



Full wwPDB NMR Structure Validation Report ⓘ

Aug 10, 2026 – 05:14 pm BST

PDB ID : 9S9X / pdb_00009s9x
BMRB ID : 35012
Title : Human WASP/WIP complex
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Deposited on : 2025-08-06

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

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
BMRB Restraints Analysis : v1.2.1
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

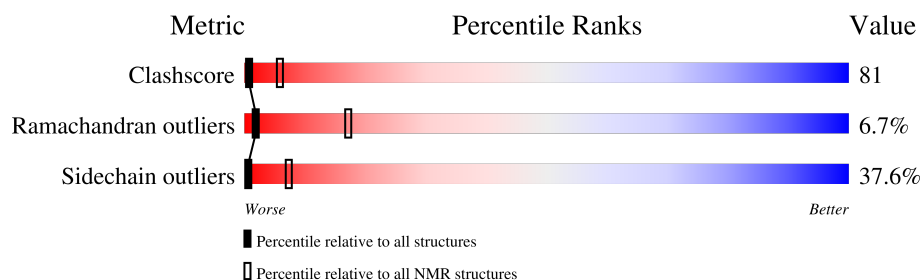
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 41%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	141	
2	B	53	

2 Ensemble composition and analysis

This entry contains 24 models. Model 1 is the overall representative, medoid model (most similar to other models).

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:24-A:149, B:444-B:481 (164)	0.83	1

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

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

The models can be grouped into 5 clusters and 1 single-model cluster was found.

Cluster number	Models
1	1, 2, 3, 9, 15, 18, 19, 21, 22, 23
2	7, 8, 11, 12, 17
3	4, 6, 13, 24
4	5, 20
5	14, 16
Single-model clusters	10

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3081 atoms, of which 1507 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Actin nucleation-promoting factor WAS.

Mol	Chain	Residues	Atoms						Trace
1	A	141	Total	C	H	N	O	S	0
			2248	718	1109	204	212	5	

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	SER	-	expression tag	UNP P42768
A	19	GLY	-	expression tag	UNP P42768

- Molecule 2 is a protein called WAS/WASL-interacting protein family member 1.

Mol	Chain	Residues	Atoms						Trace
2	B	53	Total	C	H	N	O	S	0
			833	267	398	77	90	1	

There are 2 discrepancies between the modelled and reference sequences:

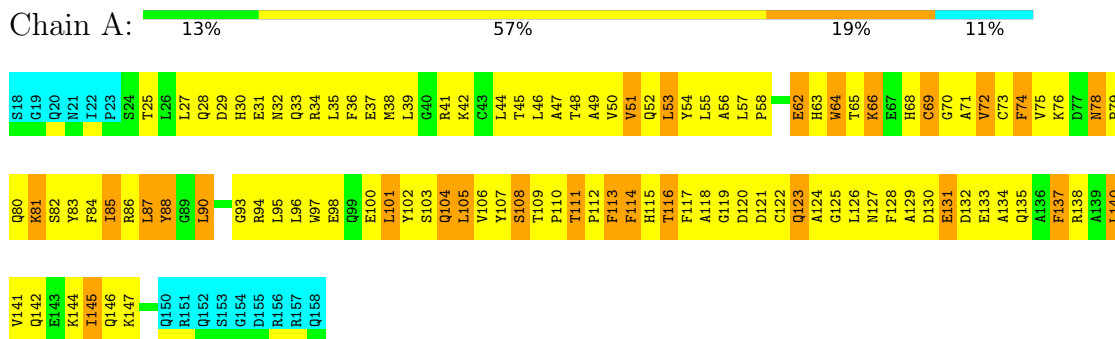
Chain	Residue	Modelled	Actual	Comment	Reference
B	440	SER	-	expression tag	UNP O43516
B	441	GLY	-	expression tag	UNP O43516

4 Residue-property plots

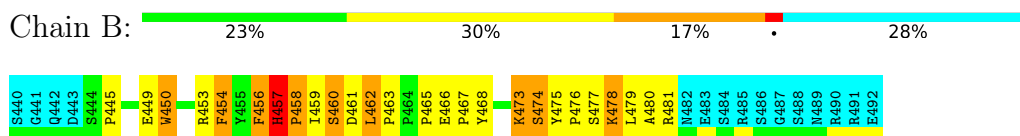
4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Actin nucleation-promoting factor WAS



- Molecule 2: WAS/WASL-interacting protein family member 1

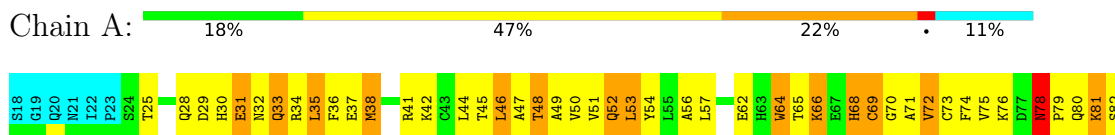


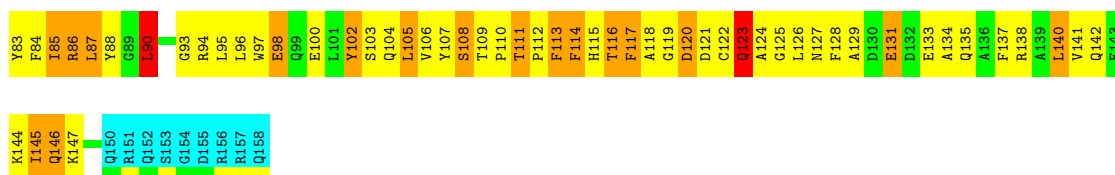
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Actin nucleation-promoting factor WAS





- Molecule 2: WAS/WASL-interacting protein family member 1

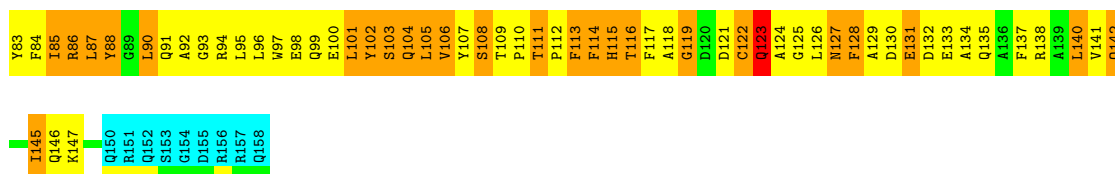
Chain B: 25% 30% 17% 28%



4.2.2 Score per residue for model 2

- Molecule 1: Actin nucleation-promoting factor WAS

Chain A: 15% 45% 29% 11%



- Molecule 2: WAS/WASL-interacting protein family member 1

Chain B: 17% 34% 19% 28%



4.2.3 Score per residue for model 3

- Molecule 1: Actin nucleation-promoting factor WAS

Chain A: 16% 47% 24% 11%



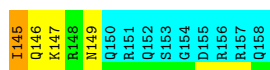
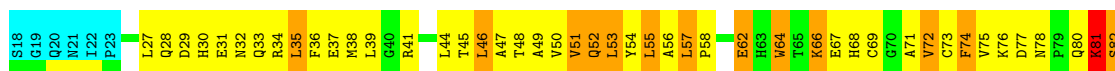
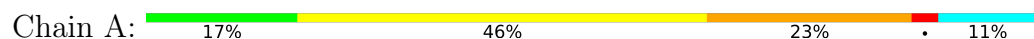


- Molecule 2: WAS/WASL-interacting protein family member 1



4.2.4 Score per residue for model 4

- Molecule 1: Actin nucleation-promoting factor WAS

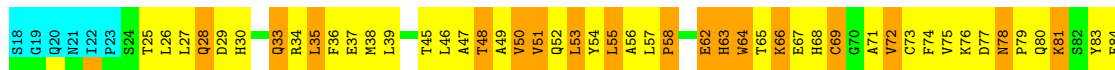
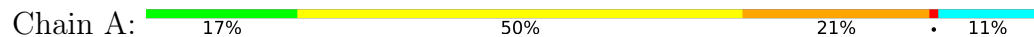


- Molecule 2: WAS/WASL-interacting protein family member 1

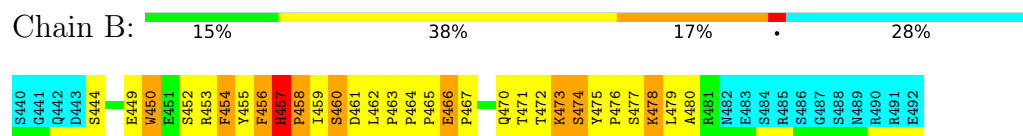


4.2.5 Score per residue for model 5

- Molecule 1: Actin nucleation-promoting factor WAS

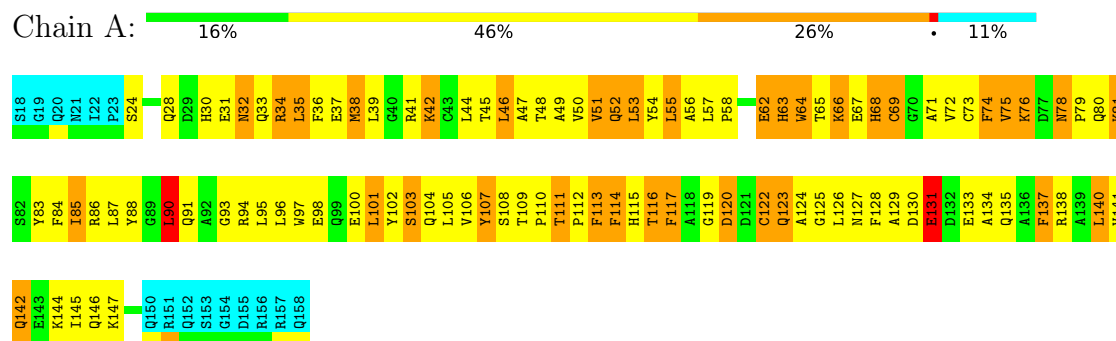


- Molecule 2: WAS/WASL-interacting protein family member 1

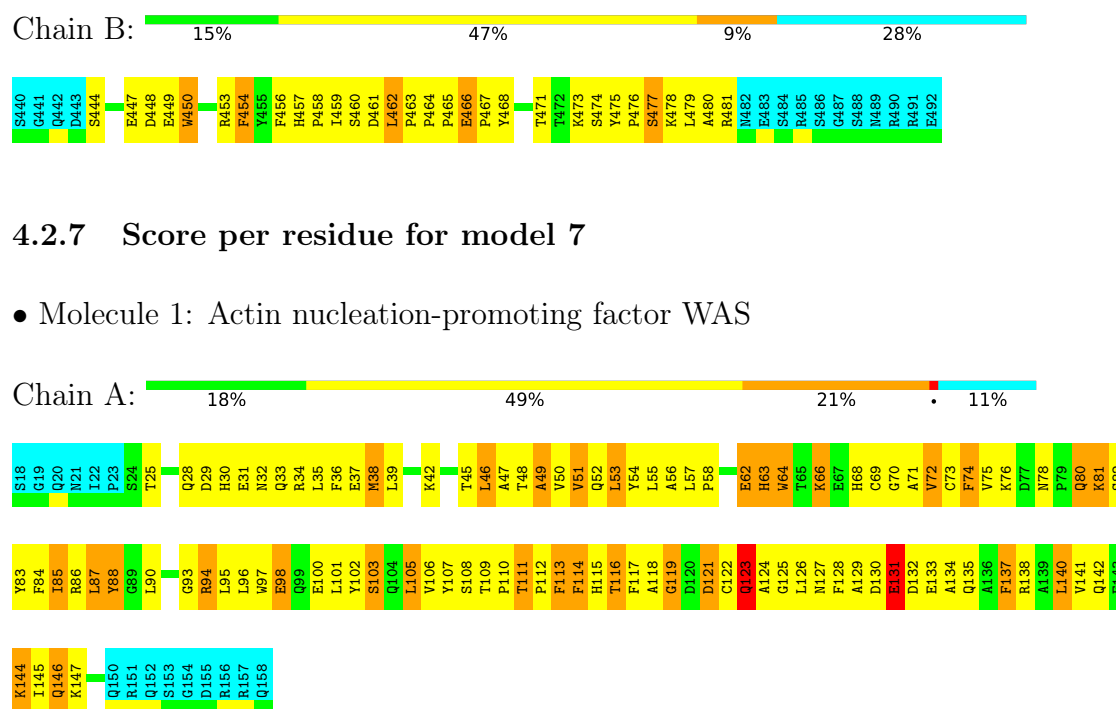


4.2.6 Score per residue for model 6

- Molecule 1: Actin nucleation-promoting factor WAS

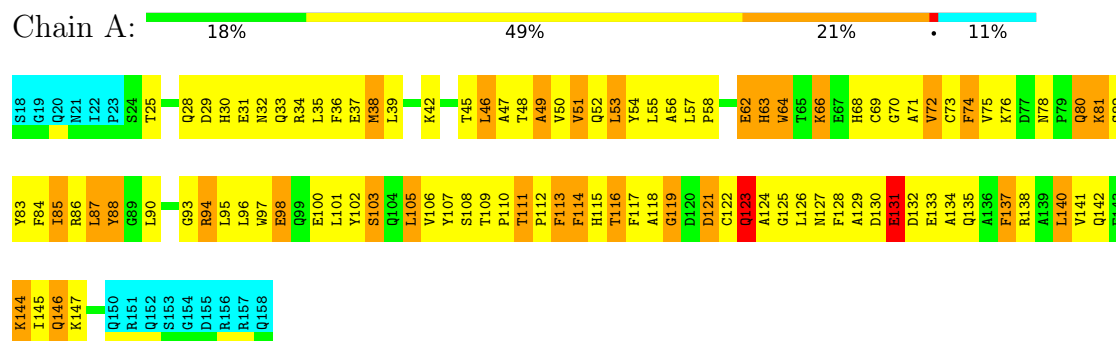


- Molecule 2: WAS/WASL-interacting protein family member 1

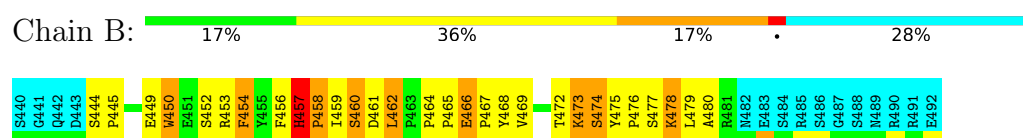


4.2.7 Score per residue for model 7

- Molecule 1: Actin nucleation-promoting factor WAS

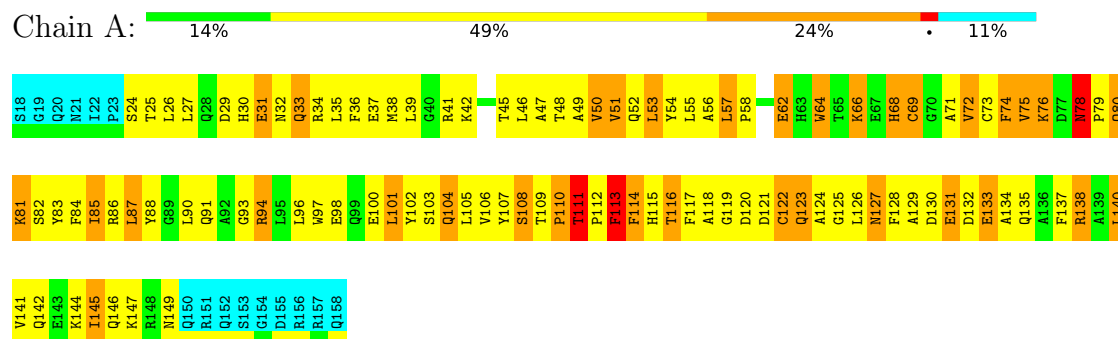


- Molecule 2: WAS/WASL-interacting protein family member 1

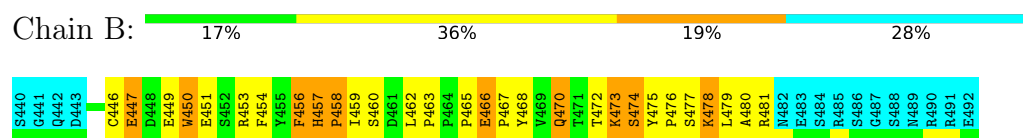


4.2.8 Score per residue for model 8

- Molecule 1: Actin nucleation-promoting factor WAS

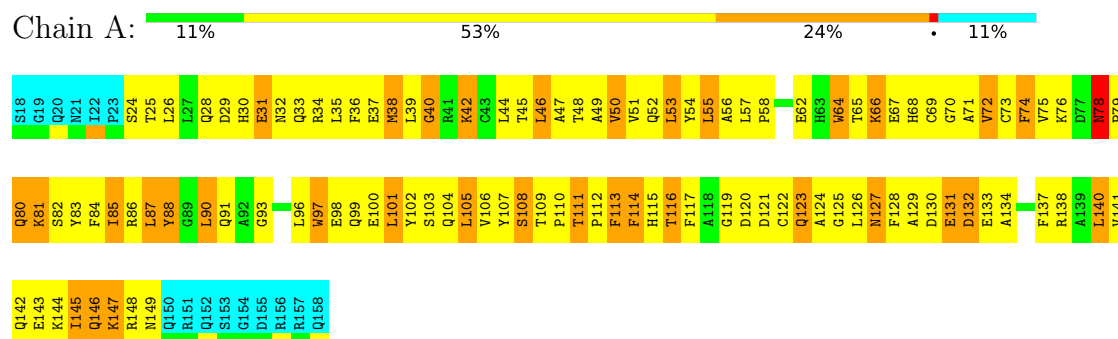


- Molecule 2: WAS/WASL-interacting protein family member 1

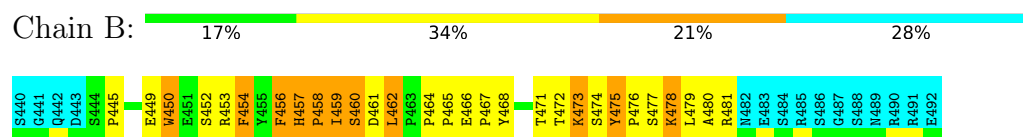


4.2.9 Score per residue for model 9

- Molecule 1: Actin nucleation-promoting factor WAS

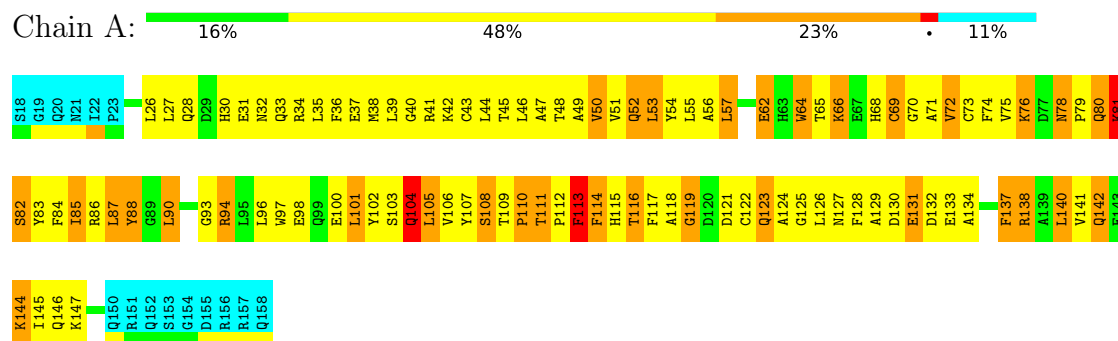


- Molecule 2: WAS/WASL-interacting protein family member 1

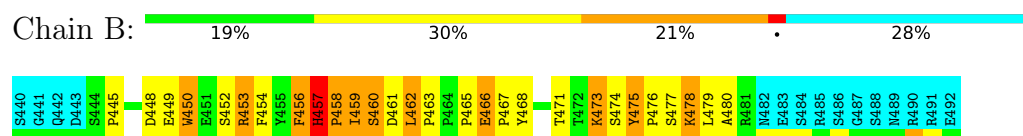


4.2.10 Score per residue for model 10

- Molecule 1: Actin nucleation-promoting factor WAS

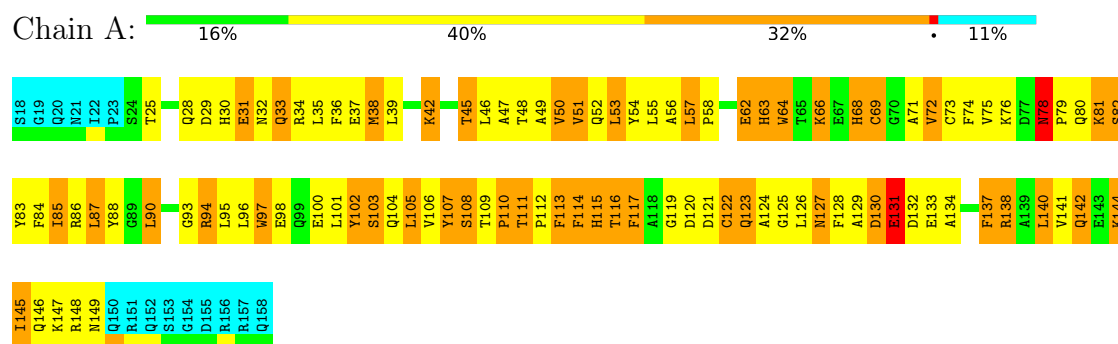


- Molecule 2: WAS/WASL-interacting protein family member 1

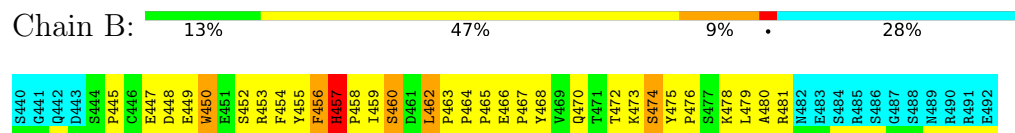


4.2.11 Score per residue for model 11

- Molecule 1: Actin nucleation-promoting factor WAS

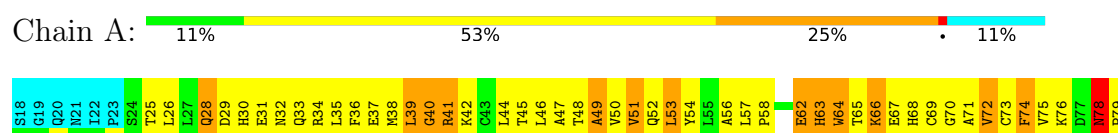


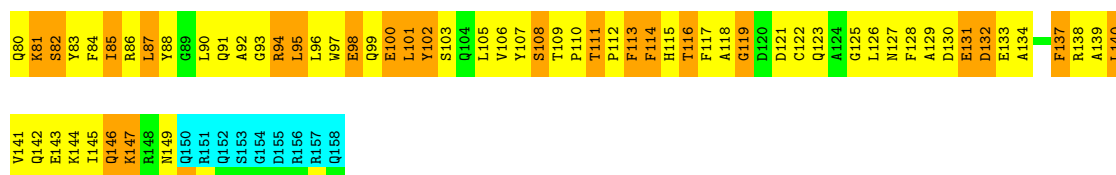
- Molecule 2: WAS/WASL-interacting protein family member 1



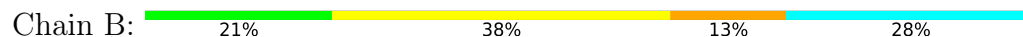
4.2.12 Score per residue for model 12

- Molecule 1: Actin nucleation-promoting factor WAS



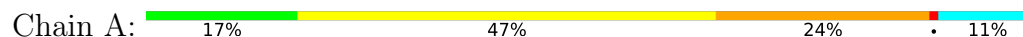


- Molecule 2: WAS/WASL-interacting protein family member 1



4.2.13 Score per residue for model 13

- Molecule 1: Actin nucleation-promoting factor WAS

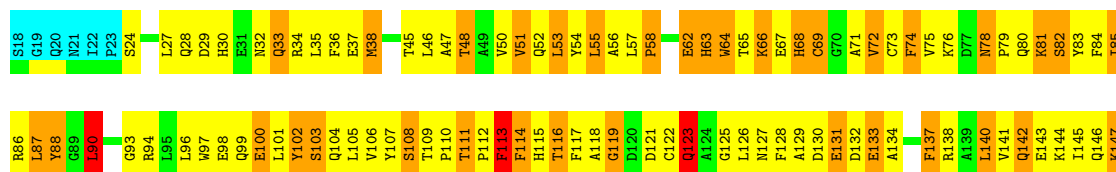
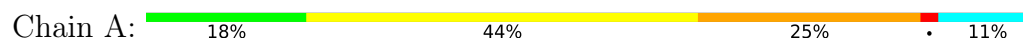


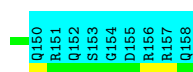
- Molecule 2: WAS/WASL-interacting protein family member 1



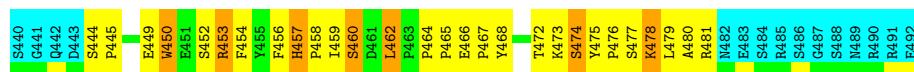
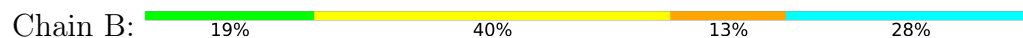
4.2.14 Score per residue for model 14

- Molecule 1: Actin nucleation-promoting factor WAS



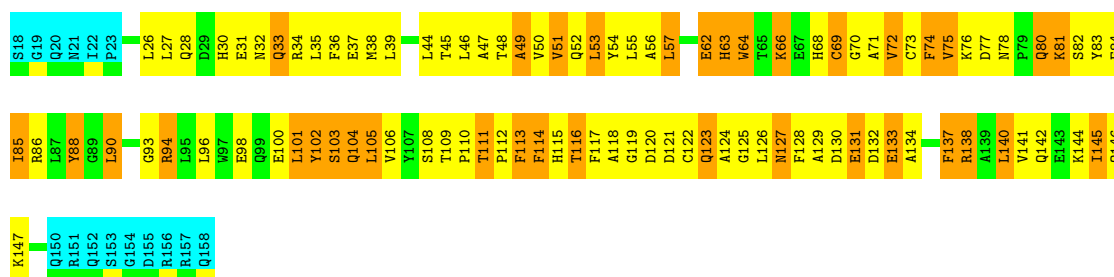
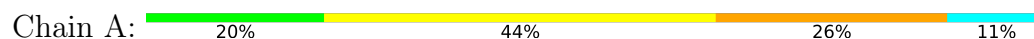


- Molecule 2: WAS/WASL-interacting protein family member 1

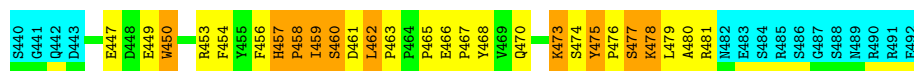


4.2.15 Score per residue for model 15

- Molecule 1: Actin nucleation-promoting factor WAS

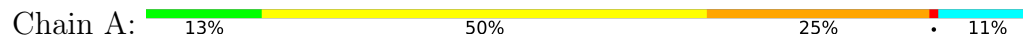


- Molecule 2: WAS/WASL-interacting protein family member 1

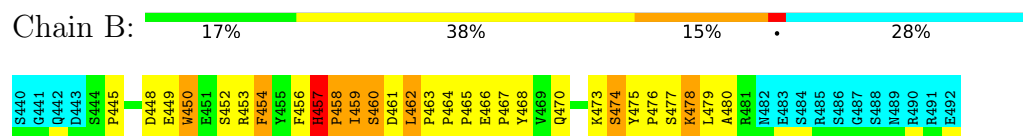


4.2.16 Score per residue for model 16

- Molecule 1: Actin nucleation-promoting factor WAS

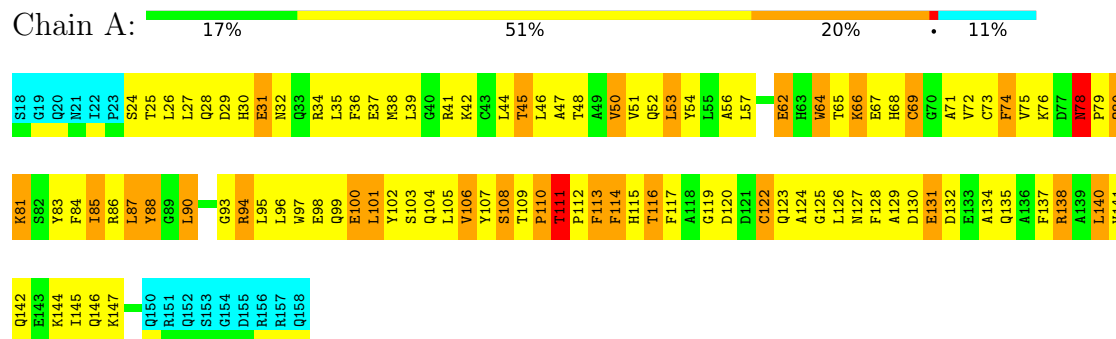


- Molecule 2: WAS/WASL-interacting protein family member 1

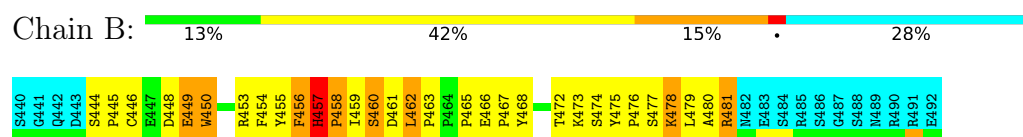


4.2.17 Score per residue for model 17

- Molecule 1: Actin nucleation-promoting factor WAS

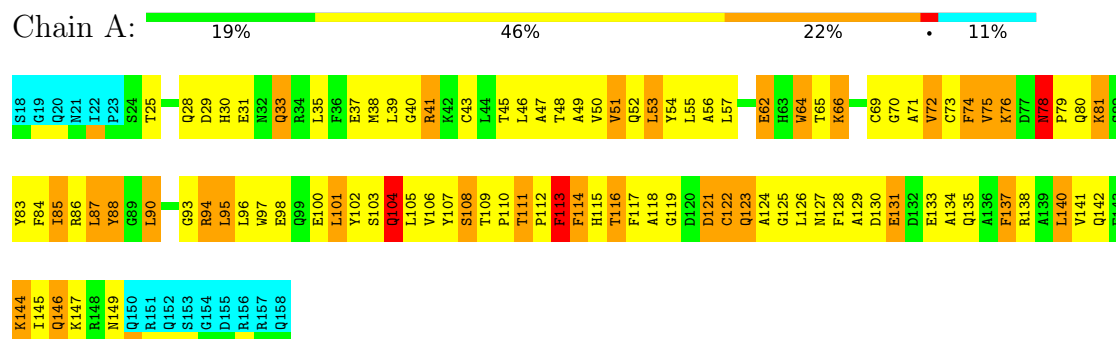


- Molecule 2: WAS/WASL-interacting protein family member 1

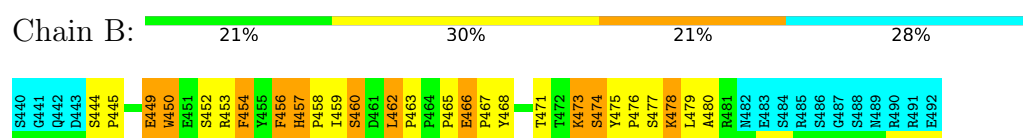


4.2.18 Score per residue for model 18

- Molecule 1: Actin nucleation-promoting factor WAS

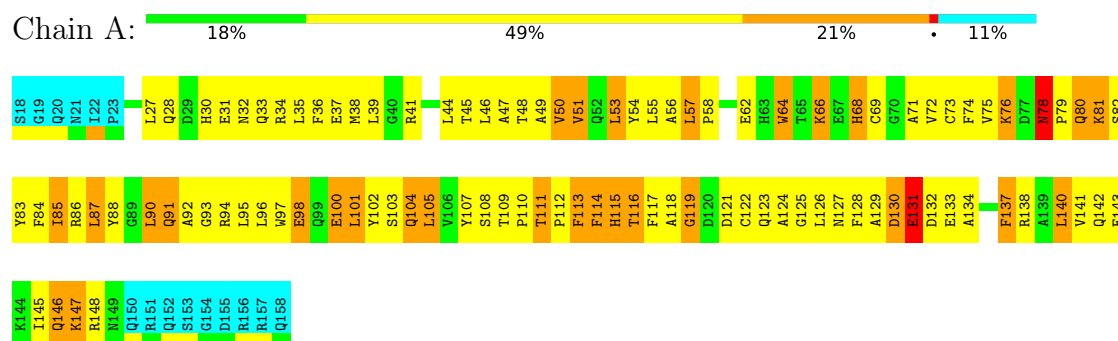


- Molecule 2: WAS/WASL-interacting protein family member 1

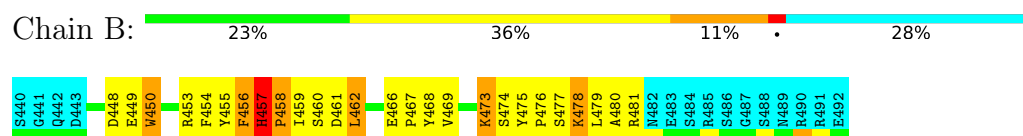


4.2.19 Score per residue for model 19

- Molecule 1: Actin nucleation-promoting factor WAS

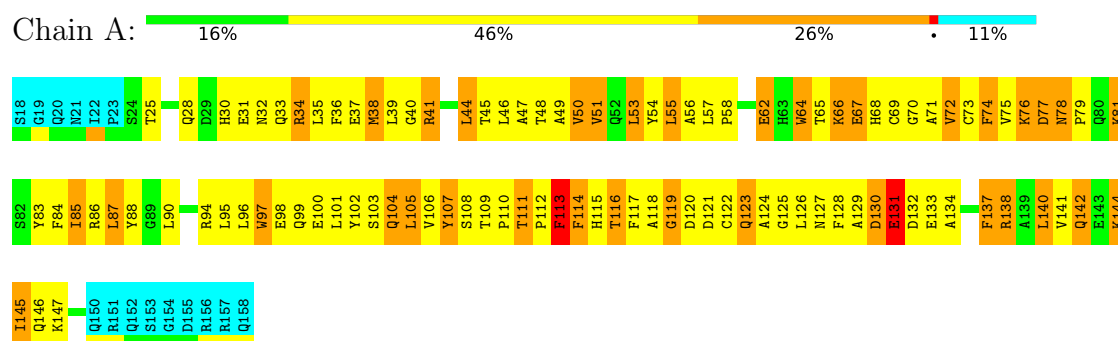


- Molecule 2: WAS/WASL-interacting protein family member 1

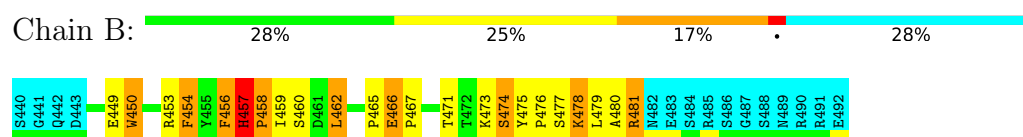


4.2.20 Score per residue for model 20

- Molecule 1: Actin nucleation-promoting factor WAS

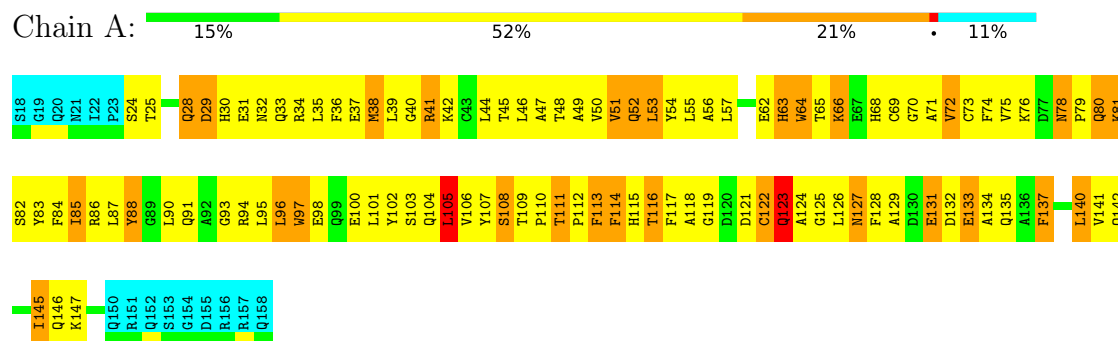


- Molecule 2: WAS/WASL-interacting protein family member 1

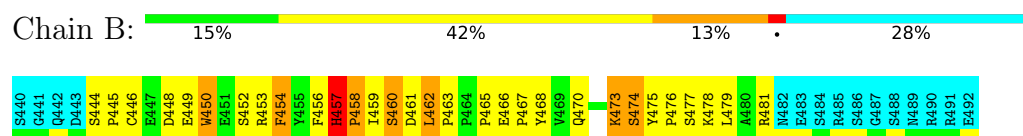


4.2.21 Score per residue for model 21

- Molecule 1: Actin nucleation-promoting factor WAS



- Molecule 2: WAS/WASL-interacting protein family member 1

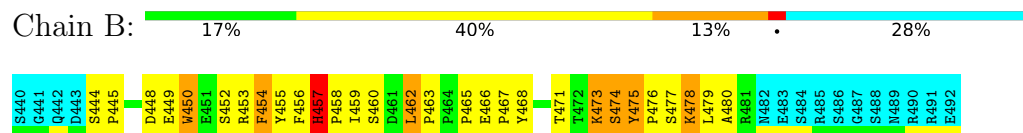


4.2.22 Score per residue for model 22

- Molecule 1: Actin nucleation-promoting factor WAS

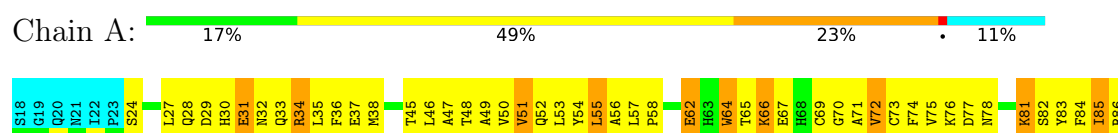


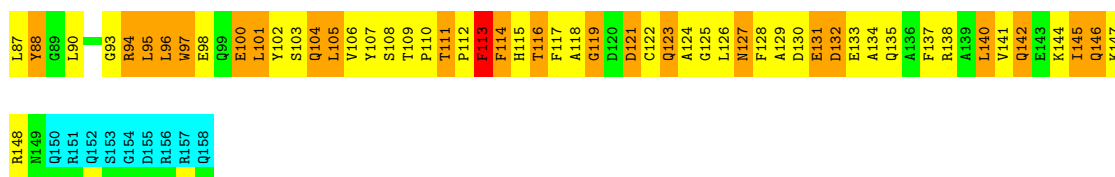
- Molecule 2: WAS/WASL-interacting protein family member 1



4.2.23 Score per residue for model 23

- Molecule 1: Actin nucleation-promoting factor WAS





- Molecule 2: WAS/WASL-interacting protein family member 1

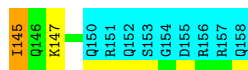
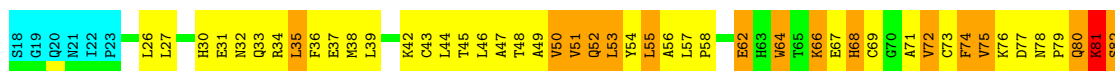
Chain B: 19% 30% 21% 28%



4.2.24 Score per residue for model 24

- Molecule 1: Actin nucleation-promoting factor WAS

Chain A: 16% 48% 24% 11%



- Molecule 2: WAS/WASL-interacting protein family member 1

Chain B: 17% 38% 15% 28%



5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 24 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CNS	structure calculation	
CNS	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1256
Number of shifts mapped to atoms	1256
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	41%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.45±0.01	0±0/1044 (0.0± 0.0%)	0.74±0.01	0±0/1416 (0.0± 0.0%)
2	B	0.48±0.01	0±0/333 (0.0± 0.0%)	0.96±0.03	2±1/458 (0.4± 0.2%)
All	All	0.45	0/33048 (0.0%)	0.80	40/44976 (0.1%)

There are no bond-length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	B	457	HIS	CA-C-N	6.34	127.77	119.84	18	20
2	B	457	HIS	C-N-CA	6.34	127.77	119.84	18	20

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1018	992	988	182±10
2	B	318	295	294	60±6
All	All	32064	30888	30768	5066

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 81.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:141:VAL:HG13	1:A:145:ILE:HD12	1.06	1.27	6	3
1:A:35:LEU:HD11	1:A:75:VAL:HG22	1.01	1.30	10	22
1:A:109:THR:HG23	1:A:128:PHE:CE2	1.00	1.92	2	2
2:B:459:ILE:HD11	2:B:462:LEU:HD13	0.99	1.31	19	2
1:A:106:VAL:HA	1:A:145:ILE:HD11	0.94	1.37	10	4
1:A:74:PHE:CD1	1:A:85:ILE:HD11	0.94	1.96	8	11
1:A:109:THR:HG22	1:A:128:PHE:CD2	0.93	1.98	12	5
1:A:122:CYS:O	1:A:123:GLN:HG3	0.91	1.65	14	13
1:A:109:THR:HG22	1:A:128:PHE:CZ	0.91	2.01	22	6
2:B:462:LEU:HD13	2:B:462:LEU:O	0.91	1.66	15	9
1:A:74:PHE:CD2	1:A:85:ILE:HD11	0.91	2.01	7	13
1:A:140:LEU:HD23	1:A:141:VAL:N	0.90	1.80	16	4
1:A:114:PHE:CD2	2:B:462:LEU:HD13	0.90	2.01	12	3
2:B:474:SER:HA	2:B:479:LEU:HD21	0.90	1.41	14	24
1:A:46:LEU:HD11	1:A:140:LEU:HD21	0.89	1.43	4	3
1:A:127:ASN:CB	2:B:459:ILE:HG22	0.89	1.98	22	7
1:A:102:TYR:CD1	2:B:473:LYS:HB2	0.89	2.02	18	7
1:A:114:PHE:CD1	2:B:462:LEU:HD13	0.89	2.03	13	1
1:A:107:TYR:O	1:A:141:VAL:HG11	0.88	1.68	7	11
1:A:47:ALA:HB1	1:A:140:LEU:HD22	0.88	1.41	12	3
1:A:56:ALA:HB2	1:A:64:TRP:CE3	0.88	2.04	22	16
1:A:127:ASN:HB2	2:B:459:ILE:HG22	0.88	1.45	21	5
1:A:38:MET:HE2	1:A:88:TYR:CE1	0.88	2.03	5	2
1:A:105:LEU:O	1:A:145:ILE:HD13	0.87	1.68	6	4
1:A:53:LEU:HD22	1:A:126:LEU:HD21	0.87	1.42	4	2
1:A:72:VAL:HG12	1:A:87:LEU:HD13	0.86	1.45	1	3
1:A:54:TYR:CD1	2:B:459:ILE:HD13	0.86	2.06	15	4
1:A:56:ALA:HB2	1:A:64:TRP:CD2	0.86	2.06	22	23
1:A:109:THR:HG23	1:A:128:PHE:CE1	0.86	2.04	18	2
1:A:47:ALA:CB	1:A:140:LEU:HD12	0.85	2.01	16	2
1:A:127:ASN:HB3	2:B:459:ILE:HG22	0.85	1.49	15	5
1:A:53:LEU:HD22	1:A:54:TYR:N	0.85	1.84	5	1
1:A:47:ALA:HB3	1:A:74:PHE:CG	0.84	2.07	12	24
1:A:53:LEU:HD23	1:A:87:LEU:HD21	0.84	1.49	4	2
1:A:51:VAL:HG13	1:A:128:PHE:HB3	0.84	1.48	20	16
1:A:109:THR:HG22	1:A:128:PHE:CE2	0.84	2.07	4	6
1:A:105:LEU:HD11	1:A:107:TYR:CE2	0.84	2.07	5	1
1:A:37:GLU:CG	1:A:90:LEU:HD21	0.83	2.03	11	5
1:A:50:VAL:HG13	1:A:71:ALA:HA	0.83	1.51	17	3
1:A:105:LEU:C	1:A:145:ILE:HD11	0.83	1.98	3	2
1:A:114:PHE:CD1	2:B:462:LEU:HD23	0.82	2.09	24	2
1:A:109:THR:HG23	1:A:128:PHE:CG	0.82	2.10	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:37:GLU:CG	1:A:90:LEU:HD11	0.82	2.03	20	1
1:A:32:ASN:HA	1:A:45:THR:HG21	0.82	1.52	17	11
1:A:81:LYS:O	1:A:81:LYS:HG3	0.82	1.73	14	13
1:A:127:ASN:OD1	2:B:459:ILE:HG22	0.81	1.75	14	4
1:A:54:TYR:C	1:A:55:LEU:HD13	0.81	2.00	5	7
2:B:459:ILE:HD12	2:B:462:LEU:HD21	0.81	1.51	12	3
1:A:35:LEU:HD22	1:A:74:PHE:O	0.81	1.76	16	22
1:A:34:ARG:HB2	1:A:48:THR:HG21	0.81	1.53	1	4
1:A:115:HIS:CE1	1:A:126:LEU:HD13	0.81	2.11	15	4
1:A:106:VAL:HG22	1:A:145:ILE:HD11	0.80	1.53	15	3
1:A:114:PHE:CE1	2:B:462:LEU:HD11	0.80	2.10	10	1
1:A:35:LEU:HD12	1:A:73:CYS:CB	0.80	2.07	8	14
2:B:450:TRP:CD2	2:B:454:PHE:HB2	0.80	2.11	24	22
1:A:81:LYS:HG3	1:A:81:LYS:O	0.80	1.75	6	10
1:A:107:TYR:CD2	1:A:117:PHE:CD1	0.80	2.70	16	1
1:A:127:ASN:OD1	2:B:459:ILE:HG23	0.80	1.77	18	1
1:A:111:THR:HG22	1:A:112:PRO:HD2	0.79	1.54	23	22
1:A:57:LEU:HD21	1:A:123:GLN:HB2	0.79	1.53	14	4
1:A:114:PHE:CD1	2:B:462:LEU:HD11	0.79	2.12	10	2
1:A:50:VAL:HG13	1:A:71:ALA:CA	0.79	2.07	17	3
1:A:38:MET:HE2	1:A:86:ARG:NH2	0.79	1.91	15	1
1:A:115:HIS:NE2	1:A:126:LEU:HD13	0.79	1.93	24	11
2:B:462:LEU:HD12	2:B:462:LEU:O	0.79	1.78	7	1
1:A:47:ALA:HB2	1:A:140:LEU:HD13	0.79	1.53	11	2
1:A:102:TYR:CD1	2:B:473:LYS:HB3	0.78	2.13	9	4
1:A:38:MET:O	1:A:38:MET:HE3	0.78	1.78	15	3
1:A:140:LEU:HD23	1:A:140:LEU:C	0.78	2.04	19	4
1:A:35:LEU:HD23	1:A:45:THR:HG23	0.78	1.56	1	5
1:A:35:LEU:CD1	1:A:75:VAL:HG22	0.77	2.09	15	21
1:A:49:ALA:HB1	1:A:133:GLU:CD	0.77	2.04	13	13
1:A:105:LEU:HD11	1:A:107:TYR:CE1	0.77	2.14	9	2
1:A:106:VAL:O	1:A:117:PHE:HB3	0.77	1.80	6	2
1:A:108:SER:O	1:A:115:HIS:HB3	0.77	1.78	24	21
1:A:105:LEU:HD21	1:A:144:LYS:CE	0.77	2.10	10	1
2:B:475:TYR:CD2	2:B:476:PRO:HD2	0.77	2.14	12	10
1:A:50:VAL:HG11	2:B:454:PHE:HB3	0.76	1.57	21	22
1:A:37:GLU:O	1:A:90:LEU:HD22	0.76	1.80	16	9
1:A:105:LEU:C	1:A:145:ILE:HD13	0.76	2.06	14	3
1:A:109:THR:HG21	1:A:133:GLU:OE1	0.75	1.80	1	3
1:A:102:TYR:CD2	2:B:473:LYS:HB3	0.75	2.17	17	4
1:A:57:LEU:HD11	1:A:123:GLN:CB	0.75	2.11	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:50:VAL:HG21	2:B:454:PHE:CB	0.75	2.11	19	3
1:A:54:TYR:CG	2:B:459:ILE:HD11	0.75	2.17	4	1
1:A:105:LEU:HD21	1:A:107:TYR:CD1	0.75	2.17	23	1
2:B:449:GLU:O	2:B:453:ARG:O	0.75	2.05	24	24
1:A:38:MET:HA	1:A:90:LEU:HD13	0.75	1.59	13	19
1:A:56:ALA:C	1:A:57:LEU:HD22	0.75	2.07	14	5
2:B:462:LEU:C	2:B:462:LEU:HD12	0.74	2.07	3	4
2:B:475:TYR:CD1	2:B:476:PRO:HD2	0.74	2.16	10	13
1:A:106:VAL:HG13	1:A:145:ILE:CD1	0.74	2.12	12	3
1:A:50:VAL:HG22	2:B:454:PHE:CD2	0.74	2.18	15	5
1:A:127:ASN:ND2	2:B:462:LEU:HD23	0.74	1.98	1	2
1:A:54:TYR:CD2	2:B:459:ILE:HD13	0.73	2.18	11	2
1:A:108:SER:HB3	1:A:110:PRO:HD3	0.73	1.60	13	23
1:A:106:VAL:HA	1:A:145:ILE:HD13	0.73	1.60	21	11
1:A:109:THR:OG1	1:A:134:ALA:HA	0.73	1.81	1	14
1:A:46:LEU:HD22	1:A:76:LYS:HD3	0.73	1.58	20	2
1:A:105:LEU:HD12	1:A:107:TYR:CD2	0.73	2.18	24	2
2:B:475:TYR:O	2:B:479:LEU:N	0.73	2.18	21	21
1:A:53:LEU:HD22	1:A:126:LEU:CD2	0.73	2.13	24	2
1:A:50:VAL:HG22	2:B:454:PHE:CD1	0.73	2.18	14	7
1:A:47:ALA:HB2	1:A:140:LEU:HD23	0.73	1.61	10	4
1:A:52:GLN:HB2	2:B:456:PHE:O	0.73	1.82	12	17
2:B:462:LEU:HD12	2:B:463:PRO:O	0.73	1.84	13	6
1:A:69:CYS:O	1:A:96:LEU:HD12	0.73	1.83	20	6
2:B:476:PRO:O	2:B:480:ALA:HB3	0.73	1.82	14	18
2:B:462:LEU:HD23	2:B:462:LEU:O	0.73	1.84	9	2
1:A:122:CYS:O	1:A:123:GLN:HG2	0.73	1.83	20	8
1:A:38:MET:HE3	1:A:86:ARG:NE	0.73	1.99	7	3
1:A:37:GLU:HG3	1:A:90:LEU:HD22	0.73	1.59	10	7
1:A:109:THR:HG23	1:A:128:PHE:CD2	0.72	2.19	11	2
1:A:87:LEU:HD12	1:A:96:LEU:HB2	0.72	1.59	2	4
1:A:37:GLU:HG2	1:A:90:LEU:HD21	0.72	1.62	19	5
1:A:46:LEU:HD11	1:A:140:LEU:CD2	0.72	2.14	4	2
1:A:37:GLU:O	1:A:90:LEU:HD13	0.72	1.85	7	2
1:A:114:PHE:CG	2:B:462:LEU:HD23	0.72	2.19	24	2
1:A:109:THR:HB	1:A:128:PHE:CE1	0.71	2.20	4	6
1:A:129:ALA:HB3	1:A:133:GLU:HG2	0.71	1.61	2	5
1:A:90:LEU:HA	1:A:94:ARG:H	0.71	1.44	15	13
1:A:35:LEU:HD12	1:A:73:CYS:HB2	0.71	1.61	8	17
1:A:37:GLU:CG	1:A:90:LEU:HD22	0.71	2.16	22	8
1:A:51:VAL:HA	1:A:127:ASN:O	0.71	1.84	18	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:122:CYS:O	1:A:123:GLN:CG	0.71	2.39	24	20
1:A:54:TYR:CD2	2:B:459:ILE:HD11	0.71	2.21	4	1
1:A:102:TYR:CD2	2:B:473:LYS:HB2	0.71	2.20	13	6
2:B:474:SER:CB	2:B:479:LEU:HD21	0.71	2.16	2	4
1:A:50:VAL:HB	2:B:454:PHE:CD1	0.70	2.21	11	1
1:A:81:LYS:O	2:B:476:PRO:HD3	0.70	1.87	21	12
1:A:114:PHE:HA	1:A:126:LEU:O	0.70	1.85	17	21
2:B:474:SER:CA	2:B:479:LEU:HD21	0.70	2.15	10	22
1:A:105:LEU:O	1:A:145:ILE:HD11	0.70	1.86	18	2
1:A:69:CYS:O	1:A:96:LEU:HD13	0.70	1.85	21	12
1:A:109:THR:HG21	1:A:133:GLU:OE2	0.70	1.87	8	1
1:A:109:THR:HG23	1:A:128:PHE:CD1	0.70	2.22	18	1
1:A:53:LEU:HD12	1:A:87:LEU:HD11	0.70	1.61	13	4
1:A:81:LYS:O	1:A:81:LYS:CG	0.70	2.39	16	21
1:A:95:LEU:O	1:A:96:LEU:HD23	0.70	1.87	18	9
1:A:131:GLU:HA	1:A:134:ALA:HB3	0.70	1.62	15	14
1:A:50:VAL:CG1	2:B:450:TRP:CZ2	0.70	2.75	23	11
1:A:105:LEU:HD21	1:A:144:LYS:HE3	0.69	1.61	10	2
1:A:112:PRO:O	1:A:113:PHE:CD1	0.69	2.45	8	3
1:A:118:ALA:HB1	2:B:468:TYR:CE2	0.69	2.22	16	2
1:A:106:VAL:HG12	1:A:117:PHE:CD2	0.69	2.23	21	1
1:A:105:LEU:HD12	1:A:145:ILE:HD11	0.69	1.63	14	4
1:A:105:LEU:HD11	1:A:107:TYR:CZ	0.69	2.21	23	1
1:A:105:LEU:O	1:A:145:ILE:HD12	0.69	1.88	9	2
1:A:50:VAL:O	1:A:51:VAL:HG13	0.69	1.88	11	6
1:A:55:LEU:HD11	1:A:67:GLU:OE2	0.69	1.87	6	3
1:A:46:LEU:HD21	1:A:144:LYS:HD2	0.69	1.63	11	1
1:A:31:GLU:HA	1:A:48:THR:OG1	0.69	1.88	19	4
1:A:112:PRO:O	1:A:113:PHE:CD2	0.69	2.46	17	7
1:A:114:PHE:CG	2:B:462:LEU:HD12	0.69	2.23	4	3
1:A:105:LEU:HD23	1:A:105:LEU:O	0.68	1.88	23	4
1:A:87:LEU:HD21	1:A:97:TRP:CE3	0.68	2.23	22	2
1:A:109:THR:N	1:A:110:PRO:CD	0.68	2.56	4	24
1:A:27:LEU:HD12	1:A:28:GLN:NE2	0.68	2.03	5	1
1:A:54:TYR:CD1	1:A:125:GLY:O	0.68	2.47	14	3
1:A:37:GLU:HG3	1:A:90:LEU:HD21	0.68	1.65	11	3
1:A:83:TYR:CE1	1:A:105:LEU:HD21	0.68	2.23	6	2
1:A:109:THR:HA	1:A:128:PHE:CE1	0.68	2.24	10	2
1:A:57:LEU:HD21	1:A:123:GLN:CB	0.68	2.19	14	1
1:A:129:ALA:HB1	2:B:454:PHE:CE2	0.68	2.24	1	8
1:A:38:MET:HE3	1:A:86:ARG:CD	0.68	2.19	7	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:34:ARG:HB3	1:A:48:THR:HG21	0.68	1.64	21	12
1:A:30:HIS:O	1:A:33:GLN:N	0.68	2.27	10	14
1:A:74:PHE:CE1	1:A:140:LEU:HD21	0.68	2.24	11	2
1:A:46:LEU:HD22	1:A:76:LYS:HG3	0.67	1.66	10	4
1:A:49:ALA:HB1	1:A:133:GLU:OE1	0.67	1.89	3	5
1:A:54:TYR:CG	1:A:125:GLY:O	0.67	2.47	14	2
2:B:459:ILE:CG1	2:B:462:LEU:HD13	0.67	2.19	9	1
1:A:38:MET:O	1:A:90:LEU:HD13	0.67	1.90	8	6
1:A:46:LEU:HD13	1:A:76:LYS:CE	0.67	2.19	14	3
1:A:119:GLY:N	1:A:122:CYS:O	0.67	2.28	17	2
1:A:101:LEU:HD23	1:A:102:TYR:N	0.67	2.05	18	1
1:A:44:LEU:HD11	1:A:77:ASP:O	0.67	1.88	20	1
1:A:109:THR:HG22	1:A:109:THR:O	0.67	1.90	18	4
1:A:109:THR:HA	1:A:128:PHE:CZ	0.67	2.25	5	12
2:B:459:ILE:O	2:B:462:LEU:HD12	0.67	1.90	18	7
1:A:81:LYS:CG	1:A:81:LYS:O	0.67	2.42	17	2
2:B:475:TYR:HB3	2:B:478:LYS:CD	0.67	2.20	2	12
1:A:140:LEU:C	1:A:140:LEU:HD13	0.67	2.15	14	12
1:A:113:PHE:O	1:A:127:ASN:HA	0.66	1.90	23	20
1:A:54:TYR:CE1	1:A:66:LYS:HB3	0.66	2.24	20	8
1:A:114:PHE:CG	2:B:462:LEU:HD22	0.66	2.25	17	3
2:B:450:TRP:CE3	2:B:454:PHE:HB2	0.66	2.25	1	21
1:A:51:VAL:HG13	1:A:128:PHE:CB	0.66	2.21	4	12
1:A:35:LEU:HG	1:A:39:LEU:HD23	0.66	1.67	13	3
2:B:462:LEU:HD12	2:B:463:PRO:N	0.66	2.05	17	3
1:A:129:ALA:HB3	1:A:133:GLU:HB2	0.66	1.65	21	9
1:A:31:GLU:OE2	1:A:45:THR:HG22	0.66	1.90	11	1
1:A:118:ALA:HB2	2:B:468:TYR:CE1	0.66	2.26	1	1
1:A:119:GLY:O	1:A:122:CYS:O	0.66	2.14	9	8
2:B:462:LEU:HD22	2:B:463:PRO:O	0.66	1.90	21	7
1:A:109:THR:HG23	1:A:128:PHE:CZ	0.66	2.26	7	1
1:A:75:VAL:HG21	1:A:86:ARG:NE	0.65	2.06	4	4
1:A:35:LEU:CD2	1:A:45:THR:HA	0.65	2.21	15	20
1:A:39:LEU:O	1:A:39:LEU:HD12	0.65	1.91	5	1
1:A:134:ALA:O	1:A:138:ARG:HB2	0.65	1.92	17	7
2:B:462:LEU:C	2:B:462:LEU:HD13	0.65	2.16	24	1
2:B:454:PHE:O	2:B:456:PHE:CE1	0.65	2.50	11	11
1:A:107:TYR:CE2	1:A:117:PHE:CD2	0.65	2.85	16	1
1:A:109:THR:HG22	1:A:128:PHE:CG	0.65	2.25	1	5
1:A:48:THR:HG22	1:A:88:TYR:CE1	0.65	2.27	1	1
1:A:32:ASN:HB2	1:A:45:THR:HG21	0.65	1.66	21	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:81:LYS:HB2	2:B:476:PRO:HD3	0.65	1.68	10	1
1:A:114:PHE:CD1	2:B:462:LEU:HD12	0.65	2.27	19	1
1:A:140:LEU:O	1:A:140:LEU:HD22	0.65	1.91	6	4
2:B:462:LEU:HD13	2:B:462:LEU:C	0.65	2.16	15	7
2:B:474:SER:CB	2:B:479:LEU:HD11	0.65	2.21	14	5
1:A:37:GLU:CD	1:A:90:LEU:HD22	0.65	2.16	15	3
1:A:87:LEU:CB	1:A:96:LEU:HD12	0.65	2.22	13	3
1:A:39:LEU:HD22	1:A:43:CYS:SG	0.65	2.31	24	1
1:A:54:TYR:CE1	2:B:459:ILE:HG23	0.65	2.27	1	3
1:A:75:VAL:O	1:A:84:PHE:O	0.65	2.15	23	23
1:A:87:LEU:HD11	1:A:97:TRP:HB3	0.65	1.68	12	3
1:A:81:LYS:HD2	2:B:479:LEU:HD12	0.65	1.67	14	3
2:B:462:LEU:HD22	2:B:463:PRO:HD2	0.65	1.67	10	2
1:A:140:LEU:HD13	1:A:141:VAL:N	0.65	2.06	1	16
2:B:475:TYR:HD2	2:B:476:PRO:HD2	0.65	1.52	22	5
1:A:141:VAL:HG13	1:A:145:ILE:CD1	0.65	2.16	6	2
1:A:53:LEU:HD12	1:A:97:TRP:CZ3	0.64	2.27	14	1
1:A:35:LEU:HD12	1:A:73:CYS:HB3	0.64	1.69	5	7
1:A:129:ALA:HB3	1:A:133:GLU:HB3	0.64	1.70	3	1
1:A:118:ALA:HA	1:A:122:CYS:O	0.64	1.92	5	8
1:A:35:LEU:CD1	1:A:73:CYS:HB2	0.64	2.23	1	7
1:A:142:GLN:O	1:A:146:GLN:HB2	0.64	1.92	6	17
1:A:114:PHE:CB	2:B:459:ILE:HG22	0.64	2.22	18	1
1:A:102:TYR:CG	2:B:473:LYS:HB3	0.64	2.28	17	8
1:A:125:GLY:C	1:A:126:LEU:HD12	0.64	2.17	1	8
1:A:126:LEU:HD12	1:A:126:LEU:N	0.64	2.07	1	6
1:A:97:TRP:C	1:A:97:TRP:CD1	0.64	2.75	3	5
1:A:46:LEU:HD13	1:A:76:LYS:HE2	0.64	1.68	14	2
1:A:51:VAL:HG12	1:A:128:PHE:HB3	0.64	1.69	9	5
1:A:108:SER:HB3	1:A:110:PRO:CD	0.64	2.22	4	2
2:B:450:TRP:CE3	2:B:450:TRP:O	0.64	2.51	10	19
1:A:113:PHE:O	1:A:128:PHE:N	0.64	2.30	6	12
1:A:106:VAL:HA	1:A:145:ILE:CD1	0.64	2.23	1	7
1:A:38:MET:HB2	1:A:90:LEU:HD22	0.64	1.67	19	2
1:A:90:LEU:HD23	1:A:90:LEU:O	0.63	1.91	20	7
1:A:114:PHE:CE2	1:A:116:THR:HG23	0.63	2.29	19	2
1:A:142:GLN:O	1:A:146:GLN:CB	0.63	2.46	14	8
2:B:450:TRP:O	2:B:450:TRP:CE3	0.63	2.51	17	5
1:A:46:LEU:HD11	1:A:144:LYS:CE	0.63	2.24	20	1
1:A:35:LEU:HD11	1:A:75:VAL:CG2	0.63	2.17	10	11
1:A:37:GLU:CB	1:A:90:LEU:HD11	0.63	2.24	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:71:ALA:O	1:A:88:TYR:O	0.63	2.17	5	15
1:A:114:PHE:CD2	2:B:462:LEU:HD12	0.63	2.28	20	3
1:A:97:TRP:CD1	1:A:97:TRP:C	0.63	2.77	23	4
1:A:32:ASN:OD1	1:A:45:THR:HG21	0.63	1.94	19	1
1:A:105:LEU:HD11	1:A:107:TYR:CD2	0.63	2.29	5	1
1:A:106:VAL:O	1:A:117:PHE:HB2	0.63	1.94	2	12
1:A:107:TYR:C	1:A:141:VAL:HG11	0.63	2.19	12	4
1:A:54:TYR:CD1	2:B:459:ILE:HD12	0.63	2.29	8	1
1:A:95:LEU:C	1:A:96:LEU:HD23	0.63	2.18	19	4
1:A:39:LEU:HD13	1:A:43:CYS:SG	0.63	2.34	24	1
2:B:457:HIS:HB2	2:B:458:PRO:HD2	0.63	1.71	20	1
1:A:81:LYS:HG3	2:B:476:PRO:HD3	0.62	1.70	17	16
2:B:475:TYR:HB3	2:B:478:LYS:HG2	0.62	1.70	18	13
1:A:53:LEU:HD13	1:A:126:LEU:HG	0.62	1.69	24	2
1:A:114:PHE:CE2	2:B:462:LEU:HD23	0.62	2.29	18	2
1:A:53:LEU:HD13	1:A:87:LEU:HD11	0.62	1.69	1	1
2:B:459:ILE:HB	2:B:462:LEU:HD22	0.62	1.70	14	1
1:A:133:GLU:OE2	1:A:136:ALA:HB3	0.62	1.94	16	1
1:A:81:LYS:CD	2:B:476:PRO:HD3	0.62	2.24	11	15
1:A:87:LEU:N	1:A:87:LEU:CD2	0.62	2.63	7	3
1:A:109:THR:HA	1:A:128:PHE:CE2	0.62	2.29	1	7
1:A:126:LEU:N	1:A:126:LEU:HD12	0.62	2.10	22	9
1:A:46:LEU:HD21	1:A:144:LYS:CD	0.62	2.24	11	1
1:A:129:ALA:HB1	2:B:454:PHE:CE1	0.62	2.29	13	5
1:A:54:TYR:CE2	1:A:64:TRP:CH2	0.62	2.88	5	2
1:A:37:GLU:HG2	1:A:90:LEU:HD22	0.62	1.71	14	3
1:A:35:LEU:N	1:A:48:THR:HG21	0.62	2.09	23	3
1:A:49:ALA:HB1	1:A:133:GLU:OE2	0.62	1.94	6	4
1:A:38:MET:HE3	1:A:86:ARG:HD2	0.62	1.70	7	3
1:A:105:LEU:O	1:A:105:LEU:HD23	0.62	1.95	9	1
1:A:80:GLN:O	1:A:81:LYS:HB2	0.62	1.94	10	1
1:A:81:LYS:HD3	2:B:476:PRO:HD3	0.62	1.71	20	16
1:A:131:GLU:O	1:A:134:ALA:HB3	0.62	1.93	21	17
1:A:114:PHE:CE2	2:B:462:LEU:HD13	0.62	2.30	16	3
1:A:109:THR:N	1:A:110:PRO:HD3	0.62	2.10	8	24
1:A:118:ALA:HB2	2:B:468:TYR:CD1	0.61	2.29	1	4
1:A:52:GLN:NE2	1:A:54:TYR:CD2	0.61	2.68	2	1
2:B:474:SER:HB3	2:B:479:LEU:HD11	0.61	1.70	10	5
1:A:105:LEU:CD1	1:A:145:ILE:HD11	0.61	2.25	11	1
2:B:454:PHE:O	2:B:456:PHE:CE2	0.61	2.54	19	8
2:B:459:ILE:HG13	2:B:462:LEU:HD13	0.61	1.72	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:54:TYR:OH	1:A:114:PHE:CD2	0.61	2.53	5	3
1:A:55:LEU:HD13	1:A:55:LEU:N	0.61	2.10	23	4
1:A:102:TYR:CE1	2:B:478:LYS:CD	0.61	2.82	18	6
1:A:47:ALA:CB	1:A:140:LEU:HD22	0.61	2.26	23	3
1:A:71:ALA:HB2	2:B:450:TRP:CH2	0.61	2.30	10	5
2:B:462:LEU:CD1	2:B:463:PRO:O	0.61	2.49	3	5
2:B:462:LEU:HD13	2:B:463:PRO:HD2	0.61	1.73	10	1
1:A:54:TYR:CD2	2:B:459:ILE:HG23	0.61	2.31	22	1
1:A:129:ALA:HB3	1:A:133:GLU:CB	0.61	2.25	21	3
1:A:47:ALA:CB	1:A:140:LEU:HD13	0.61	2.25	11	2
1:A:122:CYS:O	1:A:123:GLN:CB	0.61	2.49	6	13
1:A:109:THR:HB	1:A:128:PHE:CE2	0.61	2.30	3	4
1:A:81:LYS:O	1:A:81:LYS:HE3	0.61	1.96	6	7
1:A:55:LEU:HD11	1:A:67:GLU:HB2	0.61	1.73	20	2
1:A:127:ASN:ND2	2:B:457:HIS:O	0.61	2.33	21	1
1:A:87:LEU:HB3	1:A:96:LEU:HD12	0.61	1.73	13	2
1:A:129:ALA:CB	2:B:454:PHE:CE1	0.61	2.84	11	5
1:A:81:LYS:CB	2:B:476:PRO:HD3	0.61	2.25	10	1
1:A:118:ALA:HB1	1:A:123:GLN:OE1	0.61	1.95	1	2
1:A:54:TYR:OH	1:A:114:PHE:HB2	0.61	1.95	4	3
1:A:25:THR:HG22	1:A:29:ASP:CG	0.60	2.21	2	5
1:A:108:SER:O	1:A:115:HIS:CB	0.60	2.49	2	18
2:B:475:TYR:CD2	2:B:476:PRO:CD	0.60	2.84	14	6
1:A:38:MET:HE3	1:A:86:ARG:CZ	0.60	2.26	22	3
2:B:466:GLU:HB2	2:B:467:PRO:HD2	0.60	1.71	16	7
1:A:118:ALA:HB1	2:B:468:TYR:CD2	0.60	2.31	16	1
1:A:55:LEU:HD12	1:A:124:ALA:HA	0.60	1.72	7	10
1:A:57:LEU:HD22	1:A:62:GLU:CG	0.60	2.26	10	5
1:A:50:VAL:CG1	2:B:454:PHE:HB3	0.60	2.26	21	17
2:B:475:TYR:C	2:B:479:LEU:HG	0.60	2.21	12	15
1:A:53:LEU:HD12	1:A:54:TYR:N	0.60	2.12	24	2
1:A:54:TYR:HB3	1:A:66:LYS:HA	0.60	1.73	4	3
1:A:74:PHE:CE2	1:A:140:LEU:HD21	0.60	2.32	2	2
1:A:106:VAL:HB	1:A:117:PHE:CG	0.60	2.31	12	3
1:A:102:TYR:CB	2:B:473:LYS:HB3	0.60	2.25	15	2
1:A:32:ASN:CA	1:A:45:THR:HG21	0.60	2.27	23	12
1:A:35:LEU:HD13	1:A:74:PHE:C	0.60	2.22	6	16
1:A:49:ALA:HB1	1:A:133:GLU:CG	0.60	2.27	7	6
1:A:114:PHE:C	1:A:128:PHE:CE2	0.60	2.80	18	9
1:A:129:ALA:CB	2:B:454:PHE:CE2	0.60	2.85	19	12
1:A:54:TYR:HH	1:A:114:PHE:HB2	0.60	1.56	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:34:ARG:CB	1:A:48:THR:HG21	0.60	2.27	4	2
1:A:54:TYR:HB2	1:A:125:GLY:O	0.60	1.96	16	19
1:A:106:VAL:HG23	1:A:117:PHE:CE2	0.60	2.32	2	3
1:A:57:LEU:HD22	1:A:62:GLU:HG3	0.60	1.74	12	10
1:A:38:MET:HE1	1:A:86:ARG:NH1	0.59	2.12	1	1
1:A:53:LEU:HD12	1:A:126:LEU:HD23	0.59	1.74	1	2
2:B:457:HIS:CB	2:B:458:PRO:HD2	0.59	2.27	8	15
1:A:35:LEU:HD11	1:A:75:VAL:HB	0.59	1.72	8	1
1:A:34:ARG:HD3	1:A:48:THR:CB	0.59	2.27	6	1
2:B:459:ILE:CD1	2:B:462:LEU:HD13	0.59	2.17	19	2
1:A:54:TYR:CE1	2:B:459:ILE:HG21	0.59	2.32	19	2
2:B:459:ILE:O	2:B:462:LEU:N	0.59	2.34	2	12
1:A:114:PHE:CG	2:B:462:LEU:HD11	0.59	2.32	8	1
1:A:46:LEU:HD23	1:A:74:PHE:HB3	0.59	1.73	15	3
1:A:71:ALA:O	1:A:88:TYR:CD2	0.59	2.56	14	2
1:A:46:LEU:CD1	1:A:140:LEU:HD23	0.59	2.27	1	2
1:A:71:ALA:O	1:A:88:TYR:CD1	0.59	2.56	6	2
1:A:117:PHE:CZ	1:A:118:ALA:O	0.59	2.55	10	12
1:A:101:LEU:O	2:B:475:TYR:CE1	0.59	2.55	17	9
1:A:38:MET:HG2	1:A:90:LEU:HB2	0.59	1.75	13	2
1:A:74:PHE:CD1	1:A:140:LEU:HD11	0.59	2.33	19	2
1:A:87:LEU:HD12	1:A:97:TRP:CD1	0.59	2.32	16	8
1:A:54:TYR:CD2	1:A:64:TRP:CZ3	0.59	2.90	14	2
1:A:102:TYR:CE1	2:B:478:LYS:HD2	0.59	2.32	12	7
1:A:140:LEU:HD12	1:A:140:LEU:C	0.59	2.23	2	4
1:A:25:THR:HG22	1:A:29:ASP:OD2	0.59	1.97	8	4
1:A:35:LEU:HD13	1:A:73:CYS:HB2	0.59	1.74	23	2
2:B:462:LEU:HD22	2:B:463:PRO:N	0.59	2.12	6	1
2:B:459:ILE:HG12	2:B:462:LEU:HD22	0.59	1.73	9	2
1:A:86:ARG:CB	1:A:98:GLU:HA	0.59	2.28	6	21
1:A:80:GLN:O	1:A:81:LYS:CG	0.59	2.51	24	17
1:A:47:ALA:HB2	1:A:140:LEU:HD12	0.59	1.74	5	2
1:A:54:TYR:CE1	2:B:459:ILE:HD13	0.59	2.32	15	1
1:A:88:TYR:CD1	1:A:88:TYR:C	0.58	2.80	10	1
1:A:129:ALA:HB3	1:A:133:GLU:CG	0.58	2.27	1	5
1:A:140:LEU:HD12	1:A:140:LEU:O	0.58	1.98	11	4
1:A:54:TYR:CB	1:A:66:LYS:HA	0.58	2.28	24	4
1:A:50:VAL:HG21	2:B:454:PHE:CG	0.58	2.32	11	1
1:A:35:LEU:H	1:A:48:THR:HG21	0.58	1.58	23	2
1:A:35:LEU:HD13	1:A:74:PHE:O	0.58	1.98	6	15
1:A:102:TYR:O	1:A:105:LEU:HD23	0.58	1.99	13	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:53:LEU:HG	1:A:126:LEU:HD21	0.58	1.75	14	12
1:A:81:LYS:HD3	2:B:479:LEU:HD11	0.58	1.74	2	1
1:A:114:PHE:C	1:A:128:PHE:CE1	0.58	2.81	16	4
2:B:459:ILE:HD12	2:B:462:LEU:CD2	0.58	2.26	16	3
1:A:54:TYR:CD1	2:B:459:ILE:HG21	0.58	2.32	14	1
1:A:57:LEU:HD11	1:A:123:GLN:CG	0.58	2.28	14	1
1:A:39:LEU:C	1:A:39:LEU:HD12	0.58	2.24	9	12
1:A:106:VAL:HG22	1:A:145:ILE:CD1	0.58	2.26	15	3
1:A:107:TYR:CD2	1:A:117:PHE:CE1	0.58	2.91	16	1
1:A:106:VAL:HG23	1:A:117:PHE:CE1	0.58	2.34	10	4
1:A:106:VAL:HG23	1:A:117:PHE:CD1	0.58	2.34	13	4
1:A:46:LEU:CD1	1:A:140:LEU:HD21	0.58	2.29	17	4
1:A:50:VAL:O	1:A:51:VAL:HG22	0.58	1.99	19	15
1:A:140:LEU:C	1:A:140:LEU:CD2	0.58	2.77	19	3
1:A:57:LEU:HD13	1:A:62:GLU:HG3	0.58	1.74	19	7
1:A:25:THR:HG22	1:A:29:ASP:OD1	0.58	1.99	2	3
2:B:475:TYR:HB3	2:B:478:LYS:HG3	0.58	1.76	1	11
1:A:57:LEU:HD11	1:A:123:GLN:HB2	0.57	1.76	15	8
1:A:57:LEU:HD11	1:A:123:GLN:HB3	0.57	1.74	5	2
1:A:106:VAL:CA	1:A:145:ILE:HD11	0.57	2.24	10	1
1:A:114:PHE:CD2	1:A:115:HIS:N	0.57	2.72	5	4
1:A:101:LEU:HD11	1:A:122:CYS:SG	0.57	2.38	24	2
1:A:75:VAL:HB	1:A:84:PHE:HB3	0.57	1.75	18	14
1:A:107:TYR:CB	1:A:141:VAL:HG22	0.57	2.30	16	1
1:A:74:PHE:N	1:A:74:PHE:CD2	0.57	2.72	6	11
1:A:54:TYR:CE2	2:B:459:ILE:HG21	0.57	2.35	7	1
1:A:38:MET:HE3	1:A:90:LEU:HB3	0.57	1.76	21	1
1:A:107:TYR:HB2	1:A:141:VAL:HG22	0.57	1.75	16	1
1:A:34:ARG:NH1	1:A:38:MET:HE2	0.57	2.14	21	2
1:A:111:THR:HG22	1:A:112:PRO:CD	0.57	2.29	12	10
1:A:128:PHE:CD1	1:A:128:PHE:N	0.57	2.71	4	1
1:A:38:MET:HE3	1:A:88:TYR:CB	0.57	2.30	6	1
1:A:52:GLN:HE22	2:B:459:ILE:HG23	0.57	1.60	24	1
1:A:112:PRO:O	1:A:113:PHE:CG	0.57	2.57	24	9
1:A:37:GLU:HG3	1:A:90:LEU:HD11	0.57	1.76	19	3
2:B:462:LEU:C	2:B:462:LEU:CD1	0.56	2.78	7	6
2:B:462:LEU:HD12	2:B:462:LEU:C	0.56	2.25	7	1
1:A:106:VAL:HG13	1:A:145:ILE:HD13	0.56	1.76	12	2
2:B:474:SER:OG	2:B:479:LEU:HD11	0.56	2.00	8	2
1:A:51:VAL:HG11	1:A:115:HIS:CE1	0.56	2.35	11	2
1:A:101:LEU:HD13	1:A:102:TYR:H	0.56	1.60	24	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:75:VAL:HG21	1:A:86:ARG:HE	0.56	1.59	23	3
1:A:140:LEU:HD13	1:A:140:LEU:C	0.56	2.25	8	4
1:A:52:GLN:CD	1:A:54:TYR:CE2	0.56	2.84	21	2
1:A:52:GLN:HB3	2:B:456:PHE:O	0.56	1.99	21	3
2:B:475:TYR:HB3	2:B:478:LYS:CG	0.56	2.29	18	14
1:A:50:VAL:O	1:A:51:VAL:HG12	0.56	1.99	3	2
1:A:128:PHE:CD2	1:A:129:ALA:O	0.56	2.58	14	3
1:A:106:VAL:HG22	1:A:145:ILE:HD13	0.56	1.76	10	2
1:A:116:THR:O	1:A:117:PHE:CD1	0.56	2.57	17	1
1:A:37:GLU:HB3	1:A:90:LEU:HD11	0.56	1.77	20	1
1:A:106:VAL:HG12	1:A:117:PHE:HD2	0.56	1.57	21	1
1:A:32:ASN:HB3	1:A:45:THR:HG21	0.56	1.76	6	2
1:A:105:LEU:HD21	1:A:107:TYR:CG	0.56	2.36	23	1
2:B:475:TYR:CD1	2:B:476:PRO:CD	0.56	2.89	1	7
1:A:101:LEU:O	2:B:475:TYR:CE2	0.56	2.58	19	9
2:B:459:ILE:HG13	2:B:462:LEU:HG	0.56	1.77	12	3
1:A:102:TYR:CD2	2:B:475:TYR:HB2	0.56	2.35	8	6
1:A:115:HIS:O	1:A:125:GLY:HA2	0.56	2.00	12	13
1:A:107:TYR:CZ	1:A:117:PHE:CZ	0.56	2.93	6	1
1:A:47:ALA:O	1:A:48:THR:HG23	0.56	2.01	23	2
1:A:50:VAL:O	1:A:51:VAL:CG1	0.56	2.53	9	6
1:A:102:TYR:CD2	2:B:473:LYS:CB	0.56	2.88	2	4
1:A:50:VAL:HG13	2:B:450:TRP:CZ2	0.56	2.36	21	7
1:A:74:PHE:CD1	1:A:74:PHE:N	0.56	2.73	13	13
1:A:50:VAL:HG23	1:A:71:ALA:HA	0.56	1.77	20	7
1:A:96:LEU:O	1:A:97:TRP:HB3	0.56	2.01	4	4
1:A:52:GLN:CB	2:B:456:PHE:O	0.56	2.54	3	7
1:A:54:TYR:C	1:A:54:TYR:CD2	0.55	2.83	14	2
1:A:83:TYR:CE2	1:A:105:LEU:HD21	0.55	2.36	14	2
1:A:115:HIS:HE1	1:A:126:LEU:HD13	0.55	1.57	14	2
1:A:38:MET:HB2	1:A:88:TYR:CD1	0.55	2.37	24	3
1:A:140:LEU:HD22	1:A:140:LEU:C	0.55	2.26	6	3
1:A:101:LEU:HD22	1:A:102:TYR:O	0.55	2.01	18	1
1:A:106:VAL:HG13	1:A:106:VAL:O	0.55	2.02	21	1
1:A:55:LEU:HD12	1:A:124:ALA:CB	0.55	2.32	16	4
2:B:475:TYR:HD1	2:B:476:PRO:CD	0.55	2.15	23	8
1:A:106:VAL:O	1:A:117:PHE:CD1	0.55	2.59	9	1
1:A:113:PHE:CE2	2:B:462:LEU:HD23	0.55	2.36	10	1
1:A:74:PHE:CZ	1:A:140:LEU:HD21	0.55	2.36	11	2
1:A:101:LEU:HD23	1:A:102:TYR:H	0.55	1.62	18	1
1:A:64:TRP:CH2	2:B:459:ILE:CD1	0.55	2.89	23	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:102:TYR:CD1	1:A:102:TYR:N	0.55	2.75	2	4
1:A:62:GLU:O	1:A:63:HIS:CG	0.55	2.60	7	8
1:A:105:LEU:HD11	1:A:107:TYR:CD1	0.55	2.37	9	1
1:A:116:THR:C	1:A:117:PHE:CD1	0.55	2.85	16	2
1:A:112:PRO:C	1:A:113:PHE:CG	0.55	2.84	5	12
1:A:102:TYR:CG	2:B:473:LYS:HB2	0.55	2.37	16	9
1:A:38:MET:HE3	1:A:91:GLN:N	0.55	2.17	8	3
1:A:46:LEU:HD11	1:A:144:LYS:HD3	0.55	1.78	18	1
1:A:83:TYR:HB3	1:A:101:LEU:HB3	0.55	1.79	18	1
1:A:56:ALA:O	1:A:57:LEU:HD22	0.55	2.01	14	7
1:A:117:PHE:CG	1:A:118:ALA:N	0.55	2.74	18	16
2:B:459:ILE:HG22	2:B:462:LEU:HD21	0.55	1.77	1	1
1:A:39:LEU:HD22	1:A:43:CYS:HB2	0.55	1.78	18	2
1:A:54:TYR:CD2	1:A:64:TRP:CH2	0.55	2.95	14	3
1:A:128:PHE:HD2	1:A:129:ALA:O	0.55	1.85	16	2
1:A:87:LEU:HG	1:A:97:TRP:O	0.55	2.02	22	1
1:A:72:VAL:CG1	1:A:87:LEU:HD13	0.55	2.27	1	2
1:A:87:LEU:CD1	1:A:97:TRP:CD1	0.55	2.90	13	8
1:A:111:THR:HG21	1:A:114:PHE:CD1	0.55	2.37	6	1
2:B:462:LEU:O	2:B:462:LEU:HD23	0.55	2.01	14	1
1:A:32:ASN:O	1:A:36:PHE:CB	0.54	2.55	24	18
1:A:87:LEU:N	1:A:87:LEU:HD23	0.54	2.17	24	2
1:A:117:PHE:CE1	1:A:118:ALA:O	0.54	2.59	12	3
1:A:107:TYR:O	1:A:108:SER:CB	0.54	2.56	4	6
1:A:75:VAL:O	1:A:84:PHE:HB2	0.54	2.01	4	2
1:A:53:LEU:HD13	1:A:67:GLU:HB2	0.54	1.78	5	1
1:A:102:TYR:CG	2:B:473:LYS:CB	0.54	2.90	23	2
1:A:127:ASN:CG	2:B:459:ILE:HG22	0.54	2.26	23	1
2:B:459:ILE:CG2	2:B:462:LEU:HD23	0.54	2.32	17	2
1:A:72:VAL:CG1	1:A:87:LEU:HD22	0.54	2.32	4	4
1:A:85:ILE:HD13	1:A:105:LEU:HD11	0.54	1.79	12	2
1:A:107:TYR:CE2	1:A:117:PHE:CG	0.54	2.95	16	1
1:A:107:TYR:O	1:A:115:HIS:HB2	0.54	2.02	20	1
1:A:109:THR:O	1:A:109:THR:CG2	0.54	2.56	18	1
1:A:129:ALA:HB3	2:B:454:PHE:CE2	0.54	2.38	19	5
1:A:53:LEU:HD23	1:A:87:LEU:CD2	0.54	2.33	24	1
1:A:35:LEU:HD23	1:A:45:THR:HG22	0.54	1.79	3	1
1:A:53:LEU:CD2	1:A:126:LEU:HD21	0.54	2.31	24	2
1:A:128:PHE:CD2	1:A:128:PHE:N	0.54	2.76	2	2
1:A:127:ASN:ND2	2:B:459:ILE:HG22	0.54	2.18	23	1
1:A:81:LYS:O	1:A:81:LYS:CE	0.54	2.56	19	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:114:PHE:CD1	2:B:462:LEU:HD21	0.54	2.38	10	1
1:A:47:ALA:HB3	1:A:74:PHE:CB	0.54	2.33	8	17
1:A:101:LEU:O	2:B:475:TYR:CZ	0.54	2.61	9	5
1:A:140:LEU:HD23	1:A:141:VAL:CA	0.54	2.33	16	3
1:A:75:VAL:O	1:A:84:PHE:HB3	0.54	2.03	17	7
1:A:129:ALA:CB	2:B:454:PHE:CZ	0.54	2.91	5	17
1:A:34:ARG:HG2	1:A:88:TYR:CZ	0.54	2.38	10	1
1:A:81:LYS:HE3	1:A:103:SER:CB	0.53	2.33	2	3
1:A:83:TYR:CE1	1:A:103:SER:CB	0.53	2.91	23	3
1:A:81:LYS:HD2	2:B:479:LEU:HD11	0.53	1.80	9	4
1:A:102:TYR:CD1	2:B:473:LYS:CB	0.53	2.91	15	4
1:A:106:VAL:CG2	1:A:117:PHE:CE2	0.53	2.91	8	1
1:A:127:ASN:ND2	2:B:456:PHE:O	0.53	2.40	9	2
1:A:47:ALA:HB1	1:A:140:LEU:HD12	0.53	1.80	19	1
2:B:475:TYR:O	2:B:478:LYS:N	0.53	2.42	17	15
1:A:122:CYS:O	1:A:123:GLN:HB2	0.53	2.03	6	7
1:A:46:LEU:C	1:A:46:LEU:HD13	0.53	2.28	24	11
1:A:50:VAL:CG2	2:B:456:PHE:CD2	0.53	2.91	24	3
1:A:81:LYS:CG	2:B:476:PRO:HD3	0.53	2.33	19	15
1:A:25:THR:C	1:A:26:LEU:HD12	0.53	2.28	9	2
1:A:53:LEU:HD23	1:A:126:LEU:CD2	0.53	2.34	5	1
1:A:113:PHE:CD2	1:A:113:PHE:N	0.53	2.77	19	5
2:B:462:LEU:HD22	2:B:463:PRO:CD	0.53	2.34	24	3
1:A:39:LEU:HD12	1:A:40:GLY:N	0.53	2.19	12	2
1:A:50:VAL:HG12	1:A:71:ALA:CA	0.53	2.33	15	2
1:A:105:LEU:O	1:A:145:ILE:HG23	0.53	2.04	14	2
1:A:34:ARG:O	1:A:90:LEU:HD12	0.53	2.03	20	1
1:A:30:HIS:O	1:A:31:GLU:C	0.53	2.52	1	12
1:A:50:VAL:HG11	2:B:454:PHE:CB	0.53	2.33	1	5
1:A:106:VAL:HB	1:A:117:PHE:CD1	0.53	2.39	1	3
1:A:113:PHE:CD1	1:A:113:PHE:N	0.53	2.77	7	7
1:A:54:TYR:CE2	1:A:66:LYS:HB3	0.53	2.38	7	3
1:A:47:ALA:HB2	1:A:140:LEU:CD2	0.53	2.33	18	2
1:A:86:ARG:CD	1:A:88:TYR:CE1	0.53	2.91	13	2
1:A:48:THR:HG22	1:A:88:TYR:HE1	0.53	1.60	1	1
1:A:87:LEU:HG	1:A:97:TRP:CD1	0.53	2.39	3	8
1:A:114:PHE:CD1	2:B:462:LEU:CD2	0.53	2.92	6	2
1:A:46:LEU:HD22	1:A:76:LYS:CG	0.53	2.33	15	3
1:A:54:TYR:CE1	1:A:125:GLY:C	0.53	2.87	24	1
2:B:450:TRP:O	2:B:450:TRP:HE3	0.53	1.86	10	9
1:A:50:VAL:HG22	2:B:456:PHE:CD1	0.53	2.39	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:107:TYR:CE2	1:A:117:PHE:CE2	0.53	2.96	16	2
1:A:105:LEU:O	1:A:105:LEU:HG	0.53	2.04	24	2
1:A:142:GLN:O	1:A:146:GLN:HB3	0.53	2.03	19	2
1:A:116:THR:HG22	1:A:124:ALA:O	0.52	2.04	10	5
1:A:50:VAL:CG2	2:B:454:PHE:CG	0.52	2.92	11	1
1:A:102:TYR:CE2	2:B:478:LYS:HD2	0.52	2.39	17	2
1:A:53:LEU:HD23	1:A:126:LEU:HG	0.52	1.81	21	11
1:A:52:GLN:HA	1:A:69:CYS:HB3	0.52	1.82	3	4
1:A:69:CYS:O	1:A:96:LEU:CD1	0.52	2.57	3	8
1:A:52:GLN:CB	1:A:127:ASN:ND2	0.52	2.72	9	2
1:A:54:TYR:CD2	1:A:125:GLY:O	0.52	2.62	4	3
1:A:109:THR:CB	1:A:128:PHE:CE1	0.52	2.92	4	3
1:A:54:TYR:HB2	1:A:66:LYS:HA	0.52	1.81	5	2
1:A:83:TYR:CE2	1:A:103:SER:CB	0.52	2.91	9	5
1:A:83:TYR:O	2:B:475:TYR:OH	0.52	2.24	9	1
1:A:105:LEU:HA	1:A:117:PHE:CZ	0.52	2.39	14	1
1:A:46:LEU:HD21	1:A:140:LEU:CD2	0.52	2.35	24	1
1:A:109:THR:OG1	1:A:134:ALA:HB2	0.52	2.05	24	1
1:A:83:TYR:CE1	1:A:103:SER:HA	0.52	2.39	7	4
1:A:115:HIS:CE1	1:A:137:PHE:CZ	0.52	2.97	21	5
1:A:102:TYR:N	1:A:102:TYR:CD2	0.52	2.77	15	4
1:A:30:HIS:HB2	2:B:445:PRO:HB3	0.52	1.81	16	1
1:A:102:TYR:CD1	2:B:475:TYR:HB2	0.52	2.40	7	6
1:A:127:ASN:HB3	2:B:456:PHE:O	0.52	2.04	18	1
1:A:119:GLY:O	1:A:120:ASP:C	0.52	2.53	9	9
1:A:50:VAL:C	1:A:51:VAL:HG22	0.52	2.29	22	14
1:A:46:LEU:HD23	1:A:76:LYS:HE3	0.52	1.79	5	1
1:A:55:LEU:HD11	1:A:67:GLU:CD	0.52	2.29	6	3
1:A:109:THR:HB	1:A:128:PHE:CZ	0.52	2.39	6	1
1:A:33:GLN:O	1:A:37:GLU:HB3	0.52	2.05	2	3
2:B:446:CYS:O	2:B:447:GLU:CG	0.52	2.58	8	3
2:B:456:PHE:CD2	2:B:456:PHE:N	0.52	2.78	24	2
1:A:81:LYS:HE2	2:B:474:SER:O	0.52	2.04	6	3
2:B:459:ILE:HD11	2:B:462:LEU:HD21	0.52	1.80	7	1
1:A:128:PHE:HD1	1:A:129:ALA:O	0.52	1.88	8	2
1:A:38:MET:HB2	1:A:88:TYR:CD2	0.52	2.39	10	1
1:A:88:TYR:CZ	1:A:95:LEU:HD13	0.52	2.38	20	1
1:A:114:PHE:CG	2:B:462:LEU:CD1	0.52	2.93	8	2
1:A:50:VAL:CG2	2:B:454:PHE:CD1	0.52	2.93	14	7
2:B:462:LEU:HD22	2:B:462:LEU:C	0.52	2.30	6	2
1:A:114:PHE:CA	1:A:126:LEU:O	0.52	2.57	1	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:54:TYR:CE2	1:A:125:GLY:C	0.52	2.88	6	2
1:A:122:CYS:C	1:A:123:GLN:HG3	0.52	2.30	19	2
1:A:53:LEU:HD22	1:A:53:LEU:C	0.52	2.30	5	1
2:B:474:SER:C	2:B:479:LEU:HD21	0.52	2.30	12	1
1:A:106:VAL:CG2	1:A:145:ILE:HD11	0.52	2.33	15	1
1:A:109:THR:OG1	1:A:134:ALA:CB	0.52	2.58	24	1
1:A:26:LEU:O	1:A:30:HIS:CE1	0.52	2.63	12	2
1:A:133:GLU:O	1:A:137:PHE:HB2	0.52	2.05	12	1
1:A:64:TRP:HE3	1:A:65:THR:N	0.51	2.03	14	14
1:A:50:VAL:HG21	2:B:454:PHE:HB2	0.51	1.79	19	1
1:A:114:PHE:CD1	1:A:115:HIS:O	0.51	2.64	4	4
1:A:50:VAL:C	1:A:51:VAL:CG2	0.51	2.83	4	16
1:A:34:ARG:NH2	2:B:450:TRP:CZ2	0.51	2.78	9	3
1:A:107:TYR:CD2	1:A:115:HIS:CD2	0.51	2.98	4	1
1:A:50:VAL:HG22	2:B:456:PHE:CD2	0.51	2.41	1	1
1:A:53:LEU:CD1	1:A:126:LEU:HD23	0.51	2.35	22	2
1:A:102:TYR:CE2	2:B:473:LYS:CG	0.51	2.94	1	1
1:A:35:LEU:HD23	1:A:45:THR:HA	0.51	1.81	15	15
1:A:50:VAL:C	1:A:51:VAL:HG12	0.51	2.30	24	1
1:A:107:TYR:CD1	1:A:115:HIS:CD2	0.51	2.98	18	2
1:A:48:THR:O	1:A:49:ALA:HB2	0.51	2.04	15	4
1:A:128:PHE:CD1	1:A:129:ALA:O	0.51	2.63	6	1
1:A:34:ARG:NH2	2:B:450:TRP:CE2	0.51	2.78	20	2
1:A:81:LYS:HZ2	2:B:475:TYR:HA	0.51	1.65	2	2
1:A:39:LEU:HD12	1:A:39:LEU:C	0.51	2.30	5	4
1:A:44:LEU:HD21	1:A:77:ASP:O	0.51	2.04	15	2
2:B:450:TRP:CE2	2:B:454:PHE:HB2	0.51	2.41	15	11
1:A:50:VAL:CG2	2:B:456:PHE:CD1	0.51	2.94	3	1
2:B:459:ILE:CG1	2:B:462:LEU:CD2	0.51	2.88	7	1
1:A:81:LYS:HZ1	1:A:103:SER:CB	0.51	2.19	12	1
2:B:475:TYR:HD1	2:B:476:PRO:HD2	0.51	1.65	23	2
1:A:87:LEU:HD11	1:A:97:TRP:CB	0.51	2.35	2	3
1:A:50:VAL:C	1:A:51:VAL:CG1	0.51	2.83	3	2
2:B:475:TYR:N	2:B:479:LEU:HG	0.51	2.21	3	5
1:A:53:LEU:HD23	1:A:126:LEU:HD21	0.51	1.82	5	1
1:A:53:LEU:HA	1:A:126:LEU:HD23	0.51	1.81	19	2
1:A:87:LEU:HD21	1:A:97:TRP:HE3	0.51	1.66	17	3
1:A:105:LEU:C	1:A:145:ILE:CD1	0.51	2.84	24	6
1:A:75:VAL:N	1:A:84:PHE:O	0.51	2.43	14	15
1:A:81:LYS:O	1:A:81:LYS:CD	0.51	2.59	17	5
1:A:34:ARG:O	1:A:37:GLU:HG2	0.51	2.05	9	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:111:THR:HG21	1:A:114:PHE:CE2	0.51	2.40	16	1
1:A:83:TYR:CD2	1:A:105:LEU:CD2	0.51	2.94	24	1
1:A:55:LEU:N	1:A:55:LEU:HD22	0.51	2.21	5	4
1:A:107:TYR:H	1:A:141:VAL:HG11	0.51	1.66	23	2
1:A:50:VAL:HG12	1:A:71:ALA:HA	0.51	1.83	15	3
1:A:109:THR:OG1	1:A:134:ALA:CA	0.51	2.59	9	4
1:A:31:GLU:O	1:A:48:THR:CG2	0.51	2.58	22	14
1:A:127:ASN:ND2	1:A:127:ASN:C	0.51	2.67	21	3
1:A:114:PHE:HE1	1:A:116:THR:HG23	0.51	1.64	14	1
1:A:34:ARG:HE	1:A:48:THR:HB	0.51	1.66	19	1
1:A:102:TYR:CE1	2:B:473:LYS:HB2	0.51	2.41	19	1
1:A:32:ASN:CB	1:A:45:THR:HG21	0.50	2.36	6	3
1:A:31:GLU:HA	1:A:48:THR:CG2	0.50	2.36	19	6
1:A:90:LEU:C	1:A:93:GLY:H	0.50	2.14	18	19
1:A:107:TYR:CE1	1:A:115:HIS:CD2	0.50	2.99	13	3
1:A:107:TYR:CD1	1:A:115:HIS:CE1	0.50	3.00	24	3
1:A:35:LEU:HD11	1:A:75:VAL:CB	0.50	2.36	8	1
1:A:107:TYR:CE2	1:A:115:HIS:CD2	0.50	2.99	9	1
1:A:129:ALA:HB3	2:B:454:PHE:CE1	0.50	2.41	11	1
1:A:49:ALA:O	1:A:72:VAL:N	0.50	2.45	10	9
1:A:116:THR:OG1	1:A:117:PHE:N	0.50	2.45	8	12
1:A:54:TYR:CZ	1:A:66:LYS:HB3	0.50	2.42	12	15
1:A:50:VAL:HA	1:A:71:ALA:HA	0.50	1.84	4	14
1:A:36:PHE:HA	1:A:39:LEU:HG	0.50	1.84	13	4
1:A:54:TYR:CB	2:B:459:ILE:HD13	0.50	2.37	22	1
1:A:82:SER:O	1:A:83:TYR:CG	0.50	2.65	10	4
1:A:106:VAL:HG23	1:A:117:PHE:CD2	0.50	2.42	2	4
2:B:475:TYR:HD2	2:B:476:PRO:CD	0.50	2.20	17	8
1:A:47:ALA:C	1:A:74:PHE:CD2	0.50	2.90	6	11
1:A:39:LEU:HD12	1:A:40:GLY:C	0.50	2.32	12	2
1:A:68:HIS:C	1:A:69:CYS:SG	0.50	2.95	3	14
1:A:127:ASN:HD21	2:B:462:LEU:HD23	0.50	1.66	1	2
1:A:53:LEU:HB2	1:A:87:LEU:HD11	0.50	1.82	7	1
1:A:52:GLN:HG2	1:A:69:CYS:HB3	0.50	1.84	22	1
1:A:106:VAL:CG2	1:A:117:PHE:CD1	0.50	2.95	20	6
1:A:31:GLU:HG3	1:A:32:ASN:N	0.50	2.21	11	2
2:B:469:VAL:CG2	2:B:470:GLN:N	0.50	2.74	3	1
1:A:38:MET:CG	1:A:88:TYR:CG	0.50	2.95	22	2
1:A:28:GLN:O	1:A:31:GLU:HG2	0.50	2.05	13	3
1:A:82:SER:O	1:A:83:TYR:CD2	0.50	2.65	4	6
1:A:140:LEU:HG	1:A:141:VAL:N	0.50	2.21	12	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:459:ILE:HG22	2:B:462:LEU:HD23	0.50	1.83	3	2
1:A:50:VAL:CG1	2:B:454:PHE:CD2	0.50	2.95	8	1
1:A:109:THR:HG23	1:A:137:PHE:CG	0.50	2.42	16	4
1:A:114:PHE:CE1	1:A:116:THR:HG23	0.50	2.42	14	1
1:A:54:TYR:HB3	1:A:64:TRP:CZ3	0.49	2.41	12	12
1:A:38:MET:HE3	1:A:88:TYR:HB2	0.49	1.83	6	1
1:A:34:ARG:NH2	2:B:450:TRP:CD1	0.49	2.80	10	1
1:A:57:LEU:HB2	1:A:62:GLU:CG	0.49	2.37	8	23
1:A:105:LEU:O	1:A:145:ILE:CD1	0.49	2.60	19	5
1:A:106:VAL:HG22	1:A:145:ILE:HD12	0.49	1.84	3	2
1:A:81:LYS:CE	2:B:474:SER:O	0.49	2.60	19	3
1:A:55:LEU:HB3	1:A:124:ALA:CB	0.49	2.37	6	1
1:A:120:ASP:CG	1:A:121:ASP:N	0.49	2.70	24	1
1:A:52:GLN:O	1:A:126:LEU:HB3	0.49	2.07	23	15
1:A:115:HIS:CD2	1:A:126:LEU:HD13	0.49	2.42	1	2
1:A:50:VAL:HG23	1:A:71:ALA:CA	0.49	2.38	20	5
1:A:34:ARG:HD3	1:A:38:MET:HE1	0.49	1.83	16	1
1:A:35:LEU:CD1	1:A:73:CYS:HB3	0.49	2.36	5	8
1:A:54:TYR:OH	1:A:114:PHE:CE2	0.49	2.63	5	1
1:A:114:PHE:CZ	1:A:116:THR:HG22	0.49	2.43	6	2
1:A:52:GLN:HG2	1:A:54:TYR:CE2	0.49	2.43	13	3
1:A:54:TYR:OH	1:A:127:ASN:OD1	0.49	2.29	24	1
1:A:76:LYS:HD3	1:A:82:SER:O	0.49	2.07	4	2
1:A:109:THR:CG2	1:A:128:PHE:CE1	0.49	2.95	6	1
1:A:105:LEU:HD23	1:A:144:LYS:NZ	0.49	2.23	7	1
1:A:129:ALA:HB2	2:B:454:PHE:CE1	0.49	2.41	11	1
2:B:459:ILE:CG1	2:B:462:LEU:HB3	0.49	2.37	19	2
1:A:38:MET:CA	1:A:90:LEU:HD13	0.49	2.36	14	5
1:A:113:PHE:N	1:A:113:PHE:CD2	0.49	2.81	3	1
1:A:114:PHE:CE2	1:A:116:THR:HG22	0.49	2.42	5	2
1:A:35:LEU:CD2	1:A:74:PHE:O	0.49	2.60	2	4
1:A:53:LEU:HD22	1:A:54:TYR:H	0.49	1.64	5	1
1:A:105:LEU:HD23	1:A:144:LYS:HZ3	0.49	1.66	7	1
2:B:475:TYR:CB	2:B:478:LYS:HG3	0.49	2.37	22	4
1:A:114:PHE:CZ	1:A:116:THR:HG21	0.49	2.43	11	3
1:A:83:TYR:CE2	1:A:105:LEU:CD2	0.49	2.95	24	2
1:A:57:LEU:HD13	1:A:62:GLU:CB	0.49	2.37	12	1
1:A:118:ALA:HB1	2:B:468:TYR:HE1	0.49	1.67	14	1
1:A:133:GLU:HB3	2:B:454:PHE:CE2	0.49	2.43	15	1
1:A:50:VAL:HG21	2:B:454:PHE:HB3	0.49	1.83	21	4
1:A:106:VAL:CG2	1:A:117:PHE:CE1	0.49	2.96	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:128:PHE:CD2	1:A:133:GLU:OE1	0.49	2.66	2	1
2:B:475:TYR:CB	2:B:478:LYS:CD	0.49	2.91	3	3
2:B:476:PRO:O	2:B:480:ALA:CB	0.49	2.59	20	18
1:A:53:LEU:C	1:A:53:LEU:CD2	0.49	2.86	19	11
1:A:127:ASN:OD1	1:A:127:ASN:C	0.49	2.56	2	3
1:A:106:VAL:CG2	1:A:117:PHE:CD2	0.49	2.95	18	3
1:A:35:LEU:HD12	1:A:38:MET:SD	0.49	2.48	22	2
1:A:127:ASN:HD21	2:B:459:ILE:HD12	0.49	1.68	19	1
1:A:28:GLN:HA	1:A:31:GLU:CG	0.49	2.38	21	1
1:A:54:TYR:CE1	2:B:459:ILE:CG2	0.48	2.96	6	3
1:A:104:GLN:O	1:A:117:PHE:CE1	0.48	2.66	8	3
1:A:46:LEU:HD13	1:A:76:LYS:HE3	0.48	1.83	23	2
1:A:35:LEU:HD21	1:A:45:THR:HA	0.48	1.84	1	1
1:A:107:TYR:O	1:A:108:SER:OG	0.48	2.26	16	8
1:A:49:ALA:HB3	1:A:137:PHE:CE1	0.48	2.43	12	2
1:A:109:THR:CG2	1:A:137:PHE:CD1	0.48	2.97	17	2
1:A:76:LYS:CD	1:A:82:SER:O	0.48	2.61	24	4
1:A:100:GLU:CD	2:B:475:TYR:CE1	0.48	2.91	17	2
1:A:127:ASN:OD1	2:B:459:ILE:N	0.48	2.46	18	1
1:A:52:GLN:NE2	2:B:458:PRO:HA	0.48	2.23	21	1
1:A:115:HIS:ND1	1:A:128:PHE:CE2	0.48	2.81	21	1
2:B:462:LEU:CD2	2:B:463:PRO:O	0.48	2.61	18	3
1:A:90:LEU:HA	1:A:94:ARG:N	0.48	2.23	18	8
1:A:38:MET:CG	1:A:88:TYR:CD1	0.48	2.97	11	2
1:A:34:ARG:NH1	1:A:71:ALA:HB1	0.48	2.22	16	1
1:A:52:GLN:NE2	2:B:459:ILE:HG23	0.48	2.22	24	1
1:A:30:HIS:HA	1:A:33:GLN:HB2	0.48	1.83	2	2
1:A:35:LEU:CD1	1:A:73:CYS:CB	0.48	2.88	8	15
1:A:54:TYR:CE2	1:A:66:LYS:HB2	0.48	2.43	10	7
1:A:107:TYR:CB	1:A:141:VAL:HG21	0.48	2.38	9	6
1:A:54:TYR:CE2	2:B:459:ILE:CG2	0.48	2.96	7	2
1:A:83:TYR:CE2	1:A:103:SER:HB2	0.48	2.44	22	3
1:A:88:TYR:C	1:A:88:TYR:CD2	0.48	2.90	15	2
1:A:53:LEU:CD1	1:A:97:TRP:CZ3	0.48	2.97	10	3
2:B:462:LEU:HD23	2:B:462:LEU:C	0.48	2.33	14	3
1:A:82:SER:C	1:A:83:TYR:CG	0.48	2.90	10	1
1:A:140:LEU:CD2	1:A:141:VAL:N	0.48	2.67	16	2
1:A:113:PHE:HB2	1:A:127:ASN:OD1	0.48	2.09	21	1
1:A:31:GLU:CG	1:A:45:THR:HG22	0.48	2.39	23	1
1:A:54:TYR:CE2	1:A:126:LEU:HA	0.48	2.43	24	1
1:A:35:LEU:HD13	1:A:73:CYS:CB	0.48	2.38	2	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:112:PRO:C	1:A:113:PHE:CD1	0.48	2.92	21	3
1:A:114:PHE:CG	1:A:115:HIS:N	0.48	2.81	24	4
1:A:87:LEU:CD1	1:A:97:TRP:CE2	0.48	2.97	4	1
2:B:459:ILE:O	2:B:459:ILE:CG2	0.48	2.61	4	1
1:A:118:ALA:CA	1:A:122:CYS:O	0.48	2.62	5	1
1:A:51:VAL:CG1	1:A:128:PHE:HB3	0.48	2.38	6	3
1:A:73:CYS:HB3	1:A:88:TYR:CD1	0.48	2.43	6	1
2:B:459:ILE:O	2:B:459:ILE:HG23	0.48	2.08	10	1
2:B:462:LEU:CD2	2:B:463:PRO:HD2	0.48	2.37	10	1
1:A:114:PHE:CD2	2:B:462:LEU:CD1	0.48	2.97	20	2
1:A:101:LEU:CD2	1:A:102:TYR:N	0.48	2.75	18	1
1:A:54:TYR:CG	2:B:459:ILE:HD13	0.48	2.43	22	1
1:A:114:PHE:HB2	1:A:127:ASN:HD22	0.48	1.69	23	1
1:A:47:ALA:C	1:A:74:PHE:CD1	0.48	2.91	13	12
1:A:82:SER:O	1:A:83:TYR:CD1	0.48	2.66	24	6
1:A:26:LEU:O	1:A:30:HIS:NE2	0.48	2.47	17	2
1:A:123:GLN:HG2	2:B:468:TYR:CE2	0.48	2.44	19	1
1:A:97:TRP:CE2	1:A:98:GLU:O	0.48	2.66	7	6
1:A:117:PHE:CE2	1:A:118:ALA:O	0.48	2.67	5	7
1:A:137:PHE:O	1:A:141:VAL:HG23	0.48	2.09	17	6
2:B:459:ILE:HB	2:B:462:LEU:CD2	0.48	2.39	3	2
1:A:107:TYR:CD2	1:A:117:PHE:CE2	0.48	3.02	6	1
1:A:88:TYR:CE2	1:A:90:LEU:CB	0.48	2.96	10	1
2:B:462:LEU:HD13	2:B:463:PRO:CD	0.48	2.37	10	1
2:B:459:ILE:HG12	2:B:462:LEU:HB3	0.48	1.84	19	1
1:A:33:GLN:O	1:A:37:GLU:CB	0.48	2.62	1	7
2:B:458:PRO:C	2:B:460:SER:H	0.48	2.16	1	1
1:A:113:PHE:CE1	2:B:461:ASP:CB	0.48	2.97	6	2
1:A:109:THR:CG2	1:A:137:PHE:CB	0.48	2.91	20	9
1:A:106:VAL:HB	1:A:117:PHE:CD2	0.48	2.43	12	4
1:A:31:GLU:HB2	1:A:47:ALA:HA	0.48	1.85	21	2
1:A:75:VAL:HB	1:A:84:PHE:HB2	0.48	1.86	19	1
1:A:47:ALA:N	1:A:74:PHE:HB2	0.48	2.24	8	8
1:A:54:TYR:CE2	1:A:66:LYS:CB	0.48	2.97	7	2
1:A:102:TYR:CE2	2:B:478:LYS:HD3	0.47	2.44	2	1
1:A:106:VAL:O	1:A:117:PHE:CB	0.47	2.61	3	1
1:A:133:GLU:HB3	2:B:454:PHE:CE1	0.47	2.44	9	4
1:A:81:LYS:NZ	1:A:81:LYS:HB2	0.47	2.24	6	3
1:A:83:TYR:CZ	1:A:105:LEU:HD21	0.47	2.44	6	1
1:A:30:HIS:CD2	2:B:445:PRO:O	0.47	2.67	17	6
1:A:91:GLN:OE1	1:A:92:ALA:HB2	0.47	2.08	13	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:105:LEU:HD23	1:A:145:ILE:HD11	0.47	1.86	19	1
1:A:90:LEU:HD23	1:A:90:LEU:C	0.47	2.34	20	1
1:A:105:LEU:CD1	1:A:107:TYR:CZ	0.47	2.97	23	1
1:A:52:GLN:NE2	1:A:54:TYR:CE2	0.47	2.82	24	1
1:A:52:GLN:CD	1:A:54:TYR:CD2	0.47	2.92	2	2
1:A:47:ALA:CB	1:A:140:LEU:HG	0.47	2.39	17	4
1:A:88:TYR:CD1	1:A:95:LEU:CB	0.47	2.97	5	1
1:A:51:VAL:HG11	1:A:115:HIS:NE2	0.47	2.24	6	2
1:A:109:THR:CB	1:A:134:ALA:HA	0.47	2.39	6	4
1:A:111:THR:HG21	1:A:114:PHE:CE1	0.47	2.44	6	1
1:A:106:VAL:O	1:A:107:TYR:CD1	0.47	2.67	7	1
2:B:456:PHE:O	2:B:457:HIS:O	0.47	2.32	8	4
1:A:47:ALA:CB	1:A:140:LEU:CD1	0.47	2.91	5	2
1:A:105:LEU:HG	1:A:145:ILE:HG12	0.47	1.85	14	1
1:A:107:TYR:CB	1:A:141:VAL:CG2	0.47	2.93	16	1
1:A:48:THR:HG22	1:A:73:CYS:CB	0.47	2.40	23	2
1:A:133:GLU:HB2	2:B:454:PHE:CZ	0.47	2.45	21	1
1:A:46:LEU:HD12	1:A:140:LEU:HD21	0.47	1.86	22	1
1:A:31:GLU:HA	1:A:48:THR:HG23	0.47	1.87	3	7
1:A:50:VAL:HG21	2:B:456:PHE:CD2	0.47	2.44	24	2
1:A:106:VAL:CG1	1:A:117:PHE:CD2	0.47	2.98	7	1
1:A:143:GLU:O	1:A:147:LYS:HB2	0.47	2.08	16	5
1:A:114:PHE:HB2	2:B:459:ILE:HG22	0.47	1.85	18	1
1:A:127:ASN:CG	2:B:459:ILE:HG23	0.47	2.33	18	1
1:A:36:PHE:CD2	1:A:36:PHE:C	0.47	2.92	6	5
1:A:50:VAL:HG11	2:B:454:PHE:CG	0.47	2.45	1	3
1:A:33:GLN:O	1:A:37:GLU:CG	0.47	2.63	2	3
1:A:103:SER:O	1:A:104:GLN:CB	0.47	2.62	3	7
1:A:83:TYR:CZ	1:A:103:SER:HA	0.47	2.45	10	2
1:A:109:THR:HG1	1:A:134:ALA:HA	0.47	1.70	13	1
1:A:54:TYR:CE1	1:A:66:LYS:HB2	0.47	2.44	17	1
1:A:46:LEU:HD11	1:A:144:LYS:HE2	0.47	1.85	20	1
2:B:477:SER:O	2:B:481:ARG:HB2	0.47	2.10	17	5
1:A:57:LEU:HD23	1:A:58:PRO:HD2	0.47	1.85	19	2
1:A:71:ALA:HB3	1:A:88:TYR:O	0.47	2.09	14	2
1:A:100:GLU:O	1:A:100:GLU:HG3	0.47	2.09	12	1
1:A:50:VAL:CG2	2:B:454:PHE:CD2	0.47	2.95	18	2
1:A:107:TYR:CD2	1:A:117:PHE:CG	0.47	3.02	16	1
1:A:123:GLN:NE2	2:B:468:TYR:CD1	0.47	2.83	18	1
1:A:54:TYR:CD1	2:B:459:ILE:CD1	0.47	2.97	21	3
1:A:68:HIS:CG	1:A:87:LEU:HD11	0.47	2.44	22	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:90:LEU:O	1:A:93:GLY:N	0.47	2.48	6	15
1:A:107:TYR:HB3	1:A:141:VAL:HG21	0.47	1.86	6	3
1:A:119:GLY:O	1:A:121:ASP:N	0.47	2.47	2	13
1:A:26:LEU:HD12	1:A:26:LEU:N	0.47	2.25	3	2
1:A:29:ASP:O	1:A:33:GLN:HB2	0.47	2.10	16	5
1:A:86:ARG:HB3	1:A:98:GLU:HA	0.47	1.85	19	2
1:A:112:PRO:C	1:A:113:PHE:CD2	0.47	2.92	11	3
1:A:140:LEU:HD22	1:A:140:LEU:O	0.47	2.10	8	2
2:B:462:LEU:HD23	2:B:463:PRO:O	0.47	2.09	8	1
1:A:127:ASN:HB3	2:B:459:ILE:CG2	0.47	2.31	15	2
1:A:83:TYR:CE1	1:A:103:SER:HB2	0.47	2.45	21	2
1:A:57:LEU:HD13	1:A:62:GLU:HB2	0.47	1.87	12	1
1:A:114:PHE:CE1	2:B:462:LEU:HD13	0.47	2.45	13	1
1:A:107:TYR:CZ	1:A:117:PHE:CE2	0.47	3.03	16	1
1:A:107:TYR:CG	1:A:145:ILE:HD11	0.47	2.45	16	1
1:A:50:VAL:HB	2:B:454:PHE:CD2	0.47	2.45	19	1
1:A:44:LEU:HD12	1:A:76:LYS:HB3	0.47	1.87	20	1
1:A:81:LYS:NZ	2:B:474:SER:O	0.47	2.43	1	3
1:A:114:PHE:HB3	2:B:462:LEU:CB	0.47	2.39	1	4
1:A:30:HIS:CG	2:B:445:PRO:O	0.47	2.67	10	4
1:A:38:MET:CG	1:A:88:TYR:CD2	0.47	2.98	19	2
1:A:54:TYR:OH	1:A:114:PHE:CE1	0.47	2.56	14	1
1:A:105:LEU:HD12	1:A:145:ILE:CD1	0.47	2.38	14	1
1:A:102:TYR:CZ	2:B:478:LYS:HD3	0.47	2.44	18	1
1:A:44:LEU:HD21	1:A:77:ASP:C	0.47	2.35	20	1
1:A:52:GLN:OE1	1:A:54:TYR:CD2	0.47	2.68	21	1
1:A:113:PHE:CE2	2:B:461:ASP:CB	0.47	2.97	5	3
1:A:133:GLU:HB2	2:B:454:PHE:CE1	0.47	2.45	22	3
2:B:459:ILE:HG12	2:B:459:ILE:O	0.47	2.09	8	1
1:A:105:LEU:HD21	1:A:144:LYS:HE2	0.47	1.85	10	1
1:A:107:TYR:C	1:A:117:PHE:CE1	0.47	2.93	17	1
1:A:83:TYR:O	2:B:475:TYR:CZ	0.47	2.68	18	1
1:A:51:VAL:HG12	1:A:128:PHE:CB	0.47	2.37	9	4
2:B:473:LYS:HD2	2:B:473:LYS:N	0.47	2.26	1	1
1:A:66:LYS:HB3	2:B:459:ILE:HD12	0.47	1.87	4	1
1:A:86:ARG:HB2	1:A:98:GLU:HA	0.47	1.86	12	10
1:A:81:LYS:NZ	1:A:103:SER:HB2	0.47	2.25	9	6
2:B:445:PRO:HB2	2:B:450:TRP:CD1	0.47	2.45	18	6
1:A:50:VAL:CG1	1:A:71:ALA:HA	0.47	2.35	11	3
1:A:106:VAL:O	1:A:117:PHE:CD2	0.47	2.68	11	1
1:A:86:ARG:HD3	1:A:88:TYR:CE1	0.47	2.44	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:459:ILE:HD13	2:B:462:LEU:HD22	0.47	1.86	14	1
1:A:83:TYR:HB2	1:A:101:LEU:O	0.46	2.09	22	8
1:A:130:ASP:O	1:A:132:ASP:N	0.46	2.48	9	14
1:A:112:PRO:O	1:A:113:PHE:CB	0.46	2.63	4	2
1:A:50:VAL:CG1	2:B:450:TRP:CH2	0.46	2.98	21	2
1:A:140:LEU:C	1:A:140:LEU:CD1	0.46	2.88	22	10
1:A:107:TYR:CD1	1:A:115:HIS:ND1	0.46	2.83	7	1
1:A:114:PHE:CG	2:B:462:LEU:CD2	0.46	2.98	7	1
1:A:127:ASN:OD1	2:B:459:ILE:CG1	0.46	2.63	7	1
1:A:50:VAL:HB	2:B:450:TRP:CZ2	0.46	2.44	10	1
1:A:104:GLN:O	1:A:117:PHE:CZ	0.46	2.68	18	6
1:A:105:LEU:HD12	1:A:107:TYR:CE2	0.46	2.44	24	1
1:A:34:ARG:CD	1:A:48:THR:HB	0.46	2.40	4	2
1:A:76:LYS:HD2	1:A:82:SER:O	0.46	2.10	19	8
1:A:50:VAL:CG2	2:B:450:TRP:CZ2	0.46	2.98	19	2
1:A:114:PHE:CG	2:B:462:LEU:HD13	0.46	2.45	12	3
2:B:475:TYR:CB	2:B:478:LYS:HD2	0.46	2.40	18	1
1:A:46:LEU:CD1	1:A:140:LEU:HD13	0.46	2.39	2	1
1:A:83:TYR:CD1	1:A:105:LEU:CD2	0.46	2.98	4	3
2:B:466:GLU:CB	2:B:467:PRO:HD2	0.46	2.41	23	17
1:A:109:THR:CA	1:A:128:PHE:CZ	0.46	2.98	15	2
1:A:46:LEU:HD22	1:A:46:LEU:O	0.46	2.10	4	1
1:A:107:TYR:CE2	1:A:115:HIS:NE2	0.46	2.84	4	2
1:A:119:GLY:N	1:A:122:CYS:HB2	0.46	2.26	23	4
1:A:114:PHE:HD1	2:B:462:LEU:HD21	0.46	1.70	10	1
1:A:87:LEU:HB2	1:A:96:LEU:HD12	0.46	1.86	21	1
1:A:38:MET:CB	1:A:88:TYR:CD1	0.46	2.99	22	1
1:A:34:ARG:CG	1:A:88:TYR:OH	0.46	2.64	24	1
1:A:38:MET:C	1:A:90:LEU:HD13	0.46	2.36	2	1
1:A:55:LEU:HD22	1:A:55:LEU:N	0.46	2.25	4	1
1:A:102:TYR:CD1	2:B:473:LYS:CG	0.46	2.98	8	1
1:A:75:VAL:HG21	1:A:86:ARG:CZ	0.46	2.40	13	2
1:A:38:MET:HG2	1:A:88:TYR:CD2	0.46	2.46	19	1
1:A:38:MET:HE2	1:A:88:TYR:CD1	0.46	2.45	5	2
1:A:76:LYS:HD2	1:A:83:TYR:HA	0.46	1.88	6	2
1:A:106:VAL:HA	1:A:145:ILE:HD12	0.46	1.88	8	1
1:A:122:CYS:C	1:A:123:GLN:CG	0.46	2.89	13	1
1:A:72:VAL:HG12	1:A:87:LEU:CD1	0.46	2.40	14	1
1:A:72:VAL:CG1	1:A:87:LEU:HD12	0.46	2.40	14	1
1:A:68:HIS:CD2	1:A:87:LEU:HD11	0.46	2.45	22	1
1:A:37:GLU:C	1:A:90:LEU:HD22	0.46	2.35	24	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:38:MET:HG3	1:A:88:TYR:CB	0.46	2.41	1	2
1:A:49:ALA:O	1:A:72:VAL:HG22	0.46	2.11	2	1
1:A:112:PRO:CB	1:A:113:PHE:CE1	0.46	2.99	2	4
1:A:34:ARG:NH2	1:A:71:ALA:CB	0.46	2.79	5	1
1:A:54:TYR:CZ	1:A:125:GLY:C	0.46	2.93	5	1
1:A:109:THR:HB	1:A:134:ALA:HA	0.46	1.87	7	2
1:A:47:ALA:CB	1:A:140:LEU:HD23	0.46	2.38	10	1
1:A:78:ASN:HB3	1:A:79:PRO:CD	0.46	2.41	10	3
1:A:38:MET:HA	1:A:90:LEU:HD22	0.46	1.87	11	1
1:A:54:TYR:CE1	1:A:66:LYS:CB	0.46	2.99	17	3
1:A:127:ASN:ND2	2:B:459:ILE:CB	0.46	2.79	23	1
1:A:81:LYS:HD2	2:B:479:LEU:CD1	0.46	2.39	1	8
1:A:83:TYR:CE1	1:A:105:LEU:CD2	0.46	2.99	18	2
1:A:102:TYR:CZ	2:B:478:LYS:HD2	0.46	2.46	12	2
1:A:38:MET:CE	1:A:91:GLN:N	0.46	2.79	21	1
1:A:114:PHE:CE1	2:B:462:LEU:HD23	0.46	2.46	21	2
1:A:52:GLN:NE2	2:B:459:ILE:N	0.46	2.64	24	1
1:A:32:ASN:O	1:A:36:PHE:HB3	0.46	2.11	6	4
1:A:54:TYR:CB	1:A:125:GLY:O	0.46	2.64	3	9
2:B:458:PRO:C	2:B:460:SER:N	0.46	2.73	1	1
1:A:112:PRO:HB2	1:A:113:PHE:CD1	0.46	2.45	7	4
1:A:31:GLU:O	1:A:48:THR:HG23	0.46	2.11	20	2
1:A:71:ALA:O	1:A:88:TYR:HD2	0.46	1.94	18	2
1:A:48:THR:HG23	1:A:73:CYS:CB	0.46	2.41	14	2
1:A:38:MET:SD	1:A:88:TYR:CE1	0.46	3.09	13	2
1:A:52:GLN:CB	1:A:127:ASN:HB2	0.46	2.40	10	2
1:A:127:ASN:CG	2:B:457:HIS:O	0.46	2.59	21	3
1:A:53:LEU:HD13	1:A:126:LEU:CG	0.46	2.40	24	1
1:A:39:LEU:HD12	1:A:39:LEU:O	0.45	2.10	19	2
1:A:81:LYS:CD	2:B:479:LEU:HD11	0.45	2.40	9	1
1:A:141:VAL:HG13	1:A:145:ILE:HB	0.45	1.88	14	2
1:A:85:ILE:HD13	1:A:101:LEU:HD12	0.45	1.86	18	1
1:A:88:TYR:CE1	1:A:95:LEU:CB	0.45	3.00	23	1
1:A:50:VAL:CG1	2:B:454:PHE:CD1	0.45	2.99	1	3
1:A:63:HIS:N	1:A:63:HIS:ND1	0.45	2.64	2	2
1:A:102:TYR:CE2	2:B:473:LYS:HB3	0.45	2.46	8	2
1:A:30:HIS:CG	2:B:445:PRO:HA	0.45	2.46	9	3
1:A:52:GLN:CB	1:A:127:ASN:OD1	0.45	2.65	15	2
1:A:109:THR:CG2	1:A:137:PHE:CD2	0.45	2.98	23	2
1:A:113:PHE:HA	1:A:128:PHE:CE1	0.45	2.46	18	1
1:A:56:ALA:C	1:A:57:LEU:HD12	0.45	2.37	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:56:ALA:HB2	1:A:64:TRP:CE2	0.45	2.46	10	2
1:A:78:ASN:CB	1:A:79:PRO:CD	0.45	2.95	11	17
1:A:81:LYS:O	1:A:81:LYS:HE2	0.45	2.11	1	1
1:A:81:LYS:HD3	2:B:476:PRO:CD	0.45	2.42	8	4
1:A:126:LEU:N	1:A:126:LEU:CD1	0.45	2.76	1	2
1:A:74:PHE:CD2	1:A:140:LEU:HD21	0.45	2.47	2	1
1:A:46:LEU:CD1	1:A:140:LEU:CD2	0.45	2.94	9	4
1:A:123:GLN:OE1	2:B:468:TYR:CD2	0.45	2.70	22	4
1:A:102:TYR:CG	2:B:473:LYS:HG3	0.45	2.47	8	1
1:A:74:PHE:CZ	1:A:140:LEU:CD2	0.45	3.00	11	1
1:A:68:HIS:HB3	1:A:87:LEU:HD13	0.45	1.87	17	2
1:A:81:LYS:CD	2:B:474:SER:O	0.45	2.64	19	1
1:A:115:HIS:CD2	1:A:126:LEU:HB2	0.45	2.46	24	3
2:B:450:TRP:CE3	2:B:450:TRP:HA	0.45	2.47	14	22
2:B:475:TYR:HB2	2:B:478:LYS:HD2	0.45	1.86	14	3
1:A:34:ARG:NH2	2:B:446:CYS:HG	0.45	2.09	4	1
2:B:457:HIS:HB3	2:B:458:PRO:HD2	0.45	1.87	8	4
1:A:102:TYR:CD1	2:B:473:LYS:HG2	0.45	2.47	8	1
2:B:459:ILE:O	2:B:462:LEU:HB2	0.45	2.11	10	1
1:A:139:ALA:O	1:A:143:GLU:CB	0.45	2.64	12	1
1:A:105:LEU:HB2	1:A:107:TYR:CE2	0.45	2.47	16	1
1:A:118:ALA:CB	2:B:468:TYR:CE2	0.45	3.00	19	1
1:A:115:HIS:N	1:A:128:PHE:CE2	0.45	2.85	18	3
1:A:115:HIS:CD2	1:A:115:HIS:C	0.45	2.95	4	4
1:A:83:TYR:CE2	1:A:103:SER:OG	0.45	2.70	15	2
1:A:109:THR:HG21	1:A:137:PHE:HB2	0.45	1.88	6	2
1:A:114:PHE:CZ	1:A:116:THR:CG2	0.45	2.99	11	5
1:A:38:MET:HG3	1:A:88:TYR:CG	0.45	2.46	7	4
1:A:114:PHE:CG	2:B:459:ILE:HD11	0.45	2.47	10	1
1:A:35:LEU:HB2	1:A:73:CYS:HB3	0.45	1.89	11	1
1:A:87:LEU:CD1	1:A:97:TRP:HB3	0.45	2.42	17	2
1:A:109:THR:CG2	1:A:137:PHE:CG	0.45	2.99	15	2
1:A:109:THR:HG22	1:A:128:PHE:CE1	0.45	2.47	16	1
1:A:56:ALA:CB	1:A:64:TRP:CD2	0.45	2.96	10	6
1:A:114:PHE:CE2	1:A:115:HIS:O	0.45	2.70	22	4
1:A:86:ARG:HB3	1:A:98:GLU:CB	0.45	2.41	20	5
1:A:30:HIS:HB3	1:A:34:ARG:NH1	0.45	2.27	6	1
1:A:142:GLN:O	1:A:146:GLN:CG	0.45	2.65	11	4
1:A:102:TYR:CE1	2:B:473:LYS:CD	0.45	2.99	18	1
1:A:84:PHE:CE2	2:B:475:TYR:OH	0.45	2.69	19	1
1:A:34:ARG:NH2	2:B:450:TRP:CD2	0.45	2.84	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:88:TYR:CD2	1:A:90:LEU:HB2	0.45	2.46	10	1
1:A:74:PHE:CD2	1:A:140:LEU:HD11	0.45	2.47	16	1
1:A:107:TYR:CG	1:A:117:PHE:CE1	0.45	3.05	16	1
1:A:46:LEU:HB2	1:A:76:LYS:HG3	0.45	1.88	17	1
2:B:459:ILE:HB	2:B:462:LEU:HD23	0.45	1.89	17	1
2:B:478:LYS:N	2:B:478:LYS:HE3	0.45	2.26	19	2
1:A:34:ARG:HH12	1:A:38:MET:HE2	0.45	1.70	21	1
1:A:101:LEU:HD21	1:A:122:CYS:SG	0.45	2.52	24	1
1:A:54:TYR:CD1	2:B:459:ILE:CG2	0.45	3.00	14	2
1:A:75:VAL:O	1:A:84:PHE:N	0.45	2.50	15	5
1:A:46:LEU:HD11	1:A:140:LEU:HD23	0.45	1.87	1	1
1:A:97:TRP:CG	1:A:98:GLU:N	0.45	2.85	6	4
2:B:450:TRP:CZ3	2:B:454:PHE:HB2	0.45	2.47	8	3
1:A:129:ALA:N	2:B:455:TYR:O	0.45	2.50	5	3
2:B:459:ILE:HD13	2:B:459:ILE:C	0.45	2.37	9	1
2:B:462:LEU:CD1	2:B:463:PRO:HD2	0.45	2.41	10	1
1:A:141:VAL:O	1:A:145:ILE:N	0.45	2.50	14	2
1:A:44:LEU:HD12	1:A:44:LEU:C	0.45	2.37	15	1
1:A:117:PHE:CD2	1:A:118:ALA:N	0.45	2.85	19	1
1:A:83:TYR:CD2	1:A:105:LEU:HD22	0.45	2.47	24	1
2:B:455:TYR:CD2	2:B:455:TYR:C	0.44	2.95	2	1
1:A:52:GLN:HB3	1:A:127:ASN:HB2	0.44	1.88	6	1
1:A:72:VAL:CG1	1:A:87:LEU:CD2	0.44	2.95	9	6
1:A:72:VAL:HA	1:A:87:LEU:HA	0.44	1.89	22	4
1:A:36:PHE:HA	1:A:39:LEU:CG	0.44	2.42	13	1
1:A:55:LEU:HD12	1:A:124:ALA:CA	0.44	2.42	22	2
1:A:115:HIS:ND1	1:A:137:PHE:CZ	0.44	2.85	16	1
2:B:446:CYS:O	2:B:450:TRP:HB2	0.44	2.12	17	2
1:A:54:TYR:CD2	2:B:459:ILE:HG12	0.44	2.47	18	1
1:A:83:TYR:C	1:A:84:PHE:CD1	0.44	2.95	19	1
1:A:108:SER:H	1:A:141:VAL:HG21	0.44	1.73	15	3
1:A:47:ALA:HB2	1:A:140:LEU:CD1	0.44	2.41	5	1
1:A:114:PHE:C	1:A:128:PHE:CZ	0.44	2.95	5	2
1:A:102:TYR:CG	2:B:473:LYS:HG2	0.44	2.47	10	2
1:A:46:LEU:CD2	1:A:76:LYS:HG3	0.44	2.40	10	1
1:A:128:PHE:CD2	1:A:133:GLU:OE2	0.44	2.70	15	1
1:A:107:TYR:HB2	1:A:145:ILE:HD12	0.44	1.88	16	1
1:A:53:LEU:CD1	1:A:97:TRP:CZ2	0.44	3.00	20	1
1:A:50:VAL:C	1:A:51:VAL:HG13	0.44	2.36	1	4
1:A:69:CYS:SG	1:A:70:GLY:N	0.44	2.90	18	9
1:A:74:PHE:CE2	1:A:140:LEU:CD2	0.44	3.01	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:88:TYR:CD1	1:A:95:LEU:HB3	0.44	2.48	20	2
1:A:102:TYR:CG	2:B:473:LYS:CG	0.44	3.00	9	2
1:A:115:HIS:CD2	1:A:115:HIS:H	0.44	2.30	11	1
1:A:30:HIS:CD2	1:A:34:ARG:NH2	0.44	2.85	12	1
1:A:56:ALA:HA	1:A:63:HIS:O	0.44	2.12	14	1
2:B:477:SER:O	2:B:481:ARG:CB	0.44	2.66	14	2
1:A:50:VAL:HG13	1:A:71:ALA:N	0.44	2.26	17	1
1:A:107:TYR:CA	1:A:117:PHE:CE1	0.44	3.01	17	1
1:A:141:VAL:O	1:A:145:ILE:HG22	0.44	2.12	22	1
1:A:115:HIS:N	1:A:128:PHE:HE2	0.44	2.11	23	1
1:A:114:PHE:HB2	1:A:126:LEU:O	0.44	2.11	2	4
1:A:54:TYR:CE2	1:A:125:GLY:HA3	0.44	2.48	5	1
1:A:141:VAL:O	1:A:145:ILE:HB	0.44	2.12	6	3
1:A:86:ARG:HG3	1:A:97:TRP:O	0.44	2.13	10	1
2:B:445:PRO:HG2	2:B:450:TRP:CG	0.44	2.47	23	1
1:A:53:LEU:N	1:A:68:HIS:O	0.44	2.50	17	6
1:A:109:THR:OG1	1:A:137:PHE:HB3	0.44	2.12	5	3
1:A:30:HIS:ND1	2:B:445:PRO:O	0.44	2.51	12	2
1:A:118:ALA:HB1	2:B:468:TYR:CE1	0.44	2.48	14	1
1:A:128:PHE:HB2	1:A:133:GLU:CD	0.44	2.38	15	1
1:A:52:GLN:OE1	2:B:459:ILE:CG2	0.44	2.66	21	1
1:A:106:VAL:O	1:A:106:VAL:CG1	0.44	2.65	21	1
1:A:57:LEU:O	1:A:58:PRO:C	0.44	2.61	14	15
1:A:111:THR:CB	1:A:112:PRO:CD	0.44	2.96	4	2
1:A:71:ALA:O	1:A:88:TYR:CG	0.44	2.71	6	1
1:A:102:TYR:CE1	2:B:473:LYS:HG3	0.44	2.48	12	1
2:B:457:HIS:HB2	2:B:458:PRO:CD	0.44	2.41	20	1
1:A:31:GLU:O	1:A:48:THR:OG1	0.44	2.36	1	2
1:A:102:TYR:OH	1:A:122:CYS:N	0.44	2.50	3	1
1:A:25:THR:C	1:A:26:LEU:HD22	0.44	2.37	5	1
1:A:54:TYR:CZ	1:A:126:LEU:C	0.44	2.95	6	1
1:A:107:TYR:CE2	1:A:117:PHE:CZ	0.44	3.06	6	1
2:B:454:PHE:O	2:B:456:PHE:CD1	0.44	2.70	22	4
1:A:53:LEU:HD12	1:A:87:LEU:CD2	0.44	2.43	12	1
1:A:48:THR:CG2	1:A:73:CYS:HA	0.44	2.43	14	1
1:A:100:GLU:CD	2:B:475:TYR:CE2	0.44	2.96	23	2
1:A:114:PHE:CD1	1:A:115:HIS:N	0.44	2.86	20	1
1:A:129:ALA:O	1:A:133:GLU:OE1	0.44	2.36	2	1
1:A:87:LEU:CD1	1:A:97:TRP:NE1	0.44	2.81	9	5
1:A:127:ASN:OD1	2:B:462:LEU:HD23	0.44	2.13	13	4
2:B:459:ILE:CD1	2:B:462:LEU:HD21	0.44	2.36	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:101:LEU:O	2:B:475:TYR:CD2	0.44	2.71	18	1
1:A:105:LEU:HD23	1:A:105:LEU:H	0.44	1.73	24	2
1:A:54:TYR:HE1	2:B:459:ILE:HG21	0.44	1.71	19	1
2:B:474:SER:HA	2:B:479:LEU:CD2	0.44	2.39	1	1
1:A:52:GLN:HA	1:A:69:CYS:HA	0.44	1.90	24	8
1:A:57:LEU:CB	1:A:62:GLU:CG	0.44	2.95	11	2
1:A:109:THR:CG2	1:A:128:PHE:CZ	0.44	2.98	4	1
1:A:123:GLN:CD	2:B:468:TYR:CD1	0.44	2.96	24	4
2:B:462:LEU:HD23	2:B:463:PRO:N	0.44	2.28	8	1
1:A:81:LYS:HG3	2:B:476:PRO:HG3	0.44	1.90	9	1
1:A:127:ASN:OD1	2:B:459:ILE:HG13	0.44	2.12	10	1
2:B:459:ILE:CG1	2:B:462:LEU:HD22	0.44	2.43	20	1
1:A:54:TYR:CD1	1:A:64:TRP:CH2	0.44	3.06	24	1
1:A:102:TYR:CZ	2:B:473:LYS:HG2	0.43	2.48	1	1
1:A:107:TYR:CE1	1:A:115:HIS:NE2	0.43	2.86	1	1
1:A:112:PRO:HB3	1:A:113:PHE:CE1	0.43	2.48	21	3
2:B:446:CYS:O	2:B:447:GLU:HG2	0.43	2.13	4	2
1:A:34:ARG:CZ	1:A:71:ALA:HB1	0.43	2.43	5	1
1:A:35:LEU:HA	1:A:73:CYS:CB	0.43	2.43	18	2
1:A:30:HIS:CD2	2:B:445:PRO:HA	0.43	2.48	23	1
1:A:48:THR:HG22	1:A:73:CYS:HB3	0.43	1.90	23	1
1:A:106:VAL:HG13	1:A:145:ILE:HD11	0.43	1.88	7	1
2:B:457:HIS:CG	2:B:458:PRO:HD2	0.43	2.49	8	3
2:B:475:TYR:CB	2:B:478:LYS:HG2	0.43	2.42	17	3
1:A:38:MET:HA	1:A:38:MET:HE2	0.43	1.90	20	1
1:A:102:TYR:CE2	2:B:478:LYS:CD	0.43	3.01	2	2
1:A:81:LYS:HZ3	2:B:476:PRO:CD	0.43	2.27	4	1
1:A:127:ASN:OD1	2:B:459:ILE:CB	0.43	2.67	7	1
1:A:141:VAL:HG13	1:A:145:ILE:HG13	0.43	1.89	11	1
1:A:115:HIS:CD2	1:A:128:PHE:CD2	0.43	3.07	19	1
1:A:34:ARG:O	1:A:90:LEU:CD1	0.43	2.66	20	1
1:A:53:LEU:CD1	1:A:126:LEU:CD2	0.43	2.97	1	2
1:A:51:VAL:HG13	1:A:128:PHE:CG	0.43	2.48	2	1
1:A:34:ARG:CD	1:A:48:THR:OG1	0.43	2.67	6	1
1:A:83:TYR:CG	1:A:102:TYR:O	0.43	2.71	19	3
1:A:103:SER:N	2:B:474:SER:O	0.43	2.51	11	2
1:A:127:ASN:OD1	2:B:456:PHE:O	0.43	2.36	11	1
1:A:88:TYR:CD1	1:A:90:LEU:HB2	0.43	2.48	18	2
1:A:104:GLN:O	1:A:117:PHE:CE2	0.43	2.72	5	2
1:A:114:PHE:HB3	2:B:462:LEU:HB2	0.43	1.89	16	4
1:A:118:ALA:CB	2:B:468:TYR:CD1	0.43	3.01	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:107:TYR:HB2	1:A:141:VAL:CG2	0.43	2.42	16	3
1:A:38:MET:O	1:A:88:TYR:CZ	0.43	2.71	4	1
1:A:109:THR:HB	1:A:128:PHE:CD2	0.43	2.49	10	1
1:A:127:ASN:OD1	2:B:457:HIS:O	0.43	2.36	15	2
1:A:114:PHE:CD1	2:B:462:LEU:HD22	0.43	2.48	17	1
1:A:111:THR:HB	1:A:112:PRO:CD	0.43	2.44	24	1
1:A:70:GLY:HA3	1:A:96:LEU:HD12	0.43	1.90	1	3
1:A:133:GLU:CD	1:A:133:GLU:C	0.43	2.86	1	1
1:A:34:ARG:O	1:A:38:MET:SD	0.43	2.77	3	2
1:A:72:VAL:O	1:A:72:VAL:CG2	0.43	2.66	3	5
1:A:114:PHE:CD2	2:B:462:LEU:HD22	0.43	2.49	3	1
1:A:52:GLN:O	1:A:126:LEU:HD23	0.43	2.12	4	1
2:B:468:TYR:CD1	2:B:469:VAL:N	0.43	2.87	19	3
2:B:475:TYR:CB	2:B:478:LYS:HD3	0.43	2.43	5	1
1:A:80:GLN:O	1:A:81:LYS:HG3	0.43	2.13	17	4
1:A:25:THR:HA	1:A:29:ASP:HB2	0.43	1.90	17	3
1:A:102:TYR:CD2	1:A:102:TYR:N	0.43	2.86	19	2
1:A:57:LEU:CD1	1:A:123:GLN:CB	0.43	2.97	16	2
1:A:32:ASN:CG	1:A:45:THR:HG21	0.43	2.39	19	1
1:A:50:VAL:HG11	2:B:454:PHE:C	0.43	2.39	24	1
1:A:128:PHE:CD1	1:A:133:GLU:OE2	0.43	2.72	1	1
1:A:123:GLN:OE1	2:B:468:TYR:CD1	0.43	2.72	2	7
1:A:75:VAL:HG11	1:A:86:ARG:NE	0.43	2.28	8	1
1:A:112:PRO:CB	1:A:113:PHE:CE2	0.43	3.02	19	2
1:A:96:LEU:O	1:A:97:TRP:HB2	0.43	2.13	17	2
1:A:104:GLN:O	1:A:106:VAL:HG23	0.43	2.13	23	1
1:A:87:LEU:N	1:A:87:LEU:HD22	0.43	2.29	1	1
1:A:113:PHE:CE1	2:B:461:ASP:HB2	0.43	2.48	21	3
1:A:87:LEU:HD12	1:A:97:TRP:HB3	0.43	1.89	5	1
1:A:113:PHE:CE2	2:B:461:ASP:HB3	0.43	2.49	5	1
1:A:38:MET:HE3	1:A:91:GLN:H	0.43	1.74	8	1
1:A:109:THR:C	1:A:128:PHE:CZ	0.43	2.97	8	1
1:A:111:THR:CG2	1:A:112:PRO:HD2	0.43	2.42	8	1
1:A:53:LEU:HD11	1:A:97:TRP:CZ3	0.43	2.48	10	2
1:A:123:GLN:OE1	2:B:468:TYR:CG	0.43	2.72	24	5
2:B:459:ILE:HG13	2:B:459:ILE:O	0.43	2.12	13	2
1:A:117:PHE:O	1:A:123:GLN:HA	0.43	2.13	23	2
1:A:115:HIS:C	1:A:115:HIS:CD2	0.43	2.96	21	1
1:A:131:GLU:CA	1:A:134:ALA:HB3	0.43	2.42	3	1
1:A:34:ARG:HG2	2:B:445:PRO:HB3	0.43	1.91	4	1
1:A:105:LEU:CD1	1:A:107:TYR:CD1	0.43	3.01	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:454:PHE:O	2:B:456:PHE:CD2	0.43	2.72	5	3
2:B:455:TYR:CD1	2:B:455:TYR:C	0.43	2.97	5	2
2:B:459:ILE:HB	2:B:462:LEU:HD12	0.43	1.91	6	1
1:A:88:TYR:CE2	1:A:90:LEU:HB3	0.43	2.48	10	1
1:A:109:THR:HG21	1:A:137:PHE:CD2	0.43	2.49	10	1
1:A:80:GLN:O	1:A:80:GLN:HG2	0.43	2.13	15	1
1:A:82:SER:C	1:A:83:TYR:CD1	0.43	2.97	19	2
1:A:34:ARG:HA	1:A:90:LEU:HD13	0.43	1.89	20	1
2:B:475:TYR:C	2:B:477:SER:N	0.43	2.76	3	1
1:A:54:TYR:HB3	1:A:64:TRP:HZ3	0.43	1.74	17	2
1:A:141:VAL:CG1	1:A:145:ILE:HB	0.43	2.44	19	2
1:A:34:ARG:NH1	2:B:450:TRP:NE1	0.43	2.67	15	2
2:B:459:ILE:HG22	2:B:462:LEU:CD2	0.42	2.43	1	1
1:A:87:LEU:O	1:A:97:TRP:O	0.42	2.37	2	1
1:A:105:LEU:O	1:A:145:ILE:CG2	0.42	2.68	6	1
1:A:113:PHE:CE1	2:B:461:ASP:CG	0.42	2.97	7	1
1:A:81:LYS:CE	1:A:103:SER:HB2	0.42	2.43	9	2
1:A:81:LYS:CE	2:B:476:PRO:HD3	0.42	2.44	14	1
1:A:55:LEU:CD1	1:A:124:ALA:HB2	0.42	2.44	16	2
1:A:70:GLY:HA3	1:A:96:LEU:HD11	0.42	1.91	16	1
2:B:466:GLU:HB3	2:B:467:PRO:HD2	0.42	1.91	17	1
1:A:51:VAL:HG12	1:A:127:ASN:C	0.42	2.39	18	2
1:A:114:PHE:HB3	2:B:459:ILE:HG22	0.42	1.88	18	1
1:A:53:LEU:C	1:A:53:LEU:HD22	0.42	2.39	19	1
1:A:55:LEU:HD22	1:A:55:LEU:O	0.42	2.14	20	1
1:A:100:GLU:OE2	2:B:475:TYR:CE2	0.42	2.72	23	1
1:A:91:GLN:NE2	1:A:92:ALA:HB2	0.42	2.29	2	1
1:A:128:PHE:CE1	1:A:137:PHE:CE1	0.42	3.08	2	1
1:A:106:VAL:N	1:A:145:ILE:HD11	0.42	2.29	3	1
2:B:475:TYR:O	2:B:477:SER:N	0.42	2.52	3	2
1:A:106:VAL:O	1:A:107:TYR:CG	0.42	2.73	7	2
1:A:50:VAL:HG21	2:B:450:TRP:CZ2	0.42	2.49	11	1
1:A:47:ALA:HB3	1:A:74:PHE:CD1	0.42	2.48	17	1
1:A:128:PHE:CD1	1:A:128:PHE:C	0.42	2.97	18	2
1:A:105:LEU:CD1	1:A:107:TYR:CD2	0.42	3.01	22	1
1:A:114:PHE:CZ	1:A:116:THR:OG1	0.42	2.72	23	1
1:A:123:GLN:OE1	2:B:468:TYR:CZ	0.42	2.73	9	3
1:A:33:GLN:O	1:A:37:GLU:HB2	0.42	2.14	13	1
1:A:109:THR:HG21	1:A:137:PHE:CD1	0.42	2.49	17	1
1:A:52:GLN:HG3	2:B:457:HIS:C	0.42	2.40	22	1
1:A:87:LEU:CD2	1:A:97:TRP:CE3	0.42	3.00	22	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:111:THR:HB	1:A:112:PRO:HD2	0.42	1.89	24	1
1:A:133:GLU:HB3	2:B:454:PHE:CZ	0.42	2.49	3	2
1:A:89:GLY:O	1:A:92:ALA:N	0.42	2.53	5	1
1:A:128:PHE:CD2	1:A:128:PHE:C	0.42	2.97	16	2
1:A:112:PRO:CB	2:B:461:ASP:O	0.42	2.68	9	1
1:A:123:GLN:OE1	2:B:468:TYR:CE1	0.42	2.72	9	2
1:A:112:PRO:HG2	2:B:463:PRO:HD3	0.42	1.90	13	1
1:A:30:HIS:CD2	1:A:48:THR:OG1	0.42	2.73	16	1
1:A:116:THR:CB	1:A:124:ALA:O	0.42	2.67	20	3
1:A:115:HIS:CD2	1:A:128:PHE:CE2	0.42	3.08	19	1
1:A:82:SER:C	1:A:83:TYR:CD2	0.42	2.97	1	1
1:A:87:LEU:N	1:A:97:TRP:O	0.42	2.52	14	2
1:A:34:ARG:O	1:A:38:MET:N	0.42	2.50	2	1
1:A:48:THR:HG23	1:A:73:CYS:HA	0.42	1.91	2	1
1:A:38:MET:HG2	1:A:88:TYR:HB3	0.42	1.91	17	2
1:A:112:PRO:HB2	1:A:113:PHE:CD2	0.42	2.49	11	3
2:B:459:ILE:CB	2:B:462:LEU:HD23	0.42	2.44	17	2
1:A:54:TYR:OH	1:A:126:LEU:C	0.42	2.62	4	1
1:A:140:LEU:C	1:A:140:LEU:HD22	0.42	2.39	8	1
1:A:109:THR:OG1	1:A:137:PHE:CG	0.42	2.73	11	1
1:A:102:TYR:CE1	2:B:473:LYS:HD2	0.42	2.50	18	1
1:A:36:PHE:HB2	1:A:45:THR:CG2	0.42	2.44	20	1
1:A:52:GLN:NE2	1:A:68:HIS:O	0.42	2.53	22	1
1:A:76:LYS:CD	1:A:83:TYR:HA	0.42	2.45	2	1
1:A:109:THR:CB	1:A:128:PHE:CE2	0.42	3.01	3	1
1:A:53:LEU:CD1	1:A:54:TYR:N	0.42	2.82	4	1
1:A:113:PHE:CZ	1:A:130:ASP:CB	0.42	3.02	4	1
1:A:115:HIS:HB3	1:A:128:PHE:CZ	0.42	2.50	4	1
1:A:138:ARG:O	1:A:142:GLN:CB	0.42	2.68	4	2
1:A:145:ILE:CG2	1:A:146:GLN:N	0.42	2.82	15	3
2:B:459:ILE:CD1	2:B:462:LEU:CD2	0.42	2.97	12	2
1:A:129:ALA:CA	2:B:455:TYR:O	0.42	2.68	13	1
1:A:123:GLN:HG2	2:B:468:TYR:CE1	0.42	2.49	14	1
1:A:85:ILE:HB	1:A:101:LEU:HD12	0.42	1.91	18	1
2:B:459:ILE:HB	2:B:462:LEU:HG	0.42	1.91	18	1
1:A:37:GLU:HG2	1:A:90:LEU:CD2	0.42	2.41	19	1
1:A:83:TYR:CE2	1:A:103:SER:HA	0.42	2.49	6	4
1:A:54:TYR:C	1:A:55:LEU:CD1	0.42	2.87	4	1
1:A:30:HIS:O	1:A:34:ARG:CB	0.42	2.68	5	1
1:A:38:MET:HG2	1:A:88:TYR:CG	0.42	2.49	5	1
1:A:105:LEU:CD1	1:A:107:TYR:CE2	0.42	2.95	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:30:HIS:HA	1:A:33:GLN:CB	0.42	2.44	9	4
1:A:54:TYR:CZ	2:B:459:ILE:HG22	0.42	2.50	6	1
1:A:68:HIS:CD2	1:A:97:TRP:CE3	0.42	3.07	12	1
1:A:91:GLN:HG3	1:A:92:ALA:N	0.42	2.30	12	1
1:A:88:TYR:OH	1:A:95:LEU:HD13	0.42	2.14	20	1
1:A:102:TYR:CE2	2:B:473:LYS:HG3	0.42	2.50	20	1
1:A:123:GLN:HG2	2:B:468:TYR:CD1	0.42	2.49	23	1
1:A:30:HIS:CE1	2:B:444:SER:O	0.42	2.73	24	1
2:B:459:ILE:C	2:B:459:ILE:HD12	0.42	2.40	3	1
1:A:57:LEU:CD2	1:A:123:GLN:NE2	0.42	2.83	13	1
1:A:127:ASN:CG	2:B:459:ILE:HA	0.42	2.40	23	1
1:A:135:GLN:O	1:A:138:ARG:HG2	0.42	2.15	7	2
2:B:459:ILE:C	2:B:461:ASP:N	0.42	2.78	17	5
1:A:109:THR:CG2	1:A:128:PHE:CE2	0.42	2.97	7	1
1:A:130:ASP:O	1:A:131:GLU:C	0.42	2.63	10	2
1:A:30:HIS:CE1	2:B:445:PRO:O	0.42	2.73	14	1
1:A:54:TYR:CE2	2:B:459:ILE:HG23	0.42	2.49	17	1
1:A:69:CYS:C	1:A:87:LEU:HD12	0.42	2.39	18	1
2:B:459:ILE:CG1	2:B:462:LEU:CB	0.42	2.98	19	1
1:A:114:PHE:CE1	1:A:115:HIS:O	0.42	2.73	4	3
1:A:53:LEU:CD2	1:A:54:TYR:N	0.42	2.83	14	3
1:A:34:ARG:NH2	2:B:450:TRP:NE1	0.42	2.67	10	1
1:A:54:TYR:O	1:A:125:GLY:O	0.42	2.38	12	1
1:A:79:PRO:C	1:A:81:LYS:H	0.42	2.23	16	1
1:A:50:VAL:HB	2:B:454:PHE:HD2	0.42	1.74	19	2
2:B:466:GLU:O	2:B:468:TYR:CE1	0.42	2.73	17	1
1:A:118:ALA:HB2	1:A:123:GLN:OE1	0.42	2.14	18	1
1:A:38:MET:CB	1:A:90:LEU:HD22	0.42	2.39	19	1
1:A:84:PHE:CE1	1:A:86:ARG:NE	0.41	2.88	2	1
1:A:128:PHE:CG	1:A:133:GLU:OE1	0.41	2.73	2	1
1:A:47:ALA:HB3	1:A:74:PHE:CD2	0.41	2.50	5	2
1:A:127:ASN:OD1	2:B:459:ILE:HD12	0.41	2.15	7	1
1:A:114:PHE:CD2	2:B:462:LEU:HG	0.41	2.50	8	1
1:A:112:PRO:HB3	1:A:113:PHE:CE2	0.41	2.49	19	2
1:A:87:LEU:HD12	1:A:96:LEU:CB	0.41	2.40	12	1
2:B:475:TYR:O	2:B:478:LYS:HG2	0.41	2.14	12	1
1:A:100:GLU:OE1	2:B:475:TYR:CE2	0.41	2.73	19	1
1:A:38:MET:HE3	1:A:90:LEU:C	0.41	2.40	21	1
1:A:68:HIS:CB	1:A:87:LEU:CD1	0.41	2.98	5	1
1:A:105:LEU:CD1	1:A:107:TYR:CE1	0.41	2.98	9	1
1:A:87:LEU:O	1:A:88:TYR:CD2	0.41	2.73	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:30:HIS:C	1:A:32:ASN:N	0.41	2.78	19	1
1:A:50:VAL:HG22	2:B:450:TRP:CZ2	0.41	2.50	19	1
1:A:115:HIS:CE1	1:A:137:PHE:CE2	0.41	3.07	19	1
1:A:50:VAL:O	1:A:128:PHE:HB3	0.41	2.15	24	1
1:A:51:VAL:HG22	1:A:72:VAL:CG1	0.41	2.45	1	1
1:A:105:LEU:O	1:A:105:LEU:HD12	0.41	2.15	2	1
1:A:52:GLN:HB3	1:A:127:ASN:ND2	0.41	2.30	4	2
1:A:72:VAL:HG12	1:A:87:LEU:HD22	0.41	1.92	10	2
1:A:83:TYR:C	1:A:84:PHE:CD2	0.41	2.98	4	1
1:A:34:ARG:HD3	1:A:48:THR:CG2	0.41	2.44	5	1
1:A:97:TRP:CE3	1:A:98:GLU:O	0.41	2.74	10	2
1:A:54:TYR:CD2	2:B:459:ILE:CD1	0.41	3.00	11	1
1:A:111:THR:O	1:A:112:PRO:C	0.41	2.64	11	2
1:A:91:GLN:OE1	2:B:450:TRP:CZ3	0.41	2.73	12	1
2:B:459:ILE:HG13	2:B:462:LEU:CG	0.41	2.45	12	1
1:A:53:LEU:HD12	1:A:97:TRP:CH2	0.41	2.50	14	1
1:A:48:THR:O	1:A:49:ALA:CB	0.41	2.69	15	1
1:A:133:GLU:OE1	1:A:137:PHE:CD2	0.41	2.74	15	1
1:A:78:ASN:CB	1:A:79:PRO:HD2	0.41	2.46	17	2
1:A:113:PHE:O	1:A:127:ASN:CA	0.41	2.67	18	1
1:A:55:LEU:HD11	1:A:67:GLU:HG3	0.41	1.92	23	1
1:A:107:TYR:CG	1:A:115:HIS:CE1	0.41	3.08	24	1
1:A:115:HIS:CD2	1:A:128:PHE:CE1	0.41	3.08	24	1
1:A:105:LEU:O	1:A:105:LEU:CG	0.41	2.69	1	2
1:A:115:HIS:CE1	1:A:126:LEU:CD1	0.41	3.04	4	1
1:A:35:LEU:HB2	1:A:73:CYS:HB2	0.41	1.92	6	1
1:A:37:GLU:CD	1:A:90:LEU:HD21	0.41	2.41	6	1
1:A:112:PRO:HB2	1:A:113:PHE:CE1	0.41	2.50	6	1
1:A:128:PHE:CE1	1:A:129:ALA:O	0.41	2.73	6	1
1:A:115:HIS:N	1:A:128:PHE:CE1	0.41	2.88	7	1
1:A:37:GLU:O	1:A:90:LEU:CD1	0.41	2.69	11	1
1:A:55:LEU:CD1	1:A:124:ALA:CB	0.41	2.98	11	2
1:A:133:GLU:OE1	2:B:454:PHE:CZ	0.41	2.73	11	1
1:A:131:GLU:HA	1:A:134:ALA:CB	0.41	2.46	12	3
1:A:106:VAL:HB	1:A:117:PHE:HB2	0.41	1.92	15	1
1:A:76:LYS:HE2	1:A:83:TYR:CD1	0.41	2.49	17	1
1:A:100:GLU:OE1	2:B:475:TYR:CZ	0.41	2.73	19	1
1:A:123:GLN:HG2	2:B:468:TYR:CZ	0.41	2.50	19	1
1:A:129:ALA:HB2	2:B:454:PHE:CE2	0.41	2.49	19	1
1:A:114:PHE:CD2	1:A:115:HIS:O	0.41	2.73	22	1
1:A:32:ASN:HA	1:A:45:THR:CG2	0.41	2.45	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:102:TYR:CE2	2:B:473:LYS:HG2	0.41	2.50	1	1
1:A:34:ARG:NH1	1:A:38:MET:CE	0.41	2.84	3	1
1:A:109:THR:OG1	1:A:134:ALA:O	0.41	2.39	3	1
1:A:88:TYR:CD1	1:A:88:TYR:O	0.41	2.73	10	1
1:A:75:VAL:C	1:A:76:LYS:HG2	0.41	2.40	17	2
1:A:58:PRO:CD	1:A:123:GLN:OE1	0.41	2.69	12	1
1:A:74:PHE:CE2	1:A:140:LEU:HD11	0.41	2.51	16	1
1:A:83:TYR:CD1	1:A:105:LEU:HB2	0.41	2.50	17	1
1:A:127:ASN:OD1	2:B:459:ILE:CG2	0.41	2.68	17	1
1:A:46:LEU:CB	1:A:76:LYS:HG3	0.41	2.46	4	1
1:A:58:PRO:CG	2:B:468:TYR:CD2	0.41	3.03	7	1
2:B:459:ILE:CD1	2:B:462:LEU:HG	0.41	2.46	10	1
1:A:75:VAL:HB	1:A:84:PHE:CD1	0.41	2.51	16	3
1:A:106:VAL:HB	1:A:117:PHE:HB3	0.41	1.91	11	1
1:A:51:VAL:HG12	1:A:127:ASN:O	0.41	2.16	13	2
1:A:54:TYR:CE1	1:A:125:GLY:O	0.41	2.73	14	1
1:A:114:PHE:CD1	1:A:114:PHE:C	0.41	2.97	14	1
1:A:47:ALA:C	1:A:74:PHE:HD1	0.41	2.24	2	1
1:A:58:PRO:HG2	2:B:468:TYR:CD2	0.41	2.50	2	1
1:A:111:THR:CB	1:A:112:PRO:HD2	0.41	2.46	4	1
1:A:73:CYS:SG	1:A:88:TYR:HB2	0.41	2.56	5	1
1:A:47:ALA:O	1:A:48:THR:CG2	0.41	2.69	11	2
2:B:459:ILE:O	2:B:462:LEU:HG	0.41	2.16	7	1
1:A:34:ARG:NH2	2:B:450:TRP:CH2	0.41	2.89	9	1
1:A:105:LEU:HA	1:A:117:PHE:CE2	0.41	2.50	9	1
1:A:38:MET:HG2	1:A:88:TYR:CD1	0.41	2.51	11	1
1:A:75:VAL:CG2	1:A:86:ARG:NE	0.41	2.84	12	1
2:B:459:ILE:O	2:B:461:ASP:N	0.41	2.53	17	1
1:A:114:PHE:CZ	1:A:116:THR:HG23	0.41	2.50	19	1
1:A:38:MET:O	1:A:90:LEU:CD1	0.41	2.69	23	1
1:A:127:ASN:ND2	2:B:459:ILE:CG2	0.41	2.84	23	1
1:A:102:TYR:CZ	2:B:473:LYS:HB3	0.41	2.51	24	1
1:A:30:HIS:O	1:A:32:ASN:N	0.41	2.54	7	3
1:A:37:GLU:O	1:A:90:LEU:CD2	0.41	2.69	3	2
1:A:88:TYR:CE1	1:A:95:LEU:HB3	0.41	2.51	5	2
1:A:34:ARG:HB3	1:A:48:THR:CG2	0.41	2.45	17	1
1:A:141:VAL:HG13	1:A:145:ILE:CB	0.41	2.45	19	1
1:A:113:PHE:CZ	1:A:130:ASP:HB3	0.41	2.51	24	1
1:A:127:ASN:OD1	2:B:462:LEU:HB2	0.41	2.16	24	1
1:A:56:ALA:HB2	1:A:64:TRP:CG	0.41	2.51	4	1
1:A:118:ALA:HB1	2:B:468:TYR:CD1	0.41	2.51	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:48:THR:N	1:A:74:PHE:CD2	0.41	2.88	6	1
2:B:459:ILE:HG13	2:B:462:LEU:CD2	0.41	2.46	7	1
1:A:81:LYS:O	2:B:476:PRO:CD	0.41	2.64	8	2
1:A:86:ARG:HD2	1:A:88:TYR:CE1	0.41	2.50	9	1
1:A:86:ARG:HD3	1:A:88:TYR:CZ	0.41	2.51	9	1
1:A:102:TYR:HB2	2:B:473:LYS:HG3	0.41	1.92	9	1
1:A:114:PHE:O	1:A:114:PHE:CD2	0.41	2.74	9	1
1:A:123:GLN:OE1	2:B:468:TYR:CE2	0.41	2.74	11	2
1:A:114:PHE:CD1	2:B:462:LEU:CD1	0.41	2.97	10	1
1:A:146:GLN:OE1	1:A:146:GLN:N	0.41	2.53	12	1
1:A:115:HIS:CE1	1:A:137:PHE:CE1	0.41	3.09	13	1
1:A:26:LEU:O	1:A:30:HIS:CD2	0.41	2.74	15	1
1:A:54:TYR:CZ	1:A:66:LYS:CB	0.41	3.04	15	1
1:A:71:ALA:O	1:A:88:TYR:N	0.41	2.49	18	2
1:A:138:ARG:O	1:A:142:GLN:HB2	0.41	2.16	15	1
1:A:75:VAL:HG21	1:A:86:ARG:CD	0.41	2.46	17	1
1:A:50:VAL:HG12	1:A:71:ALA:CB	0.41	2.46	18	1
1:A:81:LYS:HE2	1:A:103:SER:HB2	0.41	1.93	18	1
1:A:47:ALA:HB3	1:A:74:PHE:HB2	0.41	1.92	19	1
1:A:127:ASN:ND2	2:B:459:ILE:HD12	0.41	2.30	19	1
1:A:131:GLU:O	1:A:132:ASP:C	0.41	2.63	21	1
1:A:52:GLN:CG	2:B:456:PHE:O	0.41	2.69	22	1
1:A:97:TRP:CD1	1:A:98:GLU:H	0.41	2.33	22	1
1:A:51:VAL:CG2	1:A:126:LEU:HB3	0.41	2.46	24	1
1:A:46:LEU:HD11	1:A:140:LEU:HD13	0.41	1.92	2	1
1:A:34:ARG:HD3	1:A:48:THR:HB	0.41	1.93	4	1
1:A:107:TYR:N	1:A:141:VAL:HG11	0.41	2.30	5	1
1:A:87:LEU:CG	1:A:97:TRP:CD1	0.41	3.04	9	3
1:A:106:VAL:O	1:A:117:PHE:CG	0.41	2.73	9	1
1:A:113:PHE:CE2	1:A:130:ASP:HA	0.41	2.51	15	1
1:A:127:ASN:HB2	2:B:456:PHE:O	0.40	2.16	1	1
1:A:114:PHE:CE2	1:A:116:THR:CG2	0.40	3.04	5	1
1:A:38:MET:CE	1:A:86:ARG:CZ	0.40	2.99	10	2
1:A:107:TYR:HB3	1:A:141:VAL:CG2	0.40	2.46	11	1
1:A:30:HIS:O	1:A:34:ARG:HB2	0.40	2.15	14	2
1:A:88:TYR:CD2	1:A:88:TYR:C	0.40	2.98	18	1
1:A:101:LEU:O	2:B:475:TYR:CD1	0.40	2.73	2	1
1:A:109:THR:CB	1:A:128:PHE:CZ	0.40	3.04	3	1
1:A:49:ALA:CB	1:A:137:PHE:CD1	0.40	3.04	11	1
2:B:450:TRP:CE3	2:B:453:ARG:C	0.40	3.00	18	2
1:A:34:ARG:NH1	1:A:49:ALA:N	0.40	2.68	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:49:ALA:CB	1:A:137:PHE:CE1	0.40	3.04	12	1
1:A:107:TYR:HA	1:A:117:PHE:CE1	0.40	2.52	17	1
1:A:47:ALA:CB	1:A:140:LEU:CD2	0.40	2.99	18	1
1:A:53:LEU:HD22	1:A:126:LEU:HD23	0.40	1.91	24	1
1:A:54:TYR:CD1	1:A:64:TRP:HH2	0.40	2.35	24	1
1:A:127:ASN:ND2	2:B:458:PRO:C	0.40	2.79	1	1
1:A:134:ALA:O	1:A:138:ARG:HG2	0.40	2.16	1	2
1:A:114:PHE:CD2	1:A:114:PHE:C	0.40	2.99	5	1
1:A:55:LEU:HD21	1:A:67:GLU:OE2	0.40	2.16	6	1
1:A:113:PHE:CE1	2:B:461:ASP:HB3	0.40	2.52	7	1
1:A:120:ASP:HA	2:B:470:GLN:HG3	0.40	1.91	8	1
1:A:36:PHE:HA	1:A:39:LEU:CD2	0.40	2.46	9	1
1:A:35:LEU:O	1:A:38:MET:HB3	0.40	2.16	10	1
1:A:80:GLN:O	1:A:81:LYS:CB	0.40	2.68	10	1
1:A:97:TRP:CD2	1:A:98:GLU:O	0.40	2.75	10	1
1:A:123:GLN:CD	2:B:468:TYR:CD2	0.40	2.99	16	1
1:A:114:PHE:CB	1:A:127:ASN:ND2	0.40	2.84	20	1
1:A:38:MET:SD	1:A:39:LEU:N	0.40	2.94	22	1
1:A:87:LEU:H	1:A:87:LEU:HD23	0.40	1.76	22	1
1:A:128:PHE:CB	1:A:133:GLU:OE1	0.40	2.69	24	1
1:A:62:GLU:O	1:A:63:HIS:O	0.40	2.40	5	1
1:A:54:TYR:CZ	1:A:126:LEU:CA	0.40	3.04	6	1
1:A:111:THR:CB	1:A:114:PHE:O	0.40	2.70	7	1
1:A:128:PHE:CD2	1:A:128:PHE:O	0.40	2.74	11	1
1:A:109:THR:OG1	1:A:137:PHE:CB	0.40	2.70	12	1
2:B:456:PHE:CD1	2:B:456:PHE:N	0.40	2.89	15	1
1:A:106:VAL:CG2	1:A:117:PHE:CB	0.40	3.00	17	1
1:A:81:LYS:NZ	1:A:103:SER:CB	0.40	2.84	22	1
1:A:38:MET:HE3	1:A:90:LEU:N	0.40	2.32	3	1
1:A:51:VAL:HG22	1:A:72:VAL:HG11	0.40	1.94	3	1
1:A:97:TRP:CZ3	1:A:98:GLU:O	0.40	2.74	5	1
1:A:38:MET:SD	1:A:88:TYR:CZ	0.40	3.14	9	1
1:A:39:LEU:HB3	1:A:86:ARG:NH2	0.40	2.32	12	1
1:A:57:LEU:HG	1:A:123:GLN:CB	0.40	2.46	12	1
1:A:75:VAL:HB	1:A:84:PHE:CD2	0.40	2.51	12	1
1:A:54:TYR:CE1	2:B:459:ILE:HB	0.40	2.52	13	1
1:A:34:ARG:NH1	2:B:445:PRO:CB	0.40	2.85	14	1
1:A:81:LYS:NZ	1:A:103:SER:OG	0.40	2.53	17	1
1:A:128:PHE:CD1	1:A:128:PHE:O	0.40	2.75	18	1
1:A:68:HIS:CE1	1:A:97:TRP:CD1	0.40	3.10	19	1
1:A:100:GLU:HG2	2:B:475:TYR:CE2	0.40	2.51	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:113:PHE:CE2	2:B:461:ASP:HB2	0.40	2.52	19	1
1:A:77:ASP:N	1:A:82:SER:HB2	0.40	2.31	24	1

