194:A:LEU:C	1:195:A:TYR:N	1:195:A:TYR:CA	1:195:A:TYR:C	6	1.48
(1,298)	1:184:C:ALA:N	1:184:C:ALA:CA	1:184:C:ALA:C	1:185:C:VAL:N	12	1.47
(1,273)	1:135:C:GLU:C	1:136:C:ALA:N	1:136:C:ALA:CA	1:136:C:ALA:C	8	1.47
(1,208)	1:194:B:LEU:N	1:194:B:LEU:CA	1:194:B:LEU:C	1:195:B:TYR:N	20	1.47
(1,167)	1:135:B:GLU:C	1:136:B:ALA:N	1:136:B:ALA:CA	1:136:B:ALA:C	2	1.47
(1,86)	1:184:A:ALA:N	1:184:A:ALA:CA	1:184:A:ALA:C	1:185:A:VAL:N	4	1.47
(1,83)	1:182:A:GLY:C	1:183:A:MET:N	1:183:A:MET:CA	1:183:A:MET:C	7	1.47
(1,54)	1:129:A:GLU:N	1:129:A:GLU:CA	1:129:A:GLU:C	1:130:A:SER:N	20	1.47
(1,265)	1:128:C:PRO:C	1:129:C:GLU:N	1:129:C:GLU:CA	1:129:C:GLU:C	18	1.46
(1,198)	1:187:B:THR:N	1:187:B:THR:CA	1:187:B:THR:C	1:188:B:LEU:N	12	1.46
(1,182)	1:143:B:ASN:N	1:143:B:ASN:CA	1:143:B:ASN:C	1:144:B:PHE:N	12	1.46
(1,175)	1:139:B:ARG:C	1:140:B:LYS:N	1:140:B:LYS:CA	1:140:B:LYS:C	8	1.46
(1,149)	1:122:B:TYR:C	1:123:B:ILE:N	1:123:B:ILE:CA	1:123:B:ILE:C	7	1.46
(1,54)	1:129:A:GLU:N	1:129:A:GLU:CA	1:129:A:GLU:C	1:130:A:SER:N	11	1.46

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,314)	1:194:C:LEU:N	1:194:C:LEU:CA	1:194:C:LEU:C	1:195:C:TYR:N	20	1.45
(1,288)	1:143:C:ASN:N	1:143:C:ASN:CA	1:143:C:ASN:C	1:144:C:PHE:N	10	1.45
(1,192)	1:184:B:ALA:N	1:184:B:ALA:CA	1:184:B:ALA:C	1:185:B:VAL:N	14	1.45
(1,69)	1:139:A:ARG:C	1:140:A:LYS:N	1:140:A:LYS:CA	1:140:A:LYS:C	14	1.45
(1,14)	1:100:A:GLY:N	1:100:A:GLY:CA	1:100:A:GLY:C	1:101:A:LEU:N	11	1.45
(1,2)	1:91:A:THR:N	1:91:A:THR:CA	1:91:A:THR:C	1:92:A:ALA:N	4	1.45
(1,266)	1:129:C:GLU:N	1:129:C:GLU:CA	1:129:C:GLU:C	1:130:C:SER:N	2	1.44
(1,243)	1:112:C:ALA:C	1:113:C:TYR:N	1:113:C:TYR:CA	1:113:C:TYR:C	20	1.44
(1,192)	1:184:B:ALA:N	1:184:B:ALA:CA	1:184:B:ALA:C	1:185:B:VAL:N	7	1.44
(1,35)	1:115:A:PRO:C	1:116:A:ALA:N	1:116:A:ALA:CA	1:116:A:ALA:C	6	1.44
(1,298)	1:184:C:ALA:N	1:184:C:ALA:CA	1:184:C:ALA:C	1:185:C:VAL:N	3	1.43
(1,281)	1:139:C:ARG:C	1:140:C:LYS:N	1:140:C:LYS:CA	1:140:C:LYS:C	6	1.43
(1,266)	1:129:C:GLU:N	1:129:C:GLU:CA	1:129:C:GLU:C	1:130:C:SER:N	15	1.43
(1,76)	1:143:A:ASN:N	1:143:A:ASN:CA	1:143:A:ASN:C	1:144:A:PHE:N	7	1.43
(1,47)	1:124:A:MET:C	1:125:A:LYS:N	1:125:A:LYS:CA	1:125:A:LYS:C	18	1.43
(1,266)	1:129:C:GLU:N	1:129:C:GLU:CA	1:129:C:GLU:C	1:130:C:SER:N	3	1.42
(1,259)	1:124:C:MET:C	1:125:C:LYS:N	1:125:C:LYS:CA	1:125:C:LYS:C	11	1.42
(1,146)	1:121:B:CYS:N	1:121:B:CYS:CA	1:121:B:CYS:C	1:122:B:TYR:N	9	1.42