6.3 Torsion angles

6.3.1 Protein backbone

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	126/141 (89%)	89±3 (71±2%)	29±3 (23±3%)	8±1 (6±1%)	2	19
2	B	38/53 (72%)	29±1 (76±4%)	6±2 (16±4%)	3±1 (9±2%)	1	12
All	All	3936/4656 (85%)	2823 (72%)	848 (22%)	265 (7%)	2	17

All 30 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	B	458	PRO	24
1	A	131	GLU	23
2	B	457	HIS	23
1	A	78	ASN	21
1	A	123	GLN	18
2	B	460	SER	17
1	A	108	SER	16
1	A	113	PHE	16
1	A	42	LYS	11
1	A	41	ARG	10
1	A	104	GLN	9
1	A	119	GLY	9
2	B	464	PRO	8
1	A	40	GLY	8
1	A	63	HIS	8
1	A	80	GLN	6
2	B	447	GLU	5
1	A	49	ALA	5
1	A	58	PRO	4

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Mol	Chain	Res	Type	Models (Total)
1	A	111	THR	4
1	A	110	PRO	4
1	A	90	LEU	3
1	A	81	LYS	3
1	A	105	LEU	3
1	A	97	TRP	2
1	A	117	PHE	1
2	B	467	PRO	1
1	A	106	VAL	1
2	B	445	PRO	1
1	A	109	THR	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	107/120 (89%)	65±5 (61±5%)	42±5 (39±5%)	0	6
2	B	37/50 (74%)	24±2 (66±5%)	12±2 (34±5%)	1	11
All	All	3456/4080 (85%)	2156 (62%)	1300 (38%)	0	7

All 119 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	53	LEU	24
1	A	64	TRP	24
1	A	66	LYS	24
1	A	72	VAL	24
1	A	81	LYS	24
1	A	85	ILE	24
1	A	100	GLU	24
1	A	114	PHE	24
1	A	116	THR	24
1	A	140	LEU	24
1	A	147	LYS	24
2	B	450	TRP	24
2	B	460	SER	24

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Mol	Chain	Res	Type	Models (Total)
1	A	111	THR	23
2	B	465	PRO	23
2	B	462	LEU	22
1	A	62	GLU	21
1	A	28	GLN	20
1	A	144	LYS	20
1	A	51	VAL	20
1	A	101	LEU	20
1	A	94	ARG	19
1	A	138	ARG	19
1	A	137	PHE	18
2	B	478	LYS	18
2	B	477	SER	17
1	A	68	HIS	16
1	A	87	LEU	16
1	A	88	TYR	16
1	A	113	PHE	16
1	A	104	GLN	16
1	A	44	LEU	15
1	A	90	LEU	15
1	A	105	LEU	15
2	B	454	PHE	15
2	B	473	LYS	15
1	A	145	ILE	14
2	B	456	PHE	14
2	B	474	SER	14
1	A	69	CYS	13
1	A	74	PHE	13
1	A	121	ASP	12
1	A	135	GLN	12
2	B	466	GLU	12
1	A	27	LEU	12
2	B	452	SER	12
1	A	38	MET	11
1	A	50	VAL	11
2	B	448	ASP	11
2	B	444	SER	11
1	A	76	LYS	11
1	A	33	GLN	10
1	A	41	ARG	10
1	A	52	GLN	10
1	A	78	ASN	10

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Mol	Chain	Res	Type	Models (Total)
2	B	481	ARG	10
1	A	122	CYS	10
1	A	142	GLN	10
1	A	95	LEU	10
1	A	123	GLN	9
1	A	146	GLN	9
1	A	127	ASN	9
2	B	470	GLN	9
2	B	471	THR	9
1	A	24	SER	9
1	A	55	LEU	9
1	A	97	TRP	9
1	A	131	GLU	9
1	A	80	GLN	9
1	A	46	LEU	8
1	A	57	LEU	8
1	A	99	GLN	8
1	A	103	SER	8
1	A	130	ASP	8
2	B	459	ILE	8
2	B	472	THR	8
1	A	31	GLU	7
1	A	102	TYR	7
1	A	82	SER	7
1	A	132	ASP	7
1	A	42	LYS	7
1	A	96	LEU	7
1	A	98	GLU	6
1	A	75	VAL	6
1	A	91	GLN	6
1	A	133	GLU	6
1	A	149	ASN	6
1	A	35	LEU	5
1	A	120	ASP	5
1	A	148	ARG	5
1	A	77	ASP	5
1	A	34	ARG	5
2	B	475	TYR	5
1	A	48	THR	4
1	A	86	ARG	4
1	A	128	PHE	4
1	A	29	ASP	4

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Mol	Chain	Res	Type	Models (Total)
2	B	447	GLU	4
1	A	67	GLU	4
1	A	115	HIS	3
2	B	453	ARG	3
1	A	107	TYR	3
1	A	117	PHE	3
2	B	461	ASP	3
2	B	455	TYR	3
1	A	63	HIS	2
1	A	109	THR	2
1	A	25	THR	2
1	A	26	LEU	2
1	A	45	THR	2
2	B	449	GLU	2
2	B	469	VAL	1
1	A	126	LEU	1
2	B	468	TYR	1
1	A	32	ASN	1
2	B	451	GLU	1
1	A	39	LEU	1
1	A	106	VAL	1
2	B	457	HIS	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 41% for the well-defined parts and 40% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	1256
Number of shifts mapped to atoms	1256
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

- Can not parse the chemical shift value. All 202 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	20	GLN	HB2	2.02	0.01	.
1	A	20	GLN	HB3	1.87	0.01	.
1	A	21	ASN	HB2	2.86	0.01	.
1	A	21	ASN	HB3	2.86	0.01	.
1	A	23	PRO	HB2	2.10	0.01	.
1	A	23	PRO	HB3	2.10	0.01	.
1	A	24	SER	HB2	3.52	0.01	.
1	A	24	SER	HB3	3.52	0.01	.
1	A	26	LEU	HB2	1.55	0.01	.
1	A	26	LEU	HB3	1.55	0.01	.
1	A	27	LEU	HB2	1.74	0.01	.
1	A	27	LEU	HB3	1.55	0.01	.
1	A	30	HIS	HB2	3.15	0.01	.
1	A	30	HIS	HB3	3.15	0.01	.
1	A	31	GLU	HB2	1.85	0.01	.
1	A	31	GLU	HB3	1.85	0.01	.
1	A	32	ASN	HB2	2.48	0.01	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	32	ASN	HB3	1.83	0.01	.
1	A	33	GLN	HB2	1.95	0.01	.
1	A	33	GLN	HB3	1.95	0.01	.
1	A	34	ARG	HB2	1.90	0.01	.
1	A	34	ARG	HB3	1.90	0.01	.
1	A	40	GLY	HA2	3.75	0.01	.
1	A	40	GLY	HA3	3.75	0.01	.
1	A	41	ARG	HB2	1.80	0.01	.
1	A	41	ARG	HB3	1.80	0.01	.
1	A	42	LYS	HB2	2.12	0.01	.
1	A	42	LYS	HB3	1.88	0.01	.
1	A	44	LEU	HB2	1.36	0.01	.
1	A	44	LEU	HB3	1.36	0.01	.
1	A	46	LEU	HB2	1.84	0.01	.
1	A	46	LEU	HB3	1.84	0.01	.
1	A	54	TYR	HB2	1.90	0.01	.
1	A	54	TYR	HB3	1.90	0.01	.
1	A	55	LEU	HB2	1.66	0.01	.
1	A	55	LEU	HB3	1.66	0.01	.
1	A	60	GLY	HA2	4.50	0.01	.
1	A	60	GLY	HA3	3.87	0.01	.
1	A	62	GLU	HB2	1.82	0.01	.
1	A	62	GLU	HB3	1.82	0.01	.
1	A	63	HIS	HB2	3.05	0.01	.
1	A	63	HIS	HB3	3.05	0.01	.
1	A	64	TRP	HB2	3.37	0.01	.
1	A	64	TRP	HB3	2.93	0.01	.
1	A	68	HIS	HB2	2.16	0.01	.
1	A	68	HIS	HB3	2.16	0.01	.
1	A	69	CYS	HB2	2.83	0.01	.
1	A	69	CYS	HB3	2.83	0.01	.
1	A	70	GLY	HA2	4.52	0.01	.
1	A	70	GLY	HA3	2.96	0.01	.
1	A	73	CYS	HB2	3.40	0.01	.
1	A	73	CYS	HB3	2.81	0.01	.
1	A	74	PHE	HB2	3.00	0.01	.
1	A	74	PHE	HB3	2.44	0.01	.
1	A	76	LYS	HB2	2.03	0.01	.
1	A	76	LYS	HB3	1.53	0.01	.
1	A	77	ASP	HB2	2.10	0.01	.
1	A	77	ASP	HB3	2.10	0.01	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	79	PRO	HB2	2.33	0.01	.
1	A	79	PRO	HB3	1.86	0.01	.
1	A	81	LYS	HB2	1.90	0.01	.
1	A	81	LYS	HB3	1.75	0.01	.
1	A	82	SER	HB2	3.54	0.01	.
1	A	82	SER	HB3	3.54	0.01	.
1	A	83	TYR	HB2	2.58	0.01	.
1	A	83	TYR	HB3	2.42	0.01	.
1	A	84	PHE	HB2	2.65	0.01	.
1	A	84	PHE	HB3	2.51	0.01	.
1	A	86	ARG	HB2	1.63	0.01	.
1	A	86	ARG	HB3	1.63	0.01	.
1	A	87	LEU	HB2	2.20	0.01	.
1	A	87	LEU	HB3	2.20	0.01	.
1	A	88	TYR	HB2	2.74	0.01	.
1	A	88	TYR	HB3	2.74	0.01	.
1	A	89	GLY	HA2	4.00	0.01	.
1	A	89	GLY	HA3	3.51	0.01	.
1	A	91	GLN	HB2	2.66	0.01	.
1	A	91	GLN	HB3	2.05	0.01	.
1	A	94	ARG	HB2	1.85	0.01	.
1	A	94	ARG	HB3	1.61	0.01	.
1	A	96	LEU	HB2	1.05	0.01	.
1	A	96	LEU	HB3	0.20	0.01	.
1	A	97	TRP	HB2	3.28	0.01	.
1	A	97	TRP	HB3	2.64	0.01	.
1	A	101	LEU	HB2	2.00	0.01	.
1	A	101	LEU	HB3	1.16	0.01	.
1	A	107	TYR	HB2	3.00	0.01	.
1	A	107	TYR	HB3	2.21	0.01	.
1	A	108	SER	HB2	3.84	0.01	.
1	A	108	SER	HB3	3.84	0.01	.
1	A	110	PRO	HB2	2.50	0.01	.
1	A	110	PRO	HB3	2.04	0.01	.
1	A	112	PRO	HB2	2.50	0.01	.
1	A	112	PRO	HB3	1.92	0.01	.
1	A	113	PHE	HB2	4.10	0.01	.
1	A	113	PHE	HB3	2.84	0.01	.
1	A	114	PHE	HB2	2.62	0.01	.
1	A	114	PHE	HB3	2.62	0.01	.
1	A	115	HIS	HB2	3.18	0.01	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	115	HIS	HB3	2.97	0.01	.
1	A	117	PHE	HB2	3.00	0.01	.
1	A	117	PHE	HB3	3.00	0.01	.
1	A	119	GLY	HA2	4.92	0.01	.
1	A	119	GLY	HA3	4.59	0.01	.
1	A	120	ASP	HB2	2.79	0.01	.
1	A	120	ASP	HB3	2.79	0.01	.
1	A	121	ASP	HB2	2.63	0.01	.
1	A	121	ASP	HB3	2.63	0.01	.
1	A	125	GLY	HA2	4.45	0.01	.
1	A	125	GLY	HA3	2.33	0.01	.
1	A	126	LEU	HB2	1.72	0.01	.
1	A	126	LEU	HB3	1.72	0.01	.
1	A	127	ASN	HB2	2.56	0.01	.
1	A	127	ASN	HB3	2.56	0.01	.
1	A	130	ASP	HB2	2.81	0.01	.
1	A	130	ASP	HB3	2.54	0.01	.
1	A	132	ASP	HB2	3.16	0.01	.
1	A	132	ASP	HB3	2.74	0.01	.
1	A	133	GLU	HB2	1.80	0.01	.
1	A	133	GLU	HB3	1.80	0.01	.
1	A	135	GLN	HB2	2.30	0.01	.
1	A	135	GLN	HB3	2.30	0.01	.
1	A	140	LEU	HB2	1.50	0.01	.
1	A	140	LEU	HB3	1.05	0.01	.
1	A	142	GLN	HB2	2.06	0.01	.
1	A	142	GLN	HB3	2.06	0.01	.
1	A	146	GLN	HB2	2.17	0.01	.
1	A	146	GLN	HB3	2.17	0.01	.
1	A	147	LYS	HB2	1.89	0.01	.
1	A	147	LYS	HB3	1.89	0.01	.
1	A	148	ARG	HB2	1.96	0.01	.
1	A	148	ARG	HB3	1.96	0.01	.
1	A	149	ASN	HB2	2.88	0.01	.
1	A	149	ASN	HB3	2.57	0.01	.
1	A	153	SER	HB2	3.90	0.01	.
1	A	153	SER	HB3	3.90	0.01	.
1	A	154	GLY	HA2	4.00	0.01	.
1	A	154	GLY	HA3	4.00	0.01	.
1	A	155	ASP	HB2	2.70	0.01	.
1	A	155	ASP	HB3	2.70	0.01	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	156	ARG	HB2	1.86	0.01	.
1	A	156	ARG	HB3	1.86	0.01	.
1	B	442	GLN	HB2	2.11	0.01	.
1	B	442	GLN	HB3	1.97	0.01	.
1	B	443	ASP	HB2	2.67	0.01	.
1	B	443	ASP	HB3	2.67	0.01	.
1	B	445	PRO	HB2	2.30	0.01	.
1	B	445	PRO	HB3	1.96	0.01	.
1	B	446	CYS	HB2	3.00	0.01	.
1	B	446	CYS	HB3	3.00	0.01	.
1	B	448	ASP	HB2	2.73	0.01	.
1	B	448	ASP	HB3	2.73	0.01	.
1	B	449	GLU	HB2	2.16	0.01	.
1	B	449	GLU	HB3	2.16	0.01	.
1	B	450	TRP	HB2	3.63	0.01	.
1	B	450	TRP	HB3	3.63	0.01	.
1	B	451	GLU	HB2	2.30	0.01	.
1	B	451	GLU	HB3	2.30	0.01	.
1	B	452	SER	HB2	4.00	0.01	.
1	B	452	SER	HB3	4.00	0.01	.
1	B	453	ARG	HB2	0.89	0.01	.
1	B	453	ARG	HB3	0.89	0.01	.
1	B	455	TYR	HB2	2.75	0.01	.
1	B	455	TYR	HB3	2.75	0.01	.
1	B	458	PRO	HB2	2.31	0.01	.
1	B	458	PRO	HB3	2.24	0.01	.
1	B	460	SER	HB2	4.08	0.01	.
1	B	460	SER	HB3	3.86	0.01	.
1	B	461	ASP	HB2	3.00	0.01	.
1	B	461	ASP	HB3	2.84	0.01	.
1	B	465	PRO	HB2	2.16	0.01	.
1	B	465	PRO	HB3	2.16	0.01	.
1	B	467	PRO	HB2	2.27	0.01	.
1	B	467	PRO	HB3	1.73	0.01	.
1	B	468	TYR	HB2	2.96	0.01	.
1	B	468	TYR	HB3	2.75	0.01	.
1	B	470	GLN	HB2	2.03	0.01	.
1	B	470	GLN	HB3	2.03	0.01	.
1	B	474	SER	HB2	3.86	0.01	.
1	B	474	SER	HB3	3.86	0.01	.
1	B	476	PRO	HB2	2.20	0.01	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	476	PRO	HB3	2.20	0.01	.
1	B	478	LYS	HB2	2.08	0.01	.
1	B	478	LYS	HB3	2.08	0.01	.
1	B	479	LEU	HB2	1.74	0.01	.
1	B	479	LEU	HB3	1.74	0.01	.
1	B	481	ARG	HB2	1.35	0.01	.
1	B	481	ARG	HB3	1.35	0.01	.
1	B	482	ASN	HB2	2.88	0.01	.
1	B	482	ASN	HB3	2.21	0.01	.
1	B	483	GLU	HB2	2.04	0.01	.
1	B	483	GLU	HB3	2.04	0.01	.
1	B	486	SER	HB2	3.91	0.01	.
1	B	486	SER	HB3	3.91	0.01	.
1	B	487	GLY	HA2	4.04	0.01	.
1	B	487	GLY	HA3	4.04	0.01	.
1	B	489	ASN	HB2	2.14	0.01	.
1	B	489	ASN	HB3	2.14	0.01	.
1	B	490	ARG	HB2	1.82	0.01	.
1	B	490	ARG	HB3	1.82	0.01	.
1	B	491	ARG	HB2	1.84	0.01	.
1	B	491	ARG	HB3	1.84	0.01	.

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	185	-0.04 ± 0.13	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	174	0.06 ± 0.17	None needed (< 0.5 ppm)
$^{13}\text{C}'$	167	0.31 ± 0.10	None needed (< 0.5 ppm)
^{15}N	167	-0.11 ± 0.29	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 41%, i.e. 929 atoms were assigned a chemical shift out of a possible 2270. 0 out of 26 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	728/803 (91%)	275/323 (85%)	307/328 (94%)	146/152 (96%)

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	Total	¹ H	¹³ C	¹⁵ N
Sidechain	201/1219 (16%)	50/789 (6%)	151/382 (40%)	0/48 (0%)
Aromatic	0/248 (0%)	0/120 (0%)	0/115 (0%)	0/13 (0%)
Overall	929/2270 (41%)	325/1232 (26%)	458/825 (56%)	146/213 (69%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 40%, i.e. 1054 atoms were assigned a chemical shift out of a possible 2663. 0 out of 26 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	830/955 (87%)	311/386 (81%)	352/388 (91%)	167/181 (92%)
Sidechain	224/1460 (15%)	50/936 (5%)	174/450 (39%)	0/74 (0%)
Aromatic	0/248 (0%)	0/120 (0%)	0/115 (0%)	0/13 (0%)
Overall	1054/2663 (40%)	361/1442 (25%)	526/953 (55%)	167/268 (62%)

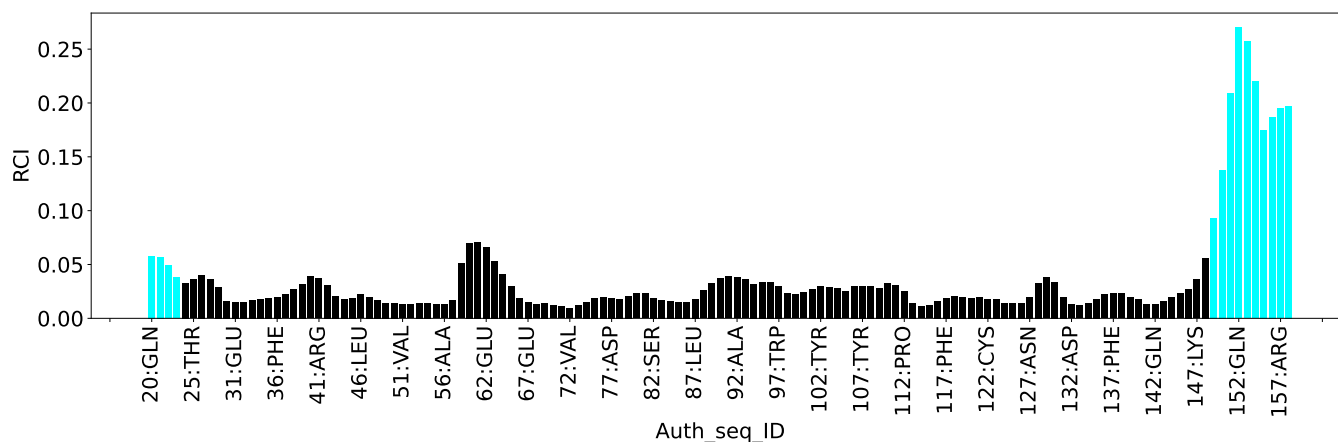
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

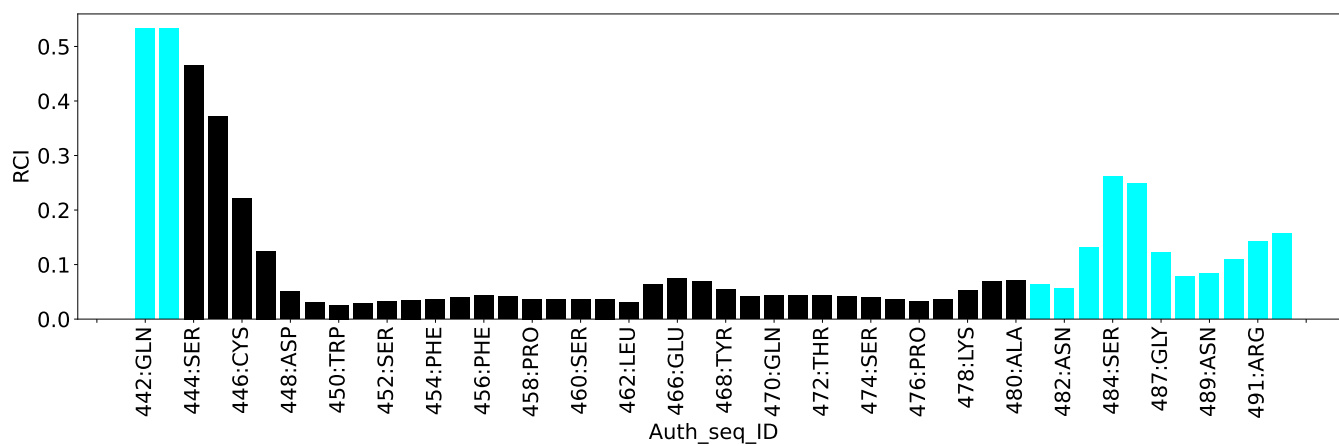
7.1.5 Random Coil Index (RCI) plots [i](#)

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:



Random coil index (RCI) for chain B:



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	1151
Intra-residue ($ i-j =0$)	4
Sequential ($ i-j =1$)	494
Medium range ($ i-j >1$ and $ i-j <5$)	192
Long range ($ i-j \geq 5$)	266
Inter-chain	63
Hydrogen bond restraints	132
Disulfide bond restraints	0
Total dihedral-angle restraints	308
Number of unmapped restraints	0
Number of restraints per residue	7.5
Number of long range restraints per residue ¹	1.7

¹Long range hydrogen bonds and disulfide bonds are counted as long range restraints while calculating the number of long range restraints per residue

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	56.5	0.2
0.2-0.5 (Medium)	30.7	0.49
>0.5 (Large)	0.4	0.83

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)	43.2	8.07
10.0-20.0 (Medium)	0.2	15.94
>20.0 (Large)	1.5	95.73

9 Distance violation analysis ⓘ

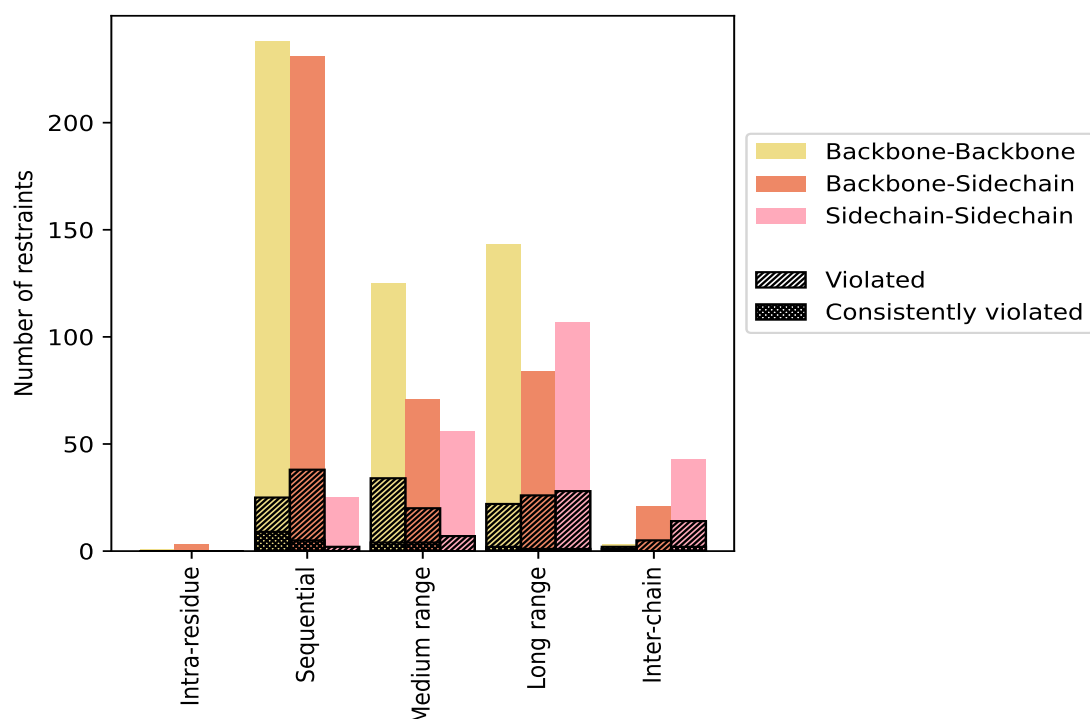
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($ i-j =0$)	4	0.3	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	1	0.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	3	0.3	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sequential ($ i-j =1$)	494	42.9	65	13.2	5.6	14	2.8	1.2
Backbone-Backbone	238	20.7	25	10.5	2.2	9	3.8	0.8
Backbone-Sidechain	231	20.1	38	16.5	3.3	5	2.2	0.4
Sidechain-Sidechain	25	2.2	2	8.0	0.2	0	0.0	0.0
Medium range ($ i-j >1$ & $ i-j <5$)	192	16.7	47	24.5	4.1	7	3.6	0.6
Backbone-Backbone	65	5.6	20	30.8	1.7	3	4.6	0.3
Backbone-Sidechain	71	6.2	20	28.2	1.7	4	5.6	0.3
Sidechain-Sidechain	56	4.9	7	12.5	0.6	0	0.0	0.0
Long range ($ i-j \geq 5$)	266	23.1	64	24.1	5.6	4	1.5	0.3
Backbone-Backbone	75	6.5	10	13.3	0.9	2	2.7	0.2
Backbone-Sidechain	84	7.3	26	31.0	2.3	1	1.2	0.1
Sidechain-Sidechain	107	9.3	28	26.2	2.4	1	0.9	0.1
Inter-chain	63	5.5	21	33.3	1.8	3	4.8	0.3
Backbone-Backbone	3	0.3	2	66.7	0.2	1	33.3	0.1
Backbone-Sidechain	21	1.8	5	23.8	0.4	0	0.0	0.0
Sidechain-Sidechain	39	3.4	14	35.9	1.2	2	5.1	0.2
Hydrogen bond	132	11.5	26	19.7	2.3	1	0.8	0.1
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1151	100.0	223	19.4	19.4	29	2.5	2.5
Backbone-Backbone	510	44.3	83	16.3	7.2	16	3.1	1.4
Backbone-Sidechain	410	35.6	89	21.7	7.7	10	2.4	0.9
Sidechain-Sidechain	231	20.1	51	22.1	4.4	3	1.3	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 [i](#)



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

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	0	37	21	33	8	99	0.19	0.45	0.09	0.16
2	0	36	22	35	9	102	0.2	0.77	0.11	0.16
3	0	28	18	37	6	89	0.19	0.44	0.09	0.16
4	0	30	21	38	6	95	0.19	0.45	0.09	0.16
5	0	30	20	36	9	95	0.21	0.79	0.11	0.18
6	0	33	27	36	7	103	0.19	0.46	0.09	0.16
7	0	31	20	26	7	84	0.2	0.44	0.09	0.16
8	0	32	18	31	5	86	0.2	0.49	0.1	0.16
9	0	31	24	34	9	98	0.19	0.44	0.09	0.16
10	0	31	16	31	13	91	0.2	0.46	0.09	0.17

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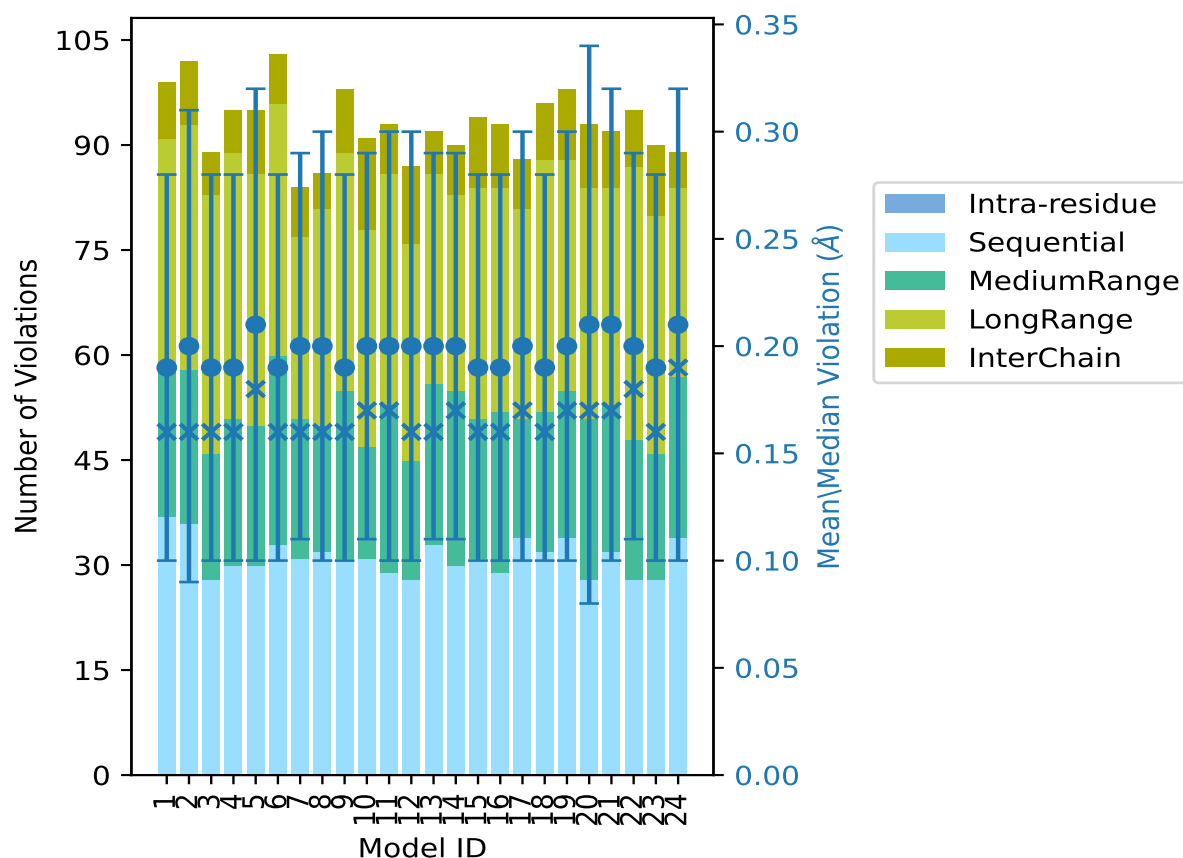
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	0	29	24	33	7	93	0.2	0.68	0.1	0.17
12	0	28	17	31	11	87	0.2	0.45	0.1	0.16
13	0	33	23	30	6	92	0.2	0.47	0.09	0.16
14	0	30	25	28	7	90	0.2	0.46	0.09	0.17
15	0	31	20	33	10	94	0.19	0.49	0.09	0.16
16	0	29	23	32	9	93	0.19	0.52	0.09	0.16
17	0	34	17	30	7	88	0.2	0.64	0.1	0.17
18	0	32	20	36	8	96	0.19	0.45	0.09	0.16
19	0	34	21	33	10	98	0.2	0.47	0.1	0.17
20	0	28	23	33	9	93	0.21	0.83	0.13	0.17
21	0	32	21	31	8	92	0.21	0.7	0.11	0.17
22	0	28	20	39	8	95	0.2	0.45	0.09	0.18
23	0	28	18	34	10	90	0.19	0.46	0.09	0.16
24	0	34	23	27	5	89	0.21	0.83	0.11	0.19

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

⁵Inter-chain restraints, ⁶Standard deviation

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



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

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

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 822(IR:4, SQ:429, MR:145, LR:202, IC:42) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	8	11	4	3	26	1	4.2
0	7	0	9	2	18	2	8.3
0	6	4	3	0	13	3	12.5
0	2	3	5	3	13	4	16.7
0	4	5	5	1	15	5	20.8
0	0	2	3	1	6	6	25.0

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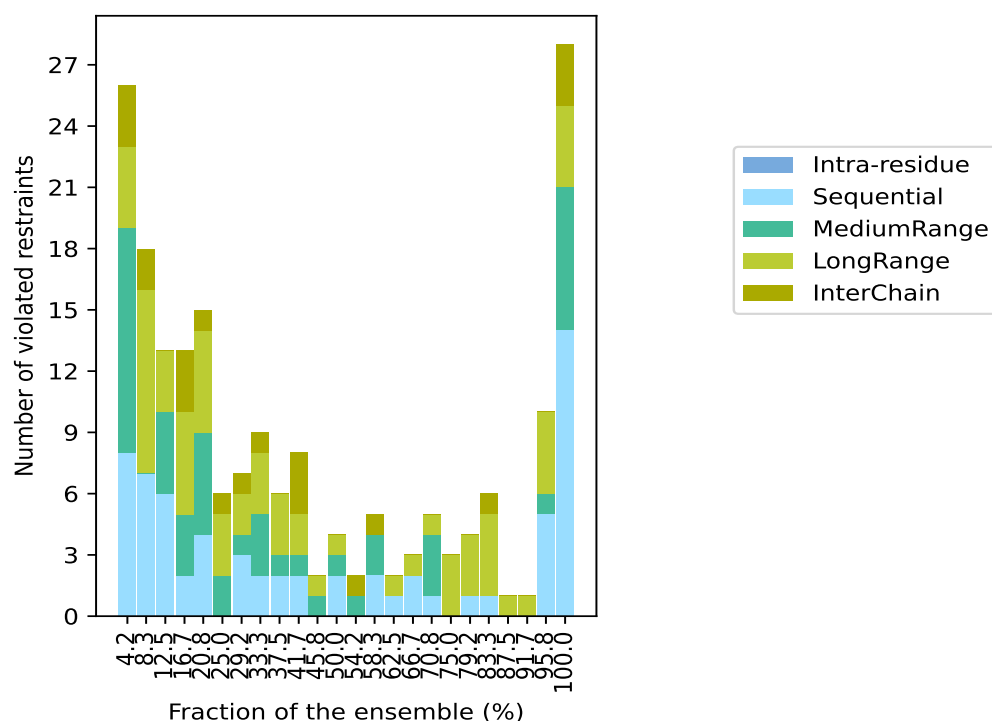
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	3	1	2	1	7	7	29.2
0	2	3	3	1	9	8	33.3
0	2	1	3	0	6	9	37.5
0	2	1	2	3	8	10	41.7
0	0	1	1	0	2	11	45.8
0	2	1	1	0	4	12	50.0
0	0	1	0	1	2	13	54.2
0	2	2	0	1	5	14	58.3
0	1	0	1	0	2	15	62.5
0	2	0	1	0	3	16	66.7
0	1	3	1	0	5	17	70.8
0	0	0	3	0	3	18	75.0
0	1	0	3	0	4	19	79.2
0	1	0	4	1	6	20	83.3
0	0	0	1	0	1	21	87.5
0	0	0	1	0	1	22	91.7
0	5	1	4	0	10	23	95.8
0	14	7	4	3	28	24	100.0

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

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

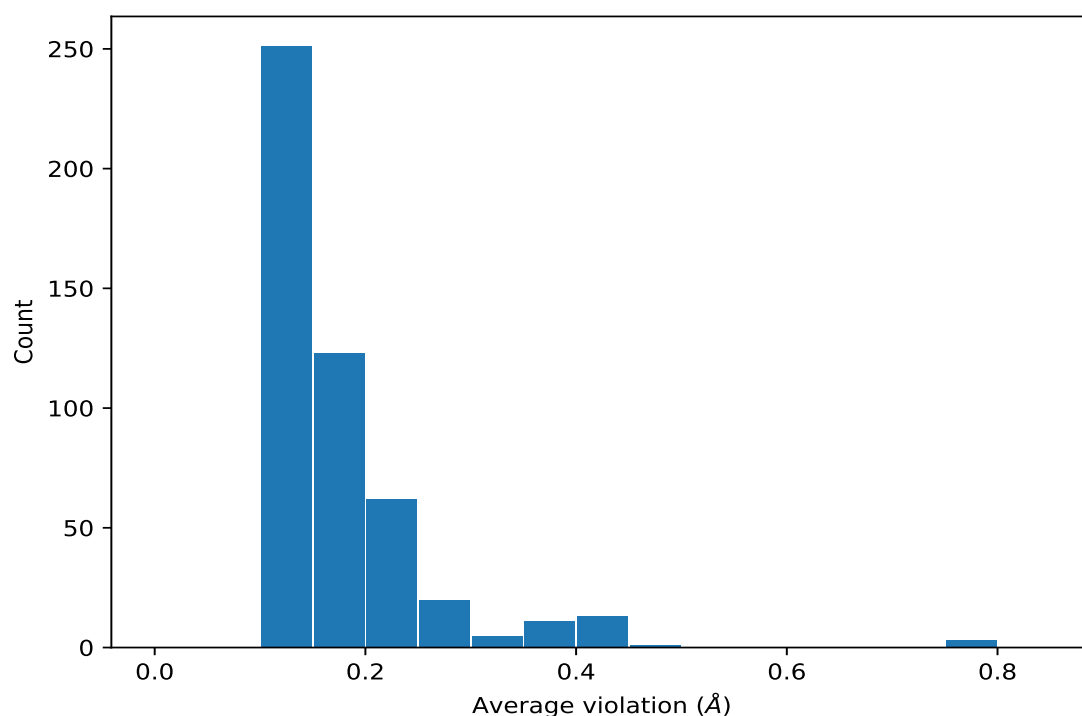
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,553)	2:450:B:TRP:H	2:449:B:GLU:HA	24	0.45	0.01	0.45
(1,787)	1:83:A:TYR:HA	1:85:A:ILE:HB	24	0.43	0.03	0.43
(1,582)	2:466:B:GLU:H	2:465:B:PRO:HG2	24	0.42	0.01	0.42
(1,582)	2:466:B:GLU:H	2:465:B:PRO:HG3	24	0.42	0.01	0.42
(1,551)	2:449:B:GLU:H	2:448:B:ASP:HA	24	0.4	0.01	0.4
(1,612)	2:479:B:LEU:H	2:475:B:TYR:HA	24	0.38	0.04	0.4
(1,396)	1:57:A:LEU:H	1:65:A:THR:HG23	24	0.38	0.02	0.37
(1,396)	1:57:A:LEU:H	1:65:A:THR:HG21	24	0.38	0.02	0.37
(1,396)	1:57:A:LEU:H	1:65:A:THR:HG22	24	0.38	0.02	0.37
(1,101)	1:62:A:GLU:H	1:61:A:ALA:HA	24	0.35	0.01	0.35
(1,75)	1:51:A:VAL:H	1:50:A:VAL:H	24	0.32	0.03	0.33
(1,191)	1:95:A:LEU:H	1:94:A:ARG:H	24	0.32	0.04	0.33
(1,167)	1:86:A:ARG:H	1:85:A:ILE:HB	24	0.32	0.02	0.32
(1,615)	2:480:B:ALA:H	2:479:B:LEU:HG	24	0.31	0.04	0.3
(1,822)	1:94:A:ARG:HA	1:90:A:LEU:HA	24	0.3	0.04	0.3
(1,465)	1:52:A:GLN:H	1:51:A:VAL:H	24	0.29	0.04	0.29

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,969)	1:71:A:ALA:HB1	2:453:B:ARG:HB2	24	0.27	0.03	0.27
(1,969)	1:71:A:ALA:HB1	2:453:B:ARG:HB3	24	0.27	0.03	0.27
(1,969)	1:71:A:ALA:HB2	2:453:B:ARG:HB2	24	0.27	0.03	0.27
(1,969)	1:71:A:ALA:HB2	2:453:B:ARG:HB3	24	0.27	0.03	0.27
(1,969)	1:71:A:ALA:HB3	2:453:B:ARG:HB2	24	0.27	0.03	0.27
(1,969)	1:71:A:ALA:HB3	2:453:B:ARG:HB3	24	0.27	0.03	0.27
(1,845)	1:108:A:SER:HB2	1:110:A:PRO:HA	24	0.26	0.05	0.26
(1,845)	1:108:A:SER:HB3	1:110:A:PRO:HA	24	0.26	0.05	0.26
(1,992)	1:129:A:ALA:H	2:457:B:HIS:H	24	0.26	0.05	0.26
(1,522)	1:116:A:THR:H	1:125:A:GLY:HA2	24	0.24	0.04	0.24
(1,522)	1:116:A:THR:H	1:125:A:GLY:HA3	24	0.24	0.04	0.24
(1,328)	1:143:A:GLU:H	1:139:A:ALA:HB1	24	0.23	0.04	0.23
(1,328)	1:143:A:GLU:H	1:139:A:ALA:HB2	24	0.23	0.04	0.23
(1,328)	1:143:A:GLU:H	1:139:A:ALA:HB3	24	0.23	0.04	0.23
(1,944)	2:458:B:PRO:HA	2:460:B:SER:HB2	24	0.22	0.07	0.2
(1,944)	2:458:B:PRO:HA	2:460:B:SER:HB3	24	0.22	0.07	0.2
(1,403)	1:74:A:PHE:H	1:47:A:ALA:HA	24	0.21	0.03	0.21
(1,635)	1:33:A:GLN:HA	1:30:A:HIS:HA	24	0.21	0.02	0.21
(1,877)	1:127:A:ASN:HB2	1:113:A:PHE:HB2	24	0.21	0.04	0.2
(1,877)	1:127:A:ASN:HB2	1:113:A:PHE:HB3	24	0.21	0.04	0.2
(1,877)	1:127:A:ASN:HB3	1:113:A:PHE:HB2	24	0.21	0.04	0.2
(1,877)	1:127:A:ASN:HB3	1:113:A:PHE:HB3	24	0.21	0.04	0.2
(1,584)	2:468:B:TYR:H	2:467:B:PRO:HG2	24	0.2	0.03	0.2
(1,584)	2:468:B:TYR:H	2:467:B:PRO:HG3	24	0.2	0.03	0.2
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD11	24	0.2	0.06	0.18
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD12	24	0.2	0.06	0.18
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD13	24	0.2	0.06	0.18
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD21	24	0.2	0.06	0.18
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD22	24	0.2	0.06	0.18
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD23	24	0.2	0.06	0.18
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD11	24	0.2	0.06	0.18
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD12	24	0.2	0.06	0.18
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD13	24	0.2	0.06	0.18
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD21	24	0.2	0.06	0.18
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD22	24	0.2	0.06	0.18
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD23	24	0.2	0.06	0.18
(1,105)	1:63:A:HIS:H	1:62:A:GLU:HA	24	0.18	0.03	0.19
(1,616)	2:480:B:ALA:H	2:479:B:LEU:HA	24	0.18	0.01	0.18
(4,92)	1:136:A:ALA:N	1:132:A:ASP:O	24	0.18	0.02	0.18
(1,556)	2:451:B:GLU:H	2:450:B:TRP:HB2	24	0.17	0.02	0.16
(1,559)	2:452:B:SER:H	2:451:B:GLU:HA	24	0.16	0.01	0.16
(1,241)	1:109:A:THR:H	1:108:A:SER:H	23	0.24	0.03	0.23

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,705)	1:53:A:LEU:HD11	1:127:A:ASN:HB2	23	0.23	0.04	0.23
(1,705)	1:53:A:LEU:HD11	1:127:A:ASN:HB3	23	0.23	0.04	0.23
(1,705)	1:53:A:LEU:HD12	1:127:A:ASN:HB2	23	0.23	0.04	0.23
(1,705)	1:53:A:LEU:HD12	1:127:A:ASN:HB3	23	0.23	0.04	0.23
(1,705)	1:53:A:LEU:HD13	1:127:A:ASN:HB2	23	0.23	0.04	0.23
(1,705)	1:53:A:LEU:HD13	1:127:A:ASN:HB3	23	0.23	0.04	0.23
(1,705)	1:53:A:LEU:HD21	1:127:A:ASN:HB2	23	0.23	0.04	0.23
(1,705)	1:53:A:LEU:HD21	1:127:A:ASN:HB3	23	0.23	0.04	0.23
(1,705)	1:53:A:LEU:HD22	1:127:A:ASN:HB2	23	0.23	0.04	0.23
(1,705)	1:53:A:LEU:HD22	1:127:A:ASN:HB3	23	0.23	0.04	0.23
(1,705)	1:53:A:LEU:HD23	1:127:A:ASN:HB2	23	0.23	0.04	0.23
(1,705)	1:53:A:LEU:HD23	1:127:A:ASN:HB3	23	0.23	0.04	0.23
(1,272)	1:124:A:ALA:H	1:123:A:GLN:HG2	23	0.18	0.03	0.18
(1,272)	1:124:A:ALA:H	1:123:A:GLN:HG3	23	0.18	0.03	0.18
(1,732)	1:65:A:THR:HB	1:56:A:ALA:HB1	23	0.17	0.02	0.17
(1,732)	1:65:A:THR:HB	1:56:A:ALA:HB2	23	0.17	0.02	0.17
(1,732)	1:65:A:THR:HB	1:56:A:ALA:HB3	23	0.17	0.02	0.17
(1,783)	1:81:A:LYS:HG2	1:80:A:GLN:HA	23	0.17	0.04	0.17
(1,783)	1:81:A:LYS:HG3	1:80:A:GLN:HA	23	0.17	0.04	0.17
(1,366)	1:35:A:LEU:H	1:32:A:ASN:HA	23	0.16	0.03	0.15
(1,477)	1:72:A:VAL:H	1:48:A:THR:HA	23	0.16	0.03	0.16
(1,268)	1:122:A:CYS:H	1:121:A:ASP:HA	23	0.15	0.01	0.15
(1,469)	1:55:A:LEU:H	1:65:A:THR:H	23	0.14	0.03	0.13
(1,336)	1:145:A:ILE:H	1:144:A:LYS:HA	23	0.12	0.01	0.12
(1,399)	1:72:A:VAL:H	1:50:A:VAL:HB	22	0.22	0.1	0.22
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD11	21	0.22	0.04	0.22
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD12	21	0.22	0.04	0.22
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD13	21	0.22	0.04	0.22
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD21	21	0.22	0.04	0.22
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD22	21	0.22	0.04	0.22
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD23	21	0.22	0.04	0.22
(1,638)	1:34:A:ARG:HB2	1:74:A:PHE:HD1	20	0.22	0.08	0.23
(1,638)	1:34:A:ARG:HB2	1:74:A:PHE:HD2	20	0.22	0.08	0.23
(1,638)	1:34:A:ARG:HB3	1:74:A:PHE:HD1	20	0.22	0.08	0.23
(1,638)	1:34:A:ARG:HB3	1:74:A:PHE:HD2	20	0.22	0.08	0.23
(1,259)	1:118:A:ALA:H	1:117:A:PHE:HB3	20	0.21	0.05	0.2
(1,846)	1:108:A:SER:HB2	1:137:A:PHE:HB2	20	0.19	0.06	0.19
(1,846)	1:108:A:SER:HB2	1:137:A:PHE:HB3	20	0.19	0.06	0.19
(1,846)	1:108:A:SER:HB3	1:137:A:PHE:HB2	20	0.19	0.06	0.19
(1,846)	1:108:A:SER:HB3	1:137:A:PHE:HB3	20	0.19	0.06	0.19
(1,741)	1:71:A:ALA:HB1	1:35:A:LEU:HB2	20	0.18	0.04	0.17
(1,741)	1:71:A:ALA:HB1	1:35:A:LEU:HB3	20	0.18	0.04	0.17

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,741)	1:71:A:ALA:HB2	1:35:A:LEU:HB2	20	0.18	0.04	0.17
(1,741)	1:71:A:ALA:HB2	1:35:A:LEU:HB3	20	0.18	0.04	0.17
(1,741)	1:71:A:ALA:HB3	1:35:A:LEU:HB2	20	0.18	0.04	0.17
(1,741)	1:71:A:ALA:HB3	1:35:A:LEU:HB3	20	0.18	0.04	0.17
(1,1016)	2:479:B:LEU:HG	1:83:A:TYR:HD1	20	0.15	0.03	0.15
(1,1016)	2:479:B:LEU:HG	1:83:A:TYR:HD2	20	0.15	0.03	0.15
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG11	20	0.14	0.02	0.14
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG12	20	0.14	0.02	0.14
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG13	20	0.14	0.02	0.14
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG21	20	0.14	0.02	0.14
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG22	20	0.14	0.02	0.14
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG23	20	0.14	0.02	0.14
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG11	20	0.14	0.02	0.14
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG12	20	0.14	0.02	0.14
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG13	20	0.14	0.02	0.14
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG21	20	0.14	0.02	0.14
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG22	20	0.14	0.02	0.14
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG23	20	0.14	0.02	0.14
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG11	20	0.14	0.02	0.14
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG12	20	0.14	0.02	0.14
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG13	20	0.14	0.02	0.14
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG21	20	0.14	0.02	0.14
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG22	20	0.14	0.02	0.14
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG23	20	0.14	0.02	0.14
(4,23)	1:68:A:HIS:H	1:53:A:LEU:O	20	0.13	0.02	0.14
(1,925)	1:145:A:ILE:HD11	1:117:A:PHE:HB3	19	0.27	0.04	0.28
(1,925)	1:145:A:ILE:HD12	1:117:A:PHE:HB3	19	0.27	0.04	0.28
(1,925)	1:145:A:ILE:HD13	1:117:A:PHE:HB3	19	0.27	0.04	0.28
(1,523)	1:116:A:THR:H	1:108:A:SER:HB2	19	0.16	0.04	0.17
(1,523)	1:116:A:THR:H	1:108:A:SER:HB3	19	0.16	0.04	0.17
(4,41)	1:71:A:ALA:H	1:88:A:TYR:O	19	0.16	0.03	0.16
(1,250)	1:116:A:THR:H	1:115:A:HIS:HB3	19	0.15	0.02	0.15
(1,669)	1:47:A:ALA:HB1	1:137:A:PHE:HA	19	0.15	0.03	0.14
(1,669)	1:47:A:ALA:HB2	1:137:A:PHE:HA	19	0.15	0.03	0.14
(1,669)	1:47:A:ALA:HB3	1:137:A:PHE:HA	19	0.15	0.03	0.14
(1,847)	1:109:A:THR:HB	1:115:A:HIS:HB2	18	0.19	0.05	0.18
(1,847)	1:109:A:THR:HB	1:115:A:HIS:HB3	18	0.19	0.05	0.18
(1,412)	1:84:A:PHE:H	1:76:A:LYS:HB2	18	0.18	0.05	0.18
(1,412)	1:84:A:PHE:H	1:76:A:LYS:HB3	18	0.18	0.05	0.18
(1,851)	1:110:A:PRO:HA	1:131:A:GLU:HB2	18	0.14	0.02	0.15
(1,851)	1:110:A:PRO:HA	1:131:A:GLU:HB3	18	0.14	0.02	0.15
(4,9)	1:74:A:PHE:H	1:47:A:ALA:O	18	0.12	0.01	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,598)	2:473:B:LYS:H	2:472:B:THR:HG22	17	0.29	0.12	0.32
(1,598)	2:473:B:LYS:H	2:472:B:THR:HG21	17	0.29	0.12	0.32
(1,598)	2:473:B:LYS:H	2:472:B:THR:HG23	17	0.29	0.12	0.32
(1,863)	1:120:A:ASP:HA	1:123:A:GLN:HG2	17	0.16	0.03	0.15
(1,863)	1:120:A:ASP:HA	1:123:A:GLN:HG3	17	0.16	0.03	0.15
(1,912)	1:141:A:VAL:HG11	1:107:A:TYR:HB3	17	0.15	0.03	0.15
(1,912)	1:141:A:VAL:HG12	1:107:A:TYR:HB3	17	0.15	0.03	0.15
(1,912)	1:141:A:VAL:HG13	1:107:A:TYR:HB3	17	0.15	0.03	0.15
(1,912)	1:141:A:VAL:HG21	1:107:A:TYR:HB3	17	0.15	0.03	0.15
(1,912)	1:141:A:VAL:HG22	1:107:A:TYR:HB3	17	0.15	0.03	0.15
(1,912)	1:141:A:VAL:HG23	1:107:A:TYR:HB3	17	0.15	0.03	0.15
(1,912)	1:141:A:VAL:HG11	1:107:A:TYR:HB2	17	0.15	0.03	0.15
(1,912)	1:141:A:VAL:HG12	1:107:A:TYR:HB2	17	0.15	0.03	0.15
(1,912)	1:141:A:VAL:HG13	1:107:A:TYR:HB2	17	0.15	0.03	0.15
(1,912)	1:141:A:VAL:HG21	1:107:A:TYR:HB2	17	0.15	0.03	0.15
(1,912)	1:141:A:VAL:HG22	1:107:A:TYR:HB2	17	0.15	0.03	0.15
(1,912)	1:141:A:VAL:HG23	1:107:A:TYR:HB2	17	0.15	0.03	0.15
(1,364)	1:34:A:ARG:H	1:31:A:GLU:HA	17	0.14	0.03	0.15
(4,40)	1:56:A:ALA:N	1:123:A:GLN:O	17	0.13	0.01	0.13
(1,786)	1:83:A:TYR:HA	1:85:A:ILE:HD11	17	0.11	0.01	0.11
(1,786)	1:83:A:TYR:HA	1:85:A:ILE:HD12	17	0.11	0.01	0.11
(1,786)	1:83:A:TYR:HA	1:85:A:ILE:HD13	17	0.11	0.01	0.11
(1,865)	1:123:A:GLN:HG2	1:122:A:CYS:HB2	16	0.26	0.08	0.3
(1,865)	1:123:A:GLN:HG2	1:122:A:CYS:HB3	16	0.26	0.08	0.3
(1,865)	1:123:A:GLN:HG3	1:122:A:CYS:HB2	16	0.26	0.08	0.3
(1,865)	1:123:A:GLN:HG3	1:122:A:CYS:HB3	16	0.26	0.08	0.3
(1,195)	1:96:A:LEU:H	1:95:A:LEU:H	16	0.16	0.04	0.15
(4,77)	1:34:A:ARG:H	1:30:A:HIS:O	16	0.15	0.04	0.16
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD11	16	0.13	0.03	0.12
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD12	16	0.13	0.03	0.12
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD13	16	0.13	0.03	0.12
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD21	16	0.13	0.03	0.12
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD22	16	0.13	0.03	0.12
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD23	16	0.13	0.03	0.12
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD11	16	0.13	0.03	0.12
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD12	16	0.13	0.03	0.12
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD13	16	0.13	0.03	0.12
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD21	16	0.13	0.03	0.12
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD22	16	0.13	0.03	0.12
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD23	16	0.13	0.03	0.12
(1,112)	1:65:A:THR:H	1:64:A:TRP:HB3	15	0.14	0.04	0.14
(1,875)	1:126:A:LEU:HG	1:114:A:PHE:HD1	15	0.13	0.02	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,875)	1:126:A:LEU:HG	1:114:A:PHE:HD2	15	0.13	0.02	0.13
(1,69)	1:49:A:ALA:H	1:48:A:THR:HG21	14	0.39	0.16	0.4
(1,69)	1:49:A:ALA:H	1:48:A:THR:HG22	14	0.39	0.16	0.4
(1,69)	1:49:A:ALA:H	1:48:A:THR:HG1	14	0.39	0.16	0.4
(1,69)	1:49:A:ALA:H	1:48:A:THR:HG23	14	0.39	0.16	0.4
(1,493)	1:97:A:TRP:H	1:95:A:LEU:HA	14	0.16	0.04	0.15
(1,972)	1:71:A:ALA:H	2:450:B:TRP:HZ2	14	0.15	0.02	0.15
(1,278)	1:127:A:ASN:H	1:126:A:LEU:HG	14	0.14	0.03	0.13
(1,531)	1:120:A:ASP:H	1:122:A:CYS:H	14	0.12	0.02	0.12
(1,1007)	2:474:B:SER:H	1:102:A:TYR:HA	13	0.15	0.05	0.12
(1,640)	1:35:A:LEU:HD11	1:31:A:GLU:HA	13	0.14	0.03	0.12
(1,640)	1:35:A:LEU:HD12	1:31:A:GLU:HA	13	0.14	0.03	0.12
(1,640)	1:35:A:LEU:HD13	1:31:A:GLU:HA	13	0.14	0.03	0.12
(1,640)	1:35:A:LEU:HD21	1:31:A:GLU:HA	13	0.14	0.03	0.12
(1,640)	1:35:A:LEU:HD22	1:31:A:GLU:HA	13	0.14	0.03	0.12
(1,640)	1:35:A:LEU:HD23	1:31:A:GLU:HA	13	0.14	0.03	0.12
(4,122)	2:452:B:SER:N	2:448:B:ASP:O	13	0.11	0.0	0.11
(1,54)	1:43:A:CYS:H	1:42:A:LYS:HB2	12	0.13	0.02	0.12
(1,54)	1:43:A:CYS:H	1:42:A:LYS:HB3	12	0.13	0.02	0.12
(1,429)	1:101:A:LEU:H	1:84:A:PHE:HB2	12	0.13	0.02	0.13
(1,429)	1:101:A:LEU:H	1:84:A:PHE:HB3	12	0.13	0.02	0.13
(1,509)	1:114:A:PHE:H	1:110:A:PRO:HD2	12	0.13	0.01	0.12
(1,509)	1:114:A:PHE:H	1:110:A:PRO:HD3	12	0.13	0.01	0.12
(1,346)	1:148:A:ARG:H	1:147:A:LYS:HA	12	0.11	0.01	0.11
(1,639)	1:34:A:ARG:HD2	1:74:A:PHE:HE1	11	0.14	0.03	0.14
(1,639)	1:34:A:ARG:HD2	1:74:A:PHE:HE2	11	0.14	0.03	0.14
(1,639)	1:34:A:ARG:HD3	1:74:A:PHE:HE1	11	0.14	0.03	0.14
(1,639)	1:34:A:ARG:HD3	1:74:A:PHE:HE2	11	0.14	0.03	0.14
(1,776)	1:75:A:VAL:HG11	1:73:A:CYS:HB2	11	0.13	0.03	0.13
(1,776)	1:75:A:VAL:HG11	1:73:A:CYS:HB3	11	0.13	0.03	0.13
(1,776)	1:75:A:VAL:HG12	1:73:A:CYS:HB2	11	0.13	0.03	0.13
(1,776)	1:75:A:VAL:HG12	1:73:A:CYS:HB3	11	0.13	0.03	0.13
(1,776)	1:75:A:VAL:HG13	1:73:A:CYS:HB2	11	0.13	0.03	0.13
(1,776)	1:75:A:VAL:HG13	1:73:A:CYS:HB3	11	0.13	0.03	0.13
(1,513)	1:114:A:PHE:H	1:113:A:PHE:HD1	10	0.4	0.04	0.42
(1,513)	1:114:A:PHE:H	1:113:A:PHE:HD2	10	0.4	0.04	0.42
(1,965)	1:56:A:ALA:HB1	2:462:B:LEU:HD11	10	0.16	0.04	0.16
(1,965)	1:56:A:ALA:HB1	2:462:B:LEU:HD12	10	0.16	0.04	0.16
(1,965)	1:56:A:ALA:HB1	2:462:B:LEU:HD13	10	0.16	0.04	0.16
(1,965)	1:56:A:ALA:HB1	2:462:B:LEU:HD21	10	0.16	0.04	0.16
(1,965)	1:56:A:ALA:HB1	2:462:B:LEU:HD22	10	0.16	0.04	0.16
(1,965)	1:56:A:ALA:HB1	2:462:B:LEU:HD23	10	0.16	0.04	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,965)	1:56:A:ALA:HB2	2:462:B:LEU:HD11	10	0.16	0.04	0.16
(1,965)	1:56:A:ALA:HB2	2:462:B:LEU:HD12	10	0.16	0.04	0.16
(1,965)	1:56:A:ALA:HB2	2:462:B:LEU:HD13	10	0.16	0.04	0.16
(1,965)	1:56:A:ALA:HB2	2:462:B:LEU:HD21	10	0.16	0.04	0.16
(1,965)	1:56:A:ALA:HB2	2:462:B:LEU:HD22	10	0.16	0.04	0.16
(1,965)	1:56:A:ALA:HB2	2:462:B:LEU:HD23	10	0.16	0.04	0.16
(1,965)	1:56:A:ALA:HB3	2:462:B:LEU:HD11	10	0.16	0.04	0.16
(1,965)	1:56:A:ALA:HB3	2:462:B:LEU:HD12	10	0.16	0.04	0.16
(1,965)	1:56:A:ALA:HB3	2:462:B:LEU:HD13	10	0.16	0.04	0.16
(1,965)	1:56:A:ALA:HB3	2:462:B:LEU:HD21	10	0.16	0.04	0.16
(1,965)	1:56:A:ALA:HB3	2:462:B:LEU:HD22	10	0.16	0.04	0.16
(1,965)	1:56:A:ALA:HB3	2:462:B:LEU:HD23	10	0.16	0.04	0.16
(1,416)	1:87:A:LEU:H	1:98:A:GLU:HB2	10	0.15	0.03	0.15
(1,416)	1:87:A:LEU:H	1:98:A:GLU:HB3	10	0.15	0.03	0.15
(1,869)	1:124:A:ALA:HB1	1:117:A:PHE:HD1	10	0.15	0.03	0.15
(1,869)	1:124:A:ALA:HB1	1:117:A:PHE:HD2	10	0.15	0.03	0.15
(1,869)	1:124:A:ALA:HB2	1:117:A:PHE:HD1	10	0.15	0.03	0.15
(1,869)	1:124:A:ALA:HB2	1:117:A:PHE:HD2	10	0.15	0.03	0.15
(1,869)	1:124:A:ALA:HB3	1:117:A:PHE:HD1	10	0.15	0.03	0.15
(1,869)	1:124:A:ALA:HB3	1:117:A:PHE:HD2	10	0.15	0.03	0.15
(1,957)	1:50:A:VAL:HG11	2:453:B:ARG:HB2	10	0.13	0.02	0.13
(1,957)	1:50:A:VAL:HG11	2:453:B:ARG:HB3	10	0.13	0.02	0.13
(1,957)	1:50:A:VAL:HG12	2:453:B:ARG:HB2	10	0.13	0.02	0.13
(1,957)	1:50:A:VAL:HG12	2:453:B:ARG:HB3	10	0.13	0.02	0.13
(1,957)	1:50:A:VAL:HG13	2:453:B:ARG:HB2	10	0.13	0.02	0.13
(1,957)	1:50:A:VAL:HG13	2:453:B:ARG:HB3	10	0.13	0.02	0.13
(1,957)	1:50:A:VAL:HG21	2:453:B:ARG:HB2	10	0.13	0.02	0.13
(1,957)	1:50:A:VAL:HG21	2:453:B:ARG:HB3	10	0.13	0.02	0.13
(1,957)	1:50:A:VAL:HG22	2:453:B:ARG:HB2	10	0.13	0.02	0.13
(1,957)	1:50:A:VAL:HG22	2:453:B:ARG:HB3	10	0.13	0.02	0.13
(1,957)	1:50:A:VAL:HG23	2:453:B:ARG:HB2	10	0.13	0.02	0.13
(1,957)	1:50:A:VAL:HG23	2:453:B:ARG:HB3	10	0.13	0.02	0.13
(1,456)	1:35:A:LEU:H	1:31:A:GLU:HA	10	0.13	0.01	0.13
(1,988)	1:129:A:ALA:HA	2:454:B:PHE:HZ	10	0.12	0.02	0.12
(4,39)	1:56:A:ALA:H	1:123:A:GLN:O	10	0.12	0.01	0.12
(1,567)	2:457:B:HIS:H	2:456:B:PHE:HB3	10	0.12	0.01	0.12
(1,439)	1:126:A:LEU:H	1:116:A:THR:HG22	9	0.23	0.13	0.17
(1,439)	1:126:A:LEU:H	1:116:A:THR:HG21	9	0.23	0.13	0.17
(1,439)	1:126:A:LEU:H	1:116:A:THR:HG23	9	0.23	0.13	0.17
(1,529)	1:126:A:LEU:H	1:125:A:GLY:H	9	0.22	0.11	0.14
(1,440)	1:127:A:ASN:H	1:53:A:LEU:HA	9	0.16	0.03	0.15
(4,31)	1:52:A:GLN:H	1:127:A:ASN:O	9	0.13	0.02	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,486)	1:89:A:GLY:H	1:94:A:ARG:HB2	9	0.12	0.01	0.12
(1,486)	1:89:A:GLY:H	1:94:A:ARG:HB3	9	0.12	0.01	0.12
(1,729)	1:63:A:HIS:HA	1:59:A:PRO:HB2	9	0.11	0.01	0.11
(1,729)	1:63:A:HIS:HA	1:59:A:PRO:HB3	9	0.11	0.01	0.11
(1,265)	1:121:A:ASP:H	1:120:A:ASP:H	9	0.11	0.01	0.11
(1,327)	1:143:A:GLU:H	1:140:A:LEU:HD11	8	0.19	0.04	0.2
(1,327)	1:143:A:GLU:H	1:140:A:LEU:HD12	8	0.19	0.04	0.2
(1,327)	1:143:A:GLU:H	1:140:A:LEU:HD13	8	0.19	0.04	0.2
(1,327)	1:143:A:GLU:H	1:140:A:LEU:HD21	8	0.19	0.04	0.2
(1,327)	1:143:A:GLU:H	1:140:A:LEU:HD22	8	0.19	0.04	0.2
(1,327)	1:143:A:GLU:H	1:140:A:LEU:HD23	8	0.19	0.04	0.2
(1,864)	1:122:A:CYS:HA	1:123:A:GLN:HB2	8	0.17	0.07	0.15
(1,864)	1:122:A:CYS:HA	1:123:A:GLN:HB3	8	0.17	0.07	0.15
(1,483)	1:87:A:LEU:H	1:97:A:TRP:HZ3	8	0.16	0.05	0.15
(1,483)	1:87:A:LEU:H	1:97:A:TRP:HZ2	8	0.16	0.05	0.15
(1,314)	1:140:A:LEU:H	1:136:A:ALA:HA	8	0.14	0.02	0.15
(1,496)	1:101:A:LEU:H	1:100:A:GLU:H	8	0.14	0.03	0.14
(1,1008)	2:474:B:SER:H	1:102:A:TYR:HE1	8	0.14	0.04	0.12
(1,1008)	2:474:B:SER:H	1:102:A:TYR:HE2	8	0.14	0.04	0.12
(1,911)	1:141:A:VAL:HA	1:107:A:TYR:HB2	8	0.12	0.02	0.12
(1,911)	1:141:A:VAL:HA	1:107:A:TYR:HB3	8	0.12	0.02	0.12
(1,880)	1:129:A:ALA:HB1	1:50:A:VAL:HB	8	0.12	0.01	0.12
(1,880)	1:129:A:ALA:HB2	1:50:A:VAL:HB	8	0.12	0.01	0.12
(1,880)	1:129:A:ALA:HB3	1:50:A:VAL:HB	8	0.12	0.01	0.12
(4,43)	1:88:A:TYR:H	1:71:A:ALA:O	8	0.12	0.01	0.12
(1,360)	1:32:A:ASN:H	1:29:A:ASP:HA	8	0.11	0.01	0.11
(1,1015)	2:475:B:TYR:HE2	1:102:A:TYR:HE1	7	0.43	0.09	0.44
(1,1015)	2:475:B:TYR:HE2	1:102:A:TYR:HE2	7	0.43	0.09	0.44
(1,1015)	2:475:B:TYR:HE1	1:102:A:TYR:HE2	7	0.43	0.09	0.44
(1,1015)	2:475:B:TYR:HE2	1:102:A:TYR:HD2	7	0.43	0.09	0.44
(1,1015)	2:475:B:TYR:HE2	1:102:A:TYR:HD1	7	0.43	0.09	0.44
(1,457)	1:38:A:MET:H	1:34:A:ARG:HD2	7	0.18	0.04	0.18
(1,457)	1:38:A:MET:H	1:34:A:ARG:HD3	7	0.18	0.04	0.18
(1,610)	2:479:B:LEU:H	2:478:B:LYS:HG2	7	0.18	0.02	0.19
(1,610)	2:479:B:LEU:H	2:478:B:LYS:HG3	7	0.18	0.02	0.19
(4,67)	1:124:A:ALA:H	1:117:A:PHE:O	7	0.14	0.02	0.12
(1,245)	1:114:A:PHE:H	1:113:A:PHE:H	7	0.12	0.02	0.12
(1,714)	1:55:A:LEU:HB2	1:126:A:LEU:HG	7	0.12	0.01	0.12
(1,714)	1:55:A:LEU:HB3	1:126:A:LEU:HG	7	0.12	0.01	0.12
(1,340)	1:146:A:GLN:H	1:145:A:ILE:HB	7	0.11	0.01	0.12
(1,797)	1:85:A:ILE:HA	1:74:A:PHE:HD1	7	0.11	0.01	0.1
(1,797)	1:85:A:ILE:HA	1:74:A:PHE:HD2	7	0.11	0.01	0.1

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,928)	1:145:A:ILE:HD11	1:117:A:PHE:HZ	6	0.2	0.06	0.2
(1,928)	1:145:A:ILE:HD12	1:117:A:PHE:HZ	6	0.2	0.06	0.2
(1,928)	1:145:A:ILE:HD13	1:117:A:PHE:HZ	6	0.2	0.06	0.2
(1,502)	1:104:A:GLN:H	1:102:A:TYR:HA	6	0.16	0.05	0.13
(1,466)	1:52:A:GLN:H	1:128:A:PHE:HB2	6	0.14	0.03	0.13
(1,466)	1:52:A:GLN:H	1:128:A:PHE:HB3	6	0.14	0.03	0.13
(1,342)	1:146:A:GLN:H	1:143:A:GLU:HA	6	0.13	0.03	0.12
(1,487)	1:89:A:GLY:H	1:94:A:ARG:H	6	0.13	0.02	0.12
(1,975)	1:91:A:GLN:HB2	2:445:B:PRO:HD2	6	0.11	0.01	0.11
(1,975)	1:91:A:GLN:HB2	2:445:B:PRO:HD3	6	0.11	0.01	0.11
(1,975)	1:91:A:GLN:HB3	2:445:B:PRO:HD2	6	0.11	0.01	0.11
(1,975)	1:91:A:GLN:HB3	2:445:B:PRO:HD3	6	0.11	0.01	0.11
(1,660)	1:45:A:THR:HG1	1:47:A:ALA:HA	5	0.44	0.3	0.24
(1,660)	1:45:A:THR:HG21	1:47:A:ALA:HA	5	0.44	0.3	0.24
(1,435)	1:125:A:GLY:H	1:54:A:TYR:HB2	5	0.24	0.04	0.26
(1,435)	1:125:A:GLY:H	1:54:A:TYR:HB3	5	0.24	0.04	0.26
(1,141)	1:77:A:ASP:H	1:76:A:LYS:HG2	5	0.15	0.03	0.15
(1,141)	1:77:A:ASP:H	1:76:A:LYS:HG3	5	0.15	0.03	0.15
(1,374)	1:38:A:MET:H	1:35:A:LEU:HG	5	0.13	0.03	0.13
(1,815)	1:88:A:TYR:HB2	1:75:A:VAL:HG11	5	0.13	0.02	0.14
(1,815)	1:88:A:TYR:HB2	1:75:A:VAL:HG12	5	0.13	0.02	0.14
(1,815)	1:88:A:TYR:HB2	1:75:A:VAL:HG13	5	0.13	0.02	0.14
(1,815)	1:88:A:TYR:HB2	1:75:A:VAL:HG21	5	0.13	0.02	0.14
(1,815)	1:88:A:TYR:HB2	1:75:A:VAL:HG22	5	0.13	0.02	0.14
(1,815)	1:88:A:TYR:HB2	1:75:A:VAL:HG23	5	0.13	0.02	0.14
(1,815)	1:88:A:TYR:HB3	1:75:A:VAL:HG11	5	0.13	0.02	0.14
(1,815)	1:88:A:TYR:HB3	1:75:A:VAL:HG12	5	0.13	0.02	0.14
(1,815)	1:88:A:TYR:HB3	1:75:A:VAL:HG13	5	0.13	0.02	0.14
(1,815)	1:88:A:TYR:HB3	1:75:A:VAL:HG21	5	0.13	0.02	0.14
(1,815)	1:88:A:TYR:HB3	1:75:A:VAL:HG22	5	0.13	0.02	0.14
(1,815)	1:88:A:TYR:HB3	1:75:A:VAL:HG23	5	0.13	0.02	0.14
(1,300)	1:136:A:ALA:H	1:132:A:ASP:HA	5	0.12	0.02	0.11
(1,482)	1:87:A:LEU:H	1:72:A:VAL:HB	5	0.12	0.01	0.12
(1,545)	2:447:B:GLU:H	2:446:B:CYS:H	5	0.12	0.01	0.12
(1,153)	1:82:A:SER:H	1:81:A:LYS:HE2	5	0.12	0.01	0.12
(1,153)	1:82:A:SER:H	1:81:A:LYS:HE3	5	0.12	0.01	0.12
(1,642)	1:36:A:PHE:HB2	1:34:A:ARG:HG2	5	0.12	0.01	0.12
(1,642)	1:36:A:PHE:HB2	1:34:A:ARG:HG3	5	0.12	0.01	0.12
(1,642)	1:36:A:PHE:HB3	1:34:A:ARG:HG2	5	0.12	0.01	0.12
(1,642)	1:36:A:PHE:HB3	1:34:A:ARG:HG3	5	0.12	0.01	0.12
(1,738)	1:69:A:CYS:HG	1:52:A:GLN:HA	5	0.12	0.02	0.11
(1,646)	1:39:A:LEU:HA	1:88:A:TYR:HB2	5	0.12	0.02	0.11

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,646)	1:39:A:LEU:HA	1:88:A:TYR:HB3	5	0.12	0.02	0.11
(1,964)	1:51:A:VAL:H	2:454:B:PHE:HD1	5	0.12	0.01	0.12
(1,964)	1:51:A:VAL:H	2:454:B:PHE:HD2	5	0.12	0.01	0.12
(1,44)	1:39:A:LEU:H	1:36:A:PHE:HE1	5	0.11	0.01	0.11
(1,44)	1:39:A:LEU:H	1:36:A:PHE:HE2	5	0.11	0.01	0.11
(1,936)	1:147:A:LYS:HB2	1:148:A:ARG:HA	5	0.11	0.01	0.1
(1,936)	1:147:A:LYS:HB3	1:148:A:ARG:HA	5	0.11	0.01	0.1
(1,735)	1:65:A:THR:HG23	1:67:A:GLU:HA	4	0.36	0.23	0.3
(1,735)	1:65:A:THR:HG22	1:67:A:GLU:HA	4	0.36	0.23	0.3
(1,926)	1:145:A:ILE:HD11	1:117:A:PHE:HB2	4	0.19	0.04	0.18
(1,926)	1:145:A:ILE:HD12	1:117:A:PHE:HB2	4	0.19	0.04	0.18
(1,926)	1:145:A:ILE:HD13	1:117:A:PHE:HB2	4	0.19	0.04	0.18
(1,453)	1:26:A:LEU:H	1:30:A:HIS:H	4	0.16	0.04	0.16
(1,333)	1:144:A:LYS:H	1:141:A:VAL:HA	4	0.15	0.0	0.15
(4,111)	1:146:A:GLN:H	1:142:A:GLN:O	4	0.15	0.02	0.16
(1,707)	1:54:A:TYR:HE1	1:127:A:ASN:H	4	0.13	0.03	0.13
(1,707)	1:54:A:TYR:HE2	1:127:A:ASN:H	4	0.13	0.03	0.13
(1,1002)	2:463:B:PRO:HG2	1:114:A:PHE:HD1	4	0.13	0.05	0.11
(1,1002)	2:463:B:PRO:HG2	1:114:A:PHE:HD2	4	0.13	0.05	0.11
(1,1002)	2:463:B:PRO:HG3	1:114:A:PHE:HD1	4	0.13	0.05	0.11
(1,1002)	2:463:B:PRO:HG3	1:114:A:PHE:HD2	4	0.13	0.05	0.11
(4,70)	1:119:A:GLY:N	1:122:A:CYS:O	4	0.13	0.01	0.12
(1,410)	1:84:A:PHE:H	1:76:A:LYS:HG2	4	0.12	0.02	0.12
(1,410)	1:84:A:PHE:H	1:76:A:LYS:HG3	4	0.12	0.02	0.12
(1,977)	1:103:A:SER:HB2	2:476:B:PRO:HD2	4	0.12	0.02	0.12
(1,977)	1:103:A:SER:HB2	2:476:B:PRO:HD3	4	0.12	0.02	0.12
(1,977)	1:103:A:SER:HB3	2:476:B:PRO:HD2	4	0.12	0.02	0.12
(1,977)	1:103:A:SER:HB3	2:476:B:PRO:HD3	4	0.12	0.02	0.12
(1,427)	1:101:A:LEU:H	1:83:A:TYR:H	4	0.12	0.03	0.11
(1,339)	1:146:A:GLN:H	1:145:A:ILE:HA	4	0.12	0.01	0.12
(4,19)	1:53:A:LEU:H	1:68:A:HIS:O	4	0.12	0.01	0.11
(1,963)	1:50:A:VAL:HG11	2:456:B:PHE:HD1	4	0.12	0.01	0.11
(1,963)	1:50:A:VAL:HG11	2:456:B:PHE:HD2	4	0.12	0.01	0.11
(1,963)	1:50:A:VAL:HG12	2:456:B:PHE:HD1	4	0.12	0.01	0.11
(1,963)	1:50:A:VAL:HG12	2:456:B:PHE:HD2	4	0.12	0.01	0.11
(1,963)	1:50:A:VAL:HG13	2:456:B:PHE:HD1	4	0.12	0.01	0.11
(1,963)	1:50:A:VAL:HG13	2:456:B:PHE:HD2	4	0.12	0.01	0.11
(1,963)	1:50:A:VAL:HG21	2:456:B:PHE:HD1	4	0.12	0.01	0.11
(1,963)	1:50:A:VAL:HG21	2:456:B:PHE:HD2	4	0.12	0.01	0.11
(1,963)	1:50:A:VAL:HG22	2:456:B:PHE:HD1	4	0.12	0.01	0.11
(1,963)	1:50:A:VAL:HG22	2:456:B:PHE:HD2	4	0.12	0.01	0.11
(1,963)	1:50:A:VAL:HG23	2:456:B:PHE:HD1	4	0.12	0.01	0.11

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,963)	1:50:A:VAL:HG23	2:456:B:PHE:HD2	4	0.12	0.01	0.11
(1,542)	2:446:B:CYS:H	2:445:B:PRO:HA	4	0.11	0.01	0.12
(1,759)	1:72:A:VAL:HG11	1:85:A:ILE:HB	4	0.11	0.01	0.11
(1,759)	1:72:A:VAL:HG12	1:85:A:ILE:HB	4	0.11	0.01	0.11
(1,759)	1:72:A:VAL:HG13	1:85:A:ILE:HB	4	0.11	0.01	0.11
(1,759)	1:72:A:VAL:HG21	1:85:A:ILE:HB	4	0.11	0.01	0.11
(1,759)	1:72:A:VAL:HG22	1:85:A:ILE:HB	4	0.11	0.01	0.11
(1,759)	1:72:A:VAL:HG23	1:85:A:ILE:HB	4	0.11	0.01	0.11
(1,734)	1:65:A:THR:HG21	1:63:A:HIS:HD1	3	0.77	0.05	0.77
(1,734)	1:65:A:THR:HG23	1:63:A:HIS:HD1	3	0.77	0.05	0.77
(1,734)	1:65:A:THR:HG22	1:63:A:HIS:HD1	3	0.77	0.05	0.77
(1,235)	1:107:A:TYR:H	1:106:A:VAL:H	3	0.19	0.02	0.19
(1,903)	1:139:A:ALA:HA	1:138:A:ARG:HB2	3	0.16	0.01	0.15
(1,903)	1:139:A:ALA:HA	1:138:A:ARG:HB3	3	0.16	0.01	0.15
(1,417)	1:88:A:TYR:H	1:71:A:ALA:H	3	0.15	0.04	0.16
(1,369)	1:37:A:GLU:H	1:34:A:ARG:HA	3	0.14	0.03	0.13
(1,370)	1:38:A:MET:H	1:34:A:ARG:HA	3	0.14	0.02	0.13
(1,41)	1:38:A:MET:H	1:37:A:GLU:HG2	3	0.14	0.01	0.13
(1,41)	1:38:A:MET:H	1:37:A:GLU:HG3	3	0.14	0.01	0.13
(1,571)	2:459:B:ILE:H	2:458:B:PRO:HB2	3	0.12	0.01	0.12
(1,688)	1:51:A:VAL:HG11	1:128:A:PHE:HB2	3	0.12	0.02	0.12
(1,688)	1:51:A:VAL:HG11	1:128:A:PHE:HB3	3	0.12	0.02	0.12
(1,688)	1:51:A:VAL:HG12	1:128:A:PHE:HB2	3	0.12	0.02	0.12
(1,688)	1:51:A:VAL:HG12	1:128:A:PHE:HB3	3	0.12	0.02	0.12
(1,688)	1:51:A:VAL:HG13	1:128:A:PHE:HB2	3	0.12	0.02	0.12
(1,688)	1:51:A:VAL:HG13	1:128:A:PHE:HB3	3	0.12	0.02	0.12
(1,688)	1:51:A:VAL:HG21	1:128:A:PHE:HB2	3	0.12	0.02	0.12
(1,688)	1:51:A:VAL:HG21	1:128:A:PHE:HB3	3	0.12	0.02	0.12
(1,688)	1:51:A:VAL:HG22	1:128:A:PHE:HB2	3	0.12	0.02	0.12
(1,688)	1:51:A:VAL:HG22	1:128:A:PHE:HB3	3	0.12	0.02	0.12
(1,688)	1:51:A:VAL:HG23	1:128:A:PHE:HB2	3	0.12	0.02	0.12
(1,688)	1:51:A:VAL:HG23	1:128:A:PHE:HB3	3	0.12	0.02	0.12
(1,512)	1:114:A:PHE:H	1:112:A:PRO:HA	3	0.12	0.01	0.11
(1,586)	2:469:B:VAL:H	2:468:B:TYR:HB3	3	0.11	0.0	0.11
(1,65)	1:47:A:ALA:H	1:46:A:LEU:HD21	3	0.11	0.0	0.11
(1,65)	1:47:A:ALA:H	1:46:A:LEU:HD22	3	0.11	0.0	0.11
(1,65)	1:47:A:ALA:H	1:46:A:LEU:HD23	3	0.11	0.0	0.11
(1,713)	1:55:A:LEU:HD11	1:126:A:LEU:HG	3	0.11	0.01	0.11
(1,713)	1:55:A:LEU:HD12	1:126:A:LEU:HG	3	0.11	0.01	0.11
(1,713)	1:55:A:LEU:HD13	1:126:A:LEU:HG	3	0.11	0.01	0.11
(1,713)	1:55:A:LEU:HD21	1:126:A:LEU:HG	3	0.11	0.01	0.11
(1,713)	1:55:A:LEU:HD22	1:126:A:LEU:HG	3	0.11	0.01	0.11

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,713)	1:55:A:LEU:HD23	1:126:A:LEU:HG	3	0.11	0.01	0.11
(4,98)	1:139:A:ALA:N	1:135:A:GLN:O	3	0.11	0.01	0.1
(1,989)	1:129:A:ALA:HB3	2:454:B:PHE:HA	2	0.24	0.03	0.24
(1,720)	1:56:A:ALA:HB1	1:123:A:GLN:HB2	2	0.18	0.01	0.18
(1,720)	1:56:A:ALA:HB1	1:123:A:GLN:HB3	2	0.18	0.01	0.18
(1,720)	1:56:A:ALA:HB2	1:123:A:GLN:HB2	2	0.18	0.01	0.18
(1,720)	1:56:A:ALA:HB2	1:123:A:GLN:HB3	2	0.18	0.01	0.18
(1,720)	1:56:A:ALA:HB3	1:123:A:GLN:HB2	2	0.18	0.01	0.18
(1,720)	1:56:A:ALA:HB3	1:123:A:GLN:HB3	2	0.18	0.01	0.18
(1,755)	1:72:A:VAL:HG11	1:53:A:LEU:HG	2	0.15	0.02	0.15
(1,755)	1:72:A:VAL:HG12	1:53:A:LEU:HG	2	0.15	0.02	0.15
(1,755)	1:72:A:VAL:HG13	1:53:A:LEU:HG	2	0.15	0.02	0.15
(1,755)	1:72:A:VAL:HG21	1:53:A:LEU:HG	2	0.15	0.02	0.15
(1,755)	1:72:A:VAL:HG22	1:53:A:LEU:HG	2	0.15	0.02	0.15
(1,755)	1:72:A:VAL:HG23	1:53:A:LEU:HG	2	0.15	0.02	0.15
(1,85)	1:54:A:TYR:H	1:53:A:LEU:HG	2	0.14	0.03	0.14
(1,255)	1:117:A:PHE:H	1:116:A:THR:HB	2	0.14	0.02	0.14
(1,691)	1:53:A:LEU:HG	1:126:A:LEU:HA	2	0.14	0.01	0.14
(1,176)	1:88:A:TYR:H	1:87:A:LEU:HD11	2	0.12	0.01	0.12
(1,176)	1:88:A:TYR:H	1:87:A:LEU:HD12	2	0.12	0.01	0.12
(1,176)	1:88:A:TYR:H	1:87:A:LEU:HD13	2	0.12	0.01	0.12
(1,176)	1:88:A:TYR:H	1:87:A:LEU:HD21	2	0.12	0.01	0.12
(1,176)	1:88:A:TYR:H	1:87:A:LEU:HD22	2	0.12	0.01	0.12
(1,176)	1:88:A:TYR:H	1:87:A:LEU:HD23	2	0.12	0.01	0.12
(1,683)	1:50:A:VAL:HA	1:71:A:ALA:HA	2	0.12	0.01	0.12
(1,715)	1:55:A:LEU:HA	1:64:A:TRP:HZ3	2	0.12	0.01	0.12
(1,140)	1:77:A:ASP:H	1:76:A:LYS:HD2	2	0.12	0.0	0.12
(1,140)	1:77:A:ASP:H	1:76:A:LYS:HD3	2	0.12	0.0	0.12
(1,392)	1:55:A:LEU:H	1:66:A:LYS:HB2	2	0.12	0.0	0.12
(1,392)	1:55:A:LEU:H	1:66:A:LYS:HB3	2	0.12	0.0	0.12
(1,408)	1:84:A:PHE:H	1:75:A:VAL:H	2	0.12	0.0	0.12
(1,425)	1:97:A:TRP:H	1:87:A:LEU:HG	2	0.11	0.0	0.11
(1,860)	1:117:A:PHE:HB2	1:122:A:CYS:HB2	2	0.11	0.0	0.11
(1,860)	1:117:A:PHE:HB2	1:122:A:CYS:HB3	2	0.11	0.0	0.11
(1,860)	1:117:A:PHE:HB3	1:122:A:CYS:HB2	2	0.11	0.0	0.11
(1,860)	1:117:A:PHE:HB3	1:122:A:CYS:HB3	2	0.11	0.0	0.11
(1,958)	1:50:A:VAL:HG11	2:455:B:TYR:HE1	2	0.11	0.01	0.11
(1,958)	1:50:A:VAL:HG11	2:455:B:TYR:HE2	2	0.11	0.01	0.11
(1,958)	1:50:A:VAL:HG12	2:455:B:TYR:HE1	2	0.11	0.01	0.11
(1,958)	1:50:A:VAL:HG12	2:455:B:TYR:HE2	2	0.11	0.01	0.11
(1,958)	1:50:A:VAL:HG13	2:455:B:TYR:HE1	2	0.11	0.01	0.11
(1,958)	1:50:A:VAL:HG13	2:455:B:TYR:HE2	2	0.11	0.01	0.11

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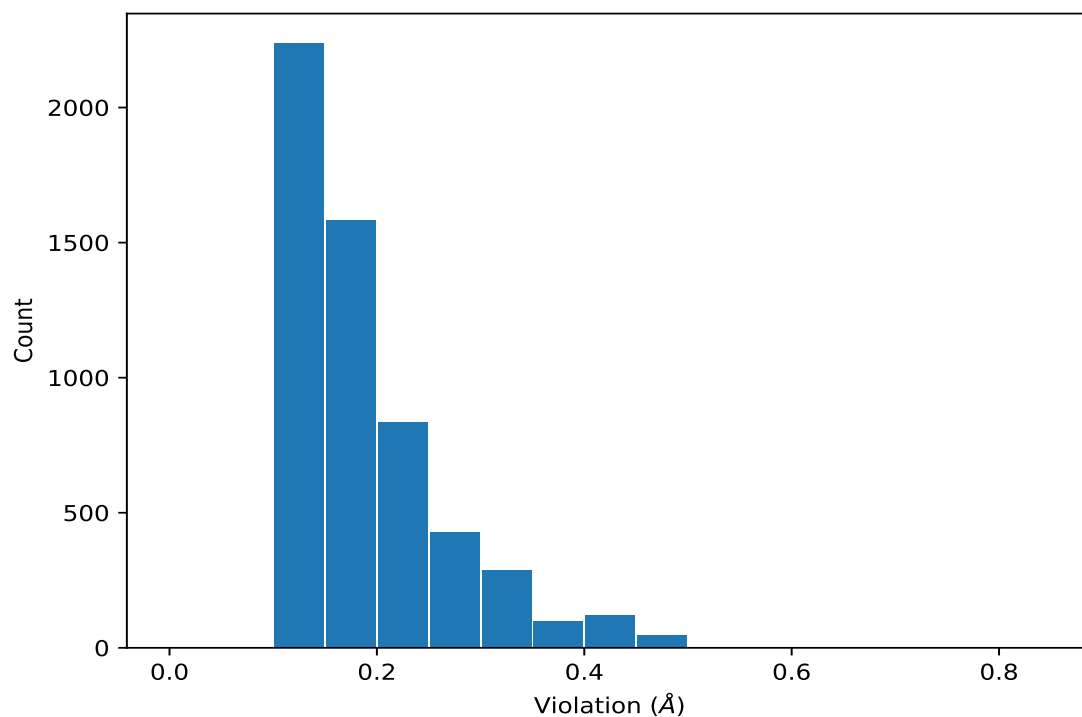
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,958)	1:50:A:VAL:HG21	2:455:B:TYR:HE1	2	0.11	0.01	0.11
(1,958)	1:50:A:VAL:HG21	2:455:B:TYR:HE2	2	0.11	0.01	0.11
(1,958)	1:50:A:VAL:HG22	2:455:B:TYR:HE1	2	0.11	0.01	0.11
(1,958)	1:50:A:VAL:HG22	2:455:B:TYR:HE2	2	0.11	0.01	0.11
(1,958)	1:50:A:VAL:HG23	2:455:B:TYR:HE1	2	0.11	0.01	0.11
(1,958)	1:50:A:VAL:HG23	2:455:B:TYR:HE2	2	0.11	0.01	0.11
(1,119)	1:70:A:GLY:H	1:69:A:CYS:HB2	2	0.11	0.0	0.11
(1,95)	1:57:A:LEU:H	1:56:A:ALA:H	2	0.1	0.0	0.1
(1,623)	2:483:B:GLU:H	2:482:B:ASN:HA	2	0.1	0.0	0.1
(4,105)	1:143:A:GLU:H	1:139:A:ALA:O	2	0.1	0.0	0.1
(4,114)	1:147:A:LYS:N	1:143:A:GLU:O	2	0.1	0.0	0.1