(1,69)	1:139:A:ARG:C	1:140:A:LYS:N	1:140:A:LYS:CA	1:140:A:LYS:C	18	1.42
(1,38)	1:118:A:GLY:N	1:118:A:GLY:CA	1:118:A:GLY:C	1:119:A:THR:N	7	1.42
(1,259)	1:124:C:MET:C	1:125:C:LYS:N	1:125:C:LYS:CA	1:125:C:LYS:C	17	1.41
(1,192)	1:184:B:ALA:N	1:184:B:ALA:CA	1:184:B:ALA:C	1:185:B:VAL:N	12	1.41
(1,189)	1:182:B:GLY:C	1:183:B:MET:N	1:183:B:MET:CA	1:183:B:MET:C	16	1.41
(1,149)	1:122:B:TYR:C	1:123:B:ILE:N	1:123:B:ILE:CA	1:123:B:ILE:C	9	1.41
(1,137)	1:112:B:ALA:C	1:113:B:TYR:N	1:113:B:TYR:CA	1:113:B:TYR:C	8	1.41
(1,76)	1:143:A:ASN:N	1:143:A:ASN:CA	1:143:A:ASN:C	1:144:A:PHE:N	12	1.41
(1,288)	1:143:C:ASN:N	1:143:C:ASN:CA	1:143:C:ASN:C	1:144:C:PHE:N	2	1.4
(1,270)	1:133:C:SER:N	1:133:C:SER:CA	1:133:C:SER:C	1:134:C:LEU:N	4	1.4
(1,255)	1:122:C:TYR:C	1:123:C:ILE:N	1:123:C:ILE:CA	1:123:C:ILE:C	7	1.4
(1,160)	1:129:B:GLU:N	1:129:B:GLU:CA	1:129:B:GLU:C	1:130:B:SER:N	13	1.4
(1,160)	1:129:B:GLU:N	1:129:B:GLU:CA	1:129:B:GLU:C	1:130:B:SER:N	15	1.4
(1,54)	1:129:A:GLU:N	1:129:A:GLU:CA	1:129:A:GLU:C	1:130:A:SER:N	15	1.4
(1,33)	1:113:A:TYR:C	1:114:A:LYS:N	1:114:A:LYS:CA	1:114:A:LYS:C	13	1.4
(1,295)	1:182:C:GLY:C	1:183:C:MET:N	1:183:C:MET:CA	1:183:C:MET:C	14	1.39
(1,281)	1:139:C:ARG:C	1:140:C:LYS:N	1:140:C:LYS:CA	1:140:C:LYS:C	2	1.39
(1,270)	1:133:C:SER:N	1:133:C:SER:CA	1:133:C:SER:C	1:134:C:LEU:N	7	1.39
(1,266)	1:129:C:GLU:N	1:129:C:GLU:CA	1:129:C:GLU:C	1:130:C:SER:N	9	1.39
(1,255)	1:122:C:TYR:C	1:123:C:ILE:N	1:123:C:ILE:CA	1:123:C:ILE:C	9	1.39
(1,245)	1:113:C:TYR:C	1:114:C:LYS:N	1:114:C:LYS:CA	1:114:C:LYS:C	3	1.39
(1,160)	1:129:B:GLU:N	1:129:B:GLU:CA	1:129:B:GLU:C	1:130:B:SER:N	9	1.39
(1,266)	1:129:C:GLU:N	1:129:C:GLU:CA	1:129:C:GLU:C	1:130:C:SER:N	19	1.38
(1,225)	1:99:C:THR:C	1:100:C:GLY:N	1:100:C:GLY:CA	1:100:C:GLY:C	13	1.38
(1,214)	1:91:C:THR:N	1:91:C:THR:CA	1:91:C:THR:C	1:92:C:ALA:N	15	1.38
(1,197)	1:186:B:SER:C	1:187:B:THR:N	1:187:B:THR:CA	1:187:B:THR:C	13	1.38
(1,160)	1:129:B:GLU:N	1:129:B:GLU:CA	1:129:B:GLU:C	1:130:B:SER:N	1	1.38
(1,160)	1:129:B:GLU:N	1:129:B:GLU:CA	1:129:B:GLU:C	1:130:B:SER:N	16	1.38
(1,69)	1:139:A:ARG:C	1:140:A:LYS:N	1:140:A:LYS:CA	1:140:A:LYS:C	9	1.38
(1,54)	1:129:A:GLU:N	1:129:A:GLU:CA	1:129:A:GLU:C	1:130:A:SER:N	14	1.38
(1,41)	1:121:A:CYS:C	1:122:A:TYR:N	1:122:A:TYR:CA	1:122:A:TYR:C	16	1.38
(1,33)	1:113:A:TYR:C	1:114:A:LYS:N	1:114:A:LYS:CA	1:114:A:LYS:C	6	1.38
(1,31)	1:112:A:ALA:C	1:113:A:TYR:N	1:113:A:TYR:CA	1:113:A:TYR:C	10	1.38