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



9.5.2 Table : All distance violations

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)
(1,734)	1:65:A:THR:HG23	1:63:A:HIS:HD1	20	0.83
(1,660)	1:45:A:THR:HG21	1:47:A:ALA:HA	24	0.83
(1,660)	1:45:A:THR:HG1	1:47:A:ALA:HA	5	0.79
(1,734)	1:65:A:THR:HG21	1:63:A:HIS:HD1	2	0.77
(1,735)	1:65:A:THR:HG22	1:67:A:GLU:HA	20	0.74
(1,734)	1:65:A:THR:HG22	1:63:A:HIS:HD1	21	0.7
(1,69)	1:49:A:ALA:H	1:48:A:THR:HG21	11	0.68
(1,69)	1:49:A:ALA:H	1:48:A:THR:HG23	17	0.64
(1,1015)	2:475:B:TYR:HE2	1:102:A:TYR:HE1	2	0.57
(1,69)	1:49:A:ALA:H	1:48:A:THR:HG23	16	0.52
(1,1015)	2:475:B:TYR:HE2	1:102:A:TYR:HE2	15	0.49
(1,69)	1:49:A:ALA:H	1:48:A:THR:HG22	8	0.49
(1,787)	1:83:A:TYR:HA	1:85:A:ILE:HB	8	0.48
(1,396)	1:57:A:LEU:H	1:65:A:THR:HG23	20	0.48
(1,1015)	2:475:B:TYR:HE2	1:102:A:TYR:HD2	19	0.47
(1,787)	1:83:A:TYR:HA	1:85:A:ILE:HB	5	0.47
(1,553)	2:450:B:TRP:H	2:449:B:GLU:HA	13	0.47
(1,439)	1:126:A:LEU:H	1:116:A:THR:HG22	2	0.47
(1,787)	1:83:A:TYR:HA	1:85:A:ILE:HB	14	0.46
(1,787)	1:83:A:TYR:HA	1:85:A:ILE:HB	21	0.46
(1,787)	1:83:A:TYR:HA	1:85:A:ILE:HB	23	0.46
(1,553)	2:450:B:TRP:H	2:449:B:GLU:HA	6	0.46
(1,553)	2:450:B:TRP:H	2:449:B:GLU:HA	8	0.46
(1,553)	2:450:B:TRP:H	2:449:B:GLU:HA	10	0.46
(1,553)	2:450:B:TRP:H	2:449:B:GLU:HA	11	0.46
(1,553)	2:450:B:TRP:H	2:449:B:GLU:HA	14	0.46
(1,553)	2:450:B:TRP:H	2:449:B:GLU:HA	15	0.46
(1,553)	2:450:B:TRP:H	2:449:B:GLU:HA	20	0.46
(1,553)	2:450:B:TRP:H	2:449:B:GLU:HA	24	0.46
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD11	18	0.45
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD12	18	0.45
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD13	18	0.45
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD21	18	0.45
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD22	18	0.45
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD23	18	0.45
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD11	18	0.45
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD12	18	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD13	18	0.45
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD21	18	0.45
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD22	18	0.45
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD23	18	0.45
(1,787)	1:83:A:TYR:HA	1:85:A:ILE:HB	18	0.45
(1,787)	1:83:A:TYR:HA	1:85:A:ILE:HB	20	0.45
(1,787)	1:83:A:TYR:HA	1:85:A:ILE:HB	22	0.45
(1,612)	2:479:B:LEU:H	2:475:B:TYR:HA	8	0.45
(1,612)	2:479:B:LEU:H	2:475:B:TYR:HA	18	0.45
(1,598)	2:473:B:LYS:H	2:472:B:THR:HG22	2	0.45
(1,553)	2:450:B:TRP:H	2:449:B:GLU:HA	1	0.45
(1,553)	2:450:B:TRP:H	2:449:B:GLU:HA	2	0.45
(1,553)	2:450:B:TRP:H	2:449:B:GLU:HA	4	0.45
(1,553)	2:450:B:TRP:H	2:449:B:GLU:HA	5	0.45
(1,553)	2:450:B:TRP:H	2:449:B:GLU:HA	12	0.45
(1,553)	2:450:B:TRP:H	2:449:B:GLU:HA	16	0.45
(1,553)	2:450:B:TRP:H	2:449:B:GLU:HA	22	0.45
(1,399)	1:72:A:VAL:H	1:50:A:VAL:HB	11	0.45
(1,69)	1:49:A:ALA:H	1:48:A:THR:HG22	24	0.45
(1,1015)	2:475:B:TYR:HE2	1:102:A:TYR:HE2	10	0.44
(1,787)	1:83:A:TYR:HA	1:85:A:ILE:HB	3	0.44
(1,787)	1:83:A:TYR:HA	1:85:A:ILE:HB	7	0.44
(1,787)	1:83:A:TYR:HA	1:85:A:ILE:HB	19	0.44
(1,612)	2:479:B:LEU:H	2:475:B:TYR:HA	5	0.44
(1,598)	2:473:B:LYS:H	2:472:B:THR:HG21	3	0.44
(1,598)	2:473:B:LYS:H	2:472:B:THR:HG21	6	0.44
(1,598)	2:473:B:LYS:H	2:472:B:THR:HG23	21	0.44
(1,582)	2:466:B:GLU:H	2:465:B:PRO:HG2	14	0.44
(1,582)	2:466:B:GLU:H	2:465:B:PRO:HG3	14	0.44
(1,553)	2:450:B:TRP:H	2:449:B:GLU:HA	3	0.44
(1,553)	2:450:B:TRP:H	2:449:B:GLU:HA	7	0.44
(1,553)	2:450:B:TRP:H	2:449:B:GLU:HA	9	0.44
(1,553)	2:450:B:TRP:H	2:449:B:GLU:HA	17	0.44
(1,553)	2:450:B:TRP:H	2:449:B:GLU:HA	18	0.44
(1,553)	2:450:B:TRP:H	2:449:B:GLU:HA	19	0.44
(1,553)	2:450:B:TRP:H	2:449:B:GLU:HA	21	0.44
(1,553)	2:450:B:TRP:H	2:449:B:GLU:HA	23	0.44
(1,551)	2:449:B:GLU:H	2:448:B:ASP:HA	13	0.44
(1,513)	1:114:A:PHE:H	1:113:A:PHE:HD1	15	0.44
(1,513)	1:114:A:PHE:H	1:113:A:PHE:HD2	15	0.44
(1,513)	1:114:A:PHE:H	1:113:A:PHE:HD1	17	0.44
(1,513)	1:114:A:PHE:H	1:113:A:PHE:HD2	17	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,399)	1:72:A:VAL:H	1:50:A:VAL:HB	17	0.44
(1,787)	1:83:A:TYR:HA	1:85:A:ILE:HB	4	0.43
(1,787)	1:83:A:TYR:HA	1:85:A:ILE:HB	9	0.43
(1,787)	1:83:A:TYR:HA	1:85:A:ILE:HB	13	0.43
(1,612)	2:479:B:LEU:H	2:475:B:TYR:HA	14	0.43
(1,582)	2:466:B:GLU:H	2:465:B:PRO:HG2	5	0.43
(1,582)	2:466:B:GLU:H	2:465:B:PRO:HG3	5	0.43
(1,582)	2:466:B:GLU:H	2:465:B:PRO:HG2	6	0.43
(1,582)	2:466:B:GLU:H	2:465:B:PRO:HG3	6	0.43
(1,582)	2:466:B:GLU:H	2:465:B:PRO:HG2	8	0.43
(1,582)	2:466:B:GLU:H	2:465:B:PRO:HG3	8	0.43
(1,582)	2:466:B:GLU:H	2:465:B:PRO:HG2	9	0.43
(1,582)	2:466:B:GLU:H	2:465:B:PRO:HG3	9	0.43
(1,582)	2:466:B:GLU:H	2:465:B:PRO:HG2	15	0.43
(1,582)	2:466:B:GLU:H	2:465:B:PRO:HG3	15	0.43
(1,582)	2:466:B:GLU:H	2:465:B:PRO:HG2	16	0.43
(1,582)	2:466:B:GLU:H	2:465:B:PRO:HG3	16	0.43
(1,582)	2:466:B:GLU:H	2:465:B:PRO:HG2	18	0.43
(1,582)	2:466:B:GLU:H	2:465:B:PRO:HG3	18	0.43
(1,582)	2:466:B:GLU:H	2:465:B:PRO:HG2	19	0.43
(1,582)	2:466:B:GLU:H	2:465:B:PRO:HG3	19	0.43
(1,582)	2:466:B:GLU:H	2:465:B:PRO:HG2	20	0.43
(1,582)	2:466:B:GLU:H	2:465:B:PRO:HG3	20	0.43
(1,582)	2:466:B:GLU:H	2:465:B:PRO:HG2	22	0.43
(1,582)	2:466:B:GLU:H	2:465:B:PRO:HG3	22	0.43
(1,582)	2:466:B:GLU:H	2:465:B:PRO:HG2	24	0.43
(1,582)	2:466:B:GLU:H	2:465:B:PRO:HG3	24	0.43
(1,513)	1:114:A:PHE:H	1:113:A:PHE:HD1	9	0.43
(1,513)	1:114:A:PHE:H	1:113:A:PHE:HD2	9	0.43
(1,69)	1:49:A:ALA:H	1:48:A:THR:HG21	10	0.43
(1,787)	1:83:A:TYR:HA	1:85:A:ILE:HB	10	0.42
(1,787)	1:83:A:TYR:HA	1:85:A:ILE:HB	15	0.42
(1,612)	2:479:B:LEU:H	2:475:B:TYR:HA	3	0.42
(1,612)	2:479:B:LEU:H	2:475:B:TYR:HA	7	0.42
(1,582)	2:466:B:GLU:H	2:465:B:PRO:HG2	1	0.42
(1,582)	2:466:B:GLU:H	2:465:B:PRO:HG3	1	0.42
(1,582)	2:466:B:GLU:H	2:465:B:PRO:HG2	2	0.42
(1,582)	2:466:B:GLU:H	2:465:B:PRO:HG3	2	0.42
(1,582)	2:466:B:GLU:H	2:465:B:PRO:HG2	4	0.42
(1,582)	2:466:B:GLU:H	2:465:B:PRO:HG3	4	0.42
(1,582)	2:466:B:GLU:H	2:465:B:PRO:HG2	7	0.42
(1,582)	2:466:B:GLU:H	2:465:B:PRO:HG3	7	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,582)	2:466:B:GLU:H	2:465:B:PRO:HG2	10	0.42
(1,582)	2:466:B:GLU:H	2:465:B:PRO:HG3	10	0.42
(1,582)	2:466:B:GLU:H	2:465:B:PRO:HG2	11	0.42
(1,582)	2:466:B:GLU:H	2:465:B:PRO:HG3	11	0.42
(1,582)	2:466:B:GLU:H	2:465:B:PRO:HG2	21	0.42
(1,582)	2:466:B:GLU:H	2:465:B:PRO:HG3	21	0.42
(1,582)	2:466:B:GLU:H	2:465:B:PRO:HG2	23	0.42
(1,582)	2:466:B:GLU:H	2:465:B:PRO:HG3	23	0.42
(1,513)	1:114:A:PHE:H	1:113:A:PHE:HD1	1	0.42
(1,513)	1:114:A:PHE:H	1:113:A:PHE:HD2	1	0.42
(1,513)	1:114:A:PHE:H	1:113:A:PHE:HD1	16	0.42
(1,513)	1:114:A:PHE:H	1:113:A:PHE:HD2	16	0.42
(1,191)	1:95:A:LEU:H	1:94:A:ARG:H	6	0.42
(1,787)	1:83:A:TYR:HA	1:85:A:ILE:HB	1	0.41
(1,787)	1:83:A:TYR:HA	1:85:A:ILE:HB	16	0.41
(1,787)	1:83:A:TYR:HA	1:85:A:ILE:HB	17	0.41
(1,787)	1:83:A:TYR:HA	1:85:A:ILE:HB	24	0.41
(1,615)	2:480:B:ALA:H	2:479:B:LEU:HG	21	0.41
(1,612)	2:479:B:LEU:H	2:475:B:TYR:HA	9	0.41
(1,612)	2:479:B:LEU:H	2:475:B:TYR:HA	13	0.41
(1,612)	2:479:B:LEU:H	2:475:B:TYR:HA	20	0.41
(1,582)	2:466:B:GLU:H	2:465:B:PRO:HG2	13	0.41
(1,582)	2:466:B:GLU:H	2:465:B:PRO:HG3	13	0.41
(1,582)	2:466:B:GLU:H	2:465:B:PRO:HG2	17	0.41
(1,582)	2:466:B:GLU:H	2:465:B:PRO:HG3	17	0.41
(1,551)	2:449:B:GLU:H	2:448:B:ASP:HA	4	0.41
(1,551)	2:449:B:GLU:H	2:448:B:ASP:HA	12	0.41
(1,551)	2:449:B:GLU:H	2:448:B:ASP:HA	17	0.41
(1,513)	1:114:A:PHE:H	1:113:A:PHE:HD1	8	0.41
(1,513)	1:114:A:PHE:H	1:113:A:PHE:HD2	8	0.41
(1,513)	1:114:A:PHE:H	1:113:A:PHE:HD1	12	0.41
(1,513)	1:114:A:PHE:H	1:113:A:PHE:HD2	12	0.41
(1,399)	1:72:A:VAL:H	1:50:A:VAL:HB	19	0.41
(1,787)	1:83:A:TYR:HA	1:85:A:ILE:HB	12	0.4
(1,612)	2:479:B:LEU:H	2:475:B:TYR:HA	12	0.4
(1,612)	2:479:B:LEU:H	2:475:B:TYR:HA	17	0.4
(1,612)	2:479:B:LEU:H	2:475:B:TYR:HA	23	0.4
(1,582)	2:466:B:GLU:H	2:465:B:PRO:HG2	3	0.4
(1,582)	2:466:B:GLU:H	2:465:B:PRO:HG3	3	0.4
(1,582)	2:466:B:GLU:H	2:465:B:PRO:HG2	12	0.4
(1,582)	2:466:B:GLU:H	2:465:B:PRO:HG3	12	0.4
(1,551)	2:449:B:GLU:H	2:448:B:ASP:HA	2	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,551)	2:449:B:GLU:H	2:448:B:ASP:HA	3	0.4
(1,551)	2:449:B:GLU:H	2:448:B:ASP:HA	6	0.4
(1,551)	2:449:B:GLU:H	2:448:B:ASP:HA	8	0.4
(1,551)	2:449:B:GLU:H	2:448:B:ASP:HA	10	0.4
(1,551)	2:449:B:GLU:H	2:448:B:ASP:HA	18	0.4
(1,551)	2:449:B:GLU:H	2:448:B:ASP:HA	19	0.4
(1,551)	2:449:B:GLU:H	2:448:B:ASP:HA	21	0.4
(1,551)	2:449:B:GLU:H	2:448:B:ASP:HA	24	0.4
(1,513)	1:114:A:PHE:H	1:113:A:PHE:HD1	13	0.4
(1,513)	1:114:A:PHE:H	1:113:A:PHE:HD2	13	0.4
(1,396)	1:57:A:LEU:H	1:65:A:THR:HG21	23	0.4
(1,69)	1:49:A:ALA:H	1:48:A:THR:HG1	12	0.4
(1,69)	1:49:A:ALA:H	1:48:A:THR:HG1	22	0.4
(1,612)	2:479:B:LEU:H	2:475:B:TYR:HA	22	0.39
(1,551)	2:449:B:GLU:H	2:448:B:ASP:HA	1	0.39
(1,551)	2:449:B:GLU:H	2:448:B:ASP:HA	5	0.39
(1,551)	2:449:B:GLU:H	2:448:B:ASP:HA	7	0.39
(1,551)	2:449:B:GLU:H	2:448:B:ASP:HA	9	0.39
(1,551)	2:449:B:GLU:H	2:448:B:ASP:HA	11	0.39
(1,551)	2:449:B:GLU:H	2:448:B:ASP:HA	14	0.39
(1,551)	2:449:B:GLU:H	2:448:B:ASP:HA	15	0.39
(1,551)	2:449:B:GLU:H	2:448:B:ASP:HA	16	0.39
(1,551)	2:449:B:GLU:H	2:448:B:ASP:HA	20	0.39
(1,551)	2:449:B:GLU:H	2:448:B:ASP:HA	22	0.39
(1,551)	2:449:B:GLU:H	2:448:B:ASP:HA	23	0.39
(1,529)	1:126:A:LEU:H	1:125:A:GLY:H	6	0.39
(1,439)	1:126:A:LEU:H	1:116:A:THR:HG23	21	0.39
(1,396)	1:57:A:LEU:H	1:65:A:THR:HG22	8	0.39
(1,396)	1:57:A:LEU:H	1:65:A:THR:HG23	9	0.39
(1,396)	1:57:A:LEU:H	1:65:A:THR:HG21	12	0.39
(1,396)	1:57:A:LEU:H	1:65:A:THR:HG23	14	0.39
(1,396)	1:57:A:LEU:H	1:65:A:THR:HG22	15	0.39
(1,1015)	2:475:B:TYR:HE1	1:102:A:TYR:HE2	12	0.38
(1,992)	1:129:A:ALA:H	2:457:B:HIS:H	9	0.38
(1,787)	1:83:A:TYR:HA	1:85:A:ILE:HB	11	0.38
(1,396)	1:57:A:LEU:H	1:65:A:THR:HG21	6	0.38
(1,396)	1:57:A:LEU:H	1:65:A:THR:HG21	22	0.38
(1,69)	1:49:A:ALA:H	1:48:A:THR:HG21	7	0.38
(1,1015)	2:475:B:TYR:HE2	1:102:A:TYR:HD2	20	0.37
(1,822)	1:94:A:ARG:HA	1:90:A:LEU:HA	13	0.37
(1,787)	1:83:A:TYR:HA	1:85:A:ILE:HB	2	0.37
(1,787)	1:83:A:TYR:HA	1:85:A:ILE:HB	6	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,612)	2:479:B:LEU:H	2:475:B:TYR:HA	10	0.37
(1,612)	2:479:B:LEU:H	2:475:B:TYR:HA	15	0.37
(1,612)	2:479:B:LEU:H	2:475:B:TYR:HA	16	0.37
(1,598)	2:473:B:LYS:H	2:472:B:THR:HG23	20	0.37
(1,396)	1:57:A:LEU:H	1:65:A:THR:HG23	1	0.37
(1,396)	1:57:A:LEU:H	1:65:A:THR:HG22	3	0.37
(1,396)	1:57:A:LEU:H	1:65:A:THR:HG21	5	0.37
(1,396)	1:57:A:LEU:H	1:65:A:THR:HG22	10	0.37
(1,396)	1:57:A:LEU:H	1:65:A:THR:HG23	11	0.37
(1,396)	1:57:A:LEU:H	1:65:A:THR:HG21	13	0.37
(1,396)	1:57:A:LEU:H	1:65:A:THR:HG23	17	0.37
(1,396)	1:57:A:LEU:H	1:65:A:THR:HG21	18	0.37
(1,396)	1:57:A:LEU:H	1:65:A:THR:HG23	19	0.37
(1,191)	1:95:A:LEU:H	1:94:A:ARG:H	24	0.37
(1,75)	1:51:A:VAL:H	1:50:A:VAL:H	19	0.37
(1,822)	1:94:A:ARG:HA	1:90:A:LEU:HA	16	0.36
(1,822)	1:94:A:ARG:HA	1:90:A:LEU:HA	23	0.36
(1,615)	2:480:B:ALA:H	2:479:B:LEU:HG	2	0.36
(1,612)	2:479:B:LEU:H	2:475:B:TYR:HA	21	0.36
(1,396)	1:57:A:LEU:H	1:65:A:THR:HG21	2	0.36
(1,396)	1:57:A:LEU:H	1:65:A:THR:HG21	4	0.36
(1,396)	1:57:A:LEU:H	1:65:A:THR:HG22	7	0.36
(1,396)	1:57:A:LEU:H	1:65:A:THR:HG21	16	0.36
(1,396)	1:57:A:LEU:H	1:65:A:THR:HG22	21	0.36
(1,396)	1:57:A:LEU:H	1:65:A:THR:HG21	24	0.36
(1,191)	1:95:A:LEU:H	1:94:A:ARG:H	5	0.36
(1,191)	1:95:A:LEU:H	1:94:A:ARG:H	20	0.36
(1,167)	1:86:A:ARG:H	1:85:A:ILE:HB	8	0.36
(1,101)	1:62:A:GLU:H	1:61:A:ALA:HA	19	0.36
(1,75)	1:51:A:VAL:H	1:50:A:VAL:H	11	0.36
(1,944)	2:458:B:PRO:HA	2:460:B:SER:HB2	1	0.35
(1,944)	2:458:B:PRO:HA	2:460:B:SER:HB3	1	0.35
(1,865)	1:123:A:GLN:HG2	1:122:A:CYS:HB2	4	0.35
(1,865)	1:123:A:GLN:HG2	1:122:A:CYS:HB3	4	0.35
(1,865)	1:123:A:GLN:HG3	1:122:A:CYS:HB2	4	0.35
(1,865)	1:123:A:GLN:HG3	1:122:A:CYS:HB3	4	0.35
(1,845)	1:108:A:SER:HB2	1:110:A:PRO:HA	8	0.35
(1,845)	1:108:A:SER:HB3	1:110:A:PRO:HA	8	0.35
(1,822)	1:94:A:ARG:HA	1:90:A:LEU:HA	12	0.35
(1,735)	1:65:A:THR:HG23	1:67:A:GLU:HA	6	0.35
(1,638)	1:34:A:ARG:HB2	1:74:A:PHE:HD1	20	0.35
(1,638)	1:34:A:ARG:HB2	1:74:A:PHE:HD2	20	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,638)	1:34:A:ARG:HB3	1:74:A:PHE:HD1	20	0.35
(1,638)	1:34:A:ARG:HB3	1:74:A:PHE:HD2	20	0.35
(1,612)	2:479:B:LEU:H	2:475:B:TYR:HA	19	0.35
(1,598)	2:473:B:LYS:H	2:472:B:THR:HG21	23	0.35
(1,465)	1:52:A:GLN:H	1:51:A:VAL:H	1	0.35
(1,465)	1:52:A:GLN:H	1:51:A:VAL:H	17	0.35
(1,465)	1:52:A:GLN:H	1:51:A:VAL:H	24	0.35
(1,439)	1:126:A:LEU:H	1:116:A:THR:HG21	18	0.35
(1,167)	1:86:A:ARG:H	1:85:A:ILE:HB	5	0.35
(1,167)	1:86:A:ARG:H	1:85:A:ILE:HB	22	0.35
(1,101)	1:62:A:GLU:H	1:61:A:ALA:HA	1	0.35
(1,101)	1:62:A:GLU:H	1:61:A:ALA:HA	3	0.35
(1,101)	1:62:A:GLU:H	1:61:A:ALA:HA	4	0.35
(1,101)	1:62:A:GLU:H	1:61:A:ALA:HA	7	0.35
(1,101)	1:62:A:GLU:H	1:61:A:ALA:HA	8	0.35
(1,101)	1:62:A:GLU:H	1:61:A:ALA:HA	9	0.35
(1,101)	1:62:A:GLU:H	1:61:A:ALA:HA	11	0.35
(1,101)	1:62:A:GLU:H	1:61:A:ALA:HA	12	0.35
(1,101)	1:62:A:GLU:H	1:61:A:ALA:HA	13	0.35
(1,101)	1:62:A:GLU:H	1:61:A:ALA:HA	15	0.35
(1,101)	1:62:A:GLU:H	1:61:A:ALA:HA	18	0.35
(1,101)	1:62:A:GLU:H	1:61:A:ALA:HA	21	0.35
(1,101)	1:62:A:GLU:H	1:61:A:ALA:HA	22	0.35
(1,101)	1:62:A:GLU:H	1:61:A:ALA:HA	23	0.35
(1,101)	1:62:A:GLU:H	1:61:A:ALA:HA	24	0.35
(1,75)	1:51:A:VAL:H	1:50:A:VAL:H	2	0.35
(1,75)	1:51:A:VAL:H	1:50:A:VAL:H	7	0.35
(1,969)	1:71:A:ALA:HB1	2:453:B:ARG:HB2	24	0.34
(1,969)	1:71:A:ALA:HB1	2:453:B:ARG:HB3	24	0.34
(1,969)	1:71:A:ALA:HB2	2:453:B:ARG:HB2	24	0.34
(1,969)	1:71:A:ALA:HB2	2:453:B:ARG:HB3	24	0.34
(1,969)	1:71:A:ALA:HB3	2:453:B:ARG:HB2	24	0.34
(1,969)	1:71:A:ALA:HB3	2:453:B:ARG:HB3	24	0.34
(1,944)	2:458:B:PRO:HA	2:460:B:SER:HB2	24	0.34
(1,944)	2:458:B:PRO:HA	2:460:B:SER:HB3	24	0.34
(1,877)	1:127:A:ASN:HB2	1:113:A:PHE:HB2	23	0.34
(1,877)	1:127:A:ASN:HB2	1:113:A:PHE:HB3	23	0.34
(1,877)	1:127:A:ASN:HB3	1:113:A:PHE:HB2	23	0.34
(1,877)	1:127:A:ASN:HB3	1:113:A:PHE:HB3	23	0.34
(1,865)	1:123:A:GLN:HG2	1:122:A:CYS:HB2	14	0.34
(1,865)	1:123:A:GLN:HG2	1:122:A:CYS:HB3	14	0.34
(1,865)	1:123:A:GLN:HG3	1:122:A:CYS:HB2	14	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,865)	1:123:A:GLN:HG3	1:122:A:CYS:HB3	14	0.34
(1,865)	1:123:A:GLN:HG2	1:122:A:CYS:HB2	19	0.34
(1,865)	1:123:A:GLN:HG2	1:122:A:CYS:HB3	19	0.34
(1,865)	1:123:A:GLN:HG3	1:122:A:CYS:HB2	19	0.34
(1,865)	1:123:A:GLN:HG3	1:122:A:CYS:HB3	19	0.34
(1,864)	1:122:A:CYS:HA	1:123:A:GLN:HB2	5	0.34
(1,864)	1:122:A:CYS:HA	1:123:A:GLN:HB3	5	0.34
(1,822)	1:94:A:ARG:HA	1:90:A:LEU:HA	11	0.34
(1,615)	2:480:B:ALA:H	2:479:B:LEU:HG	22	0.34
(1,612)	2:479:B:LEU:H	2:475:B:TYR:HA	2	0.34
(1,612)	2:479:B:LEU:H	2:475:B:TYR:HA	11	0.34
(1,598)	2:473:B:LYS:H	2:472:B:THR:HG23	7	0.34
(1,513)	1:114:A:PHE:H	1:113:A:PHE:HD1	24	0.34
(1,513)	1:114:A:PHE:H	1:113:A:PHE:HD2	24	0.34
(1,191)	1:95:A:LEU:H	1:94:A:ARG:H	9	0.34
(1,191)	1:95:A:LEU:H	1:94:A:ARG:H	12	0.34
(1,191)	1:95:A:LEU:H	1:94:A:ARG:H	19	0.34
(1,191)	1:95:A:LEU:H	1:94:A:ARG:H	21	0.34
(1,191)	1:95:A:LEU:H	1:94:A:ARG:H	23	0.34
(1,167)	1:86:A:ARG:H	1:85:A:ILE:HB	2	0.34
(1,167)	1:86:A:ARG:H	1:85:A:ILE:HB	10	0.34
(1,101)	1:62:A:GLU:H	1:61:A:ALA:HA	2	0.34
(1,101)	1:62:A:GLU:H	1:61:A:ALA:HA	6	0.34
(1,101)	1:62:A:GLU:H	1:61:A:ALA:HA	10	0.34
(1,101)	1:62:A:GLU:H	1:61:A:ALA:HA	14	0.34
(1,101)	1:62:A:GLU:H	1:61:A:ALA:HA	16	0.34
(1,101)	1:62:A:GLU:H	1:61:A:ALA:HA	17	0.34
(1,101)	1:62:A:GLU:H	1:61:A:ALA:HA	20	0.34
(1,75)	1:51:A:VAL:H	1:50:A:VAL:H	4	0.34
(1,75)	1:51:A:VAL:H	1:50:A:VAL:H	5	0.34
(1,75)	1:51:A:VAL:H	1:50:A:VAL:H	14	0.34
(1,75)	1:51:A:VAL:H	1:50:A:VAL:H	16	0.34
(1,75)	1:51:A:VAL:H	1:50:A:VAL:H	18	0.34
(1,75)	1:51:A:VAL:H	1:50:A:VAL:H	20	0.34
(1,944)	2:458:B:PRO:HA	2:460:B:SER:HB2	6	0.33
(1,944)	2:458:B:PRO:HA	2:460:B:SER:HB3	6	0.33
(1,925)	1:145:A:ILE:HD11	1:117:A:PHE:HB3	10	0.33
(1,925)	1:145:A:ILE:HD12	1:117:A:PHE:HB3	10	0.33
(1,925)	1:145:A:ILE:HD13	1:117:A:PHE:HB3	10	0.33
(1,865)	1:123:A:GLN:HG2	1:122:A:CYS:HB2	13	0.33
(1,865)	1:123:A:GLN:HG2	1:122:A:CYS:HB3	13	0.33
(1,865)	1:123:A:GLN:HG3	1:122:A:CYS:HB2	13	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,865)	1:123:A:GLN:HG3	1:122:A:CYS:HB3	13	0.33
(1,845)	1:108:A:SER:HB2	1:110:A:PRO:HA	13	0.33
(1,845)	1:108:A:SER:HB3	1:110:A:PRO:HA	13	0.33
(1,845)	1:108:A:SER:HB2	1:110:A:PRO:HA	15	0.33
(1,845)	1:108:A:SER:HB3	1:110:A:PRO:HA	15	0.33
(1,822)	1:94:A:ARG:HA	1:90:A:LEU:HA	7	0.33
(1,822)	1:94:A:ARG:HA	1:90:A:LEU:HA	15	0.33
(1,638)	1:34:A:ARG:HB2	1:74:A:PHE:HD1	10	0.33
(1,638)	1:34:A:ARG:HB2	1:74:A:PHE:HD2	10	0.33
(1,638)	1:34:A:ARG:HB3	1:74:A:PHE:HD1	10	0.33
(1,638)	1:34:A:ARG:HB3	1:74:A:PHE:HD2	10	0.33
(1,615)	2:480:B:ALA:H	2:479:B:LEU:HG	4	0.33
(1,615)	2:480:B:ALA:H	2:479:B:LEU:HG	6	0.33
(1,615)	2:480:B:ALA:H	2:479:B:LEU:HG	18	0.33
(1,615)	2:480:B:ALA:H	2:479:B:LEU:HG	19	0.33
(1,612)	2:479:B:LEU:H	2:475:B:TYR:HA	6	0.33
(1,598)	2:473:B:LYS:H	2:472:B:THR:HG22	13	0.33
(1,529)	1:126:A:LEU:H	1:125:A:GLY:H	4	0.33
(1,513)	1:114:A:PHE:H	1:113:A:PHE:HD1	4	0.33
(1,513)	1:114:A:PHE:H	1:113:A:PHE:HD2	4	0.33
(1,465)	1:52:A:GLN:H	1:51:A:VAL:H	11	0.33
(1,465)	1:52:A:GLN:H	1:51:A:VAL:H	19	0.33
(1,259)	1:118:A:ALA:H	1:117:A:PHE:HB3	19	0.33
(1,191)	1:95:A:LEU:H	1:94:A:ARG:H	1	0.33
(1,191)	1:95:A:LEU:H	1:94:A:ARG:H	7	0.33
(1,191)	1:95:A:LEU:H	1:94:A:ARG:H	11	0.33
(1,191)	1:95:A:LEU:H	1:94:A:ARG:H	14	0.33
(1,191)	1:95:A:LEU:H	1:94:A:ARG:H	16	0.33
(1,191)	1:95:A:LEU:H	1:94:A:ARG:H	22	0.33
(1,167)	1:86:A:ARG:H	1:85:A:ILE:HB	1	0.33
(1,167)	1:86:A:ARG:H	1:85:A:ILE:HB	14	0.33
(1,167)	1:86:A:ARG:H	1:85:A:ILE:HB	18	0.33
(1,167)	1:86:A:ARG:H	1:85:A:ILE:HB	19	0.33
(1,101)	1:62:A:GLU:H	1:61:A:ALA:HA	5	0.33
(1,75)	1:51:A:VAL:H	1:50:A:VAL:H	6	0.33
(1,75)	1:51:A:VAL:H	1:50:A:VAL:H	12	0.33
(1,75)	1:51:A:VAL:H	1:50:A:VAL:H	17	0.33
(1,75)	1:51:A:VAL:H	1:50:A:VAL:H	22	0.33
(1,75)	1:51:A:VAL:H	1:50:A:VAL:H	23	0.33
(1,992)	1:129:A:ALA:H	2:457:B:HIS:H	15	0.32
(1,969)	1:71:A:ALA:HB1	2:453:B:ARG:HB2	19	0.32
(1,969)	1:71:A:ALA:HB1	2:453:B:ARG:HB3	19	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,969)	1:71:A:ALA:HB2	2:453:B:ARG:HB2	19	0.32
(1,969)	1:71:A:ALA:HB2	2:453:B:ARG:HB3	19	0.32
(1,969)	1:71:A:ALA:HB3	2:453:B:ARG:HB2	19	0.32
(1,969)	1:71:A:ALA:HB3	2:453:B:ARG:HB3	19	0.32
(1,969)	1:71:A:ALA:HB1	2:453:B:ARG:HB2	21	0.32
(1,969)	1:71:A:ALA:HB1	2:453:B:ARG:HB3	21	0.32
(1,969)	1:71:A:ALA:HB2	2:453:B:ARG:HB2	21	0.32
(1,969)	1:71:A:ALA:HB2	2:453:B:ARG:HB3	21	0.32
(1,969)	1:71:A:ALA:HB3	2:453:B:ARG:HB2	21	0.32
(1,969)	1:71:A:ALA:HB3	2:453:B:ARG:HB3	21	0.32
(1,925)	1:145:A:ILE:HD11	1:117:A:PHE:HB3	1	0.32
(1,925)	1:145:A:ILE:HD12	1:117:A:PHE:HB3	1	0.32
(1,925)	1:145:A:ILE:HD13	1:117:A:PHE:HB3	1	0.32
(1,865)	1:123:A:GLN:HG2	1:122:A:CYS:HB2	8	0.32
(1,865)	1:123:A:GLN:HG2	1:122:A:CYS:HB3	8	0.32
(1,865)	1:123:A:GLN:HG3	1:122:A:CYS:HB2	8	0.32
(1,865)	1:123:A:GLN:HG3	1:122:A:CYS:HB3	8	0.32
(1,865)	1:123:A:GLN:HG2	1:122:A:CYS:HB2	10	0.32
(1,865)	1:123:A:GLN:HG2	1:122:A:CYS:HB3	10	0.32
(1,865)	1:123:A:GLN:HG3	1:122:A:CYS:HB2	10	0.32
(1,865)	1:123:A:GLN:HG3	1:122:A:CYS:HB3	10	0.32
(1,865)	1:123:A:GLN:HG2	1:122:A:CYS:HB2	24	0.32
(1,865)	1:123:A:GLN:HG2	1:122:A:CYS:HB3	24	0.32
(1,865)	1:123:A:GLN:HG3	1:122:A:CYS:HB2	24	0.32
(1,865)	1:123:A:GLN:HG3	1:122:A:CYS:HB3	24	0.32
(1,846)	1:108:A:SER:HB2	1:137:A:PHE:HB2	6	0.32
(1,846)	1:108:A:SER:HB2	1:137:A:PHE:HB3	6	0.32
(1,846)	1:108:A:SER:HB3	1:137:A:PHE:HB2	6	0.32
(1,846)	1:108:A:SER:HB3	1:137:A:PHE:HB3	6	0.32
(1,845)	1:108:A:SER:HB2	1:110:A:PRO:HA	12	0.32
(1,845)	1:108:A:SER:HB3	1:110:A:PRO:HA	12	0.32
(1,845)	1:108:A:SER:HB2	1:110:A:PRO:HA	20	0.32
(1,845)	1:108:A:SER:HB3	1:110:A:PRO:HA	20	0.32
(1,822)	1:94:A:ARG:HA	1:90:A:LEU:HA	21	0.32
(1,638)	1:34:A:ARG:HB2	1:74:A:PHE:HD1	1	0.32
(1,638)	1:34:A:ARG:HB2	1:74:A:PHE:HD2	1	0.32
(1,638)	1:34:A:ARG:HB3	1:74:A:PHE:HD1	1	0.32
(1,638)	1:34:A:ARG:HB3	1:74:A:PHE:HD2	1	0.32
(1,638)	1:34:A:ARG:HB2	1:74:A:PHE:HD1	6	0.32
(1,638)	1:34:A:ARG:HB2	1:74:A:PHE:HD2	6	0.32
(1,638)	1:34:A:ARG:HB3	1:74:A:PHE:HD1	6	0.32
(1,638)	1:34:A:ARG:HB3	1:74:A:PHE:HD2	6	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,638)	1:34:A:ARG:HB2	1:74:A:PHE:HD1	21	0.32
(1,638)	1:34:A:ARG:HB2	1:74:A:PHE:HD2	21	0.32
(1,638)	1:34:A:ARG:HB3	1:74:A:PHE:HD1	21	0.32
(1,638)	1:34:A:ARG:HB3	1:74:A:PHE:HD2	21	0.32
(1,615)	2:480:B:ALA:H	2:479:B:LEU:HG	1	0.32
(1,615)	2:480:B:ALA:H	2:479:B:LEU:HG	7	0.32
(1,615)	2:480:B:ALA:H	2:479:B:LEU:HG	9	0.32
(1,615)	2:480:B:ALA:H	2:479:B:LEU:HG	11	0.32
(1,612)	2:479:B:LEU:H	2:475:B:TYR:HA	24	0.32
(1,598)	2:473:B:LYS:H	2:472:B:THR:HG22	15	0.32
(1,529)	1:126:A:LEU:H	1:125:A:GLY:H	5	0.32
(1,167)	1:86:A:ARG:H	1:85:A:ILE:HB	3	0.32
(1,167)	1:86:A:ARG:H	1:85:A:ILE:HB	7	0.32
(1,167)	1:86:A:ARG:H	1:85:A:ILE:HB	12	0.32
(1,167)	1:86:A:ARG:H	1:85:A:ILE:HB	15	0.32
(1,167)	1:86:A:ARG:H	1:85:A:ILE:HB	17	0.32
(1,75)	1:51:A:VAL:H	1:50:A:VAL:H	13	0.32
(1,75)	1:51:A:VAL:H	1:50:A:VAL:H	21	0.32
(1,992)	1:129:A:ALA:H	2:457:B:HIS:H	8	0.31
(1,992)	1:129:A:ALA:H	2:457:B:HIS:H	21	0.31
(1,944)	2:458:B:PRO:HA	2:460:B:SER:HB2	12	0.31
(1,944)	2:458:B:PRO:HA	2:460:B:SER:HB3	12	0.31
(1,925)	1:145:A:ILE:HD11	1:117:A:PHE:HB3	14	0.31
(1,925)	1:145:A:ILE:HD12	1:117:A:PHE:HB3	14	0.31
(1,925)	1:145:A:ILE:HD13	1:117:A:PHE:HB3	14	0.31
(1,925)	1:145:A:ILE:HD11	1:117:A:PHE:HB3	19	0.31
(1,925)	1:145:A:ILE:HD12	1:117:A:PHE:HB3	19	0.31
(1,925)	1:145:A:ILE:HD13	1:117:A:PHE:HB3	19	0.31
(1,925)	1:145:A:ILE:HD11	1:117:A:PHE:HB3	23	0.31
(1,925)	1:145:A:ILE:HD12	1:117:A:PHE:HB3	23	0.31
(1,925)	1:145:A:ILE:HD13	1:117:A:PHE:HB3	23	0.31
(1,865)	1:123:A:GLN:HG2	1:122:A:CYS:HB2	20	0.31
(1,865)	1:123:A:GLN:HG2	1:122:A:CYS:HB3	20	0.31
(1,865)	1:123:A:GLN:HG3	1:122:A:CYS:HB2	20	0.31
(1,865)	1:123:A:GLN:HG3	1:122:A:CYS:HB3	20	0.31
(1,847)	1:109:A:THR:HB	1:115:A:HIS:HB2	2	0.31
(1,847)	1:109:A:THR:HB	1:115:A:HIS:HB3	2	0.31
(1,822)	1:94:A:ARG:HA	1:90:A:LEU:HA	6	0.31
(1,822)	1:94:A:ARG:HA	1:90:A:LEU:HA	10	0.31
(1,822)	1:94:A:ARG:HA	1:90:A:LEU:HA	17	0.31
(1,822)	1:94:A:ARG:HA	1:90:A:LEU:HA	22	0.31
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD11	1	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD12	1	0.31
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD13	1	0.31
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD21	1	0.31
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD22	1	0.31
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD23	1	0.31
(1,705)	1:53:A:LEU:HD11	1:127:A:ASN:HB2	12	0.31
(1,705)	1:53:A:LEU:HD11	1:127:A:ASN:HB3	12	0.31
(1,705)	1:53:A:LEU:HD12	1:127:A:ASN:HB2	12	0.31
(1,705)	1:53:A:LEU:HD12	1:127:A:ASN:HB3	12	0.31
(1,705)	1:53:A:LEU:HD13	1:127:A:ASN:HB2	12	0.31
(1,705)	1:53:A:LEU:HD13	1:127:A:ASN:HB3	12	0.31
(1,705)	1:53:A:LEU:HD21	1:127:A:ASN:HB2	12	0.31
(1,705)	1:53:A:LEU:HD21	1:127:A:ASN:HB3	12	0.31
(1,705)	1:53:A:LEU:HD22	1:127:A:ASN:HB2	12	0.31
(1,705)	1:53:A:LEU:HD22	1:127:A:ASN:HB3	12	0.31
(1,705)	1:53:A:LEU:HD23	1:127:A:ASN:HB2	12	0.31
(1,705)	1:53:A:LEU:HD23	1:127:A:ASN:HB3	12	0.31
(1,615)	2:480:B:ALA:H	2:479:B:LEU:HG	23	0.31
(1,612)	2:479:B:LEU:H	2:475:B:TYR:HA	1	0.31
(1,612)	2:479:B:LEU:H	2:475:B:TYR:HA	4	0.31
(1,598)	2:473:B:LYS:H	2:472:B:THR:HG23	19	0.31
(1,529)	1:126:A:LEU:H	1:125:A:GLY:H	24	0.31
(1,522)	1:116:A:THR:H	1:125:A:GLY:HA2	2	0.31
(1,522)	1:116:A:THR:H	1:125:A:GLY:HA3	2	0.31
(1,465)	1:52:A:GLN:H	1:51:A:VAL:H	5	0.31
(1,465)	1:52:A:GLN:H	1:51:A:VAL:H	8	0.31
(1,465)	1:52:A:GLN:H	1:51:A:VAL:H	9	0.31
(1,328)	1:143:A:GLU:H	1:139:A:ALA:HB1	21	0.31
(1,328)	1:143:A:GLU:H	1:139:A:ALA:HB2	21	0.31
(1,328)	1:143:A:GLU:H	1:139:A:ALA:HB3	21	0.31
(1,241)	1:109:A:THR:H	1:108:A:SER:H	3	0.31
(1,191)	1:95:A:LEU:H	1:94:A:ARG:H	2	0.31
(1,167)	1:86:A:ARG:H	1:85:A:ILE:HB	13	0.31
(1,167)	1:86:A:ARG:H	1:85:A:ILE:HB	16	0.31
(1,167)	1:86:A:ARG:H	1:85:A:ILE:HB	20	0.31
(1,75)	1:51:A:VAL:H	1:50:A:VAL:H	9	0.31
(1,75)	1:51:A:VAL:H	1:50:A:VAL:H	15	0.31
(1,992)	1:129:A:ALA:H	2:457:B:HIS:H	4	0.3
(1,969)	1:71:A:ALA:HB1	2:453:B:ARG:HB2	4	0.3
(1,969)	1:71:A:ALA:HB1	2:453:B:ARG:HB3	4	0.3
(1,969)	1:71:A:ALA:HB2	2:453:B:ARG:HB2	4	0.3
(1,969)	1:71:A:ALA:HB2	2:453:B:ARG:HB3	4	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,969)	1:71:A:ALA:HB3	2:453:B:ARG:HB2	4	0.3
(1,969)	1:71:A:ALA:HB3	2:453:B:ARG:HB3	4	0.3
(1,969)	1:71:A:ALA:HB1	2:453:B:ARG:HB2	7	0.3
(1,969)	1:71:A:ALA:HB1	2:453:B:ARG:HB3	7	0.3
(1,969)	1:71:A:ALA:HB2	2:453:B:ARG:HB2	7	0.3
(1,969)	1:71:A:ALA:HB2	2:453:B:ARG:HB3	7	0.3
(1,969)	1:71:A:ALA:HB3	2:453:B:ARG:HB2	7	0.3
(1,969)	1:71:A:ALA:HB3	2:453:B:ARG:HB3	7	0.3
(1,969)	1:71:A:ALA:HB1	2:453:B:ARG:HB2	13	0.3
(1,969)	1:71:A:ALA:HB1	2:453:B:ARG:HB3	13	0.3
(1,969)	1:71:A:ALA:HB2	2:453:B:ARG:HB2	13	0.3
(1,969)	1:71:A:ALA:HB2	2:453:B:ARG:HB3	13	0.3
(1,969)	1:71:A:ALA:HB3	2:453:B:ARG:HB2	13	0.3
(1,969)	1:71:A:ALA:HB3	2:453:B:ARG:HB3	13	0.3
(1,925)	1:145:A:ILE:HD11	1:117:A:PHE:HB3	12	0.3
(1,925)	1:145:A:ILE:HD12	1:117:A:PHE:HB3	12	0.3
(1,925)	1:145:A:ILE:HD13	1:117:A:PHE:HB3	12	0.3
(1,865)	1:123:A:GLN:HG2	1:122:A:CYS:HB2	12	0.3
(1,865)	1:123:A:GLN:HG2	1:122:A:CYS:HB3	12	0.3
(1,865)	1:123:A:GLN:HG3	1:122:A:CYS:HB2	12	0.3
(1,865)	1:123:A:GLN:HG3	1:122:A:CYS:HB3	12	0.3
(1,847)	1:109:A:THR:HB	1:115:A:HIS:HB2	22	0.3
(1,847)	1:109:A:THR:HB	1:115:A:HIS:HB3	22	0.3
(1,846)	1:108:A:SER:HB2	1:137:A:PHE:HB2	19	0.3
(1,846)	1:108:A:SER:HB2	1:137:A:PHE:HB3	19	0.3
(1,846)	1:108:A:SER:HB3	1:137:A:PHE:HB2	19	0.3
(1,846)	1:108:A:SER:HB3	1:137:A:PHE:HB3	19	0.3
(1,845)	1:108:A:SER:HB2	1:110:A:PRO:HA	1	0.3
(1,845)	1:108:A:SER:HB3	1:110:A:PRO:HA	1	0.3
(1,845)	1:108:A:SER:HB2	1:110:A:PRO:HA	4	0.3
(1,845)	1:108:A:SER:HB3	1:110:A:PRO:HA	4	0.3
(1,822)	1:94:A:ARG:HA	1:90:A:LEU:HA	18	0.3
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD11	24	0.3
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD12	24	0.3
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD13	24	0.3
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD21	24	0.3
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD22	24	0.3
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD23	24	0.3
(1,615)	2:480:B:ALA:H	2:479:B:LEU:HG	5	0.3
(1,615)	2:480:B:ALA:H	2:479:B:LEU:HG	8	0.3
(1,615)	2:480:B:ALA:H	2:479:B:LEU:HG	10	0.3
(1,615)	2:480:B:ALA:H	2:479:B:LEU:HG	13	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,615)	2:480:B:ALA:H	2:479:B:LEU:HG	15	0.3
(1,522)	1:116:A:THR:H	1:125:A:GLY:HA2	1	0.3
(1,522)	1:116:A:THR:H	1:125:A:GLY:HA3	1	0.3
(1,522)	1:116:A:THR:H	1:125:A:GLY:HA2	4	0.3
(1,522)	1:116:A:THR:H	1:125:A:GLY:HA3	4	0.3
(1,522)	1:116:A:THR:H	1:125:A:GLY:HA2	22	0.3
(1,522)	1:116:A:THR:H	1:125:A:GLY:HA3	22	0.3
(1,465)	1:52:A:GLN:H	1:51:A:VAL:H	10	0.3
(1,465)	1:52:A:GLN:H	1:51:A:VAL:H	14	0.3
(1,465)	1:52:A:GLN:H	1:51:A:VAL:H	22	0.3
(1,399)	1:72:A:VAL:H	1:50:A:VAL:HB	24	0.3
(1,259)	1:118:A:ALA:H	1:117:A:PHE:HB3	5	0.3
(1,241)	1:109:A:THR:H	1:108:A:SER:H	15	0.3
(1,191)	1:95:A:LEU:H	1:94:A:ARG:H	4	0.3
(1,191)	1:95:A:LEU:H	1:94:A:ARG:H	8	0.3
(1,191)	1:95:A:LEU:H	1:94:A:ARG:H	13	0.3
(1,167)	1:86:A:ARG:H	1:85:A:ILE:HB	6	0.3
(1,167)	1:86:A:ARG:H	1:85:A:ILE:HB	9	0.3
(1,167)	1:86:A:ARG:H	1:85:A:ILE:HB	11	0.3
(1,167)	1:86:A:ARG:H	1:85:A:ILE:HB	23	0.3
(1,167)	1:86:A:ARG:H	1:85:A:ILE:HB	24	0.3
(1,1015)	2:475:B:TYR:HE2	1:102:A:TYR:HD1	23	0.29
(1,992)	1:129:A:ALA:H	2:457:B:HIS:H	11	0.29
(1,944)	2:458:B:PRO:HA	2:460:B:SER:HB2	4	0.29
(1,944)	2:458:B:PRO:HA	2:460:B:SER:HB3	4	0.29
(1,944)	2:458:B:PRO:HA	2:460:B:SER:HB2	13	0.29
(1,944)	2:458:B:PRO:HA	2:460:B:SER:HB3	13	0.29
(1,944)	2:458:B:PRO:HA	2:460:B:SER:HB2	16	0.29
(1,944)	2:458:B:PRO:HA	2:460:B:SER:HB3	16	0.29
(1,928)	1:145:A:ILE:HD11	1:117:A:PHE:HZ	16	0.29
(1,928)	1:145:A:ILE:HD12	1:117:A:PHE:HZ	16	0.29
(1,928)	1:145:A:ILE:HD13	1:117:A:PHE:HZ	16	0.29
(1,925)	1:145:A:ILE:HD11	1:117:A:PHE:HB3	2	0.29
(1,925)	1:145:A:ILE:HD12	1:117:A:PHE:HB3	2	0.29
(1,925)	1:145:A:ILE:HD13	1:117:A:PHE:HB3	2	0.29
(1,925)	1:145:A:ILE:HD11	1:117:A:PHE:HB3	21	0.29
(1,925)	1:145:A:ILE:HD12	1:117:A:PHE:HB3	21	0.29
(1,925)	1:145:A:ILE:HD13	1:117:A:PHE:HB3	21	0.29
(1,925)	1:145:A:ILE:HD11	1:117:A:PHE:HB3	22	0.29
(1,925)	1:145:A:ILE:HD12	1:117:A:PHE:HB3	22	0.29
(1,925)	1:145:A:ILE:HD13	1:117:A:PHE:HB3	22	0.29
(1,865)	1:123:A:GLN:HG2	1:122:A:CYS:HB2	5	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,865)	1:123:A:GLN:HG2	1:122:A:CYS:HB3	5	0.29
(1,865)	1:123:A:GLN:HG3	1:122:A:CYS:HB2	5	0.29
(1,865)	1:123:A:GLN:HG3	1:122:A:CYS:HB3	5	0.29
(1,822)	1:94:A:ARG:HA	1:90:A:LEU:HA	9	0.29
(1,822)	1:94:A:ARG:HA	1:90:A:LEU:HA	24	0.29
(1,775)	1:75:A:VAL:HG21	1:73:A:CYS:HB2	8	0.29
(1,775)	1:75:A:VAL:HG21	1:73:A:CYS:HB3	8	0.29
(1,775)	1:75:A:VAL:HG22	1:73:A:CYS:HB2	8	0.29
(1,775)	1:75:A:VAL:HG22	1:73:A:CYS:HB3	8	0.29
(1,775)	1:75:A:VAL:HG23	1:73:A:CYS:HB2	8	0.29
(1,775)	1:75:A:VAL:HG23	1:73:A:CYS:HB3	8	0.29
(1,635)	1:33:A:GLN:HA	1:30:A:HIS:HA	2	0.29
(1,615)	2:480:B:ALA:H	2:479:B:LEU:HG	3	0.29
(1,615)	2:480:B:ALA:H	2:479:B:LEU:HG	16	0.29
(1,615)	2:480:B:ALA:H	2:479:B:LEU:HG	17	0.29
(1,615)	2:480:B:ALA:H	2:479:B:LEU:HG	24	0.29
(1,522)	1:116:A:THR:H	1:125:A:GLY:HA2	21	0.29
(1,522)	1:116:A:THR:H	1:125:A:GLY:HA3	21	0.29
(1,465)	1:52:A:GLN:H	1:51:A:VAL:H	4	0.29
(1,328)	1:143:A:GLU:H	1:139:A:ALA:HB1	5	0.29
(1,328)	1:143:A:GLU:H	1:139:A:ALA:HB2	5	0.29
(1,328)	1:143:A:GLU:H	1:139:A:ALA:HB3	5	0.29
(1,167)	1:86:A:ARG:H	1:85:A:ILE:HB	21	0.29
(1,75)	1:51:A:VAL:H	1:50:A:VAL:H	3	0.29
(1,75)	1:51:A:VAL:H	1:50:A:VAL:H	8	0.29
(1,75)	1:51:A:VAL:H	1:50:A:VAL:H	24	0.29
(1,69)	1:49:A:ALA:H	1:48:A:THR:HG22	13	0.29
(1,992)	1:129:A:ALA:H	2:457:B:HIS:H	14	0.28
(1,992)	1:129:A:ALA:H	2:457:B:HIS:H	20	0.28
(1,969)	1:71:A:ALA:HB1	2:453:B:ARG:HB2	2	0.28
(1,969)	1:71:A:ALA:HB1	2:453:B:ARG:HB3	2	0.28
(1,969)	1:71:A:ALA:HB2	2:453:B:ARG:HB2	2	0.28
(1,969)	1:71:A:ALA:HB2	2:453:B:ARG:HB3	2	0.28
(1,969)	1:71:A:ALA:HB3	2:453:B:ARG:HB2	2	0.28
(1,969)	1:71:A:ALA:HB3	2:453:B:ARG:HB3	2	0.28
(1,969)	1:71:A:ALA:HB1	2:453:B:ARG:HB2	9	0.28
(1,969)	1:71:A:ALA:HB1	2:453:B:ARG:HB3	9	0.28
(1,969)	1:71:A:ALA:HB2	2:453:B:ARG:HB2	9	0.28
(1,969)	1:71:A:ALA:HB2	2:453:B:ARG:HB3	9	0.28
(1,969)	1:71:A:ALA:HB3	2:453:B:ARG:HB2	9	0.28
(1,969)	1:71:A:ALA:HB3	2:453:B:ARG:HB3	9	0.28
(1,925)	1:145:A:ILE:HD11	1:117:A:PHE:HB3	7	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,925)	1:145:A:ILE:HD12	1:117:A:PHE:HB3	7	0.28
(1,925)	1:145:A:ILE:HD13	1:117:A:PHE:HB3	7	0.28
(1,925)	1:145:A:ILE:HD11	1:117:A:PHE:HB3	20	0.28
(1,925)	1:145:A:ILE:HD12	1:117:A:PHE:HB3	20	0.28
(1,925)	1:145:A:ILE:HD13	1:117:A:PHE:HB3	20	0.28
(1,845)	1:108:A:SER:HB2	1:110:A:PRO:HA	10	0.28
(1,845)	1:108:A:SER:HB3	1:110:A:PRO:HA	10	0.28
(1,845)	1:108:A:SER:HB2	1:110:A:PRO:HA	17	0.28
(1,845)	1:108:A:SER:HB3	1:110:A:PRO:HA	17	0.28
(1,822)	1:94:A:ARG:HA	1:90:A:LEU:HA	4	0.28
(1,705)	1:53:A:LEU:HD11	1:127:A:ASN:HB2	17	0.28
(1,705)	1:53:A:LEU:HD11	1:127:A:ASN:HB3	17	0.28
(1,705)	1:53:A:LEU:HD12	1:127:A:ASN:HB2	17	0.28
(1,705)	1:53:A:LEU:HD12	1:127:A:ASN:HB3	17	0.28
(1,705)	1:53:A:LEU:HD13	1:127:A:ASN:HB2	17	0.28
(1,705)	1:53:A:LEU:HD13	1:127:A:ASN:HB3	17	0.28
(1,705)	1:53:A:LEU:HD21	1:127:A:ASN:HB2	17	0.28
(1,705)	1:53:A:LEU:HD21	1:127:A:ASN:HB3	17	0.28
(1,705)	1:53:A:LEU:HD22	1:127:A:ASN:HB2	17	0.28
(1,705)	1:53:A:LEU:HD22	1:127:A:ASN:HB3	17	0.28
(1,705)	1:53:A:LEU:HD23	1:127:A:ASN:HB2	17	0.28
(1,705)	1:53:A:LEU:HD23	1:127:A:ASN:HB3	17	0.28
(1,522)	1:116:A:THR:H	1:125:A:GLY:HA2	11	0.28
(1,522)	1:116:A:THR:H	1:125:A:GLY:HA3	11	0.28
(1,465)	1:52:A:GLN:H	1:51:A:VAL:H	3	0.28
(1,465)	1:52:A:GLN:H	1:51:A:VAL:H	6	0.28
(1,465)	1:52:A:GLN:H	1:51:A:VAL:H	20	0.28
(1,435)	1:125:A:GLY:H	1:54:A:TYR:HB2	5	0.28
(1,435)	1:125:A:GLY:H	1:54:A:TYR:HB3	5	0.28
(1,241)	1:109:A:THR:H	1:108:A:SER:H	20	0.28
(1,191)	1:95:A:LEU:H	1:94:A:ARG:H	3	0.28
(1,191)	1:95:A:LEU:H	1:94:A:ARG:H	10	0.28
(1,75)	1:51:A:VAL:H	1:50:A:VAL:H	1	0.28
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD11	2	0.27
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD12	2	0.27
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD13	2	0.27
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD21	2	0.27
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD22	2	0.27
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD23	2	0.27
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD11	2	0.27
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD12	2	0.27
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD13	2	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD21	2	0.27
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD22	2	0.27
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD23	2	0.27
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD11	19	0.27
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD12	19	0.27
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD13	19	0.27
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD21	19	0.27
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD22	19	0.27
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD23	19	0.27
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD11	19	0.27
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD12	19	0.27
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD13	19	0.27
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD21	19	0.27
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD22	19	0.27
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD23	19	0.27
(1,992)	1:129:A:ALA:H	2:457:B:HIS:H	1	0.27
(1,992)	1:129:A:ALA:H	2:457:B:HIS:H	17	0.27
(1,992)	1:129:A:ALA:H	2:457:B:HIS:H	22	0.27
(1,989)	1:129:A:ALA:HB3	2:454:B:PHE:HA	19	0.27
(1,969)	1:71:A:ALA:HB1	2:453:B:ARG:HB2	6	0.27
(1,969)	1:71:A:ALA:HB1	2:453:B:ARG:HB3	6	0.27
(1,969)	1:71:A:ALA:HB2	2:453:B:ARG:HB2	6	0.27
(1,969)	1:71:A:ALA:HB2	2:453:B:ARG:HB3	6	0.27
(1,969)	1:71:A:ALA:HB3	2:453:B:ARG:HB2	6	0.27
(1,969)	1:71:A:ALA:HB3	2:453:B:ARG:HB3	6	0.27
(1,969)	1:71:A:ALA:HB1	2:453:B:ARG:HB2	11	0.27
(1,969)	1:71:A:ALA:HB1	2:453:B:ARG:HB3	11	0.27
(1,969)	1:71:A:ALA:HB2	2:453:B:ARG:HB2	11	0.27
(1,969)	1:71:A:ALA:HB2	2:453:B:ARG:HB3	11	0.27
(1,969)	1:71:A:ALA:HB3	2:453:B:ARG:HB2	11	0.27
(1,969)	1:71:A:ALA:HB3	2:453:B:ARG:HB3	11	0.27
(1,969)	1:71:A:ALA:HB1	2:453:B:ARG:HB2	12	0.27
(1,969)	1:71:A:ALA:HB1	2:453:B:ARG:HB3	12	0.27
(1,969)	1:71:A:ALA:HB2	2:453:B:ARG:HB2	12	0.27
(1,969)	1:71:A:ALA:HB2	2:453:B:ARG:HB3	12	0.27
(1,969)	1:71:A:ALA:HB3	2:453:B:ARG:HB2	12	0.27
(1,969)	1:71:A:ALA:HB3	2:453:B:ARG:HB3	12	0.27
(1,969)	1:71:A:ALA:HB1	2:453:B:ARG:HB2	18	0.27
(1,969)	1:71:A:ALA:HB1	2:453:B:ARG:HB3	18	0.27
(1,969)	1:71:A:ALA:HB2	2:453:B:ARG:HB2	18	0.27
(1,969)	1:71:A:ALA:HB2	2:453:B:ARG:HB3	18	0.27
(1,969)	1:71:A:ALA:HB3	2:453:B:ARG:HB2	18	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,969)	1:71:A:ALA:HB3	2:453:B:ARG:HB3	18	0.27
(1,969)	1:71:A:ALA:HB1	2:453:B:ARG:HB2	23	0.27
(1,969)	1:71:A:ALA:HB1	2:453:B:ARG:HB3	23	0.27
(1,969)	1:71:A:ALA:HB2	2:453:B:ARG:HB2	23	0.27
(1,969)	1:71:A:ALA:HB2	2:453:B:ARG:HB3	23	0.27
(1,969)	1:71:A:ALA:HB3	2:453:B:ARG:HB2	23	0.27
(1,969)	1:71:A:ALA:HB3	2:453:B:ARG:HB3	23	0.27
(1,944)	2:458:B:PRO:HA	2:460:B:SER:HB2	14	0.27
(1,944)	2:458:B:PRO:HA	2:460:B:SER:HB3	14	0.27
(1,925)	1:145:A:ILE:HD11	1:117:A:PHE:HB3	8	0.27
(1,925)	1:145:A:ILE:HD12	1:117:A:PHE:HB3	8	0.27
(1,925)	1:145:A:ILE:HD13	1:117:A:PHE:HB3	8	0.27
(1,865)	1:123:A:GLN:HG2	1:122:A:CYS:HB2	17	0.27
(1,865)	1:123:A:GLN:HG2	1:122:A:CYS:HB3	17	0.27
(1,865)	1:123:A:GLN:HG3	1:122:A:CYS:HB2	17	0.27
(1,865)	1:123:A:GLN:HG3	1:122:A:CYS:HB3	17	0.27
(1,845)	1:108:A:SER:HB2	1:110:A:PRO:HA	3	0.27
(1,845)	1:108:A:SER:HB3	1:110:A:PRO:HA	3	0.27
(1,845)	1:108:A:SER:HB2	1:110:A:PRO:HA	5	0.27
(1,845)	1:108:A:SER:HB3	1:110:A:PRO:HA	5	0.27
(1,845)	1:108:A:SER:HB2	1:110:A:PRO:HA	9	0.27
(1,845)	1:108:A:SER:HB3	1:110:A:PRO:HA	9	0.27
(1,822)	1:94:A:ARG:HA	1:90:A:LEU:HA	1	0.27
(1,822)	1:94:A:ARG:HA	1:90:A:LEU:HA	8	0.27
(1,705)	1:53:A:LEU:HD11	1:127:A:ASN:HB2	6	0.27
(1,705)	1:53:A:LEU:HD11	1:127:A:ASN:HB3	6	0.27
(1,705)	1:53:A:LEU:HD12	1:127:A:ASN:HB2	6	0.27
(1,705)	1:53:A:LEU:HD12	1:127:A:ASN:HB3	6	0.27
(1,705)	1:53:A:LEU:HD13	1:127:A:ASN:HB2	6	0.27
(1,705)	1:53:A:LEU:HD13	1:127:A:ASN:HB3	6	0.27
(1,705)	1:53:A:LEU:HD21	1:127:A:ASN:HB2	6	0.27
(1,705)	1:53:A:LEU:HD21	1:127:A:ASN:HB3	6	0.27
(1,705)	1:53:A:LEU:HD22	1:127:A:ASN:HB2	6	0.27
(1,705)	1:53:A:LEU:HD22	1:127:A:ASN:HB3	6	0.27
(1,705)	1:53:A:LEU:HD23	1:127:A:ASN:HB2	6	0.27
(1,705)	1:53:A:LEU:HD23	1:127:A:ASN:HB3	6	0.27
(1,705)	1:53:A:LEU:HD11	1:127:A:ASN:HB2	7	0.27
(1,705)	1:53:A:LEU:HD11	1:127:A:ASN:HB3	7	0.27
(1,705)	1:53:A:LEU:HD12	1:127:A:ASN:HB2	7	0.27
(1,705)	1:53:A:LEU:HD12	1:127:A:ASN:HB3	7	0.27
(1,705)	1:53:A:LEU:HD13	1:127:A:ASN:HB2	7	0.27
(1,705)	1:53:A:LEU:HD13	1:127:A:ASN:HB3	7	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,705)	1:53:A:LEU:HD21	1:127:A:ASN:HB2	7	0.27
(1,705)	1:53:A:LEU:HD21	1:127:A:ASN:HB3	7	0.27
(1,705)	1:53:A:LEU:HD22	1:127:A:ASN:HB2	7	0.27
(1,705)	1:53:A:LEU:HD22	1:127:A:ASN:HB3	7	0.27
(1,705)	1:53:A:LEU:HD23	1:127:A:ASN:HB2	7	0.27
(1,705)	1:53:A:LEU:HD23	1:127:A:ASN:HB3	7	0.27
(1,705)	1:53:A:LEU:HD11	1:127:A:ASN:HB2	10	0.27
(1,705)	1:53:A:LEU:HD11	1:127:A:ASN:HB3	10	0.27
(1,705)	1:53:A:LEU:HD12	1:127:A:ASN:HB2	10	0.27
(1,705)	1:53:A:LEU:HD12	1:127:A:ASN:HB3	10	0.27
(1,705)	1:53:A:LEU:HD13	1:127:A:ASN:HB2	10	0.27
(1,705)	1:53:A:LEU:HD13	1:127:A:ASN:HB3	10	0.27
(1,705)	1:53:A:LEU:HD21	1:127:A:ASN:HB2	10	0.27
(1,705)	1:53:A:LEU:HD21	1:127:A:ASN:HB3	10	0.27
(1,705)	1:53:A:LEU:HD22	1:127:A:ASN:HB2	10	0.27
(1,705)	1:53:A:LEU:HD22	1:127:A:ASN:HB3	10	0.27
(1,705)	1:53:A:LEU:HD23	1:127:A:ASN:HB2	10	0.27
(1,705)	1:53:A:LEU:HD23	1:127:A:ASN:HB3	10	0.27
(1,638)	1:34:A:ARG:HB2	1:74:A:PHE:HD1	22	0.27
(1,638)	1:34:A:ARG:HB2	1:74:A:PHE:HD2	22	0.27
(1,638)	1:34:A:ARG:HB3	1:74:A:PHE:HD1	22	0.27
(1,638)	1:34:A:ARG:HB3	1:74:A:PHE:HD2	22	0.27
(1,435)	1:125:A:GLY:H	1:54:A:TYR:HB2	24	0.27
(1,435)	1:125:A:GLY:H	1:54:A:TYR:HB3	24	0.27
(1,403)	1:74:A:PHE:H	1:47:A:ALA:HA	1	0.27
(1,403)	1:74:A:PHE:H	1:47:A:ALA:HA	6	0.27
(1,328)	1:143:A:GLU:H	1:139:A:ALA:HB1	2	0.27
(1,328)	1:143:A:GLU:H	1:139:A:ALA:HB2	2	0.27
(1,328)	1:143:A:GLU:H	1:139:A:ALA:HB3	2	0.27
(1,328)	1:143:A:GLU:H	1:139:A:ALA:HB1	4	0.27
(1,328)	1:143:A:GLU:H	1:139:A:ALA:HB2	4	0.27
(1,328)	1:143:A:GLU:H	1:139:A:ALA:HB3	4	0.27
(1,328)	1:143:A:GLU:H	1:139:A:ALA:HB1	14	0.27
(1,328)	1:143:A:GLU:H	1:139:A:ALA:HB2	14	0.27
(1,328)	1:143:A:GLU:H	1:139:A:ALA:HB3	14	0.27
(1,259)	1:118:A:ALA:H	1:117:A:PHE:HB3	14	0.27
(1,191)	1:95:A:LEU:H	1:94:A:ARG:H	17	0.27
(1,191)	1:95:A:LEU:H	1:94:A:ARG:H	18	0.27
(1,75)	1:51:A:VAL:H	1:50:A:VAL:H	10	0.27
(1,1007)	2:474:B:SER:H	1:102:A:TYR:HA	15	0.26
(1,992)	1:129:A:ALA:H	2:457:B:HIS:H	3	0.26
(1,992)	1:129:A:ALA:H	2:457:B:HIS:H	10	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,969)	1:71:A:ALA:HB1	2:453:B:ARG:HB2	1	0.26
(1,969)	1:71:A:ALA:HB1	2:453:B:ARG:HB3	1	0.26
(1,969)	1:71:A:ALA:HB2	2:453:B:ARG:HB2	1	0.26
(1,969)	1:71:A:ALA:HB2	2:453:B:ARG:HB3	1	0.26
(1,969)	1:71:A:ALA:HB3	2:453:B:ARG:HB2	1	0.26
(1,969)	1:71:A:ALA:HB3	2:453:B:ARG:HB3	1	0.26
(1,969)	1:71:A:ALA:HB1	2:453:B:ARG:HB2	5	0.26
(1,969)	1:71:A:ALA:HB1	2:453:B:ARG:HB3	5	0.26
(1,969)	1:71:A:ALA:HB2	2:453:B:ARG:HB2	5	0.26
(1,969)	1:71:A:ALA:HB2	2:453:B:ARG:HB3	5	0.26
(1,969)	1:71:A:ALA:HB3	2:453:B:ARG:HB2	5	0.26
(1,969)	1:71:A:ALA:HB3	2:453:B:ARG:HB3	5	0.26
(1,969)	1:71:A:ALA:HB1	2:453:B:ARG:HB2	15	0.26
(1,969)	1:71:A:ALA:HB1	2:453:B:ARG:HB3	15	0.26
(1,969)	1:71:A:ALA:HB2	2:453:B:ARG:HB2	15	0.26
(1,969)	1:71:A:ALA:HB2	2:453:B:ARG:HB3	15	0.26
(1,969)	1:71:A:ALA:HB3	2:453:B:ARG:HB2	15	0.26
(1,969)	1:71:A:ALA:HB3	2:453:B:ARG:HB3	15	0.26
(1,944)	2:458:B:PRO:HA	2:460:B:SER:HB2	3	0.26
(1,944)	2:458:B:PRO:HA	2:460:B:SER:HB3	3	0.26
(1,944)	2:458:B:PRO:HA	2:460:B:SER:HB2	17	0.26
(1,944)	2:458:B:PRO:HA	2:460:B:SER:HB3	17	0.26
(1,925)	1:145:A:ILE:HD11	1:117:A:PHE:HB3	5	0.26
(1,925)	1:145:A:ILE:HD12	1:117:A:PHE:HB3	5	0.26
(1,925)	1:145:A:ILE:HD13	1:117:A:PHE:HB3	5	0.26
(1,846)	1:108:A:SER:HB2	1:137:A:PHE:HB2	16	0.26
(1,846)	1:108:A:SER:HB2	1:137:A:PHE:HB3	16	0.26
(1,846)	1:108:A:SER:HB3	1:137:A:PHE:HB2	16	0.26
(1,846)	1:108:A:SER:HB3	1:137:A:PHE:HB3	16	0.26
(1,822)	1:94:A:ARG:HA	1:90:A:LEU:HA	5	0.26
(1,822)	1:94:A:ARG:HA	1:90:A:LEU:HA	19	0.26
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD11	12	0.26
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD12	12	0.26
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD13	12	0.26
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD21	12	0.26
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD22	12	0.26
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD23	12	0.26
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD11	19	0.26
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD12	19	0.26
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD13	19	0.26
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD21	19	0.26
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD22	19	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD23	19	0.26
(1,783)	1:81:A:LYS:HG2	1:80:A:GLN:HA	6	0.26
(1,783)	1:81:A:LYS:HG3	1:80:A:GLN:HA	6	0.26
(1,783)	1:81:A:LYS:HG2	1:80:A:GLN:HA	14	0.26
(1,783)	1:81:A:LYS:HG3	1:80:A:GLN:HA	14	0.26
(1,741)	1:71:A:ALA:HB1	1:35:A:LEU:HB2	3	0.26
(1,741)	1:71:A:ALA:HB1	1:35:A:LEU:HB3	3	0.26
(1,741)	1:71:A:ALA:HB2	1:35:A:LEU:HB2	3	0.26
(1,741)	1:71:A:ALA:HB2	1:35:A:LEU:HB3	3	0.26
(1,741)	1:71:A:ALA:HB3	1:35:A:LEU:HB2	3	0.26
(1,741)	1:71:A:ALA:HB3	1:35:A:LEU:HB3	3	0.26
(1,705)	1:53:A:LEU:HD11	1:127:A:ASN:HB2	8	0.26
(1,705)	1:53:A:LEU:HD11	1:127:A:ASN:HB3	8	0.26
(1,705)	1:53:A:LEU:HD12	1:127:A:ASN:HB2	8	0.26
(1,705)	1:53:A:LEU:HD12	1:127:A:ASN:HB3	8	0.26
(1,705)	1:53:A:LEU:HD13	1:127:A:ASN:HB2	8	0.26
(1,705)	1:53:A:LEU:HD13	1:127:A:ASN:HB3	8	0.26
(1,705)	1:53:A:LEU:HD21	1:127:A:ASN:HB2	8	0.26
(1,705)	1:53:A:LEU:HD21	1:127:A:ASN:HB3	8	0.26
(1,705)	1:53:A:LEU:HD22	1:127:A:ASN:HB2	8	0.26
(1,705)	1:53:A:LEU:HD22	1:127:A:ASN:HB3	8	0.26
(1,705)	1:53:A:LEU:HD23	1:127:A:ASN:HB2	8	0.26
(1,705)	1:53:A:LEU:HD23	1:127:A:ASN:HB3	8	0.26
(1,669)	1:47:A:ALA:HB1	1:137:A:PHE:HA	19	0.26
(1,669)	1:47:A:ALA:HB2	1:137:A:PHE:HA	19	0.26
(1,669)	1:47:A:ALA:HB3	1:137:A:PHE:HA	19	0.26
(1,638)	1:34:A:ARG:HB2	1:74:A:PHE:HD1	2	0.26
(1,638)	1:34:A:ARG:HB2	1:74:A:PHE:HD2	2	0.26
(1,638)	1:34:A:ARG:HB3	1:74:A:PHE:HD1	2	0.26
(1,638)	1:34:A:ARG:HB3	1:74:A:PHE:HD2	2	0.26
(1,584)	2:468:B:TYR:H	2:467:B:PRO:HG2	1	0.26
(1,584)	2:468:B:TYR:H	2:467:B:PRO:HG3	1	0.26
(1,522)	1:116:A:THR:H	1:125:A:GLY:HA2	7	0.26
(1,522)	1:116:A:THR:H	1:125:A:GLY:HA3	7	0.26
(1,522)	1:116:A:THR:H	1:125:A:GLY:HA2	18	0.26
(1,522)	1:116:A:THR:H	1:125:A:GLY:HA3	18	0.26
(1,483)	1:87:A:LEU:H	1:97:A:TRP:HZ2	4	0.26
(1,465)	1:52:A:GLN:H	1:51:A:VAL:H	7	0.26
(1,465)	1:52:A:GLN:H	1:51:A:VAL:H	15	0.26
(1,465)	1:52:A:GLN:H	1:51:A:VAL:H	16	0.26
(1,435)	1:125:A:GLY:H	1:54:A:TYR:HB2	14	0.26
(1,435)	1:125:A:GLY:H	1:54:A:TYR:HB3	14	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,403)	1:74:A:PHE:H	1:47:A:ALA:HA	19	0.26
(1,399)	1:72:A:VAL:H	1:50:A:VAL:HB	10	0.26
(1,328)	1:143:A:GLU:H	1:139:A:ALA:HB1	12	0.26
(1,328)	1:143:A:GLU:H	1:139:A:ALA:HB2	12	0.26
(1,328)	1:143:A:GLU:H	1:139:A:ALA:HB3	12	0.26
(1,328)	1:143:A:GLU:H	1:139:A:ALA:HB1	19	0.26
(1,328)	1:143:A:GLU:H	1:139:A:ALA:HB2	19	0.26
(1,328)	1:143:A:GLU:H	1:139:A:ALA:HB3	19	0.26
(1,328)	1:143:A:GLU:H	1:139:A:ALA:HB1	20	0.26
(1,328)	1:143:A:GLU:H	1:139:A:ALA:HB2	20	0.26
(1,328)	1:143:A:GLU:H	1:139:A:ALA:HB3	20	0.26
(1,167)	1:86:A:ARG:H	1:85:A:ILE:HB	4	0.26
(1,992)	1:129:A:ALA:H	2:457:B:HIS:H	7	0.25
(1,992)	1:129:A:ALA:H	2:457:B:HIS:H	18	0.25
(1,969)	1:71:A:ALA:HB1	2:453:B:ARG:HB2	14	0.25
(1,969)	1:71:A:ALA:HB1	2:453:B:ARG:HB3	14	0.25
(1,969)	1:71:A:ALA:HB2	2:453:B:ARG:HB2	14	0.25
(1,969)	1:71:A:ALA:HB2	2:453:B:ARG:HB3	14	0.25
(1,969)	1:71:A:ALA:HB3	2:453:B:ARG:HB2	14	0.25
(1,969)	1:71:A:ALA:HB3	2:453:B:ARG:HB3	14	0.25
(1,969)	1:71:A:ALA:HB1	2:453:B:ARG:HB2	20	0.25
(1,969)	1:71:A:ALA:HB1	2:453:B:ARG:HB3	20	0.25
(1,969)	1:71:A:ALA:HB2	2:453:B:ARG:HB2	20	0.25
(1,969)	1:71:A:ALA:HB2	2:453:B:ARG:HB3	20	0.25
(1,969)	1:71:A:ALA:HB3	2:453:B:ARG:HB2	20	0.25
(1,969)	1:71:A:ALA:HB3	2:453:B:ARG:HB3	20	0.25
(1,944)	2:458:B:PRO:HA	2:460:B:SER:HB2	5	0.25
(1,944)	2:458:B:PRO:HA	2:460:B:SER:HB3	5	0.25
(1,928)	1:145:A:ILE:HD11	1:117:A:PHE:HZ	9	0.25
(1,928)	1:145:A:ILE:HD12	1:117:A:PHE:HZ	9	0.25
(1,928)	1:145:A:ILE:HD13	1:117:A:PHE:HZ	9	0.25
(1,926)	1:145:A:ILE:HD11	1:117:A:PHE:HB2	11	0.25
(1,926)	1:145:A:ILE:HD12	1:117:A:PHE:HB2	11	0.25
(1,926)	1:145:A:ILE:HD13	1:117:A:PHE:HB2	11	0.25
(1,877)	1:127:A:ASN:HB2	1:113:A:PHE:HB2	3	0.25
(1,877)	1:127:A:ASN:HB2	1:113:A:PHE:HB3	3	0.25
(1,877)	1:127:A:ASN:HB3	1:113:A:PHE:HB2	3	0.25
(1,877)	1:127:A:ASN:HB3	1:113:A:PHE:HB3	3	0.25
(1,847)	1:109:A:THR:HB	1:115:A:HIS:HB2	11	0.25
(1,847)	1:109:A:THR:HB	1:115:A:HIS:HB3	11	0.25
(1,846)	1:108:A:SER:HB2	1:137:A:PHE:HB2	3	0.25
(1,846)	1:108:A:SER:HB2	1:137:A:PHE:HB3	3	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,846)	1:108:A:SER:HB3	1:137:A:PHE:HB2	3	0.25
(1,846)	1:108:A:SER:HB3	1:137:A:PHE:HB3	3	0.25
(1,845)	1:108:A:SER:HB2	1:110:A:PRO:HA	16	0.25
(1,845)	1:108:A:SER:HB3	1:110:A:PRO:HA	16	0.25
(1,845)	1:108:A:SER:HB2	1:110:A:PRO:HA	23	0.25
(1,845)	1:108:A:SER:HB3	1:110:A:PRO:HA	23	0.25
(1,845)	1:108:A:SER:HB2	1:110:A:PRO:HA	24	0.25
(1,845)	1:108:A:SER:HB3	1:110:A:PRO:HA	24	0.25
(1,705)	1:53:A:LEU:HD11	1:127:A:ASN:HB2	5	0.25
(1,705)	1:53:A:LEU:HD11	1:127:A:ASN:HB3	5	0.25
(1,705)	1:53:A:LEU:HD12	1:127:A:ASN:HB2	5	0.25
(1,705)	1:53:A:LEU:HD12	1:127:A:ASN:HB3	5	0.25
(1,705)	1:53:A:LEU:HD13	1:127:A:ASN:HB2	5	0.25
(1,705)	1:53:A:LEU:HD13	1:127:A:ASN:HB3	5	0.25
(1,705)	1:53:A:LEU:HD21	1:127:A:ASN:HB2	5	0.25
(1,705)	1:53:A:LEU:HD21	1:127:A:ASN:HB3	5	0.25
(1,705)	1:53:A:LEU:HD22	1:127:A:ASN:HB2	5	0.25
(1,705)	1:53:A:LEU:HD22	1:127:A:ASN:HB3	5	0.25
(1,705)	1:53:A:LEU:HD23	1:127:A:ASN:HB2	5	0.25
(1,705)	1:53:A:LEU:HD23	1:127:A:ASN:HB3	5	0.25
(1,705)	1:53:A:LEU:HD11	1:127:A:ASN:HB2	9	0.25
(1,705)	1:53:A:LEU:HD11	1:127:A:ASN:HB3	9	0.25
(1,705)	1:53:A:LEU:HD12	1:127:A:ASN:HB2	9	0.25
(1,705)	1:53:A:LEU:HD12	1:127:A:ASN:HB3	9	0.25
(1,705)	1:53:A:LEU:HD13	1:127:A:ASN:HB2	9	0.25
(1,705)	1:53:A:LEU:HD13	1:127:A:ASN:HB3	9	0.25
(1,705)	1:53:A:LEU:HD21	1:127:A:ASN:HB2	9	0.25
(1,705)	1:53:A:LEU:HD21	1:127:A:ASN:HB3	9	0.25
(1,705)	1:53:A:LEU:HD22	1:127:A:ASN:HB2	9	0.25
(1,705)	1:53:A:LEU:HD22	1:127:A:ASN:HB3	9	0.25
(1,705)	1:53:A:LEU:HD23	1:127:A:ASN:HB2	9	0.25
(1,705)	1:53:A:LEU:HD23	1:127:A:ASN:HB3	9	0.25
(1,705)	1:53:A:LEU:HD11	1:127:A:ASN:HB2	15	0.25
(1,705)	1:53:A:LEU:HD11	1:127:A:ASN:HB3	15	0.25
(1,705)	1:53:A:LEU:HD12	1:127:A:ASN:HB2	15	0.25
(1,705)	1:53:A:LEU:HD12	1:127:A:ASN:HB3	15	0.25
(1,705)	1:53:A:LEU:HD13	1:127:A:ASN:HB2	15	0.25
(1,705)	1:53:A:LEU:HD13	1:127:A:ASN:HB3	15	0.25
(1,705)	1:53:A:LEU:HD21	1:127:A:ASN:HB2	15	0.25
(1,705)	1:53:A:LEU:HD21	1:127:A:ASN:HB3	15	0.25
(1,705)	1:53:A:LEU:HD22	1:127:A:ASN:HB2	15	0.25
(1,705)	1:53:A:LEU:HD22	1:127:A:ASN:HB3	15	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,705)	1:53:A:LEU:HD23	1:127:A:ASN:HB2	15	0.25
(1,705)	1:53:A:LEU:HD23	1:127:A:ASN:HB3	15	0.25
(1,638)	1:34:A:ARG:HB2	1:74:A:PHE:HD1	23	0.25
(1,638)	1:34:A:ARG:HB2	1:74:A:PHE:HD2	23	0.25
(1,638)	1:34:A:ARG:HB3	1:74:A:PHE:HD1	23	0.25
(1,638)	1:34:A:ARG:HB3	1:74:A:PHE:HD2	23	0.25
(1,522)	1:116:A:THR:H	1:125:A:GLY:HA2	8	0.25
(1,522)	1:116:A:THR:H	1:125:A:GLY:HA3	8	0.25
(1,465)	1:52:A:GLN:H	1:51:A:VAL:H	2	0.25
(1,465)	1:52:A:GLN:H	1:51:A:VAL:H	12	0.25
(1,435)	1:125:A:GLY:H	1:54:A:TYR:HB2	4	0.25
(1,435)	1:125:A:GLY:H	1:54:A:TYR:HB3	4	0.25
(1,412)	1:84:A:PHE:H	1:76:A:LYS:HB2	14	0.25
(1,412)	1:84:A:PHE:H	1:76:A:LYS:HB3	14	0.25
(1,399)	1:72:A:VAL:H	1:50:A:VAL:HB	5	0.25
(1,399)	1:72:A:VAL:H	1:50:A:VAL:HB	8	0.25
(1,399)	1:72:A:VAL:H	1:50:A:VAL:HB	9	0.25
(1,328)	1:143:A:GLU:H	1:139:A:ALA:HB1	1	0.25
(1,328)	1:143:A:GLU:H	1:139:A:ALA:HB2	1	0.25
(1,328)	1:143:A:GLU:H	1:139:A:ALA:HB3	1	0.25
(1,328)	1:143:A:GLU:H	1:139:A:ALA:HB1	3	0.25
(1,328)	1:143:A:GLU:H	1:139:A:ALA:HB2	3	0.25
(1,328)	1:143:A:GLU:H	1:139:A:ALA:HB3	3	0.25
(1,259)	1:118:A:ALA:H	1:117:A:PHE:HB3	10	0.25
(1,259)	1:118:A:ALA:H	1:117:A:PHE:HB3	13	0.25
(1,259)	1:118:A:ALA:H	1:117:A:PHE:HB3	20	0.25
(1,241)	1:109:A:THR:H	1:108:A:SER:H	24	0.25
(1,191)	1:95:A:LEU:H	1:94:A:ARG:H	15	0.25
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD11	15	0.24
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD12	15	0.24
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD13	15	0.24
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD21	15	0.24
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD22	15	0.24
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD23	15	0.24
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD11	15	0.24
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD12	15	0.24
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD13	15	0.24
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD21	15	0.24
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD22	15	0.24
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD23	15	0.24
(1,992)	1:129:A:ALA:H	2:457:B:HIS:H	2	0.24
(1,992)	1:129:A:ALA:H	2:457:B:HIS:H	12	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,969)	1:71:A:ALA:HB1	2:453:B:ARG:HB2	3	0.24
(1,969)	1:71:A:ALA:HB1	2:453:B:ARG:HB3	3	0.24
(1,969)	1:71:A:ALA:HB2	2:453:B:ARG:HB2	3	0.24
(1,969)	1:71:A:ALA:HB2	2:453:B:ARG:HB3	3	0.24
(1,969)	1:71:A:ALA:HB3	2:453:B:ARG:HB2	3	0.24
(1,969)	1:71:A:ALA:HB3	2:453:B:ARG:HB3	3	0.24
(1,969)	1:71:A:ALA:HB1	2:453:B:ARG:HB2	17	0.24
(1,969)	1:71:A:ALA:HB1	2:453:B:ARG:HB3	17	0.24
(1,969)	1:71:A:ALA:HB2	2:453:B:ARG:HB2	17	0.24
(1,969)	1:71:A:ALA:HB2	2:453:B:ARG:HB3	17	0.24
(1,969)	1:71:A:ALA:HB3	2:453:B:ARG:HB2	17	0.24
(1,969)	1:71:A:ALA:HB3	2:453:B:ARG:HB3	17	0.24
(1,969)	1:71:A:ALA:HB1	2:453:B:ARG:HB2	22	0.24
(1,969)	1:71:A:ALA:HB1	2:453:B:ARG:HB3	22	0.24
(1,969)	1:71:A:ALA:HB2	2:453:B:ARG:HB2	22	0.24
(1,969)	1:71:A:ALA:HB2	2:453:B:ARG:HB3	22	0.24
(1,969)	1:71:A:ALA:HB3	2:453:B:ARG:HB2	22	0.24
(1,969)	1:71:A:ALA:HB3	2:453:B:ARG:HB3	22	0.24
(1,925)	1:145:A:ILE:HD11	1:117:A:PHE:HB3	3	0.24
(1,925)	1:145:A:ILE:HD12	1:117:A:PHE:HB3	3	0.24
(1,925)	1:145:A:ILE:HD13	1:117:A:PHE:HB3	3	0.24
(1,877)	1:127:A:ASN:HB2	1:113:A:PHE:HB2	22	0.24
(1,877)	1:127:A:ASN:HB2	1:113:A:PHE:HB3	22	0.24
(1,877)	1:127:A:ASN:HB3	1:113:A:PHE:HB2	22	0.24
(1,877)	1:127:A:ASN:HB3	1:113:A:PHE:HB3	22	0.24
(1,822)	1:94:A:ARG:HA	1:90:A:LEU:HA	2	0.24
(1,822)	1:94:A:ARG:HA	1:90:A:LEU:HA	3	0.24
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD11	8	0.24
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD12	8	0.24
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD13	8	0.24
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD21	8	0.24
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD22	8	0.24
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD23	8	0.24
(1,741)	1:71:A:ALA:HB1	1:35:A:LEU:HB2	9	0.24
(1,741)	1:71:A:ALA:HB1	1:35:A:LEU:HB3	9	0.24
(1,741)	1:71:A:ALA:HB2	1:35:A:LEU:HB2	9	0.24
(1,741)	1:71:A:ALA:HB2	1:35:A:LEU:HB3	9	0.24
(1,741)	1:71:A:ALA:HB3	1:35:A:LEU:HB2	9	0.24
(1,741)	1:71:A:ALA:HB3	1:35:A:LEU:HB3	9	0.24
(1,741)	1:71:A:ALA:HB1	1:35:A:LEU:HB2	10	0.24
(1,741)	1:71:A:ALA:HB1	1:35:A:LEU:HB3	10	0.24
(1,741)	1:71:A:ALA:HB2	1:35:A:LEU:HB2	10	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,741)	1:71:A:ALA:HB2	1:35:A:LEU:HB3	10	0.24
(1,741)	1:71:A:ALA:HB3	1:35:A:LEU:HB2	10	0.24
(1,741)	1:71:A:ALA:HB3	1:35:A:LEU:HB3	10	0.24
(1,735)	1:65:A:THR:HG22	1:67:A:GLU:HA	14	0.24
(1,705)	1:53:A:LEU:HD11	1:127:A:ASN:HB2	21	0.24
(1,705)	1:53:A:LEU:HD11	1:127:A:ASN:HB3	21	0.24
(1,705)	1:53:A:LEU:HD12	1:127:A:ASN:HB2	21	0.24
(1,705)	1:53:A:LEU:HD12	1:127:A:ASN:HB3	21	0.24
(1,705)	1:53:A:LEU:HD13	1:127:A:ASN:HB2	21	0.24
(1,705)	1:53:A:LEU:HD13	1:127:A:ASN:HB3	21	0.24
(1,705)	1:53:A:LEU:HD21	1:127:A:ASN:HB2	21	0.24
(1,705)	1:53:A:LEU:HD21	1:127:A:ASN:HB3	21	0.24
(1,705)	1:53:A:LEU:HD22	1:127:A:ASN:HB2	21	0.24
(1,705)	1:53:A:LEU:HD22	1:127:A:ASN:HB3	21	0.24
(1,705)	1:53:A:LEU:HD23	1:127:A:ASN:HB2	21	0.24
(1,705)	1:53:A:LEU:HD23	1:127:A:ASN:HB3	21	0.24
(1,705)	1:53:A:LEU:HD11	1:127:A:ASN:HB2	22	0.24
(1,705)	1:53:A:LEU:HD11	1:127:A:ASN:HB3	22	0.24
(1,705)	1:53:A:LEU:HD12	1:127:A:ASN:HB2	22	0.24
(1,705)	1:53:A:LEU:HD12	1:127:A:ASN:HB3	22	0.24
(1,705)	1:53:A:LEU:HD13	1:127:A:ASN:HB2	22	0.24
(1,705)	1:53:A:LEU:HD13	1:127:A:ASN:HB3	22	0.24
(1,705)	1:53:A:LEU:HD21	1:127:A:ASN:HB2	22	0.24
(1,705)	1:53:A:LEU:HD21	1:127:A:ASN:HB3	22	0.24
(1,705)	1:53:A:LEU:HD22	1:127:A:ASN:HB2	22	0.24
(1,705)	1:53:A:LEU:HD22	1:127:A:ASN:HB3	22	0.24
(1,705)	1:53:A:LEU:HD23	1:127:A:ASN:HB2	22	0.24
(1,705)	1:53:A:LEU:HD23	1:127:A:ASN:HB3	22	0.24
(1,660)	1:45:A:THR:HG21	1:47:A:ALA:HA	20	0.24
(1,638)	1:34:A:ARG:HB2	1:74:A:PHE:HD1	5	0.24
(1,638)	1:34:A:ARG:HB2	1:74:A:PHE:HD2	5	0.24
(1,638)	1:34:A:ARG:HB3	1:74:A:PHE:HD1	5	0.24
(1,638)	1:34:A:ARG:HB3	1:74:A:PHE:HD2	5	0.24
(1,638)	1:34:A:ARG:HB2	1:74:A:PHE:HD1	19	0.24
(1,638)	1:34:A:ARG:HB2	1:74:A:PHE:HD2	19	0.24
(1,638)	1:34:A:ARG:HB3	1:74:A:PHE:HD1	19	0.24
(1,638)	1:34:A:ARG:HB3	1:74:A:PHE:HD2	19	0.24
(1,635)	1:33:A:GLN:HA	1:30:A:HIS:HA	21	0.24
(1,615)	2:480:B:ALA:H	2:479:B:LEU:HG	20	0.24
(1,584)	2:468:B:TYR:H	2:467:B:PRO:HG2	15	0.24
(1,584)	2:468:B:TYR:H	2:467:B:PRO:HG3	15	0.24
(1,523)	1:116:A:THR:H	1:108:A:SER:HB2	24	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,523)	1:116:A:THR:H	1:108:A:SER:HB3	24	0.24
(1,522)	1:116:A:THR:H	1:125:A:GLY:HA2	3	0.24
(1,522)	1:116:A:THR:H	1:125:A:GLY:HA3	3	0.24
(1,522)	1:116:A:THR:H	1:125:A:GLY:HA2	13	0.24
(1,522)	1:116:A:THR:H	1:125:A:GLY:HA3	13	0.24
(1,522)	1:116:A:THR:H	1:125:A:GLY:HA2	23	0.24
(1,522)	1:116:A:THR:H	1:125:A:GLY:HA3	23	0.24
(1,502)	1:104:A:GLN:H	1:102:A:TYR:HA	16	0.24
(1,465)	1:52:A:GLN:H	1:51:A:VAL:H	13	0.24
(1,465)	1:52:A:GLN:H	1:51:A:VAL:H	18	0.24
(1,465)	1:52:A:GLN:H	1:51:A:VAL:H	23	0.24
(1,457)	1:38:A:MET:H	1:34:A:ARG:HD2	1	0.24
(1,457)	1:38:A:MET:H	1:34:A:ARG:HD3	1	0.24
(1,412)	1:84:A:PHE:H	1:76:A:LYS:HB2	4	0.24
(1,412)	1:84:A:PHE:H	1:76:A:LYS:HB3	4	0.24
(1,412)	1:84:A:PHE:H	1:76:A:LYS:HB2	10	0.24
(1,412)	1:84:A:PHE:H	1:76:A:LYS:HB3	10	0.24
(1,412)	1:84:A:PHE:H	1:76:A:LYS:HB2	24	0.24
(1,412)	1:84:A:PHE:H	1:76:A:LYS:HB3	24	0.24
(1,403)	1:74:A:PHE:H	1:47:A:ALA:HA	11	0.24
(1,399)	1:72:A:VAL:H	1:50:A:VAL:HB	20	0.24
(1,328)	1:143:A:GLU:H	1:139:A:ALA:HB1	23	0.24
(1,328)	1:143:A:GLU:H	1:139:A:ALA:HB2	23	0.24
(1,328)	1:143:A:GLU:H	1:139:A:ALA:HB3	23	0.24
(1,327)	1:143:A:GLU:H	1:140:A:LEU:HD11	16	0.24
(1,327)	1:143:A:GLU:H	1:140:A:LEU:HD12	16	0.24
(1,327)	1:143:A:GLU:H	1:140:A:LEU:HD13	16	0.24
(1,327)	1:143:A:GLU:H	1:140:A:LEU:HD21	16	0.24
(1,327)	1:143:A:GLU:H	1:140:A:LEU:HD22	16	0.24
(1,327)	1:143:A:GLU:H	1:140:A:LEU:HD23	16	0.24
(1,272)	1:124:A:ALA:H	1:123:A:GLN:HG2	6	0.24
(1,272)	1:124:A:ALA:H	1:123:A:GLN:HG3	6	0.24
(1,241)	1:109:A:THR:H	1:108:A:SER:H	2	0.24
(1,241)	1:109:A:THR:H	1:108:A:SER:H	14	0.24
(1,241)	1:109:A:THR:H	1:108:A:SER:H	16	0.24
(1,241)	1:109:A:THR:H	1:108:A:SER:H	17	0.24
(1,241)	1:109:A:THR:H	1:108:A:SER:H	22	0.24
(1,241)	1:109:A:THR:H	1:108:A:SER:H	23	0.24
(1,195)	1:96:A:LEU:H	1:95:A:LEU:H	5	0.24
(1,105)	1:63:A:HIS:H	1:62:A:GLU:HA	13	0.24
(1,69)	1:49:A:ALA:H	1:48:A:THR:HG21	18	0.24
(4,77)	1:34:A:ARG:H	1:30:A:HIS:O	24	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,992)	1:129:A:ALA:H	2:457:B:HIS:H	6	0.23
(1,992)	1:129:A:ALA:H	2:457:B:HIS:H	23	0.23
(1,969)	1:71:A:ALA:HB1	2:453:B:ARG:HB2	10	0.23
(1,969)	1:71:A:ALA:HB1	2:453:B:ARG:HB3	10	0.23
(1,969)	1:71:A:ALA:HB2	2:453:B:ARG:HB2	10	0.23
(1,969)	1:71:A:ALA:HB2	2:453:B:ARG:HB3	10	0.23
(1,969)	1:71:A:ALA:HB3	2:453:B:ARG:HB2	10	0.23
(1,969)	1:71:A:ALA:HB3	2:453:B:ARG:HB3	10	0.23
(1,925)	1:145:A:ILE:HD11	1:117:A:PHE:HB3	24	0.23
(1,925)	1:145:A:ILE:HD12	1:117:A:PHE:HB3	24	0.23
(1,925)	1:145:A:ILE:HD13	1:117:A:PHE:HB3	24	0.23
(1,912)	1:141:A:VAL:HG11	1:107:A:TYR:HB3	16	0.23
(1,912)	1:141:A:VAL:HG12	1:107:A:TYR:HB3	16	0.23
(1,912)	1:141:A:VAL:HG13	1:107:A:TYR:HB3	16	0.23
(1,912)	1:141:A:VAL:HG21	1:107:A:TYR:HB3	16	0.23
(1,912)	1:141:A:VAL:HG22	1:107:A:TYR:HB3	16	0.23
(1,912)	1:141:A:VAL:HG23	1:107:A:TYR:HB3	16	0.23
(1,912)	1:141:A:VAL:HG11	1:107:A:TYR:HB2	16	0.23
(1,912)	1:141:A:VAL:HG12	1:107:A:TYR:HB2	16	0.23
(1,912)	1:141:A:VAL:HG13	1:107:A:TYR:HB2	16	0.23
(1,912)	1:141:A:VAL:HG21	1:107:A:TYR:HB2	16	0.23
(1,912)	1:141:A:VAL:HG22	1:107:A:TYR:HB2	16	0.23
(1,912)	1:141:A:VAL:HG23	1:107:A:TYR:HB2	16	0.23
(1,877)	1:127:A:ASN:HB2	1:113:A:PHE:HB2	5	0.23
(1,877)	1:127:A:ASN:HB2	1:113:A:PHE:HB3	5	0.23
(1,877)	1:127:A:ASN:HB3	1:113:A:PHE:HB2	5	0.23
(1,877)	1:127:A:ASN:HB3	1:113:A:PHE:HB3	5	0.23
(1,877)	1:127:A:ASN:HB2	1:113:A:PHE:HB2	6	0.23
(1,877)	1:127:A:ASN:HB2	1:113:A:PHE:HB3	6	0.23
(1,877)	1:127:A:ASN:HB3	1:113:A:PHE:HB2	6	0.23
(1,877)	1:127:A:ASN:HB3	1:113:A:PHE:HB3	6	0.23
(1,877)	1:127:A:ASN:HB2	1:113:A:PHE:HB2	13	0.23
(1,877)	1:127:A:ASN:HB2	1:113:A:PHE:HB3	13	0.23
(1,877)	1:127:A:ASN:HB3	1:113:A:PHE:HB2	13	0.23
(1,877)	1:127:A:ASN:HB3	1:113:A:PHE:HB3	13	0.23
(1,877)	1:127:A:ASN:HB2	1:113:A:PHE:HB2	17	0.23
(1,877)	1:127:A:ASN:HB2	1:113:A:PHE:HB3	17	0.23
(1,877)	1:127:A:ASN:HB3	1:113:A:PHE:HB2	17	0.23
(1,877)	1:127:A:ASN:HB3	1:113:A:PHE:HB3	17	0.23
(1,846)	1:108:A:SER:HB2	1:137:A:PHE:HB2	2	0.23
(1,846)	1:108:A:SER:HB2	1:137:A:PHE:HB3	2	0.23
(1,846)	1:108:A:SER:HB3	1:137:A:PHE:HB2	2	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,846)	1:108:A:SER:HB3	1:137:A:PHE:HB3	2	0.23
(1,846)	1:108:A:SER:HB2	1:137:A:PHE:HB2	14	0.23
(1,846)	1:108:A:SER:HB2	1:137:A:PHE:HB3	14	0.23
(1,846)	1:108:A:SER:HB3	1:137:A:PHE:HB2	14	0.23
(1,846)	1:108:A:SER:HB3	1:137:A:PHE:HB3	14	0.23
(1,845)	1:108:A:SER:HB2	1:110:A:PRO:HA	7	0.23
(1,845)	1:108:A:SER:HB3	1:110:A:PRO:HA	7	0.23
(1,845)	1:108:A:SER:HB2	1:110:A:PRO:HA	14	0.23
(1,845)	1:108:A:SER:HB3	1:110:A:PRO:HA	14	0.23
(1,845)	1:108:A:SER:HB2	1:110:A:PRO:HA	21	0.23
(1,845)	1:108:A:SER:HB3	1:110:A:PRO:HA	21	0.23
(1,822)	1:94:A:ARG:HA	1:90:A:LEU:HA	20	0.23
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD11	7	0.23
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD12	7	0.23
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD13	7	0.23
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD21	7	0.23
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD22	7	0.23
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD23	7	0.23
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD11	20	0.23
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD12	20	0.23
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD13	20	0.23
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD21	20	0.23
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD22	20	0.23
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD23	20	0.23
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD11	21	0.23
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD12	21	0.23
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD13	21	0.23
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD21	21	0.23
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD22	21	0.23
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD23	21	0.23
(1,783)	1:81:A:LYS:HG2	1:80:A:GLN:HA	11	0.23
(1,783)	1:81:A:LYS:HG3	1:80:A:GLN:HA	11	0.23
(1,732)	1:65:A:THR:HB	1:56:A:ALA:HB1	20	0.23
(1,732)	1:65:A:THR:HB	1:56:A:ALA:HB2	20	0.23
(1,732)	1:65:A:THR:HB	1:56:A:ALA:HB3	20	0.23
(1,705)	1:53:A:LEU:HD11	1:127:A:ASN:HB2	3	0.23
(1,705)	1:53:A:LEU:HD11	1:127:A:ASN:HB3	3	0.23
(1,705)	1:53:A:LEU:HD12	1:127:A:ASN:HB2	3	0.23
(1,705)	1:53:A:LEU:HD12	1:127:A:ASN:HB3	3	0.23
(1,705)	1:53:A:LEU:HD13	1:127:A:ASN:HB2	3	0.23
(1,705)	1:53:A:LEU:HD13	1:127:A:ASN:HB3	3	0.23
(1,705)	1:53:A:LEU:HD21	1:127:A:ASN:HB2	3	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,705)	1:53:A:LEU:HD21	1:127:A:ASN:HB3	3	0.23
(1,705)	1:53:A:LEU:HD22	1:127:A:ASN:HB2	3	0.23
(1,705)	1:53:A:LEU:HD22	1:127:A:ASN:HB3	3	0.23
(1,705)	1:53:A:LEU:HD23	1:127:A:ASN:HB2	3	0.23
(1,705)	1:53:A:LEU:HD23	1:127:A:ASN:HB3	3	0.23
(1,705)	1:53:A:LEU:HD11	1:127:A:ASN:HB2	16	0.23
(1,705)	1:53:A:LEU:HD11	1:127:A:ASN:HB3	16	0.23
(1,705)	1:53:A:LEU:HD12	1:127:A:ASN:HB2	16	0.23
(1,705)	1:53:A:LEU:HD12	1:127:A:ASN:HB3	16	0.23
(1,705)	1:53:A:LEU:HD13	1:127:A:ASN:HB2	16	0.23
(1,705)	1:53:A:LEU:HD13	1:127:A:ASN:HB3	16	0.23
(1,705)	1:53:A:LEU:HD21	1:127:A:ASN:HB2	16	0.23
(1,705)	1:53:A:LEU:HD21	1:127:A:ASN:HB3	16	0.23
(1,705)	1:53:A:LEU:HD22	1:127:A:ASN:HB2	16	0.23
(1,705)	1:53:A:LEU:HD22	1:127:A:ASN:HB3	16	0.23
(1,705)	1:53:A:LEU:HD23	1:127:A:ASN:HB2	16	0.23
(1,705)	1:53:A:LEU:HD23	1:127:A:ASN:HB3	16	0.23
(1,705)	1:53:A:LEU:HD11	1:127:A:ASN:HB2	20	0.23
(1,705)	1:53:A:LEU:HD11	1:127:A:ASN:HB3	20	0.23
(1,705)	1:53:A:LEU:HD12	1:127:A:ASN:HB2	20	0.23
(1,705)	1:53:A:LEU:HD12	1:127:A:ASN:HB3	20	0.23
(1,705)	1:53:A:LEU:HD13	1:127:A:ASN:HB2	20	0.23
(1,705)	1:53:A:LEU:HD13	1:127:A:ASN:HB3	20	0.23
(1,705)	1:53:A:LEU:HD21	1:127:A:ASN:HB2	20	0.23
(1,705)	1:53:A:LEU:HD21	1:127:A:ASN:HB3	20	0.23
(1,705)	1:53:A:LEU:HD22	1:127:A:ASN:HB2	20	0.23
(1,705)	1:53:A:LEU:HD22	1:127:A:ASN:HB3	20	0.23
(1,705)	1:53:A:LEU:HD23	1:127:A:ASN:HB2	20	0.23
(1,705)	1:53:A:LEU:HD23	1:127:A:ASN:HB3	20	0.23
(1,635)	1:33:A:GLN:HA	1:30:A:HIS:HA	19	0.23
(1,615)	2:480:B:ALA:H	2:479:B:LEU:HG	12	0.23
(1,584)	2:468:B:TYR:H	2:467:B:PRO:HG2	3	0.23
(1,584)	2:468:B:TYR:H	2:467:B:PRO:HG3	3	0.23
(1,584)	2:468:B:TYR:H	2:467:B:PRO:HG2	16	0.23
(1,584)	2:468:B:TYR:H	2:467:B:PRO:HG3	16	0.23
(1,556)	2:451:B:GLU:H	2:450:B:TRP:HB2	17	0.23
(1,522)	1:116:A:THR:H	1:125:A:GLY:HA2	6	0.23
(1,522)	1:116:A:THR:H	1:125:A:GLY:HA3	6	0.23
(1,522)	1:116:A:THR:H	1:125:A:GLY:HA2	10	0.23
(1,522)	1:116:A:THR:H	1:125:A:GLY:HA3	10	0.23
(1,522)	1:116:A:THR:H	1:125:A:GLY:HA2	14	0.23
(1,522)	1:116:A:THR:H	1:125:A:GLY:HA3	14	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,522)	1:116:A:THR:H	1:125:A:GLY:HA2	17	0.23
(1,522)	1:116:A:THR:H	1:125:A:GLY:HA3	17	0.23
(1,522)	1:116:A:THR:H	1:125:A:GLY:HA2	24	0.23
(1,522)	1:116:A:THR:H	1:125:A:GLY:HA3	24	0.23
(1,457)	1:38:A:MET:H	1:34:A:ARG:HD2	2	0.23
(1,457)	1:38:A:MET:H	1:34:A:ARG:HD3	2	0.23
(1,412)	1:84:A:PHE:H	1:76:A:LYS:HB2	3	0.23
(1,412)	1:84:A:PHE:H	1:76:A:LYS:HB3	3	0.23
(1,412)	1:84:A:PHE:H	1:76:A:LYS:HB2	15	0.23
(1,412)	1:84:A:PHE:H	1:76:A:LYS:HB3	15	0.23
(1,403)	1:74:A:PHE:H	1:47:A:ALA:HA	8	0.23
(1,403)	1:74:A:PHE:H	1:47:A:ALA:HA	24	0.23
(1,328)	1:143:A:GLU:H	1:139:A:ALA:HB1	11	0.23
(1,328)	1:143:A:GLU:H	1:139:A:ALA:HB2	11	0.23
(1,328)	1:143:A:GLU:H	1:139:A:ALA:HB3	11	0.23
(1,328)	1:143:A:GLU:H	1:139:A:ALA:HB1	24	0.23
(1,328)	1:143:A:GLU:H	1:139:A:ALA:HB2	24	0.23
(1,328)	1:143:A:GLU:H	1:139:A:ALA:HB3	24	0.23
(1,272)	1:124:A:ALA:H	1:123:A:GLN:HG2	9	0.23
(1,272)	1:124:A:ALA:H	1:123:A:GLN:HG3	9	0.23
(1,272)	1:124:A:ALA:H	1:123:A:GLN:HG2	11	0.23
(1,272)	1:124:A:ALA:H	1:123:A:GLN:HG3	11	0.23
(1,241)	1:109:A:THR:H	1:108:A:SER:H	5	0.23
(1,241)	1:109:A:THR:H	1:108:A:SER:H	6	0.23
(1,241)	1:109:A:THR:H	1:108:A:SER:H	9	0.23
(1,241)	1:109:A:THR:H	1:108:A:SER:H	10	0.23
(1,241)	1:109:A:THR:H	1:108:A:SER:H	11	0.23
(1,241)	1:109:A:THR:H	1:108:A:SER:H	18	0.23
(1,241)	1:109:A:THR:H	1:108:A:SER:H	19	0.23
(1,241)	1:109:A:THR:H	1:108:A:SER:H	21	0.23
(1,195)	1:96:A:LEU:H	1:95:A:LEU:H	20	0.23
(1,105)	1:63:A:HIS:H	1:62:A:GLU:HA	9	0.23
(1,992)	1:129:A:ALA:H	2:457:B:HIS:H	5	0.22
(1,992)	1:129:A:ALA:H	2:457:B:HIS:H	13	0.22
(1,989)	1:129:A:ALA:HB3	2:454:B:PHE:HA	11	0.22
(1,969)	1:71:A:ALA:HB1	2:453:B:ARG:HB2	8	0.22
(1,969)	1:71:A:ALA:HB1	2:453:B:ARG:HB3	8	0.22
(1,969)	1:71:A:ALA:HB2	2:453:B:ARG:HB2	8	0.22
(1,969)	1:71:A:ALA:HB2	2:453:B:ARG:HB3	8	0.22
(1,969)	1:71:A:ALA:HB3	2:453:B:ARG:HB2	8	0.22
(1,969)	1:71:A:ALA:HB3	2:453:B:ARG:HB3	8	0.22
(1,969)	1:71:A:ALA:HB1	2:453:B:ARG:HB2	16	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,969)	1:71:A:ALA:HB1	2:453:B:ARG:HB3	16	0.22
(1,969)	1:71:A:ALA:HB2	2:453:B:ARG:HB2	16	0.22
(1,969)	1:71:A:ALA:HB2	2:453:B:ARG:HB3	16	0.22
(1,969)	1:71:A:ALA:HB3	2:453:B:ARG:HB2	16	0.22
(1,969)	1:71:A:ALA:HB3	2:453:B:ARG:HB3	16	0.22
(1,965)	1:56:A:ALA:HB1	2:462:B:LEU:HD11	10	0.22
(1,965)	1:56:A:ALA:HB1	2:462:B:LEU:HD12	10	0.22
(1,965)	1:56:A:ALA:HB1	2:462:B:LEU:HD13	10	0.22
(1,965)	1:56:A:ALA:HB1	2:462:B:LEU:HD21	10	0.22
(1,965)	1:56:A:ALA:HB1	2:462:B:LEU:HD22	10	0.22
(1,965)	1:56:A:ALA:HB1	2:462:B:LEU:HD23	10	0.22
(1,965)	1:56:A:ALA:HB2	2:462:B:LEU:HD11	10	0.22
(1,965)	1:56:A:ALA:HB2	2:462:B:LEU:HD12	10	0.22
(1,965)	1:56:A:ALA:HB2	2:462:B:LEU:HD13	10	0.22
(1,965)	1:56:A:ALA:HB2	2:462:B:LEU:HD21	10	0.22
(1,965)	1:56:A:ALA:HB2	2:462:B:LEU:HD22	10	0.22
(1,965)	1:56:A:ALA:HB2	2:462:B:LEU:HD23	10	0.22
(1,965)	1:56:A:ALA:HB3	2:462:B:LEU:HD11	10	0.22
(1,965)	1:56:A:ALA:HB3	2:462:B:LEU:HD12	10	0.22
(1,965)	1:56:A:ALA:HB3	2:462:B:LEU:HD13	10	0.22
(1,965)	1:56:A:ALA:HB3	2:462:B:LEU:HD21	10	0.22
(1,965)	1:56:A:ALA:HB3	2:462:B:LEU:HD22	10	0.22
(1,965)	1:56:A:ALA:HB3	2:462:B:LEU:HD23	10	0.22
(1,928)	1:145:A:ILE:HD11	1:117:A:PHE:HZ	14	0.22
(1,928)	1:145:A:ILE:HD12	1:117:A:PHE:HZ	14	0.22
(1,928)	1:145:A:ILE:HD13	1:117:A:PHE:HZ	14	0.22
(1,925)	1:145:A:ILE:HD11	1:117:A:PHE:HB3	4	0.22
(1,925)	1:145:A:ILE:HD12	1:117:A:PHE:HB3	4	0.22
(1,925)	1:145:A:ILE:HD13	1:117:A:PHE:HB3	4	0.22
(1,925)	1:145:A:ILE:HD11	1:117:A:PHE:HB3	18	0.22
(1,925)	1:145:A:ILE:HD12	1:117:A:PHE:HB3	18	0.22
(1,925)	1:145:A:ILE:HD13	1:117:A:PHE:HB3	18	0.22
(1,877)	1:127:A:ASN:HB2	1:113:A:PHE:HB2	1	0.22
(1,877)	1:127:A:ASN:HB2	1:113:A:PHE:HB3	1	0.22
(1,877)	1:127:A:ASN:HB3	1:113:A:PHE:HB2	1	0.22
(1,877)	1:127:A:ASN:HB3	1:113:A:PHE:HB3	1	0.22
(1,877)	1:127:A:ASN:HB2	1:113:A:PHE:HB2	4	0.22
(1,877)	1:127:A:ASN:HB2	1:113:A:PHE:HB3	4	0.22
(1,877)	1:127:A:ASN:HB3	1:113:A:PHE:HB2	4	0.22
(1,877)	1:127:A:ASN:HB3	1:113:A:PHE:HB3	4	0.22
(1,846)	1:108:A:SER:HB2	1:137:A:PHE:HB2	21	0.22
(1,846)	1:108:A:SER:HB2	1:137:A:PHE:HB3	21	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,846)	1:108:A:SER:HB3	1:137:A:PHE:HB2	21	0.22
(1,846)	1:108:A:SER:HB3	1:137:A:PHE:HB3	21	0.22
(1,845)	1:108:A:SER:HB2	1:110:A:PRO:HA	18	0.22
(1,845)	1:108:A:SER:HB3	1:110:A:PRO:HA	18	0.22
(1,822)	1:94:A:ARG:HA	1:90:A:LEU:HA	14	0.22
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD11	2	0.22
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD12	2	0.22
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD13	2	0.22
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD21	2	0.22
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD22	2	0.22
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD23	2	0.22
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD11	3	0.22
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD12	3	0.22
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD13	3	0.22
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD21	3	0.22
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD22	3	0.22
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD23	3	0.22
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD11	22	0.22
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD12	22	0.22
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD13	22	0.22
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD21	22	0.22
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD22	22	0.22
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD23	22	0.22
(1,741)	1:71:A:ALA:HB1	1:35:A:LEU:HB2	11	0.22
(1,741)	1:71:A:ALA:HB1	1:35:A:LEU:HB3	11	0.22
(1,741)	1:71:A:ALA:HB2	1:35:A:LEU:HB2	11	0.22
(1,741)	1:71:A:ALA:HB2	1:35:A:LEU:HB3	11	0.22
(1,741)	1:71:A:ALA:HB3	1:35:A:LEU:HB2	11	0.22
(1,741)	1:71:A:ALA:HB3	1:35:A:LEU:HB3	11	0.22
(1,638)	1:34:A:ARG:HB2	1:74:A:PHE:HD1	4	0.22
(1,638)	1:34:A:ARG:HB2	1:74:A:PHE:HD2	4	0.22
(1,638)	1:34:A:ARG:HB3	1:74:A:PHE:HD1	4	0.22
(1,638)	1:34:A:ARG:HB3	1:74:A:PHE:HD2	4	0.22
(1,635)	1:33:A:GLN:HA	1:30:A:HIS:HA	13	0.22
(1,635)	1:33:A:GLN:HA	1:30:A:HIS:HA	16	0.22
(1,635)	1:33:A:GLN:HA	1:30:A:HIS:HA	20	0.22
(1,635)	1:33:A:GLN:HA	1:30:A:HIS:HA	22	0.22
(1,635)	1:33:A:GLN:HA	1:30:A:HIS:HA	23	0.22
(1,635)	1:33:A:GLN:HA	1:30:A:HIS:HA	24	0.22
(1,615)	2:480:B:ALA:H	2:479:B:LEU:HG	14	0.22
(1,598)	2:473:B:LYS:H	2:472:B:THR:HG21	18	0.22
(1,598)	2:473:B:LYS:H	2:472:B:THR:HG22	24	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,584)	2:468:B:TYR:H	2:467:B:PRO:HG2	11	0.22
(1,584)	2:468:B:TYR:H	2:467:B:PRO:HG3	11	0.22
(1,584)	2:468:B:TYR:H	2:467:B:PRO:HG2	22	0.22
(1,584)	2:468:B:TYR:H	2:467:B:PRO:HG3	22	0.22
(1,523)	1:116:A:THR:H	1:108:A:SER:HB2	5	0.22
(1,523)	1:116:A:THR:H	1:108:A:SER:HB3	5	0.22
(1,523)	1:116:A:THR:H	1:108:A:SER:HB2	18	0.22
(1,523)	1:116:A:THR:H	1:108:A:SER:HB3	18	0.22
(1,510)	1:114:A:PHE:H	1:111:A:THR:HG22	8	0.22
(1,502)	1:104:A:GLN:H	1:102:A:TYR:HA	22	0.22
(1,469)	1:55:A:LEU:H	1:65:A:THR:H	24	0.22
(1,465)	1:52:A:GLN:H	1:51:A:VAL:H	21	0.22
(1,453)	1:26:A:LEU:H	1:30:A:HIS:H	12	0.22
(1,412)	1:84:A:PHE:H	1:76:A:LYS:HB2	11	0.22
(1,412)	1:84:A:PHE:H	1:76:A:LYS:HB3	11	0.22
(1,403)	1:74:A:PHE:H	1:47:A:ALA:HA	2	0.22
(1,403)	1:74:A:PHE:H	1:47:A:ALA:HA	3	0.22
(1,403)	1:74:A:PHE:H	1:47:A:ALA:HA	10	0.22
(1,403)	1:74:A:PHE:H	1:47:A:ALA:HA	14	0.22
(1,399)	1:72:A:VAL:H	1:50:A:VAL:HB	1	0.22
(1,399)	1:72:A:VAL:H	1:50:A:VAL:HB	2	0.22
(1,399)	1:72:A:VAL:H	1:50:A:VAL:HB	3	0.22
(1,366)	1:35:A:LEU:H	1:32:A:ASN:HA	16	0.22
(1,328)	1:143:A:GLU:H	1:139:A:ALA:HB1	9	0.22
(1,328)	1:143:A:GLU:H	1:139:A:ALA:HB2	9	0.22
(1,328)	1:143:A:GLU:H	1:139:A:ALA:HB3	9	0.22
(1,328)	1:143:A:GLU:H	1:139:A:ALA:HB1	15	0.22
(1,328)	1:143:A:GLU:H	1:139:A:ALA:HB2	15	0.22
(1,328)	1:143:A:GLU:H	1:139:A:ALA:HB3	15	0.22
(1,327)	1:143:A:GLU:H	1:140:A:LEU:HD11	12	0.22
(1,327)	1:143:A:GLU:H	1:140:A:LEU:HD12	12	0.22
(1,327)	1:143:A:GLU:H	1:140:A:LEU:HD13	12	0.22
(1,327)	1:143:A:GLU:H	1:140:A:LEU:HD21	12	0.22
(1,327)	1:143:A:GLU:H	1:140:A:LEU:HD22	12	0.22
(1,327)	1:143:A:GLU:H	1:140:A:LEU:HD23	12	0.22
(1,259)	1:118:A:ALA:H	1:117:A:PHE:HB3	4	0.22
(1,259)	1:118:A:ALA:H	1:117:A:PHE:HB3	21	0.22
(1,259)	1:118:A:ALA:H	1:117:A:PHE:HB3	23	0.22
(1,241)	1:109:A:THR:H	1:108:A:SER:H	13	0.22
(1,112)	1:65:A:THR:H	1:64:A:TRP:HB3	14	0.22
(1,105)	1:63:A:HIS:H	1:62:A:GLU:HA	19	0.22
(1,69)	1:49:A:ALA:H	1:48:A:THR:HG21	15	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,92)	1:136:A:ALA:N	1:132:A:ASP:O	11	0.21
(4,77)	1:34:A:ARG:H	1:30:A:HIS:O	1	0.21
(4,77)	1:34:A:ARG:H	1:30:A:HIS:O	4	0.21
(1,1008)	2:474:B:SER:H	1:102:A:TYR:HE1	18	0.21
(1,1008)	2:474:B:SER:H	1:102:A:TYR:HE2	18	0.21
(1,1007)	2:474:B:SER:H	1:102:A:TYR:HA	10	0.21
(1,1007)	2:474:B:SER:H	1:102:A:TYR:HA	23	0.21
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD11	8	0.21
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD12	8	0.21
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD13	8	0.21
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD21	8	0.21
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD22	8	0.21
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD23	8	0.21
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD11	8	0.21
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD12	8	0.21
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD13	8	0.21
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD21	8	0.21
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD22	8	0.21
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD23	8	0.21
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD11	22	0.21
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD12	22	0.21
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD13	22	0.21
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD21	22	0.21
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD22	22	0.21
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD23	22	0.21
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD11	22	0.21
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD12	22	0.21
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD13	22	0.21
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD21	22	0.21
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD22	22	0.21
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD23	22	0.21
(1,1002)	2:463:B:PRO:HG2	1:114:A:PHE:HD1	10	0.21
(1,1002)	2:463:B:PRO:HG2	1:114:A:PHE:HD2	10	0.21
(1,1002)	2:463:B:PRO:HG3	1:114:A:PHE:HD1	10	0.21
(1,1002)	2:463:B:PRO:HG3	1:114:A:PHE:HD2	10	0.21
(1,925)	1:145:A:ILE:HD11	1:117:A:PHE:HB3	13	0.21
(1,925)	1:145:A:ILE:HD12	1:117:A:PHE:HB3	13	0.21
(1,925)	1:145:A:ILE:HD13	1:117:A:PHE:HB3	13	0.21
(1,877)	1:127:A:ASN:HB2	1:113:A:PHE:HB2	12	0.21
(1,877)	1:127:A:ASN:HB2	1:113:A:PHE:HB3	12	0.21
(1,877)	1:127:A:ASN:HB3	1:113:A:PHE:HB2	12	0.21
(1,877)	1:127:A:ASN:HB3	1:113:A:PHE:HB3	12	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,877)	1:127:A:ASN:HB2	1:113:A:PHE:HB2	18	0.21
(1,877)	1:127:A:ASN:HB2	1:113:A:PHE:HB3	18	0.21
(1,877)	1:127:A:ASN:HB3	1:113:A:PHE:HB2	18	0.21
(1,877)	1:127:A:ASN:HB3	1:113:A:PHE:HB3	18	0.21
(1,869)	1:124:A:ALA:HB1	1:117:A:PHE:HD1	24	0.21
(1,869)	1:124:A:ALA:HB1	1:117:A:PHE:HD2	24	0.21
(1,869)	1:124:A:ALA:HB2	1:117:A:PHE:HD1	24	0.21
(1,869)	1:124:A:ALA:HB2	1:117:A:PHE:HD2	24	0.21
(1,869)	1:124:A:ALA:HB3	1:117:A:PHE:HD1	24	0.21
(1,869)	1:124:A:ALA:HB3	1:117:A:PHE:HD2	24	0.21
(1,863)	1:120:A:ASP:HA	1:123:A:GLN:HG2	22	0.21
(1,863)	1:120:A:ASP:HA	1:123:A:GLN:HG3	22	0.21
(1,847)	1:109:A:THR:HB	1:115:A:HIS:HB2	5	0.21
(1,847)	1:109:A:THR:HB	1:115:A:HIS:HB3	5	0.21
(1,847)	1:109:A:THR:HB	1:115:A:HIS:HB2	23	0.21
(1,847)	1:109:A:THR:HB	1:115:A:HIS:HB3	23	0.21
(1,846)	1:108:A:SER:HB2	1:137:A:PHE:HB2	15	0.21
(1,846)	1:108:A:SER:HB2	1:137:A:PHE:HB3	15	0.21
(1,846)	1:108:A:SER:HB3	1:137:A:PHE:HB2	15	0.21
(1,846)	1:108:A:SER:HB3	1:137:A:PHE:HB3	15	0.21
(1,845)	1:108:A:SER:HB2	1:110:A:PRO:HA	11	0.21
(1,845)	1:108:A:SER:HB3	1:110:A:PRO:HA	11	0.21
(1,845)	1:108:A:SER:HB2	1:110:A:PRO:HA	22	0.21
(1,845)	1:108:A:SER:HB3	1:110:A:PRO:HA	22	0.21
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD11	9	0.21
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD12	9	0.21
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD13	9	0.21
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD21	9	0.21
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD22	9	0.21
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD23	9	0.21
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD11	10	0.21
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD12	10	0.21
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD13	10	0.21
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD21	10	0.21
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD22	10	0.21
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD23	10	0.21
(1,783)	1:81:A:LYS:HG2	1:80:A:GLN:HA	16	0.21
(1,783)	1:81:A:LYS:HG3	1:80:A:GLN:HA	16	0.21
(1,741)	1:71:A:ALA:HB1	1:35:A:LEU:HB2	21	0.21
(1,741)	1:71:A:ALA:HB1	1:35:A:LEU:HB3	21	0.21
(1,741)	1:71:A:ALA:HB2	1:35:A:LEU:HB2	21	0.21
(1,741)	1:71:A:ALA:HB2	1:35:A:LEU:HB3	21	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,741)	1:71:A:ALA:HB3	1:35:A:LEU:HB2	21	0.21
(1,741)	1:71:A:ALA:HB3	1:35:A:LEU:HB3	21	0.21
(1,732)	1:65:A:THR:HB	1:56:A:ALA:HB1	22	0.21
(1,732)	1:65:A:THR:HB	1:56:A:ALA:HB2	22	0.21
(1,732)	1:65:A:THR:HB	1:56:A:ALA:HB3	22	0.21
(1,705)	1:53:A:LEU:HD11	1:127:A:ASN:HB2	1	0.21
(1,705)	1:53:A:LEU:HD11	1:127:A:ASN:HB3	1	0.21
(1,705)	1:53:A:LEU:HD12	1:127:A:ASN:HB2	1	0.21
(1,705)	1:53:A:LEU:HD12	1:127:A:ASN:HB3	1	0.21
(1,705)	1:53:A:LEU:HD13	1:127:A:ASN:HB2	1	0.21
(1,705)	1:53:A:LEU:HD13	1:127:A:ASN:HB3	1	0.21
(1,705)	1:53:A:LEU:HD21	1:127:A:ASN:HB2	1	0.21
(1,705)	1:53:A:LEU:HD21	1:127:A:ASN:HB3	1	0.21
(1,705)	1:53:A:LEU:HD22	1:127:A:ASN:HB2	1	0.21
(1,705)	1:53:A:LEU:HD22	1:127:A:ASN:HB3	1	0.21
(1,705)	1:53:A:LEU:HD23	1:127:A:ASN:HB2	1	0.21
(1,705)	1:53:A:LEU:HD23	1:127:A:ASN:HB3	1	0.21
(1,705)	1:53:A:LEU:HD11	1:127:A:ASN:HB2	13	0.21
(1,705)	1:53:A:LEU:HD11	1:127:A:ASN:HB3	13	0.21
(1,705)	1:53:A:LEU:HD12	1:127:A:ASN:HB2	13	0.21
(1,705)	1:53:A:LEU:HD12	1:127:A:ASN:HB3	13	0.21
(1,705)	1:53:A:LEU:HD13	1:127:A:ASN:HB2	13	0.21
(1,705)	1:53:A:LEU:HD13	1:127:A:ASN:HB3	13	0.21
(1,705)	1:53:A:LEU:HD21	1:127:A:ASN:HB2	13	0.21
(1,705)	1:53:A:LEU:HD21	1:127:A:ASN:HB3	13	0.21
(1,705)	1:53:A:LEU:HD22	1:127:A:ASN:HB2	13	0.21
(1,705)	1:53:A:LEU:HD22	1:127:A:ASN:HB3	13	0.21
(1,705)	1:53:A:LEU:HD23	1:127:A:ASN:HB2	13	0.21
(1,705)	1:53:A:LEU:HD23	1:127:A:ASN:HB3	13	0.21
(1,705)	1:53:A:LEU:HD11	1:127:A:ASN:HB2	14	0.21
(1,705)	1:53:A:LEU:HD11	1:127:A:ASN:HB3	14	0.21
(1,705)	1:53:A:LEU:HD12	1:127:A:ASN:HB2	14	0.21
(1,705)	1:53:A:LEU:HD12	1:127:A:ASN:HB3	14	0.21
(1,705)	1:53:A:LEU:HD13	1:127:A:ASN:HB2	14	0.21
(1,705)	1:53:A:LEU:HD13	1:127:A:ASN:HB3	14	0.21
(1,705)	1:53:A:LEU:HD21	1:127:A:ASN:HB2	14	0.21
(1,705)	1:53:A:LEU:HD21	1:127:A:ASN:HB3	14	0.21
(1,705)	1:53:A:LEU:HD22	1:127:A:ASN:HB2	14	0.21
(1,705)	1:53:A:LEU:HD22	1:127:A:ASN:HB3	14	0.21
(1,705)	1:53:A:LEU:HD23	1:127:A:ASN:HB2	14	0.21
(1,705)	1:53:A:LEU:HD23	1:127:A:ASN:HB3	14	0.21
(1,660)	1:45:A:THR:HG21	1:47:A:ALA:HA	4	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,635)	1:33:A:GLN:HA	1:30:A:HIS:HA	1	0.21
(1,635)	1:33:A:GLN:HA	1:30:A:HIS:HA	6	0.21
(1,635)	1:33:A:GLN:HA	1:30:A:HIS:HA	7	0.21
(1,635)	1:33:A:GLN:HA	1:30:A:HIS:HA	9	0.21
(1,598)	2:473:B:LYS:H	2:472:B:THR:HG21	10	0.21
(1,584)	2:468:B:TYR:H	2:467:B:PRO:HG2	4	0.21
(1,584)	2:468:B:TYR:H	2:467:B:PRO:HG3	4	0.21
(1,584)	2:468:B:TYR:H	2:467:B:PRO:HG2	7	0.21
(1,584)	2:468:B:TYR:H	2:467:B:PRO:HG3	7	0.21
(1,584)	2:468:B:TYR:H	2:467:B:PRO:HG2	13	0.21
(1,584)	2:468:B:TYR:H	2:467:B:PRO:HG3	13	0.21
(1,556)	2:451:B:GLU:H	2:450:B:TRP:HB2	19	0.21
(1,522)	1:116:A:THR:H	1:125:A:GLY:HA2	12	0.21
(1,522)	1:116:A:THR:H	1:125:A:GLY:HA3	12	0.21
(1,522)	1:116:A:THR:H	1:125:A:GLY:HA2	15	0.21
(1,522)	1:116:A:THR:H	1:125:A:GLY:HA3	15	0.21
(1,493)	1:97:A:TRP:H	1:95:A:LEU:HA	23	0.21
(1,477)	1:72:A:VAL:H	1:48:A:THR:HA	3	0.21
(1,477)	1:72:A:VAL:H	1:48:A:THR:HA	12	0.21
(1,403)	1:74:A:PHE:H	1:47:A:ALA:HA	13	0.21
(1,403)	1:74:A:PHE:H	1:47:A:ALA:HA	18	0.21
(1,403)	1:74:A:PHE:H	1:47:A:ALA:HA	21	0.21
(1,403)	1:74:A:PHE:H	1:47:A:ALA:HA	22	0.21
(1,366)	1:35:A:LEU:H	1:32:A:ASN:HA	8	0.21
(1,328)	1:143:A:GLU:H	1:139:A:ALA:HB1	16	0.21
(1,328)	1:143:A:GLU:H	1:139:A:ALA:HB2	16	0.21
(1,328)	1:143:A:GLU:H	1:139:A:ALA:HB3	16	0.21
(1,328)	1:143:A:GLU:H	1:139:A:ALA:HB1	22	0.21
(1,328)	1:143:A:GLU:H	1:139:A:ALA:HB2	22	0.21
(1,328)	1:143:A:GLU:H	1:139:A:ALA:HB3	22	0.21
(1,327)	1:143:A:GLU:H	1:140:A:LEU:HD11	5	0.21
(1,327)	1:143:A:GLU:H	1:140:A:LEU:HD12	5	0.21
(1,327)	1:143:A:GLU:H	1:140:A:LEU:HD13	5	0.21
(1,327)	1:143:A:GLU:H	1:140:A:LEU:HD21	5	0.21
(1,327)	1:143:A:GLU:H	1:140:A:LEU:HD22	5	0.21
(1,327)	1:143:A:GLU:H	1:140:A:LEU:HD23	5	0.21
(1,278)	1:127:A:ASN:H	1:126:A:LEU:HG	5	0.21
(1,272)	1:124:A:ALA:H	1:123:A:GLN:HG2	7	0.21
(1,272)	1:124:A:ALA:H	1:123:A:GLN:HG3	7	0.21
(1,272)	1:124:A:ALA:H	1:123:A:GLN:HG2	15	0.21
(1,272)	1:124:A:ALA:H	1:123:A:GLN:HG3	15	0.21
(1,259)	1:118:A:ALA:H	1:117:A:PHE:HB3	24	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,241)	1:109:A:THR:H	1:108:A:SER:H	1	0.21
(1,241)	1:109:A:THR:H	1:108:A:SER:H	7	0.21
(1,241)	1:109:A:THR:H	1:108:A:SER:H	8	0.21
(1,241)	1:109:A:THR:H	1:108:A:SER:H	12	0.21
(1,235)	1:107:A:TYR:H	1:106:A:VAL:H	7	0.21
(1,112)	1:65:A:THR:H	1:64:A:TRP:HB3	22	0.21
(1,105)	1:63:A:HIS:H	1:62:A:GLU:HA	1	0.21
(1,105)	1:63:A:HIS:H	1:62:A:GLU:HA	20	0.21
(1,105)	1:63:A:HIS:H	1:62:A:GLU:HA	21	0.21
(4,92)	1:136:A:ALA:N	1:132:A:ASP:O	2	0.2
(4,92)	1:136:A:ALA:N	1:132:A:ASP:O	4	0.2
(4,92)	1:136:A:ALA:N	1:132:A:ASP:O	19	0.2
(4,92)	1:136:A:ALA:N	1:132:A:ASP:O	20	0.2
(4,92)	1:136:A:ALA:N	1:132:A:ASP:O	21	0.2
(4,41)	1:71:A:ALA:H	1:88:A:TYR:O	10	0.2
(4,41)	1:71:A:ALA:H	1:88:A:TYR:O	13	0.2
(4,41)	1:71:A:ALA:H	1:88:A:TYR:O	22	0.2
(4,41)	1:71:A:ALA:H	1:88:A:TYR:O	24	0.2
(1,1016)	2:479:B:LEU:HG	1:83:A:TYR:HD1	19	0.2
(1,1016)	2:479:B:LEU:HG	1:83:A:TYR:HD2	19	0.2
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD11	5	0.2
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD12	5	0.2
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD13	5	0.2
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD21	5	0.2
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD22	5	0.2
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD23	5	0.2
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD11	5	0.2
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD12	5	0.2
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD13	5	0.2
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD21	5	0.2
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD22	5	0.2
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD23	5	0.2
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD11	10	0.2
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD12	10	0.2
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD13	10	0.2
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD21	10	0.2
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD22	10	0.2
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD23	10	0.2
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD11	10	0.2
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD12	10	0.2
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD13	10	0.2
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD21	10	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD22	10	0.2
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD23	10	0.2
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD11	13	0.2
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD12	13	0.2
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD13	13	0.2
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD21	13	0.2
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD22	13	0.2
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD23	13	0.2
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD11	13	0.2
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD12	13	0.2
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD13	13	0.2
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD21	13	0.2
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD22	13	0.2
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD23	13	0.2
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD11	21	0.2
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD12	21	0.2
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD13	21	0.2
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD21	21	0.2
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD22	21	0.2
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD23	21	0.2
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD11	21	0.2
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD12	21	0.2
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD13	21	0.2
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD21	21	0.2
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD22	21	0.2
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD23	21	0.2
(1,992)	1:129:A:ALA:H	2:457:B:HIS:H	16	0.2
(1,992)	1:129:A:ALA:H	2:457:B:HIS:H	19	0.2
(1,972)	1:71:A:ALA:H	2:450:B:TRP:HZ2	22	0.2
(1,965)	1:56:A:ALA:HB1	2:462:B:LEU:HD11	1	0.2
(1,965)	1:56:A:ALA:HB1	2:462:B:LEU:HD12	1	0.2
(1,965)	1:56:A:ALA:HB1	2:462:B:LEU:HD13	1	0.2
(1,965)	1:56:A:ALA:HB1	2:462:B:LEU:HD21	1	0.2
(1,965)	1:56:A:ALA:HB1	2:462:B:LEU:HD22	1	0.2
(1,965)	1:56:A:ALA:HB1	2:462:B:LEU:HD23	1	0.2
(1,965)	1:56:A:ALA:HB2	2:462:B:LEU:HD11	1	0.2
(1,965)	1:56:A:ALA:HB2	2:462:B:LEU:HD12	1	0.2
(1,965)	1:56:A:ALA:HB2	2:462:B:LEU:HD13	1	0.2
(1,965)	1:56:A:ALA:HB2	2:462:B:LEU:HD21	1	0.2
(1,965)	1:56:A:ALA:HB2	2:462:B:LEU:HD22	1	0.2
(1,965)	1:56:A:ALA:HB2	2:462:B:LEU:HD23	1	0.2
(1,965)	1:56:A:ALA:HB3	2:462:B:LEU:HD11	1	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,965)	1:56:A:ALA:HB3	2:462:B:LEU:HD12	1	0.2
(1,965)	1:56:A:ALA:HB3	2:462:B:LEU:HD13	1	0.2
(1,965)	1:56:A:ALA:HB3	2:462:B:LEU:HD21	1	0.2
(1,965)	1:56:A:ALA:HB3	2:462:B:LEU:HD22	1	0.2
(1,965)	1:56:A:ALA:HB3	2:462:B:LEU:HD23	1	0.2
(1,944)	2:458:B:PRO:HA	2:460:B:SER:HB2	18	0.2
(1,944)	2:458:B:PRO:HA	2:460:B:SER:HB3	18	0.2
(1,925)	1:145:A:ILE:HD11	1:117:A:PHE:HB3	15	0.2
(1,925)	1:145:A:ILE:HD12	1:117:A:PHE:HB3	15	0.2
(1,925)	1:145:A:ILE:HD13	1:117:A:PHE:HB3	15	0.2
(1,877)	1:127:A:ASN:HB2	1:113:A:PHE:HB2	7	0.2
(1,877)	1:127:A:ASN:HB2	1:113:A:PHE:HB3	7	0.2
(1,877)	1:127:A:ASN:HB3	1:113:A:PHE:HB2	7	0.2
(1,877)	1:127:A:ASN:HB3	1:113:A:PHE:HB3	7	0.2
(1,877)	1:127:A:ASN:HB2	1:113:A:PHE:HB2	8	0.2
(1,877)	1:127:A:ASN:HB2	1:113:A:PHE:HB3	8	0.2
(1,877)	1:127:A:ASN:HB3	1:113:A:PHE:HB2	8	0.2
(1,877)	1:127:A:ASN:HB3	1:113:A:PHE:HB3	8	0.2
(1,877)	1:127:A:ASN:HB2	1:113:A:PHE:HB2	11	0.2
(1,877)	1:127:A:ASN:HB2	1:113:A:PHE:HB3	11	0.2
(1,877)	1:127:A:ASN:HB3	1:113:A:PHE:HB2	11	0.2
(1,877)	1:127:A:ASN:HB3	1:113:A:PHE:HB3	11	0.2
(1,877)	1:127:A:ASN:HB2	1:113:A:PHE:HB2	16	0.2
(1,877)	1:127:A:ASN:HB2	1:113:A:PHE:HB3	16	0.2
(1,877)	1:127:A:ASN:HB3	1:113:A:PHE:HB2	16	0.2
(1,877)	1:127:A:ASN:HB3	1:113:A:PHE:HB3	16	0.2
(1,877)	1:127:A:ASN:HB2	1:113:A:PHE:HB2	21	0.2
(1,877)	1:127:A:ASN:HB2	1:113:A:PHE:HB3	21	0.2
(1,877)	1:127:A:ASN:HB3	1:113:A:PHE:HB2	21	0.2
(1,877)	1:127:A:ASN:HB3	1:113:A:PHE:HB3	21	0.2
(1,863)	1:120:A:ASP:HA	1:123:A:GLN:HG2	1	0.2
(1,863)	1:120:A:ASP:HA	1:123:A:GLN:HG3	1	0.2
(1,863)	1:120:A:ASP:HA	1:123:A:GLN:HG2	11	0.2
(1,863)	1:120:A:ASP:HA	1:123:A:GLN:HG3	11	0.2
(1,847)	1:109:A:THR:HB	1:115:A:HIS:HB2	7	0.2
(1,847)	1:109:A:THR:HB	1:115:A:HIS:HB3	7	0.2
(1,847)	1:109:A:THR:HB	1:115:A:HIS:HB2	18	0.2
(1,847)	1:109:A:THR:HB	1:115:A:HIS:HB3	18	0.2
(1,847)	1:109:A:THR:HB	1:115:A:HIS:HB2	21	0.2
(1,847)	1:109:A:THR:HB	1:115:A:HIS:HB3	21	0.2
(1,845)	1:108:A:SER:HB2	1:110:A:PRO:HA	19	0.2
(1,845)	1:108:A:SER:HB3	1:110:A:PRO:HA	19	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD11	4	0.2
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD12	4	0.2
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD13	4	0.2
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD21	4	0.2
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD22	4	0.2
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD23	4	0.2
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD11	5	0.2
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD12	5	0.2
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD13	5	0.2
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD21	5	0.2
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD22	5	0.2
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD23	5	0.2
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD11	6	0.2
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD12	6	0.2
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD13	6	0.2
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD21	6	0.2
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD22	6	0.2
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD23	6	0.2
(1,783)	1:81:A:LYS:HG2	1:80:A:GLN:HA	21	0.2
(1,783)	1:81:A:LYS:HG3	1:80:A:GLN:HA	21	0.2
(1,732)	1:65:A:THR:HB	1:56:A:ALA:HB1	10	0.2
(1,732)	1:65:A:THR:HB	1:56:A:ALA:HB2	10	0.2
(1,732)	1:65:A:THR:HB	1:56:A:ALA:HB3	10	0.2
(1,732)	1:65:A:THR:HB	1:56:A:ALA:HB1	15	0.2
(1,732)	1:65:A:THR:HB	1:56:A:ALA:HB2	15	0.2
(1,732)	1:65:A:THR:HB	1:56:A:ALA:HB3	15	0.2
(1,640)	1:35:A:LEU:HD11	1:31:A:GLU:HA	4	0.2
(1,640)	1:35:A:LEU:HD12	1:31:A:GLU:HA	4	0.2
(1,640)	1:35:A:LEU:HD13	1:31:A:GLU:HA	4	0.2
(1,640)	1:35:A:LEU:HD21	1:31:A:GLU:HA	4	0.2
(1,640)	1:35:A:LEU:HD22	1:31:A:GLU:HA	4	0.2
(1,640)	1:35:A:LEU:HD23	1:31:A:GLU:HA	4	0.2
(1,635)	1:33:A:GLN:HA	1:30:A:HIS:HA	3	0.2
(1,635)	1:33:A:GLN:HA	1:30:A:HIS:HA	5	0.2
(1,635)	1:33:A:GLN:HA	1:30:A:HIS:HA	8	0.2
(1,635)	1:33:A:GLN:HA	1:30:A:HIS:HA	10	0.2
(1,635)	1:33:A:GLN:HA	1:30:A:HIS:HA	14	0.2
(1,635)	1:33:A:GLN:HA	1:30:A:HIS:HA	15	0.2
(1,616)	2:480:B:ALA:H	2:479:B:LEU:HA	14	0.2
(1,616)	2:480:B:ALA:H	2:479:B:LEU:HA	20	0.2
(1,610)	2:479:B:LEU:H	2:478:B:LYS:HG2	1	0.2
(1,610)	2:479:B:LEU:H	2:478:B:LYS:HG3	1	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,610)	2:479:B:LEU:H	2:478:B:LYS:HG2	6	0.2
(1,610)	2:479:B:LEU:H	2:478:B:LYS:HG3	6	0.2
(1,610)	2:479:B:LEU:H	2:478:B:LYS:HG2	11	0.2
(1,610)	2:479:B:LEU:H	2:478:B:LYS:HG3	11	0.2
(1,584)	2:468:B:TYR:H	2:467:B:PRO:HG2	6	0.2
(1,584)	2:468:B:TYR:H	2:467:B:PRO:HG3	6	0.2
(1,584)	2:468:B:TYR:H	2:467:B:PRO:HG2	10	0.2
(1,584)	2:468:B:TYR:H	2:467:B:PRO:HG3	10	0.2
(1,584)	2:468:B:TYR:H	2:467:B:PRO:HG2	14	0.2
(1,584)	2:468:B:TYR:H	2:467:B:PRO:HG3	14	0.2
(1,584)	2:468:B:TYR:H	2:467:B:PRO:HG2	19	0.2
(1,584)	2:468:B:TYR:H	2:467:B:PRO:HG3	19	0.2
(1,584)	2:468:B:TYR:H	2:467:B:PRO:HG2	20	0.2
(1,584)	2:468:B:TYR:H	2:467:B:PRO:HG3	20	0.2
(1,584)	2:468:B:TYR:H	2:467:B:PRO:HG2	23	0.2
(1,584)	2:468:B:TYR:H	2:467:B:PRO:HG3	23	0.2
(1,584)	2:468:B:TYR:H	2:467:B:PRO:HG2	24	0.2
(1,584)	2:468:B:TYR:H	2:467:B:PRO:HG3	24	0.2
(1,523)	1:116:A:THR:H	1:108:A:SER:HB2	2	0.2
(1,523)	1:116:A:THR:H	1:108:A:SER:HB3	2	0.2
(1,522)	1:116:A:THR:H	1:125:A:GLY:HA2	9	0.2
(1,522)	1:116:A:THR:H	1:125:A:GLY:HA3	9	0.2
(1,522)	1:116:A:THR:H	1:125:A:GLY:HA2	19	0.2
(1,522)	1:116:A:THR:H	1:125:A:GLY:HA3	19	0.2
(1,496)	1:101:A:LEU:H	1:100:A:GLU:H	18	0.2
(1,493)	1:97:A:TRP:H	1:95:A:LEU:HA	11	0.2
(1,493)	1:97:A:TRP:H	1:95:A:LEU:HA	13	0.2
(1,493)	1:97:A:TRP:H	1:95:A:LEU:HA	16	0.2
(1,483)	1:87:A:LEU:H	1:97:A:TRP:HZ3	17	0.2
(1,477)	1:72:A:VAL:H	1:48:A:THR:HA	7	0.2
(1,466)	1:52:A:GLN:H	1:128:A:PHE:HB2	18	0.2
(1,466)	1:52:A:GLN:H	1:128:A:PHE:HB3	18	0.2
(1,440)	1:127:A:ASN:H	1:53:A:LEU:HA	6	0.2
(1,440)	1:127:A:ASN:H	1:53:A:LEU:HA	22	0.2
(1,439)	1:126:A:LEU:H	1:116:A:THR:HG22	24	0.2
(1,417)	1:88:A:TYR:H	1:71:A:ALA:H	20	0.2
(1,403)	1:74:A:PHE:H	1:47:A:ALA:HA	4	0.2
(1,403)	1:74:A:PHE:H	1:47:A:ALA:HA	7	0.2
(1,403)	1:74:A:PHE:H	1:47:A:ALA:HA	16	0.2
(1,403)	1:74:A:PHE:H	1:47:A:ALA:HA	23	0.2
(1,366)	1:35:A:LEU:H	1:32:A:ASN:HA	11	0.2
(1,366)	1:35:A:LEU:H	1:32:A:ASN:HA	17	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,327)	1:143:A:GLU:H	1:140:A:LEU:HD11	11	0.2
(1,327)	1:143:A:GLU:H	1:140:A:LEU:HD12	11	0.2
(1,327)	1:143:A:GLU:H	1:140:A:LEU:HD13	11	0.2
(1,327)	1:143:A:GLU:H	1:140:A:LEU:HD21	11	0.2
(1,327)	1:143:A:GLU:H	1:140:A:LEU:HD22	11	0.2
(1,327)	1:143:A:GLU:H	1:140:A:LEU:HD23	11	0.2
(1,327)	1:143:A:GLU:H	1:140:A:LEU:HD11	21	0.2
(1,327)	1:143:A:GLU:H	1:140:A:LEU:HD12	21	0.2
(1,327)	1:143:A:GLU:H	1:140:A:LEU:HD13	21	0.2
(1,327)	1:143:A:GLU:H	1:140:A:LEU:HD21	21	0.2
(1,327)	1:143:A:GLU:H	1:140:A:LEU:HD22	21	0.2
(1,327)	1:143:A:GLU:H	1:140:A:LEU:HD23	21	0.2
(1,259)	1:118:A:ALA:H	1:117:A:PHE:HB3	8	0.2
(1,259)	1:118:A:ALA:H	1:117:A:PHE:HB3	18	0.2
(1,259)	1:118:A:ALA:H	1:117:A:PHE:HB3	22	0.2
(1,195)	1:96:A:LEU:H	1:95:A:LEU:H	6	0.2
(1,112)	1:65:A:THR:H	1:64:A:TRP:HB3	5	0.2
(1,105)	1:63:A:HIS:H	1:62:A:GLU:HA	2	0.2
(1,105)	1:63:A:HIS:H	1:62:A:GLU:HA	18	0.2
(1,105)	1:63:A:HIS:H	1:62:A:GLU:HA	22	0.2
(1,69)	1:49:A:ALA:H	1:48:A:THR:HG21	6	0.2
(4,92)	1:136:A:ALA:N	1:132:A:ASP:O	5	0.19
(4,92)	1:136:A:ALA:N	1:132:A:ASP:O	9	0.19
(4,92)	1:136:A:ALA:N	1:132:A:ASP:O	12	0.19
(4,92)	1:136:A:ALA:N	1:132:A:ASP:O	24	0.19
(4,41)	1:71:A:ALA:H	1:88:A:TYR:O	1	0.19
(1,1016)	2:479:B:LEU:HG	1:83:A:TYR:HD1	2	0.19
(1,1016)	2:479:B:LEU:HG	1:83:A:TYR:HD2	2	0.19
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD11	24	0.19
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD12	24	0.19
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD13	24	0.19
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD21	24	0.19
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD22	24	0.19
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD23	24	0.19
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD11	24	0.19
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD12	24	0.19
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD13	24	0.19
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD21	24	0.19
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD22	24	0.19
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD23	24	0.19
(1,972)	1:71:A:ALA:H	2:450:B:TRP:HZ2	13	0.19
(1,972)	1:71:A:ALA:H	2:450:B:TRP:HZ2	16	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,965)	1:56:A:ALA:HB1	2:462:B:LEU:HD11	14	0.19
(1,965)	1:56:A:ALA:HB1	2:462:B:LEU:HD12	14	0.19
(1,965)	1:56:A:ALA:HB1	2:462:B:LEU:HD13	14	0.19
(1,965)	1:56:A:ALA:HB1	2:462:B:LEU:HD21	14	0.19
(1,965)	1:56:A:ALA:HB1	2:462:B:LEU:HD22	14	0.19
(1,965)	1:56:A:ALA:HB1	2:462:B:LEU:HD23	14	0.19
(1,965)	1:56:A:ALA:HB2	2:462:B:LEU:HD11	14	0.19
(1,965)	1:56:A:ALA:HB2	2:462:B:LEU:HD12	14	0.19
(1,965)	1:56:A:ALA:HB2	2:462:B:LEU:HD13	14	0.19
(1,965)	1:56:A:ALA:HB2	2:462:B:LEU:HD21	14	0.19
(1,965)	1:56:A:ALA:HB2	2:462:B:LEU:HD22	14	0.19
(1,965)	1:56:A:ALA:HB2	2:462:B:LEU:HD23	14	0.19
(1,965)	1:56:A:ALA:HB3	2:462:B:LEU:HD11	14	0.19
(1,965)	1:56:A:ALA:HB3	2:462:B:LEU:HD12	14	0.19
(1,965)	1:56:A:ALA:HB3	2:462:B:LEU:HD13	14	0.19
(1,965)	1:56:A:ALA:HB3	2:462:B:LEU:HD21	14	0.19
(1,965)	1:56:A:ALA:HB3	2:462:B:LEU:HD22	14	0.19
(1,965)	1:56:A:ALA:HB3	2:462:B:LEU:HD23	14	0.19
(1,965)	1:56:A:ALA:HB1	2:462:B:LEU:HD11	22	0.19
(1,965)	1:56:A:ALA:HB1	2:462:B:LEU:HD12	22	0.19
(1,965)	1:56:A:ALA:HB1	2:462:B:LEU:HD13	22	0.19
(1,965)	1:56:A:ALA:HB1	2:462:B:LEU:HD21	22	0.19
(1,965)	1:56:A:ALA:HB1	2:462:B:LEU:HD22	22	0.19
(1,965)	1:56:A:ALA:HB1	2:462:B:LEU:HD23	22	0.19
(1,965)	1:56:A:ALA:HB2	2:462:B:LEU:HD11	22	0.19
(1,965)	1:56:A:ALA:HB2	2:462:B:LEU:HD12	22	0.19
(1,965)	1:56:A:ALA:HB2	2:462:B:LEU:HD13	22	0.19
(1,965)	1:56:A:ALA:HB2	2:462:B:LEU:HD21	22	0.19
(1,965)	1:56:A:ALA:HB2	2:462:B:LEU:HD22	22	0.19
(1,965)	1:56:A:ALA:HB2	2:462:B:LEU:HD23	22	0.19
(1,965)	1:56:A:ALA:HB3	2:462:B:LEU:HD11	22	0.19
(1,965)	1:56:A:ALA:HB3	2:462:B:LEU:HD12	22	0.19
(1,965)	1:56:A:ALA:HB3	2:462:B:LEU:HD13	22	0.19
(1,965)	1:56:A:ALA:HB3	2:462:B:LEU:HD21	22	0.19
(1,965)	1:56:A:ALA:HB3	2:462:B:LEU:HD22	22	0.19
(1,965)	1:56:A:ALA:HB3	2:462:B:LEU:HD23	22	0.19
(1,944)	2:458:B:PRO:HA	2:460:B:SER:HB2	8	0.19
(1,944)	2:458:B:PRO:HA	2:460:B:SER:HB3	8	0.19
(1,926)	1:145:A:ILE:HD11	1:117:A:PHE:HB2	17	0.19
(1,926)	1:145:A:ILE:HD12	1:117:A:PHE:HB2	17	0.19
(1,926)	1:145:A:ILE:HD13	1:117:A:PHE:HB2	17	0.19
(1,912)	1:141:A:VAL:HG11	1:107:A:TYR:HB3	2	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,912)	1:141:A:VAL:HG12	1:107:A:TYR:HB3	2	0.19
(1,912)	1:141:A:VAL:HG13	1:107:A:TYR:HB3	2	0.19
(1,912)	1:141:A:VAL:HG21	1:107:A:TYR:HB3	2	0.19
(1,912)	1:141:A:VAL:HG22	1:107:A:TYR:HB3	2	0.19
(1,912)	1:141:A:VAL:HG23	1:107:A:TYR:HB3	2	0.19
(1,912)	1:141:A:VAL:HG11	1:107:A:TYR:HB2	2	0.19
(1,912)	1:141:A:VAL:HG12	1:107:A:TYR:HB2	2	0.19
(1,912)	1:141:A:VAL:HG13	1:107:A:TYR:HB2	2	0.19
(1,912)	1:141:A:VAL:HG21	1:107:A:TYR:HB2	2	0.19
(1,912)	1:141:A:VAL:HG22	1:107:A:TYR:HB2	2	0.19
(1,912)	1:141:A:VAL:HG23	1:107:A:TYR:HB2	2	0.19
(1,912)	1:141:A:VAL:HG11	1:107:A:TYR:HB3	6	0.19
(1,912)	1:141:A:VAL:HG12	1:107:A:TYR:HB3	6	0.19
(1,912)	1:141:A:VAL:HG13	1:107:A:TYR:HB3	6	0.19
(1,912)	1:141:A:VAL:HG21	1:107:A:TYR:HB3	6	0.19
(1,912)	1:141:A:VAL:HG22	1:107:A:TYR:HB3	6	0.19
(1,912)	1:141:A:VAL:HG23	1:107:A:TYR:HB3	6	0.19
(1,912)	1:141:A:VAL:HG11	1:107:A:TYR:HB2	6	0.19
(1,912)	1:141:A:VAL:HG12	1:107:A:TYR:HB2	6	0.19
(1,912)	1:141:A:VAL:HG13	1:107:A:TYR:HB2	6	0.19
(1,912)	1:141:A:VAL:HG21	1:107:A:TYR:HB2	6	0.19
(1,912)	1:141:A:VAL:HG22	1:107:A:TYR:HB2	6	0.19
(1,912)	1:141:A:VAL:HG23	1:107:A:TYR:HB2	6	0.19
(1,877)	1:127:A:ASN:HB2	1:113:A:PHE:HB2	14	0.19
(1,877)	1:127:A:ASN:HB2	1:113:A:PHE:HB3	14	0.19