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,160)	1:129:B:GLU:N	1:129:B:GLU:CA	1:129:B:GLU:C	1:130:B:SER:N	4	1.37
(1,83)	1:182:A:GLY:C	1:183:A:MET:N	1:183:A:MET:CA	1:183:A:MET:C	12	1.37
(1,69)	1:139:A:ARG:C	1:140:A:LYS:N	1:140:A:LYS:CA	1:140:A:LYS:C	10	1.37
(1,69)	1:139:A:ARG:C	1:140:A:LYS:N	1:140:A:LYS:CA	1:140:A:LYS:C	19	1.37
(1,44)	1:123:A:ILE:N	1:123:A:ILE:CA	1:123:A:ILE:C	1:124:A:MET:N	12	1.37
(1,38)	1:118:A:GLY:N	1:118:A:GLY:CA	1:118:A:GLY:C	1:119:A:THR:N	2	1.37
(1,4)	1:92:A:ALA:N	1:92:A:ALA:CA	1:92:A:ALA:C	1:93:A:THR:N	11	1.37
(1,281)	1:139:C:ARG:C	1:140:C:LYS:N	1:140:C:LYS:CA	1:140:C:LYS:C	8	1.36
(1,266)	1:129:C:GLU:N	1:129:C:GLU:CA	1:129:C:GLU:C	1:130:C:SER:N	13	1.36
(1,153)	1:124:B:MET:C	1:125:B:LYS:N	1:125:B:LYS:CA	1:125:B:LYS:C	11	1.36
(1,147)	1:121:B:CYS:C	1:122:B:TYR:N	1:122:B:TYR:CA	1:122:B:TYR:C	18	1.36
(1,53)	1:128:A:PRO:C	1:129:A:GLU:N	1:129:A:GLU:CA	1:129:A:GLU:C	18	1.36
(1,266)	1:129:C:GLU:N	1:129:C:GLU:CA	1:129:C:GLU:C	1:130:C:SER:N	7	1.35
(1,76)	1:143:A:ASN:N	1:143:A:ASN:CA	1:143:A:ASN:C	1:144:A:PHE:N	19	1.35
(1,54)	1:129:A:GLU:N	1:129:A:GLU:CA	1:129:A:GLU:C	1:130:A:SER:N	12	1.35
(1,270)	1:133:C:SER:N	1:133:C:SER:CA	1:133:C:SER:C	1:134:C:LEU:N	10	1.34
(1,255)	1:122:C:TYR:C	1:123:C:ILE:N	1:123:C:ILE:CA	1:123:C:ILE:C	16	1.34
(1,91)	1:186:A:SER:C	1:187:A:THR:N	1:187:A:THR:CA	1:187:A:THR:C	5	1.34
(1,76)	1:143:A:ASN:N	1:143:A:ASN:CA	1:143:A:ASN:C	1:144:A:PHE:N	2	1.34
(1,41)	1:121:A:CYS:C	1:122:A:TYR:N	1:122:A:TYR:CA	1:122:A:TYR:C	18	1.34
(1,160)	1:129:B:GLU:N	1:129:B:GLU:CA	1:129:B:GLU:C	1:130:B:SER:N	3	1.33
(1,86)	1:184:A:ALA:N	1:184:A:ALA:CA	1:184:A:ALA:C	1:185:A:VAL:N	15	1.33
(1,54)	1:129:A:GLU:N	1:129:A:GLU:CA	1:129:A:GLU:C	1:130:A:SER:N	7	1.33
(1,24)	1:109:A:LEU:N	1:109:A:LEU:CA	1:109:A:LEU:C	1:110:A:LEU:N	3	1.33
(1,266)	1:129:C:GLU:N	1:129:C:GLU:CA	1:129:C:GLU:C	1:130:C:SER:N	16	1.32
(1,247)	1:115:C:PRO:C	1:116:C:ALA:N	1:116:C:ALA:CA	1:116:C:ALA:C	16	1.32
(1,220)	1:94:C:PHE:N	1:94:C:PHE:CA	1:94:C:PHE:C	1:95:C:SER:N	9	1.32
(1,192)	1:184:B:ALA:N	1:184:B:ALA:CA	1:184:B:ALA:C	1:185:B:VAL:N	2	1.32
(1,86)	1:184:A:ALA:N	1:184:A:ALA:CA	1:184:A:ALA:C	1:185:A:VAL:N	14	1.32
(1,54)	1:129:A:GLU:N	1:129:A:GLU:CA	1:129:A:GLU:C	1:130:A:SER:N	9	1.32
(1,35)	1:115:A:PRO:C	1:116:A:ALA:N	1:116:A:ALA:CA	1:116:A:ALA:C	3	1.32
(1,288)	1:143:C:ASN:N	1:143:C:ASN:CA	1:143:C:ASN:C	1:144:C:PHE:N	20	1.31