(1,877)	1:127:A:ASN:HB3	1:113:A:PHE:HB2	14	0.19
(1,877)	1:127:A:ASN:HB3	1:113:A:PHE:HB3	14	0.19
(1,877)	1:127:A:ASN:HB2	1:113:A:PHE:HB2	20	0.19
(1,877)	1:127:A:ASN:HB2	1:113:A:PHE:HB3	20	0.19
(1,877)	1:127:A:ASN:HB3	1:113:A:PHE:HB2	20	0.19
(1,877)	1:127:A:ASN:HB3	1:113:A:PHE:HB3	20	0.19
(1,877)	1:127:A:ASN:HB2	1:113:A:PHE:HB2	24	0.19
(1,877)	1:127:A:ASN:HB2	1:113:A:PHE:HB3	24	0.19
(1,877)	1:127:A:ASN:HB3	1:113:A:PHE:HB2	24	0.19
(1,877)	1:127:A:ASN:HB3	1:113:A:PHE:HB3	24	0.19
(1,863)	1:120:A:ASP:HA	1:123:A:GLN:HG2	9	0.19
(1,863)	1:120:A:ASP:HA	1:123:A:GLN:HG3	9	0.19
(1,863)	1:120:A:ASP:HA	1:123:A:GLN:HG2	15	0.19
(1,863)	1:120:A:ASP:HA	1:123:A:GLN:HG3	15	0.19
(1,863)	1:120:A:ASP:HA	1:123:A:GLN:HG2	16	0.19
(1,863)	1:120:A:ASP:HA	1:123:A:GLN:HG3	16	0.19
(1,847)	1:109:A:THR:HB	1:115:A:HIS:HB2	9	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,847)	1:109:A:THR:HB	1:115:A:HIS:HB3	9	0.19
(1,846)	1:108:A:SER:HB2	1:137:A:PHE:HB2	9	0.19
(1,846)	1:108:A:SER:HB2	1:137:A:PHE:HB3	9	0.19
(1,846)	1:108:A:SER:HB3	1:137:A:PHE:HB2	9	0.19
(1,846)	1:108:A:SER:HB3	1:137:A:PHE:HB3	9	0.19
(1,846)	1:108:A:SER:HB2	1:137:A:PHE:HB2	20	0.19
(1,846)	1:108:A:SER:HB2	1:137:A:PHE:HB3	20	0.19
(1,846)	1:108:A:SER:HB3	1:137:A:PHE:HB2	20	0.19
(1,846)	1:108:A:SER:HB3	1:137:A:PHE:HB3	20	0.19
(1,846)	1:108:A:SER:HB2	1:137:A:PHE:HB2	22	0.19
(1,846)	1:108:A:SER:HB2	1:137:A:PHE:HB3	22	0.19
(1,846)	1:108:A:SER:HB3	1:137:A:PHE:HB2	22	0.19
(1,846)	1:108:A:SER:HB3	1:137:A:PHE:HB3	22	0.19
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD11	13	0.19
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD12	13	0.19
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD13	13	0.19
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD21	13	0.19
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD22	13	0.19
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD23	13	0.19
(1,783)	1:81:A:LYS:HG2	1:80:A:GLN:HA	1	0.19
(1,783)	1:81:A:LYS:HG3	1:80:A:GLN:HA	1	0.19
(1,783)	1:81:A:LYS:HG2	1:80:A:GLN:HA	18	0.19
(1,783)	1:81:A:LYS:HG3	1:80:A:GLN:HA	18	0.19
(1,776)	1:75:A:VAL:HG11	1:73:A:CYS:HB2	1	0.19
(1,776)	1:75:A:VAL:HG11	1:73:A:CYS:HB3	1	0.19
(1,776)	1:75:A:VAL:HG12	1:73:A:CYS:HB2	1	0.19
(1,776)	1:75:A:VAL:HG12	1:73:A:CYS:HB3	1	0.19
(1,776)	1:75:A:VAL:HG13	1:73:A:CYS:HB2	1	0.19
(1,776)	1:75:A:VAL:HG13	1:73:A:CYS:HB3	1	0.19
(1,741)	1:71:A:ALA:HB1	1:35:A:LEU:HB2	18	0.19
(1,741)	1:71:A:ALA:HB1	1:35:A:LEU:HB3	18	0.19
(1,741)	1:71:A:ALA:HB2	1:35:A:LEU:HB2	18	0.19
(1,741)	1:71:A:ALA:HB2	1:35:A:LEU:HB3	18	0.19
(1,741)	1:71:A:ALA:HB3	1:35:A:LEU:HB2	18	0.19
(1,741)	1:71:A:ALA:HB3	1:35:A:LEU:HB3	18	0.19
(1,741)	1:71:A:ALA:HB1	1:35:A:LEU:HB2	23	0.19
(1,741)	1:71:A:ALA:HB1	1:35:A:LEU:HB3	23	0.19
(1,741)	1:71:A:ALA:HB2	1:35:A:LEU:HB2	23	0.19
(1,741)	1:71:A:ALA:HB2	1:35:A:LEU:HB3	23	0.19
(1,741)	1:71:A:ALA:HB3	1:35:A:LEU:HB2	23	0.19
(1,741)	1:71:A:ALA:HB3	1:35:A:LEU:HB3	23	0.19
(1,732)	1:65:A:THR:HB	1:56:A:ALA:HB1	9	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,732)	1:65:A:THR:HB	1:56:A:ALA:HB2	9	0.19
(1,732)	1:65:A:THR:HB	1:56:A:ALA:HB3	9	0.19
(1,732)	1:65:A:THR:HB	1:56:A:ALA:HB1	21	0.19
(1,732)	1:65:A:THR:HB	1:56:A:ALA:HB2	21	0.19
(1,732)	1:65:A:THR:HB	1:56:A:ALA:HB3	21	0.19
(1,720)	1:56:A:ALA:HB1	1:123:A:GLN:HB2	5	0.19
(1,720)	1:56:A:ALA:HB1	1:123:A:GLN:HB3	5	0.19
(1,720)	1:56:A:ALA:HB2	1:123:A:GLN:HB2	5	0.19
(1,720)	1:56:A:ALA:HB2	1:123:A:GLN:HB3	5	0.19
(1,720)	1:56:A:ALA:HB3	1:123:A:GLN:HB2	5	0.19
(1,720)	1:56:A:ALA:HB3	1:123:A:GLN:HB3	5	0.19
(1,705)	1:53:A:LEU:HD11	1:127:A:ASN:HB2	4	0.19
(1,705)	1:53:A:LEU:HD11	1:127:A:ASN:HB3	4	0.19
(1,705)	1:53:A:LEU:HD12	1:127:A:ASN:HB2	4	0.19
(1,705)	1:53:A:LEU:HD12	1:127:A:ASN:HB3	4	0.19
(1,705)	1:53:A:LEU:HD13	1:127:A:ASN:HB2	4	0.19
(1,705)	1:53:A:LEU:HD13	1:127:A:ASN:HB3	4	0.19
(1,705)	1:53:A:LEU:HD21	1:127:A:ASN:HB2	4	0.19
(1,705)	1:53:A:LEU:HD21	1:127:A:ASN:HB3	4	0.19
(1,705)	1:53:A:LEU:HD22	1:127:A:ASN:HB2	4	0.19
(1,705)	1:53:A:LEU:HD22	1:127:A:ASN:HB3	4	0.19
(1,705)	1:53:A:LEU:HD23	1:127:A:ASN:HB2	4	0.19
(1,705)	1:53:A:LEU:HD23	1:127:A:ASN:HB3	4	0.19
(1,705)	1:53:A:LEU:HD11	1:127:A:ASN:HB2	23	0.19
(1,705)	1:53:A:LEU:HD11	1:127:A:ASN:HB3	23	0.19
(1,705)	1:53:A:LEU:HD12	1:127:A:ASN:HB2	23	0.19
(1,705)	1:53:A:LEU:HD12	1:127:A:ASN:HB3	23	0.19
(1,705)	1:53:A:LEU:HD13	1:127:A:ASN:HB2	23	0.19
(1,705)	1:53:A:LEU:HD13	1:127:A:ASN:HB3	23	0.19
(1,705)	1:53:A:LEU:HD21	1:127:A:ASN:HB2	23	0.19
(1,705)	1:53:A:LEU:HD21	1:127:A:ASN:HB3	23	0.19
(1,705)	1:53:A:LEU:HD22	1:127:A:ASN:HB2	23	0.19
(1,705)	1:53:A:LEU:HD22	1:127:A:ASN:HB3	23	0.19
(1,705)	1:53:A:LEU:HD23	1:127:A:ASN:HB2	23	0.19
(1,705)	1:53:A:LEU:HD23	1:127:A:ASN:HB3	23	0.19
(1,669)	1:47:A:ALA:HB1	1:137:A:PHE:HA	11	0.19
(1,669)	1:47:A:ALA:HB2	1:137:A:PHE:HA	11	0.19
(1,669)	1:47:A:ALA:HB3	1:137:A:PHE:HA	11	0.19
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD11	19	0.19
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD12	19	0.19
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD13	19	0.19
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD21	19	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD22	19	0.19
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD23	19	0.19
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD11	19	0.19
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD12	19	0.19
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD13	19	0.19
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD21	19	0.19
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD22	19	0.19
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD23	19	0.19
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD11	20	0.19
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD12	20	0.19
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD13	20	0.19
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD21	20	0.19
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD22	20	0.19
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD23	20	0.19
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD11	20	0.19
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD12	20	0.19
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD13	20	0.19
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD21	20	0.19
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD22	20	0.19
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD23	20	0.19
(1,640)	1:35:A:LEU:HD11	1:31:A:GLU:HA	20	0.19
(1,640)	1:35:A:LEU:HD12	1:31:A:GLU:HA	20	0.19
(1,640)	1:35:A:LEU:HD13	1:31:A:GLU:HA	20	0.19
(1,640)	1:35:A:LEU:HD21	1:31:A:GLU:HA	20	0.19
(1,640)	1:35:A:LEU:HD22	1:31:A:GLU:HA	20	0.19
(1,640)	1:35:A:LEU:HD23	1:31:A:GLU:HA	20	0.19
(1,638)	1:34:A:ARG:HB2	1:74:A:PHE:HD1	3	0.19
(1,638)	1:34:A:ARG:HB2	1:74:A:PHE:HD2	3	0.19
(1,638)	1:34:A:ARG:HB3	1:74:A:PHE:HD1	3	0.19
(1,638)	1:34:A:ARG:HB3	1:74:A:PHE:HD2	3	0.19
(1,638)	1:34:A:ARG:HB2	1:74:A:PHE:HD1	9	0.19
(1,638)	1:34:A:ARG:HB2	1:74:A:PHE:HD2	9	0.19
(1,638)	1:34:A:ARG:HB3	1:74:A:PHE:HD1	9	0.19
(1,638)	1:34:A:ARG:HB3	1:74:A:PHE:HD2	9	0.19
(1,635)	1:33:A:GLN:HA	1:30:A:HIS:HA	4	0.19
(1,635)	1:33:A:GLN:HA	1:30:A:HIS:HA	11	0.19
(1,635)	1:33:A:GLN:HA	1:30:A:HIS:HA	12	0.19
(1,635)	1:33:A:GLN:HA	1:30:A:HIS:HA	17	0.19
(1,616)	2:480:B:ALA:H	2:479:B:LEU:HA	8	0.19
(1,616)	2:480:B:ALA:H	2:479:B:LEU:HA	12	0.19
(1,616)	2:480:B:ALA:H	2:479:B:LEU:HA	24	0.19
(1,610)	2:479:B:LEU:H	2:478:B:LYS:HG2	16	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,610)	2:479:B:LEU:H	2:478:B:LYS:HG3	16	0.19
(1,610)	2:479:B:LEU:H	2:478:B:LYS:HG2	21	0.19
(1,610)	2:479:B:LEU:H	2:478:B:LYS:HG3	21	0.19
(1,584)	2:468:B:TYR:H	2:467:B:PRO:HG2	9	0.19
(1,584)	2:468:B:TYR:H	2:467:B:PRO:HG3	9	0.19
(1,584)	2:468:B:TYR:H	2:467:B:PRO:HG2	18	0.19
(1,584)	2:468:B:TYR:H	2:467:B:PRO:HG3	18	0.19
(1,556)	2:451:B:GLU:H	2:450:B:TRP:HB2	11	0.19
(1,556)	2:451:B:GLU:H	2:450:B:TRP:HB2	21	0.19
(1,522)	1:116:A:THR:H	1:125:A:GLY:HA2	16	0.19
(1,522)	1:116:A:THR:H	1:125:A:GLY:HA3	16	0.19
(1,522)	1:116:A:THR:H	1:125:A:GLY:HA2	20	0.19
(1,522)	1:116:A:THR:H	1:125:A:GLY:HA3	20	0.19
(1,477)	1:72:A:VAL:H	1:48:A:THR:HA	11	0.19
(1,457)	1:38:A:MET:H	1:34:A:ARG:HD2	4	0.19
(1,457)	1:38:A:MET:H	1:34:A:ARG:HD3	4	0.19
(1,416)	1:87:A:LEU:H	1:98:A:GLU:HB2	13	0.19
(1,416)	1:87:A:LEU:H	1:98:A:GLU:HB3	13	0.19
(1,403)	1:74:A:PHE:H	1:47:A:ALA:HA	5	0.19
(1,403)	1:74:A:PHE:H	1:47:A:ALA:HA	9	0.19
(1,403)	1:74:A:PHE:H	1:47:A:ALA:HA	15	0.19
(1,403)	1:74:A:PHE:H	1:47:A:ALA:HA	17	0.19
(1,399)	1:72:A:VAL:H	1:50:A:VAL:HB	22	0.19
(1,369)	1:37:A:GLU:H	1:34:A:ARG:HA	19	0.19
(1,366)	1:35:A:LEU:H	1:32:A:ASN:HA	3	0.19
(1,366)	1:35:A:LEU:H	1:32:A:ASN:HA	19	0.19
(1,366)	1:35:A:LEU:H	1:32:A:ASN:HA	23	0.19
(1,364)	1:34:A:ARG:H	1:31:A:GLU:HA	15	0.19
(1,328)	1:143:A:GLU:H	1:139:A:ALA:HB1	6	0.19
(1,328)	1:143:A:GLU:H	1:139:A:ALA:HB2	6	0.19
(1,328)	1:143:A:GLU:H	1:139:A:ALA:HB3	6	0.19
(1,328)	1:143:A:GLU:H	1:139:A:ALA:HB1	7	0.19
(1,328)	1:143:A:GLU:H	1:139:A:ALA:HB2	7	0.19
(1,328)	1:143:A:GLU:H	1:139:A:ALA:HB3	7	0.19
(1,328)	1:143:A:GLU:H	1:139:A:ALA:HB1	13	0.19
(1,328)	1:143:A:GLU:H	1:139:A:ALA:HB2	13	0.19
(1,328)	1:143:A:GLU:H	1:139:A:ALA:HB3	13	0.19
(1,328)	1:143:A:GLU:H	1:139:A:ALA:HB1	18	0.19
(1,328)	1:143:A:GLU:H	1:139:A:ALA:HB2	18	0.19
(1,328)	1:143:A:GLU:H	1:139:A:ALA:HB3	18	0.19
(1,272)	1:124:A:ALA:H	1:123:A:GLN:HG2	1	0.19
(1,272)	1:124:A:ALA:H	1:123:A:GLN:HG3	1	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,272)	1:124:A:ALA:H	1:123:A:GLN:HG2	2	0.19
(1,272)	1:124:A:ALA:H	1:123:A:GLN:HG3	2	0.19
(1,272)	1:124:A:ALA:H	1:123:A:GLN:HG2	14	0.19
(1,272)	1:124:A:ALA:H	1:123:A:GLN:HG3	14	0.19
(1,272)	1:124:A:ALA:H	1:123:A:GLN:HG2	16	0.19
(1,272)	1:124:A:ALA:H	1:123:A:GLN:HG3	16	0.19
(1,272)	1:124:A:ALA:H	1:123:A:GLN:HG2	18	0.19
(1,272)	1:124:A:ALA:H	1:123:A:GLN:HG3	18	0.19
(1,272)	1:124:A:ALA:H	1:123:A:GLN:HG2	22	0.19
(1,272)	1:124:A:ALA:H	1:123:A:GLN:HG3	22	0.19
(1,259)	1:118:A:ALA:H	1:117:A:PHE:HB3	2	0.19
(1,250)	1:116:A:THR:H	1:115:A:HIS:HB3	4	0.19
(1,250)	1:116:A:THR:H	1:115:A:HIS:HB3	13	0.19
(1,235)	1:107:A:TYR:H	1:106:A:VAL:H	17	0.19
(1,195)	1:96:A:LEU:H	1:95:A:LEU:H	1	0.19
(1,141)	1:77:A:ASP:H	1:76:A:LYS:HG2	11	0.19
(1,141)	1:77:A:ASP:H	1:76:A:LYS:HG3	11	0.19
(1,105)	1:63:A:HIS:H	1:62:A:GLU:HA	3	0.19
(1,105)	1:63:A:HIS:H	1:62:A:GLU:HA	4	0.19
(1,105)	1:63:A:HIS:H	1:62:A:GLU:HA	8	0.19
(1,105)	1:63:A:HIS:H	1:62:A:GLU:HA	23	0.19
(1,105)	1:63:A:HIS:H	1:62:A:GLU:HA	24	0.19
(1,54)	1:43:A:CYS:H	1:42:A:LYS:HB2	8	0.19
(1,54)	1:43:A:CYS:H	1:42:A:LYS:HB3	8	0.19
(4,92)	1:136:A:ALA:N	1:132:A:ASP:O	1	0.18
(4,92)	1:136:A:ALA:N	1:132:A:ASP:O	10	0.18
(4,92)	1:136:A:ALA:N	1:132:A:ASP:O	18	0.18
(4,92)	1:136:A:ALA:N	1:132:A:ASP:O	22	0.18
(4,41)	1:71:A:ALA:H	1:88:A:TYR:O	14	0.18
(4,23)	1:68:A:HIS:H	1:53:A:LEU:O	5	0.18
(1,1016)	2:479:B:LEU:HG	1:83:A:TYR:HD1	22	0.18
(1,1016)	2:479:B:LEU:HG	1:83:A:TYR:HD2	22	0.18
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD11	1	0.18
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD12	1	0.18
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD13	1	0.18
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD21	1	0.18
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD22	1	0.18
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD23	1	0.18
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD11	1	0.18
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD12	1	0.18
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD13	1	0.18
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD21	1	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD22	1	0.18
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD23	1	0.18
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD11	3	0.18
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD12	3	0.18
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD13	3	0.18
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD21	3	0.18
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD22	3	0.18
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD23	3	0.18
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD11	3	0.18
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD12	3	0.18
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD13	3	0.18
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD21	3	0.18
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD22	3	0.18
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD23	3	0.18
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD11	12	0.18
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD12	12	0.18
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD13	12	0.18
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD21	12	0.18
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD22	12	0.18
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD23	12	0.18
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD11	12	0.18
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD12	12	0.18
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD13	12	0.18
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD21	12	0.18
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD22	12	0.18
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD23	12	0.18
(1,944)	2:458:B:PRO:HA	2:460:B:SER:HB2	2	0.18
(1,944)	2:458:B:PRO:HA	2:460:B:SER:HB3	2	0.18
(1,944)	2:458:B:PRO:HA	2:460:B:SER:HB2	7	0.18
(1,944)	2:458:B:PRO:HA	2:460:B:SER:HB3	7	0.18
(1,944)	2:458:B:PRO:HA	2:460:B:SER:HB2	15	0.18
(1,944)	2:458:B:PRO:HA	2:460:B:SER:HB3	15	0.18
(1,928)	1:145:A:ILE:HD11	1:117:A:PHE:HZ	6	0.18
(1,928)	1:145:A:ILE:HD12	1:117:A:PHE:HZ	6	0.18
(1,928)	1:145:A:ILE:HD13	1:117:A:PHE:HZ	6	0.18
(1,912)	1:141:A:VAL:HG11	1:107:A:TYR:HB3	9	0.18
(1,912)	1:141:A:VAL:HG12	1:107:A:TYR:HB3	9	0.18
(1,912)	1:141:A:VAL:HG13	1:107:A:TYR:HB3	9	0.18
(1,912)	1:141:A:VAL:HG21	1:107:A:TYR:HB3	9	0.18
(1,912)	1:141:A:VAL:HG22	1:107:A:TYR:HB3	9	0.18
(1,912)	1:141:A:VAL:HG23	1:107:A:TYR:HB3	9	0.18
(1,912)	1:141:A:VAL:HG11	1:107:A:TYR:HB2	9	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,912)	1:141:A:VAL:HG12	1:107:A:TYR:HB2	9	0.18
(1,912)	1:141:A:VAL:HG13	1:107:A:TYR:HB2	9	0.18
(1,912)	1:141:A:VAL:HG21	1:107:A:TYR:HB2	9	0.18
(1,912)	1:141:A:VAL:HG22	1:107:A:TYR:HB2	9	0.18
(1,912)	1:141:A:VAL:HG23	1:107:A:TYR:HB2	9	0.18
(1,877)	1:127:A:ASN:HB2	1:113:A:PHE:HB2	9	0.18
(1,877)	1:127:A:ASN:HB2	1:113:A:PHE:HB3	9	0.18
(1,877)	1:127:A:ASN:HB3	1:113:A:PHE:HB2	9	0.18
(1,877)	1:127:A:ASN:HB3	1:113:A:PHE:HB3	9	0.18
(1,877)	1:127:A:ASN:HB2	1:113:A:PHE:HB2	10	0.18
(1,877)	1:127:A:ASN:HB2	1:113:A:PHE:HB3	10	0.18
(1,877)	1:127:A:ASN:HB3	1:113:A:PHE:HB2	10	0.18
(1,877)	1:127:A:ASN:HB3	1:113:A:PHE:HB3	10	0.18
(1,875)	1:126:A:LEU:HG	1:114:A:PHE:HD1	10	0.18
(1,875)	1:126:A:LEU:HG	1:114:A:PHE:HD2	10	0.18
(1,865)	1:123:A:GLN:HG2	1:122:A:CYS:HB2	21	0.18
(1,865)	1:123:A:GLN:HG2	1:122:A:CYS:HB3	21	0.18
(1,865)	1:123:A:GLN:HG3	1:122:A:CYS:HB2	21	0.18
(1,865)	1:123:A:GLN:HG3	1:122:A:CYS:HB3	21	0.18
(1,864)	1:122:A:CYS:HA	1:123:A:GLN:HB2	17	0.18
(1,864)	1:122:A:CYS:HA	1:123:A:GLN:HB3	17	0.18
(1,851)	1:110:A:PRO:HA	1:131:A:GLU:HB2	7	0.18
(1,851)	1:110:A:PRO:HA	1:131:A:GLU:HB3	7	0.18
(1,851)	1:110:A:PRO:HA	1:131:A:GLU:HB2	15	0.18
(1,851)	1:110:A:PRO:HA	1:131:A:GLU:HB3	15	0.18
(1,847)	1:109:A:THR:HB	1:115:A:HIS:HB2	1	0.18
(1,847)	1:109:A:THR:HB	1:115:A:HIS:HB3	1	0.18
(1,847)	1:109:A:THR:HB	1:115:A:HIS:HB2	13	0.18
(1,847)	1:109:A:THR:HB	1:115:A:HIS:HB3	13	0.18
(1,845)	1:108:A:SER:HB2	1:110:A:PRO:HA	6	0.18
(1,845)	1:108:A:SER:HB3	1:110:A:PRO:HA	6	0.18
(1,783)	1:81:A:LYS:HG2	1:80:A:GLN:HA	4	0.18
(1,783)	1:81:A:LYS:HG3	1:80:A:GLN:HA	4	0.18
(1,783)	1:81:A:LYS:HG2	1:80:A:GLN:HA	17	0.18
(1,783)	1:81:A:LYS:HG3	1:80:A:GLN:HA	17	0.18
(1,741)	1:71:A:ALA:HB1	1:35:A:LEU:HB2	12	0.18
(1,741)	1:71:A:ALA:HB1	1:35:A:LEU:HB3	12	0.18
(1,741)	1:71:A:ALA:HB2	1:35:A:LEU:HB2	12	0.18
(1,741)	1:71:A:ALA:HB2	1:35:A:LEU:HB3	12	0.18
(1,741)	1:71:A:ALA:HB3	1:35:A:LEU:HB2	12	0.18
(1,741)	1:71:A:ALA:HB3	1:35:A:LEU:HB3	12	0.18
(1,741)	1:71:A:ALA:HB1	1:35:A:LEU:HB2	17	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,741)	1:71:A:ALA:HB1	1:35:A:LEU:HB3	17	0.18
(1,741)	1:71:A:ALA:HB2	1:35:A:LEU:HB2	17	0.18
(1,741)	1:71:A:ALA:HB2	1:35:A:LEU:HB3	17	0.18
(1,741)	1:71:A:ALA:HB3	1:35:A:LEU:HB2	17	0.18
(1,741)	1:71:A:ALA:HB3	1:35:A:LEU:HB3	17	0.18
(1,732)	1:65:A:THR:HB	1:56:A:ALA:HB1	5	0.18
(1,732)	1:65:A:THR:HB	1:56:A:ALA:HB2	5	0.18
(1,732)	1:65:A:THR:HB	1:56:A:ALA:HB3	5	0.18
(1,732)	1:65:A:THR:HB	1:56:A:ALA:HB1	12	0.18
(1,732)	1:65:A:THR:HB	1:56:A:ALA:HB2	12	0.18
(1,732)	1:65:A:THR:HB	1:56:A:ALA:HB3	12	0.18
(1,732)	1:65:A:THR:HB	1:56:A:ALA:HB1	18	0.18
(1,732)	1:65:A:THR:HB	1:56:A:ALA:HB2	18	0.18
(1,732)	1:65:A:THR:HB	1:56:A:ALA:HB3	18	0.18
(1,720)	1:56:A:ALA:HB1	1:123:A:GLN:HB2	14	0.18
(1,720)	1:56:A:ALA:HB1	1:123:A:GLN:HB3	14	0.18
(1,720)	1:56:A:ALA:HB2	1:123:A:GLN:HB2	14	0.18
(1,720)	1:56:A:ALA:HB2	1:123:A:GLN:HB3	14	0.18
(1,720)	1:56:A:ALA:HB3	1:123:A:GLN:HB2	14	0.18
(1,720)	1:56:A:ALA:HB3	1:123:A:GLN:HB3	14	0.18
(1,705)	1:53:A:LEU:HD11	1:127:A:ASN:HB2	2	0.18
(1,705)	1:53:A:LEU:HD11	1:127:A:ASN:HB3	2	0.18
(1,705)	1:53:A:LEU:HD12	1:127:A:ASN:HB2	2	0.18
(1,705)	1:53:A:LEU:HD12	1:127:A:ASN:HB3	2	0.18
(1,705)	1:53:A:LEU:HD13	1:127:A:ASN:HB2	2	0.18
(1,705)	1:53:A:LEU:HD13	1:127:A:ASN:HB3	2	0.18
(1,705)	1:53:A:LEU:HD21	1:127:A:ASN:HB2	2	0.18
(1,705)	1:53:A:LEU:HD21	1:127:A:ASN:HB3	2	0.18
(1,705)	1:53:A:LEU:HD22	1:127:A:ASN:HB2	2	0.18
(1,705)	1:53:A:LEU:HD22	1:127:A:ASN:HB3	2	0.18
(1,705)	1:53:A:LEU:HD23	1:127:A:ASN:HB2	2	0.18
(1,705)	1:53:A:LEU:HD23	1:127:A:ASN:HB3	2	0.18
(1,669)	1:47:A:ALA:HB1	1:137:A:PHE:HA	2	0.18
(1,669)	1:47:A:ALA:HB2	1:137:A:PHE:HA	2	0.18
(1,669)	1:47:A:ALA:HB3	1:137:A:PHE:HA	2	0.18
(1,669)	1:47:A:ALA:HB1	1:137:A:PHE:HA	5	0.18
(1,669)	1:47:A:ALA:HB2	1:137:A:PHE:HA	5	0.18
(1,669)	1:47:A:ALA:HB3	1:137:A:PHE:HA	5	0.18
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG11	17	0.18
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG12	17	0.18
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG13	17	0.18
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG21	17	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG22	17	0.18
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG23	17	0.18
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG11	17	0.18
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG12	17	0.18
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG13	17	0.18
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG21	17	0.18
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG22	17	0.18
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG23	17	0.18
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG11	17	0.18
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG12	17	0.18
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG13	17	0.18
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG21	17	0.18
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG22	17	0.18
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG23	17	0.18
(1,639)	1:34:A:ARG:HD2	1:74:A:PHE:HE1	6	0.18
(1,639)	1:34:A:ARG:HD2	1:74:A:PHE:HE2	6	0.18
(1,639)	1:34:A:ARG:HD3	1:74:A:PHE:HE1	6	0.18
(1,639)	1:34:A:ARG:HD3	1:74:A:PHE:HE2	6	0.18
(1,638)	1:34:A:ARG:HB2	1:74:A:PHE:HD1	16	0.18
(1,638)	1:34:A:ARG:HB2	1:74:A:PHE:HD2	16	0.18
(1,638)	1:34:A:ARG:HB3	1:74:A:PHE:HD1	16	0.18
(1,638)	1:34:A:ARG:HB3	1:74:A:PHE:HD2	16	0.18
(1,616)	2:480:B:ALA:H	2:479:B:LEU:HA	1	0.18
(1,616)	2:480:B:ALA:H	2:479:B:LEU:HA	3	0.18
(1,616)	2:480:B:ALA:H	2:479:B:LEU:HA	4	0.18
(1,616)	2:480:B:ALA:H	2:479:B:LEU:HA	5	0.18
(1,616)	2:480:B:ALA:H	2:479:B:LEU:HA	6	0.18
(1,616)	2:480:B:ALA:H	2:479:B:LEU:HA	7	0.18
(1,616)	2:480:B:ALA:H	2:479:B:LEU:HA	9	0.18
(1,616)	2:480:B:ALA:H	2:479:B:LEU:HA	10	0.18
(1,616)	2:480:B:ALA:H	2:479:B:LEU:HA	11	0.18
(1,616)	2:480:B:ALA:H	2:479:B:LEU:HA	13	0.18
(1,616)	2:480:B:ALA:H	2:479:B:LEU:HA	15	0.18
(1,616)	2:480:B:ALA:H	2:479:B:LEU:HA	16	0.18
(1,616)	2:480:B:ALA:H	2:479:B:LEU:HA	17	0.18
(1,616)	2:480:B:ALA:H	2:479:B:LEU:HA	18	0.18
(1,616)	2:480:B:ALA:H	2:479:B:LEU:HA	19	0.18
(1,616)	2:480:B:ALA:H	2:479:B:LEU:HA	22	0.18
(1,616)	2:480:B:ALA:H	2:479:B:LEU:HA	23	0.18
(1,584)	2:468:B:TYR:H	2:467:B:PRO:HG2	2	0.18
(1,584)	2:468:B:TYR:H	2:467:B:PRO:HG3	2	0.18
(1,584)	2:468:B:TYR:H	2:467:B:PRO:HG2	12	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,584)	2:468:B:TYR:H	2:467:B:PRO:HG3	12	0.18
(1,556)	2:451:B:GLU:H	2:450:B:TRP:HB2	13	0.18
(1,556)	2:451:B:GLU:H	2:450:B:TRP:HB2	23	0.18
(1,523)	1:116:A:THR:H	1:108:A:SER:HB2	6	0.18
(1,523)	1:116:A:THR:H	1:108:A:SER:HB3	6	0.18
(1,523)	1:116:A:THR:H	1:108:A:SER:HB2	20	0.18
(1,523)	1:116:A:THR:H	1:108:A:SER:HB3	20	0.18
(1,522)	1:116:A:THR:H	1:125:A:GLY:HA2	5	0.18
(1,522)	1:116:A:THR:H	1:125:A:GLY:HA3	5	0.18
(1,493)	1:97:A:TRP:H	1:95:A:LEU:HA	21	0.18
(1,493)	1:97:A:TRP:H	1:95:A:LEU:HA	22	0.18
(1,477)	1:72:A:VAL:H	1:48:A:THR:HA	18	0.18
(1,477)	1:72:A:VAL:H	1:48:A:THR:HA	19	0.18
(1,469)	1:55:A:LEU:H	1:65:A:THR:H	5	0.18
(1,469)	1:55:A:LEU:H	1:65:A:THR:H	17	0.18
(1,466)	1:52:A:GLN:H	1:128:A:PHE:HB2	10	0.18
(1,466)	1:52:A:GLN:H	1:128:A:PHE:HB3	10	0.18
(1,457)	1:38:A:MET:H	1:34:A:ARG:HD2	15	0.18
(1,457)	1:38:A:MET:H	1:34:A:ARG:HD3	15	0.18
(1,429)	1:101:A:LEU:H	1:84:A:PHE:HB2	19	0.18
(1,429)	1:101:A:LEU:H	1:84:A:PHE:HB3	19	0.18
(1,416)	1:87:A:LEU:H	1:98:A:GLU:HB2	4	0.18
(1,416)	1:87:A:LEU:H	1:98:A:GLU:HB3	4	0.18
(1,412)	1:84:A:PHE:H	1:76:A:LYS:HB2	21	0.18
(1,412)	1:84:A:PHE:H	1:76:A:LYS:HB3	21	0.18
(1,412)	1:84:A:PHE:H	1:76:A:LYS:HB2	22	0.18
(1,412)	1:84:A:PHE:H	1:76:A:LYS:HB3	22	0.18
(1,403)	1:74:A:PHE:H	1:47:A:ALA:HA	12	0.18
(1,403)	1:74:A:PHE:H	1:47:A:ALA:HA	20	0.18
(1,399)	1:72:A:VAL:H	1:50:A:VAL:HB	6	0.18
(1,374)	1:38:A:MET:H	1:35:A:LEU:HG	9	0.18
(1,366)	1:35:A:LEU:H	1:32:A:ASN:HA	12	0.18
(1,364)	1:34:A:ARG:H	1:31:A:GLU:HA	8	0.18
(1,342)	1:146:A:GLN:H	1:143:A:GLU:HA	19	0.18
(1,328)	1:143:A:GLU:H	1:139:A:ALA:HB1	10	0.18
(1,328)	1:143:A:GLU:H	1:139:A:ALA:HB2	10	0.18
(1,328)	1:143:A:GLU:H	1:139:A:ALA:HB3	10	0.18
(1,328)	1:143:A:GLU:H	1:139:A:ALA:HB1	17	0.18
(1,328)	1:143:A:GLU:H	1:139:A:ALA:HB2	17	0.18
(1,328)	1:143:A:GLU:H	1:139:A:ALA:HB3	17	0.18
(1,272)	1:124:A:ALA:H	1:123:A:GLN:HG2	3	0.18
(1,272)	1:124:A:ALA:H	1:123:A:GLN:HG3	3	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,272)	1:124:A:ALA:H	1:123:A:GLN:HG2	23	0.18
(1,272)	1:124:A:ALA:H	1:123:A:GLN:HG3	23	0.18
(1,250)	1:116:A:THR:H	1:115:A:HIS:HB3	8	0.18
(1,112)	1:65:A:THR:H	1:64:A:TRP:HB3	9	0.18
(1,105)	1:63:A:HIS:H	1:62:A:GLU:HA	17	0.18
(4,111)	1:146:A:GLN:H	1:142:A:GLN:O	14	0.17
(4,111)	1:146:A:GLN:H	1:142:A:GLN:O	19	0.17
(4,92)	1:136:A:ALA:N	1:132:A:ASP:O	3	0.17
(4,92)	1:136:A:ALA:N	1:132:A:ASP:O	13	0.17
(4,77)	1:34:A:ARG:H	1:30:A:HIS:O	5	0.17
(4,77)	1:34:A:ARG:H	1:30:A:HIS:O	7	0.17
(4,41)	1:71:A:ALA:H	1:88:A:TYR:O	7	0.17
(4,41)	1:71:A:ALA:H	1:88:A:TYR:O	8	0.17
(1,1016)	2:479:B:LEU:HG	1:83:A:TYR:HD1	23	0.17
(1,1016)	2:479:B:LEU:HG	1:83:A:TYR:HD2	23	0.17
(1,1008)	2:474:B:SER:H	1:102:A:TYR:HE1	12	0.17
(1,1008)	2:474:B:SER:H	1:102:A:TYR:HE2	12	0.17
(1,1007)	2:474:B:SER:H	1:102:A:TYR:HA	9	0.17
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD11	14	0.17
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD12	14	0.17
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD13	14	0.17
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD21	14	0.17
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD22	14	0.17
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD23	14	0.17
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD11	14	0.17
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD12	14	0.17
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD13	14	0.17
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD21	14	0.17
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD22	14	0.17
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD23	14	0.17
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD11	17	0.17
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD12	17	0.17
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD13	17	0.17
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD21	17	0.17
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD22	17	0.17
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD23	17	0.17
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD11	17	0.17
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD12	17	0.17
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD13	17	0.17
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD21	17	0.17
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD22	17	0.17
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD23	17	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD11	20	0.17
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD12	20	0.17
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD13	20	0.17
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD21	20	0.17
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD22	20	0.17
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD23	20	0.17
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD11	20	0.17
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD12	20	0.17
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD13	20	0.17
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD21	20	0.17
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD22	20	0.17
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD23	20	0.17
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD11	23	0.17
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD12	23	0.17
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD13	23	0.17
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD21	23	0.17
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD22	23	0.17
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD23	23	0.17
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD11	23	0.17
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD12	23	0.17
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD13	23	0.17
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD21	23	0.17
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD22	23	0.17
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD23	23	0.17
(1,965)	1:56:A:ALA:HB1	2:462:B:LEU:HD11	5	0.17
(1,965)	1:56:A:ALA:HB1	2:462:B:LEU:HD12	5	0.17
(1,965)	1:56:A:ALA:HB1	2:462:B:LEU:HD13	5	0.17
(1,965)	1:56:A:ALA:HB1	2:462:B:LEU:HD21	5	0.17
(1,965)	1:56:A:ALA:HB1	2:462:B:LEU:HD22	5	0.17
(1,965)	1:56:A:ALA:HB1	2:462:B:LEU:HD23	5	0.17
(1,965)	1:56:A:ALA:HB2	2:462:B:LEU:HD11	5	0.17
(1,965)	1:56:A:ALA:HB2	2:462:B:LEU:HD12	5	0.17
(1,965)	1:56:A:ALA:HB2	2:462:B:LEU:HD13	5	0.17
(1,965)	1:56:A:ALA:HB2	2:462:B:LEU:HD21	5	0.17
(1,965)	1:56:A:ALA:HB2	2:462:B:LEU:HD22	5	0.17
(1,965)	1:56:A:ALA:HB2	2:462:B:LEU:HD23	5	0.17
(1,965)	1:56:A:ALA:HB3	2:462:B:LEU:HD11	5	0.17
(1,965)	1:56:A:ALA:HB3	2:462:B:LEU:HD12	5	0.17
(1,965)	1:56:A:ALA:HB3	2:462:B:LEU:HD13	5	0.17
(1,965)	1:56:A:ALA:HB3	2:462:B:LEU:HD21	5	0.17
(1,965)	1:56:A:ALA:HB3	2:462:B:LEU:HD22	5	0.17
(1,965)	1:56:A:ALA:HB3	2:462:B:LEU:HD23	5	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,957)	1:50:A:VAL:HG11	2:453:B:ARG:HB2	11	0.17
(1,957)	1:50:A:VAL:HG11	2:453:B:ARG:HB3	11	0.17
(1,957)	1:50:A:VAL:HG12	2:453:B:ARG:HB2	11	0.17
(1,957)	1:50:A:VAL:HG12	2:453:B:ARG:HB3	11	0.17
(1,957)	1:50:A:VAL:HG13	2:453:B:ARG:HB2	11	0.17
(1,957)	1:50:A:VAL:HG13	2:453:B:ARG:HB3	11	0.17
(1,957)	1:50:A:VAL:HG21	2:453:B:ARG:HB2	11	0.17
(1,957)	1:50:A:VAL:HG21	2:453:B:ARG:HB3	11	0.17
(1,957)	1:50:A:VAL:HG22	2:453:B:ARG:HB2	11	0.17
(1,957)	1:50:A:VAL:HG22	2:453:B:ARG:HB3	11	0.17
(1,957)	1:50:A:VAL:HG23	2:453:B:ARG:HB2	11	0.17
(1,957)	1:50:A:VAL:HG23	2:453:B:ARG:HB3	11	0.17
(1,957)	1:50:A:VAL:HG11	2:453:B:ARG:HB2	22	0.17
(1,957)	1:50:A:VAL:HG11	2:453:B:ARG:HB3	22	0.17
(1,957)	1:50:A:VAL:HG12	2:453:B:ARG:HB2	22	0.17
(1,957)	1:50:A:VAL:HG12	2:453:B:ARG:HB3	22	0.17
(1,957)	1:50:A:VAL:HG13	2:453:B:ARG:HB2	22	0.17
(1,957)	1:50:A:VAL:HG13	2:453:B:ARG:HB3	22	0.17
(1,957)	1:50:A:VAL:HG21	2:453:B:ARG:HB2	22	0.17
(1,957)	1:50:A:VAL:HG21	2:453:B:ARG:HB3	22	0.17
(1,957)	1:50:A:VAL:HG22	2:453:B:ARG:HB2	22	0.17
(1,957)	1:50:A:VAL:HG22	2:453:B:ARG:HB3	22	0.17
(1,957)	1:50:A:VAL:HG23	2:453:B:ARG:HB2	22	0.17
(1,957)	1:50:A:VAL:HG23	2:453:B:ARG:HB3	22	0.17
(1,944)	2:458:B:PRO:HA	2:460:B:SER:HB2	21	0.17
(1,944)	2:458:B:PRO:HA	2:460:B:SER:HB3	21	0.17
(1,944)	2:458:B:PRO:HA	2:460:B:SER:HB2	23	0.17
(1,944)	2:458:B:PRO:HA	2:460:B:SER:HB3	23	0.17
(1,912)	1:141:A:VAL:HG11	1:107:A:TYR:HB3	5	0.17
(1,912)	1:141:A:VAL:HG12	1:107:A:TYR:HB3	5	0.17
(1,912)	1:141:A:VAL:HG13	1:107:A:TYR:HB3	5	0.17
(1,912)	1:141:A:VAL:HG21	1:107:A:TYR:HB3	5	0.17
(1,912)	1:141:A:VAL:HG22	1:107:A:TYR:HB3	5	0.17
(1,912)	1:141:A:VAL:HG23	1:107:A:TYR:HB3	5	0.17
(1,912)	1:141:A:VAL:HG11	1:107:A:TYR:HB2	5	0.17
(1,912)	1:141:A:VAL:HG12	1:107:A:TYR:HB2	5	0.17
(1,912)	1:141:A:VAL:HG13	1:107:A:TYR:HB2	5	0.17
(1,912)	1:141:A:VAL:HG21	1:107:A:TYR:HB2	5	0.17
(1,912)	1:141:A:VAL:HG22	1:107:A:TYR:HB2	5	0.17
(1,912)	1:141:A:VAL:HG23	1:107:A:TYR:HB2	5	0.17
(1,912)	1:141:A:VAL:HG11	1:107:A:TYR:HB3	20	0.17
(1,912)	1:141:A:VAL:HG12	1:107:A:TYR:HB3	20	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,912)	1:141:A:VAL:HG13	1:107:A:TYR:HB3	20	0.17
(1,912)	1:141:A:VAL:HG21	1:107:A:TYR:HB3	20	0.17
(1,912)	1:141:A:VAL:HG22	1:107:A:TYR:HB3	20	0.17
(1,912)	1:141:A:VAL:HG23	1:107:A:TYR:HB3	20	0.17
(1,912)	1:141:A:VAL:HG11	1:107:A:TYR:HB2	20	0.17
(1,912)	1:141:A:VAL:HG12	1:107:A:TYR:HB2	20	0.17
(1,912)	1:141:A:VAL:HG13	1:107:A:TYR:HB2	20	0.17
(1,912)	1:141:A:VAL:HG21	1:107:A:TYR:HB2	20	0.17
(1,912)	1:141:A:VAL:HG22	1:107:A:TYR:HB2	20	0.17
(1,912)	1:141:A:VAL:HG23	1:107:A:TYR:HB2	20	0.17
(1,903)	1:139:A:ALA:HA	1:138:A:ARG:HB2	19	0.17
(1,903)	1:139:A:ALA:HA	1:138:A:ARG:HB3	19	0.17
(1,901)	1:138:A:ARG:HA	1:140:A:LEU:HD11	11	0.17
(1,901)	1:138:A:ARG:HA	1:140:A:LEU:HD12	11	0.17
(1,901)	1:138:A:ARG:HA	1:140:A:LEU:HD13	11	0.17
(1,901)	1:138:A:ARG:HA	1:140:A:LEU:HD21	11	0.17
(1,901)	1:138:A:ARG:HA	1:140:A:LEU:HD22	11	0.17
(1,901)	1:138:A:ARG:HA	1:140:A:LEU:HD23	11	0.17
(1,877)	1:127:A:ASN:HB2	1:113:A:PHE:HB2	2	0.17
(1,877)	1:127:A:ASN:HB2	1:113:A:PHE:HB3	2	0.17
(1,877)	1:127:A:ASN:HB3	1:113:A:PHE:HB2	2	0.17
(1,877)	1:127:A:ASN:HB3	1:113:A:PHE:HB3	2	0.17
(1,875)	1:126:A:LEU:HG	1:114:A:PHE:HD1	1	0.17
(1,875)	1:126:A:LEU:HG	1:114:A:PHE:HD2	1	0.17
(1,869)	1:124:A:ALA:HB1	1:117:A:PHE:HD1	12	0.17
(1,869)	1:124:A:ALA:HB1	1:117:A:PHE:HD2	12	0.17
(1,869)	1:124:A:ALA:HB2	1:117:A:PHE:HD1	12	0.17
(1,869)	1:124:A:ALA:HB2	1:117:A:PHE:HD2	12	0.17
(1,869)	1:124:A:ALA:HB3	1:117:A:PHE:HD1	12	0.17
(1,869)	1:124:A:ALA:HB3	1:117:A:PHE:HD2	12	0.17
(1,865)	1:123:A:GLN:HG2	1:122:A:CYS:HB2	23	0.17
(1,865)	1:123:A:GLN:HG2	1:122:A:CYS:HB3	23	0.17
(1,865)	1:123:A:GLN:HG3	1:122:A:CYS:HB2	23	0.17
(1,865)	1:123:A:GLN:HG3	1:122:A:CYS:HB3	23	0.17
(1,864)	1:122:A:CYS:HA	1:123:A:GLN:HB2	19	0.17
(1,864)	1:122:A:CYS:HA	1:123:A:GLN:HB3	19	0.17
(1,863)	1:120:A:ASP:HA	1:123:A:GLN:HG2	3	0.17
(1,863)	1:120:A:ASP:HA	1:123:A:GLN:HG3	3	0.17
(1,863)	1:120:A:ASP:HA	1:123:A:GLN:HG2	6	0.17
(1,863)	1:120:A:ASP:HA	1:123:A:GLN:HG3	6	0.17
(1,851)	1:110:A:PRO:HA	1:131:A:GLU:HB2	9	0.17
(1,851)	1:110:A:PRO:HA	1:131:A:GLU:HB3	9	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,851)	1:110:A:PRO:HA	1:131:A:GLU:HB2	16	0.17
(1,851)	1:110:A:PRO:HA	1:131:A:GLU:HB3	16	0.17
(1,846)	1:108:A:SER:HB2	1:137:A:PHE:HB2	7	0.17
(1,846)	1:108:A:SER:HB2	1:137:A:PHE:HB3	7	0.17
(1,846)	1:108:A:SER:HB3	1:137:A:PHE:HB2	7	0.17
(1,846)	1:108:A:SER:HB3	1:137:A:PHE:HB3	7	0.17
(1,845)	1:108:A:SER:HB2	1:110:A:PRO:HA	2	0.17
(1,845)	1:108:A:SER:HB3	1:110:A:PRO:HA	2	0.17
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD11	14	0.17
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD12	14	0.17
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD13	14	0.17
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD21	14	0.17
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD22	14	0.17
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD23	14	0.17
(1,783)	1:81:A:LYS:HG2	1:80:A:GLN:HA	3	0.17
(1,783)	1:81:A:LYS:HG3	1:80:A:GLN:HA	3	0.17
(1,783)	1:81:A:LYS:HG2	1:80:A:GLN:HA	7	0.17
(1,783)	1:81:A:LYS:HG3	1:80:A:GLN:HA	7	0.17
(1,783)	1:81:A:LYS:HG2	1:80:A:GLN:HA	13	0.17
(1,783)	1:81:A:LYS:HG3	1:80:A:GLN:HA	13	0.17
(1,741)	1:71:A:ALA:HB1	1:35:A:LEU:HB2	16	0.17
(1,741)	1:71:A:ALA:HB1	1:35:A:LEU:HB3	16	0.17
(1,741)	1:71:A:ALA:HB2	1:35:A:LEU:HB2	16	0.17
(1,741)	1:71:A:ALA:HB2	1:35:A:LEU:HB3	16	0.17
(1,741)	1:71:A:ALA:HB3	1:35:A:LEU:HB2	16	0.17
(1,741)	1:71:A:ALA:HB3	1:35:A:LEU:HB3	16	0.17
(1,741)	1:71:A:ALA:HB1	1:35:A:LEU:HB2	24	0.17
(1,741)	1:71:A:ALA:HB1	1:35:A:LEU:HB3	24	0.17
(1,741)	1:71:A:ALA:HB2	1:35:A:LEU:HB2	24	0.17
(1,741)	1:71:A:ALA:HB2	1:35:A:LEU:HB3	24	0.17
(1,741)	1:71:A:ALA:HB3	1:35:A:LEU:HB2	24	0.17
(1,741)	1:71:A:ALA:HB3	1:35:A:LEU:HB3	24	0.17
(1,732)	1:65:A:THR:HB	1:56:A:ALA:HB1	2	0.17
(1,732)	1:65:A:THR:HB	1:56:A:ALA:HB2	2	0.17
(1,732)	1:65:A:THR:HB	1:56:A:ALA:HB3	2	0.17
(1,732)	1:65:A:THR:HB	1:56:A:ALA:HB1	3	0.17
(1,732)	1:65:A:THR:HB	1:56:A:ALA:HB2	3	0.17
(1,732)	1:65:A:THR:HB	1:56:A:ALA:HB3	3	0.17
(1,732)	1:65:A:THR:HB	1:56:A:ALA:HB1	6	0.17
(1,732)	1:65:A:THR:HB	1:56:A:ALA:HB2	6	0.17
(1,732)	1:65:A:THR:HB	1:56:A:ALA:HB3	6	0.17
(1,732)	1:65:A:THR:HB	1:56:A:ALA:HB1	14	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,732)	1:65:A:THR:HB	1:56:A:ALA:HB2	14	0.17
(1,732)	1:65:A:THR:HB	1:56:A:ALA:HB3	14	0.17
(1,707)	1:54:A:TYR:HE1	1:127:A:ASN:H	2	0.17
(1,707)	1:54:A:TYR:HE2	1:127:A:ASN:H	2	0.17
(1,705)	1:53:A:LEU:HD11	1:127:A:ASN:HB2	11	0.17
(1,705)	1:53:A:LEU:HD11	1:127:A:ASN:HB3	11	0.17
(1,705)	1:53:A:LEU:HD12	1:127:A:ASN:HB2	11	0.17
(1,705)	1:53:A:LEU:HD12	1:127:A:ASN:HB3	11	0.17
(1,705)	1:53:A:LEU:HD13	1:127:A:ASN:HB2	11	0.17
(1,705)	1:53:A:LEU:HD13	1:127:A:ASN:HB3	11	0.17
(1,705)	1:53:A:LEU:HD21	1:127:A:ASN:HB2	11	0.17
(1,705)	1:53:A:LEU:HD21	1:127:A:ASN:HB3	11	0.17
(1,705)	1:53:A:LEU:HD22	1:127:A:ASN:HB2	11	0.17
(1,705)	1:53:A:LEU:HD22	1:127:A:ASN:HB3	11	0.17
(1,705)	1:53:A:LEU:HD23	1:127:A:ASN:HB2	11	0.17
(1,705)	1:53:A:LEU:HD23	1:127:A:ASN:HB3	11	0.17
(1,705)	1:53:A:LEU:HD11	1:127:A:ASN:HB2	18	0.17
(1,705)	1:53:A:LEU:HD11	1:127:A:ASN:HB3	18	0.17
(1,705)	1:53:A:LEU:HD12	1:127:A:ASN:HB2	18	0.17
(1,705)	1:53:A:LEU:HD12	1:127:A:ASN:HB3	18	0.17
(1,705)	1:53:A:LEU:HD13	1:127:A:ASN:HB2	18	0.17
(1,705)	1:53:A:LEU:HD13	1:127:A:ASN:HB3	18	0.17
(1,705)	1:53:A:LEU:HD21	1:127:A:ASN:HB2	18	0.17
(1,705)	1:53:A:LEU:HD21	1:127:A:ASN:HB3	18	0.17
(1,705)	1:53:A:LEU:HD22	1:127:A:ASN:HB2	18	0.17
(1,705)	1:53:A:LEU:HD22	1:127:A:ASN:HB3	18	0.17
(1,705)	1:53:A:LEU:HD23	1:127:A:ASN:HB2	18	0.17
(1,705)	1:53:A:LEU:HD23	1:127:A:ASN:HB3	18	0.17
(1,705)	1:53:A:LEU:HD11	1:127:A:ASN:HB2	19	0.17
(1,705)	1:53:A:LEU:HD11	1:127:A:ASN:HB3	19	0.17
(1,705)	1:53:A:LEU:HD12	1:127:A:ASN:HB2	19	0.17
(1,705)	1:53:A:LEU:HD12	1:127:A:ASN:HB3	19	0.17
(1,705)	1:53:A:LEU:HD13	1:127:A:ASN:HB2	19	0.17
(1,705)	1:53:A:LEU:HD13	1:127:A:ASN:HB3	19	0.17
(1,705)	1:53:A:LEU:HD21	1:127:A:ASN:HB2	19	0.17
(1,705)	1:53:A:LEU:HD21	1:127:A:ASN:HB3	19	0.17
(1,705)	1:53:A:LEU:HD22	1:127:A:ASN:HB2	19	0.17
(1,705)	1:53:A:LEU:HD22	1:127:A:ASN:HB3	19	0.17
(1,705)	1:53:A:LEU:HD23	1:127:A:ASN:HB2	19	0.17
(1,705)	1:53:A:LEU:HD23	1:127:A:ASN:HB3	19	0.17
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG11	11	0.17
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG12	11	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG13	11	0.17
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG21	11	0.17
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG22	11	0.17
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG23	11	0.17
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG11	11	0.17
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG12	11	0.17
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG13	11	0.17
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG21	11	0.17
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG22	11	0.17
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG23	11	0.17
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG11	11	0.17
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG12	11	0.17
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG13	11	0.17
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG21	11	0.17
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG22	11	0.17
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG23	11	0.17
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG11	20	0.17
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG12	20	0.17
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG13	20	0.17
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG21	20	0.17
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG22	20	0.17
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG23	20	0.17
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG11	20	0.17
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG12	20	0.17
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG13	20	0.17
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG21	20	0.17
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG22	20	0.17
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG23	20	0.17
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG11	20	0.17
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG12	20	0.17
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG13	20	0.17
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG21	20	0.17
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG22	20	0.17
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG23	20	0.17
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD11	11	0.17
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD12	11	0.17
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD13	11	0.17
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD21	11	0.17
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD22	11	0.17
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD23	11	0.17
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD11	11	0.17
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD12	11	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD13	11	0.17
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD21	11	0.17
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD22	11	0.17
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD23	11	0.17
(1,639)	1:34:A:ARG:HD2	1:74:A:PHE:HE1	11	0.17
(1,639)	1:34:A:ARG:HD2	1:74:A:PHE:HE2	11	0.17
(1,639)	1:34:A:ARG:HD3	1:74:A:PHE:HE1	11	0.17
(1,639)	1:34:A:ARG:HD3	1:74:A:PHE:HE2	11	0.17
(1,639)	1:34:A:ARG:HD2	1:74:A:PHE:HE1	14	0.17
(1,639)	1:34:A:ARG:HD2	1:74:A:PHE:HE2	14	0.17
(1,639)	1:34:A:ARG:HD3	1:74:A:PHE:HE1	14	0.17
(1,639)	1:34:A:ARG:HD3	1:74:A:PHE:HE2	14	0.17
(1,616)	2:480:B:ALA:H	2:479:B:LEU:HA	2	0.17
(1,616)	2:480:B:ALA:H	2:479:B:LEU:HA	21	0.17
(1,584)	2:468:B:TYR:H	2:467:B:PRO:HG2	17	0.17
(1,584)	2:468:B:TYR:H	2:467:B:PRO:HG3	17	0.17
(1,584)	2:468:B:TYR:H	2:467:B:PRO:HG2	21	0.17
(1,584)	2:468:B:TYR:H	2:467:B:PRO:HG3	21	0.17
(1,559)	2:452:B:SER:H	2:451:B:GLU:HA	10	0.17
(1,559)	2:452:B:SER:H	2:451:B:GLU:HA	13	0.17
(1,559)	2:452:B:SER:H	2:451:B:GLU:HA	21	0.17
(1,556)	2:451:B:GLU:H	2:450:B:TRP:HB2	1	0.17
(1,556)	2:451:B:GLU:H	2:450:B:TRP:HB2	4	0.17
(1,556)	2:451:B:GLU:H	2:450:B:TRP:HB2	7	0.17
(1,556)	2:451:B:GLU:H	2:450:B:TRP:HB2	20	0.17
(1,556)	2:451:B:GLU:H	2:450:B:TRP:HB2	24	0.17
(1,523)	1:116:A:THR:H	1:108:A:SER:HB2	4	0.17
(1,523)	1:116:A:THR:H	1:108:A:SER:HB3	4	0.17
(1,523)	1:116:A:THR:H	1:108:A:SER:HB2	11	0.17
(1,523)	1:116:A:THR:H	1:108:A:SER:HB3	11	0.17
(1,523)	1:116:A:THR:H	1:108:A:SER:HB2	13	0.17
(1,523)	1:116:A:THR:H	1:108:A:SER:HB3	13	0.17
(1,523)	1:116:A:THR:H	1:108:A:SER:HB2	21	0.17
(1,523)	1:116:A:THR:H	1:108:A:SER:HB3	21	0.17
(1,477)	1:72:A:VAL:H	1:48:A:THR:HA	8	0.17
(1,477)	1:72:A:VAL:H	1:48:A:THR:HA	9	0.17
(1,477)	1:72:A:VAL:H	1:48:A:THR:HA	17	0.17
(1,469)	1:55:A:LEU:H	1:65:A:THR:H	19	0.17
(1,457)	1:38:A:MET:H	1:34:A:ARG:HD2	6	0.17
(1,457)	1:38:A:MET:H	1:34:A:ARG:HD3	6	0.17
(1,457)	1:38:A:MET:H	1:34:A:ARG:HD2	18	0.17
(1,457)	1:38:A:MET:H	1:34:A:ARG:HD3	18	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,453)	1:26:A:LEU:H	1:30:A:HIS:H	8	0.17
(1,440)	1:127:A:ASN:H	1:53:A:LEU:HA	4	0.17
(1,439)	1:126:A:LEU:H	1:116:A:THR:HG21	15	0.17
(1,439)	1:126:A:LEU:H	1:116:A:THR:HG21	20	0.17
(1,427)	1:101:A:LEU:H	1:83:A:TYR:H	24	0.17
(1,412)	1:84:A:PHE:H	1:76:A:LYS:HB2	5	0.17
(1,412)	1:84:A:PHE:H	1:76:A:LYS:HB3	5	0.17
(1,412)	1:84:A:PHE:H	1:76:A:LYS:HB2	17	0.17
(1,412)	1:84:A:PHE:H	1:76:A:LYS:HB3	17	0.17
(1,370)	1:38:A:MET:H	1:34:A:ARG:HA	24	0.17
(1,366)	1:35:A:LEU:H	1:32:A:ASN:HA	14	0.17
(1,364)	1:34:A:ARG:H	1:31:A:GLU:HA	11	0.17
(1,364)	1:34:A:ARG:H	1:31:A:GLU:HA	17	0.17
(1,328)	1:143:A:GLU:H	1:139:A:ALA:HB1	8	0.17
(1,328)	1:143:A:GLU:H	1:139:A:ALA:HB2	8	0.17
(1,328)	1:143:A:GLU:H	1:139:A:ALA:HB3	8	0.17
(1,314)	1:140:A:LEU:H	1:136:A:ALA:HA	10	0.17
(1,314)	1:140:A:LEU:H	1:136:A:ALA:HA	11	0.17
(1,278)	1:127:A:ASN:H	1:126:A:LEU:HG	14	0.17
(1,278)	1:127:A:ASN:H	1:126:A:LEU:HG	24	0.17
(1,272)	1:124:A:ALA:H	1:123:A:GLN:HG2	21	0.17
(1,272)	1:124:A:ALA:H	1:123:A:GLN:HG3	21	0.17
(1,259)	1:118:A:ALA:H	1:117:A:PHE:HB3	3	0.17
(1,259)	1:118:A:ALA:H	1:117:A:PHE:HB3	12	0.17
(1,245)	1:114:A:PHE:H	1:113:A:PHE:H	17	0.17
(1,105)	1:63:A:HIS:H	1:62:A:GLU:HA	6	0.17
(1,105)	1:63:A:HIS:H	1:62:A:GLU:HA	14	0.17
(1,85)	1:54:A:TYR:H	1:53:A:LEU:HG	5	0.17
(4,92)	1:136:A:ALA:N	1:132:A:ASP:O	8	0.16
(4,92)	1:136:A:ALA:N	1:132:A:ASP:O	15	0.16
(4,92)	1:136:A:ALA:N	1:132:A:ASP:O	17	0.16
(4,92)	1:136:A:ALA:N	1:132:A:ASP:O	23	0.16
(4,77)	1:34:A:ARG:H	1:30:A:HIS:O	2	0.16
(4,77)	1:34:A:ARG:H	1:30:A:HIS:O	21	0.16
(4,77)	1:34:A:ARG:H	1:30:A:HIS:O	22	0.16
(4,67)	1:124:A:ALA:H	1:117:A:PHE:O	5	0.16
(4,67)	1:124:A:ALA:H	1:117:A:PHE:O	13	0.16
(4,41)	1:71:A:ALA:H	1:88:A:TYR:O	2	0.16
(4,41)	1:71:A:ALA:H	1:88:A:TYR:O	6	0.16
(4,41)	1:71:A:ALA:H	1:88:A:TYR:O	11	0.16
(4,23)	1:68:A:HIS:H	1:53:A:LEU:O	3	0.16
(4,23)	1:68:A:HIS:H	1:53:A:LEU:O	8	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,23)	1:68:A:HIS:H	1:53:A:LEU:O	16	0.16
(4,23)	1:68:A:HIS:H	1:53:A:LEU:O	23	0.16
(1,1016)	2:479:B:LEU:HG	1:83:A:TYR:HD1	5	0.16
(1,1016)	2:479:B:LEU:HG	1:83:A:TYR:HD2	5	0.16
(1,1016)	2:479:B:LEU:HG	1:83:A:TYR:HD1	10	0.16
(1,1016)	2:479:B:LEU:HG	1:83:A:TYR:HD2	10	0.16
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD11	7	0.16
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD12	7	0.16
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD13	7	0.16
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD21	7	0.16
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD22	7	0.16
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD23	7	0.16
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD11	7	0.16
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD12	7	0.16
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD13	7	0.16
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD21	7	0.16
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD22	7	0.16
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD23	7	0.16
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD11	9	0.16
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD12	9	0.16
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD13	9	0.16
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD21	9	0.16
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD22	9	0.16
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD23	9	0.16
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD11	9	0.16
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD12	9	0.16
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD13	9	0.16
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD21	9	0.16
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD22	9	0.16
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD23	9	0.16
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD11	16	0.16
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD12	16	0.16
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD13	16	0.16
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD21	16	0.16
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD22	16	0.16
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD23	16	0.16
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD11	16	0.16
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD12	16	0.16
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD13	16	0.16
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD21	16	0.16
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD22	16	0.16
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD23	16	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,977)	1:103:A:SER:HB2	2:476:B:PRO:HD2	2	0.16
(1,977)	1:103:A:SER:HB2	2:476:B:PRO:HD3	2	0.16
(1,977)	1:103:A:SER:HB3	2:476:B:PRO:HD2	2	0.16
(1,977)	1:103:A:SER:HB3	2:476:B:PRO:HD3	2	0.16
(1,972)	1:71:A:ALA:H	2:450:B:TRP:HZ2	6	0.16
(1,972)	1:71:A:ALA:H	2:450:B:TRP:HZ2	14	0.16
(1,965)	1:56:A:ALA:HB1	2:462:B:LEU:HD11	15	0.16
(1,965)	1:56:A:ALA:HB1	2:462:B:LEU:HD12	15	0.16
(1,965)	1:56:A:ALA:HB1	2:462:B:LEU:HD13	15	0.16
(1,965)	1:56:A:ALA:HB1	2:462:B:LEU:HD21	15	0.16
(1,965)	1:56:A:ALA:HB1	2:462:B:LEU:HD22	15	0.16
(1,965)	1:56:A:ALA:HB1	2:462:B:LEU:HD23	15	0.16
(1,965)	1:56:A:ALA:HB2	2:462:B:LEU:HD11	15	0.16
(1,965)	1:56:A:ALA:HB2	2:462:B:LEU:HD12	15	0.16
(1,965)	1:56:A:ALA:HB2	2:462:B:LEU:HD13	15	0.16
(1,965)	1:56:A:ALA:HB2	2:462:B:LEU:HD21	15	0.16
(1,965)	1:56:A:ALA:HB2	2:462:B:LEU:HD22	15	0.16
(1,965)	1:56:A:ALA:HB2	2:462:B:LEU:HD23	15	0.16
(1,965)	1:56:A:ALA:HB3	2:462:B:LEU:HD11	15	0.16
(1,965)	1:56:A:ALA:HB3	2:462:B:LEU:HD12	15	0.16
(1,965)	1:56:A:ALA:HB3	2:462:B:LEU:HD13	15	0.16
(1,965)	1:56:A:ALA:HB3	2:462:B:LEU:HD21	15	0.16
(1,965)	1:56:A:ALA:HB3	2:462:B:LEU:HD22	15	0.16
(1,965)	1:56:A:ALA:HB3	2:462:B:LEU:HD23	15	0.16
(1,944)	2:458:B:PRO:HA	2:460:B:SER:HB2	22	0.16
(1,944)	2:458:B:PRO:HA	2:460:B:SER:HB3	22	0.16
(1,928)	1:145:A:ILE:HD11	1:117:A:PHE:HZ	11	0.16
(1,928)	1:145:A:ILE:HD12	1:117:A:PHE:HZ	11	0.16
(1,928)	1:145:A:ILE:HD13	1:117:A:PHE:HZ	11	0.16
(1,926)	1:145:A:ILE:HD11	1:117:A:PHE:HB2	9	0.16
(1,926)	1:145:A:ILE:HD12	1:117:A:PHE:HB2	9	0.16
(1,926)	1:145:A:ILE:HD13	1:117:A:PHE:HB2	9	0.16
(1,926)	1:145:A:ILE:HD11	1:117:A:PHE:HB2	16	0.16
(1,926)	1:145:A:ILE:HD12	1:117:A:PHE:HB2	16	0.16
(1,926)	1:145:A:ILE:HD13	1:117:A:PHE:HB2	16	0.16
(1,911)	1:141:A:VAL:HA	1:107:A:TYR:HB2	23	0.16
(1,911)	1:141:A:VAL:HA	1:107:A:TYR:HB3	23	0.16
(1,877)	1:127:A:ASN:HB2	1:113:A:PHE:HB2	15	0.16
(1,877)	1:127:A:ASN:HB2	1:113:A:PHE:HB3	15	0.16
(1,877)	1:127:A:ASN:HB3	1:113:A:PHE:HB2	15	0.16
(1,877)	1:127:A:ASN:HB3	1:113:A:PHE:HB3	15	0.16
(1,875)	1:126:A:LEU:HG	1:114:A:PHE:HD1	23	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,875)	1:126:A:LEU:HG	1:114:A:PHE:HD2	23	0.16
(1,869)	1:124:A:ALA:HB1	1:117:A:PHE:HD1	4	0.16
(1,869)	1:124:A:ALA:HB1	1:117:A:PHE:HD2	4	0.16
(1,869)	1:124:A:ALA:HB2	1:117:A:PHE:HD1	4	0.16
(1,869)	1:124:A:ALA:HB2	1:117:A:PHE:HD2	4	0.16
(1,869)	1:124:A:ALA:HB3	1:117:A:PHE:HD1	4	0.16
(1,869)	1:124:A:ALA:HB3	1:117:A:PHE:HD2	4	0.16
(1,851)	1:110:A:PRO:HA	1:131:A:GLU:HB2	12	0.16
(1,851)	1:110:A:PRO:HA	1:131:A:GLU:HB3	12	0.16
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD11	11	0.16
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD12	11	0.16
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD13	11	0.16
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD21	11	0.16
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD22	11	0.16
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD23	11	0.16
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD11	17	0.16
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD12	17	0.16
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD13	17	0.16
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD21	17	0.16
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD22	17	0.16
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD23	17	0.16
(1,783)	1:81:A:LYS:HG2	1:80:A:GLN:HA	8	0.16
(1,783)	1:81:A:LYS:HG3	1:80:A:GLN:HA	8	0.16
(1,783)	1:81:A:LYS:HG2	1:80:A:GLN:HA	9	0.16
(1,783)	1:81:A:LYS:HG3	1:80:A:GLN:HA	9	0.16
(1,783)	1:81:A:LYS:HG2	1:80:A:GLN:HA	12	0.16
(1,783)	1:81:A:LYS:HG3	1:80:A:GLN:HA	12	0.16
(1,783)	1:81:A:LYS:HG2	1:80:A:GLN:HA	24	0.16
(1,783)	1:81:A:LYS:HG3	1:80:A:GLN:HA	24	0.16
(1,776)	1:75:A:VAL:HG11	1:73:A:CYS:HB2	24	0.16
(1,776)	1:75:A:VAL:HG11	1:73:A:CYS:HB3	24	0.16
(1,776)	1:75:A:VAL:HG12	1:73:A:CYS:HB2	24	0.16
(1,776)	1:75:A:VAL:HG12	1:73:A:CYS:HB3	24	0.16
(1,776)	1:75:A:VAL:HG13	1:73:A:CYS:HB2	24	0.16
(1,776)	1:75:A:VAL:HG13	1:73:A:CYS:HB3	24	0.16
(1,755)	1:72:A:VAL:HG11	1:53:A:LEU:HG	24	0.16
(1,755)	1:72:A:VAL:HG12	1:53:A:LEU:HG	24	0.16
(1,755)	1:72:A:VAL:HG13	1:53:A:LEU:HG	24	0.16
(1,755)	1:72:A:VAL:HG21	1:53:A:LEU:HG	24	0.16
(1,755)	1:72:A:VAL:HG22	1:53:A:LEU:HG	24	0.16
(1,755)	1:72:A:VAL:HG23	1:53:A:LEU:HG	24	0.16
(1,741)	1:71:A:ALA:HB1	1:35:A:LEU:HB2	13	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,741)	1:71:A:ALA:HB1	1:35:A:LEU:HB3	13	0.16
(1,741)	1:71:A:ALA:HB2	1:35:A:LEU:HB2	13	0.16
(1,741)	1:71:A:ALA:HB2	1:35:A:LEU:HB3	13	0.16
(1,741)	1:71:A:ALA:HB3	1:35:A:LEU:HB2	13	0.16
(1,741)	1:71:A:ALA:HB3	1:35:A:LEU:HB3	13	0.16
(1,738)	1:69:A:CYS:HG	1:52:A:GLN:HA	3	0.16
(1,732)	1:65:A:THR:HB	1:56:A:ALA:HB1	1	0.16
(1,732)	1:65:A:THR:HB	1:56:A:ALA:HB2	1	0.16
(1,732)	1:65:A:THR:HB	1:56:A:ALA:HB3	1	0.16
(1,732)	1:65:A:THR:HB	1:56:A:ALA:HB1	7	0.16
(1,732)	1:65:A:THR:HB	1:56:A:ALA:HB2	7	0.16
(1,732)	1:65:A:THR:HB	1:56:A:ALA:HB3	7	0.16
(1,732)	1:65:A:THR:HB	1:56:A:ALA:HB1	8	0.16
(1,732)	1:65:A:THR:HB	1:56:A:ALA:HB2	8	0.16
(1,732)	1:65:A:THR:HB	1:56:A:ALA:HB3	8	0.16
(1,732)	1:65:A:THR:HB	1:56:A:ALA:HB1	11	0.16
(1,732)	1:65:A:THR:HB	1:56:A:ALA:HB2	11	0.16
(1,732)	1:65:A:THR:HB	1:56:A:ALA:HB3	11	0.16
(1,732)	1:65:A:THR:HB	1:56:A:ALA:HB1	13	0.16
(1,732)	1:65:A:THR:HB	1:56:A:ALA:HB2	13	0.16
(1,732)	1:65:A:THR:HB	1:56:A:ALA:HB3	13	0.16
(1,732)	1:65:A:THR:HB	1:56:A:ALA:HB1	17	0.16
(1,732)	1:65:A:THR:HB	1:56:A:ALA:HB2	17	0.16
(1,732)	1:65:A:THR:HB	1:56:A:ALA:HB3	17	0.16
(1,732)	1:65:A:THR:HB	1:56:A:ALA:HB1	19	0.16
(1,732)	1:65:A:THR:HB	1:56:A:ALA:HB2	19	0.16
(1,732)	1:65:A:THR:HB	1:56:A:ALA:HB3	19	0.16
(1,669)	1:47:A:ALA:HB1	1:137:A:PHE:HA	21	0.16
(1,669)	1:47:A:ALA:HB2	1:137:A:PHE:HA	21	0.16
(1,669)	1:47:A:ALA:HB3	1:137:A:PHE:HA	21	0.16
(1,669)	1:47:A:ALA:HB1	1:137:A:PHE:HA	24	0.16
(1,669)	1:47:A:ALA:HB2	1:137:A:PHE:HA	24	0.16
(1,669)	1:47:A:ALA:HB3	1:137:A:PHE:HA	24	0.16
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG11	3	0.16
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG12	3	0.16
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG13	3	0.16
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG21	3	0.16
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG22	3	0.16
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG23	3	0.16
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG11	3	0.16
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG12	3	0.16
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG13	3	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG21	3	0.16
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG22	3	0.16
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG23	3	0.16
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG11	3	0.16
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG12	3	0.16
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG13	3	0.16
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG21	3	0.16
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG22	3	0.16
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG23	3	0.16
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG11	19	0.16
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG12	19	0.16
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG13	19	0.16
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG21	19	0.16
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG22	19	0.16
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG23	19	0.16
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG11	19	0.16
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG12	19	0.16
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG13	19	0.16
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG21	19	0.16
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG22	19	0.16
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG23	19	0.16
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG11	19	0.16
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG12	19	0.16
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG13	19	0.16
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG21	19	0.16
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG22	19	0.16
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG23	19	0.16
(1,646)	1:39:A:LEU:HA	1:88:A:TYR:HB2	15	0.16
(1,646)	1:39:A:LEU:HA	1:88:A:TYR:HB3	15	0.16
(1,640)	1:35:A:LEU:HD11	1:31:A:GLU:HA	19	0.16
(1,640)	1:35:A:LEU:HD12	1:31:A:GLU:HA	19	0.16
(1,640)	1:35:A:LEU:HD13	1:31:A:GLU:HA	19	0.16
(1,640)	1:35:A:LEU:HD21	1:31:A:GLU:HA	19	0.16
(1,640)	1:35:A:LEU:HD22	1:31:A:GLU:HA	19	0.16
(1,640)	1:35:A:LEU:HD23	1:31:A:GLU:HA	19	0.16
(1,639)	1:34:A:ARG:HD2	1:74:A:PHE:HE1	15	0.16
(1,639)	1:34:A:ARG:HD2	1:74:A:PHE:HE2	15	0.16
(1,639)	1:34:A:ARG:HD3	1:74:A:PHE:HE1	15	0.16
(1,639)	1:34:A:ARG:HD3	1:74:A:PHE:HE2	15	0.16
(1,638)	1:34:A:ARG:HB2	1:74:A:PHE:HD1	12	0.16
(1,638)	1:34:A:ARG:HB2	1:74:A:PHE:HD2	12	0.16
(1,638)	1:34:A:ARG:HB3	1:74:A:PHE:HD1	12	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,638)	1:34:A:ARG:HB3	1:74:A:PHE:HD2	12	0.16
(1,638)	1:34:A:ARG:HB2	1:74:A:PHE:HD1	17	0.16
(1,638)	1:34:A:ARG:HB2	1:74:A:PHE:HD2	17	0.16
(1,638)	1:34:A:ARG:HB3	1:74:A:PHE:HD1	17	0.16
(1,638)	1:34:A:ARG:HB3	1:74:A:PHE:HD2	17	0.16
(1,635)	1:33:A:GLN:HA	1:30:A:HIS:HA	18	0.16
(1,610)	2:479:B:LEU:H	2:478:B:LYS:HG2	4	0.16
(1,610)	2:479:B:LEU:H	2:478:B:LYS:HG3	4	0.16
(1,584)	2:468:B:TYR:H	2:467:B:PRO:HG2	8	0.16
(1,584)	2:468:B:TYR:H	2:467:B:PRO:HG3	8	0.16
(1,559)	2:452:B:SER:H	2:451:B:GLU:HA	1	0.16
(1,559)	2:452:B:SER:H	2:451:B:GLU:HA	2	0.16
(1,559)	2:452:B:SER:H	2:451:B:GLU:HA	4	0.16
(1,559)	2:452:B:SER:H	2:451:B:GLU:HA	6	0.16
(1,559)	2:452:B:SER:H	2:451:B:GLU:HA	7	0.16
(1,559)	2:452:B:SER:H	2:451:B:GLU:HA	9	0.16
(1,559)	2:452:B:SER:H	2:451:B:GLU:HA	11	0.16
(1,559)	2:452:B:SER:H	2:451:B:GLU:HA	12	0.16
(1,559)	2:452:B:SER:H	2:451:B:GLU:HA	15	0.16
(1,559)	2:452:B:SER:H	2:451:B:GLU:HA	16	0.16
(1,559)	2:452:B:SER:H	2:451:B:GLU:HA	18	0.16
(1,559)	2:452:B:SER:H	2:451:B:GLU:HA	19	0.16
(1,559)	2:452:B:SER:H	2:451:B:GLU:HA	20	0.16
(1,559)	2:452:B:SER:H	2:451:B:GLU:HA	22	0.16
(1,559)	2:452:B:SER:H	2:451:B:GLU:HA	23	0.16
(1,559)	2:452:B:SER:H	2:451:B:GLU:HA	24	0.16
(1,556)	2:451:B:GLU:H	2:450:B:TRP:HB2	2	0.16
(1,556)	2:451:B:GLU:H	2:450:B:TRP:HB2	8	0.16
(1,556)	2:451:B:GLU:H	2:450:B:TRP:HB2	14	0.16
(1,523)	1:116:A:THR:H	1:108:A:SER:HB2	19	0.16
(1,523)	1:116:A:THR:H	1:108:A:SER:HB3	19	0.16
(1,496)	1:101:A:LEU:H	1:100:A:GLU:H	14	0.16
(1,493)	1:97:A:TRP:H	1:95:A:LEU:HA	9	0.16
(1,487)	1:89:A:GLY:H	1:94:A:ARG:H	18	0.16
(1,483)	1:87:A:LEU:H	1:97:A:TRP:HZ3	2	0.16
(1,483)	1:87:A:LEU:H	1:97:A:TRP:HZ2	11	0.16
(1,477)	1:72:A:VAL:H	1:48:A:THR:HA	16	0.16
(1,477)	1:72:A:VAL:H	1:48:A:THR:HA	21	0.16
(1,477)	1:72:A:VAL:H	1:48:A:THR:HA	22	0.16
(1,477)	1:72:A:VAL:H	1:48:A:THR:HA	23	0.16
(1,469)	1:55:A:LEU:H	1:65:A:THR:H	4	0.16
(1,469)	1:55:A:LEU:H	1:65:A:THR:H	7	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,453)	1:26:A:LEU:H	1:30:A:HIS:H	17	0.16
(1,440)	1:127:A:ASN:H	1:53:A:LEU:HA	18	0.16
(1,435)	1:125:A:GLY:H	1:54:A:TYR:HB2	6	0.16
(1,435)	1:125:A:GLY:H	1:54:A:TYR:HB3	6	0.16
(1,429)	1:101:A:LEU:H	1:84:A:PHE:HB2	5	0.16
(1,429)	1:101:A:LEU:H	1:84:A:PHE:HB3	5	0.16
(1,417)	1:88:A:TYR:H	1:71:A:ALA:H	19	0.16
(1,416)	1:87:A:LEU:H	1:98:A:GLU:HB2	16	0.16
(1,416)	1:87:A:LEU:H	1:98:A:GLU:HB3	16	0.16
(1,416)	1:87:A:LEU:H	1:98:A:GLU:HB2	20	0.16
(1,416)	1:87:A:LEU:H	1:98:A:GLU:HB3	20	0.16
(1,412)	1:84:A:PHE:H	1:76:A:LYS:HB2	2	0.16
(1,412)	1:84:A:PHE:H	1:76:A:LYS:HB3	2	0.16
(1,412)	1:84:A:PHE:H	1:76:A:LYS:HB2	23	0.16
(1,412)	1:84:A:PHE:H	1:76:A:LYS:HB3	23	0.16
(1,410)	1:84:A:PHE:H	1:76:A:LYS:HG2	6	0.16
(1,410)	1:84:A:PHE:H	1:76:A:LYS:HG3	6	0.16
(1,399)	1:72:A:VAL:H	1:50:A:VAL:HB	21	0.16
(1,366)	1:35:A:LEU:H	1:32:A:ASN:HA	18	0.16
(1,366)	1:35:A:LEU:H	1:32:A:ASN:HA	20	0.16
(1,364)	1:34:A:ARG:H	1:31:A:GLU:HA	9	0.16
(1,364)	1:34:A:ARG:H	1:31:A:GLU:HA	13	0.16
(1,364)	1:34:A:ARG:H	1:31:A:GLU:HA	16	0.16
(1,364)	1:34:A:ARG:H	1:31:A:GLU:HA	23	0.16
(1,327)	1:143:A:GLU:H	1:140:A:LEU:HD11	19	0.16
(1,327)	1:143:A:GLU:H	1:140:A:LEU:HD12	19	0.16
(1,327)	1:143:A:GLU:H	1:140:A:LEU:HD13	19	0.16
(1,327)	1:143:A:GLU:H	1:140:A:LEU:HD21	19	0.16
(1,327)	1:143:A:GLU:H	1:140:A:LEU:HD22	19	0.16
(1,327)	1:143:A:GLU:H	1:140:A:LEU:HD23	19	0.16
(1,300)	1:136:A:ALA:H	1:132:A:ASP:HA	14	0.16
(1,272)	1:124:A:ALA:H	1:123:A:GLN:HG2	4	0.16
(1,272)	1:124:A:ALA:H	1:123:A:GLN:HG3	4	0.16
(1,272)	1:124:A:ALA:H	1:123:A:GLN:HG2	10	0.16
(1,272)	1:124:A:ALA:H	1:123:A:GLN:HG3	10	0.16
(1,272)	1:124:A:ALA:H	1:123:A:GLN:HG2	24	0.16
(1,272)	1:124:A:ALA:H	1:123:A:GLN:HG3	24	0.16
(1,268)	1:122:A:CYS:H	1:121:A:ASP:HA	1	0.16
(1,268)	1:122:A:CYS:H	1:121:A:ASP:HA	2	0.16
(1,268)	1:122:A:CYS:H	1:121:A:ASP:HA	11	0.16
(1,268)	1:122:A:CYS:H	1:121:A:ASP:HA	22	0.16
(1,259)	1:118:A:ALA:H	1:117:A:PHE:HB3	1	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,250)	1:116:A:THR:H	1:115:A:HIS:HB3	5	0.16
(1,250)	1:116:A:THR:H	1:115:A:HIS:HB3	18	0.16
(1,250)	1:116:A:THR:H	1:115:A:HIS:HB3	23	0.16
(1,235)	1:107:A:TYR:H	1:106:A:VAL:H	10	0.16
(1,195)	1:96:A:LEU:H	1:95:A:LEU:H	9	0.16
(1,195)	1:96:A:LEU:H	1:95:A:LEU:H	14	0.16
(1,112)	1:65:A:THR:H	1:64:A:TRP:HB3	20	0.16
(1,105)	1:63:A:HIS:H	1:62:A:GLU:HA	10	0.16
(1,54)	1:43:A:CYS:H	1:42:A:LYS:HB2	22	0.16
(1,54)	1:43:A:CYS:H	1:42:A:LYS:HB3	22	0.16
(4,92)	1:136:A:ALA:N	1:132:A:ASP:O	7	0.15
(4,92)	1:136:A:ALA:N	1:132:A:ASP:O	14	0.15
(4,77)	1:34:A:ARG:H	1:30:A:HIS:O	20	0.15
(4,70)	1:119:A:GLY:N	1:122:A:CYS:O	3	0.15
(4,67)	1:124:A:ALA:H	1:117:A:PHE:O	17	0.15
(4,41)	1:71:A:ALA:H	1:88:A:TYR:O	9	0.15
(4,40)	1:56:A:ALA:N	1:123:A:GLN:O	1	0.15
(4,31)	1:52:A:GLN:H	1:127:A:ASN:O	7	0.15
(4,31)	1:52:A:GLN:H	1:127:A:ASN:O	23	0.15
(4,23)	1:68:A:HIS:H	1:53:A:LEU:O	13	0.15
(4,23)	1:68:A:HIS:H	1:53:A:LEU:O	14	0.15
(1,1016)	2:479:B:LEU:HG	1:83:A:TYR:HD1	1	0.15
(1,1016)	2:479:B:LEU:HG	1:83:A:TYR:HD2	1	0.15
(1,1016)	2:479:B:LEU:HG	1:83:A:TYR:HD1	4	0.15
(1,1016)	2:479:B:LEU:HG	1:83:A:TYR:HD2	4	0.15
(1,1016)	2:479:B:LEU:HG	1:83:A:TYR:HD1	9	0.15
(1,1016)	2:479:B:LEU:HG	1:83:A:TYR:HD2	9	0.15
(1,1016)	2:479:B:LEU:HG	1:83:A:TYR:HD1	17	0.15
(1,1016)	2:479:B:LEU:HG	1:83:A:TYR:HD2	17	0.15
(1,1016)	2:479:B:LEU:HG	1:83:A:TYR:HD1	20	0.15
(1,1016)	2:479:B:LEU:HG	1:83:A:TYR:HD2	20	0.15
(1,1008)	2:474:B:SER:H	1:102:A:TYR:HE1	2	0.15
(1,1008)	2:474:B:SER:H	1:102:A:TYR:HE2	2	0.15
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD11	6	0.15
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD12	6	0.15
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD13	6	0.15
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD21	6	0.15
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD22	6	0.15
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD23	6	0.15
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD11	6	0.15
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD12	6	0.15
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD13	6	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD21	6	0.15
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD22	6	0.15
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD23	6	0.15
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD11	11	0.15
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD12	11	0.15
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD13	11	0.15
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD21	11	0.15
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD22	11	0.15
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD23	11	0.15
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD11	11	0.15
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD12	11	0.15
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD13	11	0.15
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD21	11	0.15
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD22	11	0.15
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD23	11	0.15
(1,992)	1:129:A:ALA:H	2:457:B:HIS:H	24	0.15
(1,988)	1:129:A:ALA:HA	2:454:B:PHE:HZ	9	0.15
(1,972)	1:71:A:ALA:H	2:450:B:TRP:HZ2	4	0.15
(1,972)	1:71:A:ALA:H	2:450:B:TRP:HZ2	20	0.15
(1,972)	1:71:A:ALA:H	2:450:B:TRP:HZ2	23	0.15
(1,945)	2:459:B:ILE:HG13	2:462:B:LEU:HD11	9	0.15
(1,945)	2:459:B:ILE:HG13	2:462:B:LEU:HD12	9	0.15
(1,945)	2:459:B:ILE:HG13	2:462:B:LEU:HD13	9	0.15
(1,945)	2:459:B:ILE:HG13	2:462:B:LEU:HD21	9	0.15
(1,945)	2:459:B:ILE:HG13	2:462:B:LEU:HD22	9	0.15
(1,945)	2:459:B:ILE:HG13	2:462:B:LEU:HD23	9	0.15
(1,945)	2:459:B:ILE:HG12	2:462:B:LEU:HD11	9	0.15
(1,945)	2:459:B:ILE:HG12	2:462:B:LEU:HD12	9	0.15
(1,945)	2:459:B:ILE:HG12	2:462:B:LEU:HD13	9	0.15
(1,945)	2:459:B:ILE:HG12	2:462:B:LEU:HD21	9	0.15
(1,945)	2:459:B:ILE:HG12	2:462:B:LEU:HD22	9	0.15
(1,945)	2:459:B:ILE:HG12	2:462:B:LEU:HD23	9	0.15
(1,944)	2:458:B:PRO:HA	2:460:B:SER:HB2	20	0.15
(1,944)	2:458:B:PRO:HA	2:460:B:SER:HB3	20	0.15
(1,912)	1:141:A:VAL:HG11	1:107:A:TYR:HB3	11	0.15
(1,912)	1:141:A:VAL:HG12	1:107:A:TYR:HB3	11	0.15
(1,912)	1:141:A:VAL:HG13	1:107:A:TYR:HB3	11	0.15
(1,912)	1:141:A:VAL:HG21	1:107:A:TYR:HB3	11	0.15
(1,912)	1:141:A:VAL:HG22	1:107:A:TYR:HB3	11	0.15
(1,912)	1:141:A:VAL:HG23	1:107:A:TYR:HB3	11	0.15
(1,912)	1:141:A:VAL:HG11	1:107:A:TYR:HB2	11	0.15
(1,912)	1:141:A:VAL:HG12	1:107:A:TYR:HB2	11	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,912)	1:141:A:VAL:HG13	1:107:A:TYR:HB2	11	0.15
(1,912)	1:141:A:VAL:HG21	1:107:A:TYR:HB2	11	0.15
(1,912)	1:141:A:VAL:HG22	1:107:A:TYR:HB2	11	0.15
(1,912)	1:141:A:VAL:HG23	1:107:A:TYR:HB2	11	0.15
(1,912)	1:141:A:VAL:HG11	1:107:A:TYR:HB3	23	0.15
(1,912)	1:141:A:VAL:HG12	1:107:A:TYR:HB3	23	0.15
(1,912)	1:141:A:VAL:HG13	1:107:A:TYR:HB3	23	0.15
(1,912)	1:141:A:VAL:HG21	1:107:A:TYR:HB3	23	0.15
(1,912)	1:141:A:VAL:HG22	1:107:A:TYR:HB3	23	0.15
(1,912)	1:141:A:VAL:HG23	1:107:A:TYR:HB3	23	0.15
(1,912)	1:141:A:VAL:HG11	1:107:A:TYR:HB2	23	0.15
(1,912)	1:141:A:VAL:HG12	1:107:A:TYR:HB2	23	0.15
(1,912)	1:141:A:VAL:HG13	1:107:A:TYR:HB2	23	0.15
(1,912)	1:141:A:VAL:HG21	1:107:A:TYR:HB2	23	0.15
(1,912)	1:141:A:VAL:HG22	1:107:A:TYR:HB2	23	0.15
(1,912)	1:141:A:VAL:HG23	1:107:A:TYR:HB2	23	0.15
(1,912)	1:141:A:VAL:HG11	1:107:A:TYR:HB3	24	0.15
(1,912)	1:141:A:VAL:HG12	1:107:A:TYR:HB3	24	0.15
(1,912)	1:141:A:VAL:HG13	1:107:A:TYR:HB3	24	0.15
(1,912)	1:141:A:VAL:HG21	1:107:A:TYR:HB3	24	0.15
(1,912)	1:141:A:VAL:HG22	1:107:A:TYR:HB3	24	0.15
(1,912)	1:141:A:VAL:HG23	1:107:A:TYR:HB3	24	0.15
(1,912)	1:141:A:VAL:HG11	1:107:A:TYR:HB2	24	0.15
(1,912)	1:141:A:VAL:HG12	1:107:A:TYR:HB2	24	0.15
(1,912)	1:141:A:VAL:HG13	1:107:A:TYR:HB2	24	0.15
(1,912)	1:141:A:VAL:HG21	1:107:A:TYR:HB2	24	0.15
(1,912)	1:141:A:VAL:HG22	1:107:A:TYR:HB2	24	0.15
(1,912)	1:141:A:VAL:HG23	1:107:A:TYR:HB2	24	0.15
(1,911)	1:141:A:VAL:HA	1:107:A:TYR:HB2	21	0.15
(1,911)	1:141:A:VAL:HA	1:107:A:TYR:HB3	21	0.15
(1,903)	1:139:A:ALA:HA	1:138:A:ARG:HB2	1	0.15
(1,903)	1:139:A:ALA:HA	1:138:A:ARG:HB3	1	0.15
(1,903)	1:139:A:ALA:HA	1:138:A:ARG:HB2	7	0.15
(1,903)	1:139:A:ALA:HA	1:138:A:ARG:HB3	7	0.15
(1,875)	1:126:A:LEU:HG	1:114:A:PHE:HD1	4	0.15
(1,875)	1:126:A:LEU:HG	1:114:A:PHE:HD2	4	0.15
(1,869)	1:124:A:ALA:HB1	1:117:A:PHE:HD1	5	0.15
(1,869)	1:124:A:ALA:HB1	1:117:A:PHE:HD2	5	0.15
(1,869)	1:124:A:ALA:HB2	1:117:A:PHE:HD1	5	0.15
(1,869)	1:124:A:ALA:HB2	1:117:A:PHE:HD2	5	0.15
(1,869)	1:124:A:ALA:HB3	1:117:A:PHE:HD1	5	0.15
(1,869)	1:124:A:ALA:HB3	1:117:A:PHE:HD2	5	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,869)	1:124:A:ALA:HB1	1:117:A:PHE:HD1	8	0.15
(1,869)	1:124:A:ALA:HB1	1:117:A:PHE:HD2	8	0.15
(1,869)	1:124:A:ALA:HB2	1:117:A:PHE:HD1	8	0.15
(1,869)	1:124:A:ALA:HB2	1:117:A:PHE:HD2	8	0.15
(1,869)	1:124:A:ALA:HB3	1:117:A:PHE:HD1	8	0.15
(1,869)	1:124:A:ALA:HB3	1:117:A:PHE:HD2	8	0.15
(1,864)	1:122:A:CYS:HA	1:123:A:GLN:HB2	20	0.15
(1,864)	1:122:A:CYS:HA	1:123:A:GLN:HB3	20	0.15
(1,863)	1:120:A:ASP:HA	1:123:A:GLN:HG2	21	0.15
(1,863)	1:120:A:ASP:HA	1:123:A:GLN:HG3	21	0.15
(1,851)	1:110:A:PRO:HA	1:131:A:GLU:HB2	1	0.15
(1,851)	1:110:A:PRO:HA	1:131:A:GLU:HB3	1	0.15
(1,851)	1:110:A:PRO:HA	1:131:A:GLU:HB2	8	0.15
(1,851)	1:110:A:PRO:HA	1:131:A:GLU:HB3	8	0.15
(1,851)	1:110:A:PRO:HA	1:131:A:GLU:HB2	21	0.15
(1,851)	1:110:A:PRO:HA	1:131:A:GLU:HB3	21	0.15
(1,851)	1:110:A:PRO:HA	1:131:A:GLU:HB2	22	0.15
(1,851)	1:110:A:PRO:HA	1:131:A:GLU:HB3	22	0.15
(1,847)	1:109:A:THR:HB	1:115:A:HIS:HB2	8	0.15
(1,847)	1:109:A:THR:HB	1:115:A:HIS:HB3	8	0.15
(1,847)	1:109:A:THR:HB	1:115:A:HIS:HB2	10	0.15
(1,847)	1:109:A:THR:HB	1:115:A:HIS:HB3	10	0.15
(1,846)	1:108:A:SER:HB2	1:137:A:PHE:HB2	5	0.15
(1,846)	1:108:A:SER:HB2	1:137:A:PHE:HB3	5	0.15
(1,846)	1:108:A:SER:HB3	1:137:A:PHE:HB2	5	0.15
(1,846)	1:108:A:SER:HB3	1:137:A:PHE:HB3	5	0.15
(1,846)	1:108:A:SER:HB2	1:137:A:PHE:HB2	24	0.15
(1,846)	1:108:A:SER:HB2	1:137:A:PHE:HB3	24	0.15
(1,846)	1:108:A:SER:HB3	1:137:A:PHE:HB2	24	0.15
(1,846)	1:108:A:SER:HB3	1:137:A:PHE:HB3	24	0.15
(1,815)	1:88:A:TYR:HB2	1:75:A:VAL:HG11	19	0.15
(1,815)	1:88:A:TYR:HB2	1:75:A:VAL:HG12	19	0.15
(1,815)	1:88:A:TYR:HB2	1:75:A:VAL:HG13	19	0.15
(1,815)	1:88:A:TYR:HB2	1:75:A:VAL:HG21	19	0.15
(1,815)	1:88:A:TYR:HB2	1:75:A:VAL:HG22	19	0.15
(1,815)	1:88:A:TYR:HB2	1:75:A:VAL:HG23	19	0.15
(1,815)	1:88:A:TYR:HB3	1:75:A:VAL:HG11	19	0.15
(1,815)	1:88:A:TYR:HB3	1:75:A:VAL:HG12	19	0.15
(1,815)	1:88:A:TYR:HB3	1:75:A:VAL:HG13	19	0.15
(1,815)	1:88:A:TYR:HB3	1:75:A:VAL:HG21	19	0.15
(1,815)	1:88:A:TYR:HB3	1:75:A:VAL:HG22	19	0.15
(1,815)	1:88:A:TYR:HB3	1:75:A:VAL:HG23	19	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD11	16	0.15
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD12	16	0.15
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD13	16	0.15
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD21	16	0.15
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD22	16	0.15
(1,811)	1:88:A:TYR:HA	1:35:A:LEU:HD23	16	0.15
(1,783)	1:81:A:LYS:HG2	1:80:A:GLN:HA	19	0.15
(1,783)	1:81:A:LYS:HG3	1:80:A:GLN:HA	19	0.15
(1,776)	1:75:A:VAL:HG11	1:73:A:CYS:HB2	6	0.15
(1,776)	1:75:A:VAL:HG11	1:73:A:CYS:HB3	6	0.15
(1,776)	1:75:A:VAL:HG12	1:73:A:CYS:HB2	6	0.15
(1,776)	1:75:A:VAL:HG12	1:73:A:CYS:HB3	6	0.15
(1,776)	1:75:A:VAL:HG13	1:73:A:CYS:HB2	6	0.15
(1,776)	1:75:A:VAL:HG13	1:73:A:CYS:HB3	6	0.15
(1,741)	1:71:A:ALA:HB1	1:35:A:LEU:HB2	6	0.15
(1,741)	1:71:A:ALA:HB1	1:35:A:LEU:HB3	6	0.15
(1,741)	1:71:A:ALA:HB2	1:35:A:LEU:HB2	6	0.15
(1,741)	1:71:A:ALA:HB2	1:35:A:LEU:HB3	6	0.15
(1,741)	1:71:A:ALA:HB3	1:35:A:LEU:HB2	6	0.15
(1,741)	1:71:A:ALA:HB3	1:35:A:LEU:HB3	6	0.15
(1,741)	1:71:A:ALA:HB1	1:35:A:LEU:HB2	7	0.15
(1,741)	1:71:A:ALA:HB1	1:35:A:LEU:HB3	7	0.15
(1,741)	1:71:A:ALA:HB2	1:35:A:LEU:HB2	7	0.15
(1,741)	1:71:A:ALA:HB2	1:35:A:LEU:HB3	7	0.15
(1,741)	1:71:A:ALA:HB3	1:35:A:LEU:HB2	7	0.15
(1,741)	1:71:A:ALA:HB3	1:35:A:LEU:HB3	7	0.15
(1,732)	1:65:A:THR:HB	1:56:A:ALA:HB1	16	0.15
(1,732)	1:65:A:THR:HB	1:56:A:ALA:HB2	16	0.15
(1,732)	1:65:A:THR:HB	1:56:A:ALA:HB3	16	0.15
(1,732)	1:65:A:THR:HB	1:56:A:ALA:HB1	23	0.15
(1,732)	1:65:A:THR:HB	1:56:A:ALA:HB2	23	0.15
(1,732)	1:65:A:THR:HB	1:56:A:ALA:HB3	23	0.15
(1,714)	1:55:A:LEU:HB2	1:126:A:LEU:HG	14	0.15
(1,714)	1:55:A:LEU:HB3	1:126:A:LEU:HG	14	0.15
(1,707)	1:54:A:TYR:HE1	1:127:A:ASN:H	21	0.15
(1,707)	1:54:A:TYR:HE2	1:127:A:ASN:H	21	0.15
(1,669)	1:47:A:ALA:HB1	1:137:A:PHE:HA	9	0.15
(1,669)	1:47:A:ALA:HB2	1:137:A:PHE:HA	9	0.15
(1,669)	1:47:A:ALA:HB3	1:137:A:PHE:HA	9	0.15
(1,669)	1:47:A:ALA:HB1	1:137:A:PHE:HA	17	0.15
(1,669)	1:47:A:ALA:HB2	1:137:A:PHE:HA	17	0.15
(1,669)	1:47:A:ALA:HB3	1:137:A:PHE:HA	17	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG11	5	0.15
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG12	5	0.15
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG13	5	0.15
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG21	5	0.15
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG22	5	0.15
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG23	5	0.15
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG11	5	0.15
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG12	5	0.15
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG13	5	0.15
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG21	5	0.15
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG22	5	0.15
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG23	5	0.15
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG11	5	0.15
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG12	5	0.15
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG13	5	0.15
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG21	5	0.15
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG22	5	0.15
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG23	5	0.15
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG11	9	0.15
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG12	9	0.15
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG13	9	0.15
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG21	9	0.15
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG22	9	0.15
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG23	9	0.15
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG11	9	0.15
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG12	9	0.15
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG13	9	0.15
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG21	9	0.15
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG22	9	0.15
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG23	9	0.15
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG11	9	0.15
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG12	9	0.15
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG13	9	0.15
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG21	9	0.15
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG22	9	0.15
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG23	9	0.15
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG11	12	0.15
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG12	12	0.15
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG13	12	0.15
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG21	12	0.15
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG22	12	0.15
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG23	12	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG11	12	0.15
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG12	12	0.15
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG13	12	0.15
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG21	12	0.15
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG22	12	0.15
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG23	12	0.15
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG11	12	0.15
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG12	12	0.15
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG13	12	0.15
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG21	12	0.15
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG22	12	0.15
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG23	12	0.15
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG11	21	0.15
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG12	21	0.15
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG13	21	0.15
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG21	21	0.15
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG22	21	0.15
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG23	21	0.15
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG11	21	0.15
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG12	21	0.15
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG13	21	0.15
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG21	21	0.15
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG22	21	0.15
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG23	21	0.15
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG11	21	0.15
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG12	21	0.15
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG13	21	0.15
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG21	21	0.15
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG22	21	0.15
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG23	21	0.15
(1,660)	1:45:A:THR:HG1	1:47:A:ALA:HA	3	0.15
(1,640)	1:35:A:LEU:HD11	1:31:A:GLU:HA	2	0.15
(1,640)	1:35:A:LEU:HD12	1:31:A:GLU:HA	2	0.15
(1,640)	1:35:A:LEU:HD13	1:31:A:GLU:HA	2	0.15
(1,640)	1:35:A:LEU:HD21	1:31:A:GLU:HA	2	0.15
(1,640)	1:35:A:LEU:HD22	1:31:A:GLU:HA	2	0.15
(1,640)	1:35:A:LEU:HD23	1:31:A:GLU:HA	2	0.15
(1,640)	1:35:A:LEU:HD11	1:31:A:GLU:HA	5	0.15
(1,640)	1:35:A:LEU:HD12	1:31:A:GLU:HA	5	0.15
(1,640)	1:35:A:LEU:HD13	1:31:A:GLU:HA	5	0.15
(1,640)	1:35:A:LEU:HD21	1:31:A:GLU:HA	5	0.15
(1,640)	1:35:A:LEU:HD22	1:31:A:GLU:HA	5	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,640)	1:35:A:LEU:HD23	1:31:A:GLU:HA	5	0.15
(1,639)	1:34:A:ARG:HD2	1:74:A:PHE:HE1	1	0.15
(1,639)	1:34:A:ARG:HD2	1:74:A:PHE:HE2	1	0.15
(1,639)	1:34:A:ARG:HD3	1:74:A:PHE:HE1	1	0.15
(1,639)	1:34:A:ARG:HD3	1:74:A:PHE:HE2	1	0.15
(1,598)	2:473:B:LYS:H	2:472:B:THR:HG22	16	0.15
(1,559)	2:452:B:SER:H	2:451:B:GLU:HA	3	0.15
(1,559)	2:452:B:SER:H	2:451:B:GLU:HA	5	0.15
(1,559)	2:452:B:SER:H	2:451:B:GLU:HA	8	0.15
(1,559)	2:452:B:SER:H	2:451:B:GLU:HA	14	0.15
(1,559)	2:452:B:SER:H	2:451:B:GLU:HA	17	0.15
(1,556)	2:451:B:GLU:H	2:450:B:TRP:HB2	5	0.15
(1,556)	2:451:B:GLU:H	2:450:B:TRP:HB2	6	0.15
(1,556)	2:451:B:GLU:H	2:450:B:TRP:HB2	9	0.15
(1,556)	2:451:B:GLU:H	2:450:B:TRP:HB2	10	0.15
(1,556)	2:451:B:GLU:H	2:450:B:TRP:HB2	16	0.15
(1,556)	2:451:B:GLU:H	2:450:B:TRP:HB2	18	0.15
(1,556)	2:451:B:GLU:H	2:450:B:TRP:HB2	22	0.15
(1,531)	1:120:A:ASP:H	1:122:A:CYS:H	23	0.15
(1,523)	1:116:A:THR:H	1:108:A:SER:HB2	12	0.15
(1,523)	1:116:A:THR:H	1:108:A:SER:HB3	12	0.15
(1,523)	1:116:A:THR:H	1:108:A:SER:HB2	15	0.15
(1,523)	1:116:A:THR:H	1:108:A:SER:HB3	15	0.15
(1,509)	1:114:A:PHE:H	1:110:A:PRO:HD2	16	0.15
(1,509)	1:114:A:PHE:H	1:110:A:PRO:HD3	16	0.15
(1,509)	1:114:A:PHE:H	1:110:A:PRO:HD2	19	0.15
(1,509)	1:114:A:PHE:H	1:110:A:PRO:HD3	19	0.15
(1,496)	1:101:A:LEU:H	1:100:A:GLU:H	2	0.15
(1,496)	1:101:A:LEU:H	1:100:A:GLU:H	10	0.15
(1,486)	1:89:A:GLY:H	1:94:A:ARG:HB2	9	0.15
(1,486)	1:89:A:GLY:H	1:94:A:ARG:HB3	9	0.15
(1,482)	1:87:A:LEU:H	1:72:A:VAL:HB	1	0.15
(1,477)	1:72:A:VAL:H	1:48:A:THR:HA	13	0.15
(1,469)	1:55:A:LEU:H	1:65:A:THR:H	2	0.15
(1,440)	1:127:A:ASN:H	1:53:A:LEU:HA	12	0.15
(1,440)	1:127:A:ASN:H	1:53:A:LEU:HA	21	0.15
(1,429)	1:101:A:LEU:H	1:84:A:PHE:HB2	1	0.15
(1,429)	1:101:A:LEU:H	1:84:A:PHE:HB3	1	0.15
(1,416)	1:87:A:LEU:H	1:98:A:GLU:HB2	11	0.15
(1,416)	1:87:A:LEU:H	1:98:A:GLU:HB3	11	0.15
(1,366)	1:35:A:LEU:H	1:32:A:ASN:HA	5	0.15
(1,366)	1:35:A:LEU:H	1:32:A:ASN:HA	9	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,366)	1:35:A:LEU:H	1:32:A:ASN:HA	13	0.15
(1,366)	1:35:A:LEU:H	1:32:A:ASN:HA	21	0.15
(1,364)	1:34:A:ARG:H	1:31:A:GLU:HA	5	0.15
(1,342)	1:146:A:GLN:H	1:143:A:GLU:HA	14	0.15
(1,333)	1:144:A:LYS:H	1:141:A:VAL:HA	14	0.15
(1,333)	1:144:A:LYS:H	1:141:A:VAL:HA	16	0.15
(1,333)	1:144:A:LYS:H	1:141:A:VAL:HA	19	0.15
(1,314)	1:140:A:LEU:H	1:136:A:ALA:HA	8	0.15
(1,314)	1:140:A:LEU:H	1:136:A:ALA:HA	19	0.15
(1,314)	1:140:A:LEU:H	1:136:A:ALA:HA	20	0.15
(1,278)	1:127:A:ASN:H	1:126:A:LEU:HG	16	0.15
(1,272)	1:124:A:ALA:H	1:123:A:GLN:HG2	13	0.15
(1,272)	1:124:A:ALA:H	1:123:A:GLN:HG3	13	0.15
(1,272)	1:124:A:ALA:H	1:123:A:GLN:HG2	19	0.15
(1,272)	1:124:A:ALA:H	1:123:A:GLN:HG3	19	0.15
(1,268)	1:122:A:CYS:H	1:121:A:ASP:HA	3	0.15
(1,268)	1:122:A:CYS:H	1:121:A:ASP:HA	4	0.15
(1,268)	1:122:A:CYS:H	1:121:A:ASP:HA	7	0.15
(1,268)	1:122:A:CYS:H	1:121:A:ASP:HA	9	0.15
(1,268)	1:122:A:CYS:H	1:121:A:ASP:HA	13	0.15
(1,268)	1:122:A:CYS:H	1:121:A:ASP:HA	15	0.15
(1,268)	1:122:A:CYS:H	1:121:A:ASP:HA	16	0.15
(1,268)	1:122:A:CYS:H	1:121:A:ASP:HA	18	0.15
(1,268)	1:122:A:CYS:H	1:121:A:ASP:HA	21	0.15
(1,268)	1:122:A:CYS:H	1:121:A:ASP:HA	23	0.15
(1,259)	1:118:A:ALA:H	1:117:A:PHE:HB3	7	0.15
(1,255)	1:117:A:PHE:H	1:116:A:THR:HB	17	0.15
(1,250)	1:116:A:THR:H	1:115:A:HIS:HB3	2	0.15
(1,250)	1:116:A:THR:H	1:115:A:HIS:HB3	3	0.15
(1,250)	1:116:A:THR:H	1:115:A:HIS:HB3	7	0.15
(1,250)	1:116:A:THR:H	1:115:A:HIS:HB3	14	0.15
(1,250)	1:116:A:THR:H	1:115:A:HIS:HB3	15	0.15
(1,250)	1:116:A:THR:H	1:115:A:HIS:HB3	17	0.15
(1,250)	1:116:A:THR:H	1:115:A:HIS:HB3	22	0.15
(1,195)	1:96:A:LEU:H	1:95:A:LEU:H	4	0.15
(1,195)	1:96:A:LEU:H	1:95:A:LEU:H	19	0.15
(1,141)	1:77:A:ASP:H	1:76:A:LYS:HG2	8	0.15
(1,141)	1:77:A:ASP:H	1:76:A:LYS:HG3	8	0.15
(1,141)	1:77:A:ASP:H	1:76:A:LYS:HG2	17	0.15
(1,141)	1:77:A:ASP:H	1:76:A:LYS:HG3	17	0.15
(1,112)	1:65:A:THR:H	1:64:A:TRP:HB3	15	0.15
(1,105)	1:63:A:HIS:H	1:62:A:GLU:HA	7	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,105)	1:63:A:HIS:H	1:62:A:GLU:HA	12	0.15
(1,105)	1:63:A:HIS:H	1:62:A:GLU:HA	15	0.15
(1,54)	1:43:A:CYS:H	1:42:A:LYS:HB2	17	0.15
(1,54)	1:43:A:CYS:H	1:42:A:LYS:HB3	17	0.15
(1,41)	1:38:A:MET:H	1:37:A:GLU:HG2	1	0.15
(1,41)	1:38:A:MET:H	1:37:A:GLU:HG3	1	0.15
(4,111)	1:146:A:GLN:H	1:142:A:GLN:O	16	0.14
(4,92)	1:136:A:ALA:N	1:132:A:ASP:O	6	0.14
(4,88)	1:134:A:ALA:N	1:130:A:ASP:O	11	0.14
(4,77)	1:34:A:ARG:H	1:30:A:HIS:O	15	0.14
(4,43)	1:88:A:TYR:H	1:71:A:ALA:O	1	0.14
(4,43)	1:88:A:TYR:H	1:71:A:ALA:O	3	0.14
(4,40)	1:56:A:ALA:N	1:123:A:GLN:O	7	0.14
(4,40)	1:56:A:ALA:N	1:123:A:GLN:O	18	0.14
(4,40)	1:56:A:ALA:N	1:123:A:GLN:O	21	0.14
(4,39)	1:56:A:ALA:H	1:123:A:GLN:O	3	0.14
(4,35)	1:54:A:TYR:H	1:125:A:GLY:O	20	0.14
(4,31)	1:52:A:GLN:H	1:127:A:ASN:O	4	0.14
(4,31)	1:52:A:GLN:H	1:127:A:ASN:O	22	0.14
(4,23)	1:68:A:HIS:H	1:53:A:LEU:O	10	0.14
(4,23)	1:68:A:HIS:H	1:53:A:LEU:O	15	0.14
(4,23)	1:68:A:HIS:H	1:53:A:LEU:O	21	0.14
(4,23)	1:68:A:HIS:H	1:53:A:LEU:O	24	0.14
(4,9)	1:74:A:PHE:H	1:47:A:ALA:O	21	0.14
(1,1016)	2:479:B:LEU:HG	1:83:A:TYR:HD1	7	0.14
(1,1016)	2:479:B:LEU:HG	1:83:A:TYR:HD2	7	0.14
(1,1016)	2:479:B:LEU:HG	1:83:A:TYR:HD1	13	0.14
(1,1016)	2:479:B:LEU:HG	1:83:A:TYR:HD2	13	0.14
(1,1016)	2:479:B:LEU:HG	1:83:A:TYR:HD1	15	0.14
(1,1016)	2:479:B:LEU:HG	1:83:A:TYR:HD2	15	0.14
(1,1007)	2:474:B:SER:H	1:102:A:TYR:HA	16	0.14
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD11	4	0.14
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD12	4	0.14
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD13	4	0.14
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD21	4	0.14
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD22	4	0.14
(1,1005)	2:478:B:LYS:HD2	1:101:A:LEU:HD23	4	0.14
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD11	4	0.14
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD12	4	0.14
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD13	4	0.14
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD21	4	0.14
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD22	4	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1005)	2:478:B:LYS:HD3	1:101:A:LEU:HD23	4	0.14
(1,988)	1:129:A:ALA:HA	2:454:B:PHE:HZ	17	0.14
(1,972)	1:71:A:ALA:H	2:450:B:TRP:HZ2	15	0.14
(1,972)	1:71:A:ALA:H	2:450:B:TRP:HZ2	21	0.14
(1,957)	1:50:A:VAL:HG11	2:453:B:ARG:HB2	18	0.14
(1,957)	1:50:A:VAL:HG11	2:453:B:ARG:HB3	18	0.14
(1,957)	1:50:A:VAL:HG12	2:453:B:ARG:HB2	18	0.14
(1,957)	1:50:A:VAL:HG12	2:453:B:ARG:HB3	18	0.14
(1,957)	1:50:A:VAL:HG13	2:453:B:ARG:HB2	18	0.14
(1,957)	1:50:A:VAL:HG13	2:453:B:ARG:HB3	18	0.14
(1,957)	1:50:A:VAL:HG21	2:453:B:ARG:HB2	18	0.14
(1,957)	1:50:A:VAL:HG21	2:453:B:ARG:HB3	18	0.14
(1,957)	1:50:A:VAL:HG22	2:453:B:ARG:HB2	18	0.14
(1,957)	1:50:A:VAL:HG22	2:453:B:ARG:HB3	18	0.14
(1,957)	1:50:A:VAL:HG23	2:453:B:ARG:HB2	18	0.14
(1,957)	1:50:A:VAL:HG23	2:453:B:ARG:HB3	18	0.14
(1,944)	2:458:B:PRO:HA	2:460:B:SER:HB2	9	0.14
(1,944)	2:458:B:PRO:HA	2:460:B:SER:HB3	9	0.14
(1,944)	2:458:B:PRO:HA	2:460:B:SER:HB2	11	0.14
(1,944)	2:458:B:PRO:HA	2:460:B:SER:HB3	11	0.14
(1,912)	1:141:A:VAL:HG11	1:107:A:TYR:HB3	1	0.14
(1,912)	1:141:A:VAL:HG12	1:107:A:TYR:HB3	1	0.14
(1,912)	1:141:A:VAL:HG13	1:107:A:TYR:HB3	1	0.14
(1,912)	1:141:A:VAL:HG21	1:107:A:TYR:HB3	1	0.14
(1,912)	1:141:A:VAL:HG22	1:107:A:TYR:HB3	1	0.14
(1,912)	1:141:A:VAL:HG23	1:107:A:TYR:HB3	1	0.14
(1,912)	1:141:A:VAL:HG11	1:107:A:TYR:HB2	1	0.14
(1,912)	1:141:A:VAL:HG12	1:107:A:TYR:HB2	1	0.14
(1,912)	1:141:A:VAL:HG13	1:107:A:TYR:HB2	1	0.14
(1,912)	1:141:A:VAL:HG21	1:107:A:TYR:HB2	1	0.14
(1,912)	1:141:A:VAL:HG22	1:107:A:TYR:HB2	1	0.14
(1,912)	1:141:A:VAL:HG23	1:107:A:TYR:HB2	1	0.14
(1,912)	1:141:A:VAL:HG11	1:107:A:TYR:HB3	13	0.14
(1,912)	1:141:A:VAL:HG12	1:107:A:TYR:HB3	13	0.14
(1,912)	1:141:A:VAL:HG13	1:107:A:TYR:HB3	13	0.14
(1,912)	1:141:A:VAL:HG21	1:107:A:TYR:HB3	13	0.14
(1,912)	1:141:A:VAL:HG22	1:107:A:TYR:HB3	13	0.14
(1,912)	1:141:A:VAL:HG23	1:107:A:TYR:HB3	13	0.14
(1,912)	1:141:A:VAL:HG11	1:107:A:TYR:HB2	13	0.14
(1,912)	1:141:A:VAL:HG12	1:107:A:TYR:HB2	13	0.14
(1,912)	1:141:A:VAL:HG13	1:107:A:TYR:HB2	13	0.14
(1,912)	1:141:A:VAL:HG21	1:107:A:TYR:HB2	13	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,912)	1:141:A:VAL:HG22	1:107:A:TYR:HB2	13	0.14
(1,912)	1:141:A:VAL:HG23	1:107:A:TYR:HB2	13	0.14
(1,880)	1:129:A:ALA:HB1	1:50:A:VAL:HB	22	0.14
(1,880)	1:129:A:ALA:HB2	1:50:A:VAL:HB	22	0.14
(1,880)	1:129:A:ALA:HB3	1:50:A:VAL:HB	22	0.14
(1,875)	1:126:A:LEU:HG	1:114:A:PHE:HD1	5	0.14
(1,875)	1:126:A:LEU:HG	1:114:A:PHE:HD2	5	0.14
(1,875)	1:126:A:LEU:HG	1:114:A:PHE:HD1	11	0.14
(1,875)	1:126:A:LEU:HG	1:114:A:PHE:HD2	11	0.14
(1,869)	1:124:A:ALA:HB1	1:117:A:PHE:HD1	2	0.14
(1,869)	1:124:A:ALA:HB1	1:117:A:PHE:HD2	2	0.14
(1,869)	1:124:A:ALA:HB2	1:117:A:PHE:HD1	2	0.14
(1,869)	1:124:A:ALA:HB2	1:117:A:PHE:HD2	2	0.14
(1,869)	1:124:A:ALA:HB3	1:117:A:PHE:HD1	2	0.14
(1,869)	1:124:A:ALA:HB3	1:117:A:PHE:HD2	2	0.14
(1,865)	1:123:A:GLN:HG2	1:122:A:CYS:HB2	2	0.14
(1,865)	1:123:A:GLN:HG2	1:122:A:CYS:HB3	2	0.14
(1,865)	1:123:A:GLN:HG3	1:122:A:CYS:HB2	2	0.14
(1,865)	1:123:A:GLN:HG3	1:122:A:CYS:HB3	2	0.14
(1,864)	1:122:A:CYS:HA	1:123:A:GLN:HB2	13	0.14
(1,864)	1:122:A:CYS:HA	1:123:A:GLN:HB3	13	0.14
(1,863)	1:120:A:ASP:HA	1:123:A:GLN:HG2	2	0.14
(1,863)	1:120:A:ASP:HA	1:123:A:GLN:HG3	2	0.14
(1,863)	1:120:A:ASP:HA	1:123:A:GLN:HG2	7	0.14
(1,863)	1:120:A:ASP:HA	1:123:A:GLN:HG3	7	0.14
(1,863)	1:120:A:ASP:HA	1:123:A:GLN:HG2	18	0.14
(1,863)	1:120:A:ASP:HA	1:123:A:GLN:HG3	18	0.14
(1,851)	1:110:A:PRO:HA	1:131:A:GLU:HB2	3	0.14
(1,851)	1:110:A:PRO:HA	1:131:A:GLU:HB3	3	0.14
(1,851)	1:110:A:PRO:HA	1:131:A:GLU:HB2	14	0.14
(1,851)	1:110:A:PRO:HA	1:131:A:GLU:HB3	14	0.14
(1,847)	1:109:A:THR:HB	1:115:A:HIS:HB2	3	0.14
(1,847)	1:109:A:THR:HB	1:115:A:HIS:HB3	3	0.14
(1,847)	1:109:A:THR:HB	1:115:A:HIS:HB2	6	0.14
(1,847)	1:109:A:THR:HB	1:115:A:HIS:HB3	6	0.14
(1,846)	1:108:A:SER:HB2	1:137:A:PHE:HB2	4	0.14
(1,846)	1:108:A:SER:HB2	1:137:A:PHE:HB3	4	0.14
(1,846)	1:108:A:SER:HB3	1:137:A:PHE:HB2	4	0.14
(1,846)	1:108:A:SER:HB3	1:137:A:PHE:HB3	4	0.14
(1,815)	1:88:A:TYR:HB2	1:75:A:VAL:HG11	6	0.14
(1,815)	1:88:A:TYR:HB2	1:75:A:VAL:HG12	6	0.14
(1,815)	1:88:A:TYR:HB2	1:75:A:VAL:HG13	6	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,815)	1:88:A:TYR:HB2	1:75:A:VAL:HG21	6	0.14
(1,815)	1:88:A:TYR:HB2	1:75:A:VAL:HG22	6	0.14
(1,815)	1:88:A:TYR:HB2	1:75:A:VAL:HG23	6	0.14
(1,815)	1:88:A:TYR:HB3	1:75:A:VAL:HG11	6	0.14
(1,815)	1:88:A:TYR:HB3	1:75:A:VAL:HG12	6	0.14
(1,815)	1:88:A:TYR:HB3	1:75:A:VAL:HG13	6	0.14
(1,815)	1:88:A:TYR:HB3	1:75:A:VAL:HG21	6	0.14
(1,815)	1:88:A:TYR:HB3	1:75:A:VAL:HG22	6	0.14
(1,815)	1:88:A:TYR:HB3	1:75:A:VAL:HG23	6	0.14
(1,815)	1:88:A:TYR:HB2	1:75:A:VAL:HG11	9	0.14
(1,815)	1:88:A:TYR:HB2	1:75:A:VAL:HG12	9	0.14
(1,815)	1:88:A:TYR:HB2	1:75:A:VAL:HG13	9	0.14
(1,815)	1:88:A:TYR:HB2	1:75:A:VAL:HG21	9	0.14
(1,815)	1:88:A:TYR:HB2	1:75:A:VAL:HG22	9	0.14
(1,815)	1:88:A:TYR:HB2	1:75:A:VAL:HG23	9	0.14
(1,815)	1:88:A:TYR:HB3	1:75:A:VAL:HG11	9	0.14
(1,815)	1:88:A:TYR:HB3	1:75:A:VAL:HG12	9	0.14
(1,815)	1:88:A:TYR:HB3	1:75:A:VAL:HG13	9	0.14
(1,815)	1:88:A:TYR:HB3	1:75:A:VAL:HG21	9	0.14
(1,815)	1:88:A:TYR:HB3	1:75:A:VAL:HG22	9	0.14
(1,815)	1:88:A:TYR:HB3	1:75:A:VAL:HG23	9	0.14
(1,783)	1:81:A:LYS:HG2	1:80:A:GLN:HA	2	0.14
(1,783)	1:81:A:LYS:HG3	1:80:A:GLN:HA	2	0.14
(1,776)	1:75:A:VAL:HG11	1:73:A:CYS:HB2	15	0.14
(1,776)	1:75:A:VAL:HG11	1:73:A:CYS:HB3	15	0.14
(1,776)	1:75:A:VAL:HG12	1:73:A:CYS:HB2	15	0.14
(1,776)	1:75:A:VAL:HG12	1:73:A:CYS:HB3	15	0.14
(1,776)	1:75:A:VAL:HG13	1:73:A:CYS:HB2	15	0.14
(1,776)	1:75:A:VAL:HG13	1:73:A:CYS:HB3	15	0.14
(1,741)	1:71:A:ALA:HB1	1:35:A:LEU:HB2	8	0.14
(1,741)	1:71:A:ALA:HB1	1:35:A:LEU:HB3	8	0.14
(1,741)	1:71:A:ALA:HB2	1:35:A:LEU:HB2	8	0.14
(1,741)	1:71:A:ALA:HB2	1:35:A:LEU:HB3	8	0.14
(1,741)	1:71:A:ALA:HB3	1:35:A:LEU:HB2	8	0.14
(1,741)	1:71:A:ALA:HB3	1:35:A:LEU:HB3	8	0.14
(1,741)	1:71:A:ALA:HB1	1:35:A:LEU:HB2	15	0.14
(1,741)	1:71:A:ALA:HB1	1:35:A:LEU:HB3	15	0.14
(1,741)	1:71:A:ALA:HB2	1:35:A:LEU:HB2	15	0.14
(1,741)	1:71:A:ALA:HB2	1:35:A:LEU:HB3	15	0.14
(1,741)	1:71:A:ALA:HB3	1:35:A:LEU:HB2	15	0.14
(1,741)	1:71:A:ALA:HB3	1:35:A:LEU:HB3	15	0.14
(1,741)	1:71:A:ALA:HB1	1:35:A:LEU:HB2	20	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,741)	1:71:A:ALA:HB1	1:35:A:LEU:HB3	20	0.14
(1,741)	1:71:A:ALA:HB2	1:35:A:LEU:HB2	20	0.14
(1,741)	1:71:A:ALA:HB2	1:35:A:LEU:HB3	20	0.14
(1,741)	1:71:A:ALA:HB3	1:35:A:LEU:HB2	20	0.14
(1,741)	1:71:A:ALA:HB3	1:35:A:LEU:HB3	20	0.14
(1,741)	1:71:A:ALA:HB1	1:35:A:LEU:HB2	22	0.14
(1,741)	1:71:A:ALA:HB1	1:35:A:LEU:HB3	22	0.14
(1,741)	1:71:A:ALA:HB2	1:35:A:LEU:HB2	22	0.14
(1,741)	1:71:A:ALA:HB2	1:35:A:LEU:HB3	22	0.14
(1,741)	1:71:A:ALA:HB3	1:35:A:LEU:HB2	22	0.14
(1,741)	1:71:A:ALA:HB3	1:35:A:LEU:HB3	22	0.14
(1,691)	1:53:A:LEU:HG	1:126:A:LEU:HA	4	0.14
(1,688)	1:51:A:VAL:HG11	1:128:A:PHE:HB2	2	0.14
(1,688)	1:51:A:VAL:HG11	1:128:A:PHE:HB3	2	0.14
(1,688)	1:51:A:VAL:HG12	1:128:A:PHE:HB2	2	0.14
(1,688)	1:51:A:VAL:HG12	1:128:A:PHE:HB3	2	0.14
(1,688)	1:51:A:VAL:HG13	1:128:A:PHE:HB2	2	0.14
(1,688)	1:51:A:VAL:HG13	1:128:A:PHE:HB3	2	0.14
(1,688)	1:51:A:VAL:HG21	1:128:A:PHE:HB2	2	0.14
(1,688)	1:51:A:VAL:HG21	1:128:A:PHE:HB3	2	0.14
(1,688)	1:51:A:VAL:HG22	1:128:A:PHE:HB2	2	0.14
(1,688)	1:51:A:VAL:HG22	1:128:A:PHE:HB3	2	0.14
(1,688)	1:51:A:VAL:HG23	1:128:A:PHE:HB2	2	0.14
(1,688)	1:51:A:VAL:HG23	1:128:A:PHE:HB3	2	0.14
(1,669)	1:47:A:ALA:HB1	1:137:A:PHE:HA	18	0.14
(1,669)	1:47:A:ALA:HB2	1:137:A:PHE:HA	18	0.14
(1,669)	1:47:A:ALA:HB3	1:137:A:PHE:HA	18	0.14
(1,669)	1:47:A:ALA:HB1	1:137:A:PHE:HA	20	0.14
(1,669)	1:47:A:ALA:HB2	1:137:A:PHE:HA	20	0.14
(1,669)	1:47:A:ALA:HB3	1:137:A:PHE:HA	20	0.14
(1,669)	1:47:A:ALA:HB1	1:137:A:PHE:HA	22	0.14
(1,669)	1:47:A:ALA:HB2	1:137:A:PHE:HA	22	0.14
(1,669)	1:47:A:ALA:HB3	1:137:A:PHE:HA	22	0.14
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG11	2	0.14
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG12	2	0.14
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG13	2	0.14
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG21	2	0.14
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG22	2	0.14
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG23	2	0.14
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG11	2	0.14
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG12	2	0.14
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG13	2	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG21	2	0.14
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG22	2	0.14
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG23	2	0.14
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG11	2	0.14
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG12	2	0.14
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG13	2	0.14
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG21	2	0.14
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG22	2	0.14
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG23	2	0.14
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD11	5	0.14
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD12	5	0.14
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD13	5	0.14
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD21	5	0.14
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD22	5	0.14
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD23	5	0.14
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD11	5	0.14
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD12	5	0.14
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD13	5	0.14
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD21	5	0.14
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD22	5	0.14
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD23	5	0.14
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD11	15	0.14
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD12	15	0.14
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD13	15	0.14
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD21	15	0.14
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD22	15	0.14
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD23	15	0.14
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD11	15	0.14
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD12	15	0.14
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD13	15	0.14
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD21	15	0.14
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD22	15	0.14
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD23	15	0.14
(1,640)	1:35:A:LEU:HD11	1:31:A:GLU:HA	24	0.14
(1,640)	1:35:A:LEU:HD12	1:31:A:GLU:HA	24	0.14
(1,640)	1:35:A:LEU:HD13	1:31:A:GLU:HA	24	0.14
(1,640)	1:35:A:LEU:HD21	1:31:A:GLU:HA	24	0.14
(1,640)	1:35:A:LEU:HD22	1:31:A:GLU:HA	24	0.14
(1,640)	1:35:A:LEU:HD23	1:31:A:GLU:HA	24	0.14
(1,639)	1:34:A:ARG:HD2	1:74:A:PHE:HE1	18	0.14
(1,639)	1:34:A:ARG:HD2	1:74:A:PHE:HE2	18	0.14
(1,639)	1:34:A:ARG:HD3	1:74:A:PHE:HE1	18	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,639)	1:34:A:ARG:HD3	1:74:A:PHE:HE2	18	0.14
(1,631)	1:30:A:HIS:HA	1:33:A:GLN:HB2	2	0.14
(1,631)	1:30:A:HIS:HA	1:33:A:GLN:HB3	2	0.14
(1,610)	2:479:B:LEU:H	2:478:B:LYS:HG2	24	0.14
(1,610)	2:479:B:LEU:H	2:478:B:LYS:HG3	24	0.14
(1,590)	2:470:B:GLN:H	2:469:B:VAL:HB	3	0.14
(1,584)	2:468:B:TYR:H	2:467:B:PRO:HG2	5	0.14
(1,584)	2:468:B:TYR:H	2:467:B:PRO:HG3	5	0.14
(1,571)	2:459:B:ILE:H	2:458:B:PRO:HB2	19	0.14
(1,567)	2:457:B:HIS:H	2:456:B:PHE:HB3	11	0.14
(1,556)	2:451:B:GLU:H	2:450:B:TRP:HB2	3	0.14
(1,556)	2:451:B:GLU:H	2:450:B:TRP:HB2	15	0.14
(1,545)	2:447:B:GLU:H	2:446:B:CYS:H	11	0.14
(1,531)	1:120:A:ASP:H	1:122:A:CYS:H	5	0.14
(1,531)	1:120:A:ASP:H	1:122:A:CYS:H	7	0.14
(1,531)	1:120:A:ASP:H	1:122:A:CYS:H	12	0.14
(1,529)	1:126:A:LEU:H	1:125:A:GLY:H	14	0.14
(1,523)	1:116:A:THR:H	1:108:A:SER:HB2	8	0.14
(1,523)	1:116:A:THR:H	1:108:A:SER:HB3	8	0.14
(1,509)	1:114:A:PHE:H	1:110:A:PRO:HD2	3	0.14
(1,509)	1:114:A:PHE:H	1:110:A:PRO:HD3	3	0.14
(1,502)	1:104:A:GLN:H	1:102:A:TYR:HA	24	0.14
(1,493)	1:97:A:TRP:H	1:95:A:LEU:HA	24	0.14
(1,487)	1:89:A:GLY:H	1:94:A:ARG:H	12	0.14
(1,477)	1:72:A:VAL:H	1:48:A:THR:HA	2	0.14
(1,477)	1:72:A:VAL:H	1:48:A:THR:HA	14	0.14
(1,477)	1:72:A:VAL:H	1:48:A:THR:HA	24	0.14
(1,469)	1:55:A:LEU:H	1:65:A:THR:H	12	0.14
(1,469)	1:55:A:LEU:H	1:65:A:THR:H	20	0.14
(1,456)	1:35:A:LEU:H	1:31:A:GLU:HA	1	0.14
(1,456)	1:35:A:LEU:H	1:31:A:GLU:HA	9	0.14
(1,456)	1:35:A:LEU:H	1:31:A:GLU:HA	15	0.14
(1,440)	1:127:A:ASN:H	1:53:A:LEU:HA	23	0.14
(1,439)	1:126:A:LEU:H	1:116:A:THR:HG22	8	0.14
(1,429)	1:101:A:LEU:H	1:84:A:PHE:HB2	22	0.14
(1,429)	1:101:A:LEU:H	1:84:A:PHE:HB3	22	0.14
(1,416)	1:87:A:LEU:H	1:98:A:GLU:HB2	9	0.14
(1,416)	1:87:A:LEU:H	1:98:A:GLU:HB3	9	0.14
(1,416)	1:87:A:LEU:H	1:98:A:GLU:HB2	21	0.14
(1,416)	1:87:A:LEU:H	1:98:A:GLU:HB3	21	0.14
(1,416)	1:87:A:LEU:H	1:98:A:GLU:HB2	23	0.14
(1,416)	1:87:A:LEU:H	1:98:A:GLU:HB3	23	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,399)	1:72:A:VAL:H	1:50:A:VAL:HB	4	0.14
(1,399)	1:72:A:VAL:H	1:50:A:VAL:HB	7	0.14
(1,399)	1:72:A:VAL:H	1:50:A:VAL:HB	14	0.14
(1,399)	1:72:A:VAL:H	1:50:A:VAL:HB	23	0.14
(1,374)	1:38:A:MET:H	1:35:A:LEU:HG	20	0.14
(1,366)	1:35:A:LEU:H	1:32:A:ASN:HA	22	0.14
(1,333)	1:144:A:LYS:H	1:141:A:VAL:HA	6	0.14
(1,327)	1:143:A:GLU:H	1:140:A:LEU:HD11	2	0.14
(1,327)	1:143:A:GLU:H	1:140:A:LEU:HD12	2	0.14
(1,327)	1:143:A:GLU:H	1:140:A:LEU:HD13	2	0.14
(1,327)	1:143:A:GLU:H	1:140:A:LEU:HD21	2	0.14
(1,327)	1:143:A:GLU:H	1:140:A:LEU:HD22	2	0.14
(1,327)	1:143:A:GLU:H	1:140:A:LEU:HD23	2	0.14
(1,327)	1:143:A:GLU:H	1:140:A:LEU:HD11	23	0.14
(1,327)	1:143:A:GLU:H	1:140:A:LEU:HD12	23	0.14
(1,327)	1:143:A:GLU:H	1:140:A:LEU:HD13	23	0.14
(1,327)	1:143:A:GLU:H	1:140:A:LEU:HD21	23	0.14
(1,327)	1:143:A:GLU:H	1:140:A:LEU:HD22	23	0.14
(1,327)	1:143:A:GLU:H	1:140:A:LEU:HD23	23	0.14
(1,300)	1:136:A:ALA:H	1:132:A:ASP:HA	6	0.14
(1,278)	1:127:A:ASN:H	1:126:A:LEU:HG	2	0.14
(1,278)	1:127:A:ASN:H	1:126:A:LEU:HG	6	0.14
(1,272)	1:124:A:ALA:H	1:123:A:GLN:HG2	8	0.14
(1,272)	1:124:A:ALA:H	1:123:A:GLN:HG3	8	0.14
(1,272)	1:124:A:ALA:H	1:123:A:GLN:HG2	12	0.14
(1,272)	1:124:A:ALA:H	1:123:A:GLN:HG3	12	0.14
(1,272)	1:124:A:ALA:H	1:123:A:GLN:HG2	20	0.14
(1,272)	1:124:A:ALA:H	1:123:A:GLN:HG3	20	0.14
(1,268)	1:122:A:CYS:H	1:121:A:ASP:HA	6	0.14
(1,268)	1:122:A:CYS:H	1:121:A:ASP:HA	8	0.14
(1,268)	1:122:A:CYS:H	1:121:A:ASP:HA	10	0.14
(1,268)	1:122:A:CYS:H	1:121:A:ASP:HA	14	0.14
(1,268)	1:122:A:CYS:H	1:121:A:ASP:HA	20	0.14
(1,268)	1:122:A:CYS:H	1:121:A:ASP:HA	24	0.14
(1,250)	1:116:A:THR:H	1:115:A:HIS:HB3	9	0.14
(1,250)	1:116:A:THR:H	1:115:A:HIS:HB3	12	0.14
(1,245)	1:114:A:PHE:H	1:113:A:PHE:H	12	0.14
(1,195)	1:96:A:LEU:H	1:95:A:LEU:H	2	0.14
(1,195)	1:96:A:LEU:H	1:95:A:LEU:H	24	0.14
(1,153)	1:82:A:SER:H	1:81:A:LYS:HE2	1	0.14
(1,153)	1:82:A:SER:H	1:81:A:LYS:HE3	1	0.14
(1,112)	1:65:A:THR:H	1:64:A:TRP:HB3	19	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,112)	1:65:A:THR:H	1:64:A:TRP:HB3	24	0.14
(1,106)	1:63:A:HIS:H	1:62:A:GLU:HG2	16	0.14
(1,106)	1:63:A:HIS:H	1:62:A:GLU:HG3	16	0.14
(1,105)	1:63:A:HIS:H	1:62:A:GLU:HA	5	0.14
(1,69)	1:49:A:ALA:H	1:48:A:THR:HG23	21	0.14
(1,54)	1:43:A:CYS:H	1:42:A:LYS:HB2	13	0.14
(1,54)	1:43:A:CYS:H	1:42:A:LYS:HB3	13	0.14
(4,77)	1:34:A:ARG:H	1:30:A:HIS:O	10	0.13
(4,70)	1:119:A:GLY:N	1:122:A:CYS:O	6	0.13
(4,41)	1:71:A:ALA:H	1:88:A:TYR:O	15	0.13
(4,41)	1:71:A:ALA:H	1:88:A:TYR:O	16	0.13
(4,41)	1:71:A:ALA:H	1:88:A:TYR:O	23	0.13
(4,40)	1:56:A:ALA:N	1:123:A:GLN:O	3	0.13
(4,40)	1:56:A:ALA:N	1:123:A:GLN:O	8	0.13