(1,273)	1:135:C:GLU:C	1:136:C:ALA:N	1:136:C:ALA:CA	1:136:C:ALA:C	4	1.31
(1,266)	1:129:C:GLU:N	1:129:C:GLU:CA	1:129:C:GLU:C	1:130:C:SER:N	4	1.31
(1,243)	1:112:C:ALA:C	1:113:C:TYR:N	1:113:C:TYR:CA	1:113:C:TYR:C	12	1.31
(1,189)	1:182:B:GLY:C	1:183:B:MET:N	1:183:B:MET:CA	1:183:B:MET:C	2	1.31
(1,175)	1:139:B:ARG:C	1:140:B:LYS:N	1:140:B:LYS:CA	1:140:B:LYS:C	6	1.31
(1,103)	1:194:A:LEU:C	1:195:A:TYR:N	1:195:A:TYR:CA	1:195:A:TYR:C	13	1.31
(1,266)	1:129:C:GLU:N	1:129:C:GLU:CA	1:129:C:GLU:C	1:130:C:SER:N	20	1.3
(1,288)	1:143:C:ASN:N	1:143:C:ASN:CA	1:143:C:ASN:C	1:144:C:PHE:N	12	1.29
(1,197)	1:186:B:SER:C	1:187:B:THR:N	1:187:B:THR:CA	1:187:B:THR:C	2	1.29
(1,189)	1:182:B:GLY:C	1:183:B:MET:N	1:183:B:MET:CA	1:183:B:MET:C	12	1.29
(1,24)	1:109:A:LEU:N	1:109:A:LEU:CA	1:109:A:LEU:C	1:110:A:LEU:N	4	1.29
(1,255)	1:122:C:TYR:C	1:123:C:ILE:N	1:123:C:ILE:CA	1:123:C:ILE:C	3	1.28
(1,243)	1:112:C:ALA:C	1:113:C:TYR:N	1:113:C:TYR:CA	1:113:C:TYR:C	8	1.28
(1,86)	1:184:A:ALA:N	1:184:A:ALA:CA	1:184:A:ALA:C	1:185:A:VAL:N	11	1.28
(1,54)	1:129:A:GLU:N	1:129:A:GLU:CA	1:129:A:GLU:C	1:130:A:SER:N	3	1.28
(1,54)	1:129:A:GLU:N	1:129:A:GLU:CA	1:129:A:GLU:C	1:130:A:SER:N	4	1.28
(1,2)	1:91:A:THR:N	1:91:A:THR:CA	1:91:A:THR:C	1:92:A:ALA:N	2	1.28
(1,298)	1:184:C:ALA:N	1:184:C:ALA:CA	1:184:C:ALA:C	1:185:C:VAL:N	10	1.27
(1,255)	1:122:C:TYR:C	1:123:C:ILE:N	1:123:C:ILE:CA	1:123:C:ILE:C	19	1.27

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Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,92)	1:187:A:THR:N	1:187:A:THR:CA	1:187:A:THR:C	1:188:A:LEU:N	13	1.27
(1,295)	1:182:C:GLY:C	1:183:C:MET:N	1:183:C:MET:CA	1:183:C:MET:C	5	1.26
(1,260)	1:125:C:LYS:N	1:125:C:LYS:CA	1:125:C:LYS:C	1:126:C:ILE:N	3	1.26
(1,160)	1:129:B:GLU:N	1:129:B:GLU:CA	1:129:B:GLU:C	1:130:B:SER:N	12	1.26
(1,92)	1:187:A:THR:N	1:187:A:THR:CA	1:187:A:THR:C	1:188:A:LEU:N	17	1.26
(1,54)	1:129:A:GLU:N	1:129:A:GLU:CA	1:129:A:GLU:C	1:130:A:SER:N	16	1.26
(1,43)	1:122:A:TYR:C	1:123:A:ILE:N	1:123:A:ILE:CA	1:123:A:ILE:C	15	1.26
(1,40)	1:121:A:CYS:N	1:121:A:CYS:CA	1:121:A:CYS:C	1:122:A:TYR:N	12	1.26
(1,266)	1:129:C:GLU:N	1:129:C:GLU:CA	1:129:C:GLU:C	1:130:C:SER:N	1	1.25
(1,164)	1:133:B:SER:N	1:133:B:SER:CA	1:133:B:SER:C	1:134:B:LEU:N	7	1.25
(1,298)	1:184:C:ALA:N	1:184:C:ALA:CA	1:184:C:ALA:C	1:185:C:VAL:N	2	1.24
(1,189)	1:182:B:GLY:C	1:183:B:MET:N	1:183:B:MET:CA	1:183:B:MET:C	5	1.24