(4,40)	1:56:A:ALA:N	1:123:A:GLN:O	10	0.13
(4,40)	1:56:A:ALA:N	1:123:A:GLN:O	16	0.13
(4,40)	1:56:A:ALA:N	1:123:A:GLN:O	22	0.13
(4,39)	1:56:A:ALA:H	1:123:A:GLN:O	10	0.13
(4,31)	1:52:A:GLN:H	1:127:A:ASN:O	12	0.13
(4,31)	1:52:A:GLN:H	1:127:A:ASN:O	18	0.13
(4,19)	1:53:A:LEU:H	1:68:A:HIS:O	22	0.13
(4,9)	1:74:A:PHE:H	1:47:A:ALA:O	6	0.13
(4,9)	1:74:A:PHE:H	1:47:A:ALA:O	15	0.13
(4,9)	1:74:A:PHE:H	1:47:A:ALA:O	20	0.13
(1,1016)	2:479:B:LEU:HG	1:83:A:TYR:HD1	3	0.13
(1,1016)	2:479:B:LEU:HG	1:83:A:TYR:HD2	3	0.13
(1,1008)	2:474:B:SER:H	1:102:A:TYR:HE1	1	0.13
(1,1008)	2:474:B:SER:H	1:102:A:TYR:HE2	1	0.13
(1,1007)	2:474:B:SER:H	1:102:A:TYR:HA	18	0.13
(1,1003)	2:463:B:PRO:HD2	1:114:A:PHE:HE1	10	0.13
(1,988)	1:129:A:ALA:HA	2:454:B:PHE:HZ	8	0.13
(1,988)	1:129:A:ALA:HA	2:454:B:PHE:HZ	19	0.13
(1,972)	1:71:A:ALA:H	2:450:B:TRP:HZ2	7	0.13
(1,972)	1:71:A:ALA:H	2:450:B:TRP:HZ2	12	0.13
(1,964)	1:51:A:VAL:H	2:454:B:PHE:HD1	21	0.13
(1,964)	1:51:A:VAL:H	2:454:B:PHE:HD2	21	0.13
(1,963)	1:50:A:VAL:HG11	2:456:B:PHE:HD1	2	0.13
(1,963)	1:50:A:VAL:HG11	2:456:B:PHE:HD2	2	0.13
(1,963)	1:50:A:VAL:HG12	2:456:B:PHE:HD1	2	0.13
(1,963)	1:50:A:VAL:HG12	2:456:B:PHE:HD2	2	0.13
(1,963)	1:50:A:VAL:HG13	2:456:B:PHE:HD1	2	0.13
(1,963)	1:50:A:VAL:HG13	2:456:B:PHE:HD2	2	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,963)	1:50:A:VAL:HG21	2:456:B:PHE:HD1	2	0.13
(1,963)	1:50:A:VAL:HG21	2:456:B:PHE:HD2	2	0.13
(1,963)	1:50:A:VAL:HG22	2:456:B:PHE:HD1	2	0.13
(1,963)	1:50:A:VAL:HG22	2:456:B:PHE:HD2	2	0.13
(1,963)	1:50:A:VAL:HG23	2:456:B:PHE:HD1	2	0.13
(1,963)	1:50:A:VAL:HG23	2:456:B:PHE:HD2	2	0.13
(1,962)	1:50:A:VAL:HG11	2:450:B:TRP:HE3	9	0.13
(1,962)	1:50:A:VAL:HG12	2:450:B:TRP:HE3	9	0.13
(1,962)	1:50:A:VAL:HG13	2:450:B:TRP:HE3	9	0.13
(1,962)	1:50:A:VAL:HG21	2:450:B:TRP:HE3	9	0.13
(1,962)	1:50:A:VAL:HG22	2:450:B:TRP:HE3	9	0.13
(1,962)	1:50:A:VAL:HG23	2:450:B:TRP:HE3	9	0.13
(1,957)	1:50:A:VAL:HG11	2:453:B:ARG:HB2	6	0.13
(1,957)	1:50:A:VAL:HG11	2:453:B:ARG:HB3	6	0.13
(1,957)	1:50:A:VAL:HG12	2:453:B:ARG:HB2	6	0.13
(1,957)	1:50:A:VAL:HG12	2:453:B:ARG:HB3	6	0.13
(1,957)	1:50:A:VAL:HG13	2:453:B:ARG:HB2	6	0.13
(1,957)	1:50:A:VAL:HG13	2:453:B:ARG:HB3	6	0.13
(1,957)	1:50:A:VAL:HG21	2:453:B:ARG:HB2	6	0.13
(1,957)	1:50:A:VAL:HG21	2:453:B:ARG:HB3	6	0.13
(1,957)	1:50:A:VAL:HG22	2:453:B:ARG:HB2	6	0.13
(1,957)	1:50:A:VAL:HG22	2:453:B:ARG:HB3	6	0.13
(1,957)	1:50:A:VAL:HG23	2:453:B:ARG:HB2	6	0.13
(1,957)	1:50:A:VAL:HG23	2:453:B:ARG:HB3	6	0.13
(1,957)	1:50:A:VAL:HG11	2:453:B:ARG:HB2	12	0.13
(1,957)	1:50:A:VAL:HG11	2:453:B:ARG:HB3	12	0.13
(1,957)	1:50:A:VAL:HG12	2:453:B:ARG:HB2	12	0.13
(1,957)	1:50:A:VAL:HG12	2:453:B:ARG:HB3	12	0.13
(1,957)	1:50:A:VAL:HG13	2:453:B:ARG:HB2	12	0.13
(1,957)	1:50:A:VAL:HG13	2:453:B:ARG:HB3	12	0.13
(1,957)	1:50:A:VAL:HG21	2:453:B:ARG:HB2	12	0.13
(1,957)	1:50:A:VAL:HG21	2:453:B:ARG:HB3	12	0.13
(1,957)	1:50:A:VAL:HG22	2:453:B:ARG:HB2	12	0.13
(1,957)	1:50:A:VAL:HG22	2:453:B:ARG:HB3	12	0.13
(1,957)	1:50:A:VAL:HG23	2:453:B:ARG:HB2	12	0.13
(1,957)	1:50:A:VAL:HG23	2:453:B:ARG:HB3	12	0.13
(1,957)	1:50:A:VAL:HG11	2:453:B:ARG:HB2	16	0.13
(1,957)	1:50:A:VAL:HG11	2:453:B:ARG:HB3	16	0.13
(1,957)	1:50:A:VAL:HG12	2:453:B:ARG:HB2	16	0.13
(1,957)	1:50:A:VAL:HG12	2:453:B:ARG:HB3	16	0.13
(1,957)	1:50:A:VAL:HG13	2:453:B:ARG:HB2	16	0.13
(1,957)	1:50:A:VAL:HG13	2:453:B:ARG:HB3	16	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,957)	1:50:A:VAL:HG21	2:453:B:ARG:HB2	16	0.13
(1,957)	1:50:A:VAL:HG21	2:453:B:ARG:HB3	16	0.13
(1,957)	1:50:A:VAL:HG22	2:453:B:ARG:HB2	16	0.13
(1,957)	1:50:A:VAL:HG22	2:453:B:ARG:HB3	16	0.13
(1,957)	1:50:A:VAL:HG23	2:453:B:ARG:HB2	16	0.13
(1,957)	1:50:A:VAL:HG23	2:453:B:ARG:HB3	16	0.13
(1,957)	1:50:A:VAL:HG11	2:453:B:ARG:HB2	23	0.13
(1,957)	1:50:A:VAL:HG11	2:453:B:ARG:HB3	23	0.13
(1,957)	1:50:A:VAL:HG12	2:453:B:ARG:HB2	23	0.13
(1,957)	1:50:A:VAL:HG12	2:453:B:ARG:HB3	23	0.13
(1,957)	1:50:A:VAL:HG13	2:453:B:ARG:HB2	23	0.13
(1,957)	1:50:A:VAL:HG13	2:453:B:ARG:HB3	23	0.13
(1,957)	1:50:A:VAL:HG21	2:453:B:ARG:HB2	23	0.13
(1,957)	1:50:A:VAL:HG21	2:453:B:ARG:HB3	23	0.13
(1,957)	1:50:A:VAL:HG22	2:453:B:ARG:HB2	23	0.13
(1,957)	1:50:A:VAL:HG22	2:453:B:ARG:HB3	23	0.13
(1,957)	1:50:A:VAL:HG23	2:453:B:ARG:HB2	23	0.13
(1,957)	1:50:A:VAL:HG23	2:453:B:ARG:HB3	23	0.13
(1,944)	2:458:B:PRO:HA	2:460:B:SER:HB2	10	0.13
(1,944)	2:458:B:PRO:HA	2:460:B:SER:HB3	10	0.13
(1,944)	2:458:B:PRO:HA	2:460:B:SER:HB2	19	0.13
(1,944)	2:458:B:PRO:HA	2:460:B:SER:HB3	19	0.13
(1,912)	1:141:A:VAL:HG11	1:107:A:TYR:HB3	4	0.13
(1,912)	1:141:A:VAL:HG12	1:107:A:TYR:HB3	4	0.13
(1,912)	1:141:A:VAL:HG13	1:107:A:TYR:HB3	4	0.13
(1,912)	1:141:A:VAL:HG21	1:107:A:TYR:HB3	4	0.13
(1,912)	1:141:A:VAL:HG22	1:107:A:TYR:HB3	4	0.13
(1,912)	1:141:A:VAL:HG23	1:107:A:TYR:HB3	4	0.13
(1,912)	1:141:A:VAL:HG11	1:107:A:TYR:HB2	4	0.13
(1,912)	1:141:A:VAL:HG12	1:107:A:TYR:HB2	4	0.13
(1,912)	1:141:A:VAL:HG13	1:107:A:TYR:HB2	4	0.13
(1,912)	1:141:A:VAL:HG21	1:107:A:TYR:HB2	4	0.13
(1,912)	1:141:A:VAL:HG22	1:107:A:TYR:HB2	4	0.13
(1,912)	1:141:A:VAL:HG23	1:107:A:TYR:HB2	4	0.13
(1,912)	1:141:A:VAL:HG11	1:107:A:TYR:HB3	8	0.13
(1,912)	1:141:A:VAL:HG12	1:107:A:TYR:HB3	8	0.13
(1,912)	1:141:A:VAL:HG13	1:107:A:TYR:HB3	8	0.13
(1,912)	1:141:A:VAL:HG21	1:107:A:TYR:HB3	8	0.13
(1,912)	1:141:A:VAL:HG22	1:107:A:TYR:HB3	8	0.13
(1,912)	1:141:A:VAL:HG23	1:107:A:TYR:HB3	8	0.13
(1,912)	1:141:A:VAL:HG11	1:107:A:TYR:HB2	8	0.13
(1,912)	1:141:A:VAL:HG12	1:107:A:TYR:HB2	8	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,912)	1:141:A:VAL:HG13	1:107:A:TYR:HB2	8	0.13
(1,912)	1:141:A:VAL:HG21	1:107:A:TYR:HB2	8	0.13
(1,912)	1:141:A:VAL:HG22	1:107:A:TYR:HB2	8	0.13
(1,912)	1:141:A:VAL:HG23	1:107:A:TYR:HB2	8	0.13
(1,912)	1:141:A:VAL:HG11	1:107:A:TYR:HB3	22	0.13
(1,912)	1:141:A:VAL:HG12	1:107:A:TYR:HB3	22	0.13
(1,912)	1:141:A:VAL:HG13	1:107:A:TYR:HB3	22	0.13
(1,912)	1:141:A:VAL:HG21	1:107:A:TYR:HB3	22	0.13
(1,912)	1:141:A:VAL:HG22	1:107:A:TYR:HB3	22	0.13
(1,912)	1:141:A:VAL:HG23	1:107:A:TYR:HB3	22	0.13
(1,912)	1:141:A:VAL:HG11	1:107:A:TYR:HB2	22	0.13
(1,912)	1:141:A:VAL:HG12	1:107:A:TYR:HB2	22	0.13
(1,912)	1:141:A:VAL:HG13	1:107:A:TYR:HB2	22	0.13
(1,912)	1:141:A:VAL:HG21	1:107:A:TYR:HB2	22	0.13
(1,912)	1:141:A:VAL:HG22	1:107:A:TYR:HB2	22	0.13
(1,912)	1:141:A:VAL:HG23	1:107:A:TYR:HB2	22	0.13
(1,911)	1:141:A:VAL:HA	1:107:A:TYR:HB2	15	0.13
(1,911)	1:141:A:VAL:HA	1:107:A:TYR:HB3	15	0.13
(1,911)	1:141:A:VAL:HA	1:107:A:TYR:HB2	17	0.13
(1,911)	1:141:A:VAL:HA	1:107:A:TYR:HB3	17	0.13
(1,880)	1:129:A:ALA:HB1	1:50:A:VAL:HB	4	0.13
(1,880)	1:129:A:ALA:HB2	1:50:A:VAL:HB	4	0.13
(1,880)	1:129:A:ALA:HB3	1:50:A:VAL:HB	4	0.13
(1,880)	1:129:A:ALA:HB1	1:50:A:VAL:HB	6	0.13
(1,880)	1:129:A:ALA:HB2	1:50:A:VAL:HB	6	0.13
(1,880)	1:129:A:ALA:HB3	1:50:A:VAL:HB	6	0.13
(1,880)	1:129:A:ALA:HB1	1:50:A:VAL:HB	23	0.13
(1,880)	1:129:A:ALA:HB2	1:50:A:VAL:HB	23	0.13
(1,880)	1:129:A:ALA:HB3	1:50:A:VAL:HB	23	0.13
(1,878)	1:128:A:PHE:HB2	1:113:A:PHE:HB2	15	0.13
(1,878)	1:128:A:PHE:HB2	1:113:A:PHE:HB3	15	0.13
(1,878)	1:128:A:PHE:HB3	1:113:A:PHE:HB2	15	0.13
(1,878)	1:128:A:PHE:HB3	1:113:A:PHE:HB3	15	0.13
(1,877)	1:127:A:ASN:HB2	1:113:A:PHE:HB2	19	0.13
(1,877)	1:127:A:ASN:HB2	1:113:A:PHE:HB3	19	0.13
(1,877)	1:127:A:ASN:HB3	1:113:A:PHE:HB2	19	0.13
(1,877)	1:127:A:ASN:HB3	1:113:A:PHE:HB3	19	0.13
(1,875)	1:126:A:LEU:HG	1:114:A:PHE:HD1	6	0.13
(1,875)	1:126:A:LEU:HG	1:114:A:PHE:HD2	6	0.13
(1,875)	1:126:A:LEU:HG	1:114:A:PHE:HD1	18	0.13
(1,875)	1:126:A:LEU:HG	1:114:A:PHE:HD2	18	0.13
(1,869)	1:124:A:ALA:HB1	1:117:A:PHE:HD1	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,869)	1:124:A:ALA:HB1	1:117:A:PHE:HD2	7	0.13
(1,869)	1:124:A:ALA:HB2	1:117:A:PHE:HD1	7	0.13
(1,869)	1:124:A:ALA:HB2	1:117:A:PHE:HD2	7	0.13
(1,869)	1:124:A:ALA:HB3	1:117:A:PHE:HD1	7	0.13
(1,869)	1:124:A:ALA:HB3	1:117:A:PHE:HD2	7	0.13
(1,869)	1:124:A:ALA:HB1	1:117:A:PHE:HD1	23	0.13
(1,869)	1:124:A:ALA:HB1	1:117:A:PHE:HD2	23	0.13
(1,869)	1:124:A:ALA:HB2	1:117:A:PHE:HD1	23	0.13
(1,869)	1:124:A:ALA:HB2	1:117:A:PHE:HD2	23	0.13
(1,869)	1:124:A:ALA:HB3	1:117:A:PHE:HD1	23	0.13
(1,869)	1:124:A:ALA:HB3	1:117:A:PHE:HD2	23	0.13
(1,865)	1:123:A:GLN:HG2	1:122:A:CYS:HB2	18	0.13
(1,865)	1:123:A:GLN:HG2	1:122:A:CYS:HB3	18	0.13
(1,865)	1:123:A:GLN:HG3	1:122:A:CYS:HB2	18	0.13
(1,865)	1:123:A:GLN:HG3	1:122:A:CYS:HB3	18	0.13
(1,864)	1:122:A:CYS:HA	1:123:A:GLN:HB2	12	0.13
(1,864)	1:122:A:CYS:HA	1:123:A:GLN:HB3	12	0.13
(1,863)	1:120:A:ASP:HA	1:123:A:GLN:HG2	13	0.13
(1,863)	1:120:A:ASP:HA	1:123:A:GLN:HG3	13	0.13
(1,863)	1:120:A:ASP:HA	1:123:A:GLN:HG2	17	0.13
(1,863)	1:120:A:ASP:HA	1:123:A:GLN:HG3	17	0.13
(1,847)	1:109:A:THR:HB	1:115:A:HIS:HB2	15	0.13
(1,847)	1:109:A:THR:HB	1:115:A:HIS:HB3	15	0.13
(1,846)	1:108:A:SER:HB2	1:137:A:PHE:HB2	11	0.13
(1,846)	1:108:A:SER:HB2	1:137:A:PHE:HB3	11	0.13
(1,846)	1:108:A:SER:HB3	1:137:A:PHE:HB2	11	0.13
(1,846)	1:108:A:SER:HB3	1:137:A:PHE:HB3	11	0.13
(1,846)	1:108:A:SER:HB2	1:137:A:PHE:HB2	23	0.13
(1,846)	1:108:A:SER:HB2	1:137:A:PHE:HB3	23	0.13
(1,846)	1:108:A:SER:HB3	1:137:A:PHE:HB2	23	0.13
(1,846)	1:108:A:SER:HB3	1:137:A:PHE:HB3	23	0.13
(1,797)	1:85:A:ILE:HA	1:74:A:PHE:HD1	15	0.13
(1,797)	1:85:A:ILE:HA	1:74:A:PHE:HD2	15	0.13
(1,786)	1:83:A:TYR:HA	1:85:A:ILE:HD11	5	0.13
(1,786)	1:83:A:TYR:HA	1:85:A:ILE:HD12	5	0.13
(1,786)	1:83:A:TYR:HA	1:85:A:ILE:HD13	5	0.13
(1,783)	1:81:A:LYS:HG2	1:80:A:GLN:HA	15	0.13
(1,783)	1:81:A:LYS:HG3	1:80:A:GLN:HA	15	0.13
(1,783)	1:81:A:LYS:HG2	1:80:A:GLN:HA	20	0.13
(1,783)	1:81:A:LYS:HG3	1:80:A:GLN:HA	20	0.13
(1,783)	1:81:A:LYS:HG2	1:80:A:GLN:HA	22	0.13
(1,783)	1:81:A:LYS:HG3	1:80:A:GLN:HA	22	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,776)	1:75:A:VAL:HG11	1:73:A:CYS:HB2	13	0.13
(1,776)	1:75:A:VAL:HG11	1:73:A:CYS:HB3	13	0.13
(1,776)	1:75:A:VAL:HG12	1:73:A:CYS:HB2	13	0.13
(1,776)	1:75:A:VAL:HG12	1:73:A:CYS:HB3	13	0.13
(1,776)	1:75:A:VAL:HG13	1:73:A:CYS:HB2	13	0.13
(1,776)	1:75:A:VAL:HG13	1:73:A:CYS:HB3	13	0.13
(1,776)	1:75:A:VAL:HG11	1:73:A:CYS:HB2	18	0.13
(1,776)	1:75:A:VAL:HG11	1:73:A:CYS:HB3	18	0.13
(1,776)	1:75:A:VAL:HG12	1:73:A:CYS:HB2	18	0.13
(1,776)	1:75:A:VAL:HG12	1:73:A:CYS:HB3	18	0.13
(1,776)	1:75:A:VAL:HG13	1:73:A:CYS:HB2	18	0.13
(1,776)	1:75:A:VAL:HG13	1:73:A:CYS:HB3	18	0.13
(1,759)	1:72:A:VAL:HG11	1:85:A:ILE:HB	5	0.13
(1,759)	1:72:A:VAL:HG12	1:85:A:ILE:HB	5	0.13
(1,759)	1:72:A:VAL:HG13	1:85:A:ILE:HB	5	0.13
(1,759)	1:72:A:VAL:HG21	1:85:A:ILE:HB	5	0.13
(1,759)	1:72:A:VAL:HG22	1:85:A:ILE:HB	5	0.13
(1,759)	1:72:A:VAL:HG23	1:85:A:ILE:HB	5	0.13
(1,755)	1:72:A:VAL:HG11	1:53:A:LEU:HG	4	0.13
(1,755)	1:72:A:VAL:HG12	1:53:A:LEU:HG	4	0.13
(1,755)	1:72:A:VAL:HG13	1:53:A:LEU:HG	4	0.13
(1,755)	1:72:A:VAL:HG21	1:53:A:LEU:HG	4	0.13
(1,755)	1:72:A:VAL:HG22	1:53:A:LEU:HG	4	0.13
(1,755)	1:72:A:VAL:HG23	1:53:A:LEU:HG	4	0.13
(1,741)	1:71:A:ALA:HB1	1:35:A:LEU:HB2	19	0.13
(1,741)	1:71:A:ALA:HB1	1:35:A:LEU:HB3	19	0.13
(1,741)	1:71:A:ALA:HB2	1:35:A:LEU:HB2	19	0.13
(1,741)	1:71:A:ALA:HB2	1:35:A:LEU:HB3	19	0.13
(1,741)	1:71:A:ALA:HB3	1:35:A:LEU:HB2	19	0.13
(1,741)	1:71:A:ALA:HB3	1:35:A:LEU:HB3	19	0.13
(1,738)	1:69:A:CYS:HG	1:52:A:GLN:HA	10	0.13
(1,715)	1:55:A:LEU:HA	1:64:A:TRP:HZ3	5	0.13
(1,714)	1:55:A:LEU:HB2	1:126:A:LEU:HG	5	0.13
(1,714)	1:55:A:LEU:HB3	1:126:A:LEU:HG	5	0.13
(1,691)	1:53:A:LEU:HG	1:126:A:LEU:HA	24	0.13
(1,683)	1:50:A:VAL:HA	1:71:A:ALA:HA	18	0.13
(1,669)	1:47:A:ALA:HB1	1:137:A:PHE:HA	6	0.13
(1,669)	1:47:A:ALA:HB2	1:137:A:PHE:HA	6	0.13
(1,669)	1:47:A:ALA:HB3	1:137:A:PHE:HA	6	0.13
(1,669)	1:47:A:ALA:HB1	1:137:A:PHE:HA	7	0.13
(1,669)	1:47:A:ALA:HB2	1:137:A:PHE:HA	7	0.13
(1,669)	1:47:A:ALA:HB3	1:137:A:PHE:HA	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,669)	1:47:A:ALA:HB1	1:137:A:PHE:HA	8	0.13
(1,669)	1:47:A:ALA:HB2	1:137:A:PHE:HA	8	0.13
(1,669)	1:47:A:ALA:HB3	1:137:A:PHE:HA	8	0.13
(1,669)	1:47:A:ALA:HB1	1:137:A:PHE:HA	12	0.13
(1,669)	1:47:A:ALA:HB2	1:137:A:PHE:HA	12	0.13
(1,669)	1:47:A:ALA:HB3	1:137:A:PHE:HA	12	0.13
(1,669)	1:47:A:ALA:HB1	1:137:A:PHE:HA	23	0.13
(1,669)	1:47:A:ALA:HB2	1:137:A:PHE:HA	23	0.13
(1,669)	1:47:A:ALA:HB3	1:137:A:PHE:HA	23	0.13
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG11	7	0.13
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG12	7	0.13
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG13	7	0.13
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG21	7	0.13
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG22	7	0.13
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG23	7	0.13
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG11	7	0.13
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG12	7	0.13
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG13	7	0.13
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG21	7	0.13
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG22	7	0.13
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG23	7	0.13
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG11	7	0.13
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG12	7	0.13
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG13	7	0.13
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG21	7	0.13
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG22	7	0.13
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG23	7	0.13
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG11	8	0.13
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG12	8	0.13
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG13	8	0.13
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG21	8	0.13
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG22	8	0.13
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG23	8	0.13
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG11	8	0.13
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG12	8	0.13
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG13	8	0.13
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG21	8	0.13
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG22	8	0.13
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG23	8	0.13
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG11	8	0.13
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG12	8	0.13
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG13	8	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG21	8	0.13
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG22	8	0.13
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG23	8	0.13
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG11	13	0.13
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG12	13	0.13
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG13	13	0.13
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG21	13	0.13
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG22	13	0.13
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG23	13	0.13
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG11	13	0.13
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG12	13	0.13
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG13	13	0.13
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG21	13	0.13
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG22	13	0.13
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG23	13	0.13
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG11	13	0.13
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG12	13	0.13
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG13	13	0.13
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG21	13	0.13
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG22	13	0.13
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG23	13	0.13
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD11	1	0.13
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD12	1	0.13
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD13	1	0.13
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD21	1	0.13
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD22	1	0.13
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD23	1	0.13
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD11	1	0.13
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD12	1	0.13
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD13	1	0.13
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD21	1	0.13
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD22	1	0.13
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD23	1	0.13
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD11	16	0.13
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD12	16	0.13
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD13	16	0.13
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD21	16	0.13
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD22	16	0.13
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD23	16	0.13
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD11	16	0.13
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD12	16	0.13
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD13	16	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD21	16	0.13
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD22	16	0.13
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD23	16	0.13
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD11	17	0.13
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD12	17	0.13
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD13	17	0.13
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD21	17	0.13
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD22	17	0.13
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD23	17	0.13
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD11	17	0.13
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD12	17	0.13
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD13	17	0.13
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD21	17	0.13
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD22	17	0.13
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD23	17	0.13
(1,642)	1:36:A:PHE:HB2	1:34:A:ARG:HG2	7	0.13
(1,642)	1:36:A:PHE:HB2	1:34:A:ARG:HG3	7	0.13
(1,642)	1:36:A:PHE:HB3	1:34:A:ARG:HG2	7	0.13
(1,642)	1:36:A:PHE:HB3	1:34:A:ARG:HG3	7	0.13
(1,642)	1:36:A:PHE:HB2	1:34:A:ARG:HG2	11	0.13
(1,642)	1:36:A:PHE:HB2	1:34:A:ARG:HG3	11	0.13
(1,642)	1:36:A:PHE:HB3	1:34:A:ARG:HG2	11	0.13
(1,642)	1:36:A:PHE:HB3	1:34:A:ARG:HG3	11	0.13
(1,639)	1:34:A:ARG:HD2	1:74:A:PHE:HE1	24	0.13
(1,639)	1:34:A:ARG:HD2	1:74:A:PHE:HE2	24	0.13
(1,639)	1:34:A:ARG:HD3	1:74:A:PHE:HE1	24	0.13
(1,639)	1:34:A:ARG:HD3	1:74:A:PHE:HE2	24	0.13
(1,638)	1:34:A:ARG:HB2	1:74:A:PHE:HD1	7	0.13
(1,638)	1:34:A:ARG:HB2	1:74:A:PHE:HD2	7	0.13
(1,638)	1:34:A:ARG:HB3	1:74:A:PHE:HD1	7	0.13
(1,638)	1:34:A:ARG:HB3	1:74:A:PHE:HD2	7	0.13
(1,638)	1:34:A:ARG:HB2	1:74:A:PHE:HD1	8	0.13
(1,638)	1:34:A:ARG:HB2	1:74:A:PHE:HD2	8	0.13
(1,638)	1:34:A:ARG:HB3	1:74:A:PHE:HD1	8	0.13
(1,638)	1:34:A:ARG:HB3	1:74:A:PHE:HD2	8	0.13
(1,556)	2:451:B:GLU:H	2:450:B:TRP:HB2	12	0.13
(1,531)	1:120:A:ASP:H	1:122:A:CYS:H	13	0.13
(1,531)	1:120:A:ASP:H	1:122:A:CYS:H	20	0.13
(1,529)	1:126:A:LEU:H	1:125:A:GLY:H	20	0.13
(1,527)	1:119:A:GLY:H	1:122:A:CYS:H	17	0.13
(1,523)	1:116:A:THR:H	1:108:A:SER:HB2	3	0.13
(1,523)	1:116:A:THR:H	1:108:A:SER:HB3	3	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,523)	1:116:A:THR:H	1:108:A:SER:HB2	9	0.13
(1,523)	1:116:A:THR:H	1:108:A:SER:HB3	9	0.13
(1,523)	1:116:A:THR:H	1:108:A:SER:HB2	14	0.13
(1,523)	1:116:A:THR:H	1:108:A:SER:HB3	14	0.13
(1,512)	1:114:A:PHE:H	1:112:A:PRO:HA	18	0.13
(1,509)	1:114:A:PHE:H	1:110:A:PRO:HD2	7	0.13
(1,509)	1:114:A:PHE:H	1:110:A:PRO:HD3	7	0.13
(1,509)	1:114:A:PHE:H	1:110:A:PRO:HD2	11	0.13
(1,509)	1:114:A:PHE:H	1:110:A:PRO:HD3	11	0.13
(1,509)	1:114:A:PHE:H	1:110:A:PRO:HD2	21	0.13
(1,509)	1:114:A:PHE:H	1:110:A:PRO:HD3	21	0.13
(1,496)	1:101:A:LEU:H	1:100:A:GLU:H	5	0.13
(1,493)	1:97:A:TRP:H	1:95:A:LEU:HA	12	0.13
(1,486)	1:89:A:GLY:H	1:94:A:ARG:HB2	5	0.13
(1,486)	1:89:A:GLY:H	1:94:A:ARG:HB3	5	0.13
(1,486)	1:89:A:GLY:H	1:94:A:ARG:HB2	8	0.13
(1,486)	1:89:A:GLY:H	1:94:A:ARG:HB3	8	0.13
(1,483)	1:87:A:LEU:H	1:97:A:TRP:HZ2	23	0.13
(1,482)	1:87:A:LEU:H	1:72:A:VAL:HB	18	0.13
(1,477)	1:72:A:VAL:H	1:48:A:THR:HA	4	0.13
(1,469)	1:55:A:LEU:H	1:65:A:THR:H	1	0.13
(1,469)	1:55:A:LEU:H	1:65:A:THR:H	3	0.13
(1,469)	1:55:A:LEU:H	1:65:A:THR:H	8	0.13
(1,469)	1:55:A:LEU:H	1:65:A:THR:H	9	0.13
(1,469)	1:55:A:LEU:H	1:65:A:THR:H	13	0.13
(1,469)	1:55:A:LEU:H	1:65:A:THR:H	21	0.13
(1,469)	1:55:A:LEU:H	1:65:A:THR:H	22	0.13
(1,469)	1:55:A:LEU:H	1:65:A:THR:H	23	0.13
(1,466)	1:52:A:GLN:H	1:128:A:PHE:HB2	13	0.13
(1,466)	1:52:A:GLN:H	1:128:A:PHE:HB3	13	0.13
(1,466)	1:52:A:GLN:H	1:128:A:PHE:HB2	16	0.13
(1,466)	1:52:A:GLN:H	1:128:A:PHE:HB3	16	0.13
(1,456)	1:35:A:LEU:H	1:31:A:GLU:HA	5	0.13
(1,456)	1:35:A:LEU:H	1:31:A:GLU:HA	6	0.13
(1,456)	1:35:A:LEU:H	1:31:A:GLU:HA	14	0.13
(1,429)	1:101:A:LEU:H	1:84:A:PHE:HB2	7	0.13
(1,429)	1:101:A:LEU:H	1:84:A:PHE:HB3	7	0.13
(1,429)	1:101:A:LEU:H	1:84:A:PHE:HB2	8	0.13
(1,429)	1:101:A:LEU:H	1:84:A:PHE:HB3	8	0.13
(1,429)	1:101:A:LEU:H	1:84:A:PHE:HB2	16	0.13
(1,429)	1:101:A:LEU:H	1:84:A:PHE:HB3	16	0.13
(1,374)	1:38:A:MET:H	1:35:A:LEU:HG	13	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,370)	1:38:A:MET:H	1:34:A:ARG:HA	9	0.13
(1,370)	1:38:A:MET:H	1:34:A:ARG:HA	13	0.13
(1,369)	1:37:A:GLU:H	1:34:A:ARG:HA	2	0.13
(1,366)	1:35:A:LEU:H	1:32:A:ASN:HA	6	0.13
(1,366)	1:35:A:LEU:H	1:32:A:ASN:HA	15	0.13
(1,364)	1:34:A:ARG:H	1:31:A:GLU:HA	7	0.13
(1,364)	1:34:A:ARG:H	1:31:A:GLU:HA	12	0.13
(1,364)	1:34:A:ARG:H	1:31:A:GLU:HA	18	0.13
(1,342)	1:146:A:GLN:H	1:143:A:GLU:HA	16	0.13
(1,339)	1:146:A:GLN:H	1:145:A:ILE:HA	19	0.13
(1,336)	1:145:A:ILE:H	1:144:A:LYS:HA	3	0.13
(1,336)	1:145:A:ILE:H	1:144:A:LYS:HA	7	0.13
(1,336)	1:145:A:ILE:H	1:144:A:LYS:HA	10	0.13
(1,336)	1:145:A:ILE:H	1:144:A:LYS:HA	18	0.13
(1,278)	1:127:A:ASN:H	1:126:A:LEU:HG	3	0.13
(1,278)	1:127:A:ASN:H	1:126:A:LEU:HG	7	0.13
(1,278)	1:127:A:ASN:H	1:126:A:LEU:HG	21	0.13
(1,278)	1:127:A:ASN:H	1:126:A:LEU:HG	22	0.13
(1,268)	1:122:A:CYS:H	1:121:A:ASP:HA	12	0.13
(1,268)	1:122:A:CYS:H	1:121:A:ASP:HA	19	0.13
(1,259)	1:118:A:ALA:H	1:117:A:PHE:HB3	15	0.13
(1,250)	1:116:A:THR:H	1:115:A:HIS:HB3	1	0.13
(1,250)	1:116:A:THR:H	1:115:A:HIS:HB3	6	0.13
(1,250)	1:116:A:THR:H	1:115:A:HIS:HB3	21	0.13
(1,195)	1:96:A:LEU:H	1:95:A:LEU:H	8	0.13
(1,195)	1:96:A:LEU:H	1:95:A:LEU:H	13	0.13
(1,176)	1:88:A:TYR:H	1:87:A:LEU:HD11	17	0.13
(1,176)	1:88:A:TYR:H	1:87:A:LEU:HD12	17	0.13
(1,176)	1:88:A:TYR:H	1:87:A:LEU:HD13	17	0.13
(1,176)	1:88:A:TYR:H	1:87:A:LEU:HD21	17	0.13
(1,176)	1:88:A:TYR:H	1:87:A:LEU:HD22	17	0.13
(1,176)	1:88:A:TYR:H	1:87:A:LEU:HD23	17	0.13
(1,141)	1:77:A:ASP:H	1:76:A:LYS:HG2	1	0.13
(1,141)	1:77:A:ASP:H	1:76:A:LYS:HG3	1	0.13
(1,105)	1:63:A:HIS:H	1:62:A:GLU:HA	11	0.13
(1,54)	1:43:A:CYS:H	1:42:A:LYS:HB2	1	0.13
(1,54)	1:43:A:CYS:H	1:42:A:LYS:HB3	1	0.13
(1,54)	1:43:A:CYS:H	1:42:A:LYS:HB2	11	0.13
(1,54)	1:43:A:CYS:H	1:42:A:LYS:HB3	11	0.13
(1,41)	1:38:A:MET:H	1:37:A:GLU:HG2	6	0.13
(1,41)	1:38:A:MET:H	1:37:A:GLU:HG3	6	0.13
(1,41)	1:38:A:MET:H	1:37:A:GLU:HG2	11	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,41)	1:38:A:MET:H	1:37:A:GLU:HG3	11	0.13
(4,98)	1:139:A:ALA:N	1:135:A:GLN:O	7	0.12
(4,92)	1:136:A:ALA:N	1:132:A:ASP:O	16	0.12
(4,70)	1:119:A:GLY:N	1:122:A:CYS:O	15	0.12
(4,67)	1:124:A:ALA:H	1:117:A:PHE:O	10	0.12
(4,67)	1:124:A:ALA:H	1:117:A:PHE:O	12	0.12
(4,67)	1:124:A:ALA:H	1:117:A:PHE:O	19	0.12
(4,67)	1:124:A:ALA:H	1:117:A:PHE:O	20	0.12
(4,43)	1:88:A:TYR:H	1:71:A:ALA:O	9	0.12
(4,43)	1:88:A:TYR:H	1:71:A:ALA:O	10	0.12
(4,43)	1:88:A:TYR:H	1:71:A:ALA:O	18	0.12
(4,41)	1:71:A:ALA:H	1:88:A:TYR:O	4	0.12
(4,40)	1:56:A:ALA:N	1:123:A:GLN:O	9	0.12
(4,40)	1:56:A:ALA:N	1:123:A:GLN:O	12	0.12
(4,40)	1:56:A:ALA:N	1:123:A:GLN:O	13	0.12
(4,40)	1:56:A:ALA:N	1:123:A:GLN:O	15	0.12
(4,40)	1:56:A:ALA:N	1:123:A:GLN:O	17	0.12
(4,39)	1:56:A:ALA:H	1:123:A:GLN:O	1	0.12
(4,39)	1:56:A:ALA:H	1:123:A:GLN:O	9	0.12
(4,39)	1:56:A:ALA:H	1:123:A:GLN:O	11	0.12
(4,39)	1:56:A:ALA:H	1:123:A:GLN:O	15	0.12
(4,39)	1:56:A:ALA:H	1:123:A:GLN:O	16	0.12
(4,23)	1:68:A:HIS:H	1:53:A:LEU:O	1	0.12
(4,23)	1:68:A:HIS:H	1:53:A:LEU:O	4	0.12
(4,23)	1:68:A:HIS:H	1:53:A:LEU:O	11	0.12
(4,9)	1:74:A:PHE:H	1:47:A:ALA:O	2	0.12
(4,9)	1:74:A:PHE:H	1:47:A:ALA:O	4	0.12
(4,9)	1:74:A:PHE:H	1:47:A:ALA:O	5	0.12
(4,9)	1:74:A:PHE:H	1:47:A:ALA:O	12	0.12
(4,9)	1:74:A:PHE:H	1:47:A:ALA:O	13	0.12
(4,9)	1:74:A:PHE:H	1:47:A:ALA:O	16	0.12
(4,9)	1:74:A:PHE:H	1:47:A:ALA:O	22	0.12
(4,9)	1:74:A:PHE:H	1:47:A:ALA:O	23	0.12
(1,1016)	2:479:B:LEU:HG	1:83:A:TYR:HD1	12	0.12
(1,1016)	2:479:B:LEU:HG	1:83:A:TYR:HD2	12	0.12
(1,1016)	2:479:B:LEU:HG	1:83:A:TYR:HD1	24	0.12
(1,1016)	2:479:B:LEU:HG	1:83:A:TYR:HD2	24	0.12
(1,1007)	2:474:B:SER:H	1:102:A:TYR:HA	2	0.12
(1,1007)	2:474:B:SER:H	1:102:A:TYR:HA	3	0.12
(1,1007)	2:474:B:SER:H	1:102:A:TYR:HA	12	0.12
(1,988)	1:129:A:ALA:HA	2:454:B:PHE:HZ	7	0.12
(1,977)	1:103:A:SER:HB2	2:476:B:PRO:HD2	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,977)	1:103:A:SER:HB2	2:476:B:PRO:HD3	9	0.12
(1,977)	1:103:A:SER:HB3	2:476:B:PRO:HD2	9	0.12
(1,977)	1:103:A:SER:HB3	2:476:B:PRO:HD3	9	0.12
(1,977)	1:103:A:SER:HB2	2:476:B:PRO:HD2	10	0.12
(1,977)	1:103:A:SER:HB2	2:476:B:PRO:HD3	10	0.12
(1,977)	1:103:A:SER:HB3	2:476:B:PRO:HD2	10	0.12
(1,977)	1:103:A:SER:HB3	2:476:B:PRO:HD3	10	0.12
(1,975)	1:91:A:GLN:HB2	2:445:B:PRO:HD2	5	0.12
(1,975)	1:91:A:GLN:HB2	2:445:B:PRO:HD3	5	0.12
(1,975)	1:91:A:GLN:HB3	2:445:B:PRO:HD2	5	0.12
(1,975)	1:91:A:GLN:HB3	2:445:B:PRO:HD3	5	0.12
(1,975)	1:91:A:GLN:HB2	2:445:B:PRO:HD2	15	0.12
(1,975)	1:91:A:GLN:HB2	2:445:B:PRO:HD3	15	0.12
(1,975)	1:91:A:GLN:HB3	2:445:B:PRO:HD2	15	0.12
(1,975)	1:91:A:GLN:HB3	2:445:B:PRO:HD3	15	0.12
(1,972)	1:71:A:ALA:H	2:450:B:TRP:HZ2	18	0.12
(1,972)	1:71:A:ALA:H	2:450:B:TRP:HZ2	19	0.12
(1,965)	1:56:A:ALA:HB1	2:462:B:LEU:HD11	21	0.12
(1,965)	1:56:A:ALA:HB1	2:462:B:LEU:HD12	21	0.12
(1,965)	1:56:A:ALA:HB1	2:462:B:LEU:HD13	21	0.12
(1,965)	1:56:A:ALA:HB1	2:462:B:LEU:HD21	21	0.12
(1,965)	1:56:A:ALA:HB1	2:462:B:LEU:HD22	21	0.12
(1,965)	1:56:A:ALA:HB1	2:462:B:LEU:HD23	21	0.12
(1,965)	1:56:A:ALA:HB2	2:462:B:LEU:HD11	21	0.12
(1,965)	1:56:A:ALA:HB2	2:462:B:LEU:HD12	21	0.12
(1,965)	1:56:A:ALA:HB2	2:462:B:LEU:HD13	21	0.12
(1,965)	1:56:A:ALA:HB2	2:462:B:LEU:HD21	21	0.12
(1,965)	1:56:A:ALA:HB2	2:462:B:LEU:HD22	21	0.12
(1,965)	1:56:A:ALA:HB2	2:462:B:LEU:HD23	21	0.12
(1,965)	1:56:A:ALA:HB3	2:462:B:LEU:HD11	21	0.12
(1,965)	1:56:A:ALA:HB3	2:462:B:LEU:HD12	21	0.12
(1,965)	1:56:A:ALA:HB3	2:462:B:LEU:HD13	21	0.12
(1,965)	1:56:A:ALA:HB3	2:462:B:LEU:HD21	21	0.12
(1,965)	1:56:A:ALA:HB3	2:462:B:LEU:HD22	21	0.12
(1,965)	1:56:A:ALA:HB3	2:462:B:LEU:HD23	21	0.12
(1,964)	1:51:A:VAL:H	2:454:B:PHE:HD1	12	0.12
(1,964)	1:51:A:VAL:H	2:454:B:PHE:HD2	12	0.12
(1,964)	1:51:A:VAL:H	2:454:B:PHE:HD1	23	0.12
(1,964)	1:51:A:VAL:H	2:454:B:PHE:HD2	23	0.12
(1,958)	1:50:A:VAL:HG11	2:455:B:TYR:HE1	17	0.12
(1,958)	1:50:A:VAL:HG11	2:455:B:TYR:HE2	17	0.12
(1,958)	1:50:A:VAL:HG12	2:455:B:TYR:HE1	17	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,958)	1:50:A:VAL:HG12	2:455:B:TYR:HE2	17	0.12
(1,958)	1:50:A:VAL:HG13	2:455:B:TYR:HE1	17	0.12
(1,958)	1:50:A:VAL:HG13	2:455:B:TYR:HE2	17	0.12
(1,958)	1:50:A:VAL:HG21	2:455:B:TYR:HE1	17	0.12
(1,958)	1:50:A:VAL:HG21	2:455:B:TYR:HE2	17	0.12
(1,958)	1:50:A:VAL:HG22	2:455:B:TYR:HE1	17	0.12
(1,958)	1:50:A:VAL:HG22	2:455:B:TYR:HE2	17	0.12
(1,958)	1:50:A:VAL:HG23	2:455:B:TYR:HE1	17	0.12
(1,958)	1:50:A:VAL:HG23	2:455:B:TYR:HE2	17	0.12
(1,936)	1:147:A:LYS:HB2	1:148:A:ARG:HA	1	0.12
(1,936)	1:147:A:LYS:HB3	1:148:A:ARG:HA	1	0.12
(1,928)	1:145:A:ILE:HD11	1:117:A:PHE:HZ	5	0.12
(1,928)	1:145:A:ILE:HD12	1:117:A:PHE:HZ	5	0.12
(1,928)	1:145:A:ILE:HD13	1:117:A:PHE:HZ	5	0.12
(1,916)	1:141:A:VAL:HB	1:137:A:PHE:HD1	16	0.12
(1,916)	1:141:A:VAL:HB	1:137:A:PHE:HD2	16	0.12
(1,912)	1:141:A:VAL:HG11	1:107:A:TYR:HB3	3	0.12
(1,912)	1:141:A:VAL:HG12	1:107:A:TYR:HB3	3	0.12
(1,912)	1:141:A:VAL:HG13	1:107:A:TYR:HB3	3	0.12
(1,912)	1:141:A:VAL:HG21	1:107:A:TYR:HB3	3	0.12
(1,912)	1:141:A:VAL:HG22	1:107:A:TYR:HB3	3	0.12
(1,912)	1:141:A:VAL:HG23	1:107:A:TYR:HB3	3	0.12
(1,912)	1:141:A:VAL:HG11	1:107:A:TYR:HB2	3	0.12
(1,912)	1:141:A:VAL:HG12	1:107:A:TYR:HB2	3	0.12
(1,912)	1:141:A:VAL:HG13	1:107:A:TYR:HB2	3	0.12
(1,912)	1:141:A:VAL:HG21	1:107:A:TYR:HB2	3	0.12
(1,912)	1:141:A:VAL:HG22	1:107:A:TYR:HB2	3	0.12
(1,912)	1:141:A:VAL:HG23	1:107:A:TYR:HB2	3	0.12
(1,880)	1:129:A:ALA:HB1	1:50:A:VAL:HB	7	0.12
(1,880)	1:129:A:ALA:HB2	1:50:A:VAL:HB	7	0.12
(1,880)	1:129:A:ALA:HB3	1:50:A:VAL:HB	7	0.12
(1,875)	1:126:A:LEU:HG	1:114:A:PHE:HD1	9	0.12
(1,875)	1:126:A:LEU:HG	1:114:A:PHE:HD2	9	0.12
(1,875)	1:126:A:LEU:HG	1:114:A:PHE:HD1	13	0.12
(1,875)	1:126:A:LEU:HG	1:114:A:PHE:HD2	13	0.12
(1,875)	1:126:A:LEU:HG	1:114:A:PHE:HD1	17	0.12
(1,875)	1:126:A:LEU:HG	1:114:A:PHE:HD2	17	0.12
(1,875)	1:126:A:LEU:HG	1:114:A:PHE:HD1	22	0.12
(1,875)	1:126:A:LEU:HG	1:114:A:PHE:HD2	22	0.12
(1,864)	1:122:A:CYS:HA	1:123:A:GLN:HB2	6	0.12
(1,864)	1:122:A:CYS:HA	1:123:A:GLN:HB3	6	0.12
(1,863)	1:120:A:ASP:HA	1:123:A:GLN:HG2	14	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,863)	1:120:A:ASP:HA	1:123:A:GLN:HG3	14	0.12
(1,851)	1:110:A:PRO:HA	1:131:A:GLU:HB2	6	0.12
(1,851)	1:110:A:PRO:HA	1:131:A:GLU:HB3	6	0.12
(1,851)	1:110:A:PRO:HA	1:131:A:GLU:HB2	13	0.12
(1,851)	1:110:A:PRO:HA	1:131:A:GLU:HB3	13	0.12
(1,851)	1:110:A:PRO:HA	1:131:A:GLU:HB2	18	0.12
(1,851)	1:110:A:PRO:HA	1:131:A:GLU:HB3	18	0.12
(1,851)	1:110:A:PRO:HA	1:131:A:GLU:HB2	20	0.12
(1,851)	1:110:A:PRO:HA	1:131:A:GLU:HB3	20	0.12
(1,851)	1:110:A:PRO:HA	1:131:A:GLU:HB2	23	0.12
(1,851)	1:110:A:PRO:HA	1:131:A:GLU:HB3	23	0.12
(1,847)	1:109:A:THR:HB	1:115:A:HIS:HB2	4	0.12
(1,847)	1:109:A:THR:HB	1:115:A:HIS:HB3	4	0.12
(1,847)	1:109:A:THR:HB	1:115:A:HIS:HB2	20	0.12
(1,847)	1:109:A:THR:HB	1:115:A:HIS:HB3	20	0.12
(1,846)	1:108:A:SER:HB2	1:137:A:PHE:HB2	1	0.12
(1,846)	1:108:A:SER:HB2	1:137:A:PHE:HB3	1	0.12
(1,846)	1:108:A:SER:HB3	1:137:A:PHE:HB2	1	0.12
(1,846)	1:108:A:SER:HB3	1:137:A:PHE:HB3	1	0.12
(1,846)	1:108:A:SER:HB2	1:137:A:PHE:HB2	12	0.12
(1,846)	1:108:A:SER:HB2	1:137:A:PHE:HB3	12	0.12
(1,846)	1:108:A:SER:HB3	1:137:A:PHE:HB2	12	0.12
(1,846)	1:108:A:SER:HB3	1:137:A:PHE:HB3	12	0.12
(1,846)	1:108:A:SER:HB2	1:137:A:PHE:HB2	18	0.12
(1,846)	1:108:A:SER:HB2	1:137:A:PHE:HB3	18	0.12
(1,846)	1:108:A:SER:HB3	1:137:A:PHE:HB2	18	0.12
(1,846)	1:108:A:SER:HB3	1:137:A:PHE:HB3	18	0.12
(1,800)	1:87:A:LEU:HD11	1:53:A:LEU:HD11	1	0.12
(1,800)	1:87:A:LEU:HD11	1:53:A:LEU:HD12	1	0.12
(1,800)	1:87:A:LEU:HD11	1:53:A:LEU:HD13	1	0.12
(1,800)	1:87:A:LEU:HD11	1:53:A:LEU:HD21	1	0.12
(1,800)	1:87:A:LEU:HD11	1:53:A:LEU:HD22	1	0.12
(1,800)	1:87:A:LEU:HD11	1:53:A:LEU:HD23	1	0.12
(1,800)	1:87:A:LEU:HD12	1:53:A:LEU:HD11	1	0.12
(1,800)	1:87:A:LEU:HD12	1:53:A:LEU:HD12	1	0.12
(1,800)	1:87:A:LEU:HD12	1:53:A:LEU:HD13	1	0.12
(1,800)	1:87:A:LEU:HD12	1:53:A:LEU:HD21	1	0.12
(1,800)	1:87:A:LEU:HD12	1:53:A:LEU:HD22	1	0.12
(1,800)	1:87:A:LEU:HD12	1:53:A:LEU:HD23	1	0.12
(1,800)	1:87:A:LEU:HD13	1:53:A:LEU:HD11	1	0.12
(1,800)	1:87:A:LEU:HD13	1:53:A:LEU:HD12	1	0.12
(1,800)	1:87:A:LEU:HD13	1:53:A:LEU:HD13	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,800)	1:87:A:LEU:HD13	1:53:A:LEU:HD21	1	0.12
(1,800)	1:87:A:LEU:HD13	1:53:A:LEU:HD22	1	0.12
(1,800)	1:87:A:LEU:HD13	1:53:A:LEU:HD23	1	0.12
(1,800)	1:87:A:LEU:HD21	1:53:A:LEU:HD11	1	0.12
(1,800)	1:87:A:LEU:HD21	1:53:A:LEU:HD12	1	0.12
(1,800)	1:87:A:LEU:HD21	1:53:A:LEU:HD13	1	0.12
(1,800)	1:87:A:LEU:HD21	1:53:A:LEU:HD21	1	0.12
(1,800)	1:87:A:LEU:HD21	1:53:A:LEU:HD22	1	0.12
(1,800)	1:87:A:LEU:HD21	1:53:A:LEU:HD23	1	0.12
(1,800)	1:87:A:LEU:HD22	1:53:A:LEU:HD11	1	0.12
(1,800)	1:87:A:LEU:HD22	1:53:A:LEU:HD12	1	0.12
(1,800)	1:87:A:LEU:HD22	1:53:A:LEU:HD13	1	0.12
(1,800)	1:87:A:LEU:HD22	1:53:A:LEU:HD21	1	0.12
(1,800)	1:87:A:LEU:HD22	1:53:A:LEU:HD22	1	0.12
(1,800)	1:87:A:LEU:HD22	1:53:A:LEU:HD23	1	0.12
(1,800)	1:87:A:LEU:HD23	1:53:A:LEU:HD11	1	0.12
(1,800)	1:87:A:LEU:HD23	1:53:A:LEU:HD12	1	0.12
(1,800)	1:87:A:LEU:HD23	1:53:A:LEU:HD13	1	0.12
(1,800)	1:87:A:LEU:HD23	1:53:A:LEU:HD21	1	0.12
(1,800)	1:87:A:LEU:HD23	1:53:A:LEU:HD22	1	0.12
(1,800)	1:87:A:LEU:HD23	1:53:A:LEU:HD23	1	0.12
(1,797)	1:85:A:ILE:HA	1:74:A:PHE:HD1	1	0.12
(1,797)	1:85:A:ILE:HA	1:74:A:PHE:HD2	1	0.12
(1,797)	1:85:A:ILE:HA	1:74:A:PHE:HD1	23	0.12
(1,797)	1:85:A:ILE:HA	1:74:A:PHE:HD2	23	0.12
(1,786)	1:83:A:TYR:HA	1:85:A:ILE:HD11	3	0.12
(1,786)	1:83:A:TYR:HA	1:85:A:ILE:HD12	3	0.12
(1,786)	1:83:A:TYR:HA	1:85:A:ILE:HD13	3	0.12
(1,786)	1:83:A:TYR:HA	1:85:A:ILE:HD11	13	0.12
(1,786)	1:83:A:TYR:HA	1:85:A:ILE:HD12	13	0.12
(1,786)	1:83:A:TYR:HA	1:85:A:ILE:HD13	13	0.12
(1,786)	1:83:A:TYR:HA	1:85:A:ILE:HD11	18	0.12
(1,786)	1:83:A:TYR:HA	1:85:A:ILE:HD12	18	0.12
(1,786)	1:83:A:TYR:HA	1:85:A:ILE:HD13	18	0.12
(1,783)	1:81:A:LYS:HG2	1:80:A:GLN:HA	5	0.12
(1,783)	1:81:A:LYS:HG3	1:80:A:GLN:HA	5	0.12
(1,776)	1:75:A:VAL:HG11	1:73:A:CYS:HB2	16	0.12
(1,776)	1:75:A:VAL:HG11	1:73:A:CYS:HB3	16	0.12
(1,776)	1:75:A:VAL:HG12	1:73:A:CYS:HB2	16	0.12
(1,776)	1:75:A:VAL:HG12	1:73:A:CYS:HB3	16	0.12
(1,776)	1:75:A:VAL:HG13	1:73:A:CYS:HB2	16	0.12
(1,776)	1:75:A:VAL:HG13	1:73:A:CYS:HB3	16	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,736)	1:66:A:LYS:HA	1:64:A:TRP:HH2	24	0.12
(1,735)	1:65:A:THR:HG23	1:67:A:GLU:HA	4	0.12
(1,732)	1:65:A:THR:HB	1:56:A:ALA:HB1	4	0.12
(1,732)	1:65:A:THR:HB	1:56:A:ALA:HB2	4	0.12
(1,732)	1:65:A:THR:HB	1:56:A:ALA:HB3	4	0.12
(1,729)	1:63:A:HIS:HA	1:59:A:PRO:HB2	13	0.12
(1,729)	1:63:A:HIS:HA	1:59:A:PRO:HB3	13	0.12
(1,729)	1:63:A:HIS:HA	1:59:A:PRO:HB2	14	0.12
(1,729)	1:63:A:HIS:HA	1:59:A:PRO:HB3	14	0.12
(1,729)	1:63:A:HIS:HA	1:59:A:PRO:HB2	18	0.12
(1,729)	1:63:A:HIS:HA	1:59:A:PRO:HB3	18	0.12
(1,729)	1:63:A:HIS:HA	1:59:A:PRO:HB2	20	0.12
(1,729)	1:63:A:HIS:HA	1:59:A:PRO:HB3	20	0.12
(1,714)	1:55:A:LEU:HB2	1:126:A:LEU:HG	10	0.12
(1,714)	1:55:A:LEU:HB3	1:126:A:LEU:HG	10	0.12
(1,714)	1:55:A:LEU:HB2	1:126:A:LEU:HG	16	0.12
(1,714)	1:55:A:LEU:HB3	1:126:A:LEU:HG	16	0.12
(1,714)	1:55:A:LEU:HB2	1:126:A:LEU:HG	22	0.12
(1,714)	1:55:A:LEU:HB3	1:126:A:LEU:HG	22	0.12
(1,713)	1:55:A:LEU:HD11	1:126:A:LEU:HG	6	0.12
(1,713)	1:55:A:LEU:HD12	1:126:A:LEU:HG	6	0.12
(1,713)	1:55:A:LEU:HD13	1:126:A:LEU:HG	6	0.12
(1,713)	1:55:A:LEU:HD21	1:126:A:LEU:HG	6	0.12
(1,713)	1:55:A:LEU:HD22	1:126:A:LEU:HG	6	0.12
(1,713)	1:55:A:LEU:HD23	1:126:A:LEU:HG	6	0.12
(1,688)	1:51:A:VAL:HG11	1:128:A:PHE:HB2	19	0.12
(1,688)	1:51:A:VAL:HG11	1:128:A:PHE:HB3	19	0.12
(1,688)	1:51:A:VAL:HG12	1:128:A:PHE:HB2	19	0.12
(1,688)	1:51:A:VAL:HG12	1:128:A:PHE:HB3	19	0.12
(1,688)	1:51:A:VAL:HG13	1:128:A:PHE:HB2	19	0.12
(1,688)	1:51:A:VAL:HG13	1:128:A:PHE:HB3	19	0.12
(1,688)	1:51:A:VAL:HG21	1:128:A:PHE:HB2	19	0.12
(1,688)	1:51:A:VAL:HG21	1:128:A:PHE:HB3	19	0.12
(1,688)	1:51:A:VAL:HG22	1:128:A:PHE:HB2	19	0.12
(1,688)	1:51:A:VAL:HG22	1:128:A:PHE:HB3	19	0.12
(1,688)	1:51:A:VAL:HG23	1:128:A:PHE:HB2	19	0.12
(1,688)	1:51:A:VAL:HG23	1:128:A:PHE:HB3	19	0.12
(1,669)	1:47:A:ALA:HB1	1:137:A:PHE:HA	16	0.12
(1,669)	1:47:A:ALA:HB2	1:137:A:PHE:HA	16	0.12
(1,669)	1:47:A:ALA:HB3	1:137:A:PHE:HA	16	0.12
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG11	1	0.12
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG12	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG13	1	0.12
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG21	1	0.12
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG22	1	0.12
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG23	1	0.12
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG11	1	0.12
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG12	1	0.12
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG13	1	0.12
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG21	1	0.12
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG22	1	0.12
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG23	1	0.12
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG11	1	0.12
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG12	1	0.12
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG13	1	0.12
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG21	1	0.12
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG22	1	0.12
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG23	1	0.12
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG11	6	0.12
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG12	6	0.12
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG13	6	0.12
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG21	6	0.12
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG22	6	0.12
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG23	6	0.12
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG11	6	0.12
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG12	6	0.12
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG13	6	0.12
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG21	6	0.12
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG22	6	0.12
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG23	6	0.12
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG11	6	0.12
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG12	6	0.12
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG13	6	0.12
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG21	6	0.12
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG22	6	0.12
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG23	6	0.12
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG11	15	0.12
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG12	15	0.12
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG13	15	0.12
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG21	15	0.12
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG22	15	0.12
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG23	15	0.12
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG11	15	0.12
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG12	15	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG13	15	0.12
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG21	15	0.12
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG22	15	0.12
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG23	15	0.12
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG11	15	0.12
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG12	15	0.12
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG13	15	0.12
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG21	15	0.12
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG22	15	0.12
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG23	15	0.12
(1,646)	1:39:A:LEU:HA	1:88:A:TYR:HB2	18	0.12
(1,646)	1:39:A:LEU:HA	1:88:A:TYR:HB3	18	0.12
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD11	10	0.12
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD12	10	0.12
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD13	10	0.12
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD21	10	0.12
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD22	10	0.12
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD23	10	0.12
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD11	10	0.12
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD12	10	0.12
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD13	10	0.12
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD21	10	0.12
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD22	10	0.12
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD23	10	0.12
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD11	14	0.12
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD12	14	0.12
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD13	14	0.12
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD21	14	0.12
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD22	14	0.12
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD23	14	0.12
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD11	14	0.12
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD12	14	0.12
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD13	14	0.12
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD21	14	0.12
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD22	14	0.12
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD23	14	0.12
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD11	23	0.12
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD12	23	0.12
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD13	23	0.12
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD21	23	0.12
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD22	23	0.12
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD23	23	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD11	23	0.12
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD12	23	0.12
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD13	23	0.12
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD21	23	0.12
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD22	23	0.12
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD23	23	0.12
(1,642)	1:36:A:PHE:HB2	1:34:A:ARG:HG2	22	0.12
(1,642)	1:36:A:PHE:HB2	1:34:A:ARG:HG3	22	0.12
(1,642)	1:36:A:PHE:HB3	1:34:A:ARG:HG2	22	0.12
(1,642)	1:36:A:PHE:HB3	1:34:A:ARG:HG3	22	0.12
(1,640)	1:35:A:LEU:HD11	1:31:A:GLU:HA	14	0.12
(1,640)	1:35:A:LEU:HD12	1:31:A:GLU:HA	14	0.12
(1,640)	1:35:A:LEU:HD13	1:31:A:GLU:HA	14	0.12
(1,640)	1:35:A:LEU:HD21	1:31:A:GLU:HA	14	0.12
(1,640)	1:35:A:LEU:HD22	1:31:A:GLU:HA	14	0.12
(1,640)	1:35:A:LEU:HD23	1:31:A:GLU:HA	14	0.12
(1,640)	1:35:A:LEU:HD11	1:31:A:GLU:HA	23	0.12
(1,640)	1:35:A:LEU:HD12	1:31:A:GLU:HA	23	0.12
(1,640)	1:35:A:LEU:HD13	1:31:A:GLU:HA	23	0.12
(1,640)	1:35:A:LEU:HD21	1:31:A:GLU:HA	23	0.12
(1,640)	1:35:A:LEU:HD22	1:31:A:GLU:HA	23	0.12
(1,640)	1:35:A:LEU:HD23	1:31:A:GLU:HA	23	0.12
(1,639)	1:34:A:ARG:HD2	1:74:A:PHE:HE1	13	0.12
(1,639)	1:34:A:ARG:HD2	1:74:A:PHE:HE2	13	0.12
(1,639)	1:34:A:ARG:HD3	1:74:A:PHE:HE1	13	0.12
(1,639)	1:34:A:ARG:HD3	1:74:A:PHE:HE2	13	0.12
(1,636)	1:33:A:GLN:HG2	1:37:A:GLU:HB2	2	0.12
(1,636)	1:33:A:GLN:HG2	1:37:A:GLU:HB3	2	0.12
(1,636)	1:33:A:GLN:HG3	1:37:A:GLU:HB2	2	0.12
(1,636)	1:33:A:GLN:HG3	1:37:A:GLU:HB3	2	0.12
(1,598)	2:473:B:LYS:H	2:472:B:THR:HG22	1	0.12
(1,598)	2:473:B:LYS:H	2:472:B:THR:HG22	4	0.12
(1,598)	2:473:B:LYS:H	2:472:B:THR:HG22	12	0.12
(1,586)	2:469:B:VAL:H	2:468:B:TYR:HB3	7	0.12
(1,578)	2:461:B:ASP:H	2:460:B:SER:H	10	0.12
(1,571)	2:459:B:ILE:H	2:458:B:PRO:HB2	9	0.12
(1,567)	2:457:B:HIS:H	2:456:B:PHE:HB3	2	0.12
(1,567)	2:457:B:HIS:H	2:456:B:PHE:HB3	8	0.12
(1,567)	2:457:B:HIS:H	2:456:B:PHE:HB3	9	0.12
(1,567)	2:457:B:HIS:H	2:456:B:PHE:HB3	18	0.12
(1,567)	2:457:B:HIS:H	2:456:B:PHE:HB3	19	0.12
(1,545)	2:447:B:GLU:H	2:446:B:CYS:H	2	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,545)	2:447:B:GLU:H	2:446:B:CYS:H	4	0.12
(1,545)	2:447:B:GLU:H	2:446:B:CYS:H	24	0.12
(1,542)	2:446:B:CYS:H	2:445:B:PRO:HA	23	0.12
(1,542)	2:446:B:CYS:H	2:445:B:PRO:HA	24	0.12
(1,531)	1:120:A:ASP:H	1:122:A:CYS:H	9	0.12
(1,531)	1:120:A:ASP:H	1:122:A:CYS:H	22	0.12
(1,523)	1:116:A:THR:H	1:108:A:SER:HB2	22	0.12
(1,523)	1:116:A:THR:H	1:108:A:SER:HB3	22	0.12
(1,509)	1:114:A:PHE:H	1:110:A:PRO:HD2	14	0.12
(1,509)	1:114:A:PHE:H	1:110:A:PRO:HD3	14	0.12
(1,509)	1:114:A:PHE:H	1:110:A:PRO:HD2	20	0.12
(1,509)	1:114:A:PHE:H	1:110:A:PRO:HD3	20	0.12
(1,509)	1:114:A:PHE:H	1:110:A:PRO:HD2	22	0.12
(1,509)	1:114:A:PHE:H	1:110:A:PRO:HD3	22	0.12
(1,502)	1:104:A:GLN:H	1:102:A:TYR:HA	4	0.12
(1,500)	1:103:A:SER:H	1:102:A:TYR:HE1	1	0.12
(1,500)	1:103:A:SER:H	1:102:A:TYR:HE2	1	0.12
(1,496)	1:101:A:LEU:H	1:100:A:GLU:H	6	0.12
(1,493)	1:97:A:TRP:H	1:95:A:LEU:HA	3	0.12
(1,493)	1:97:A:TRP:H	1:95:A:LEU:HA	4	0.12
(1,493)	1:97:A:TRP:H	1:95:A:LEU:HA	6	0.12
(1,487)	1:89:A:GLY:H	1:94:A:ARG:H	11	0.12
(1,487)	1:89:A:GLY:H	1:94:A:ARG:H	15	0.12
(1,486)	1:89:A:GLY:H	1:94:A:ARG:HB2	3	0.12
(1,486)	1:89:A:GLY:H	1:94:A:ARG:HB3	3	0.12
(1,486)	1:89:A:GLY:H	1:94:A:ARG:HB2	10	0.12
(1,486)	1:89:A:GLY:H	1:94:A:ARG:HB3	10	0.12
(1,486)	1:89:A:GLY:H	1:94:A:ARG:HB2	19	0.12
(1,486)	1:89:A:GLY:H	1:94:A:ARG:HB3	19	0.12
(1,483)	1:87:A:LEU:H	1:97:A:TRP:HZ3	12	0.12
(1,483)	1:87:A:LEU:H	1:97:A:TRP:HZ2	16	0.12
(1,482)	1:87:A:LEU:H	1:72:A:VAL:HB	19	0.12
(1,477)	1:72:A:VAL:H	1:48:A:THR:HA	1	0.12
(1,477)	1:72:A:VAL:H	1:48:A:THR:HA	5	0.12
(1,477)	1:72:A:VAL:H	1:48:A:THR:HA	10	0.12
(1,477)	1:72:A:VAL:H	1:48:A:THR:HA	15	0.12
(1,469)	1:55:A:LEU:H	1:65:A:THR:H	6	0.12
(1,469)	1:55:A:LEU:H	1:65:A:THR:H	10	0.12
(1,469)	1:55:A:LEU:H	1:65:A:THR:H	14	0.12
(1,469)	1:55:A:LEU:H	1:65:A:THR:H	15	0.12
(1,466)	1:52:A:GLN:H	1:128:A:PHE:HB2	7	0.12
(1,466)	1:52:A:GLN:H	1:128:A:PHE:HB3	7	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,456)	1:35:A:LEU:H	1:31:A:GLU:HA	4	0.12
(1,456)	1:35:A:LEU:H	1:31:A:GLU:HA	18	0.12
(1,440)	1:127:A:ASN:H	1:53:A:LEU:HA	24	0.12
(1,429)	1:101:A:LEU:H	1:84:A:PHE:HB2	12	0.12
(1,429)	1:101:A:LEU:H	1:84:A:PHE:HB3	12	0.12
(1,429)	1:101:A:LEU:H	1:84:A:PHE:HB2	23	0.12
(1,429)	1:101:A:LEU:H	1:84:A:PHE:HB3	23	0.12
(1,427)	1:101:A:LEU:H	1:83:A:TYR:H	4	0.12
(1,424)	1:97:A:TRP:H	1:87:A:LEU:HB2	22	0.12
(1,424)	1:97:A:TRP:H	1:87:A:LEU:HB3	22	0.12
(1,412)	1:84:A:PHE:H	1:76:A:LYS:HB2	6	0.12
(1,412)	1:84:A:PHE:H	1:76:A:LYS:HB3	6	0.12
(1,410)	1:84:A:PHE:H	1:76:A:LYS:HG2	16	0.12
(1,410)	1:84:A:PHE:H	1:76:A:LYS:HG3	16	0.12
(1,408)	1:84:A:PHE:H	1:75:A:VAL:H	19	0.12
(1,399)	1:72:A:VAL:H	1:50:A:VAL:HB	16	0.12
(1,392)	1:55:A:LEU:H	1:66:A:LYS:HB2	20	0.12
(1,392)	1:55:A:LEU:H	1:66:A:LYS:HB3	20	0.12
(1,366)	1:35:A:LEU:H	1:32:A:ASN:HA	1	0.12
(1,366)	1:35:A:LEU:H	1:32:A:ASN:HA	7	0.12
(1,366)	1:35:A:LEU:H	1:32:A:ASN:HA	10	0.12
(1,364)	1:34:A:ARG:H	1:31:A:GLU:HA	3	0.12
(1,364)	1:34:A:ARG:H	1:31:A:GLU:HA	6	0.12
(1,360)	1:32:A:ASN:H	1:29:A:ASP:HA	1	0.12
(1,346)	1:148:A:ARG:H	1:147:A:LYS:HA	1	0.12
(1,346)	1:148:A:ARG:H	1:147:A:LYS:HA	3	0.12
(1,346)	1:148:A:ARG:H	1:147:A:LYS:HA	15	0.12
(1,346)	1:148:A:ARG:H	1:147:A:LYS:HA	17	0.12
(1,346)	1:148:A:ARG:H	1:147:A:LYS:HA	21	0.12
(1,340)	1:146:A:GLN:H	1:145:A:ILE:HB	1	0.12
(1,340)	1:146:A:GLN:H	1:145:A:ILE:HB	4	0.12
(1,340)	1:146:A:GLN:H	1:145:A:ILE:HB	9	0.12
(1,340)	1:146:A:GLN:H	1:145:A:ILE:HB	22	0.12
(1,339)	1:146:A:GLN:H	1:145:A:ILE:HA	14	0.12
(1,339)	1:146:A:GLN:H	1:145:A:ILE:HA	16	0.12
(1,336)	1:145:A:ILE:H	1:144:A:LYS:HA	1	0.12
(1,336)	1:145:A:ILE:H	1:144:A:LYS:HA	2	0.12
(1,336)	1:145:A:ILE:H	1:144:A:LYS:HA	4	0.12
(1,336)	1:145:A:ILE:H	1:144:A:LYS:HA	5	0.12
(1,336)	1:145:A:ILE:H	1:144:A:LYS:HA	8	0.12
(1,336)	1:145:A:ILE:H	1:144:A:LYS:HA	9	0.12
(1,336)	1:145:A:ILE:H	1:144:A:LYS:HA	11	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,336)	1:145:A:ILE:H	1:144:A:LYS:HA	12	0.12
(1,336)	1:145:A:ILE:H	1:144:A:LYS:HA	13	0.12
(1,336)	1:145:A:ILE:H	1:144:A:LYS:HA	14	0.12
(1,336)	1:145:A:ILE:H	1:144:A:LYS:HA	17	0.12
(1,336)	1:145:A:ILE:H	1:144:A:LYS:HA	20	0.12
(1,336)	1:145:A:ILE:H	1:144:A:LYS:HA	21	0.12
(1,336)	1:145:A:ILE:H	1:144:A:LYS:HA	23	0.12
(1,336)	1:145:A:ILE:H	1:144:A:LYS:HA	24	0.12
(1,278)	1:127:A:ASN:H	1:126:A:LEU:HG	13	0.12
(1,278)	1:127:A:ASN:H	1:126:A:LEU:HG	23	0.12
(1,268)	1:122:A:CYS:H	1:121:A:ASP:HA	5	0.12
(1,265)	1:121:A:ASP:H	1:120:A:ASP:H	14	0.12
(1,265)	1:121:A:ASP:H	1:120:A:ASP:H	23	0.12
(1,259)	1:118:A:ALA:H	1:117:A:PHE:HB3	9	0.12
(1,255)	1:117:A:PHE:H	1:116:A:THR:HB	16	0.12
(1,245)	1:114:A:PHE:H	1:113:A:PHE:H	1	0.12
(1,245)	1:114:A:PHE:H	1:113:A:PHE:H	9	0.12
(1,195)	1:96:A:LEU:H	1:95:A:LEU:H	3	0.12
(1,195)	1:96:A:LEU:H	1:95:A:LEU:H	10	0.12
(1,195)	1:96:A:LEU:H	1:95:A:LEU:H	17	0.12
(1,153)	1:82:A:SER:H	1:81:A:LYS:HE2	8	0.12
(1,153)	1:82:A:SER:H	1:81:A:LYS:HE3	8	0.12
(1,153)	1:82:A:SER:H	1:81:A:LYS:HE2	15	0.12
(1,153)	1:82:A:SER:H	1:81:A:LYS:HE3	15	0.12
(1,153)	1:82:A:SER:H	1:81:A:LYS:HE2	22	0.12
(1,153)	1:82:A:SER:H	1:81:A:LYS:HE3	22	0.12
(1,140)	1:77:A:ASP:H	1:76:A:LYS:HD2	6	0.12
(1,140)	1:77:A:ASP:H	1:76:A:LYS:HD3	6	0.12
(1,112)	1:65:A:THR:H	1:64:A:TRP:HB3	7	0.12
(1,112)	1:65:A:THR:H	1:64:A:TRP:HB3	18	0.12
(1,105)	1:63:A:HIS:H	1:62:A:GLU:HA	16	0.12
(1,54)	1:43:A:CYS:H	1:42:A:LYS:HB2	6	0.12
(1,54)	1:43:A:CYS:H	1:42:A:LYS:HB3	6	0.12
(1,54)	1:43:A:CYS:H	1:42:A:LYS:HB2	7	0.12
(1,54)	1:43:A:CYS:H	1:42:A:LYS:HB3	7	0.12
(1,44)	1:39:A:LEU:H	1:36:A:PHE:HE1	15	0.12
(1,44)	1:39:A:LEU:H	1:36:A:PHE:HE2	15	0.12
(4,122)	2:452:B:SER:N	2:448:B:ASP:O	6	0.11
(4,122)	2:452:B:SER:N	2:448:B:ASP:O	8	0.11
(4,122)	2:452:B:SER:N	2:448:B:ASP:O	10	0.11
(4,122)	2:452:B:SER:N	2:448:B:ASP:O	12	0.11
(4,122)	2:452:B:SER:N	2:448:B:ASP:O	13	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,122)	2:452:B:SER:N	2:448:B:ASP:O	16	0.11
(4,122)	2:452:B:SER:N	2:448:B:ASP:O	17	0.11
(4,122)	2:452:B:SER:N	2:448:B:ASP:O	18	0.11
(4,122)	2:452:B:SER:N	2:448:B:ASP:O	21	0.11
(4,111)	1:146:A:GLN:H	1:142:A:GLN:O	6	0.11
(4,101)	1:141:A:VAL:H	1:137:A:PHE:O	12	0.11
(4,89)	1:135:A:GLN:H	1:131:A:GLU:O	9	0.11
(4,77)	1:34:A:ARG:H	1:30:A:HIS:O	13	0.11
(4,77)	1:34:A:ARG:H	1:30:A:HIS:O	14	0.11
(4,77)	1:34:A:ARG:H	1:30:A:HIS:O	18	0.11
(4,74)	1:32:A:ASN:N	1:28:A:GLN:O	21	0.11
(4,70)	1:119:A:GLY:N	1:122:A:CYS:O	1	0.11
(4,69)	1:119:A:GLY:H	1:122:A:CYS:O	9	0.11
(4,43)	1:88:A:TYR:H	1:71:A:ALA:O	15	0.11
(4,43)	1:88:A:TYR:H	1:71:A:ALA:O	19	0.11
(4,41)	1:71:A:ALA:H	1:88:A:TYR:O	12	0.11
(4,41)	1:71:A:ALA:H	1:88:A:TYR:O	17	0.11
(4,41)	1:71:A:ALA:H	1:88:A:TYR:O	21	0.11
(4,40)	1:56:A:ALA:N	1:123:A:GLN:O	2	0.11
(4,40)	1:56:A:ALA:N	1:123:A:GLN:O	11	0.11
(4,40)	1:56:A:ALA:N	1:123:A:GLN:O	19	0.11
(4,39)	1:56:A:ALA:H	1:123:A:GLN:O	5	0.11
(4,39)	1:56:A:ALA:H	1:123:A:GLN:O	13	0.11
(4,39)	1:56:A:ALA:H	1:123:A:GLN:O	17	0.11
(4,38)	1:125:A:GLY:N	1:54:A:TYR:O	17	0.11
(4,31)	1:52:A:GLN:H	1:127:A:ASN:O	10	0.11
(4,23)	1:68:A:HIS:H	1:53:A:LEU:O	2	0.11
(4,23)	1:68:A:HIS:H	1:53:A:LEU:O	12	0.11
(4,23)	1:68:A:HIS:H	1:53:A:LEU:O	18	0.11
(4,19)	1:53:A:LEU:H	1:68:A:HIS:O	1	0.11
(4,19)	1:53:A:LEU:H	1:68:A:HIS:O	10	0.11
(4,19)	1:53:A:LEU:H	1:68:A:HIS:O	16	0.11
(4,9)	1:74:A:PHE:H	1:47:A:ALA:O	3	0.11
(4,9)	1:74:A:PHE:H	1:47:A:ALA:O	11	0.11
(4,9)	1:74:A:PHE:H	1:47:A:ALA:O	14	0.11
(4,9)	1:74:A:PHE:H	1:47:A:ALA:O	17	0.11
(4,9)	1:74:A:PHE:H	1:47:A:ALA:O	18	0.11
(1,1016)	2:479:B:LEU:HG	1:83:A:TYR:HD1	6	0.11
(1,1016)	2:479:B:LEU:HG	1:83:A:TYR:HD2	6	0.11
(1,1008)	2:474:B:SER:H	1:102:A:TYR:HE1	5	0.11
(1,1008)	2:474:B:SER:H	1:102:A:TYR:HE2	5	0.11
(1,1008)	2:474:B:SER:H	1:102:A:TYR:HE1	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1008)	2:474:B:SER:H	1:102:A:TYR:HE2	7	0.11
(1,1008)	2:474:B:SER:H	1:102:A:TYR:HE1	17	0.11
(1,1008)	2:474:B:SER:H	1:102:A:TYR:HE2	17	0.11
(1,1007)	2:474:B:SER:H	1:102:A:TYR:HA	4	0.11
(1,1007)	2:474:B:SER:H	1:102:A:TYR:HA	5	0.11
(1,1007)	2:474:B:SER:H	1:102:A:TYR:HA	11	0.11
(1,1002)	2:463:B:PRO:HG2	1:114:A:PHE:HD1	13	0.11
(1,1002)	2:463:B:PRO:HG2	1:114:A:PHE:HD2	13	0.11
(1,1002)	2:463:B:PRO:HG3	1:114:A:PHE:HD1	13	0.11
(1,1002)	2:463:B:PRO:HG3	1:114:A:PHE:HD2	13	0.11
(1,988)	1:129:A:ALA:HA	2:454:B:PHE:HZ	12	0.11
(1,988)	1:129:A:ALA:HA	2:454:B:PHE:HZ	15	0.11
(1,988)	1:129:A:ALA:HA	2:454:B:PHE:HZ	18	0.11
(1,975)	1:91:A:GLN:HB2	2:445:B:PRO:HD2	10	0.11
(1,975)	1:91:A:GLN:HB2	2:445:B:PRO:HD3	10	0.11
(1,975)	1:91:A:GLN:HB3	2:445:B:PRO:HD2	10	0.11
(1,975)	1:91:A:GLN:HB3	2:445:B:PRO:HD3	10	0.11
(1,975)	1:91:A:GLN:HB2	2:445:B:PRO:HD2	19	0.11
(1,975)	1:91:A:GLN:HB2	2:445:B:PRO:HD3	19	0.11
(1,975)	1:91:A:GLN:HB3	2:445:B:PRO:HD2	19	0.11
(1,975)	1:91:A:GLN:HB3	2:445:B:PRO:HD3	19	0.11
(1,968)	1:64:A:TRP:HD1	2:464:B:PRO:HG2	6	0.11
(1,968)	1:64:A:TRP:HD1	2:464:B:PRO:HG3	6	0.11
(1,965)	1:56:A:ALA:HB1	2:462:B:LEU:HD11	3	0.11
(1,965)	1:56:A:ALA:HB1	2:462:B:LEU:HD12	3	0.11
(1,965)	1:56:A:ALA:HB1	2:462:B:LEU:HD13	3	0.11
(1,965)	1:56:A:ALA:HB1	2:462:B:LEU:HD21	3	0.11
(1,965)	1:56:A:ALA:HB1	2:462:B:LEU:HD22	3	0.11
(1,965)	1:56:A:ALA:HB1	2:462:B:LEU:HD23	3	0.11
(1,965)	1:56:A:ALA:HB2	2:462:B:LEU:HD11	3	0.11
(1,965)	1:56:A:ALA:HB2	2:462:B:LEU:HD12	3	0.11
(1,965)	1:56:A:ALA:HB2	2:462:B:LEU:HD13	3	0.11
(1,965)	1:56:A:ALA:HB2	2:462:B:LEU:HD21	3	0.11
(1,965)	1:56:A:ALA:HB2	2:462:B:LEU:HD22	3	0.11
(1,965)	1:56:A:ALA:HB2	2:462:B:LEU:HD23	3	0.11
(1,965)	1:56:A:ALA:HB3	2:462:B:LEU:HD11	3	0.11
(1,965)	1:56:A:ALA:HB3	2:462:B:LEU:HD12	3	0.11
(1,965)	1:56:A:ALA:HB3	2:462:B:LEU:HD13	3	0.11
(1,965)	1:56:A:ALA:HB3	2:462:B:LEU:HD21	3	0.11
(1,965)	1:56:A:ALA:HB3	2:462:B:LEU:HD22	3	0.11
(1,965)	1:56:A:ALA:HB3	2:462:B:LEU:HD23	3	0.11
(1,965)	1:56:A:ALA:HB1	2:462:B:LEU:HD11	20	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,965)	1:56:A:ALA:HB1	2:462:B:LEU:HD12	20	0.11
(1,965)	1:56:A:ALA:HB1	2:462:B:LEU:HD13	20	0.11
(1,965)	1:56:A:ALA:HB1	2:462:B:LEU:HD21	20	0.11
(1,965)	1:56:A:ALA:HB1	2:462:B:LEU:HD22	20	0.11
(1,965)	1:56:A:ALA:HB1	2:462:B:LEU:HD23	20	0.11
(1,965)	1:56:A:ALA:HB2	2:462:B:LEU:HD11	20	0.11
(1,965)	1:56:A:ALA:HB2	2:462:B:LEU:HD12	20	0.11
(1,965)	1:56:A:ALA:HB2	2:462:B:LEU:HD13	20	0.11
(1,965)	1:56:A:ALA:HB2	2:462:B:LEU:HD21	20	0.11
(1,965)	1:56:A:ALA:HB2	2:462:B:LEU:HD22	20	0.11
(1,965)	1:56:A:ALA:HB2	2:462:B:LEU:HD23	20	0.11
(1,965)	1:56:A:ALA:HB3	2:462:B:LEU:HD11	20	0.11
(1,965)	1:56:A:ALA:HB3	2:462:B:LEU:HD12	20	0.11
(1,965)	1:56:A:ALA:HB3	2:462:B:LEU:HD13	20	0.11
(1,965)	1:56:A:ALA:HB3	2:462:B:LEU:HD21	20	0.11
(1,965)	1:56:A:ALA:HB3	2:462:B:LEU:HD22	20	0.11
(1,965)	1:56:A:ALA:HB3	2:462:B:LEU:HD23	20	0.11
(1,965)	1:56:A:ALA:HB1	2:462:B:LEU:HD11	23	0.11
(1,965)	1:56:A:ALA:HB1	2:462:B:LEU:HD12	23	0.11
(1,965)	1:56:A:ALA:HB1	2:462:B:LEU:HD13	23	0.11
(1,965)	1:56:A:ALA:HB1	2:462:B:LEU:HD21	23	0.11
(1,965)	1:56:A:ALA:HB1	2:462:B:LEU:HD22	23	0.11
(1,965)	1:56:A:ALA:HB1	2:462:B:LEU:HD23	23	0.11
(1,965)	1:56:A:ALA:HB2	2:462:B:LEU:HD11	23	0.11
(1,965)	1:56:A:ALA:HB2	2:462:B:LEU:HD12	23	0.11
(1,965)	1:56:A:ALA:HB2	2:462:B:LEU:HD13	23	0.11
(1,965)	1:56:A:ALA:HB2	2:462:B:LEU:HD21	23	0.11
(1,965)	1:56:A:ALA:HB2	2:462:B:LEU:HD22	23	0.11
(1,965)	1:56:A:ALA:HB2	2:462:B:LEU:HD23	23	0.11
(1,965)	1:56:A:ALA:HB3	2:462:B:LEU:HD11	23	0.11
(1,965)	1:56:A:ALA:HB3	2:462:B:LEU:HD12	23	0.11
(1,965)	1:56:A:ALA:HB3	2:462:B:LEU:HD13	23	0.11
(1,965)	1:56:A:ALA:HB3	2:462:B:LEU:HD21	23	0.11
(1,965)	1:56:A:ALA:HB3	2:462:B:LEU:HD22	23	0.11
(1,965)	1:56:A:ALA:HB3	2:462:B:LEU:HD23	23	0.11
(1,964)	1:51:A:VAL:H	2:454:B:PHE:HD1	16	0.11
(1,964)	1:51:A:VAL:H	2:454:B:PHE:HD2	16	0.11
(1,963)	1:50:A:VAL:HG11	2:456:B:PHE:HD1	5	0.11
(1,963)	1:50:A:VAL:HG11	2:456:B:PHE:HD2	5	0.11
(1,963)	1:50:A:VAL:HG12	2:456:B:PHE:HD1	5	0.11
(1,963)	1:50:A:VAL:HG12	2:456:B:PHE:HD2	5	0.11
(1,963)	1:50:A:VAL:HG13	2:456:B:PHE:HD1	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,963)	1:50:A:VAL:HG13	2:456:B:PHE:HD2	5	0.11
(1,963)	1:50:A:VAL:HG21	2:456:B:PHE:HD1	5	0.11
(1,963)	1:50:A:VAL:HG21	2:456:B:PHE:HD2	5	0.11
(1,963)	1:50:A:VAL:HG22	2:456:B:PHE:HD1	5	0.11
(1,963)	1:50:A:VAL:HG22	2:456:B:PHE:HD2	5	0.11
(1,963)	1:50:A:VAL:HG23	2:456:B:PHE:HD1	5	0.11
(1,963)	1:50:A:VAL:HG23	2:456:B:PHE:HD2	5	0.11
(1,963)	1:50:A:VAL:HG11	2:456:B:PHE:HD1	10	0.11
(1,963)	1:50:A:VAL:HG11	2:456:B:PHE:HD2	10	0.11
(1,963)	1:50:A:VAL:HG12	2:456:B:PHE:HD1	10	0.11
(1,963)	1:50:A:VAL:HG12	2:456:B:PHE:HD2	10	0.11
(1,963)	1:50:A:VAL:HG13	2:456:B:PHE:HD1	10	0.11
(1,963)	1:50:A:VAL:HG13	2:456:B:PHE:HD2	10	0.11
(1,963)	1:50:A:VAL:HG21	2:456:B:PHE:HD1	10	0.11
(1,963)	1:50:A:VAL:HG21	2:456:B:PHE:HD2	10	0.11
(1,963)	1:50:A:VAL:HG22	2:456:B:PHE:HD1	10	0.11
(1,963)	1:50:A:VAL:HG22	2:456:B:PHE:HD2	10	0.11
(1,963)	1:50:A:VAL:HG23	2:456:B:PHE:HD1	10	0.11
(1,963)	1:50:A:VAL:HG23	2:456:B:PHE:HD2	10	0.11
(1,963)	1:50:A:VAL:HG11	2:456:B:PHE:HD1	20	0.11
(1,963)	1:50:A:VAL:HG11	2:456:B:PHE:HD2	20	0.11
(1,963)	1:50:A:VAL:HG12	2:456:B:PHE:HD1	20	0.11
(1,963)	1:50:A:VAL:HG12	2:456:B:PHE:HD2	20	0.11
(1,963)	1:50:A:VAL:HG13	2:456:B:PHE:HD1	20	0.11
(1,963)	1:50:A:VAL:HG13	2:456:B:PHE:HD2	20	0.11
(1,963)	1:50:A:VAL:HG21	2:456:B:PHE:HD1	20	0.11
(1,963)	1:50:A:VAL:HG21	2:456:B:PHE:HD2	20	0.11
(1,963)	1:50:A:VAL:HG22	2:456:B:PHE:HD1	20	0.11
(1,963)	1:50:A:VAL:HG22	2:456:B:PHE:HD2	20	0.11
(1,963)	1:50:A:VAL:HG23	2:456:B:PHE:HD1	20	0.11
(1,963)	1:50:A:VAL:HG23	2:456:B:PHE:HD2	20	0.11
(1,957)	1:50:A:VAL:HG11	2:453:B:ARG:HB2	1	0.11
(1,957)	1:50:A:VAL:HG11	2:453:B:ARG:HB3	1	0.11
(1,957)	1:50:A:VAL:HG12	2:453:B:ARG:HB2	1	0.11
(1,957)	1:50:A:VAL:HG12	2:453:B:ARG:HB3	1	0.11
(1,957)	1:50:A:VAL:HG13	2:453:B:ARG:HB2	1	0.11
(1,957)	1:50:A:VAL:HG13	2:453:B:ARG:HB3	1	0.11
(1,957)	1:50:A:VAL:HG21	2:453:B:ARG:HB2	1	0.11
(1,957)	1:50:A:VAL:HG21	2:453:B:ARG:HB3	1	0.11
(1,957)	1:50:A:VAL:HG22	2:453:B:ARG:HB2	1	0.11
(1,957)	1:50:A:VAL:HG22	2:453:B:ARG:HB3	1	0.11
(1,957)	1:50:A:VAL:HG23	2:453:B:ARG:HB2	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,957)	1:50:A:VAL:HG23	2:453:B:ARG:HB3	1	0.11
(1,957)	1:50:A:VAL:HG11	2:453:B:ARG:HB2	9	0.11
(1,957)	1:50:A:VAL:HG11	2:453:B:ARG:HB3	9	0.11
(1,957)	1:50:A:VAL:HG12	2:453:B:ARG:HB2	9	0.11
(1,957)	1:50:A:VAL:HG12	2:453:B:ARG:HB3	9	0.11
(1,957)	1:50:A:VAL:HG13	2:453:B:ARG:HB2	9	0.11
(1,957)	1:50:A:VAL:HG13	2:453:B:ARG:HB3	9	0.11
(1,957)	1:50:A:VAL:HG21	2:453:B:ARG:HB2	9	0.11
(1,957)	1:50:A:VAL:HG21	2:453:B:ARG:HB3	9	0.11
(1,957)	1:50:A:VAL:HG22	2:453:B:ARG:HB2	9	0.11
(1,957)	1:50:A:VAL:HG22	2:453:B:ARG:HB3	9	0.11
(1,957)	1:50:A:VAL:HG23	2:453:B:ARG:HB2	9	0.11
(1,957)	1:50:A:VAL:HG23	2:453:B:ARG:HB3	9	0.11
(1,957)	1:50:A:VAL:HG11	2:453:B:ARG:HB2	21	0.11
(1,957)	1:50:A:VAL:HG11	2:453:B:ARG:HB3	21	0.11
(1,957)	1:50:A:VAL:HG12	2:453:B:ARG:HB2	21	0.11
(1,957)	1:50:A:VAL:HG12	2:453:B:ARG:HB3	21	0.11
(1,957)	1:50:A:VAL:HG13	2:453:B:ARG:HB2	21	0.11
(1,957)	1:50:A:VAL:HG13	2:453:B:ARG:HB3	21	0.11
(1,957)	1:50:A:VAL:HG21	2:453:B:ARG:HB2	21	0.11
(1,957)	1:50:A:VAL:HG21	2:453:B:ARG:HB3	21	0.11
(1,957)	1:50:A:VAL:HG22	2:453:B:ARG:HB2	21	0.11
(1,957)	1:50:A:VAL:HG22	2:453:B:ARG:HB3	21	0.11
(1,957)	1:50:A:VAL:HG23	2:453:B:ARG:HB2	21	0.11
(1,957)	1:50:A:VAL:HG23	2:453:B:ARG:HB3	21	0.11
(1,936)	1:147:A:LYS:HB2	1:148:A:ARG:HA	2	0.11
(1,936)	1:147:A:LYS:HB3	1:148:A:ARG:HA	2	0.11
(1,912)	1:141:A:VAL:HG11	1:107:A:TYR:HB3	14	0.11
(1,912)	1:141:A:VAL:HG12	1:107:A:TYR:HB3	14	0.11
(1,912)	1:141:A:VAL:HG13	1:107:A:TYR:HB3	14	0.11
(1,912)	1:141:A:VAL:HG21	1:107:A:TYR:HB3	14	0.11
(1,912)	1:141:A:VAL:HG22	1:107:A:TYR:HB3	14	0.11
(1,912)	1:141:A:VAL:HG23	1:107:A:TYR:HB3	14	0.11
(1,912)	1:141:A:VAL:HG11	1:107:A:TYR:HB2	14	0.11
(1,912)	1:141:A:VAL:HG12	1:107:A:TYR:HB2	14	0.11
(1,912)	1:141:A:VAL:HG13	1:107:A:TYR:HB2	14	0.11
(1,912)	1:141:A:VAL:HG21	1:107:A:TYR:HB2	14	0.11
(1,912)	1:141:A:VAL:HG22	1:107:A:TYR:HB2	14	0.11
(1,912)	1:141:A:VAL:HG23	1:107:A:TYR:HB2	14	0.11
(1,912)	1:141:A:VAL:HG11	1:107:A:TYR:HB3	19	0.11
(1,912)	1:141:A:VAL:HG12	1:107:A:TYR:HB3	19	0.11
(1,912)	1:141:A:VAL:HG13	1:107:A:TYR:HB3	19	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,912)	1:141:A:VAL:HG21	1:107:A:TYR:HB3	19	0.11
(1,912)	1:141:A:VAL:HG22	1:107:A:TYR:HB3	19	0.11
(1,912)	1:141:A:VAL:HG23	1:107:A:TYR:HB3	19	0.11
(1,912)	1:141:A:VAL:HG11	1:107:A:TYR:HB2	19	0.11
(1,912)	1:141:A:VAL:HG12	1:107:A:TYR:HB2	19	0.11
(1,912)	1:141:A:VAL:HG13	1:107:A:TYR:HB2	19	0.11
(1,912)	1:141:A:VAL:HG21	1:107:A:TYR:HB2	19	0.11
(1,912)	1:141:A:VAL:HG22	1:107:A:TYR:HB2	19	0.11
(1,912)	1:141:A:VAL:HG23	1:107:A:TYR:HB2	19	0.11
(1,911)	1:141:A:VAL:HA	1:107:A:TYR:HB2	22	0.11
(1,911)	1:141:A:VAL:HA	1:107:A:TYR:HB3	22	0.11
(1,880)	1:129:A:ALA:HB1	1:50:A:VAL:HB	16	0.11
(1,880)	1:129:A:ALA:HB2	1:50:A:VAL:HB	16	0.11
(1,880)	1:129:A:ALA:HB3	1:50:A:VAL:HB	16	0.11
(1,880)	1:129:A:ALA:HB1	1:50:A:VAL:HB	18	0.11
(1,880)	1:129:A:ALA:HB2	1:50:A:VAL:HB	18	0.11
(1,880)	1:129:A:ALA:HB3	1:50:A:VAL:HB	18	0.11
(1,875)	1:126:A:LEU:HG	1:114:A:PHE:HD1	19	0.11
(1,875)	1:126:A:LEU:HG	1:114:A:PHE:HD2	19	0.11
(1,875)	1:126:A:LEU:HG	1:114:A:PHE:HD1	20	0.11
(1,875)	1:126:A:LEU:HG	1:114:A:PHE:HD2	20	0.11
(1,869)	1:124:A:ALA:HB1	1:117:A:PHE:HD1	1	0.11
(1,869)	1:124:A:ALA:HB1	1:117:A:PHE:HD2	1	0.11
(1,869)	1:124:A:ALA:HB2	1:117:A:PHE:HD1	1	0.11
(1,869)	1:124:A:ALA:HB2	1:117:A:PHE:HD2	1	0.11
(1,869)	1:124:A:ALA:HB3	1:117:A:PHE:HD1	1	0.11
(1,869)	1:124:A:ALA:HB3	1:117:A:PHE:HD2	1	0.11
(1,869)	1:124:A:ALA:HB1	1:117:A:PHE:HD1	3	0.11
(1,869)	1:124:A:ALA:HB1	1:117:A:PHE:HD2	3	0.11
(1,869)	1:124:A:ALA:HB2	1:117:A:PHE:HD1	3	0.11
(1,869)	1:124:A:ALA:HB2	1:117:A:PHE:HD2	3	0.11
(1,869)	1:124:A:ALA:HB3	1:117:A:PHE:HD1	3	0.11
(1,869)	1:124:A:ALA:HB3	1:117:A:PHE:HD2	3	0.11
(1,865)	1:123:A:GLN:HG2	1:122:A:CYS:HB2	7	0.11
(1,865)	1:123:A:GLN:HG2	1:122:A:CYS:HB3	7	0.11
(1,865)	1:123:A:GLN:HG3	1:122:A:CYS:HB2	7	0.11
(1,865)	1:123:A:GLN:HG3	1:122:A:CYS:HB3	7	0.11
(1,864)	1:122:A:CYS:HA	1:123:A:GLN:HB2	14	0.11
(1,864)	1:122:A:CYS:HA	1:123:A:GLN:HB3	14	0.11
(1,863)	1:120:A:ASP:HA	1:123:A:GLN:HG2	4	0.11
(1,863)	1:120:A:ASP:HA	1:123:A:GLN:HG3	4	0.11
(1,863)	1:120:A:ASP:HA	1:123:A:GLN:HG2	19	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,863)	1:120:A:ASP:HA	1:123:A:GLN:HG3	19	0.11
(1,860)	1:117:A:PHE:HB2	1:122:A:CYS:HB2	1	0.11
(1,860)	1:117:A:PHE:HB2	1:122:A:CYS:HB3	1	0.11
(1,860)	1:117:A:PHE:HB3	1:122:A:CYS:HB2	1	0.11
(1,860)	1:117:A:PHE:HB3	1:122:A:CYS:HB3	1	0.11
(1,860)	1:117:A:PHE:HB2	1:122:A:CYS:HB2	2	0.11
(1,860)	1:117:A:PHE:HB2	1:122:A:CYS:HB3	2	0.11
(1,860)	1:117:A:PHE:HB3	1:122:A:CYS:HB2	2	0.11
(1,860)	1:117:A:PHE:HB3	1:122:A:CYS:HB3	2	0.11
(1,851)	1:110:A:PRO:HA	1:131:A:GLU:HB2	24	0.11
(1,851)	1:110:A:PRO:HA	1:131:A:GLU:HB3	24	0.11
(1,815)	1:88:A:TYR:HB2	1:75:A:VAL:HG11	2	0.11
(1,815)	1:88:A:TYR:HB2	1:75:A:VAL:HG12	2	0.11
(1,815)	1:88:A:TYR:HB2	1:75:A:VAL:HG13	2	0.11
(1,815)	1:88:A:TYR:HB2	1:75:A:VAL:HG21	2	0.11
(1,815)	1:88:A:TYR:HB2	1:75:A:VAL:HG22	2	0.11
(1,815)	1:88:A:TYR:HB2	1:75:A:VAL:HG23	2	0.11
(1,815)	1:88:A:TYR:HB3	1:75:A:VAL:HG11	2	0.11
(1,815)	1:88:A:TYR:HB3	1:75:A:VAL:HG12	2	0.11
(1,815)	1:88:A:TYR:HB3	1:75:A:VAL:HG13	2	0.11
(1,815)	1:88:A:TYR:HB3	1:75:A:VAL:HG21	2	0.11
(1,815)	1:88:A:TYR:HB3	1:75:A:VAL:HG22	2	0.11
(1,815)	1:88:A:TYR:HB3	1:75:A:VAL:HG23	2	0.11
(1,786)	1:83:A:TYR:HA	1:85:A:ILE:HD11	4	0.11
(1,786)	1:83:A:TYR:HA	1:85:A:ILE:HD12	4	0.11
(1,786)	1:83:A:TYR:HA	1:85:A:ILE:HD13	4	0.11
(1,786)	1:83:A:TYR:HA	1:85:A:ILE:HD11	10	0.11
(1,786)	1:83:A:TYR:HA	1:85:A:ILE:HD12	10	0.11
(1,786)	1:83:A:TYR:HA	1:85:A:ILE:HD13	10	0.11
(1,786)	1:83:A:TYR:HA	1:85:A:ILE:HD11	14	0.11
(1,786)	1:83:A:TYR:HA	1:85:A:ILE:HD12	14	0.11
(1,786)	1:83:A:TYR:HA	1:85:A:ILE:HD13	14	0.11
(1,786)	1:83:A:TYR:HA	1:85:A:ILE:HD11	15	0.11
(1,786)	1:83:A:TYR:HA	1:85:A:ILE:HD12	15	0.11
(1,786)	1:83:A:TYR:HA	1:85:A:ILE:HD13	15	0.11
(1,786)	1:83:A:TYR:HA	1:85:A:ILE:HD11	20	0.11
(1,786)	1:83:A:TYR:HA	1:85:A:ILE:HD12	20	0.11
(1,786)	1:83:A:TYR:HA	1:85:A:ILE:HD13	20	0.11
(1,786)	1:83:A:TYR:HA	1:85:A:ILE:HD11	21	0.11
(1,786)	1:83:A:TYR:HA	1:85:A:ILE:HD12	21	0.11
(1,786)	1:83:A:TYR:HA	1:85:A:ILE:HD13	21	0.11
(1,786)	1:83:A:TYR:HA	1:85:A:ILE:HD11	23	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,786)	1:83:A:TYR:HA	1:85:A:ILE:HD12	23	0.11
(1,786)	1:83:A:TYR:HA	1:85:A:ILE:HD13	23	0.11
(1,783)	1:81:A:LYS:HG2	1:80:A:GLN:HA	23	0.11
(1,783)	1:81:A:LYS:HG3	1:80:A:GLN:HA	23	0.11
(1,777)	1:75:A:VAL:HG11	1:77:A:ASP:HA	19	0.11
(1,777)	1:75:A:VAL:HG12	1:77:A:ASP:HA	19	0.11
(1,777)	1:75:A:VAL:HG13	1:77:A:ASP:HA	19	0.11
(1,777)	1:75:A:VAL:HG21	1:77:A:ASP:HA	19	0.11
(1,777)	1:75:A:VAL:HG22	1:77:A:ASP:HA	19	0.11
(1,777)	1:75:A:VAL:HG23	1:77:A:ASP:HA	19	0.11
(1,759)	1:72:A:VAL:HG11	1:85:A:ILE:HB	24	0.11
(1,759)	1:72:A:VAL:HG12	1:85:A:ILE:HB	24	0.11
(1,759)	1:72:A:VAL:HG13	1:85:A:ILE:HB	24	0.11
(1,759)	1:72:A:VAL:HG21	1:85:A:ILE:HB	24	0.11
(1,759)	1:72:A:VAL:HG22	1:85:A:ILE:HB	24	0.11
(1,759)	1:72:A:VAL:HG23	1:85:A:ILE:HB	24	0.11
(1,741)	1:71:A:ALA:HB1	1:35:A:LEU:HB2	2	0.11
(1,741)	1:71:A:ALA:HB1	1:35:A:LEU:HB3	2	0.11
(1,741)	1:71:A:ALA:HB2	1:35:A:LEU:HB2	2	0.11
(1,741)	1:71:A:ALA:HB2	1:35:A:LEU:HB3	2	0.11
(1,741)	1:71:A:ALA:HB3	1:35:A:LEU:HB2	2	0.11
(1,741)	1:71:A:ALA:HB3	1:35:A:LEU:HB3	2	0.11
(1,738)	1:69:A:CYS:HG	1:52:A:GLN:HA	16	0.11
(1,729)	1:63:A:HIS:HA	1:59:A:PRO:HB2	5	0.11
(1,729)	1:63:A:HIS:HA	1:59:A:PRO:HB3	5	0.11
(1,729)	1:63:A:HIS:HA	1:59:A:PRO:HB2	17	0.11
(1,729)	1:63:A:HIS:HA	1:59:A:PRO:HB3	17	0.11
(1,729)	1:63:A:HIS:HA	1:59:A:PRO:HB2	23	0.11
(1,729)	1:63:A:HIS:HA	1:59:A:PRO:HB3	23	0.11
(1,715)	1:55:A:LEU:HA	1:64:A:TRP:HZ3	14	0.11
(1,714)	1:55:A:LEU:HB2	1:126:A:LEU:HG	15	0.11
(1,714)	1:55:A:LEU:HB3	1:126:A:LEU:HG	15	0.11
(1,713)	1:55:A:LEU:HD11	1:126:A:LEU:HG	5	0.11
(1,713)	1:55:A:LEU:HD12	1:126:A:LEU:HG	5	0.11
(1,713)	1:55:A:LEU:HD13	1:126:A:LEU:HG	5	0.11
(1,713)	1:55:A:LEU:HD21	1:126:A:LEU:HG	5	0.11
(1,713)	1:55:A:LEU:HD22	1:126:A:LEU:HG	5	0.11
(1,713)	1:55:A:LEU:HD23	1:126:A:LEU:HG	5	0.11
(1,707)	1:54:A:TYR:HE1	1:127:A:ASN:H	23	0.11
(1,707)	1:54:A:TYR:HE2	1:127:A:ASN:H	23	0.11
(1,683)	1:50:A:VAL:HA	1:71:A:ALA:HA	4	0.11
(1,669)	1:47:A:ALA:HB1	1:137:A:PHE:HA	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,669)	1:47:A:ALA:HB2	1:137:A:PHE:HA	3	0.11
(1,669)	1:47:A:ALA:HB3	1:137:A:PHE:HA	3	0.11
(1,669)	1:47:A:ALA:HB1	1:137:A:PHE:HA	4	0.11
(1,669)	1:47:A:ALA:HB2	1:137:A:PHE:HA	4	0.11
(1,669)	1:47:A:ALA:HB3	1:137:A:PHE:HA	4	0.11
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG11	4	0.11
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG12	4	0.11
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG13	4	0.11
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG21	4	0.11
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG22	4	0.11
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG23	4	0.11
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG11	4	0.11
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG12	4	0.11
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG13	4	0.11
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG21	4	0.11
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG22	4	0.11
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG23	4	0.11
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG11	4	0.11
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG12	4	0.11
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG13	4	0.11
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG21	4	0.11
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG22	4	0.11
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG23	4	0.11
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG11	10	0.11
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG12	10	0.11
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG13	10	0.11
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG21	10	0.11
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG22	10	0.11
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG23	10	0.11
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG11	10	0.11
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG12	10	0.11
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG13	10	0.11
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG21	10	0.11
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG22	10	0.11
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG23	10	0.11
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG11	10	0.11
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG12	10	0.11
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG13	10	0.11
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG21	10	0.11
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG22	10	0.11
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG23	10	0.11
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG11	18	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG12	18	0.11
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG13	18	0.11
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG21	18	0.11
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG22	18	0.11
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG23	18	0.11
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG11	18	0.11
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG12	18	0.11
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG13	18	0.11
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG21	18	0.11
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG22	18	0.11
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG23	18	0.11
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG11	18	0.11
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG12	18	0.11
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG13	18	0.11
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG21	18	0.11
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG22	18	0.11
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG23	18	0.11
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG11	22	0.11
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG12	22	0.11
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG13	22	0.11
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG21	22	0.11
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG22	22	0.11
(1,668)	1:47:A:ALA:HB1	1:75:A:VAL:HG23	22	0.11
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG11	22	0.11
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG12	22	0.11
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG13	22	0.11
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG21	22	0.11
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG22	22	0.11
(1,668)	1:47:A:ALA:HB2	1:75:A:VAL:HG23	22	0.11
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG11	22	0.11
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG12	22	0.11
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG13	22	0.11
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG21	22	0.11
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG22	22	0.11
(1,668)	1:47:A:ALA:HB3	1:75:A:VAL:HG23	22	0.11
(1,646)	1:39:A:LEU:HA	1:88:A:TYR:HB2	13	0.11
(1,646)	1:39:A:LEU:HA	1:88:A:TYR:HB3	13	0.11
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD11	2	0.11
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD12	2	0.11
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD13	2	0.11
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD21	2	0.11
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD22	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD23	2	0.11
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD11	2	0.11
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD12	2	0.11
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD13	2	0.11
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD21	2	0.11
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD22	2	0.11
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD23	2	0.11
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD11	6	0.11
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD12	6	0.11
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD13	6	0.11
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD21	6	0.11
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD22	6	0.11
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD23	6	0.11
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD11	6	0.11
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD12	6	0.11
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD13	6	0.11
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD21	6	0.11
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD22	6	0.11
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD23	6	0.11
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD11	8	0.11
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD12	8	0.11
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD13	8	0.11
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD21	8	0.11
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD22	8	0.11
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD23	8	0.11
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD11	8	0.11
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD12	8	0.11
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD13	8	0.11
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD21	8	0.11
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD22	8	0.11
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD23	8	0.11
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD11	9	0.11
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD12	9	0.11
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD13	9	0.11
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD21	9	0.11
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD22	9	0.11
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD23	9	0.11
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD11	9	0.11
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD12	9	0.11
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD13	9	0.11
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD21	9	0.11
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD22	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD23	9	0.11
(1,642)	1:36:A:PHE:HB2	1:34:A:ARG:HG2	14	0.11
(1,642)	1:36:A:PHE:HB2	1:34:A:ARG:HG3	14	0.11
(1,642)	1:36:A:PHE:HB3	1:34:A:ARG:HG2	14	0.11
(1,642)	1:36:A:PHE:HB3	1:34:A:ARG:HG3	14	0.11
(1,642)	1:36:A:PHE:HB2	1:34:A:ARG:HG2	19	0.11
(1,642)	1:36:A:PHE:HB2	1:34:A:ARG:HG3	19	0.11
(1,642)	1:36:A:PHE:HB3	1:34:A:ARG:HG2	19	0.11
(1,642)	1:36:A:PHE:HB3	1:34:A:ARG:HG3	19	0.11
(1,640)	1:35:A:LEU:HD11	1:31:A:GLU:HA	1	0.11
(1,640)	1:35:A:LEU:HD12	1:31:A:GLU:HA	1	0.11
(1,640)	1:35:A:LEU:HD13	1:31:A:GLU:HA	1	0.11
(1,640)	1:35:A:LEU:HD21	1:31:A:GLU:HA	1	0.11
(1,640)	1:35:A:LEU:HD22	1:31:A:GLU:HA	1	0.11
(1,640)	1:35:A:LEU:HD23	1:31:A:GLU:HA	1	0.11
(1,640)	1:35:A:LEU:HD11	1:31:A:GLU:HA	7	0.11
(1,640)	1:35:A:LEU:HD12	1:31:A:GLU:HA	7	0.11
(1,640)	1:35:A:LEU:HD13	1:31:A:GLU:HA	7	0.11
(1,640)	1:35:A:LEU:HD21	1:31:A:GLU:HA	7	0.11
(1,640)	1:35:A:LEU:HD22	1:31:A:GLU:HA	7	0.11
(1,640)	1:35:A:LEU:HD23	1:31:A:GLU:HA	7	0.11
(1,640)	1:35:A:LEU:HD11	1:31:A:GLU:HA	10	0.11
(1,640)	1:35:A:LEU:HD12	1:31:A:GLU:HA	10	0.11
(1,640)	1:35:A:LEU:HD13	1:31:A:GLU:HA	10	0.11
(1,640)	1:35:A:LEU:HD21	1:31:A:GLU:HA	10	0.11
(1,640)	1:35:A:LEU:HD22	1:31:A:GLU:HA	10	0.11
(1,640)	1:35:A:LEU:HD23	1:31:A:GLU:HA	10	0.11
(1,640)	1:35:A:LEU:HD11	1:31:A:GLU:HA	11	0.11
(1,640)	1:35:A:LEU:HD12	1:31:A:GLU:HA	11	0.11
(1,640)	1:35:A:LEU:HD13	1:31:A:GLU:HA	11	0.11
(1,640)	1:35:A:LEU:HD21	1:31:A:GLU:HA	11	0.11
(1,640)	1:35:A:LEU:HD22	1:31:A:GLU:HA	11	0.11
(1,640)	1:35:A:LEU:HD23	1:31:A:GLU:HA	11	0.11
(1,640)	1:35:A:LEU:HD11	1:31:A:GLU:HA	21	0.11
(1,640)	1:35:A:LEU:HD12	1:31:A:GLU:HA	21	0.11
(1,640)	1:35:A:LEU:HD13	1:31:A:GLU:HA	21	0.11
(1,640)	1:35:A:LEU:HD21	1:31:A:GLU:HA	21	0.11
(1,640)	1:35:A:LEU:HD22	1:31:A:GLU:HA	21	0.11
(1,640)	1:35:A:LEU:HD23	1:31:A:GLU:HA	21	0.11
(1,639)	1:34:A:ARG:HD2	1:74:A:PHE:HE1	2	0.11
(1,639)	1:34:A:ARG:HD2	1:74:A:PHE:HE2	2	0.11
(1,639)	1:34:A:ARG:HD3	1:74:A:PHE:HE1	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,639)	1:34:A:ARG:HD3	1:74:A:PHE:HE2	2	0.11
(1,639)	1:34:A:ARG:HD2	1:74:A:PHE:HE1	4	0.11
(1,639)	1:34:A:ARG:HD2	1:74:A:PHE:HE2	4	0.11
(1,639)	1:34:A:ARG:HD3	1:74:A:PHE:HE1	4	0.11
(1,639)	1:34:A:ARG:HD3	1:74:A:PHE:HE2	4	0.11
(1,638)	1:34:A:ARG:HB2	1:74:A:PHE:HD1	13	0.11
(1,638)	1:34:A:ARG:HB2	1:74:A:PHE:HD2	13	0.11
(1,638)	1:34:A:ARG:HB3	1:74:A:PHE:HD1	13	0.11
(1,638)	1:34:A:ARG:HB3	1:74:A:PHE:HD2	13	0.11
(1,587)	2:469:B:VAL:H	2:468:B:TYR:HB2	9	0.11
(1,586)	2:469:B:VAL:H	2:468:B:TYR:HB3	2	0.11
(1,586)	2:469:B:VAL:H	2:468:B:TYR:HB3	21	0.11
(1,571)	2:459:B:ILE:H	2:458:B:PRO:HB2	10	0.11
(1,567)	2:457:B:HIS:H	2:456:B:PHE:HB3	1	0.11
(1,567)	2:457:B:HIS:H	2:456:B:PHE:HB3	17	0.11
(1,545)	2:447:B:GLU:H	2:446:B:CYS:H	8	0.11
(1,542)	2:446:B:CYS:H	2:445:B:PRO:HA	13	0.11
(1,531)	1:120:A:ASP:H	1:122:A:CYS:H	2	0.11
(1,531)	1:120:A:ASP:H	1:122:A:CYS:H	11	0.11
(1,531)	1:120:A:ASP:H	1:122:A:CYS:H	18	0.11
(1,529)	1:126:A:LEU:H	1:125:A:GLY:H	9	0.11
(1,529)	1:126:A:LEU:H	1:125:A:GLY:H	19	0.11
(1,512)	1:114:A:PHE:H	1:112:A:PRO:HA	4	0.11
(1,512)	1:114:A:PHE:H	1:112:A:PRO:HA	24	0.11
(1,509)	1:114:A:PHE:H	1:110:A:PRO:HD2	2	0.11
(1,509)	1:114:A:PHE:H	1:110:A:PRO:HD3	2	0.11
(1,509)	1:114:A:PHE:H	1:110:A:PRO:HD2	15	0.11
(1,509)	1:114:A:PHE:H	1:110:A:PRO:HD3	15	0.11
(1,502)	1:104:A:GLN:H	1:102:A:TYR:HA	2	0.11
(1,496)	1:101:A:LEU:H	1:100:A:GLU:H	19	0.11
(1,493)	1:97:A:TRP:H	1:95:A:LEU:HA	7	0.11
(1,493)	1:97:A:TRP:H	1:95:A:LEU:HA	20	0.11
(1,487)	1:89:A:GLY:H	1:94:A:ARG:H	17	0.11
(1,487)	1:89:A:GLY:H	1:94:A:ARG:H	22	0.11
(1,486)	1:89:A:GLY:H	1:94:A:ARG:HB2	14	0.11
(1,486)	1:89:A:GLY:H	1:94:A:ARG:HB3	14	0.11
(1,486)	1:89:A:GLY:H	1:94:A:ARG:HB2	20	0.11
(1,486)	1:89:A:GLY:H	1:94:A:ARG:HB3	20	0.11
(1,483)	1:87:A:LEU:H	1:97:A:TRP:HZ2	21	0.11
(1,482)	1:87:A:LEU:H	1:72:A:VAL:HB	3	0.11
(1,482)	1:87:A:LEU:H	1:72:A:VAL:HB	9	0.11
(1,477)	1:72:A:VAL:H	1:48:A:THR:HA	6	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,469)	1:55:A:LEU:H	1:65:A:THR:H	11	0.11
(1,469)	1:55:A:LEU:H	1:65:A:THR:H	18	0.11
(1,456)	1:35:A:LEU:H	1:31:A:GLU:HA	20	0.11
(1,440)	1:127:A:ASN:H	1:53:A:LEU:HA	13	0.11
(1,429)	1:101:A:LEU:H	1:84:A:PHE:HB2	6	0.11
(1,429)	1:101:A:LEU:H	1:84:A:PHE:HB3	6	0.11
(1,425)	1:97:A:TRP:H	1:87:A:LEU:HG	3	0.11
(1,425)	1:97:A:TRP:H	1:87:A:LEU:HG	20	0.11
(1,416)	1:87:A:LEU:H	1:98:A:GLU:HB2	3	0.11
(1,416)	1:87:A:LEU:H	1:98:A:GLU:HB3	3	0.11
(1,412)	1:84:A:PHE:H	1:76:A:LYS:HB2	1	0.11
(1,412)	1:84:A:PHE:H	1:76:A:LYS:HB3	1	0.11
(1,412)	1:84:A:PHE:H	1:76:A:LYS:HB2	8	0.11
(1,412)	1:84:A:PHE:H	1:76:A:LYS:HB3	8	0.11
(1,412)	1:84:A:PHE:H	1:76:A:LYS:HB2	18	0.11
(1,412)	1:84:A:PHE:H	1:76:A:LYS:HB3	18	0.11
(1,410)	1:84:A:PHE:H	1:76:A:LYS:HG2	7	0.11
(1,410)	1:84:A:PHE:H	1:76:A:LYS:HG3	7	0.11
(1,410)	1:84:A:PHE:H	1:76:A:LYS:HG2	12	0.11
(1,410)	1:84:A:PHE:H	1:76:A:LYS:HG3	12	0.11
(1,408)	1:84:A:PHE:H	1:75:A:VAL:H	20	0.11
(1,399)	1:72:A:VAL:H	1:50:A:VAL:HB	18	0.11
(1,392)	1:55:A:LEU:H	1:66:A:LYS:HB2	4	0.11
(1,392)	1:55:A:LEU:H	1:66:A:LYS:HB3	4	0.11
(1,374)	1:38:A:MET:H	1:35:A:LEU:HG	6	0.11
(1,369)	1:37:A:GLU:H	1:34:A:ARG:HA	11	0.11
(1,366)	1:35:A:LEU:H	1:32:A:ASN:HA	2	0.11
(1,364)	1:34:A:ARG:H	1:31:A:GLU:HA	14	0.11
(1,364)	1:34:A:ARG:H	1:31:A:GLU:HA	22	0.11
(1,364)	1:34:A:ARG:H	1:31:A:GLU:HA	24	0.11
(1,360)	1:32:A:ASN:H	1:29:A:ASP:HA	8	0.11
(1,360)	1:32:A:ASN:H	1:29:A:ASP:HA	10	0.11
(1,360)	1:32:A:ASN:H	1:29:A:ASP:HA	22	0.11
(1,360)	1:32:A:ASN:H	1:29:A:ASP:HA	24	0.11
(1,346)	1:148:A:ARG:H	1:147:A:LYS:HA	4	0.11
(1,346)	1:148:A:ARG:H	1:147:A:LYS:HA	5	0.11
(1,346)	1:148:A:ARG:H	1:147:A:LYS:HA	6	0.11
(1,346)	1:148:A:ARG:H	1:147:A:LYS:HA	11	0.11
(1,346)	1:148:A:ARG:H	1:147:A:LYS:HA	16	0.11
(1,346)	1:148:A:ARG:H	1:147:A:LYS:HA	18	0.11
(1,342)	1:146:A:GLN:H	1:143:A:GLU:HA	9	0.11
(1,340)	1:146:A:GLN:H	1:145:A:ILE:HB	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,340)	1:146:A:GLN:H	1:145:A:ILE:HB	15	0.11
(1,339)	1:146:A:GLN:H	1:145:A:ILE:HA	13	0.11
(1,336)	1:145:A:ILE:H	1:144:A:LYS:HA	6	0.11
(1,336)	1:145:A:ILE:H	1:144:A:LYS:HA	16	0.11
(1,336)	1:145:A:ILE:H	1:144:A:LYS:HA	22	0.11
(1,314)	1:140:A:LEU:H	1:136:A:ALA:HA	5	0.11
(1,314)	1:140:A:LEU:H	1:136:A:ALA:HA	6	0.11
(1,314)	1:140:A:LEU:H	1:136:A:ALA:HA	13	0.11
(1,300)	1:136:A:ALA:H	1:132:A:ASP:HA	3	0.11
(1,300)	1:136:A:ALA:H	1:132:A:ASP:HA	15	0.11
(1,278)	1:127:A:ASN:H	1:126:A:LEU:HG	15	0.11
(1,278)	1:127:A:ASN:H	1:126:A:LEU:HG	17	0.11
(1,272)	1:124:A:ALA:H	1:123:A:GLN:HG2	17	0.11
(1,272)	1:124:A:ALA:H	1:123:A:GLN:HG3	17	0.11
(1,265)	1:121:A:ASP:H	1:120:A:ASP:H	7	0.11
(1,265)	1:121:A:ASP:H	1:120:A:ASP:H	8	0.11
(1,265)	1:121:A:ASP:H	1:120:A:ASP:H	10	0.11
(1,265)	1:121:A:ASP:H	1:120:A:ASP:H	18	0.11
(1,265)	1:121:A:ASP:H	1:120:A:ASP:H	19	0.11
(1,265)	1:121:A:ASP:H	1:120:A:ASP:H	21	0.11
(1,245)	1:114:A:PHE:H	1:113:A:PHE:H	4	0.11
(1,245)	1:114:A:PHE:H	1:113:A:PHE:H	15	0.11
(1,195)	1:96:A:LEU:H	1:95:A:LEU:H	11	0.11
(1,176)	1:88:A:TYR:H	1:87:A:LEU:HD11	2	0.11
(1,176)	1:88:A:TYR:H	1:87:A:LEU:HD12	2	0.11
(1,176)	1:88:A:TYR:H	1:87:A:LEU:HD13	2	0.11
(1,176)	1:88:A:TYR:H	1:87:A:LEU:HD21	2	0.11
(1,176)	1:88:A:TYR:H	1:87:A:LEU:HD22	2	0.11
(1,176)	1:88:A:TYR:H	1:87:A:LEU:HD23	2	0.11
(1,141)	1:77:A:ASP:H	1:76:A:LYS:HG2	10	0.11
(1,141)	1:77:A:ASP:H	1:76:A:LYS:HG3	10	0.11
(1,140)	1:77:A:ASP:H	1:76:A:LYS:HD2	18	0.11
(1,140)	1:77:A:ASP:H	1:76:A:LYS:HD3	18	0.11
(1,120)	1:70:A:GLY:H	1:69:A:CYS:HB3	21	0.11
(1,119)	1:70:A:GLY:H	1:69:A:CYS:HB2	2	0.11
(1,112)	1:65:A:THR:H	1:64:A:TRP:HB3	6	0.11
(1,112)	1:65:A:THR:H	1:64:A:TRP:HB3	12	0.11
(1,112)	1:65:A:THR:H	1:64:A:TRP:HB3	21	0.11
(1,85)	1:54:A:TYR:H	1:53:A:LEU:HG	18	0.11
(1,65)	1:47:A:ALA:H	1:46:A:LEU:HD21	1	0.11
(1,65)	1:47:A:ALA:H	1:46:A:LEU:HD22	1	0.11
(1,65)	1:47:A:ALA:H	1:46:A:LEU:HD23	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,65)	1:47:A:ALA:H	1:46:A:LEU:HD21	3	0.11
(1,65)	1:47:A:ALA:H	1:46:A:LEU:HD22	3	0.11
(1,65)	1:47:A:ALA:H	1:46:A:LEU:HD23	3	0.11
(1,65)	1:47:A:ALA:H	1:46:A:LEU:HD21	22	0.11
(1,65)	1:47:A:ALA:H	1:46:A:LEU:HD22	22	0.11
(1,65)	1:47:A:ALA:H	1:46:A:LEU:HD23	22	0.11
(1,54)	1:43:A:CYS:H	1:42:A:LYS:HB2	15	0.11
(1,54)	1:43:A:CYS:H	1:42:A:LYS:HB3	15	0.11
(1,54)	1:43:A:CYS:H	1:42:A:LYS:HB2	19	0.11
(1,54)	1:43:A:CYS:H	1:42:A:LYS:HB3	19	0.11
(1,54)	1:43:A:CYS:H	1:42:A:LYS:HB2	24	0.11
(1,54)	1:43:A:CYS:H	1:42:A:LYS:HB3	24	0.11
(1,44)	1:39:A:LEU:H	1:36:A:PHE:HE1	6	0.11
(1,44)	1:39:A:LEU:H	1:36:A:PHE:HE2	6	0.11
(1,44)	1:39:A:LEU:H	1:36:A:PHE:HE1	7	0.11
(1,44)	1:39:A:LEU:H	1:36:A:PHE:HE2	7	0.11
(4,122)	2:452:B:SER:N	2:448:B:ASP:O	1	0.1
(4,122)	2:452:B:SER:N	2:448:B:ASP:O	9	0.1
(4,122)	2:452:B:SER:N	2:448:B:ASP:O	20	0.1
(4,122)	2:452:B:SER:N	2:448:B:ASP:O	24	0.1
(4,114)	1:147:A:LYS:N	1:143:A:GLU:O	6	0.1
(4,114)	1:147:A:LYS:N	1:143:A:GLU:O	14	0.1
(4,105)	1:143:A:GLU:H	1:139:A:ALA:O	5	0.1
(4,105)	1:143:A:GLU:H	1:139:A:ALA:O	19	0.1
(4,98)	1:139:A:ALA:N	1:135:A:GLN:O	1	0.1
(4,98)	1:139:A:ALA:N	1:135:A:GLN:O	2	0.1
(4,95)	1:138:A:ARG:H	1:134:A:ALA:O	4	0.1
(4,77)	1:34:A:ARG:H	1:30:A:HIS:O	11	0.1
(4,77)	1:34:A:ARG:H	1:30:A:HIS:O	23	0.1
(4,43)	1:88:A:TYR:H	1:71:A:ALA:O	8	0.1
(4,31)	1:52:A:GLN:H	1:127:A:ASN:O	3	0.1
(4,31)	1:52:A:GLN:H	1:127:A:ASN:O	20	0.1
(4,23)	1:68:A:HIS:H	1:53:A:LEU:O	6	0.1
(4,23)	1:68:A:HIS:H	1:53:A:LEU:O	17	0.1
(4,23)	1:68:A:HIS:H	1:53:A:LEU:O	22	0.1
(4,17)	1:70:A:GLY:H	1:51:A:VAL:O	18	0.1
(4,9)	1:74:A:PHE:H	1:47:A:ALA:O	9	0.1
(1,1016)	2:479:B:LEU:HG	1:83:A:TYR:HD1	8	0.1
(1,1016)	2:479:B:LEU:HG	1:83:A:TYR:HD2	8	0.1
(1,1016)	2:479:B:LEU:HG	1:83:A:TYR:HD1	14	0.1
(1,1016)	2:479:B:LEU:HG	1:83:A:TYR:HD2	14	0.1
(1,1008)	2:474:B:SER:H	1:102:A:TYR:HE1	10	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1008)	2:474:B:SER:H	1:102:A:TYR:HE2	10	0.1
(1,1007)	2:474:B:SER:H	1:102:A:TYR:HA	20	0.1
(1,1002)	2:463:B:PRO:HG2	1:114:A:PHE:HD1	1	0.1
(1,1002)	2:463:B:PRO:HG2	1:114:A:PHE:HD2	1	0.1
(1,1002)	2:463:B:PRO:HG3	1:114:A:PHE:HD1	1	0.1
(1,1002)	2:463:B:PRO:HG3	1:114:A:PHE:HD2	1	0.1
(1,1002)	2:463:B:PRO:HG2	1:114:A:PHE:HD1	16	0.1
(1,1002)	2:463:B:PRO:HG2	1:114:A:PHE:HD2	16	0.1
(1,1002)	2:463:B:PRO:HG3	1:114:A:PHE:HD1	16	0.1
(1,1002)	2:463:B:PRO:HG3	1:114:A:PHE:HD2	16	0.1
(1,988)	1:129:A:ALA:HA	2:454:B:PHE:HZ	11	0.1
(1,988)	1:129:A:ALA:HA	2:454:B:PHE:HZ	21	0.1
(1,977)	1:103:A:SER:HB2	2:476:B:PRO:HD2	22	0.1
(1,977)	1:103:A:SER:HB2	2:476:B:PRO:HD3	22	0.1
(1,977)	1:103:A:SER:HB3	2:476:B:PRO:HD2	22	0.1
(1,977)	1:103:A:SER:HB3	2:476:B:PRO:HD3	22	0.1
(1,975)	1:91:A:GLN:HB2	2:445:B:PRO:HD2	16	0.1
(1,975)	1:91:A:GLN:HB2	2:445:B:PRO:HD3	16	0.1
(1,975)	1:91:A:GLN:HB3	2:445:B:PRO:HD2	16	0.1
(1,975)	1:91:A:GLN:HB3	2:445:B:PRO:HD3	16	0.1
(1,975)	1:91:A:GLN:HB2	2:445:B:PRO:HD2	24	0.1
(1,975)	1:91:A:GLN:HB2	2:445:B:PRO:HD3	24	0.1
(1,975)	1:91:A:GLN:HB3	2:445:B:PRO:HD2	24	0.1
(1,975)	1:91:A:GLN:HB3	2:445:B:PRO:HD3	24	0.1
(1,964)	1:51:A:VAL:H	2:454:B:PHE:HD1	14	0.1
(1,964)	1:51:A:VAL:H	2:454:B:PHE:HD2	14	0.1
(1,958)	1:50:A:VAL:HG11	2:455:B:TYR:HE1	19	0.1
(1,958)	1:50:A:VAL:HG11	2:455:B:TYR:HE2	19	0.1
(1,958)	1:50:A:VAL:HG12	2:455:B:TYR:HE1	19	0.1
(1,958)	1:50:A:VAL:HG12	2:455:B:TYR:HE2	19	0.1
(1,958)	1:50:A:VAL:HG13	2:455:B:TYR:HE1	19	0.1
(1,958)	1:50:A:VAL:HG13	2:455:B:TYR:HE2	19	0.1
(1,958)	1:50:A:VAL:HG21	2:455:B:TYR:HE1	19	0.1
(1,958)	1:50:A:VAL:HG21	2:455:B:TYR:HE2	19	0.1
(1,958)	1:50:A:VAL:HG22	2:455:B:TYR:HE1	19	0.1
(1,958)	1:50:A:VAL:HG22	2:455:B:TYR:HE2	19	0.1
(1,958)	1:50:A:VAL:HG23	2:455:B:TYR:HE1	19	0.1
(1,958)	1:50:A:VAL:HG23	2:455:B:TYR:HE2	19	0.1
(1,936)	1:147:A:LYS:HB2	1:148:A:ARG:HA	13	0.1
(1,936)	1:147:A:LYS:HB3	1:148:A:ARG:HA	13	0.1
(1,936)	1:147:A:LYS:HB2	1:148:A:ARG:HA	19	0.1
(1,936)	1:147:A:LYS:HB3	1:148:A:ARG:HA	19	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,936)	1:147:A:LYS:HB2	1:148:A:ARG:HA	20	0.1
(1,936)	1:147:A:LYS:HB3	1:148:A:ARG:HA	20	0.1
(1,911)	1:141:A:VAL:HA	1:107:A:TYR:HB2	3	0.1
(1,911)	1:141:A:VAL:HA	1:107:A:TYR:HB3	3	0.1
(1,911)	1:141:A:VAL:HA	1:107:A:TYR:HB2	9	0.1
(1,911)	1:141:A:VAL:HA	1:107:A:TYR:HB3	9	0.1
(1,911)	1:141:A:VAL:HA	1:107:A:TYR:HB2	18	0.1
(1,911)	1:141:A:VAL:HA	1:107:A:TYR:HB3	18	0.1
(1,880)	1:129:A:ALA:HB1	1:50:A:VAL:HB	21	0.1
(1,880)	1:129:A:ALA:HB2	1:50:A:VAL:HB	21	0.1
(1,880)	1:129:A:ALA:HB3	1:50:A:VAL:HB	21	0.1
(1,875)	1:126:A:LEU:HG	1:114:A:PHE:HD1	8	0.1
(1,875)	1:126:A:LEU:HG	1:114:A:PHE:HD2	8	0.1
(1,851)	1:110:A:PRO:HA	1:131:A:GLU:HB2	19	0.1
(1,851)	1:110:A:PRO:HA	1:131:A:GLU:HB3	19	0.1
(1,827)	1:95:A:LEU:HD11	1:94:A:ARG:HB2	15	0.1
(1,827)	1:95:A:LEU:HD12	1:94:A:ARG:HB2	15	0.1
(1,827)	1:95:A:LEU:HD13	1:94:A:ARG:HB2	15	0.1
(1,827)	1:95:A:LEU:HD21	1:94:A:ARG:HB2	15	0.1
(1,827)	1:95:A:LEU:HD22	1:94:A:ARG:HB2	15	0.1
(1,827)	1:95:A:LEU:HD23	1:94:A:ARG:HB2	15	0.1
(1,815)	1:88:A:TYR:HB2	1:75:A:VAL:HG11	4	0.1
(1,815)	1:88:A:TYR:HB2	1:75:A:VAL:HG12	4	0.1
(1,815)	1:88:A:TYR:HB2	1:75:A:VAL:HG13	4	0.1
(1,815)	1:88:A:TYR:HB2	1:75:A:VAL:HG21	4	0.1
(1,815)	1:88:A:TYR:HB2	1:75:A:VAL:HG22	4	0.1
(1,815)	1:88:A:TYR:HB2	1:75:A:VAL:HG23	4	0.1
(1,815)	1:88:A:TYR:HB3	1:75:A:VAL:HG11	4	0.1
(1,815)	1:88:A:TYR:HB3	1:75:A:VAL:HG12	4	0.1
(1,815)	1:88:A:TYR:HB3	1:75:A:VAL:HG13	4	0.1
(1,815)	1:88:A:TYR:HB3	1:75:A:VAL:HG21	4	0.1
(1,815)	1:88:A:TYR:HB3	1:75:A:VAL:HG22	4	0.1
(1,815)	1:88:A:TYR:HB3	1:75:A:VAL:HG23	4	0.1
(1,797)	1:85:A:ILE:HA	1:74:A:PHE:HD1	3	0.1
(1,797)	1:85:A:ILE:HA	1:74:A:PHE:HD2	3	0.1
(1,797)	1:85:A:ILE:HA	1:74:A:PHE:HD1	8	0.1
(1,797)	1:85:A:ILE:HA	1:74:A:PHE:HD2	8	0.1
(1,797)	1:85:A:ILE:HA	1:74:A:PHE:HD1	14	0.1
(1,797)	1:85:A:ILE:HA	1:74:A:PHE:HD2	14	0.1
(1,797)	1:85:A:ILE:HA	1:74:A:PHE:HD1	22	0.1
(1,797)	1:85:A:ILE:HA	1:74:A:PHE:HD2	22	0.1
(1,786)	1:83:A:TYR:HA	1:85:A:ILE:HD11	1	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,786)	1:83:A:TYR:HA	1:85:A:ILE:HD12	1	0.1
(1,786)	1:83:A:TYR:HA	1:85:A:ILE:HD13	1	0.1
(1,786)	1:83:A:TYR:HA	1:85:A:ILE:HD11	6	0.1
(1,786)	1:83:A:TYR:HA	1:85:A:ILE:HD12	6	0.1
(1,786)	1:83:A:TYR:HA	1:85:A:ILE:HD13	6	0.1
(1,786)	1:83:A:TYR:HA	1:85:A:ILE:HD11	7	0.1
(1,786)	1:83:A:TYR:HA	1:85:A:ILE:HD12	7	0.1
(1,786)	1:83:A:TYR:HA	1:85:A:ILE:HD13	7	0.1
(1,786)	1:83:A:TYR:HA	1:85:A:ILE:HD11	9	0.1
(1,786)	1:83:A:TYR:HA	1:85:A:ILE:HD12	9	0.1
(1,786)	1:83:A:TYR:HA	1:85:A:ILE:HD13	9	0.1
(1,786)	1:83:A:TYR:HA	1:85:A:ILE:HD11	22	0.1
(1,786)	1:83:A:TYR:HA	1:85:A:ILE:HD12	22	0.1
(1,786)	1:83:A:TYR:HA	1:85:A:ILE:HD13	22	0.1
(1,786)	1:83:A:TYR:HA	1:85:A:ILE:HD11	24	0.1
(1,786)	1:83:A:TYR:HA	1:85:A:ILE:HD12	24	0.1
(1,786)	1:83:A:TYR:HA	1:85:A:ILE:HD13	24	0.1
(1,776)	1:75:A:VAL:HG11	1:73:A:CYS:HB2	9	0.1
(1,776)	1:75:A:VAL:HG11	1:73:A:CYS:HB3	9	0.1
(1,776)	1:75:A:VAL:HG12	1:73:A:CYS:HB2	9	0.1
(1,776)	1:75:A:VAL:HG12	1:73:A:CYS:HB3	9	0.1
(1,776)	1:75:A:VAL:HG13	1:73:A:CYS:HB2	9	0.1
(1,776)	1:75:A:VAL:HG13	1:73:A:CYS:HB3	9	0.1
(1,776)	1:75:A:VAL:HG11	1:73:A:CYS:HB2	12	0.1
(1,776)	1:75:A:VAL:HG11	1:73:A:CYS:HB3	12	0.1
(1,776)	1:75:A:VAL:HG12	1:73:A:CYS:HB2	12	0.1
(1,776)	1:75:A:VAL:HG12	1:73:A:CYS:HB3	12	0.1
(1,776)	1:75:A:VAL:HG13	1:73:A:CYS:HB2	12	0.1
(1,776)	1:75:A:VAL:HG13	1:73:A:CYS:HB3	12	0.1
(1,776)	1:75:A:VAL:HG11	1:73:A:CYS:HB2	14	0.1
(1,776)	1:75:A:VAL:HG11	1:73:A:CYS:HB3	14	0.1
(1,776)	1:75:A:VAL:HG12	1:73:A:CYS:HB2	14	0.1
(1,776)	1:75:A:VAL:HG12	1:73:A:CYS:HB3	14	0.1
(1,776)	1:75:A:VAL:HG13	1:73:A:CYS:HB2	14	0.1
(1,776)	1:75:A:VAL:HG13	1:73:A:CYS:HB3	14	0.1
(1,776)	1:75:A:VAL:HG11	1:73:A:CYS:HB2	17	0.1
(1,776)	1:75:A:VAL:HG11	1:73:A:CYS:HB3	17	0.1
(1,776)	1:75:A:VAL:HG12	1:73:A:CYS:HB2	17	0.1
(1,776)	1:75:A:VAL:HG12	1:73:A:CYS:HB3	17	0.1
(1,776)	1:75:A:VAL:HG13	1:73:A:CYS:HB2	17	0.1
(1,776)	1:75:A:VAL:HG13	1:73:A:CYS:HB3	17	0.1
(1,759)	1:72:A:VAL:HG11	1:85:A:ILE:HB	6	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,759)	1:72:A:VAL:HG12	1:85:A:ILE:HB	6	0.1
(1,759)	1:72:A:VAL:HG13	1:85:A:ILE:HB	6	0.1
(1,759)	1:72:A:VAL:HG21	1:85:A:ILE:HB	6	0.1
(1,759)	1:72:A:VAL:HG22	1:85:A:ILE:HB	6	0.1
(1,759)	1:72:A:VAL:HG23	1:85:A:ILE:HB	6	0.1
(1,759)	1:72:A:VAL:HG11	1:85:A:ILE:HB	11	0.1
(1,759)	1:72:A:VAL:HG12	1:85:A:ILE:HB	11	0.1
(1,759)	1:72:A:VAL:HG13	1:85:A:ILE:HB	11	0.1
(1,759)	1:72:A:VAL:HG21	1:85:A:ILE:HB	11	0.1
(1,759)	1:72:A:VAL:HG22	1:85:A:ILE:HB	11	0.1
(1,759)	1:72:A:VAL:HG23	1:85:A:ILE:HB	11	0.1
(1,738)	1:69:A:CYS:HG	1:52:A:GLN:HA	17	0.1
(1,738)	1:69:A:CYS:HG	1:52:A:GLN:HA	22	0.1
(1,729)	1:63:A:HIS:HA	1:59:A:PRO:HB2	6	0.1
(1,729)	1:63:A:HIS:HA	1:59:A:PRO:HB3	6	0.1
(1,729)	1:63:A:HIS:HA	1:59:A:PRO:HB2	8	0.1
(1,729)	1:63:A:HIS:HA	1:59:A:PRO:HB3	8	0.1
(1,714)	1:55:A:LEU:HB2	1:126:A:LEU:HG	3	0.1
(1,714)	1:55:A:LEU:HB3	1:126:A:LEU:HG	3	0.1
(1,713)	1:55:A:LEU:HD11	1:126:A:LEU:HG	4	0.1
(1,713)	1:55:A:LEU:HD12	1:126:A:LEU:HG	4	0.1
(1,713)	1:55:A:LEU:HD13	1:126:A:LEU:HG	4	0.1
(1,713)	1:55:A:LEU:HD21	1:126:A:LEU:HG	4	0.1
(1,713)	1:55:A:LEU:HD22	1:126:A:LEU:HG	4	0.1
(1,713)	1:55:A:LEU:HD23	1:126:A:LEU:HG	4	0.1
(1,707)	1:54:A:TYR:HE1	1:127:A:ASN:H	15	0.1
(1,707)	1:54:A:TYR:HE2	1:127:A:ASN:H	15	0.1
(1,688)	1:51:A:VAL:HG11	1:128:A:PHE:HB2	20	0.1
(1,688)	1:51:A:VAL:HG11	1:128:A:PHE:HB3	20	0.1
(1,688)	1:51:A:VAL:HG12	1:128:A:PHE:HB2	20	0.1
(1,688)	1:51:A:VAL:HG12	1:128:A:PHE:HB3	20	0.1
(1,688)	1:51:A:VAL:HG13	1:128:A:PHE:HB2	20	0.1
(1,688)	1:51:A:VAL:HG13	1:128:A:PHE:HB3	20	0.1
(1,688)	1:51:A:VAL:HG21	1:128:A:PHE:HB2	20	0.1
(1,688)	1:51:A:VAL:HG21	1:128:A:PHE:HB3	20	0.1
(1,688)	1:51:A:VAL:HG22	1:128:A:PHE:HB2	20	0.1
(1,688)	1:51:A:VAL:HG22	1:128:A:PHE:HB3	20	0.1
(1,688)	1:51:A:VAL:HG23	1:128:A:PHE:HB2	20	0.1
(1,688)	1:51:A:VAL:HG23	1:128:A:PHE:HB3	20	0.1
(1,654)	1:39:A:LEU:HD11	1:88:A:TYR:HE1	6	0.1
(1,654)	1:39:A:LEU:HD11	1:88:A:TYR:HE2	6	0.1
(1,654)	1:39:A:LEU:HD12	1:88:A:TYR:HE1	6	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,654)	1:39:A:LEU:HD12	1:88:A:TYR:HE2	6	0.1
(1,654)	1:39:A:LEU:HD13	1:88:A:TYR:HE1	6	0.1
(1,654)	1:39:A:LEU:HD13	1:88:A:TYR:HE2	6	0.1
(1,654)	1:39:A:LEU:HD21	1:88:A:TYR:HE1	6	0.1
(1,654)	1:39:A:LEU:HD21	1:88:A:TYR:HE2	6	0.1
(1,654)	1:39:A:LEU:HD22	1:88:A:TYR:HE1	6	0.1
(1,654)	1:39:A:LEU:HD22	1:88:A:TYR:HE2	6	0.1
(1,654)	1:39:A:LEU:HD23	1:88:A:TYR:HE1	6	0.1
(1,654)	1:39:A:LEU:HD23	1:88:A:TYR:HE2	6	0.1
(1,646)	1:39:A:LEU:HA	1:88:A:TYR:HB2	10	0.1
(1,646)	1:39:A:LEU:HA	1:88:A:TYR:HB3	10	0.1
(1,646)	1:39:A:LEU:HA	1:88:A:TYR:HB2	11	0.1
(1,646)	1:39:A:LEU:HA	1:88:A:TYR:HB3	11	0.1
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD11	22	0.1
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD12	22	0.1
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD13	22	0.1
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD21	22	0.1
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD22	22	0.1
(1,644)	1:36:A:PHE:HE1	1:90:A:LEU:HD23	22	0.1
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD11	22	0.1
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD12	22	0.1
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD13	22	0.1
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD21	22	0.1
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD22	22	0.1
(1,644)	1:36:A:PHE:HE2	1:90:A:LEU:HD23	22	0.1
(1,639)	1:34:A:ARG:HD2	1:74:A:PHE:HE1	19	0.1
(1,639)	1:34:A:ARG:HD2	1:74:A:PHE:HE2	19	0.1
(1,639)	1:34:A:ARG:HD3	1:74:A:PHE:HE1	19	0.1
(1,639)	1:34:A:ARG:HD3	1:74:A:PHE:HE2	19	0.1
(1,638)	1:34:A:ARG:HB2	1:74:A:PHE:HD1	18	0.1
(1,638)	1:34:A:ARG:HB2	1:74:A:PHE:HD2	18	0.1
(1,638)	1:34:A:ARG:HB3	1:74:A:PHE:HD1	18	0.1
(1,638)	1:34:A:ARG:HB3	1:74:A:PHE:HD2	18	0.1
(1,623)	2:483:B:GLU:H	2:482:B:ASN:HA	11	0.1
(1,623)	2:483:B:GLU:H	2:482:B:ASN:HA	16	0.1
(1,567)	2:457:B:HIS:H	2:456:B:PHE:HB3	10	0.1
(1,567)	2:457:B:HIS:H	2:456:B:PHE:HB3	20	0.1
(1,542)	2:446:B:CYS:H	2:445:B:PRO:HA	2	0.1
(1,531)	1:120:A:ASP:H	1:122:A:CYS:H	1	0.1
(1,531)	1:120:A:ASP:H	1:122:A:CYS:H	4	0.1
(1,531)	1:120:A:ASP:H	1:122:A:CYS:H	8	0.1
(1,529)	1:126:A:LEU:H	1:125:A:GLY:H	23	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,523)	1:116:A:THR:H	1:108:A:SER:HB2	23	0.1
(1,523)	1:116:A:THR:H	1:108:A:SER:HB3	23	0.1
(1,509)	1:114:A:PHE:H	1:110:A:PRO:HD2	9	0.1
(1,509)	1:114:A:PHE:H	1:110:A:PRO:HD3	9	0.1
(1,502)	1:104:A:GLN:H	1:102:A:TYR:HA	10	0.1
(1,496)	1:101:A:LEU:H	1:100:A:GLU:H	24	0.1
(1,486)	1:89:A:GLY:H	1:94:A:ARG:HB2	2	0.1
(1,486)	1:89:A:GLY:H	1:94:A:ARG:HB3	2	0.1
(1,466)	1:52:A:GLN:H	1:128:A:PHE:HB2	17	0.1
(1,466)	1:52:A:GLN:H	1:128:A:PHE:HB3	17	0.1
(1,457)	1:38:A:MET:H	1:34:A:ARG:HD2	11	0.1
(1,457)	1:38:A:MET:H	1:34:A:ARG:HD3	11	0.1
(1,456)	1:35:A:LEU:H	1:31:A:GLU:HA	24	0.1
(1,453)	1:26:A:LEU:H	1:30:A:HIS:H	16	0.1
(1,439)	1:126:A:LEU:H	1:116:A:THR:HG22	5	0.1
(1,439)	1:126:A:LEU:H	1:116:A:THR:HG22	12	0.1
(1,429)	1:101:A:LEU:H	1:84:A:PHE:HB2	2	0.1
(1,429)	1:101:A:LEU:H	1:84:A:PHE:HB3	2	0.1
(1,429)	1:101:A:LEU:H	1:84:A:PHE:HB2	13	0.1
(1,429)	1:101:A:LEU:H	1:84:A:PHE:HB3	13	0.1
(1,427)	1:101:A:LEU:H	1:83:A:TYR:H	9	0.1
(1,427)	1:101:A:LEU:H	1:83:A:TYR:H	22	0.1
(1,417)	1:88:A:TYR:H	1:71:A:ALA:H	3	0.1
(1,416)	1:87:A:LEU:H	1:98:A:GLU:HB2	12	0.1
(1,416)	1:87:A:LEU:H	1:98:A:GLU:HB3	12	0.1
(1,412)	1:84:A:PHE:H	1:76:A:LYS:HB2	19	0.1
(1,412)	1:84:A:PHE:H	1:76:A:LYS:HB3	19	0.1
(1,399)	1:72:A:VAL:H	1:50:A:VAL:HB	15	0.1
(1,374)	1:38:A:MET:H	1:35:A:LEU:HG	11	0.1
(1,366)	1:35:A:LEU:H	1:32:A:ASN:HA	24	0.1
(1,360)	1:32:A:ASN:H	1:29:A:ASP:HA	13	0.1
(1,360)	1:32:A:ASN:H	1:29:A:ASP:HA	17	0.1
(1,360)	1:32:A:ASN:H	1:29:A:ASP:HA	21	0.1
(1,346)	1:148:A:ARG:H	1:147:A:LYS:HA	24	0.1
(1,342)	1:146:A:GLN:H	1:143:A:GLU:HA	21	0.1
(1,342)	1:146:A:GLN:H	1:143:A:GLU:HA	23	0.1
(1,340)	1:146:A:GLN:H	1:145:A:ILE:HB	5	0.1
(1,336)	1:145:A:ILE:H	1:144:A:LYS:HA	19	0.1
(1,320)	1:141:A:VAL:H	1:138:A:ARG:HA	3	0.1
(1,300)	1:136:A:ALA:H	1:132:A:ASP:HA	16	0.1
(1,265)	1:121:A:ASP:H	1:120:A:ASP:H	2	0.1
(1,250)	1:116:A:THR:H	1:115:A:HIS:HB3	10	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,245)	1:114:A:PHE:H	1:113:A:PHE:H	13	0.1
(1,153)	1:82:A:SER:H	1:81:A:LYS:HE2	21	0.1
(1,153)	1:82:A:SER:H	1:81:A:LYS:HE3	21	0.1
(1,119)	1:70:A:GLY:H	1:69:A:CYS:HB2	23	0.1
(1,112)	1:65:A:THR:H	1:64:A:TRP:HB3	2	0.1
(1,112)	1:65:A:THR:H	1:64:A:TRP:HB3	3	0.1
(1,95)	1:57:A:LEU:H	1:56:A:ALA:H	8	0.1
(1,95)	1:57:A:LEU:H	1:56:A:ALA:H	17	0.1
(1,84)	1:54:A:TYR:H	1:53:A:LEU:HB2	18	0.1
(1,84)	1:54:A:TYR:H	1:53:A:LEU:HB3	18	0.1
(1,54)	1:43:A:CYS:H	1:42:A:LYS:HB2	9	0.1
(1,54)	1:43:A:CYS:H	1:42:A:LYS:HB3	9	0.1
(1,44)	1:39:A:LEU:H	1:36:A:PHE:HE1	13	0.1
(1,44)	1:39:A:LEU:H	1:36:A:PHE:HE2	13	0.1
(1,44)	1:39:A:LEU:H	1:36:A:PHE:HE1	22	0.1
(1,44)	1:39:A:LEU:H	1:36:A:PHE:HE2	22	0.1

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

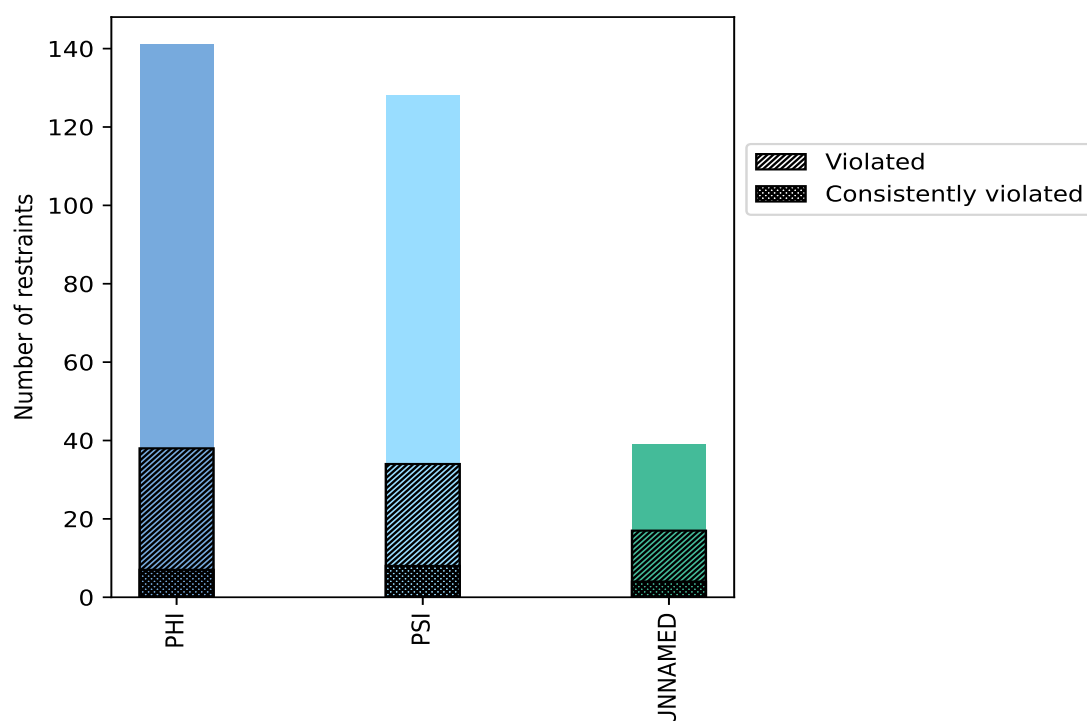
10.1 Summary of dihedral-angle violations [i](#)

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

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PHI	141	45.8	38	27.0	12.3	7	5.0	2.3
PSI	128	41.6	34	26.6	11.0	8	6.2	2.6
UNNAMED	39	12.7	17	43.6	5.5	4	10.3	1.3
Total	308	100.0	89	28.9	28.9	19	6.2	6.2

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

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



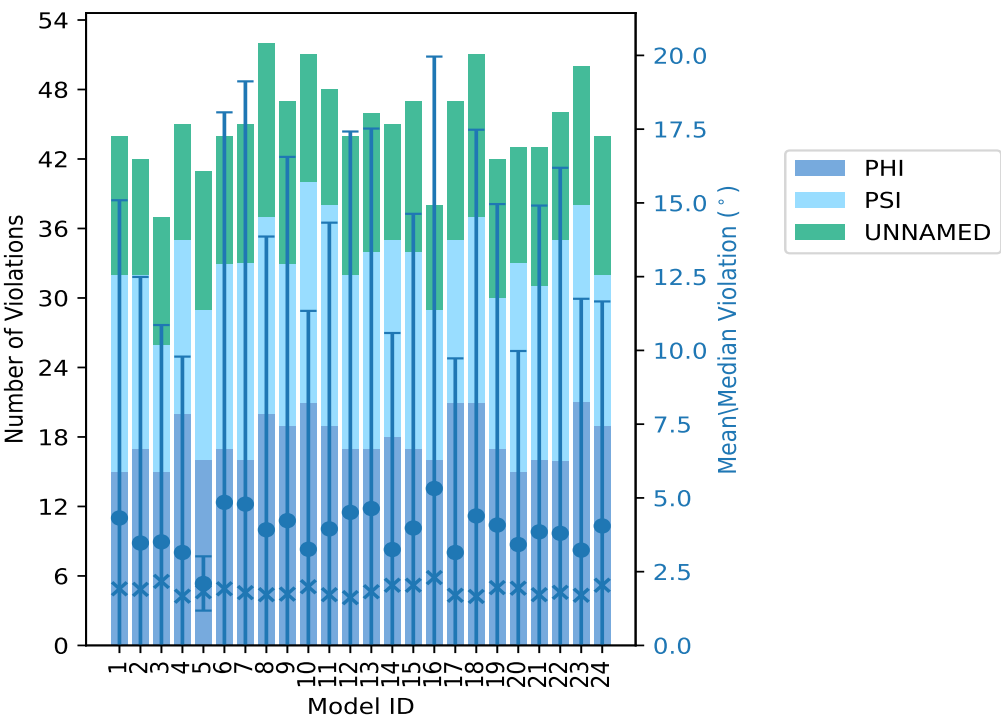
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model

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

Model ID	Number of violations				Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	UNNAMED	Total				
1	15	17	12	44	4.32	59.41	10.77	1.92
2	17	15	10	42	3.47	61.02	9.02	1.9
3	15	11	11	37	3.51	47.23	7.35	2.17
4	20	15	10	45	3.15	45.55	6.64	1.67
5	16	13	12	41	2.1	4.88	0.92	1.82
6	17	16	11	44	4.85	79.34	13.22	1.92
7	16	17	12	45	4.79	95.73	14.33	1.79
8	20	17	15	52	3.92	60.38	9.94	1.72
9	19	14	14	47	4.23	83.93	12.33	1.74
10	21	19	11	51	3.26	60.05	8.08	1.99
11	19	19	10	48	3.95	71.57	10.38	1.72
12	17	15	12	44	4.51	85.72	12.91	1.62
13	17	17	12	46	4.64	81.12	12.88	1.82
14	18	17	10	45	3.25	51.57	7.34	2.04
15	17	17	13	47	3.98	74.72	10.65	2.04
16	16	13	9	38	5.32	88.16	14.64	2.3
17	21	14	12	47	3.15	46.31	6.58	1.7
18	21	16	14	51	4.39	87.3	13.09	1.66
19	17	13	12	42	4.08	72.76	10.88	1.96
20	15	18	10	43	3.42	40.2	6.56	1.94
21	16	15	12	43	3.85	75.07	11.06	1.72
22	16	19	11	46	3.8	86.7	12.39	1.8
23	21	17	12	50	3.23	62.55	8.52	1.7
24	19	13	12	44	4.05	38.34	7.61	2.04

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	UNNAMED	Total	Count ¹	%
7	5	0	12	1	4.2
1	4	2	7	2	8.3
2	1	1	4	3	12.5
2	1	0	3	4	16.7
0	2	1	3	5	20.8
4	1	0	5	6	25.0
0	1	0	1	7	29.2
2	2	1	5	8	33.3
2	1	0	3	9	37.5
0	2	0	2	10	41.7
2	0	0	2	11	45.8

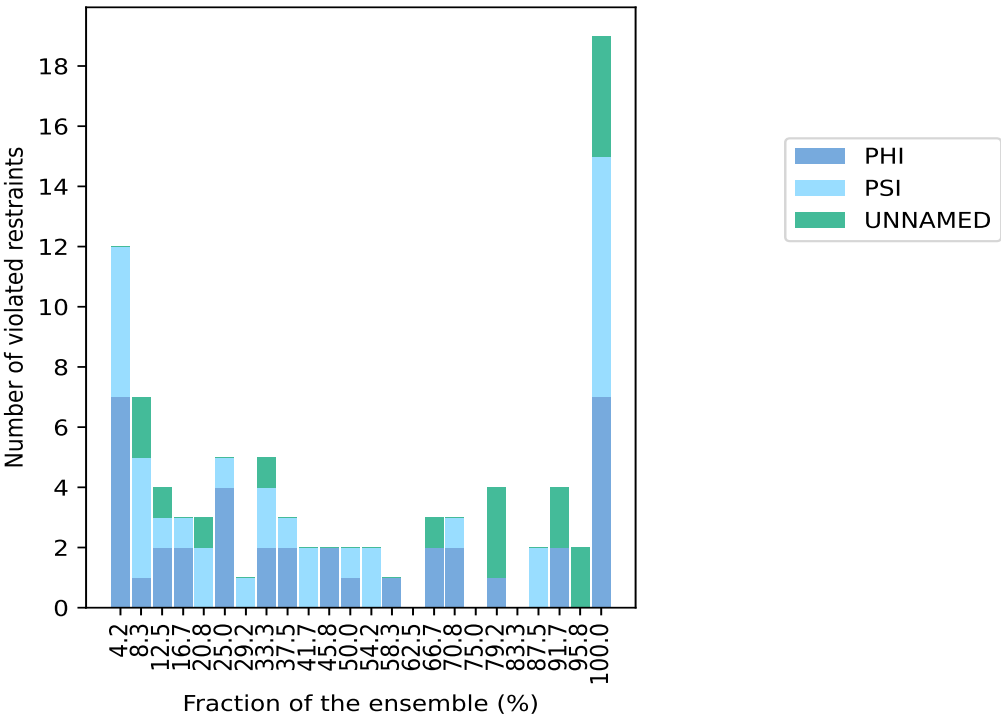
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Number of violated restraints				Fraction of the ensemble	
PHI	PSI	UNNAMED	Total	Count ¹	%
1	1	0	2	12	50.0
0	2	0	2	13	54.2
1	0	0	1	14	58.3
0	0	0	0	15	62.5
2	0	1	3	16	66.7
2	1	0	3	17	70.8
0	0	0	0	18	75.0
1	0	3	4	19	79.2
0	0	0	0	20	83.3
0	2	0	2	21	87.5
2	0	2	4	22	91.7
0	0	2	2	23	95.8
7	8	4	19	24	100.0

¹ Number of models with violations

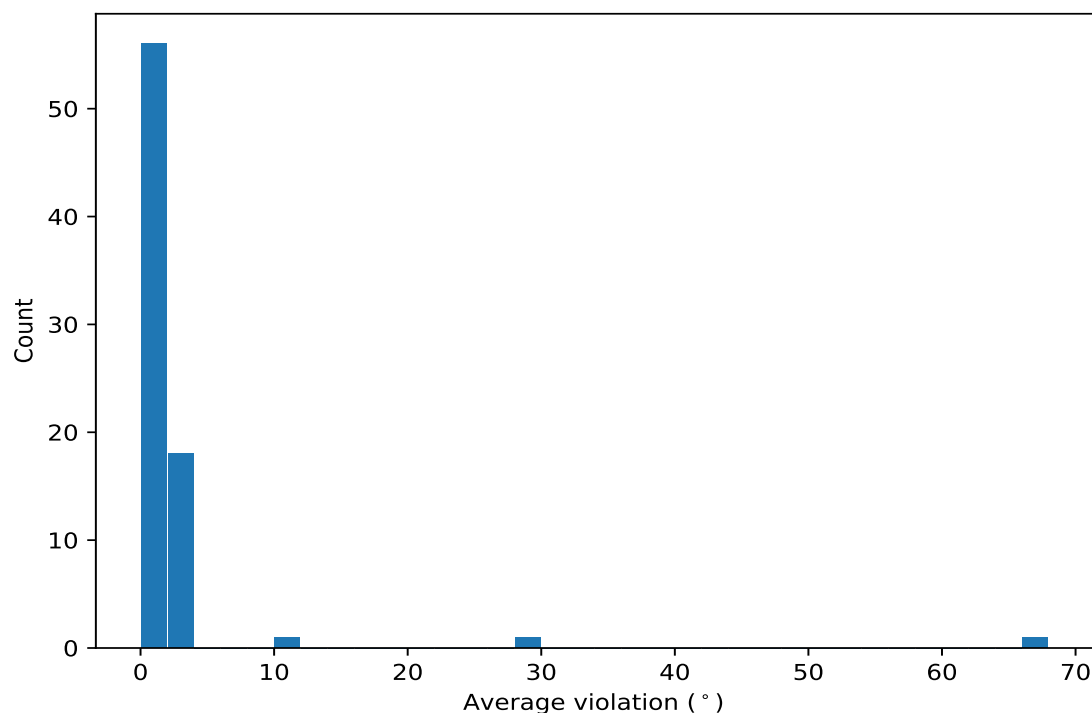
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble ⓘ



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

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

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



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,260)	2:452:B:SER:C	2:453:B:ARG:N	2:453:B:ARG:CA	2:453:B:ARG:C	24	3.93	0.29	3.88
(1,142)	1:83:A:TYR:N	1:83:A:TYR:CA	1:83:A:TYR:C	1:84:A:PHE:N	24	3.62	0.47	3.63
(1,279)	1:75:A:VAL:H	1:75:A:VAL:N	1:111:A:THR:N	1:111:A:THR:H	24	3.52	1.09	3.7
(1,242)	2:465:B:PRO:N	2:465:B:PRO:CA	2:465:B:PRO:C	2:466:B:GLU:N	24	3.35	0.33	3.28
(1,222)	2:474:B:SER:C	2:475:B:TYR:N	2:475:B:TYR:CA	2:475:B:TYR:C	24	3.25	0.59	3.28
(1,203)	2:450:B:TRP:C	2:451:B:GLU:N	2:451:B:GLU:CA	2:451:B:GLU:C	24	3.24	0.3	3.24
(1,167)	1:129:A:ALA:N	1:129:A:ALA:CA	1:129:A:ALA:C	1:130:A:ASP:N	24	2.84	0.35	2.76
(1,270)	1:51:A:VAL:H	1:51:A:VAL:N	1:60:A:GLY:N	1:60:A:GLY:H	24	2.77	0.72	2.77
(1,80)	1:129:A:ALA:C	1:130:A:ASP:N	1:130:A:ASP:CA	1:130:A:ASP:C	24	2.67	0.41	2.63
(1,231)	2:450:B:TRP:N	2:450:B:TRP:CA	2:450:B:TRP:C	2:451:B:GLU:N	24	2.66	0.33	2.66
(1,265)	2:455:B:TYR:N	2:455:B:TYR:CA	2:455:B:TYR:C	2:456:B:PHE:N	24	2.64	0.62	2.76
(1,233)	2:452:B:SER:N	2:452:B:SER:CA	2:452:B:SER:C	2:453:B:ARG:N	24	2.62	0.2	2.62
(1,205)	2:456:B:PHE:C	2:457:B:HIS:N	2:457:B:HIS:CA	2:457:B:HIS:C	24	2.51	0.3	2.54

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,267)	2:456:B:PHE:N	2:456:B:PHE:CA	2:456:B:PHE:C	2:457:B:HIS:N	24	2.49	0.36	2.4
(1,232)	2:451:B:GLU:N	2:451:B:GLU:CA	2:451:B:GLU:C	2:452:B:SER:N	24	2.22	0.31	2.28
(1,26)	1:52:A:GLN:C	1:53:A:LEU:N	1:53:A:LEU:CA	1:53:A:LEU:C	24	1.82	0.47	1.68
(1,280)	1:51:A:VAL:H	1:51:A:VAL:N	1:122:A:CYS:N	1:122:A:CYS:H	24	1.8	0.41	1.68
(1,285)	1:60:A:GLY:H	1:60:A:GLY:N	1:93:A:GLY:N	1:93:A:GLY:H	24	1.58	0.32	1.58
(1,204)	2:451:B:GLU:C	2:452:B:SER:N	2:452:B:SER:CA	2:452:B:SER:C	24	1.51	0.08	1.51
(1,308)	1:35:A:LEU:H	1:35:A:LEU:N	1:75:A:VAL:N	1:75:A:VAL:H	23	1.89	0.51	1.81
(1,307)	1:31:A:GLU:H	1:31:A:GLU:N	1:51:A:VAL:N	1:51:A:VAL:H	23	1.8	0.24	1.78
(1,276)	1:64:A:TRP:H	1:64:A:TRP:N	1:75:A:VAL:N	1:75:A:VAL:H	22	67.65	17.42	72.16
(1,288)	1:75:A:VAL:H	1:75:A:VAL:N	1:127:A:ASN:N	1:127:A:ASN:H	22	1.99	0.65	1.84
(1,266)	2:455:B:TYR:C	2:456:B:PHE:N	2:456:B:PHE:CA	2:456:B:PHE:C	22	1.73	0.29	1.72
(1,34)	1:63:A:HIS:C	1:64:A:TRP:N	1:64:A:TRP:CA	1:64:A:TRP:C	22	1.39	0.22	1.31
(1,230)	2:449:B:GLU:N	2:449:B:GLU:CA	2:449:B:GLU:C	2:450:B:TRP:N	21	1.95	0.65	1.84
(1,244)	2:467:B:PRO:N	2:467:B:PRO:CA	2:467:B:PRO:C	2:468:B:TYR:N	21	1.43	0.19	1.43
(1,274)	1:61:A:ALA:H	1:61:A:ALA:N	1:75:A:VAL:N	1:75:A:VAL:H	19	28.4	16.37	26.51
(1,278)	1:75:A:VAL:H	1:75:A:VAL:N	1:114:A:PHE:N	1:114:A:PHE:H	19	2.17	0.47	2.17
(1,273)	1:60:A:GLY:H	1:60:A:GLY:N	1:89:A:GLY:N	1:89:A:GLY:H	19	1.92	0.47	1.81
(1,37)	1:67:A:GLU:C	1:68:A:HIS:N	1:68:A:HIS:CA	1:68:A:HIS:C	19	1.36	0.22	1.3
(1,206)	2:457:B:HIS:C	2:458:B:PRO:N	2:458:B:PRO:CA	2:458:B:PRO:C	17	2.13	0.93	1.86
(1,268)	2:469:B:VAL:C	2:470:B:GLN:N	2:470:B:GLN:CA	2:470:B:GLN:C	17	1.46	0.43	1.34
(1,263)	2:454:B:PHE:N	2:454:B:PHE:CA	2:454:B:PHE:C	2:455:B:TYR:N	17	1.31	0.24	1.25
(1,284)	1:60:A:GLY:H	1:60:A:GLY:N	1:111:A:THR:N	1:111:A:THR:H	16	1.63	0.33	1.63
(1,79)	1:128:A:PHE:C	1:129:A:ALA:N	1:129:A:ALA:CA	1:129:A:ALA:C	16	1.63	0.37	1.72
(1,81)	1:130:A:ASP:C	1:131:A:GLU:N	1:131:A:GLU:CA	1:131:A:GLU:C	16	1.6	0.45	1.46
(1,55)	1:92:A:ALA:C	1:93:A:GLY:N	1:93:A:GLY:CA	1:93:A:GLY:C	14	1.29	0.21	1.25
(1,236)	2:459:B:ILE:N	2:459:B:ILE:CA	2:459:B:ILE:C	2:460:B:SER:N	13	1.77	0.46	1.71
(1,250)	2:474:B:SER:N	2:474:B:SER:CA	2:474:B:SER:C	2:475:B:TYR:N	13	1.68	0.55	1.52
(1,25)	1:50:A:VAL:C	1:51:A:VAL:N	1:51:A:VAL:CA	1:51:A:VAL:C	12	1.67	0.4	1.76
(1,129)	1:63:A:HIS:N	1:63:A:HIS:CA	1:63:A:HIS:C	1:64:A:TRP:N	12	1.2	0.14	1.17
(1,28)	1:55:A:LEU:C	1:56:A:ALA:N	1:56:A:ALA:CA	1:56:A:ALA:C	11	1.28	0.19	1.23
(1,264)	2:454:B:PHE:C	2:455:B:TYR:N	2:455:B:TYR:CA	2:455:B:TYR:C	11	1.17	0.13	1.15
(1,139)	1:80:A:GLN:N	1:80:A:GLN:CA	1:80:A:GLN:C	1:81:A:LYS:N	10	1.34	0.22	1.33
(1,125)	1:57:A:LEU:N	1:57:A:LEU:CA	1:57:A:LEU:C	1:58:A:PRO:N	10	1.19	0.19	1.1
(1,223)	2:475:B:TYR:C	2:476:B:PRO:N	2:476:B:PRO:CA	2:476:B:PRO:C	9	1.45	0.31	1.38
(1,72)	1:115:A:HIS:C	1:116:A:THR:N	1:116:A:THR:CA	1:116:A:THR:C	9	1.23	0.21	1.15
(1,254)	2:479:B:LEU:N	2:479:B:LEU:CA	2:479:B:LEU:C	2:480:B:ALA:N	9	1.2	0.19	1.16
(1,24)	1:47:A:ALA:C	1:48:A:THR:N	1:48:A:THR:CA	1:48:A:THR:C	8	1.76	0.48	1.86
(1,221)	2:473:B:LYS:C	2:474:B:SER:N	2:474:B:SER:CA	2:474:B:SER:C	8	1.25	0.21	1.18
(1,153)	1:101:A:LEU:N	1:101:A:LEU:CA	1:101:A:LEU:C	1:102:A:TYR:N	8	1.2	0.15	1.16
(1,120)	1:47:A:ALA:N	1:47:A:ALA:CA	1:47:A:ALA:C	1:48:A:THR:N	8	1.19	0.18	1.16
(1,305)	1:85:A:ILE:H	1:85:A:ILE:N	2:479:B:LEU:N	2:479:B:LEU:H	8	1.12	0.07	1.12
(1,261)	2:453:B:ARG:N	2:453:B:ARG:CA	2:453:B:ARG:C	2:454:B:PHE:N	7	1.13	0.19	1.06
(1,156)	1:105:A:LEU:N	1:105:A:LEU:CA	1:105:A:LEU:C	1:106:A:VAL:N	6	1.41	0.35	1.36
(1,225)	2:477:B:SER:C	2:478:B:LYS:N	2:478:B:LYS:CA	2:478:B:LYS:C	6	1.36	0.17	1.32
(1,202)	2:449:B:GLU:C	2:450:B:TRP:N	2:450:B:TRP:CA	2:450:B:TRP:C	6	1.36	0.19	1.4
(1,207)	2:458:B:PRO:C	2:459:B:ILE:N	2:459:B:ILE:CA	2:459:B:ILE:C	6	1.28	0.35	1.13
(1,208)	2:459:B:ILE:C	2:460:B:SER:N	2:460:B:SER:CA	2:460:B:SER:C	6	1.16	0.09	1.15
(1,275)	1:63:A:HIS:H	1:63:A:HIS:N	1:75:A:VAL:N	1:75:A:VAL:H	5	10.3	10.74	6.44
(1,145)	1:86:A:ARG:N	1:86:A:ARG:CA	1:86:A:ARG:C	1:87:A:LEU:N	5	1.41	0.24	1.37
(1,249)	2:473:B:LYS:N	2:473:B:LYS:CA	2:473:B:LYS:C	2:474:B:SER:N	5	1.4	0.26	1.52
(1,51)	1:86:A:ARG:C	1:87:A:LEU:N	1:87:A:LEU:CA	1:87:A:LEU:C	4	1.32	0.21	1.36

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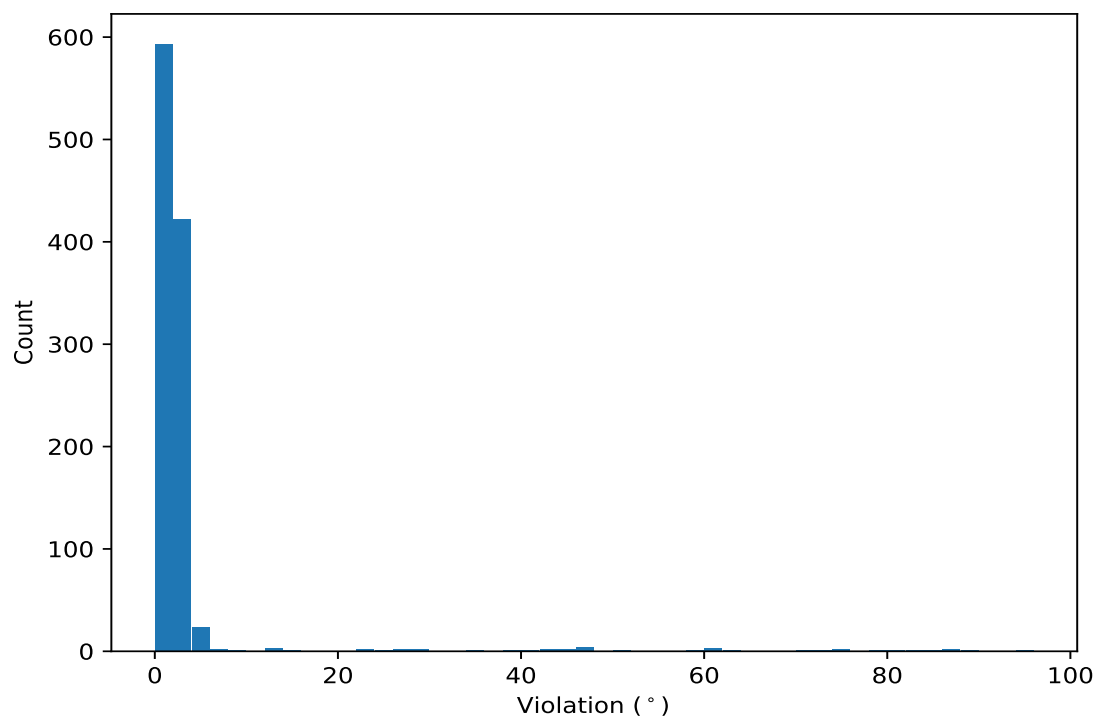
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,70)	1:113:A:PHE:C	1:114:A:PHE:N	1:114:A:PHE:CA	1:114:A:PHE:C	4	1.14	0.08	1.16
(1,151)	1:97:A:TRP:N	1:97:A:TRP:CA	1:97:A:TRP:C	1:98:A:GLU:N	4	1.12	0.09	1.12
(1,157)	1:108:A:SER:N	1:108:A:SER:CA	1:108:A:SER:C	1:109:A:THR:N	3	1.46	0.24	1.59
(1,46)	1:81:A:LYS:C	1:82:A:SER:N	1:82:A:SER:CA	1:82:A:SER:C	3	1.24	0.19	1.26
(1,47)	1:82:A:SER:C	1:83:A:TYR:N	1:83:A:TYR:CA	1:83:A:TYR:C	3	1.18	0.13	1.21
(1,281)	1:52:A:GLN:H	1:52:A:GLN:N	1:75:A:VAL:N	1:75:A:VAL:H	3	1.12	0.06	1.1
(1,65)	1:105:A:LEU:C	1:106:A:VAL:N	1:106:A:VAL:CA	1:106:A:VAL:C	2	2.06	0.19	2.06
(1,239)	2:462:B:LEU:N	2:462:B:LEU:CA	2:462:B:LEU:C	2:463:B:PRO:N	2	1.38	0.28	1.38
(1,292)	1:60:A:GLY:H	1:60:A:GLY:N	1:64:A:TRP:N	1:64:A:TRP:H	2	1.31	0.03	1.31
(1,122)	1:51:A:VAL:N	1:51:A:VAL:CA	1:51:A:VAL:C	1:52:A:GLN:N	2	1.24	0.05	1.24
(1,140)	1:81:A:LYS:N	1:81:A:LYS:CA	1:81:A:LYS:C	1:82:A:SER:N	2	1.2	0.05	1.2
(1,302)	1:51:A:VAL:H	1:51:A:VAL:N	2:470:B:GLN:N	2:470:B:GLN:H	2	1.11	0.1	1.11
(1,131)	1:66:A:LYS:N	1:66:A:LYS:CA	1:66:A:LYS:C	1:67:A:GLU:N	2	1.09	0.09	1.09

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

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

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

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



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,276)	1:64:A:TRP:H	1:64:A:TRP:N	1:75:A:VAL:N	1:75:A:VAL:H	7	95.73
(1,276)	1:64:A:TRP:H	1:64:A:TRP:N	1:75:A:VAL:N	1:75:A:VAL:H	16	88.16
(1,276)	1:64:A:TRP:H	1:64:A:TRP:N	1:75:A:VAL:N	1:75:A:VAL:H	18	87.3
(1,276)	1:64:A:TRP:H	1:64:A:TRP:N	1:75:A:VAL:N	1:75:A:VAL:H	22	86.7
(1,276)	1:64:A:TRP:H	1:64:A:TRP:N	1:75:A:VAL:N	1:75:A:VAL:H	12	85.72
(1,276)	1:64:A:TRP:H	1:64:A:TRP:N	1:75:A:VAL:N	1:75:A:VAL:H	9	83.93
(1,276)	1:64:A:TRP:H	1:64:A:TRP:N	1:75:A:VAL:N	1:75:A:VAL:H	13	81.12
(1,276)	1:64:A:TRP:H	1:64:A:TRP:N	1:75:A:VAL:N	1:75:A:VAL:H	6	79.34
(1,276)	1:64:A:TRP:H	1:64:A:TRP:N	1:75:A:VAL:N	1:75:A:VAL:H	21	75.07
(1,276)	1:64:A:TRP:H	1:64:A:TRP:N	1:75:A:VAL:N	1:75:A:VAL:H	15	74.72
(1,276)	1:64:A:TRP:H	1:64:A:TRP:N	1:75:A:VAL:N	1:75:A:VAL:H	19	72.76
(1,276)	1:64:A:TRP:H	1:64:A:TRP:N	1:75:A:VAL:N	1:75:A:VAL:H	11	71.57
(1,276)	1:64:A:TRP:H	1:64:A:TRP:N	1:75:A:VAL:N	1:75:A:VAL:H	23	62.55
(1,276)	1:64:A:TRP:H	1:64:A:TRP:N	1:75:A:VAL:N	1:75:A:VAL:H	2	61.02
(1,274)	1:61:A:ALA:H	1:61:A:ALA:N	1:75:A:VAL:N	1:75:A:VAL:H	8	60.38
(1,276)	1:64:A:TRP:H	1:64:A:TRP:N	1:75:A:VAL:N	1:75:A:VAL:H	10	60.05
(1,276)	1:64:A:TRP:H	1:64:A:TRP:N	1:75:A:VAL:N	1:75:A:VAL:H	1	59.41
(1,274)	1:61:A:ALA:H	1:61:A:ALA:N	1:75:A:VAL:N	1:75:A:VAL:H	14	51.57
(1,276)	1:64:A:TRP:H	1:64:A:TRP:N	1:75:A:VAL:N	1:75:A:VAL:H	3	47.23
(1,274)	1:61:A:ALA:H	1:61:A:ALA:N	1:75:A:VAL:N	1:75:A:VAL:H	6	47.12
(1,274)	1:61:A:ALA:H	1:61:A:ALA:N	1:75:A:VAL:N	1:75:A:VAL:H	1	46.9
(1,276)	1:64:A:TRP:H	1:64:A:TRP:N	1:75:A:VAL:N	1:75:A:VAL:H	17	46.31
(1,276)	1:64:A:TRP:H	1:64:A:TRP:N	1:75:A:VAL:N	1:75:A:VAL:H	4	45.55
(1,276)	1:64:A:TRP:H	1:64:A:TRP:N	1:75:A:VAL:N	1:75:A:VAL:H	8	45.47
(1,274)	1:61:A:ALA:H	1:61:A:ALA:N	1:75:A:VAL:N	1:75:A:VAL:H	18	43.4
(1,274)	1:61:A:ALA:H	1:61:A:ALA:N	1:75:A:VAL:N	1:75:A:VAL:H	13	42.79
(1,276)	1:64:A:TRP:H	1:64:A:TRP:N	1:75:A:VAL:N	1:75:A:VAL:H	20	40.2
(1,276)	1:64:A:TRP:H	1:64:A:TRP:N	1:75:A:VAL:N	1:75:A:VAL:H	24	38.34
(1,274)	1:61:A:ALA:H	1:61:A:ALA:N	1:75:A:VAL:N	1:75:A:VAL:H	16	35.36
(1,275)	1:63:A:HIS:H	1:63:A:HIS:N	1:75:A:VAL:N	1:75:A:VAL:H	24	29.92
(1,274)	1:61:A:ALA:H	1:61:A:ALA:N	1:75:A:VAL:N	1:75:A:VAL:H	7	29.65
(1,274)	1:61:A:ALA:H	1:61:A:ALA:N	1:75:A:VAL:N	1:75:A:VAL:H	9	27.21
(1,274)	1:61:A:ALA:H	1:61:A:ALA:N	1:75:A:VAL:N	1:75:A:VAL:H	24	26.51
(1,274)	1:61:A:ALA:H	1:61:A:ALA:N	1:75:A:VAL:N	1:75:A:VAL:H	12	25.53
(1,274)	1:61:A:ALA:H	1:61:A:ALA:N	1:75:A:VAL:N	1:75:A:VAL:H	11	23.79
(1,274)	1:61:A:ALA:H	1:61:A:ALA:N	1:75:A:VAL:N	1:75:A:VAL:H	20	23.14
(1,274)	1:61:A:ALA:H	1:61:A:ALA:N	1:75:A:VAL:N	1:75:A:VAL:H	15	15.94
(1,275)	1:63:A:HIS:H	1:63:A:HIS:N	1:75:A:VAL:N	1:75:A:VAL:H	4	12.97
(1,274)	1:61:A:ALA:H	1:61:A:ALA:N	1:75:A:VAL:N	1:75:A:VAL:H	19	12.51
(1,274)	1:61:A:ALA:H	1:61:A:ALA:N	1:75:A:VAL:N	1:75:A:VAL:H	17	12.08
(1,274)	1:61:A:ALA:H	1:61:A:ALA:N	1:75:A:VAL:N	1:75:A:VAL:H	21	8.07
(1,275)	1:63:A:HIS:H	1:63:A:HIS:N	1:75:A:VAL:N	1:75:A:VAL:H	12	6.44
(1,279)	1:75:A:VAL:H	1:75:A:VAL:N	1:111:A:THR:N	1:111:A:THR:H	7	6.11
(1,279)	1:75:A:VAL:H	1:75:A:VAL:N	1:111:A:THR:N	1:111:A:THR:H	5	4.88
(1,279)	1:75:A:VAL:H	1:75:A:VAL:N	1:111:A:THR:N	1:111:A:THR:H	23	4.6
(1,279)	1:75:A:VAL:H	1:75:A:VAL:N	1:111:A:THR:N	1:111:A:THR:H	3	4.55
(1,142)	1:83:A:TYR:N	1:83:A:TYR:CA	1:83:A:TYR:C	1:84:A:PHE:N	10	4.53

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,142)	1:83:A:TYR:N	1:83:A:TYR:CA	1:83:A:TYR:C	1:84:A:PHE:N	4	4.47
(1,222)	2:474:B:SER:C	2:475:B:TYR:N	2:475:B:TYR:CA	2:475:B:TYR:C	3	4.43
(1,260)	2:452:B:SER:C	2:453:B:ARG:N	2:453:B:ARG:CA	2:453:B:ARG:C	6	4.37
(1,260)	2:452:B:SER:C	2:453:B:ARG:N	2:453:B:ARG:CA	2:453:B:ARG:C	19	4.34
(1,260)	2:452:B:SER:C	2:453:B:ARG:N	2:453:B:ARG:CA	2:453:B:ARG:C	21	4.33
(1,260)	2:452:B:SER:C	2:453:B:ARG:N	2:453:B:ARG:CA	2:453:B:ARG:C	12	4.29
(1,260)	2:452:B:SER:C	2:453:B:ARG:N	2:453:B:ARG:CA	2:453:B:ARG:C	13	4.29
(1,142)	1:83:A:TYR:N	1:83:A:TYR:CA	1:83:A:TYR:C	1:84:A:PHE:N	24	4.29
(1,270)	1:51:A:VAL:H	1:51:A:VAL:N	1:60:A:GLY:N	1:60:A:GLY:H	13	4.25
(1,279)	1:75:A:VAL:H	1:75:A:VAL:N	1:111:A:THR:N	1:111:A:THR:H	2	4.24
(1,142)	1:83:A:TYR:N	1:83:A:TYR:CA	1:83:A:TYR:C	1:84:A:PHE:N	14	4.23
(1,279)	1:75:A:VAL:H	1:75:A:VAL:N	1:111:A:THR:N	1:111:A:THR:H	19	4.22
(1,260)	2:452:B:SER:C	2:453:B:ARG:N	2:453:B:ARG:CA	2:453:B:ARG:C	7	4.22
(1,260)	2:452:B:SER:C	2:453:B:ARG:N	2:453:B:ARG:CA	2:453:B:ARG:C	16	4.18
(1,260)	2:452:B:SER:C	2:453:B:ARG:N	2:453:B:ARG:CA	2:453:B:ARG:C	17	4.14
(1,260)	2:452:B:SER:C	2:453:B:ARG:N	2:453:B:ARG:CA	2:453:B:ARG:C	18	4.1
(1,260)	2:452:B:SER:C	2:453:B:ARG:N	2:453:B:ARG:CA	2:453:B:ARG:C	23	4.09
(1,260)	2:452:B:SER:C	2:453:B:ARG:N	2:453:B:ARG:CA	2:453:B:ARG:C	24	4.07
(1,270)	1:51:A:VAL:H	1:51:A:VAL:N	1:60:A:GLY:N	1:60:A:GLY:H	10	4.05
(1,142)	1:83:A:TYR:N	1:83:A:TYR:CA	1:83:A:TYR:C	1:84:A:PHE:N	18	4.0
(1,222)	2:474:B:SER:C	2:475:B:TYR:N	2:475:B:TYR:CA	2:475:B:TYR:C	14	3.99
(1,279)	1:75:A:VAL:H	1:75:A:VAL:N	1:111:A:THR:N	1:111:A:THR:H	20	3.98
(1,279)	1:75:A:VAL:H	1:75:A:VAL:N	1:111:A:THR:N	1:111:A:THR:H	17	3.97
(1,274)	1:61:A:ALA:H	1:61:A:ALA:N	1:75:A:VAL:N	1:75:A:VAL:H	23	3.94
(1,270)	1:51:A:VAL:H	1:51:A:VAL:N	1:60:A:GLY:N	1:60:A:GLY:H	15	3.94
(1,203)	2:450:B:TRP:C	2:451:B:GLU:N	2:451:B:GLU:CA	2:451:B:GLU:C	19	3.94
(1,222)	2:474:B:SER:C	2:475:B:TYR:N	2:475:B:TYR:CA	2:475:B:TYR:C	10	3.93
(1,260)	2:452:B:SER:C	2:453:B:ARG:N	2:453:B:ARG:CA	2:453:B:ARG:C	15	3.89
(1,142)	1:83:A:TYR:N	1:83:A:TYR:CA	1:83:A:TYR:C	1:84:A:PHE:N	6	3.89
(1,260)	2:452:B:SER:C	2:453:B:ARG:N	2:453:B:ARG:CA	2:453:B:ARG:C	22	3.87
(1,142)	1:83:A:TYR:N	1:83:A:TYR:CA	1:83:A:TYR:C	1:84:A:PHE:N	2	3.87
(1,279)	1:75:A:VAL:H	1:75:A:VAL:N	1:111:A:THR:N	1:111:A:THR:H	10	3.84
(1,203)	2:450:B:TRP:C	2:451:B:GLU:N	2:451:B:GLU:CA	2:451:B:GLU:C	11	3.84
(1,142)	1:83:A:TYR:N	1:83:A:TYR:CA	1:83:A:TYR:C	1:84:A:PHE:N	3	3.84
(1,260)	2:452:B:SER:C	2:453:B:ARG:N	2:453:B:ARG:CA	2:453:B:ARG:C	14	3.83
(1,242)	2:465:B:PRO:N	2:465:B:PRO:CA	2:465:B:PRO:C	2:466:B:GLU:N	18	3.83
(1,242)	2:465:B:PRO:N	2:465:B:PRO:CA	2:465:B:PRO:C	2:466:B:GLU:N	21	3.82
(1,222)	2:474:B:SER:C	2:475:B:TYR:N	2:475:B:TYR:CA	2:475:B:TYR:C	23	3.82
(1,142)	1:83:A:TYR:N	1:83:A:TYR:CA	1:83:A:TYR:C	1:84:A:PHE:N	12	3.81
(1,242)	2:465:B:PRO:N	2:465:B:PRO:CA	2:465:B:PRO:C	2:466:B:GLU:N	7	3.8
(1,260)	2:452:B:SER:C	2:453:B:ARG:N	2:453:B:ARG:CA	2:453:B:ARG:C	4	3.79
(1,206)	2:457:B:HIS:C	2:458:B:PRO:N	2:458:B:PRO:CA	2:458:B:PRO:C	8	3.79
(1,260)	2:452:B:SER:C	2:453:B:ARG:N	2:453:B:ARG:CA	2:453:B:ARG:C	1	3.78
(1,242)	2:465:B:PRO:N	2:465:B:PRO:CA	2:465:B:PRO:C	2:466:B:GLU:N	11	3.77
(1,242)	2:465:B:PRO:N	2:465:B:PRO:CA	2:465:B:PRO:C	2:466:B:GLU:N	23	3.77
(1,242)	2:465:B:PRO:N	2:465:B:PRO:CA	2:465:B:PRO:C	2:466:B:GLU:N	2	3.75
(1,222)	2:474:B:SER:C	2:475:B:TYR:N	2:475:B:TYR:CA	2:475:B:TYR:C	5	3.75
(1,279)	1:75:A:VAL:H	1:75:A:VAL:N	1:111:A:THR:N	1:111:A:THR:H	21	3.73
(1,279)	1:75:A:VAL:H	1:75:A:VAL:N	1:111:A:THR:N	1:111:A:THR:H	8	3.72
(1,274)	1:61:A:ALA:H	1:61:A:ALA:N	1:75:A:VAL:N	1:75:A:VAL:H	22	3.72
(1,279)	1:75:A:VAL:H	1:75:A:VAL:N	1:111:A:THR:N	1:111:A:THR:H	1	3.71

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,260)	2:452:B:SER:C	2:453:B:ARG:N	2:453:B:ARG:CA	2:453:B:ARG:C	10	3.71
(1,203)	2:450:B:TRP:C	2:451:B:GLU:N	2:451:B:GLU:CA	2:451:B:GLU:C	17	3.71
(1,279)	1:75:A:VAL:H	1:75:A:VAL:N	1:111:A:THR:N	1:111:A:THR:H	11	3.7
(1,167)	1:129:A:ALA:N	1:129:A:ALA:CA	1:129:A:ALA:C	1:130:A:ASP:N	11	3.7
(1,142)	1:83:A:TYR:N	1:83:A:TYR:CA	1:83:A:TYR:C	1:84:A:PHE:N	9	3.7
(1,260)	2:452:B:SER:C	2:453:B:ARG:N	2:453:B:ARG:CA	2:453:B:ARG:C	9	3.69
(1,260)	2:452:B:SER:C	2:453:B:ARG:N	2:453:B:ARG:CA	2:453:B:ARG:C	3	3.67
(1,260)	2:452:B:SER:C	2:453:B:ARG:N	2:453:B:ARG:CA	2:453:B:ARG:C	5	3.67
(1,142)	1:83:A:TYR:N	1:83:A:TYR:CA	1:83:A:TYR:C	1:84:A:PHE:N	15	3.67
(1,142)	1:83:A:TYR:N	1:83:A:TYR:CA	1:83:A:TYR:C	1:84:A:PHE:N	13	3.64
(1,288)	1:75:A:VAL:H	1:75:A:VAL:N	1:127:A:ASN:N	1:127:A:ASN:H	14	3.63
(1,260)	2:452:B:SER:C	2:453:B:ARG:N	2:453:B:ARG:CA	2:453:B:ARG:C	20	3.63
(1,222)	2:474:B:SER:C	2:475:B:TYR:N	2:475:B:TYR:CA	2:475:B:TYR:C	20	3.63
(1,242)	2:465:B:PRO:N	2:465:B:PRO:CA	2:465:B:PRO:C	2:466:B:GLU:N	3	3.62
(1,222)	2:474:B:SER:C	2:475:B:TYR:N	2:475:B:TYR:CA	2:475:B:TYR:C	18	3.62
(1,206)	2:457:B:HIS:C	2:458:B:PRO:N	2:458:B:PRO:CA	2:458:B:PRO:C	20	3.62
(1,142)	1:83:A:TYR:N	1:83:A:TYR:CA	1:83:A:TYR:C	1:84:A:PHE:N	11	3.62
(1,80)	1:129:A:ALA:C	1:130:A:ASP:N	1:130:A:ASP:CA	1:130:A:ASP:C	11	3.61
(1,242)	2:465:B:PRO:N	2:465:B:PRO:CA	2:465:B:PRO:C	2:466:B:GLU:N	10	3.58
(1,265)	2:455:B:TYR:N	2:455:B:TYR:CA	2:455:B:TYR:C	2:456:B:PHE:N	14	3.57
(1,222)	2:474:B:SER:C	2:475:B:TYR:N	2:475:B:TYR:CA	2:475:B:TYR:C	9	3.57
(1,279)	1:75:A:VAL:H	1:75:A:VAL:N	1:111:A:THR:N	1:111:A:THR:H	9	3.56
(1,242)	2:465:B:PRO:N	2:465:B:PRO:CA	2:465:B:PRO:C	2:466:B:GLU:N	19	3.56
(1,260)	2:452:B:SER:C	2:453:B:ARG:N	2:453:B:ARG:CA	2:453:B:ARG:C	2	3.54
(1,142)	1:83:A:TYR:N	1:83:A:TYR:CA	1:83:A:TYR:C	1:84:A:PHE:N	5	3.54
(1,242)	2:465:B:PRO:N	2:465:B:PRO:CA	2:465:B:PRO:C	2:466:B:GLU:N	22	3.53
(1,242)	2:465:B:PRO:N	2:465:B:PRO:CA	2:465:B:PRO:C	2:466:B:GLU:N	8	3.51
(1,270)	1:51:A:VAL:H	1:51:A:VAL:N	1:60:A:GLY:N	1:60:A:GLY:H	5	3.5
(1,270)	1:51:A:VAL:H	1:51:A:VAL:N	1:60:A:GLY:N	1:60:A:GLY:H	18	3.5
(1,265)	2:455:B:TYR:N	2:455:B:TYR:CA	2:455:B:TYR:C	2:456:B:PHE:N	6	3.5
(1,222)	2:474:B:SER:C	2:475:B:TYR:N	2:475:B:TYR:CA	2:475:B:TYR:C	15	3.49
(1,260)	2:452:B:SER:C	2:453:B:ARG:N	2:453:B:ARG:CA	2:453:B:ARG:C	8	3.47
(1,260)	2:452:B:SER:C	2:453:B:ARG:N	2:453:B:ARG:CA	2:453:B:ARG:C	11	3.47
(1,206)	2:457:B:HIS:C	2:458:B:PRO:N	2:458:B:PRO:CA	2:458:B:PRO:C	17	3.46
(1,222)	2:474:B:SER:C	2:475:B:TYR:N	2:475:B:TYR:CA	2:475:B:TYR:C	22	3.45
(1,222)	2:474:B:SER:C	2:475:B:TYR:N	2:475:B:TYR:CA	2:475:B:TYR:C	24	3.45
(1,265)	2:455:B:TYR:N	2:455:B:TYR:CA	2:455:B:TYR:C	2:456:B:PHE:N	3	3.43
(1,167)	1:129:A:ALA:N	1:129:A:ALA:CA	1:129:A:ALA:C	1:130:A:ASP:N	19	3.43
(1,142)	1:83:A:TYR:N	1:83:A:TYR:CA	1:83:A:TYR:C	1:84:A:PHE:N	23	3.43
(1,203)	2:450:B:TRP:C	2:451:B:GLU:N	2:451:B:GLU:CA	2:451:B:GLU:C	23	3.42
(1,142)	1:83:A:TYR:N	1:83:A:TYR:CA	1:83:A:TYR:C	1:84:A:PHE:N	7	3.41
(1,279)	1:75:A:VAL:H	1:75:A:VAL:N	1:111:A:THR:N	1:111:A:THR:H	12	3.4
(1,203)	2:450:B:TRP:C	2:451:B:GLU:N	2:451:B:GLU:CA	2:451:B:GLU:C	21	3.4
(1,167)	1:129:A:ALA:N	1:129:A:ALA:CA	1:129:A:ALA:C	1:130:A:ASP:N	14	3.39
(1,231)	2:450:B:TRP:N	2:450:B:TRP:CA	2:450:B:TRP:C	2:451:B:GLU:N	11	3.38
(1,167)	1:129:A:ALA:N	1:129:A:ALA:CA	1:129:A:ALA:C	1:130:A:ASP:N	15	3.38
(1,222)	2:474:B:SER:C	2:475:B:TYR:N	2:475:B:TYR:CA	2:475:B:TYR:C	16	3.37
(1,230)	2:449:B:GLU:N	2:449:B:GLU:CA	2:449:B:GLU:C	2:450:B:TRP:N	13	3.36
(1,265)	2:455:B:TYR:N	2:455:B:TYR:CA	2:455:B:TYR:C	2:456:B:PHE:N	5	3.35
(1,203)	2:450:B:TRP:C	2:451:B:GLU:N	2:451:B:GLU:CA	2:451:B:GLU:C	7	3.35
(1,203)	2:450:B:TRP:C	2:451:B:GLU:N	2:451:B:GLU:CA	2:451:B:GLU:C	18	3.34

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,203)	2:450:B:TRP:C	2:451:B:GLU:N	2:451:B:GLU:CA	2:451:B:GLU:C	4	3.32
(1,80)	1:129:A:ALA:C	1:130:A:ASP:N	1:130:A:ASP:CA	1:130:A:ASP:C	15	3.32
(1,203)	2:450:B:TRP:C	2:451:B:GLU:N	2:451:B:GLU:CA	2:451:B:GLU:C	1	3.31
(1,142)	1:83:A:TYR:N	1:83:A:TYR:CA	1:83:A:TYR:C	1:84:A:PHE:N	17	3.3
(1,242)	2:465:B:PRO:N	2:465:B:PRO:CA	2:465:B:PRO:C	2:466:B:GLU:N	12	3.28
(1,242)	2:465:B:PRO:N	2:465:B:PRO:CA	2:465:B:PRO:C	2:466:B:GLU:N	16	3.28
(1,142)	1:83:A:TYR:N	1:83:A:TYR:CA	1:83:A:TYR:C	1:84:A:PHE:N	8	3.28
(1,80)	1:129:A:ALA:C	1:130:A:ASP:N	1:130:A:ASP:CA	1:130:A:ASP:C	8	3.28
(1,308)	1:35:A:LEU:H	1:35:A:LEU:N	1:75:A:VAL:N	1:75:A:VAL:H	23	3.27
(1,279)	1:75:A:VAL:H	1:75:A:VAL:N	1:111:A:THR:N	1:111:A:THR:H	14	3.27
(1,267)	2:456:B:PHE:N	2:456:B:PHE:CA	2:456:B:PHE:C	2:457:B:HIS:N	8	3.27
(1,203)	2:450:B:TRP:C	2:451:B:GLU:N	2:451:B:GLU:CA	2:451:B:GLU:C	12	3.27
(1,142)	1:83:A:TYR:N	1:83:A:TYR:CA	1:83:A:TYR:C	1:84:A:PHE:N	16	3.27
(1,80)	1:129:A:ALA:C	1:130:A:ASP:N	1:130:A:ASP:CA	1:130:A:ASP:C	14	3.27
(1,250)	2:474:B:SER:N	2:474:B:SER:CA	2:474:B:SER:C	2:475:B:TYR:N	3	3.26
(1,203)	2:450:B:TRP:C	2:451:B:GLU:N	2:451:B:GLU:CA	2:451:B:GLU:C	15	3.26
(1,242)	2:465:B:PRO:N	2:465:B:PRO:CA	2:465:B:PRO:C	2:466:B:GLU:N	4	3.24
(1,203)	2:450:B:TRP:C	2:451:B:GLU:N	2:451:B:GLU:CA	2:451:B:GLU:C	9	3.24
(1,203)	2:450:B:TRP:C	2:451:B:GLU:N	2:451:B:GLU:CA	2:451:B:GLU:C	13	3.24
(1,231)	2:450:B:TRP:N	2:450:B:TRP:CA	2:450:B:TRP:C	2:451:B:GLU:N	19	3.23
(1,267)	2:456:B:PHE:N	2:456:B:PHE:CA	2:456:B:PHE:C	2:457:B:HIS:N	9	3.21
(1,203)	2:450:B:TRP:C	2:451:B:GLU:N	2:451:B:GLU:CA	2:451:B:GLU:C	24	3.21
(1,203)	2:450:B:TRP:C	2:451:B:GLU:N	2:451:B:GLU:CA	2:451:B:GLU:C	22	3.2
(1,222)	2:474:B:SER:C	2:475:B:TYR:N	2:475:B:TYR:CA	2:475:B:TYR:C	2	3.19
(1,222)	2:474:B:SER:C	2:475:B:TYR:N	2:475:B:TYR:CA	2:475:B:TYR:C	13	3.19
(1,205)	2:456:B:PHE:C	2:457:B:HIS:N	2:457:B:HIS:CA	2:457:B:HIS:C	3	3.19
(1,142)	1:83:A:TYR:N	1:83:A:TYR:CA	1:83:A:TYR:C	1:84:A:PHE:N	22	3.19
(1,279)	1:75:A:VAL:H	1:75:A:VAL:N	1:111:A:THR:N	1:111:A:THR:H	16	3.18
(1,203)	2:450:B:TRP:C	2:451:B:GLU:N	2:451:B:GLU:CA	2:451:B:GLU:C	16	3.17
(1,265)	2:455:B:TYR:N	2:455:B:TYR:CA	2:455:B:TYR:C	2:456:B:PHE:N	22	3.16
(1,142)	1:83:A:TYR:N	1:83:A:TYR:CA	1:83:A:TYR:C	1:84:A:PHE:N	21	3.16
(1,279)	1:75:A:VAL:H	1:75:A:VAL:N	1:111:A:THR:N	1:111:A:THR:H	22	3.15
(1,265)	2:455:B:TYR:N	2:455:B:TYR:CA	2:455:B:TYR:C	2:456:B:PHE:N	19	3.15
(1,242)	2:465:B:PRO:N	2:465:B:PRO:CA	2:465:B:PRO:C	2:466:B:GLU:N	13	3.15
(1,206)	2:457:B:HIS:C	2:458:B:PRO:N	2:458:B:PRO:CA	2:458:B:PRO:C	7	3.15
(1,270)	1:51:A:VAL:H	1:51:A:VAL:N	1:60:A:GLY:N	1:60:A:GLY:H	21	3.14
(1,203)	2:450:B:TRP:C	2:451:B:GLU:N	2:451:B:GLU:CA	2:451:B:GLU:C	2	3.12
(1,167)	1:129:A:ALA:N	1:129:A:ALA:CA	1:129:A:ALA:C	1:130:A:ASP:N	20	3.12
(1,270)	1:51:A:VAL:H	1:51:A:VAL:N	1:60:A:GLY:N	1:60:A:GLY:H	7	3.11
(1,242)	2:465:B:PRO:N	2:465:B:PRO:CA	2:465:B:PRO:C	2:466:B:GLU:N	20	3.11
(1,222)	2:474:B:SER:C	2:475:B:TYR:N	2:475:B:TYR:CA	2:475:B:TYR:C	17	3.11
(1,203)	2:450:B:TRP:C	2:451:B:GLU:N	2:451:B:GLU:CA	2:451:B:GLU:C	3	3.11
(1,80)	1:129:A:ALA:C	1:130:A:ASP:N	1:130:A:ASP:CA	1:130:A:ASP:C	19	3.11
(1,279)	1:75:A:VAL:H	1:75:A:VAL:N	1:111:A:THR:N	1:111:A:THR:H	15	3.1
(1,231)	2:450:B:TRP:N	2:450:B:TRP:CA	2:450:B:TRP:C	2:451:B:GLU:N	15	3.1
(1,203)	2:450:B:TRP:C	2:451:B:GLU:N	2:451:B:GLU:CA	2:451:B:GLU:C	6	3.1
(1,288)	1:75:A:VAL:H	1:75:A:VAL:N	1:127:A:ASN:N	1:127:A:ASN:H	6	3.09
(1,167)	1:129:A:ALA:N	1:129:A:ALA:CA	1:129:A:ALA:C	1:130:A:ASP:N	1	3.09
(1,203)	2:450:B:TRP:C	2:451:B:GLU:N	2:451:B:GLU:CA	2:451:B:GLU:C	5	3.08
(1,242)	2:465:B:PRO:N	2:465:B:PRO:CA	2:465:B:PRO:C	2:466:B:GLU:N	9	3.06
(1,242)	2:465:B:PRO:N	2:465:B:PRO:CA	2:465:B:PRO:C	2:466:B:GLU:N	24	3.06