(1,38)	1:118:A:GLY:N	1:118:A:GLY:CA	1:118:A:GLY:C	1:119:A:THR:N	10	1.24
(1,15)	1:100:A:GLY:C	1:101:A:LEU:N	1:101:A:LEU:CA	1:101:A:LEU:C	14	1.24
(1,314)	1:194:C:LEU:N	1:194:C:LEU:CA	1:194:C:LEU:C	1:195:C:TYR:N	16	1.23
(1,288)	1:143:C:ASN:N	1:143:C:ASN:CA	1:143:C:ASN:C	1:144:C:PHE:N	17	1.23
(1,232)	1:103:C:VAL:N	1:103:C:VAL:CA	1:103:C:VAL:C	1:104:C:TYR:N	20	1.23
(1,38)	1:118:A:GLY:N	1:118:A:GLY:CA	1:118:A:GLY:C	1:119:A:THR:N	20	1.23
(1,270)	1:133:C:SER:N	1:133:C:SER:CA	1:133:C:SER:C	1:134:C:LEU:N	5	1.22
(1,182)	1:143:B:ASN:N	1:143:B:ASN:CA	1:143:B:ASN:C	1:144:B:PHE:N	9	1.22
(1,266)	1:129:C:GLU:N	1:129:C:GLU:CA	1:129:C:GLU:C	1:130:C:SER:N	12	1.21
(1,247)	1:115:C:PRO:C	1:116:C:ALA:N	1:116:C:ALA:CA	1:116:C:ALA:C	15	1.21
(1,208)	1:194:B:LEU:N	1:194:B:LEU:CA	1:194:B:LEU:C	1:195:B:TYR:N	16	1.21
(1,141)	1:115:B:PRO:C	1:116:B:ALA:N	1:116:B:ALA:CA	1:116:B:ALA:C	16	1.21
(1,93)	1:187:A:THR:C	1:188:A:LEU:N	1:188:A:LEU:CA	1:188:A:LEU:C	6	1.21
(1,58)	1:133:A:SER:N	1:133:A:SER:CA	1:133:A:SER:C	1:134:A:LEU:N	16	1.21
(1,192)	1:184:B:ALA:N	1:184:B:ALA:CA	1:184:B:ALA:C	1:185:B:VAL:N	10	1.2
(1,108)	1:91:B:THR:N	1:91:B:THR:CA	1:91:B:THR:C	1:92:B:ALA:N	4	1.2
(1,76)	1:143:A:ASN:N	1:143:A:ASN:CA	1:143:A:ASN:C	1:144:A:PHE:N	15	1.2
(1,48)	1:125:A:LYS:N	1:125:A:LYS:CA	1:125:A:LYS:C	1:126:A:ILE:N	9	1.2
(1,47)	1:124:A:MET:C	1:125:A:LYS:N	1:125:A:LYS:CA	1:125:A:LYS:C	7	1.2
(1,44)	1:123:A:ILE:N	1:123:A:ILE:CA	1:123:A:ILE:C	1:124:A:MET:N	10	1.2
(1,200)	1:188:B:LEU:N	1:188:B:LEU:CA	1:188:B:LEU:C	1:189:B:CYS:N	20	1.19
(1,167)	1:135:B:GLU:C	1:136:B:ALA:N	1:136:B:ALA:CA	1:136:B:ALA:C	15	1.19
(1,126)	1:103:B:VAL:N	1:103:B:VAL:CA	1:103:B:VAL:C	1:104:B:TYR:N	20	1.19
(1,103)	1:194:A:LEU:C	1:195:A:TYR:N	1:195:A:TYR:CA	1:195:A:TYR:C	11	1.19
(1,182)	1:143:B:ASN:N	1:143:B:ASN:CA	1:143:B:ASN:C	1:144:B:PHE:N	17	1.18
(1,149)	1:122:B:TYR:C	1:123:B:ILE:N	1:123:B:ILE:CA	1:123:B:ILE:C	20	1.18
(1,137)	1:112:B:ALA:C	1:113:B:TYR:N	1:113:B:TYR:CA	1:113:B:TYR:C	12	1.18
(1,314)	1:194:C:LEU:N	1:194:C:LEU:CA	1:194:C:LEU:C	1:195:C:TYR:N	7	1.17
(1,266)	1:129:C:GLU:N	1:129:C:GLU:CA	1:129:C:GLU:C	1:130:C:SER:N	11	1.17
(1,266)	1:129:C:GLU:N	1:129:C:GLU:CA	1:129:C:GLU:C	1:130:C:SER:N	14	1.17
(1,167)	1:135:B:GLU:C	1:136:B:ALA:N	1:136:B:ALA:CA	1:136:B:ALA:C	7	1.17
(1,147)	1:121:B:CYS:C	1:122:B:TYR:N	1:122:B:TYR:CA	1:122:B:TYR:C	16	1.17
(1,91)	1:186:A:SER:C	1:187:A:THR:N	1:187:A:THR:CA	1:187:A:THR:C	2	1.17
(1,20)	1:103:A:VAL:N	1:103:A:VAL:CA	1:103:A:VAL:C	1:104:A:TYR:N	20	1.17
(1,306)	1:188:C:LEU:N	1:188:C:LEU:CA	1:188:C:LEU:C	1:189:C:CYS:N	14	1.16
(1,197)	1:186:B:SER:C	1:187:B:THR:N	1:187:B:THR:CA	1:187:B:THR:C	9	1.16
(1,192)	1:184:B:ALA:N	1:184:B:ALA:CA	1:184:B:ALA:C	1:185:B:VAL:N	13	1.16
(1,164)	1:133:B:SER:N	1:133:B:SER:CA	1:133:B:SER:C	1:134:B:LEU:N	18	1.16
(1,91)	1:186:A:SER:C	1:187:A:THR:N	1:187:A:THR:CA	1:187:A:THR:C	18	1.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,76)	1:143:A:ASN:N	1:143:A:ASN:CA	1:143:A:ASN:C	1:144:A:PHE:N	16	1.16
(1,2)	1:91:A:THR:N	1:91:A:THR:CA	1:91:A:THR:C	1:92:A:ALA:N	14	1.16
(1,295)	1:182:C:GLY:C	1:183:C:MET:N	1:183:C:MET:CA	1:183:C:MET:C	18	1.15
(1,281)	1:139:C:ARG:C	1:140:C:LYS:N	1:140:C:LYS:CA	1:140:C:LYS:C	3	1.15
(1,51)	1:126:A:ILE:C	1:127:A:ALA:N	1:127:A:ALA:CA	1:127:A:ALA:C	17	1.15
(1,281)	1:139:C:ARG:C	1:140:C:LYS:N	1:140:C:LYS:CA	1:140:C:LYS:C	7	1.14
(1,243)	1:112:C:ALA:C	1:113:C:TYR:N	1:113:C:TYR:CA	1:113:C:TYR:C	2	1.14
(1,243)	1:112:C:ALA:C	1:113:C:TYR:N	1:113:C:TYR:CA	1:113:C:TYR:C	17	1.14
(1,214)	1:91:C:THR:N	1:91:C:THR:CA	1:91:C:THR:C	1:92:C:ALA:N	4	1.14
(1,153)	1:124:B:MET:C	1:125:B:LYS:N	1:125:B:LYS:CA	1:125:B:LYS:C	17	1.14
(1,76)	1:143:A:ASN:N	1:143:A:ASN:CA	1:143:A:ASN:C	1:144:A:PHE:N	20	1.14
(1,208)	1:194:B:LEU:N	1:194:B:LEU:CA	1:194:B:LEU:C	1:195:B:TYR:N	4	1.13
(1,51)	1:126:A:ILE:C	1:127:A:ALA:N	1:127:A:ALA:CA	1:127:A:ALA:C	10	1.13
(1,243)	1:112:C:ALA:C	1:113:C:TYR:N	1:113:C:TYR:CA	1:113:C:TYR:C	14	1.12
(1,160)	1:129:B:GLU:N	1:129:B:GLU:CA	1:129:B:GLU:C	1:130:B:SER:N	14	1.12
(1,157)	1:126:B:ILE:C	1:127:B:ALA:N	1:127:B:ALA:CA	1:127:B:ALA:C	17	1.12
(1,137)	1:112:B:ALA:C	1:113:B:TYR:N	1:113:B:TYR:CA	1:113:B:TYR:C	17	1.12
(1,40)	1:121:A:CYS:N	1:121:A:CYS:CA	1:121:A:CYS:C	1:122:A:TYR:N	5	1.12
(1,270)	1:133:C:SER:N	1:133:C:SER:CA	1:133:C:SER:C	1:134:C:LEU:N	18	1.11
(1,265)	1:128:C:PRO:C	1:129:C:GLU:N	1:129:C:GLU:CA	1:129:C:GLU:C	10	1.11
(1,93)	1:187:A:THR:C	1:188:A:LEU:N	1:188:A:LEU:CA	1:188:A:LEU:C	14	1.11
(1,91)	1:186:A:SER:C	1:187:A:THR:N	1:187:A:THR:CA	1:187:A:THR:C	13	1.11
(1,86)	1:184:A:ALA:N	1:184:A:ALA:CA	1:184:A:ALA:C	1:185:A:VAL:N	1	1.11
(1,20)	1:103:A:VAL:N	1:103:A:VAL:CA	1:103:A:VAL:C	1:104:A:TYR:N	8	1.11
(1,13)	1:99:A:THR:C	1:100:A:GLY:N	1:100:A:GLY:CA	1:100:A:GLY:C	11	1.11
(1,154)	1:125:B:LYS:N	1:125:B:LYS:CA	1:125:B:LYS:C	1:126:B:ILE:N	3	1.1
(1,139)	1:113:B:TYR:C	1:114:B:LYS:N	1:114:B:LYS:CA	1:114:B:LYS:C	6	1.1
(1,137)	1:112:B:ALA:C	1:113:B:TYR:N	1:113:B:TYR:CA	1:113:B:TYR:C	14	1.1
(1,31)	1:112:A:ALA:C	1:113:A:TYR:N	1:113:A:TYR:CA	1:113:A:TYR:C	11	1.1
(1,303)	1:186:C:SER:C	1:187:C:THR:N	1:187:C:THR:CA	1:187:C:THR:C	13	1.09
(1,298)	1:184:C:ALA:N	1:184:C:ALA:CA	1:184:C:ALA:C	1:185:C:VAL:N	13	1.09
(1,266)	1:129:C:GLU:N	1:129:C:GLU:CA	1:129:C:GLU:C	1:130:C:SER:N	6	1.09
(1,265)	1:128:C:PRO:C	1:129:C:GLU:N	1:129:C:GLU:CA	1:129:C:GLU:C	5	1.09
(1,220)	1:94:C:PHE:N	1:94:C:PHE:CA	1:94:C:PHE:C	1:95:C:SER:N	19	1.09
(1,175)	1:139:B:ARG:C	1:140:B:LYS:N	1:140:B:LYS:CA	1:140:B:LYS:C	4	1.09
(1,91)	1:186:A:SER:C	1:187:A:THR:N	1:187:A:THR:CA	1:187:A:THR:C	12	1.09
(1,64)	1:137:A:LEU:N	1:137:A:LEU:CA	1:137:A:LEU:C	1:138:A:THR:N	3	1.09
(1,149)	1:122:B:TYR:C	1:123:B:ILE:N	1:123:B:ILE:CA	1:123:B:ILE:C	8	1.08
(1,141)	1:115:B:PRO:C	1:116:B:ALA:N	1:116:B:ALA:CA	1:116:B:ALA:C	15	1.08
(1,139)	1:113:B:TYR:C	1:114:B:LYS:N	1:114:B:LYS:CA	1:114:B:LYS:C	1	1.08
(1,76)	1:143:A:ASN:N	1:143:A:ASN:CA	1:143:A:ASN:C	1:144:A:PHE:N	10	1.08
(1,295)	1:182:C:GLY:C	1:183:C:MET:N	1:183:C:MET:CA	1:183:C:MET:C	12	1.07
(1,197)	1:186:B:SER:C	1:187:B:THR:N	1:187:B:THR:CA	1:187:B:THR:C	8	1.07
(1,197)	1:186:B:SER:C	1:187:B:THR:N	1:187:B:THR:CA	1:187:B:THR:C	19	1.07
(1,157)	1:126:B:ILE:C	1:127:B:ALA:N	1:127:B:ALA:CA	1:127:B:ALA:C	10	1.07
(1,109)	1:91:B:THR:C	1:92:B:ALA:N	1:92:B:ALA:CA	1:92:B:ALA:C	17	1.07
(1,91)	1:186:A:SER:C	1:187:A:THR:N	1:187:A:THR:CA	1:187:A:THR:C	16	1.07
(1,314)	1:194:C:LEU:N	1:194:C:LEU:CA	1:194:C:LEU:C	1:195:C:TYR:N	4	1.06
(1,295)	1:182:C:GLY:C	1:183:C:MET:N	1:183:C:MET:CA	1:183:C:MET:C	2	1.06
(1,255)	1:122:C:TYR:C	1:123:C:ILE:N	1:123:C:ILE:CA	1:123:C:ILE:C	18	1.06
(1,245)	1:113:C:TYR:C	1:114:C:LYS:N	1:114:C:LYS:CA	1:114:C:LYS:C	1	1.06

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,200)	1:188:B:LEU:N	1:188:B:LEU:CA	1:188:B:LEU:C	1:189:B:CYS:N	14	1.06
(1,192)	1:184:B:ALA:N	1:184:B:ALA:CA	1:184:B:ALA:C	1:185:B:VAL:N	9	1.06
(1,152)	1:124:B:MET:N	1:124:B:MET:CA	1:124:B:MET:C	1:125:B:LYS:N	9	1.06
(1,38)	1:118:A:GLY:N	1:118:A:GLY:CA	1:118:A:GLY:C	1:119:A:THR:N	5	1.06
(1,303)	1:186:C:SER:C	1:187:C:THR:N	1:187:C:THR:CA	1:187:C:THR:C	8	1.05
(1,298)	1:184:C:ALA:N	1:184:C:ALA:CA	1:184:C:ALA:C	1:185:C:VAL:N	9	1.05
(1,245)	1:113:C:TYR:C	1:114:C:LYS:N	1:114:C:LYS:CA	1:114:C:LYS:C	6	1.05
(1,119)	1:99:B:THR:C	1:100:B:GLY:N	1:100:B:GLY:CA	1:100:B:GLY:C	14	1.05
(1,91)	1:186:A:SER:C	1:187:A:THR:N	1:187:A:THR:CA	1:187:A:THR:C	20	1.05
(1,298)	1:184:C:ALA:N	1:184:C:ALA:CA	1:184:C:ALA:C	1:185:C:VAL:N	20	1.04
(1,288)	1:143:C:ASN:N	1:143:C:ASN:CA	1:143:C:ASN:C	1:144:C:PHE:N	9	1.04
(1,214)	1:91:C:THR:N	1:91:C:THR:CA	1:91:C:THR:C	1:92:C:ALA:N	2	1.04
(1,166)	1:135:B:GLU:N	1:135:B:GLU:CA	1:135:B:GLU:C	1:136:B:ALA:N	3	1.04
(1,43)	1:122:A:TYR:C	1:123:A:ILE:N	1:123:A:ILE:CA	1:123:A:ILE:C	18	1.04
(1,41)	1:121:A:CYS:C	1:122:A:TYR:N	1:122:A:TYR:CA	1:122:A:TYR:C	1	1.04
(1,41)	1:121:A:CYS:C	1:122:A:TYR:N	1:122:A:TYR:CA	1:122:A:TYR:C	14	1.04
(1,200)	1:188:B:LEU:N	1:188:B:LEU:CA	1:188:B:LEU:C	1:189:B:CYS:N	9	1.03
(1,189)	1:182:B:GLY:C	1:183:B:MET:N	1:183:B:MET:CA	1:183:B:MET:C	3	1.03
(1,175)	1:139:B:ARG:C	1:140:B:LYS:N	1:140:B:LYS:CA	1:140:B:LYS:C	7	1.03
(1,167)	1:135:B:GLU:C	1:136:B:ALA:N	1:136:B:ALA:CA	1:136:B:ALA:C	6	1.03
(1,255)	1:122:C:TYR:C	1:123:C:ILE:N	1:123:C:ILE:CA	1:123:C:ILE:C	1	1.02
(1,253)	1:121:C:CYS:C	1:122:C:TYR:N	1:122:C:TYR:CA	1:122:C:TYR:C	16	1.02
(1,225)	1:99:C:THR:C	1:100:C:GLY:N	1:100:C:GLY:CA	1:100:C:GLY:C	14	1.02
(1,160)	1:129:B:GLU:N	1:129:B:GLU:CA	1:129:B:GLU:C	1:130:B:SER:N	11	1.02
(1,149)	1:122:B:TYR:C	1:123:B:ILE:N	1:123:B:ILE:CA	1:123:B:ILE:C	1	1.02
(1,83)	1:182:A:GLY:C	1:183:A:MET:N	1:183:A:MET:CA	1:183:A:MET:C	14	1.02
(1,33)	1:113:A:TYR:C	1:114:A:LYS:N	1:114:A:LYS:CA	1:114:A:LYS:C	16	1.02
(1,306)	1:188:C:LEU:N	1:188:C:LEU:CA	1:188:C:LEU:C	1:189:C:CYS:N	6	1.01
(1,304)	1:187:C:THR:N	1:187:C:THR:CA	1:187:C:THR:C	1:188:C:LEU:N	19	1.01
(1,240)	1:111:C:ILE:N	1:111:C:ILE:CA	1:111:C:ILE:C	1:112:C:ALA:N	8	1.01
(1,225)	1:99:C:THR:C	1:100:C:GLY:N	1:100:C:GLY:CA	1:100:C:GLY:C	11	1.01
(1,198)	1:187:B:THR:N	1:187:B:THR:CA	1:187:B:THR:C	1:188:B:LEU:N	4	1.01
(1,182)	1:143:B:ASN:N	1:143:B:ASN:CA	1:143:B:ASN:C	1:144:B:PHE:N	4	1.01
(1,167)	1:135:B:GLU:C	1:136:B:ALA:N	1:136:B:ALA:CA	1:136:B:ALA:C	18	1.01
(1,160)	1:129:B:GLU:N	1:129:B:GLU:CA	1:129:B:GLU:C	1:130:B:SER:N	10	1.01
(1,43)	1:122:A:TYR:C	1:123:A:ILE:N	1:123:A:ILE:CA	1:123:A:ILE:C	3	1.01
(1,189)	1:182:B:GLY:C	1:183:B:MET:N	1:183:B:MET:CA	1:183:B:MET:C	4	1.0
(1,175)	1:139:B:ARG:C	1:140:B:LYS:N	1:140:B:LYS:CA	1:140:B:LYS:C	3	1.0
(1,58)	1:133:A:SER:N	1:133:A:SER:CA	1:133:A:SER:C	1:134:A:LEU:N	10	1.0