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,270)	1:51:A:VAL:H	1:51:A:VAL:N	1:60:A:GLY:N	1:60:A:GLY:H	14	3.05
(1,265)	2:455:B:TYR:N	2:455:B:TYR:CA	2:455:B:TYR:C	2:456:B:PHE:N	1	3.03
(1,242)	2:465:B:PRO:N	2:465:B:PRO:CA	2:465:B:PRO:C	2:466:B:GLU:N	14	3.03
(1,242)	2:465:B:PRO:N	2:465:B:PRO:CA	2:465:B:PRO:C	2:466:B:GLU:N	17	3.03
(1,142)	1:83:A:TYR:N	1:83:A:TYR:CA	1:83:A:TYR:C	1:84:A:PHE:N	19	3.03
(1,267)	2:456:B:PHE:N	2:456:B:PHE:CA	2:456:B:PHE:C	2:457:B:HIS:N	20	3.02
(1,222)	2:474:B:SER:C	2:475:B:TYR:N	2:475:B:TYR:CA	2:475:B:TYR:C	6	3.02
(1,222)	2:474:B:SER:C	2:475:B:TYR:N	2:475:B:TYR:CA	2:475:B:TYR:C	19	3.02
(1,167)	1:129:A:ALA:N	1:129:A:ALA:CA	1:129:A:ALA:C	1:130:A:ASP:N	8	3.02
(1,231)	2:450:B:TRP:N	2:450:B:TRP:CA	2:450:B:TRP:C	2:451:B:GLU:N	7	2.99
(1,26)	1:52:A:GLN:C	1:53:A:LEU:N	1:53:A:LEU:CA	1:53:A:LEU:C	16	2.99
(1,222)	2:474:B:SER:C	2:475:B:TYR:N	2:475:B:TYR:CA	2:475:B:TYR:C	11	2.97
(1,242)	2:465:B:PRO:N	2:465:B:PRO:CA	2:465:B:PRO:C	2:466:B:GLU:N	5	2.96
(1,279)	1:75:A:VAL:H	1:75:A:VAL:N	1:111:A:THR:N	1:111:A:THR:H	24	2.95
(1,265)	2:455:B:TYR:N	2:455:B:TYR:CA	2:455:B:TYR:C	2:456:B:PHE:N	13	2.95
(1,242)	2:465:B:PRO:N	2:465:B:PRO:CA	2:465:B:PRO:C	2:466:B:GLU:N	15	2.94
(1,233)	2:452:B:SER:N	2:452:B:SER:CA	2:452:B:SER:C	2:453:B:ARG:N	13	2.94
(1,270)	1:51:A:VAL:H	1:51:A:VAL:N	1:60:A:GLY:N	1:60:A:GLY:H	2	2.93
(1,236)	2:459:B:ILE:N	2:459:B:ILE:CA	2:459:B:ILE:C	2:460:B:SER:N	18	2.93
(1,167)	1:129:A:ALA:N	1:129:A:ALA:CA	1:129:A:ALA:C	1:130:A:ASP:N	9	2.93
(1,167)	1:129:A:ALA:N	1:129:A:ALA:CA	1:129:A:ALA:C	1:130:A:ASP:N	21	2.93
(1,267)	2:456:B:PHE:N	2:456:B:PHE:CA	2:456:B:PHE:C	2:457:B:HIS:N	7	2.92
(1,265)	2:455:B:TYR:N	2:455:B:TYR:CA	2:455:B:TYR:C	2:456:B:PHE:N	4	2.92
(1,203)	2:450:B:TRP:C	2:451:B:GLU:N	2:451:B:GLU:CA	2:451:B:GLU:C	10	2.92
(1,80)	1:129:A:ALA:C	1:130:A:ASP:N	1:130:A:ASP:CA	1:130:A:ASP:C	9	2.91
(1,242)	2:465:B:PRO:N	2:465:B:PRO:CA	2:465:B:PRO:C	2:466:B:GLU:N	1	2.9
(1,265)	2:455:B:TYR:N	2:455:B:TYR:CA	2:455:B:TYR:C	2:456:B:PHE:N	16	2.89
(1,233)	2:452:B:SER:N	2:452:B:SER:CA	2:452:B:SER:C	2:453:B:ARG:N	12	2.89
(1,230)	2:449:B:GLU:N	2:449:B:GLU:CA	2:449:B:GLU:C	2:450:B:TRP:N	6	2.89
(1,270)	1:51:A:VAL:H	1:51:A:VAL:N	1:60:A:GLY:N	1:60:A:GLY:H	23	2.88
(1,233)	2:452:B:SER:N	2:452:B:SER:CA	2:452:B:SER:C	2:453:B:ARG:N	16	2.88
(1,205)	2:456:B:PHE:C	2:457:B:HIS:N	2:457:B:HIS:CA	2:457:B:HIS:C	8	2.88
(1,167)	1:129:A:ALA:N	1:129:A:ALA:CA	1:129:A:ALA:C	1:130:A:ASP:N	3	2.88
(1,233)	2:452:B:SER:N	2:452:B:SER:CA	2:452:B:SER:C	2:453:B:ARG:N	6	2.87
(1,233)	2:452:B:SER:N	2:452:B:SER:CA	2:452:B:SER:C	2:453:B:ARG:N	21	2.87
(1,230)	2:449:B:GLU:N	2:449:B:GLU:CA	2:449:B:GLU:C	2:450:B:TRP:N	10	2.86
(1,222)	2:474:B:SER:C	2:475:B:TYR:N	2:475:B:TYR:CA	2:475:B:TYR:C	12	2.86
(1,205)	2:456:B:PHE:C	2:457:B:HIS:N	2:457:B:HIS:CA	2:457:B:HIS:C	20	2.86
(1,280)	1:51:A:VAL:H	1:51:A:VAL:N	1:122:A:CYS:N	1:122:A:CYS:H	9	2.85
(1,265)	2:455:B:TYR:N	2:455:B:TYR:CA	2:455:B:TYR:C	2:456:B:PHE:N	17	2.85
(1,231)	2:450:B:TRP:N	2:450:B:TRP:CA	2:450:B:TRP:C	2:451:B:GLU:N	17	2.85
(1,230)	2:449:B:GLU:N	2:449:B:GLU:CA	2:449:B:GLU:C	2:450:B:TRP:N	24	2.85
(1,278)	1:75:A:VAL:H	1:75:A:VAL:N	1:114:A:PHE:N	1:114:A:PHE:H	6	2.84
(1,80)	1:129:A:ALA:C	1:130:A:ASP:N	1:130:A:ASP:CA	1:130:A:ASP:C	7	2.84
(1,205)	2:456:B:PHE:C	2:457:B:HIS:N	2:457:B:HIS:CA	2:457:B:HIS:C	11	2.83
(1,270)	1:51:A:VAL:H	1:51:A:VAL:N	1:60:A:GLY:N	1:60:A:GLY:H	1	2.82
(1,242)	2:465:B:PRO:N	2:465:B:PRO:CA	2:465:B:PRO:C	2:466:B:GLU:N	6	2.82
(1,231)	2:450:B:TRP:N	2:450:B:TRP:CA	2:450:B:TRP:C	2:451:B:GLU:N	21	2.82
(1,203)	2:450:B:TRP:C	2:451:B:GLU:N	2:451:B:GLU:CA	2:451:B:GLU:C	20	2.82
(1,167)	1:129:A:ALA:N	1:129:A:ALA:CA	1:129:A:ALA:C	1:130:A:ASP:N	5	2.82
(1,142)	1:83:A:TYR:N	1:83:A:TYR:CA	1:83:A:TYR:C	1:84:A:PHE:N	20	2.82

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,222)	2:474:B:SER:C	2:475:B:TYR:N	2:475:B:TYR:CA	2:475:B:TYR:C	4	2.81
(1,206)	2:457:B:HIS:C	2:458:B:PRO:N	2:458:B:PRO:CA	2:458:B:PRO:C	15	2.81
(1,205)	2:456:B:PHE:C	2:457:B:HIS:N	2:457:B:HIS:CA	2:457:B:HIS:C	19	2.81
(1,167)	1:129:A:ALA:N	1:129:A:ALA:CA	1:129:A:ALA:C	1:130:A:ASP:N	6	2.81
(1,80)	1:129:A:ALA:C	1:130:A:ASP:N	1:130:A:ASP:CA	1:130:A:ASP:C	21	2.81
(1,231)	2:450:B:TRP:N	2:450:B:TRP:CA	2:450:B:TRP:C	2:451:B:GLU:N	13	2.8
(1,273)	1:60:A:GLY:H	1:60:A:GLY:N	1:89:A:GLY:N	1:89:A:GLY:H	10	2.79
(1,233)	2:452:B:SER:N	2:452:B:SER:CA	2:452:B:SER:C	2:453:B:ARG:N	7	2.79
(1,203)	2:450:B:TRP:C	2:451:B:GLU:N	2:451:B:GLU:CA	2:451:B:GLU:C	14	2.79
(1,81)	1:130:A:ASP:C	1:131:A:GLU:N	1:131:A:GLU:CA	1:131:A:GLU:C	11	2.79
(1,270)	1:51:A:VAL:H	1:51:A:VAL:N	1:60:A:GLY:N	1:60:A:GLY:H	24	2.78
(1,233)	2:452:B:SER:N	2:452:B:SER:CA	2:452:B:SER:C	2:453:B:ARG:N	23	2.78
(1,142)	1:83:A:TYR:N	1:83:A:TYR:CA	1:83:A:TYR:C	1:84:A:PHE:N	1	2.78
(1,265)	2:455:B:TYR:N	2:455:B:TYR:CA	2:455:B:TYR:C	2:456:B:PHE:N	24	2.77
(1,205)	2:456:B:PHE:C	2:457:B:HIS:N	2:457:B:HIS:CA	2:457:B:HIS:C	17	2.77
(1,270)	1:51:A:VAL:H	1:51:A:VAL:N	1:60:A:GLY:N	1:60:A:GLY:H	8	2.76
(1,265)	2:455:B:TYR:N	2:455:B:TYR:CA	2:455:B:TYR:C	2:456:B:PHE:N	11	2.76
(1,222)	2:474:B:SER:C	2:475:B:TYR:N	2:475:B:TYR:CA	2:475:B:TYR:C	8	2.76
(1,270)	1:51:A:VAL:H	1:51:A:VAL:N	1:60:A:GLY:N	1:60:A:GLY:H	6	2.75
(1,267)	2:456:B:PHE:N	2:456:B:PHE:CA	2:456:B:PHE:C	2:457:B:HIS:N	17	2.75
(1,233)	2:452:B:SER:N	2:452:B:SER:CA	2:452:B:SER:C	2:453:B:ARG:N	18	2.75
(1,267)	2:456:B:PHE:N	2:456:B:PHE:CA	2:456:B:PHE:C	2:457:B:HIS:N	19	2.74
(1,205)	2:456:B:PHE:C	2:457:B:HIS:N	2:457:B:HIS:CA	2:457:B:HIS:C	12	2.73
(1,278)	1:75:A:VAL:H	1:75:A:VAL:N	1:114:A:PHE:N	1:114:A:PHE:H	5	2.72
(1,278)	1:75:A:VAL:H	1:75:A:VAL:N	1:114:A:PHE:N	1:114:A:PHE:H	20	2.72
(1,267)	2:456:B:PHE:N	2:456:B:PHE:CA	2:456:B:PHE:C	2:457:B:HIS:N	11	2.72
(1,265)	2:455:B:TYR:N	2:455:B:TYR:CA	2:455:B:TYR:C	2:456:B:PHE:N	12	2.71
(1,232)	2:451:B:GLU:N	2:451:B:GLU:CA	2:451:B:GLU:C	2:452:B:SER:N	12	2.71
(1,231)	2:450:B:TRP:N	2:450:B:TRP:CA	2:450:B:TRP:C	2:451:B:GLU:N	1	2.71
(1,206)	2:457:B:HIS:C	2:458:B:PRO:N	2:458:B:PRO:CA	2:458:B:PRO:C	19	2.71
(1,205)	2:456:B:PHE:C	2:457:B:HIS:N	2:457:B:HIS:CA	2:457:B:HIS:C	10	2.71
(1,167)	1:129:A:ALA:N	1:129:A:ALA:CA	1:129:A:ALA:C	1:130:A:ASP:N	12	2.71
(1,267)	2:456:B:PHE:N	2:456:B:PHE:CA	2:456:B:PHE:C	2:457:B:HIS:N	10	2.7
(1,233)	2:452:B:SER:N	2:452:B:SER:CA	2:452:B:SER:C	2:453:B:ARG:N	17	2.7
(1,233)	2:452:B:SER:N	2:452:B:SER:CA	2:452:B:SER:C	2:453:B:ARG:N	19	2.7
(1,80)	1:129:A:ALA:C	1:130:A:ASP:N	1:130:A:ASP:CA	1:130:A:ASP:C	22	2.7
(1,288)	1:75:A:VAL:H	1:75:A:VAL:N	1:127:A:ASN:N	1:127:A:ASN:H	2	2.69
(1,267)	2:456:B:PHE:N	2:456:B:PHE:CA	2:456:B:PHE:C	2:457:B:HIS:N	12	2.69
(1,231)	2:450:B:TRP:N	2:450:B:TRP:CA	2:450:B:TRP:C	2:451:B:GLU:N	24	2.69
(1,80)	1:129:A:ALA:C	1:130:A:ASP:N	1:130:A:ASP:CA	1:130:A:ASP:C	1	2.69
(1,231)	2:450:B:TRP:N	2:450:B:TRP:CA	2:450:B:TRP:C	2:451:B:GLU:N	16	2.68
(1,231)	2:450:B:TRP:N	2:450:B:TRP:CA	2:450:B:TRP:C	2:451:B:GLU:N	9	2.67
(1,80)	1:129:A:ALA:C	1:130:A:ASP:N	1:130:A:ASP:CA	1:130:A:ASP:C	20	2.67
(1,270)	1:51:A:VAL:H	1:51:A:VAL:N	1:60:A:GLY:N	1:60:A:GLY:H	12	2.66
(1,231)	2:450:B:TRP:N	2:450:B:TRP:CA	2:450:B:TRP:C	2:451:B:GLU:N	5	2.66
(1,231)	2:450:B:TRP:N	2:450:B:TRP:CA	2:450:B:TRP:C	2:451:B:GLU:N	6	2.66
(1,167)	1:129:A:ALA:N	1:129:A:ALA:CA	1:129:A:ALA:C	1:130:A:ASP:N	16	2.66
(1,231)	2:450:B:TRP:N	2:450:B:TRP:CA	2:450:B:TRP:C	2:451:B:GLU:N	22	2.65
(1,167)	1:129:A:ALA:N	1:129:A:ALA:CA	1:129:A:ALA:C	1:130:A:ASP:N	4	2.65
(1,80)	1:129:A:ALA:C	1:130:A:ASP:N	1:130:A:ASP:CA	1:130:A:ASP:C	16	2.65
(1,278)	1:75:A:VAL:H	1:75:A:VAL:N	1:114:A:PHE:N	1:114:A:PHE:H	10	2.64

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,268)	2:469:B:VAL:C	2:470:B:GLN:N	2:470:B:GLN:CA	2:470:B:GLN:C	8	2.64
(1,233)	2:452:B:SER:N	2:452:B:SER:CA	2:452:B:SER:C	2:453:B:ARG:N	24	2.63
(1,232)	2:451:B:GLU:N	2:451:B:GLU:CA	2:451:B:GLU:C	2:452:B:SER:N	15	2.63
(1,167)	1:129:A:ALA:N	1:129:A:ALA:CA	1:129:A:ALA:C	1:130:A:ASP:N	22	2.63
(1,279)	1:75:A:VAL:H	1:75:A:VAL:N	1:111:A:THR:N	1:111:A:THR:H	13	2.62
(1,278)	1:75:A:VAL:H	1:75:A:VAL:N	1:114:A:PHE:N	1:114:A:PHE:H	14	2.62
(1,233)	2:452:B:SER:N	2:452:B:SER:CA	2:452:B:SER:C	2:453:B:ARG:N	15	2.62
(1,232)	2:451:B:GLU:N	2:451:B:GLU:CA	2:451:B:GLU:C	2:452:B:SER:N	10	2.62
(1,231)	2:450:B:TRP:N	2:450:B:TRP:CA	2:450:B:TRP:C	2:451:B:GLU:N	12	2.62
(1,233)	2:452:B:SER:N	2:452:B:SER:CA	2:452:B:SER:C	2:453:B:ARG:N	4	2.61
(1,231)	2:450:B:TRP:N	2:450:B:TRP:CA	2:450:B:TRP:C	2:451:B:GLU:N	4	2.61
(1,231)	2:450:B:TRP:N	2:450:B:TRP:CA	2:450:B:TRP:C	2:451:B:GLU:N	23	2.61
(1,205)	2:456:B:PHE:C	2:457:B:HIS:N	2:457:B:HIS:CA	2:457:B:HIS:C	5	2.61
(1,167)	1:129:A:ALA:N	1:129:A:ALA:CA	1:129:A:ALA:C	1:130:A:ASP:N	23	2.61
(1,167)	1:129:A:ALA:N	1:129:A:ALA:CA	1:129:A:ALA:C	1:130:A:ASP:N	24	2.61
(1,80)	1:129:A:ALA:C	1:130:A:ASP:N	1:130:A:ASP:CA	1:130:A:ASP:C	3	2.61
(1,222)	2:474:B:SER:C	2:475:B:TYR:N	2:475:B:TYR:CA	2:475:B:TYR:C	7	2.6
(1,203)	2:450:B:TRP:C	2:451:B:GLU:N	2:451:B:GLU:CA	2:451:B:GLU:C	8	2.6
(1,232)	2:451:B:GLU:N	2:451:B:GLU:CA	2:451:B:GLU:C	2:452:B:SER:N	13	2.59
(1,205)	2:456:B:PHE:C	2:457:B:HIS:N	2:457:B:HIS:CA	2:457:B:HIS:C	16	2.58
(1,205)	2:456:B:PHE:C	2:457:B:HIS:N	2:457:B:HIS:CA	2:457:B:HIS:C	24	2.58
(1,26)	1:52:A:GLN:C	1:53:A:LEU:N	1:53:A:LEU:CA	1:53:A:LEU:C	10	2.58
(1,273)	1:60:A:GLY:H	1:60:A:GLY:N	1:89:A:GLY:N	1:89:A:GLY:H	1	2.57
(1,265)	2:455:B:TYR:N	2:455:B:TYR:CA	2:455:B:TYR:C	2:456:B:PHE:N	23	2.57
(1,233)	2:452:B:SER:N	2:452:B:SER:CA	2:452:B:SER:C	2:453:B:ARG:N	1	2.57
(1,167)	1:129:A:ALA:N	1:129:A:ALA:CA	1:129:A:ALA:C	1:130:A:ASP:N	2	2.57
(1,167)	1:129:A:ALA:N	1:129:A:ALA:CA	1:129:A:ALA:C	1:130:A:ASP:N	7	2.57
(1,308)	1:35:A:LEU:H	1:35:A:LEU:N	1:75:A:VAL:N	1:75:A:VAL:H	16	2.56
(1,288)	1:75:A:VAL:H	1:75:A:VAL:N	1:127:A:ASN:N	1:127:A:ASN:H	4	2.56
(1,267)	2:456:B:PHE:N	2:456:B:PHE:CA	2:456:B:PHE:C	2:457:B:HIS:N	18	2.56
(1,231)	2:450:B:TRP:N	2:450:B:TRP:CA	2:450:B:TRP:C	2:451:B:GLU:N	10	2.56
(1,80)	1:129:A:ALA:C	1:130:A:ASP:N	1:130:A:ASP:CA	1:130:A:ASP:C	23	2.56
(1,270)	1:51:A:VAL:H	1:51:A:VAL:N	1:60:A:GLY:N	1:60:A:GLY:H	20	2.55
(1,233)	2:452:B:SER:N	2:452:B:SER:CA	2:452:B:SER:C	2:453:B:ARG:N	5	2.55
(1,230)	2:449:B:GLU:N	2:449:B:GLU:CA	2:449:B:GLU:C	2:450:B:TRP:N	8	2.55
(1,205)	2:456:B:PHE:C	2:457:B:HIS:N	2:457:B:HIS:CA	2:457:B:HIS:C	1	2.55
(1,167)	1:129:A:ALA:N	1:129:A:ALA:CA	1:129:A:ALA:C	1:130:A:ASP:N	10	2.55
(1,288)	1:75:A:VAL:H	1:75:A:VAL:N	1:127:A:ASN:N	1:127:A:ASN:H	1	2.54
(1,278)	1:75:A:VAL:H	1:75:A:VAL:N	1:114:A:PHE:N	1:114:A:PHE:H	1	2.54
(1,233)	2:452:B:SER:N	2:452:B:SER:CA	2:452:B:SER:C	2:453:B:ARG:N	14	2.54
(1,233)	2:452:B:SER:N	2:452:B:SER:CA	2:452:B:SER:C	2:453:B:ARG:N	22	2.54
(1,233)	2:452:B:SER:N	2:452:B:SER:CA	2:452:B:SER:C	2:453:B:ARG:N	10	2.52
(1,232)	2:451:B:GLU:N	2:451:B:GLU:CA	2:451:B:GLU:C	2:452:B:SER:N	21	2.52
(1,205)	2:456:B:PHE:C	2:457:B:HIS:N	2:457:B:HIS:CA	2:457:B:HIS:C	7	2.52
(1,80)	1:129:A:ALA:C	1:130:A:ASP:N	1:130:A:ASP:CA	1:130:A:ASP:C	10	2.52
(1,308)	1:35:A:LEU:H	1:35:A:LEU:N	1:75:A:VAL:N	1:75:A:VAL:H	8	2.51
(1,278)	1:75:A:VAL:H	1:75:A:VAL:N	1:114:A:PHE:N	1:114:A:PHE:H	13	2.51
(1,273)	1:60:A:GLY:H	1:60:A:GLY:N	1:89:A:GLY:N	1:89:A:GLY:H	4	2.51
(1,265)	2:455:B:TYR:N	2:455:B:TYR:CA	2:455:B:TYR:C	2:456:B:PHE:N	2	2.51
(1,80)	1:129:A:ALA:C	1:130:A:ASP:N	1:130:A:ASP:CA	1:130:A:ASP:C	5	2.5
(1,206)	2:457:B:HIS:C	2:458:B:PRO:N	2:458:B:PRO:CA	2:458:B:PRO:C	3	2.49

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,205)	2:456:B:PHE:C	2:457:B:HIS:N	2:457:B:HIS:CA	2:457:B:HIS:C	6	2.49
(1,167)	1:129:A:ALA:N	1:129:A:ALA:CA	1:129:A:ALA:C	1:130:A:ASP:N	17	2.49
(1,273)	1:60:A:GLY:H	1:60:A:GLY:N	1:89:A:GLY:N	1:89:A:GLY:H	15	2.48
(1,26)	1:52:A:GLN:C	1:53:A:LEU:N	1:53:A:LEU:CA	1:53:A:LEU:C	8	2.48
(1,24)	1:47:A:ALA:C	1:48:A:THR:N	1:48:A:THR:CA	1:48:A:THR:C	14	2.48
(1,278)	1:75:A:VAL:H	1:75:A:VAL:N	1:114:A:PHE:N	1:114:A:PHE:H	3	2.47
(1,267)	2:456:B:PHE:N	2:456:B:PHE:CA	2:456:B:PHE:C	2:457:B:HIS:N	3	2.47
(1,232)	2:451:B:GLU:N	2:451:B:GLU:CA	2:451:B:GLU:C	2:452:B:SER:N	16	2.47
(1,141)	1:82:A:SER:N	1:82:A:SER:CA	1:82:A:SER:C	1:83:A:TYR:N	10	2.47
(1,80)	1:129:A:ALA:C	1:130:A:ASP:N	1:130:A:ASP:CA	1:130:A:ASP:C	17	2.47
(1,288)	1:75:A:VAL:H	1:75:A:VAL:N	1:127:A:ASN:N	1:127:A:ASN:H	16	2.46
(1,231)	2:450:B:TRP:N	2:450:B:TRP:CA	2:450:B:TRP:C	2:451:B:GLU:N	18	2.46
(1,270)	1:51:A:VAL:H	1:51:A:VAL:N	1:60:A:GLY:N	1:60:A:GLY:H	4	2.45
(1,265)	2:455:B:TYR:N	2:455:B:TYR:CA	2:455:B:TYR:C	2:456:B:PHE:N	15	2.45
(1,233)	2:452:B:SER:N	2:452:B:SER:CA	2:452:B:SER:C	2:453:B:ARG:N	3	2.45
(1,308)	1:35:A:LEU:H	1:35:A:LEU:N	1:75:A:VAL:N	1:75:A:VAL:H	9	2.44
(1,265)	2:455:B:TYR:N	2:455:B:TYR:CA	2:455:B:TYR:C	2:456:B:PHE:N	7	2.43
(1,280)	1:51:A:VAL:H	1:51:A:VAL:N	1:122:A:CYS:N	1:122:A:CYS:H	7	2.42
(1,273)	1:60:A:GLY:H	1:60:A:GLY:N	1:89:A:GLY:N	1:89:A:GLY:H	24	2.42
(1,267)	2:456:B:PHE:N	2:456:B:PHE:CA	2:456:B:PHE:C	2:457:B:HIS:N	15	2.42
(1,233)	2:452:B:SER:N	2:452:B:SER:CA	2:452:B:SER:C	2:453:B:ARG:N	9	2.42
(1,222)	2:474:B:SER:C	2:475:B:TYR:N	2:475:B:TYR:CA	2:475:B:TYR:C	1	2.42
(1,288)	1:75:A:VAL:H	1:75:A:VAL:N	1:127:A:ASN:N	1:127:A:ASN:H	21	2.41
(1,232)	2:451:B:GLU:N	2:451:B:GLU:CA	2:451:B:GLU:C	2:452:B:SER:N	5	2.41
(1,231)	2:450:B:TRP:N	2:450:B:TRP:CA	2:450:B:TRP:C	2:451:B:GLU:N	2	2.41
(1,80)	1:129:A:ALA:C	1:130:A:ASP:N	1:130:A:ASP:CA	1:130:A:ASP:C	6	2.41
(1,26)	1:52:A:GLN:C	1:53:A:LEU:N	1:53:A:LEU:CA	1:53:A:LEU:C	15	2.41
(1,25)	1:50:A:VAL:C	1:51:A:VAL:N	1:51:A:VAL:CA	1:51:A:VAL:C	11	2.41
(1,80)	1:129:A:ALA:C	1:130:A:ASP:N	1:130:A:ASP:CA	1:130:A:ASP:C	4	2.4
(1,232)	2:451:B:GLU:N	2:451:B:GLU:CA	2:451:B:GLU:C	2:452:B:SER:N	7	2.39
(1,232)	2:451:B:GLU:N	2:451:B:GLU:CA	2:451:B:GLU:C	2:452:B:SER:N	19	2.39
(1,205)	2:456:B:PHE:C	2:457:B:HIS:N	2:457:B:HIS:CA	2:457:B:HIS:C	13	2.39
(1,167)	1:129:A:ALA:N	1:129:A:ALA:CA	1:129:A:ALA:C	1:130:A:ASP:N	13	2.39
(1,79)	1:128:A:PHE:C	1:129:A:ALA:N	1:129:A:ALA:CA	1:129:A:ALA:C	14	2.39
(1,267)	2:456:B:PHE:N	2:456:B:PHE:CA	2:456:B:PHE:C	2:457:B:HIS:N	4	2.38
(1,205)	2:456:B:PHE:C	2:457:B:HIS:N	2:457:B:HIS:CA	2:457:B:HIS:C	9	2.38
(1,267)	2:456:B:PHE:N	2:456:B:PHE:CA	2:456:B:PHE:C	2:457:B:HIS:N	2	2.36
(1,233)	2:452:B:SER:N	2:452:B:SER:CA	2:452:B:SER:C	2:453:B:ARG:N	20	2.36
(1,231)	2:450:B:TRP:N	2:450:B:TRP:CA	2:450:B:TRP:C	2:451:B:GLU:N	3	2.36
(1,233)	2:452:B:SER:N	2:452:B:SER:CA	2:452:B:SER:C	2:453:B:ARG:N	2	2.35
(1,230)	2:449:B:GLU:N	2:449:B:GLU:CA	2:449:B:GLU:C	2:450:B:TRP:N	4	2.35
(1,205)	2:456:B:PHE:C	2:457:B:HIS:N	2:457:B:HIS:CA	2:457:B:HIS:C	14	2.35
(1,80)	1:129:A:ALA:C	1:130:A:ASP:N	1:130:A:ASP:CA	1:130:A:ASP:C	18	2.34
(1,267)	2:456:B:PHE:N	2:456:B:PHE:CA	2:456:B:PHE:C	2:457:B:HIS:N	16	2.33
(1,233)	2:452:B:SER:N	2:452:B:SER:CA	2:452:B:SER:C	2:453:B:ARG:N	11	2.33
(1,232)	2:451:B:GLU:N	2:451:B:GLU:CA	2:451:B:GLU:C	2:452:B:SER:N	6	2.33
(1,285)	1:60:A:GLY:H	1:60:A:GLY:N	1:93:A:GLY:N	1:93:A:GLY:H	4	2.32
(1,80)	1:129:A:ALA:C	1:130:A:ASP:N	1:130:A:ASP:CA	1:130:A:ASP:C	12	2.32
(1,308)	1:35:A:LEU:H	1:35:A:LEU:N	1:75:A:VAL:N	1:75:A:VAL:H	18	2.31
(1,280)	1:51:A:VAL:H	1:51:A:VAL:N	1:122:A:CYS:N	1:122:A:CYS:H	22	2.31
(1,280)	1:51:A:VAL:H	1:51:A:VAL:N	1:122:A:CYS:N	1:122:A:CYS:H	23	2.31

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,232)	2:451:B:GLU:N	2:451:B:GLU:CA	2:451:B:GLU:C	2:452:B:SER:N	11	2.31
(1,26)	1:52:A:GLN:C	1:53:A:LEU:N	1:53:A:LEU:CA	1:53:A:LEU:C	3	2.31
(1,205)	2:456:B:PHE:C	2:457:B:HIS:N	2:457:B:HIS:CA	2:457:B:HIS:C	2	2.3
(1,232)	2:451:B:GLU:N	2:451:B:GLU:CA	2:451:B:GLU:C	2:452:B:SER:N	24	2.29
(1,267)	2:456:B:PHE:N	2:456:B:PHE:CA	2:456:B:PHE:C	2:457:B:HIS:N	1	2.28
(1,250)	2:474:B:SER:N	2:474:B:SER:CA	2:474:B:SER:C	2:475:B:TYR:N	16	2.27
(1,231)	2:450:B:TRP:N	2:450:B:TRP:CA	2:450:B:TRP:C	2:451:B:GLU:N	14	2.27
(1,167)	1:129:A:ALA:N	1:129:A:ALA:CA	1:129:A:ALA:C	1:130:A:ASP:N	18	2.27
(1,278)	1:75:A:VAL:H	1:75:A:VAL:N	1:114:A:PHE:N	1:114:A:PHE:H	24	2.26
(1,232)	2:451:B:GLU:N	2:451:B:GLU:CA	2:451:B:GLU:C	2:452:B:SER:N	18	2.26
(1,232)	2:451:B:GLU:N	2:451:B:GLU:CA	2:451:B:GLU:C	2:452:B:SER:N	23	2.26
(1,230)	2:449:B:GLU:N	2:449:B:GLU:CA	2:449:B:GLU:C	2:450:B:TRP:N	20	2.26
(1,308)	1:35:A:LEU:H	1:35:A:LEU:N	1:75:A:VAL:N	1:75:A:VAL:H	11	2.25
(1,308)	1:35:A:LEU:H	1:35:A:LEU:N	1:75:A:VAL:N	1:75:A:VAL:H	15	2.25
(1,65)	1:105:A:LEU:C	1:106:A:VAL:N	1:106:A:VAL:CA	1:106:A:VAL:C	19	2.25
(1,307)	1:31:A:GLU:H	1:31:A:GLU:N	1:51:A:VAL:N	1:51:A:VAL:H	13	2.24
(1,288)	1:75:A:VAL:H	1:75:A:VAL:N	1:127:A:ASN:N	1:127:A:ASN:H	22	2.24
(1,284)	1:60:A:GLY:H	1:60:A:GLY:N	1:111:A:THR:N	1:111:A:THR:H	5	2.24
(1,270)	1:51:A:VAL:H	1:51:A:VAL:N	1:60:A:GLY:N	1:60:A:GLY:H	17	2.24
(1,288)	1:75:A:VAL:H	1:75:A:VAL:N	1:127:A:ASN:N	1:127:A:ASN:H	20	2.23
(1,273)	1:60:A:GLY:H	1:60:A:GLY:N	1:89:A:GLY:N	1:89:A:GLY:H	14	2.22
(1,267)	2:456:B:PHE:N	2:456:B:PHE:CA	2:456:B:PHE:C	2:457:B:HIS:N	13	2.22
(1,26)	1:52:A:GLN:C	1:53:A:LEU:N	1:53:A:LEU:CA	1:53:A:LEU:C	11	2.22
(1,284)	1:60:A:GLY:H	1:60:A:GLY:N	1:111:A:THR:N	1:111:A:THR:H	10	2.21
(1,270)	1:51:A:VAL:H	1:51:A:VAL:N	1:60:A:GLY:N	1:60:A:GLY:H	16	2.21
(1,267)	2:456:B:PHE:N	2:456:B:PHE:CA	2:456:B:PHE:C	2:457:B:HIS:N	21	2.21
(1,267)	2:456:B:PHE:N	2:456:B:PHE:CA	2:456:B:PHE:C	2:457:B:HIS:N	24	2.2
(1,266)	2:455:B:TYR:C	2:456:B:PHE:N	2:456:B:PHE:CA	2:456:B:PHE:C	14	2.2
(1,231)	2:450:B:TRP:N	2:450:B:TRP:CA	2:450:B:TRP:C	2:451:B:GLU:N	20	2.2
(1,205)	2:456:B:PHE:C	2:457:B:HIS:N	2:457:B:HIS:CA	2:457:B:HIS:C	22	2.2
(1,307)	1:31:A:GLU:H	1:31:A:GLU:N	1:51:A:VAL:N	1:51:A:VAL:H	17	2.19
(1,280)	1:51:A:VAL:H	1:51:A:VAL:N	1:122:A:CYS:N	1:122:A:CYS:H	15	2.19
(1,233)	2:452:B:SER:N	2:452:B:SER:CA	2:452:B:SER:C	2:453:B:ARG:N	8	2.19
(1,205)	2:456:B:PHE:C	2:457:B:HIS:N	2:457:B:HIS:CA	2:457:B:HIS:C	23	2.19
(1,267)	2:456:B:PHE:N	2:456:B:PHE:CA	2:456:B:PHE:C	2:457:B:HIS:N	6	2.18
(1,236)	2:459:B:ILE:N	2:459:B:ILE:CA	2:459:B:ILE:C	2:460:B:SER:N	2	2.18
(1,230)	2:449:B:GLU:N	2:449:B:GLU:CA	2:449:B:GLU:C	2:450:B:TRP:N	15	2.18
(1,81)	1:130:A:ASP:C	1:131:A:GLU:N	1:131:A:GLU:CA	1:131:A:GLU:C	10	2.18
(1,80)	1:129:A:ALA:C	1:130:A:ASP:N	1:130:A:ASP:CA	1:130:A:ASP:C	13	2.18
(1,26)	1:52:A:GLN:C	1:53:A:LEU:N	1:53:A:LEU:CA	1:53:A:LEU:C	7	2.18
(1,308)	1:35:A:LEU:H	1:35:A:LEU:N	1:75:A:VAL:N	1:75:A:VAL:H	24	2.17
(1,278)	1:75:A:VAL:H	1:75:A:VAL:N	1:114:A:PHE:N	1:114:A:PHE:H	8	2.17
(1,266)	2:455:B:TYR:C	2:456:B:PHE:N	2:456:B:PHE:CA	2:456:B:PHE:C	3	2.17
(1,307)	1:31:A:GLU:H	1:31:A:GLU:N	1:51:A:VAL:N	1:51:A:VAL:H	9	2.16
(1,265)	2:455:B:TYR:N	2:455:B:TYR:CA	2:455:B:TYR:C	2:456:B:PHE:N	10	2.16
(1,24)	1:47:A:ALA:C	1:48:A:THR:N	1:48:A:THR:CA	1:48:A:THR:C	4	2.16
(1,280)	1:51:A:VAL:H	1:51:A:VAL:N	1:122:A:CYS:N	1:122:A:CYS:H	11	2.14
(1,278)	1:75:A:VAL:H	1:75:A:VAL:N	1:114:A:PHE:N	1:114:A:PHE:H	23	2.14
(1,205)	2:456:B:PHE:C	2:457:B:HIS:N	2:457:B:HIS:CA	2:457:B:HIS:C	18	2.14
(1,307)	1:31:A:GLU:H	1:31:A:GLU:N	1:51:A:VAL:N	1:51:A:VAL:H	19	2.12
(1,273)	1:60:A:GLY:H	1:60:A:GLY:N	1:89:A:GLY:N	1:89:A:GLY:H	21	2.12

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,268)	2:469:B:VAL:C	2:470:B:GLN:N	2:470:B:GLN:CA	2:470:B:GLN:C	18	2.12
(1,232)	2:451:B:GLU:N	2:451:B:GLU:CA	2:451:B:GLU:C	2:452:B:SER:N	14	2.12
(1,205)	2:456:B:PHE:C	2:457:B:HIS:N	2:457:B:HIS:CA	2:457:B:HIS:C	15	2.12
(1,270)	1:51:A:VAL:H	1:51:A:VAL:N	1:60:A:GLY:N	1:60:A:GLY:H	9	2.11
(1,268)	2:469:B:VAL:C	2:470:B:GLN:N	2:470:B:GLN:CA	2:470:B:GLN:C	5	2.11
(1,267)	2:456:B:PHE:N	2:456:B:PHE:CA	2:456:B:PHE:C	2:457:B:HIS:N	14	2.11
(1,236)	2:459:B:ILE:N	2:459:B:ILE:CA	2:459:B:ILE:C	2:460:B:SER:N	24	2.11
(1,273)	1:60:A:GLY:H	1:60:A:GLY:N	1:89:A:GLY:N	1:89:A:GLY:H	6	2.1
(1,223)	2:475:B:TYR:C	2:476:B:PRO:N	2:476:B:PRO:CA	2:476:B:PRO:C	18	2.1
(1,24)	1:47:A:ALA:C	1:48:A:THR:N	1:48:A:THR:CA	1:48:A:THR:C	21	2.1
(1,285)	1:60:A:GLY:H	1:60:A:GLY:N	1:93:A:GLY:N	1:93:A:GLY:H	6	2.09
(1,280)	1:51:A:VAL:H	1:51:A:VAL:N	1:122:A:CYS:N	1:122:A:CYS:H	1	2.09
(1,278)	1:75:A:VAL:H	1:75:A:VAL:N	1:114:A:PHE:N	1:114:A:PHE:H	18	2.09
(1,25)	1:50:A:VAL:C	1:51:A:VAL:N	1:51:A:VAL:CA	1:51:A:VAL:C	22	2.09
(1,284)	1:60:A:GLY:H	1:60:A:GLY:N	1:111:A:THR:N	1:111:A:THR:H	8	2.08
(1,232)	2:451:B:GLU:N	2:451:B:GLU:CA	2:451:B:GLU:C	2:452:B:SER:N	3	2.07
(1,232)	2:451:B:GLU:N	2:451:B:GLU:CA	2:451:B:GLU:C	2:452:B:SER:N	17	2.07
(1,267)	2:456:B:PHE:N	2:456:B:PHE:CA	2:456:B:PHE:C	2:457:B:HIS:N	22	2.06
(1,205)	2:456:B:PHE:C	2:457:B:HIS:N	2:457:B:HIS:CA	2:457:B:HIS:C	21	2.06
(1,267)	2:456:B:PHE:N	2:456:B:PHE:CA	2:456:B:PHE:C	2:457:B:HIS:N	5	2.05
(1,266)	2:455:B:TYR:C	2:456:B:PHE:N	2:456:B:PHE:CA	2:456:B:PHE:C	1	2.05
(1,207)	2:458:B:PRO:C	2:459:B:ILE:N	2:459:B:ILE:CA	2:459:B:ILE:C	10	2.05
(1,307)	1:31:A:GLU:H	1:31:A:GLU:N	1:51:A:VAL:N	1:51:A:VAL:H	15	2.04
(1,278)	1:75:A:VAL:H	1:75:A:VAL:N	1:114:A:PHE:N	1:114:A:PHE:H	19	2.04
(1,250)	2:474:B:SER:N	2:474:B:SER:CA	2:474:B:SER:C	2:475:B:TYR:N	14	2.04
(1,79)	1:128:A:PHE:C	1:129:A:ALA:N	1:129:A:ALA:CA	1:129:A:ALA:C	9	2.04
(1,267)	2:456:B:PHE:N	2:456:B:PHE:CA	2:456:B:PHE:C	2:457:B:HIS:N	23	2.02
(1,266)	2:455:B:TYR:C	2:456:B:PHE:N	2:456:B:PHE:CA	2:456:B:PHE:C	5	2.02
(1,230)	2:449:B:GLU:N	2:449:B:GLU:CA	2:449:B:GLU:C	2:450:B:TRP:N	2	2.02
(1,266)	2:455:B:TYR:C	2:456:B:PHE:N	2:456:B:PHE:CA	2:456:B:PHE:C	6	2.01
(1,81)	1:130:A:ASP:C	1:131:A:GLU:N	1:131:A:GLU:CA	1:131:A:GLU:C	5	2.01
(1,307)	1:31:A:GLU:H	1:31:A:GLU:N	1:51:A:VAL:N	1:51:A:VAL:H	10	2.0
(1,265)	2:455:B:TYR:N	2:455:B:TYR:CA	2:455:B:TYR:C	2:456:B:PHE:N	20	2.0
(1,156)	1:105:A:LEU:N	1:105:A:LEU:CA	1:105:A:LEU:C	1:106:A:VAL:N	9	2.0
(1,285)	1:60:A:GLY:H	1:60:A:GLY:N	1:93:A:GLY:N	1:93:A:GLY:H	10	1.99
(1,280)	1:51:A:VAL:H	1:51:A:VAL:N	1:122:A:CYS:N	1:122:A:CYS:H	18	1.99
(1,278)	1:75:A:VAL:H	1:75:A:VAL:N	1:114:A:PHE:N	1:114:A:PHE:H	15	1.99
(1,232)	2:451:B:GLU:N	2:451:B:GLU:CA	2:451:B:GLU:C	2:452:B:SER:N	20	1.99
(1,79)	1:128:A:PHE:C	1:129:A:ALA:N	1:129:A:ALA:CA	1:129:A:ALA:C	3	1.99
(1,81)	1:130:A:ASP:C	1:131:A:GLU:N	1:131:A:GLU:CA	1:131:A:GLU:C	19	1.98
(1,25)	1:50:A:VAL:C	1:51:A:VAL:N	1:51:A:VAL:CA	1:51:A:VAL:C	9	1.98
(1,285)	1:60:A:GLY:H	1:60:A:GLY:N	1:93:A:GLY:N	1:93:A:GLY:H	3	1.97
(1,265)	2:455:B:TYR:N	2:455:B:TYR:CA	2:455:B:TYR:C	2:456:B:PHE:N	21	1.97
(1,232)	2:451:B:GLU:N	2:451:B:GLU:CA	2:451:B:GLU:C	2:452:B:SER:N	4	1.97
(1,205)	2:456:B:PHE:C	2:457:B:HIS:N	2:457:B:HIS:CA	2:457:B:HIS:C	4	1.97
(1,80)	1:129:A:ALA:C	1:130:A:ASP:N	1:130:A:ASP:CA	1:130:A:ASP:C	2	1.97
(1,308)	1:35:A:LEU:H	1:35:A:LEU:N	1:75:A:VAL:N	1:75:A:VAL:H	2	1.96
(1,266)	2:455:B:TYR:C	2:456:B:PHE:N	2:456:B:PHE:CA	2:456:B:PHE:C	16	1.96
(1,80)	1:129:A:ALA:C	1:130:A:ASP:N	1:130:A:ASP:CA	1:130:A:ASP:C	24	1.96
(1,26)	1:52:A:GLN:C	1:53:A:LEU:N	1:53:A:LEU:CA	1:53:A:LEU:C	22	1.96
(1,26)	1:52:A:GLN:C	1:53:A:LEU:N	1:53:A:LEU:CA	1:53:A:LEU:C	19	1.95

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,307)	1:31:A:GLU:H	1:31:A:GLU:N	1:51:A:VAL:N	1:51:A:VAL:H	24	1.94
(1,280)	1:51:A:VAL:H	1:51:A:VAL:N	1:122:A:CYS:N	1:122:A:CYS:H	2	1.94
(1,236)	2:459:B:ILE:N	2:459:B:ILE:CA	2:459:B:ILE:C	2:460:B:SER:N	10	1.94
(1,232)	2:451:B:GLU:N	2:451:B:GLU:CA	2:451:B:GLU:C	2:452:B:SER:N	22	1.94
(1,81)	1:130:A:ASP:C	1:131:A:GLU:N	1:131:A:GLU:CA	1:131:A:GLU:C	20	1.94
(1,270)	1:51:A:VAL:H	1:51:A:VAL:N	1:60:A:GLY:N	1:60:A:GLY:H	19	1.93
(1,266)	2:455:B:TYR:C	2:456:B:PHE:N	2:456:B:PHE:CA	2:456:B:PHE:C	13	1.93
(1,232)	2:451:B:GLU:N	2:451:B:GLU:CA	2:451:B:GLU:C	2:452:B:SER:N	1	1.93
(1,230)	2:449:B:GLU:N	2:449:B:GLU:CA	2:449:B:GLU:C	2:450:B:TRP:N	14	1.92
(1,308)	1:35:A:LEU:H	1:35:A:LEU:N	1:75:A:VAL:N	1:75:A:VAL:H	7	1.91
(1,79)	1:128:A:PHE:C	1:129:A:ALA:N	1:129:A:ALA:CA	1:129:A:ALA:C	21	1.91
(1,273)	1:60:A:GLY:H	1:60:A:GLY:N	1:89:A:GLY:N	1:89:A:GLY:H	2	1.9
(1,266)	2:455:B:TYR:C	2:456:B:PHE:N	2:456:B:PHE:CA	2:456:B:PHE:C	24	1.9
(1,244)	2:467:B:PRO:N	2:467:B:PRO:CA	2:467:B:PRO:C	2:468:B:TYR:N	1	1.9
(1,25)	1:50:A:VAL:C	1:51:A:VAL:N	1:51:A:VAL:CA	1:51:A:VAL:C	19	1.9
(1,24)	1:47:A:ALA:C	1:48:A:THR:N	1:48:A:THR:CA	1:48:A:THR:C	2	1.9
(1,308)	1:35:A:LEU:H	1:35:A:LEU:N	1:75:A:VAL:N	1:75:A:VAL:H	13	1.89
(1,232)	2:451:B:GLU:N	2:451:B:GLU:CA	2:451:B:GLU:C	2:452:B:SER:N	2	1.89
(1,206)	2:457:B:HIS:C	2:458:B:PRO:N	2:458:B:PRO:CA	2:458:B:PRO:C	2	1.89
(1,266)	2:455:B:TYR:C	2:456:B:PHE:N	2:456:B:PHE:CA	2:456:B:PHE:C	19	1.88
(1,236)	2:459:B:ILE:N	2:459:B:ILE:CA	2:459:B:ILE:C	2:460:B:SER:N	21	1.87
(1,285)	1:60:A:GLY:H	1:60:A:GLY:N	1:93:A:GLY:N	1:93:A:GLY:H	14	1.86
(1,263)	2:454:B:PHE:N	2:454:B:PHE:CA	2:454:B:PHE:C	2:455:B:TYR:N	8	1.86
(1,206)	2:457:B:HIS:C	2:458:B:PRO:N	2:458:B:PRO:CA	2:458:B:PRO:C	10	1.86
(1,79)	1:128:A:PHE:C	1:129:A:ALA:N	1:129:A:ALA:CA	1:129:A:ALA:C	22	1.86
(1,65)	1:105:A:LEU:C	1:106:A:VAL:N	1:106:A:VAL:CA	1:106:A:VAL:C	14	1.86
(1,288)	1:75:A:VAL:H	1:75:A:VAL:N	1:127:A:ASN:N	1:127:A:ASN:H	15	1.85
(1,223)	2:475:B:TYR:C	2:476:B:PRO:N	2:476:B:PRO:CA	2:476:B:PRO:C	23	1.85
(1,288)	1:75:A:VAL:H	1:75:A:VAL:N	1:127:A:ASN:N	1:127:A:ASN:H	13	1.84
(1,284)	1:60:A:GLY:H	1:60:A:GLY:N	1:111:A:THR:N	1:111:A:THR:H	20	1.84
(1,230)	2:449:B:GLU:N	2:449:B:GLU:CA	2:449:B:GLU:C	2:450:B:TRP:N	22	1.84
(1,25)	1:50:A:VAL:C	1:51:A:VAL:N	1:51:A:VAL:CA	1:51:A:VAL:C	6	1.84
(1,288)	1:75:A:VAL:H	1:75:A:VAL:N	1:127:A:ASN:N	1:127:A:ASN:H	18	1.83
(1,288)	1:75:A:VAL:H	1:75:A:VAL:N	1:127:A:ASN:N	1:127:A:ASN:H	23	1.83
(1,34)	1:63:A:HIS:C	1:64:A:TRP:N	1:64:A:TRP:CA	1:64:A:TRP:C	15	1.83
(1,26)	1:52:A:GLN:C	1:53:A:LEU:N	1:53:A:LEU:CA	1:53:A:LEU:C	1	1.83
(1,25)	1:50:A:VAL:C	1:51:A:VAL:N	1:51:A:VAL:CA	1:51:A:VAL:C	17	1.83
(1,307)	1:31:A:GLU:H	1:31:A:GLU:N	1:51:A:VAL:N	1:51:A:VAL:H	2	1.82
(1,307)	1:31:A:GLU:H	1:31:A:GLU:N	1:51:A:VAL:N	1:51:A:VAL:H	5	1.82
(1,266)	2:455:B:TYR:C	2:456:B:PHE:N	2:456:B:PHE:CA	2:456:B:PHE:C	17	1.82
(1,34)	1:63:A:HIS:C	1:64:A:TRP:N	1:64:A:TRP:CA	1:64:A:TRP:C	7	1.82
(1,24)	1:47:A:ALA:C	1:48:A:THR:N	1:48:A:THR:CA	1:48:A:THR:C	23	1.82
(1,308)	1:35:A:LEU:H	1:35:A:LEU:N	1:75:A:VAL:N	1:75:A:VAL:H	22	1.81
(1,273)	1:60:A:GLY:H	1:60:A:GLY:N	1:89:A:GLY:N	1:89:A:GLY:H	23	1.81
(1,236)	2:459:B:ILE:N	2:459:B:ILE:CA	2:459:B:ILE:C	2:460:B:SER:N	9	1.81
(1,79)	1:128:A:PHE:C	1:129:A:ALA:N	1:129:A:ALA:CA	1:129:A:ALA:C	6	1.81
(1,307)	1:31:A:GLU:H	1:31:A:GLU:N	1:51:A:VAL:N	1:51:A:VAL:H	11	1.8
(1,270)	1:51:A:VAL:H	1:51:A:VAL:N	1:60:A:GLY:N	1:60:A:GLY:H	11	1.8
(1,79)	1:128:A:PHE:C	1:129:A:ALA:N	1:129:A:ALA:CA	1:129:A:ALA:C	8	1.8
(1,285)	1:60:A:GLY:H	1:60:A:GLY:N	1:93:A:GLY:N	1:93:A:GLY:H	15	1.79
(1,280)	1:51:A:VAL:H	1:51:A:VAL:N	1:122:A:CYS:N	1:122:A:CYS:H	13	1.79

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,278)	1:75:A:VAL:H	1:75:A:VAL:N	1:114:A:PHE:N	1:114:A:PHE:H	7	1.79
(1,37)	1:67:A:GLU:C	1:68:A:HIS:N	1:68:A:HIS:CA	1:68:A:HIS:C	17	1.79
(1,307)	1:31:A:GLU:H	1:31:A:GLU:N	1:51:A:VAL:N	1:51:A:VAL:H	7	1.78
(1,307)	1:31:A:GLU:H	1:31:A:GLU:N	1:51:A:VAL:N	1:51:A:VAL:H	22	1.78
(1,231)	2:450:B:TRP:N	2:450:B:TRP:CA	2:450:B:TRP:C	2:451:B:GLU:N	8	1.78
(1,145)	1:86:A:ARG:N	1:86:A:ARG:CA	1:86:A:ARG:C	1:87:A:LEU:N	14	1.78
(1,79)	1:128:A:PHE:C	1:129:A:ALA:N	1:129:A:ALA:CA	1:129:A:ALA:C	15	1.78
(1,26)	1:52:A:GLN:C	1:53:A:LEU:N	1:53:A:LEU:CA	1:53:A:LEU:C	13	1.78
(1,280)	1:51:A:VAL:H	1:51:A:VAL:N	1:122:A:CYS:N	1:122:A:CYS:H	8	1.77
(1,230)	2:449:B:GLU:N	2:449:B:GLU:CA	2:449:B:GLU:C	2:450:B:TRP:N	1	1.77
(1,307)	1:31:A:GLU:H	1:31:A:GLU:N	1:51:A:VAL:N	1:51:A:VAL:H	6	1.76
(1,284)	1:60:A:GLY:H	1:60:A:GLY:N	1:111:A:THR:N	1:111:A:THR:H	23	1.76
(1,279)	1:75:A:VAL:H	1:75:A:VAL:N	1:111:A:THR:N	1:111:A:THR:H	4	1.76
(1,308)	1:35:A:LEU:H	1:35:A:LEU:N	1:75:A:VAL:N	1:75:A:VAL:H	17	1.75
(1,307)	1:31:A:GLU:H	1:31:A:GLU:N	1:51:A:VAL:N	1:51:A:VAL:H	1	1.75
(1,232)	2:451:B:GLU:N	2:451:B:GLU:CA	2:451:B:GLU:C	2:452:B:SER:N	9	1.75
(1,37)	1:67:A:GLU:C	1:68:A:HIS:N	1:68:A:HIS:CA	1:68:A:HIS:C	8	1.75
(1,266)	2:455:B:TYR:C	2:456:B:PHE:N	2:456:B:PHE:CA	2:456:B:PHE:C	11	1.74
(1,249)	2:473:B:LYS:N	2:473:B:LYS:CA	2:473:B:LYS:C	2:474:B:SER:N	10	1.74
(1,206)	2:457:B:HIS:C	2:458:B:PRO:N	2:458:B:PRO:CA	2:458:B:PRO:C	9	1.74
(1,307)	1:31:A:GLU:H	1:31:A:GLU:N	1:51:A:VAL:N	1:51:A:VAL:H	18	1.73
(1,284)	1:60:A:GLY:H	1:60:A:GLY:N	1:111:A:THR:N	1:111:A:THR:H	1	1.72
(1,250)	2:474:B:SER:N	2:474:B:SER:CA	2:474:B:SER:C	2:475:B:TYR:N	20	1.72
(1,139)	1:80:A:GLN:N	1:80:A:GLN:CA	1:80:A:GLN:C	1:81:A:LYS:N	10	1.72
(1,26)	1:52:A:GLN:C	1:53:A:LEU:N	1:53:A:LEU:CA	1:53:A:LEU:C	21	1.72
(1,285)	1:60:A:GLY:H	1:60:A:GLY:N	1:93:A:GLY:N	1:93:A:GLY:H	1	1.71
(1,236)	2:459:B:ILE:N	2:459:B:ILE:CA	2:459:B:ILE:C	2:460:B:SER:N	11	1.71
(1,308)	1:35:A:LEU:H	1:35:A:LEU:N	1:75:A:VAL:N	1:75:A:VAL:H	10	1.7
(1,288)	1:75:A:VAL:H	1:75:A:VAL:N	1:127:A:ASN:N	1:127:A:ASN:H	10	1.7
(1,284)	1:60:A:GLY:H	1:60:A:GLY:N	1:111:A:THR:N	1:111:A:THR:H	2	1.7
(1,284)	1:60:A:GLY:H	1:60:A:GLY:N	1:111:A:THR:N	1:111:A:THR:H	17	1.7
(1,230)	2:449:B:GLU:N	2:449:B:GLU:CA	2:449:B:GLU:C	2:450:B:TRP:N	11	1.7
(1,280)	1:51:A:VAL:H	1:51:A:VAL:N	1:122:A:CYS:N	1:122:A:CYS:H	17	1.69
(1,273)	1:60:A:GLY:H	1:60:A:GLY:N	1:89:A:GLY:N	1:89:A:GLY:H	5	1.69
(1,273)	1:60:A:GLY:H	1:60:A:GLY:N	1:89:A:GLY:N	1:89:A:GLY:H	18	1.69
(1,266)	2:455:B:TYR:C	2:456:B:PHE:N	2:456:B:PHE:CA	2:456:B:PHE:C	12	1.69
(1,263)	2:454:B:PHE:N	2:454:B:PHE:CA	2:454:B:PHE:C	2:455:B:TYR:N	9	1.69
(1,25)	1:50:A:VAL:C	1:51:A:VAL:N	1:51:A:VAL:CA	1:51:A:VAL:C	24	1.69
(1,307)	1:31:A:GLU:H	1:31:A:GLU:N	1:51:A:VAL:N	1:51:A:VAL:H	8	1.68
(1,280)	1:51:A:VAL:H	1:51:A:VAL:N	1:122:A:CYS:N	1:122:A:CYS:H	3	1.68
(1,273)	1:60:A:GLY:H	1:60:A:GLY:N	1:89:A:GLY:N	1:89:A:GLY:H	22	1.68
(1,244)	2:467:B:PRO:N	2:467:B:PRO:CA	2:467:B:PRO:C	2:468:B:TYR:N	16	1.68
(1,37)	1:67:A:GLU:C	1:68:A:HIS:N	1:68:A:HIS:CA	1:68:A:HIS:C	15	1.68
(1,266)	2:455:B:TYR:C	2:456:B:PHE:N	2:456:B:PHE:CA	2:456:B:PHE:C	2	1.67
(1,157)	1:108:A:SER:N	1:108:A:SER:CA	1:108:A:SER:C	1:109:A:THR:N	2	1.67
(1,81)	1:130:A:ASP:C	1:131:A:GLU:N	1:131:A:GLU:CA	1:131:A:GLU:C	8	1.67
(1,79)	1:128:A:PHE:C	1:129:A:ALA:N	1:129:A:ALA:CA	1:129:A:ALA:C	4	1.67
(1,288)	1:75:A:VAL:H	1:75:A:VAL:N	1:127:A:ASN:N	1:127:A:ASN:H	12	1.66
(1,285)	1:60:A:GLY:H	1:60:A:GLY:N	1:93:A:GLY:N	1:93:A:GLY:H	18	1.66
(1,254)	2:479:B:LEU:N	2:479:B:LEU:CA	2:479:B:LEU:C	2:480:B:ALA:N	21	1.66
(1,239)	2:462:B:LEU:N	2:462:B:LEU:CA	2:462:B:LEU:C	2:463:B:PRO:N	7	1.66

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,72)	1:115:A:HIS:C	1:116:A:THR:N	1:116:A:THR:CA	1:116:A:THR:C	18	1.66
(1,37)	1:67:A:GLU:C	1:68:A:HIS:N	1:68:A:HIS:CA	1:68:A:HIS:C	3	1.66
(1,34)	1:63:A:HIS:C	1:64:A:TRP:N	1:64:A:TRP:CA	1:64:A:TRP:C	12	1.66
(1,34)	1:63:A:HIS:C	1:64:A:TRP:N	1:64:A:TRP:CA	1:64:A:TRP:C	16	1.66
(1,285)	1:60:A:GLY:H	1:60:A:GLY:N	1:93:A:GLY:N	1:93:A:GLY:H	11	1.65
(1,270)	1:51:A:VAL:H	1:51:A:VAL:N	1:60:A:GLY:N	1:60:A:GLY:H	22	1.65
(1,266)	2:455:B:TYR:C	2:456:B:PHE:N	2:456:B:PHE:CA	2:456:B:PHE:C	10	1.65
(1,266)	2:455:B:TYR:C	2:456:B:PHE:N	2:456:B:PHE:CA	2:456:B:PHE:C	23	1.65
(1,221)	2:473:B:LYS:C	2:474:B:SER:N	2:474:B:SER:CA	2:474:B:SER:C	10	1.65
(1,204)	2:451:B:GLU:C	2:452:B:SER:N	2:452:B:SER:CA	2:452:B:SER:C	24	1.65
(1,28)	1:55:A:LEU:C	1:56:A:ALA:N	1:56:A:ALA:CA	1:56:A:ALA:C	3	1.65
(1,26)	1:52:A:GLN:C	1:53:A:LEU:N	1:53:A:LEU:CA	1:53:A:LEU:C	17	1.65
(1,307)	1:31:A:GLU:H	1:31:A:GLU:N	1:51:A:VAL:N	1:51:A:VAL:H	14	1.64
(1,288)	1:75:A:VAL:H	1:75:A:VAL:N	1:127:A:ASN:N	1:127:A:ASN:H	9	1.64
(1,285)	1:60:A:GLY:H	1:60:A:GLY:N	1:93:A:GLY:N	1:93:A:GLY:H	2	1.64
(1,280)	1:51:A:VAL:H	1:51:A:VAL:N	1:122:A:CYS:N	1:122:A:CYS:H	4	1.64
(1,156)	1:105:A:LEU:N	1:105:A:LEU:CA	1:105:A:LEU:C	1:106:A:VAL:N	22	1.64
(1,125)	1:57:A:LEU:N	1:57:A:LEU:CA	1:57:A:LEU:C	1:58:A:PRO:N	5	1.64
(1,280)	1:51:A:VAL:H	1:51:A:VAL:N	1:122:A:CYS:N	1:122:A:CYS:H	21	1.63
(1,266)	2:455:B:TYR:C	2:456:B:PHE:N	2:456:B:PHE:CA	2:456:B:PHE:C	22	1.63
(1,265)	2:455:B:TYR:N	2:455:B:TYR:CA	2:455:B:TYR:C	2:456:B:PHE:N	18	1.63
(1,225)	2:477:B:SER:C	2:478:B:LYS:N	2:478:B:LYS:CA	2:478:B:LYS:C	12	1.63
(1,55)	1:92:A:ALA:C	1:93:A:GLY:N	1:93:A:GLY:CA	1:93:A:GLY:C	15	1.63
(1,25)	1:50:A:VAL:C	1:51:A:VAL:N	1:51:A:VAL:CA	1:51:A:VAL:C	8	1.63
(1,308)	1:35:A:LEU:H	1:35:A:LEU:N	1:75:A:VAL:N	1:75:A:VAL:H	19	1.62
(1,285)	1:60:A:GLY:H	1:60:A:GLY:N	1:93:A:GLY:N	1:93:A:GLY:H	23	1.62
(1,280)	1:51:A:VAL:H	1:51:A:VAL:N	1:122:A:CYS:N	1:122:A:CYS:H	12	1.62
(1,244)	2:467:B:PRO:N	2:467:B:PRO:CA	2:467:B:PRO:C	2:468:B:TYR:N	15	1.62
(1,26)	1:52:A:GLN:C	1:53:A:LEU:N	1:53:A:LEU:CA	1:53:A:LEU:C	5	1.62
(1,285)	1:60:A:GLY:H	1:60:A:GLY:N	1:93:A:GLY:N	1:93:A:GLY:H	16	1.61
(1,268)	2:469:B:VAL:C	2:470:B:GLN:N	2:470:B:GLN:CA	2:470:B:GLN:C	23	1.61
(1,244)	2:467:B:PRO:N	2:467:B:PRO:CA	2:467:B:PRO:C	2:468:B:TYR:N	7	1.61
(1,204)	2:451:B:GLU:C	2:452:B:SER:N	2:452:B:SER:CA	2:452:B:SER:C	3	1.61
(1,204)	2:451:B:GLU:C	2:452:B:SER:N	2:452:B:SER:CA	2:452:B:SER:C	12	1.61
(1,34)	1:63:A:HIS:C	1:64:A:TRP:N	1:64:A:TRP:CA	1:64:A:TRP:C	6	1.61
(1,273)	1:60:A:GLY:H	1:60:A:GLY:N	1:89:A:GLY:N	1:89:A:GLY:H	8	1.6
(1,263)	2:454:B:PHE:N	2:454:B:PHE:CA	2:454:B:PHE:C	2:455:B:TYR:N	11	1.6
(1,236)	2:459:B:ILE:N	2:459:B:ILE:CA	2:459:B:ILE:C	2:460:B:SER:N	15	1.6
(1,230)	2:449:B:GLU:N	2:449:B:GLU:CA	2:449:B:GLU:C	2:450:B:TRP:N	16	1.6
(1,206)	2:457:B:HIS:C	2:458:B:PRO:N	2:458:B:PRO:CA	2:458:B:PRO:C	5	1.6
(1,204)	2:451:B:GLU:C	2:452:B:SER:N	2:452:B:SER:CA	2:452:B:SER:C	6	1.6
(1,34)	1:63:A:HIS:C	1:64:A:TRP:N	1:64:A:TRP:CA	1:64:A:TRP:C	11	1.6
(1,308)	1:35:A:LEU:H	1:35:A:LEU:N	1:75:A:VAL:N	1:75:A:VAL:H	12	1.59
(1,307)	1:31:A:GLU:H	1:31:A:GLU:N	1:51:A:VAL:N	1:51:A:VAL:H	20	1.59
(1,261)	2:453:B:ARG:N	2:453:B:ARG:CA	2:453:B:ARG:C	2:454:B:PHE:N	11	1.59
(1,236)	2:459:B:ILE:N	2:459:B:ILE:CA	2:459:B:ILE:C	2:460:B:SER:N	14	1.59
(1,204)	2:451:B:GLU:C	2:452:B:SER:N	2:452:B:SER:CA	2:452:B:SER:C	15	1.59
(1,157)	1:108:A:SER:N	1:108:A:SER:CA	1:108:A:SER:C	1:109:A:THR:N	6	1.59
(1,81)	1:130:A:ASP:C	1:131:A:GLU:N	1:131:A:GLU:CA	1:131:A:GLU:C	17	1.59
(1,55)	1:92:A:ALA:C	1:93:A:GLY:N	1:93:A:GLY:CA	1:93:A:GLY:C	17	1.59
(1,307)	1:31:A:GLU:H	1:31:A:GLU:N	1:51:A:VAL:N	1:51:A:VAL:H	4	1.58

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,273)	1:60:A:GLY:H	1:60:A:GLY:N	1:89:A:GLY:N	1:89:A:GLY:H	3	1.58
(1,273)	1:60:A:GLY:H	1:60:A:GLY:N	1:89:A:GLY:N	1:89:A:GLY:H	7	1.58
(1,250)	2:474:B:SER:N	2:474:B:SER:CA	2:474:B:SER:C	2:475:B:TYR:N	6	1.58
(1,37)	1:67:A:GLU:C	1:68:A:HIS:N	1:68:A:HIS:CA	1:68:A:HIS:C	5	1.58
(1,204)	2:451:B:GLU:C	2:452:B:SER:N	2:452:B:SER:CA	2:452:B:SER:C	22	1.57
(1,202)	2:449:B:GLU:C	2:450:B:TRP:N	2:450:B:TRP:CA	2:450:B:TRP:C	13	1.57
(1,120)	1:47:A:ALA:N	1:47:A:ALA:CA	1:47:A:ALA:C	1:48:A:THR:N	18	1.57
(1,285)	1:60:A:GLY:H	1:60:A:GLY:N	1:93:A:GLY:N	1:93:A:GLY:H	8	1.56
(1,284)	1:60:A:GLY:H	1:60:A:GLY:N	1:111:A:THR:N	1:111:A:THR:H	11	1.56
(1,268)	2:469:B:VAL:C	2:470:B:GLN:N	2:470:B:GLN:CA	2:470:B:GLN:C	24	1.56
(1,236)	2:459:B:ILE:N	2:459:B:ILE:CA	2:459:B:ILE:C	2:460:B:SER:N	6	1.56
(1,222)	2:474:B:SER:C	2:475:B:TYR:N	2:475:B:TYR:CA	2:475:B:TYR:C	21	1.56
(1,204)	2:451:B:GLU:C	2:452:B:SER:N	2:452:B:SER:CA	2:452:B:SER:C	7	1.56
(1,204)	2:451:B:GLU:C	2:452:B:SER:N	2:452:B:SER:CA	2:452:B:SER:C	19	1.56
(1,204)	2:451:B:GLU:C	2:452:B:SER:N	2:452:B:SER:CA	2:452:B:SER:C	21	1.56
(1,139)	1:80:A:GLN:N	1:80:A:GLN:CA	1:80:A:GLN:C	1:81:A:LYS:N	4	1.56
(1,139)	1:80:A:GLN:N	1:80:A:GLN:CA	1:80:A:GLN:C	1:81:A:LYS:N	14	1.56
(1,266)	2:455:B:TYR:C	2:456:B:PHE:N	2:456:B:PHE:CA	2:456:B:PHE:C	7	1.55
(1,263)	2:454:B:PHE:N	2:454:B:PHE:CA	2:454:B:PHE:C	2:455:B:TYR:N	7	1.55
(1,263)	2:454:B:PHE:N	2:454:B:PHE:CA	2:454:B:PHE:C	2:455:B:TYR:N	18	1.55
(1,249)	2:473:B:LYS:N	2:473:B:LYS:CA	2:473:B:LYS:C	2:474:B:SER:N	20	1.55
(1,244)	2:467:B:PRO:N	2:467:B:PRO:CA	2:467:B:PRO:C	2:468:B:TYR:N	11	1.55
(1,55)	1:92:A:ALA:C	1:93:A:GLY:N	1:93:A:GLY:CA	1:93:A:GLY:C	16	1.55
(1,51)	1:86:A:ARG:C	1:87:A:LEU:N	1:87:A:LEU:CA	1:87:A:LEU:C	18	1.55
(1,26)	1:52:A:GLN:C	1:53:A:LEU:N	1:53:A:LEU:CA	1:53:A:LEU:C	6	1.55
(1,307)	1:31:A:GLU:H	1:31:A:GLU:N	1:51:A:VAL:N	1:51:A:VAL:H	21	1.54
(1,250)	2:474:B:SER:N	2:474:B:SER:CA	2:474:B:SER:C	2:475:B:TYR:N	23	1.54
(1,244)	2:467:B:PRO:N	2:467:B:PRO:CA	2:467:B:PRO:C	2:468:B:TYR:N	18	1.54
(1,225)	2:477:B:SER:C	2:478:B:LYS:N	2:478:B:LYS:CA	2:478:B:LYS:C	17	1.54
(1,156)	1:105:A:LEU:N	1:105:A:LEU:CA	1:105:A:LEU:C	1:106:A:VAL:N	13	1.54
(1,28)	1:55:A:LEU:C	1:56:A:ALA:N	1:56:A:ALA:CA	1:56:A:ALA:C	16	1.54
(1,26)	1:52:A:GLN:C	1:53:A:LEU:N	1:53:A:LEU:CA	1:53:A:LEU:C	20	1.54
(1,308)	1:35:A:LEU:H	1:35:A:LEU:N	1:75:A:VAL:N	1:75:A:VAL:H	5	1.53
(1,285)	1:60:A:GLY:H	1:60:A:GLY:N	1:93:A:GLY:N	1:93:A:GLY:H	17	1.53
(1,285)	1:60:A:GLY:H	1:60:A:GLY:N	1:93:A:GLY:N	1:93:A:GLY:H	24	1.53
(1,206)	2:457:B:HIS:C	2:458:B:PRO:N	2:458:B:PRO:CA	2:458:B:PRO:C	22	1.53
(1,204)	2:451:B:GLU:C	2:452:B:SER:N	2:452:B:SER:CA	2:452:B:SER:C	10	1.53
(1,202)	2:449:B:GLU:C	2:450:B:TRP:N	2:450:B:TRP:CA	2:450:B:TRP:C	10	1.53
(1,280)	1:51:A:VAL:H	1:51:A:VAL:N	1:122:A:CYS:N	1:122:A:CYS:H	20	1.52
(1,250)	2:474:B:SER:N	2:474:B:SER:CA	2:474:B:SER:C	2:475:B:TYR:N	11	1.52
(1,249)	2:473:B:LYS:N	2:473:B:LYS:CA	2:473:B:LYS:C	2:474:B:SER:N	12	1.52
(1,204)	2:451:B:GLU:C	2:452:B:SER:N	2:452:B:SER:CA	2:452:B:SER:C	11	1.52
(1,307)	1:31:A:GLU:H	1:31:A:GLU:N	1:51:A:VAL:N	1:51:A:VAL:H	3	1.51
(1,307)	1:31:A:GLU:H	1:31:A:GLU:N	1:51:A:VAL:N	1:51:A:VAL:H	23	1.51
(1,268)	2:469:B:VAL:C	2:470:B:GLN:N	2:470:B:GLN:CA	2:470:B:GLN:C	17	1.51
(1,244)	2:467:B:PRO:N	2:467:B:PRO:CA	2:467:B:PRO:C	2:468:B:TYR:N	14	1.51
(1,204)	2:451:B:GLU:C	2:452:B:SER:N	2:452:B:SER:CA	2:452:B:SER:C	2	1.51
(1,204)	2:451:B:GLU:C	2:452:B:SER:N	2:452:B:SER:CA	2:452:B:SER:C	16	1.51
(1,202)	2:449:B:GLU:C	2:450:B:TRP:N	2:450:B:TRP:CA	2:450:B:TRP:C	8	1.51
(1,285)	1:60:A:GLY:H	1:60:A:GLY:N	1:93:A:GLY:N	1:93:A:GLY:H	21	1.5
(1,244)	2:467:B:PRO:N	2:467:B:PRO:CA	2:467:B:PRO:C	2:468:B:TYR:N	3	1.5

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,223)	2:475:B:TYR:C	2:476:B:PRO:N	2:476:B:PRO:CA	2:476:B:PRO:C	17	1.5
(1,221)	2:473:B:LYS:C	2:474:B:SER:N	2:474:B:SER:CA	2:474:B:SER:C	12	1.5
(1,204)	2:451:B:GLU:C	2:452:B:SER:N	2:452:B:SER:CA	2:452:B:SER:C	18	1.5
(1,145)	1:86:A:ARG:N	1:86:A:ARG:CA	1:86:A:ARG:C	1:87:A:LEU:N	15	1.5
(1,280)	1:51:A:VAL:H	1:51:A:VAL:N	1:122:A:CYS:N	1:122:A:CYS:H	24	1.49
(1,204)	2:451:B:GLU:C	2:452:B:SER:N	2:452:B:SER:CA	2:452:B:SER:C	4	1.49
(1,204)	2:451:B:GLU:C	2:452:B:SER:N	2:452:B:SER:CA	2:452:B:SER:C	14	1.49
(1,55)	1:92:A:ALA:C	1:93:A:GLY:N	1:93:A:GLY:CA	1:93:A:GLY:C	10	1.49
(1,28)	1:55:A:LEU:C	1:56:A:ALA:N	1:56:A:ALA:CA	1:56:A:ALA:C	11	1.49
(1,250)	2:474:B:SER:N	2:474:B:SER:CA	2:474:B:SER:C	2:475:B:TYR:N	24	1.48
(1,236)	2:459:B:ILE:N	2:459:B:ILE:CA	2:459:B:ILE:C	2:460:B:SER:N	23	1.48
(1,153)	1:101:A:LEU:N	1:101:A:LEU:CA	1:101:A:LEU:C	1:102:A:TYR:N	13	1.48
(1,79)	1:128:A:PHE:C	1:129:A:ALA:N	1:129:A:ALA:CA	1:129:A:ALA:C	2	1.48
(1,308)	1:35:A:LEU:H	1:35:A:LEU:N	1:75:A:VAL:N	1:75:A:VAL:H	21	1.47
(1,284)	1:60:A:GLY:H	1:60:A:GLY:N	1:111:A:THR:N	1:111:A:THR:H	15	1.47
(1,244)	2:467:B:PRO:N	2:467:B:PRO:CA	2:467:B:PRO:C	2:468:B:TYR:N	20	1.47
(1,223)	2:475:B:TYR:C	2:476:B:PRO:N	2:476:B:PRO:CA	2:476:B:PRO:C	19	1.47
(1,204)	2:451:B:GLU:C	2:452:B:SER:N	2:452:B:SER:CA	2:452:B:SER:C	5	1.47
(1,81)	1:130:A:ASP:C	1:131:A:GLU:N	1:131:A:GLU:CA	1:131:A:GLU:C	23	1.47
(1,72)	1:115:A:HIS:C	1:116:A:THR:N	1:116:A:THR:CA	1:116:A:THR:C	21	1.47
(1,51)	1:86:A:ARG:C	1:87:A:LEU:N	1:87:A:LEU:CA	1:87:A:LEU:C	14	1.47
(1,278)	1:75:A:VAL:H	1:75:A:VAL:N	1:114:A:PHE:N	1:114:A:PHE:H	16	1.46
(1,278)	1:75:A:VAL:H	1:75:A:VAL:N	1:114:A:PHE:N	1:114:A:PHE:H	17	1.46
(1,266)	2:455:B:TYR:C	2:456:B:PHE:N	2:456:B:PHE:CA	2:456:B:PHE:C	4	1.46
(1,264)	2:454:B:PHE:C	2:455:B:TYR:N	2:455:B:TYR:CA	2:455:B:TYR:C	8	1.46
(1,204)	2:451:B:GLU:C	2:452:B:SER:N	2:452:B:SER:CA	2:452:B:SER:C	13	1.46
(1,204)	2:451:B:GLU:C	2:452:B:SER:N	2:452:B:SER:CA	2:452:B:SER:C	20	1.46
(1,204)	2:451:B:GLU:C	2:452:B:SER:N	2:452:B:SER:CA	2:452:B:SER:C	23	1.46
(1,46)	1:81:A:LYS:C	1:82:A:SER:N	1:82:A:SER:CA	1:82:A:SER:C	13	1.46
(1,278)	1:75:A:VAL:H	1:75:A:VAL:N	1:114:A:PHE:N	1:114:A:PHE:H	12	1.45
(1,244)	2:467:B:PRO:N	2:467:B:PRO:CA	2:467:B:PRO:C	2:468:B:TYR:N	23	1.45
(1,81)	1:130:A:ASP:C	1:131:A:GLU:N	1:131:A:GLU:CA	1:131:A:GLU:C	13	1.44
(1,55)	1:92:A:ALA:C	1:93:A:GLY:N	1:93:A:GLY:CA	1:93:A:GLY:C	3	1.44
(1,34)	1:63:A:HIS:C	1:64:A:TRP:N	1:64:A:TRP:CA	1:64:A:TRP:C	21	1.44
(1,288)	1:75:A:VAL:H	1:75:A:VAL:N	1:127:A:ASN:N	1:127:A:ASN:H	17	1.43
(1,285)	1:60:A:GLY:H	1:60:A:GLY:N	1:93:A:GLY:N	1:93:A:GLY:H	7	1.43
(1,284)	1:60:A:GLY:H	1:60:A:GLY:N	1:111:A:THR:N	1:111:A:THR:H	12	1.43
(1,280)	1:51:A:VAL:H	1:51:A:VAL:N	1:122:A:CYS:N	1:122:A:CYS:H	5	1.43
(1,244)	2:467:B:PRO:N	2:467:B:PRO:CA	2:467:B:PRO:C	2:468:B:TYR:N	13	1.43
(1,204)	2:451:B:GLU:C	2:452:B:SER:N	2:452:B:SER:CA	2:452:B:SER:C	1	1.43
(1,204)	2:451:B:GLU:C	2:452:B:SER:N	2:452:B:SER:CA	2:452:B:SER:C	17	1.43
(1,81)	1:130:A:ASP:C	1:131:A:GLU:N	1:131:A:GLU:CA	1:131:A:GLU:C	4	1.43
(1,308)	1:35:A:LEU:H	1:35:A:LEU:N	1:75:A:VAL:N	1:75:A:VAL:H	4	1.42
(1,284)	1:60:A:GLY:H	1:60:A:GLY:N	1:111:A:THR:N	1:111:A:THR:H	19	1.42
(1,250)	2:474:B:SER:N	2:474:B:SER:CA	2:474:B:SER:C	2:475:B:TYR:N	15	1.42
(1,129)	1:63:A:HIS:N	1:63:A:HIS:CA	1:63:A:HIS:C	1:64:A:TRP:N	11	1.42
(1,34)	1:63:A:HIS:C	1:64:A:TRP:N	1:64:A:TRP:CA	1:64:A:TRP:C	18	1.42
(1,273)	1:60:A:GLY:H	1:60:A:GLY:N	1:89:A:GLY:N	1:89:A:GLY:H	9	1.41
(1,270)	1:51:A:VAL:H	1:51:A:VAL:N	1:60:A:GLY:N	1:60:A:GLY:H	3	1.41
(1,268)	2:469:B:VAL:C	2:470:B:GLN:N	2:470:B:GLN:CA	2:470:B:GLN:C	16	1.41
(1,244)	2:467:B:PRO:N	2:467:B:PRO:CA	2:467:B:PRO:C	2:468:B:TYR:N	9	1.41

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,129)	1:63:A:HIS:N	1:63:A:HIS:CA	1:63:A:HIS:C	1:64:A:TRP:N	15	1.41
(1,26)	1:52:A:GLN:C	1:53:A:LEU:N	1:53:A:LEU:CA	1:53:A:LEU:C	18	1.41
(1,278)	1:75:A:VAL:H	1:75:A:VAL:N	1:114:A:PHE:N	1:114:A:PHE:H	9	1.4
(1,268)	2:469:B:VAL:C	2:470:B:GLN:N	2:470:B:GLN:CA	2:470:B:GLN:C	3	1.4
(1,244)	2:467:B:PRO:N	2:467:B:PRO:CA	2:467:B:PRO:C	2:468:B:TYR:N	19	1.4
(1,204)	2:451:B:GLU:C	2:452:B:SER:N	2:452:B:SER:CA	2:452:B:SER:C	9	1.4
(1,79)	1:128:A:PHE:C	1:129:A:ALA:N	1:129:A:ALA:CA	1:129:A:ALA:C	20	1.4
(1,26)	1:52:A:GLN:C	1:53:A:LEU:N	1:53:A:LEU:CA	1:53:A:LEU:C	4	1.4
(1,288)	1:75:A:VAL:H	1:75:A:VAL:N	1:127:A:ASN:N	1:127:A:ASN:H	5	1.39
(1,285)	1:60:A:GLY:H	1:60:A:GLY:N	1:93:A:GLY:N	1:93:A:GLY:H	22	1.39
(1,284)	1:60:A:GLY:H	1:60:A:GLY:N	1:111:A:THR:N	1:111:A:THR:H	13	1.39
(1,280)	1:51:A:VAL:H	1:51:A:VAL:N	1:122:A:CYS:N	1:122:A:CYS:H	16	1.39
(1,232)	2:451:B:GLU:N	2:451:B:GLU:CA	2:451:B:GLU:C	2:452:B:SER:N	8	1.39
(1,34)	1:63:A:HIS:C	1:64:A:TRP:N	1:64:A:TRP:CA	1:64:A:TRP:C	10	1.39
(1,34)	1:63:A:HIS:C	1:64:A:TRP:N	1:64:A:TRP:CA	1:64:A:TRP:C	13	1.39
(1,26)	1:52:A:GLN:C	1:53:A:LEU:N	1:53:A:LEU:CA	1:53:A:LEU:C	2	1.39
(1,26)	1:52:A:GLN:C	1:53:A:LEU:N	1:53:A:LEU:CA	1:53:A:LEU:C	23	1.39
(1,26)	1:52:A:GLN:C	1:53:A:LEU:N	1:53:A:LEU:CA	1:53:A:LEU:C	24	1.39
(1,24)	1:47:A:ALA:C	1:48:A:THR:N	1:48:A:THR:CA	1:48:A:THR:C	5	1.39
(1,285)	1:60:A:GLY:H	1:60:A:GLY:N	1:93:A:GLY:N	1:93:A:GLY:H	12	1.38
(1,284)	1:60:A:GLY:H	1:60:A:GLY:N	1:111:A:THR:N	1:111:A:THR:H	9	1.38
(1,280)	1:51:A:VAL:H	1:51:A:VAL:N	1:122:A:CYS:N	1:122:A:CYS:H	6	1.38
(1,250)	2:474:B:SER:N	2:474:B:SER:CA	2:474:B:SER:C	2:475:B:TYR:N	10	1.38
(1,244)	2:467:B:PRO:N	2:467:B:PRO:CA	2:467:B:PRO:C	2:468:B:TYR:N	2	1.38
(1,223)	2:475:B:TYR:C	2:476:B:PRO:N	2:476:B:PRO:CA	2:476:B:PRO:C	2	1.38
(1,139)	1:80:A:GLN:N	1:80:A:GLN:CA	1:80:A:GLN:C	1:81:A:LYS:N	24	1.38
(1,129)	1:63:A:HIS:N	1:63:A:HIS:CA	1:63:A:HIS:C	1:64:A:TRP:N	12	1.38
(1,37)	1:67:A:GLU:C	1:68:A:HIS:N	1:68:A:HIS:CA	1:68:A:HIS:C	16	1.38
(1,288)	1:75:A:VAL:H	1:75:A:VAL:N	1:127:A:ASN:N	1:127:A:ASN:H	8	1.37
(1,145)	1:86:A:ARG:N	1:86:A:ARG:CA	1:86:A:ARG:C	1:87:A:LEU:N	1	1.37
(1,125)	1:57:A:LEU:N	1:57:A:LEU:CA	1:57:A:LEU:C	1:58:A:PRO:N	6	1.37
(1,38)	1:71:A:ALA:C	1:72:A:VAL:N	1:72:A:VAL:CA	1:72:A:VAL:C	4	1.37
(1,37)	1:67:A:GLU:C	1:68:A:HIS:N	1:68:A:HIS:CA	1:68:A:HIS:C	21	1.37
(1,266)	2:455:B:TYR:C	2:456:B:PHE:N	2:456:B:PHE:CA	2:456:B:PHE:C	15	1.36
(1,265)	2:455:B:TYR:N	2:455:B:TYR:CA	2:455:B:TYR:C	2:456:B:PHE:N	8	1.36
(1,265)	2:455:B:TYR:N	2:455:B:TYR:CA	2:455:B:TYR:C	2:456:B:PHE:N	9	1.36
(1,244)	2:467:B:PRO:N	2:467:B:PRO:CA	2:467:B:PRO:C	2:468:B:TYR:N	17	1.36
(1,153)	1:101:A:LEU:N	1:101:A:LEU:CA	1:101:A:LEU:C	1:102:A:TYR:N	20	1.36
(1,139)	1:80:A:GLN:N	1:80:A:GLN:CA	1:80:A:GLN:C	1:81:A:LYS:N	11	1.36
(1,264)	2:454:B:PHE:C	2:455:B:TYR:N	2:455:B:TYR:CA	2:455:B:TYR:C	7	1.35
(1,81)	1:130:A:ASP:C	1:131:A:GLU:N	1:131:A:GLU:CA	1:131:A:GLU:C	6	1.35
(1,26)	1:52:A:GLN:C	1:53:A:LEU:N	1:53:A:LEU:CA	1:53:A:LEU:C	12	1.35
(1,308)	1:35:A:LEU:H	1:35:A:LEU:N	1:75:A:VAL:N	1:75:A:VAL:H	3	1.34
(1,307)	1:31:A:GLU:H	1:31:A:GLU:N	1:51:A:VAL:N	1:51:A:VAL:H	12	1.34
(1,280)	1:51:A:VAL:H	1:51:A:VAL:N	1:122:A:CYS:N	1:122:A:CYS:H	10	1.34
(1,268)	2:469:B:VAL:C	2:470:B:GLN:N	2:470:B:GLN:CA	2:470:B:GLN:C	13	1.34
(1,230)	2:449:B:GLU:N	2:449:B:GLU:CA	2:449:B:GLU:C	2:450:B:TRP:N	19	1.34
(1,230)	2:449:B:GLU:N	2:449:B:GLU:CA	2:449:B:GLU:C	2:450:B:TRP:N	23	1.34
(1,223)	2:475:B:TYR:C	2:476:B:PRO:N	2:476:B:PRO:CA	2:476:B:PRO:C	5	1.34
(1,72)	1:115:A:HIS:C	1:116:A:THR:N	1:116:A:THR:CA	1:116:A:THR:C	5	1.34
(1,37)	1:67:A:GLU:C	1:68:A:HIS:N	1:68:A:HIS:CA	1:68:A:HIS:C	4	1.34

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,26)	1:52:A:GLN:C	1:53:A:LEU:N	1:53:A:LEU:CA	1:53:A:LEU:C	9	1.34
(1,292)	1:60:A:GLY:H	1:60:A:GLY:N	1:64:A:TRP:N	1:64:A:TRP:H	18	1.33
(1,253)	2:478:B:LYS:N	2:478:B:LYS:CA	2:478:B:LYS:C	2:479:B:LEU:N	18	1.33
(1,244)	2:467:B:PRO:N	2:467:B:PRO:CA	2:467:B:PRO:C	2:468:B:TYR:N	8	1.33
(1,230)	2:449:B:GLU:N	2:449:B:GLU:CA	2:449:B:GLU:C	2:450:B:TRP:N	12	1.33
(1,145)	1:86:A:ARG:N	1:86:A:ARG:CA	1:86:A:ARG:C	1:87:A:LEU:N	18	1.33
(1,34)	1:63:A:HIS:C	1:64:A:TRP:N	1:64:A:TRP:CA	1:64:A:TRP:C	23	1.33
(1,263)	2:454:B:PHE:N	2:454:B:PHE:CA	2:454:B:PHE:C	2:455:B:TYR:N	19	1.32
(1,225)	2:477:B:SER:C	2:478:B:LYS:N	2:478:B:LYS:CA	2:478:B:LYS:C	2	1.32
(1,225)	2:477:B:SER:C	2:478:B:LYS:N	2:478:B:LYS:CA	2:478:B:LYS:C	9	1.32
(1,47)	1:82:A:SER:C	1:83:A:TYR:N	1:83:A:TYR:CA	1:83:A:TYR:C	10	1.32
(1,266)	2:455:B:TYR:C	2:456:B:PHE:N	2:456:B:PHE:CA	2:456:B:PHE:C	21	1.31
(1,207)	2:458:B:PRO:C	2:459:B:ILE:N	2:459:B:ILE:CA	2:459:B:ILE:C	9	1.31
(1,37)	1:67:A:GLU:C	1:68:A:HIS:N	1:68:A:HIS:CA	1:68:A:HIS:C	24	1.31
(1,280)	1:51:A:VAL:H	1:51:A:VAL:N	1:122:A:CYS:N	1:122:A:CYS:H	19	1.3
(1,244)	2:467:B:PRO:N	2:467:B:PRO:CA	2:467:B:PRO:C	2:468:B:TYR:N	21	1.3
(1,221)	2:473:B:LYS:C	2:474:B:SER:N	2:474:B:SER:CA	2:474:B:SER:C	15	1.3
(1,208)	2:459:B:ILE:C	2:460:B:SER:N	2:460:B:SER:CA	2:460:B:SER:C	6	1.3
(1,204)	2:451:B:GLU:C	2:452:B:SER:N	2:452:B:SER:CA	2:452:B:SER:C	8	1.3
(1,129)	1:63:A:HIS:N	1:63:A:HIS:CA	1:63:A:HIS:C	1:64:A:TRP:N	7	1.3
(1,125)	1:57:A:LEU:N	1:57:A:LEU:CA	1:57:A:LEU:C	1:58:A:PRO:N	14	1.3
(1,120)	1:47:A:ALA:N	1:47:A:ALA:CA	1:47:A:ALA:C	1:48:A:THR:N	20	1.3
(1,81)	1:130:A:ASP:C	1:131:A:GLU:N	1:131:A:GLU:CA	1:131:A:GLU:C	21	1.3
(1,55)	1:92:A:ALA:C	1:93:A:GLY:N	1:93:A:GLY:CA	1:93:A:GLY:C	18	1.3
(1,37)	1:67:A:GLU:C	1:68:A:HIS:N	1:68:A:HIS:CA	1:68:A:HIS:C	13	1.3
(1,308)	1:35:A:LEU:H	1:35:A:LEU:N	1:75:A:VAL:N	1:75:A:VAL:H	14	1.29
(1,273)	1:60:A:GLY:H	1:60:A:GLY:N	1:89:A:GLY:N	1:89:A:GLY:H	13	1.29
(1,254)	2:479:B:LEU:N	2:479:B:LEU:CA	2:479:B:LEU:C	2:480:B:ALA:N	1	1.29
(1,244)	2:467:B:PRO:N	2:467:B:PRO:CA	2:467:B:PRO:C	2:468:B:TYR:N	10	1.29
(1,206)	2:457:B:HIS:C	2:458:B:PRO:N	2:458:B:PRO:CA	2:458:B:PRO:C	11	1.29
(1,139)	1:80:A:GLN:N	1:80:A:GLN:CA	1:80:A:GLN:C	1:81:A:LYS:N	19	1.29
(1,122)	1:51:A:VAL:N	1:51:A:VAL:CA	1:51:A:VAL:C	1:52:A:GLN:N	21	1.29
(1,120)	1:47:A:ALA:N	1:47:A:ALA:CA	1:47:A:ALA:C	1:48:A:THR:N	7	1.29
(1,34)	1:63:A:HIS:C	1:64:A:TRP:N	1:64:A:TRP:CA	1:64:A:TRP:C	22	1.29
(1,292)	1:60:A:GLY:H	1:60:A:GLY:N	1:64:A:TRP:N	1:64:A:TRP:H	7	1.28
(1,202)	2:449:B:GLU:C	2:450:B:TRP:N	2:450:B:TRP:CA	2:450:B:TRP:C	4	1.28
(1,139)	1:80:A:GLN:N	1:80:A:GLN:CA	1:80:A:GLN:C	1:81:A:LYS:N	6	1.28
(1,55)	1:92:A:ALA:C	1:93:A:GLY:N	1:93:A:GLY:CA	1:93:A:GLY:C	4	1.28
(1,34)	1:63:A:HIS:C	1:64:A:TRP:N	1:64:A:TRP:CA	1:64:A:TRP:C	8	1.28
(1,25)	1:50:A:VAL:C	1:51:A:VAL:N	1:51:A:VAL:CA	1:51:A:VAL:C	4	1.28
(1,263)	2:454:B:PHE:N	2:454:B:PHE:CA	2:454:B:PHE:C	2:455:B:TYR:N	20	1.27
(1,250)	2:474:B:SER:N	2:474:B:SER:CA	2:474:B:SER:C	2:475:B:TYR:N	1	1.27
(1,79)	1:128:A:PHE:C	1:129:A:ALA:N	1:129:A:ALA:CA	1:129:A:ALA:C	17	1.27
(1,79)	1:128:A:PHE:C	1:129:A:ALA:N	1:129:A:ALA:CA	1:129:A:ALA:C	19	1.27
(1,79)	1:128:A:PHE:C	1:129:A:ALA:N	1:129:A:ALA:CA	1:129:A:ALA:C	23	1.27
(1,28)	1:55:A:LEU:C	1:56:A:ALA:N	1:56:A:ALA:CA	1:56:A:ALA:C	17	1.27
(1,254)	2:479:B:LEU:N	2:479:B:LEU:CA	2:479:B:LEU:C	2:480:B:ALA:N	7	1.26
(1,250)	2:474:B:SER:N	2:474:B:SER:CA	2:474:B:SER:C	2:475:B:TYR:N	22	1.26
(1,225)	2:477:B:SER:C	2:478:B:LYS:N	2:478:B:LYS:CA	2:478:B:LYS:C	23	1.26
(1,153)	1:101:A:LEU:N	1:101:A:LEU:CA	1:101:A:LEU:C	1:102:A:TYR:N	21	1.26
(1,46)	1:81:A:LYS:C	1:82:A:SER:N	1:82:A:SER:CA	1:82:A:SER:C	16	1.26

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,34)	1:63:A:HIS:C	1:64:A:TRP:N	1:64:A:TRP:CA	1:64:A:TRP:C	1	1.26
(1,28)	1:55:A:LEU:C	1:56:A:ALA:N	1:56:A:ALA:CA	1:56:A:ALA:C	12	1.26
(1,305)	1:85:A:ILE:H	1:85:A:ILE:N	2:479:B:LEU:N	2:479:B:LEU:H	21	1.25
(1,285)	1:60:A:GLY:H	1:60:A:GLY:N	1:93:A:GLY:N	1:93:A:GLY:H	9	1.25
(1,268)	2:469:B:VAL:C	2:470:B:GLN:N	2:470:B:GLN:CA	2:470:B:GLN:C	14	1.25
(1,263)	2:454:B:PHE:N	2:454:B:PHE:CA	2:454:B:PHE:C	2:455:B:TYR:N	2	1.25
(1,263)	2:454:B:PHE:N	2:454:B:PHE:CA	2:454:B:PHE:C	2:455:B:TYR:N	15	1.25
(1,254)	2:479:B:LEU:N	2:479:B:LEU:CA	2:479:B:LEU:C	2:480:B:ALA:N	13	1.25
(1,140)	1:81:A:LYS:N	1:81:A:LYS:CA	1:81:A:LYS:C	1:82:A:SER:N	6	1.25
(1,125)	1:57:A:LEU:N	1:57:A:LEU:CA	1:57:A:LEU:C	1:58:A:PRO:N	20	1.25
(1,37)	1:67:A:GLU:C	1:68:A:HIS:N	1:68:A:HIS:CA	1:68:A:HIS:C	2	1.25
(1,34)	1:63:A:HIS:C	1:64:A:TRP:N	1:64:A:TRP:CA	1:64:A:TRP:C	14	1.25
(1,263)	2:454:B:PHE:N	2:454:B:PHE:CA	2:454:B:PHE:C	2:455:B:TYR:N	12	1.24
(1,230)	2:449:B:GLU:N	2:449:B:GLU:CA	2:449:B:GLU:C	2:450:B:TRP:N	17	1.24
(1,223)	2:475:B:TYR:C	2:476:B:PRO:N	2:476:B:PRO:CA	2:476:B:PRO:C	16	1.24
(1,129)	1:63:A:HIS:N	1:63:A:HIS:CA	1:63:A:HIS:C	1:64:A:TRP:N	8	1.24
(1,70)	1:113:A:PHE:C	1:114:A:PHE:N	1:114:A:PHE:CA	1:114:A:PHE:C	16	1.24
(1,51)	1:86:A:ARG:C	1:87:A:LEU:N	1:87:A:LEU:CA	1:87:A:LEU:C	1	1.24
(1,37)	1:67:A:GLU:C	1:68:A:HIS:N	1:68:A:HIS:CA	1:68:A:HIS:C	11	1.24
(1,37)	1:67:A:GLU:C	1:68:A:HIS:N	1:68:A:HIS:CA	1:68:A:HIS:C	12	1.24
(1,37)	1:67:A:GLU:C	1:68:A:HIS:N	1:68:A:HIS:CA	1:68:A:HIS:C	22	1.24
(1,34)	1:63:A:HIS:C	1:64:A:TRP:N	1:64:A:TRP:CA	1:64:A:TRP:C	4	1.24
(1,25)	1:50:A:VAL:C	1:51:A:VAL:N	1:51:A:VAL:CA	1:51:A:VAL:C	14	1.24
(1,308)	1:35:A:LEU:H	1:35:A:LEU:N	1:75:A:VAL:N	1:75:A:VAL:H	6	1.23
(1,288)	1:75:A:VAL:H	1:75:A:VAL:N	1:127:A:ASN:N	1:127:A:ASN:H	3	1.23
(1,266)	2:455:B:TYR:C	2:456:B:PHE:N	2:456:B:PHE:CA	2:456:B:PHE:C	18	1.23
(1,264)	2:454:B:PHE:C	2:455:B:TYR:N	2:455:B:TYR:CA	2:455:B:TYR:C	9	1.23
(1,221)	2:473:B:LYS:C	2:474:B:SER:N	2:474:B:SER:CA	2:474:B:SER:C	20	1.23
(1,151)	1:97:A:TRP:N	1:97:A:TRP:CA	1:97:A:TRP:C	1:98:A:GLU:N	23	1.23
(1,55)	1:92:A:ALA:C	1:93:A:GLY:N	1:93:A:GLY:CA	1:93:A:GLY:C	12	1.23
(1,28)	1:55:A:LEU:C	1:56:A:ALA:N	1:56:A:ALA:CA	1:56:A:ALA:C	8	1.23
(1,268)	2:469:B:VAL:C	2:470:B:GLN:N	2:470:B:GLN:CA	2:470:B:GLN:C	7	1.22
(1,263)	2:454:B:PHE:N	2:454:B:PHE:CA	2:454:B:PHE:C	2:455:B:TYR:N	21	1.22
(1,238)	2:461:B:ASP:N	2:461:B:ASP:CA	2:461:B:ASP:C	2:462:B:LEU:N	10	1.22
(1,34)	1:63:A:HIS:C	1:64:A:TRP:N	1:64:A:TRP:CA	1:64:A:TRP:C	2	1.22
(1,302)	1:51:A:VAL:H	1:51:A:VAL:N	2:470:B:GLN:N	2:470:B:GLN:H	8	1.21
(1,280)	1:51:A:VAL:H	1:51:A:VAL:N	1:122:A:CYS:N	1:122:A:CYS:H	14	1.21
(1,139)	1:80:A:GLN:N	1:80:A:GLN:CA	1:80:A:GLN:C	1:81:A:LYS:N	1	1.21
(1,47)	1:82:A:SER:C	1:83:A:TYR:N	1:83:A:TYR:CA	1:83:A:TYR:C	14	1.21
(1,34)	1:63:A:HIS:C	1:64:A:TRP:N	1:64:A:TRP:CA	1:64:A:TRP:C	19	1.21
(1,28)	1:55:A:LEU:C	1:56:A:ALA:N	1:56:A:ALA:CA	1:56:A:ALA:C	13	1.21
(1,28)	1:55:A:LEU:C	1:56:A:ALA:N	1:56:A:ALA:CA	1:56:A:ALA:C	23	1.21
(1,305)	1:85:A:ILE:H	1:85:A:ILE:N	2:479:B:LEU:N	2:479:B:LEU:H	18	1.2
(1,281)	1:52:A:GLN:H	1:52:A:GLN:N	1:75:A:VAL:N	1:75:A:VAL:H	8	1.2
(1,264)	2:454:B:PHE:C	2:455:B:TYR:N	2:455:B:TYR:CA	2:455:B:TYR:C	12	1.2
(1,264)	2:454:B:PHE:C	2:455:B:TYR:N	2:455:B:TYR:CA	2:455:B:TYR:C	18	1.2
(1,230)	2:449:B:GLU:N	2:449:B:GLU:CA	2:449:B:GLU:C	2:450:B:TRP:N	9	1.2
(1,208)	2:459:B:ILE:C	2:460:B:SER:N	2:460:B:SER:CA	2:460:B:SER:C	10	1.2
(1,70)	1:113:A:PHE:C	1:114:A:PHE:N	1:114:A:PHE:CA	1:114:A:PHE:C	9	1.2
(1,37)	1:67:A:GLU:C	1:68:A:HIS:N	1:68:A:HIS:CA	1:68:A:HIS:C	10	1.2
(1,34)	1:63:A:HIS:C	1:64:A:TRP:N	1:64:A:TRP:CA	1:64:A:TRP:C	3	1.2

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,34)	1:63:A:HIS:C	1:64:A:TRP:N	1:64:A:TRP:CA	1:64:A:TRP:C	24	1.2
(1,268)	2:469:B:VAL:C	2:470:B:GLN:N	2:470:B:GLN:CA	2:470:B:GLN:C	10	1.19
(1,266)	2:455:B:TYR:C	2:456:B:PHE:N	2:456:B:PHE:CA	2:456:B:PHE:C	20	1.19
(1,156)	1:105:A:LEU:N	1:105:A:LEU:CA	1:105:A:LEU:C	1:106:A:VAL:N	2	1.19
(1,130)	1:65:A:THR:N	1:65:A:THR:CA	1:65:A:THR:C	1:66:A:LYS:N	23	1.19
(1,122)	1:51:A:VAL:N	1:51:A:VAL:CA	1:51:A:VAL:C	1:52:A:GLN:N	23	1.19
(1,26)	1:52:A:GLN:C	1:53:A:LEU:N	1:53:A:LEU:CA	1:53:A:LEU:C	14	1.19
(1,263)	2:454:B:PHE:N	2:454:B:PHE:CA	2:454:B:PHE:C	2:455:B:TYR:N	22	1.18
(1,230)	2:449:B:GLU:N	2:449:B:GLU:CA	2:449:B:GLU:C	2:450:B:TRP:N	7	1.18
(1,153)	1:101:A:LEU:N	1:101:A:LEU:CA	1:101:A:LEU:C	1:102:A:TYR:N	8	1.18
(1,151)	1:97:A:TRP:N	1:97:A:TRP:CA	1:97:A:TRP:C	1:98:A:GLU:N	13	1.18
(1,131)	1:66:A:LYS:N	1:66:A:LYS:CA	1:66:A:LYS:C	1:67:A:GLU:N	20	1.18
(1,129)	1:63:A:HIS:N	1:63:A:HIS:CA	1:63:A:HIS:C	1:64:A:TRP:N	1	1.18
(1,120)	1:47:A:ALA:N	1:47:A:ALA:CA	1:47:A:ALA:C	1:48:A:THR:N	17	1.18
(1,81)	1:130:A:ASP:C	1:131:A:GLU:N	1:131:A:GLU:CA	1:131:A:GLU:C	14	1.18
(1,72)	1:115:A:HIS:C	1:116:A:THR:N	1:116:A:THR:CA	1:116:A:THR:C	13	1.18
(1,55)	1:92:A:ALA:C	1:93:A:GLY:N	1:93:A:GLY:CA	1:93:A:GLY:C	8	1.18
(1,55)	1:92:A:ALA:C	1:93:A:GLY:N	1:93:A:GLY:CA	1:93:A:GLY:C	23	1.18
(1,285)	1:60:A:GLY:H	1:60:A:GLY:N	1:93:A:GLY:N	1:93:A:GLY:H	13	1.17
(1,268)	2:469:B:VAL:C	2:470:B:GLN:N	2:470:B:GLN:CA	2:470:B:GLN:C	9	1.17
(1,202)	2:449:B:GLU:C	2:450:B:TRP:N	2:450:B:TRP:CA	2:450:B:TRP:C	6	1.17
(1,129)	1:63:A:HIS:N	1:63:A:HIS:CA	1:63:A:HIS:C	1:64:A:TRP:N	16	1.17
(1,81)	1:130:A:ASP:C	1:131:A:GLU:N	1:131:A:GLU:CA	1:131:A:GLU:C	24	1.17
(1,37)	1:67:A:GLU:C	1:68:A:HIS:N	1:68:A:HIS:CA	1:68:A:HIS:C	7	1.17
(1,37)	1:67:A:GLU:C	1:68:A:HIS:N	1:68:A:HIS:CA	1:68:A:HIS:C	14	1.17
(1,254)	2:479:B:LEU:N	2:479:B:LEU:CA	2:479:B:LEU:C	2:480:B:ALA:N	22	1.16
(1,208)	2:459:B:ILE:C	2:460:B:SER:N	2:460:B:SER:CA	2:460:B:SER:C	18	1.16
(1,207)	2:458:B:PRO:C	2:459:B:ILE:N	2:459:B:ILE:CA	2:459:B:ILE:C	19	1.16
(1,305)	1:85:A:ILE:H	1:85:A:ILE:N	2:479:B:LEU:N	2:479:B:LEU:H	3	1.15
(1,305)	1:85:A:ILE:H	1:85:A:ILE:N	2:479:B:LEU:N	2:479:B:LEU:H	22	1.15
(1,279)	1:75:A:VAL:H	1:75:A:VAL:N	1:111:A:THR:N	1:111:A:THR:H	6	1.15
(1,264)	2:454:B:PHE:C	2:455:B:TYR:N	2:455:B:TYR:CA	2:455:B:TYR:C	20	1.15
(1,249)	2:473:B:LYS:N	2:473:B:LYS:CA	2:473:B:LYS:C	2:474:B:SER:N	13	1.15
(1,244)	2:467:B:PRO:N	2:467:B:PRO:CA	2:467:B:PRO:C	2:468:B:TYR:N	22	1.15
(1,230)	2:449:B:GLU:N	2:449:B:GLU:CA	2:449:B:GLU:C	2:450:B:TRP:N	5	1.15
(1,217)	2:468:B:TYR:C	2:469:B:VAL:N	2:469:B:VAL:CA	2:469:B:VAL:C	9	1.15
(1,153)	1:101:A:LEU:N	1:101:A:LEU:CA	1:101:A:LEU:C	1:102:A:TYR:N	15	1.15
(1,140)	1:81:A:LYS:N	1:81:A:LYS:CA	1:81:A:LYS:C	1:82:A:SER:N	14	1.15
(1,120)	1:47:A:ALA:N	1:47:A:ALA:CA	1:47:A:ALA:C	1:48:A:THR:N	8	1.15
(1,72)	1:115:A:HIS:C	1:116:A:THR:N	1:116:A:THR:CA	1:116:A:THR:C	11	1.15
(1,34)	1:63:A:HIS:C	1:64:A:TRP:N	1:64:A:TRP:CA	1:64:A:TRP:C	9	1.15
(1,221)	2:473:B:LYS:C	2:474:B:SER:N	2:474:B:SER:CA	2:474:B:SER:C	18	1.14
(1,208)	2:459:B:ILE:C	2:460:B:SER:N	2:460:B:SER:CA	2:460:B:SER:C	9	1.14
(1,208)	2:459:B:ILE:C	2:460:B:SER:N	2:460:B:SER:CA	2:460:B:SER:C	24	1.14
(1,288)	1:75:A:VAL:H	1:75:A:VAL:N	1:127:A:ASN:N	1:127:A:ASN:H	19	1.13
(1,284)	1:60:A:GLY:H	1:60:A:GLY:N	1:111:A:THR:N	1:111:A:THR:H	21	1.13
(1,279)	1:75:A:VAL:H	1:75:A:VAL:N	1:111:A:THR:N	1:111:A:THR:H	18	1.13
(1,275)	1:63:A:HIS:H	1:63:A:HIS:N	1:75:A:VAL:N	1:75:A:VAL:H	17	1.13
(1,236)	2:459:B:ILE:N	2:459:B:ILE:CA	2:459:B:ILE:C	2:460:B:SER:N	17	1.13
(1,157)	1:108:A:SER:N	1:108:A:SER:CA	1:108:A:SER:C	1:109:A:THR:N	22	1.13
(1,25)	1:50:A:VAL:C	1:51:A:VAL:N	1:51:A:VAL:CA	1:51:A:VAL:C	5	1.13

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,24)	1:47:A:ALA:C	1:48:A:THR:N	1:48:A:THR:CA	1:48:A:THR:C	1	1.13
(1,268)	2:469:B:VAL:C	2:470:B:GLN:N	2:470:B:GLN:CA	2:470:B:GLN:C	4	1.12
(1,268)	2:469:B:VAL:C	2:470:B:GLN:N	2:470:B:GLN:CA	2:470:B:GLN:C	21	1.12
(1,250)	2:474:B:SER:N	2:474:B:SER:CA	2:474:B:SER:C	2:475:B:TYR:N	5	1.12
(1,244)	2:467:B:PRO:N	2:467:B:PRO:CA	2:467:B:PRO:C	2:468:B:TYR:N	12	1.12
(1,223)	2:475:B:TYR:C	2:476:B:PRO:N	2:476:B:PRO:CA	2:476:B:PRO:C	20	1.12
(1,129)	1:63:A:HIS:N	1:63:A:HIS:CA	1:63:A:HIS:C	1:64:A:TRP:N	10	1.12
(1,125)	1:57:A:LEU:N	1:57:A:LEU:CA	1:57:A:LEU:C	1:58:A:PRO:N	12	1.12
(1,81)	1:130:A:ASP:C	1:131:A:GLU:N	1:131:A:GLU:CA	1:131:A:GLU:C	18	1.12
(1,37)	1:67:A:GLU:C	1:68:A:HIS:N	1:68:A:HIS:CA	1:68:A:HIS:C	6	1.12
(1,285)	1:60:A:GLY:H	1:60:A:GLY:N	1:93:A:GLY:N	1:93:A:GLY:H	5	1.11
(1,225)	2:477:B:SER:C	2:478:B:LYS:N	2:478:B:LYS:CA	2:478:B:LYS:C	20	1.11
(1,206)	2:457:B:HIS:C	2:458:B:PRO:N	2:458:B:PRO:CA	2:458:B:PRO:C	23	1.11
(1,153)	1:101:A:LEU:N	1:101:A:LEU:CA	1:101:A:LEU:C	1:102:A:TYR:N	10	1.11
(1,129)	1:63:A:HIS:N	1:63:A:HIS:CA	1:63:A:HIS:C	1:64:A:TRP:N	13	1.11
(1,70)	1:113:A:PHE:C	1:114:A:PHE:N	1:114:A:PHE:CA	1:114:A:PHE:C	4	1.11
(1,308)	1:35:A:LEU:H	1:35:A:LEU:N	1:75:A:VAL:N	1:75:A:VAL:H	1	1.1
(1,284)	1:60:A:GLY:H	1:60:A:GLY:N	1:111:A:THR:N	1:111:A:THR:H	24	1.1
(1,281)	1:52:A:GLN:H	1:52:A:GLN:N	1:75:A:VAL:N	1:75:A:VAL:H	9	1.1
(1,264)	2:454:B:PHE:C	2:455:B:TYR:N	2:455:B:TYR:CA	2:455:B:TYR:C	4	1.1
(1,263)	2:454:B:PHE:N	2:454:B:PHE:CA	2:454:B:PHE:C	2:455:B:TYR:N	17	1.1
(1,261)	2:453:B:ARG:N	2:453:B:ARG:CA	2:453:B:ARG:C	2:454:B:PHE:N	21	1.1
(1,261)	2:453:B:ARG:N	2:453:B:ARG:CA	2:453:B:ARG:C	2:454:B:PHE:N	22	1.1
(1,254)	2:479:B:LEU:N	2:479:B:LEU:CA	2:479:B:LEU:C	2:480:B:ALA:N	2	1.1
(1,221)	2:473:B:LYS:C	2:474:B:SER:N	2:474:B:SER:CA	2:474:B:SER:C	17	1.1
(1,207)	2:458:B:PRO:C	2:459:B:ILE:N	2:459:B:ILE:CA	2:459:B:ILE:C	11	1.1
(1,28)	1:55:A:LEU:C	1:56:A:ALA:N	1:56:A:ALA:CA	1:56:A:ALA:C	2	1.1
(1,305)	1:85:A:ILE:H	1:85:A:ILE:N	2:479:B:LEU:N	2:479:B:LEU:H	8	1.09
(1,254)	2:479:B:LEU:N	2:479:B:LEU:CA	2:479:B:LEU:C	2:480:B:ALA:N	4	1.09
(1,239)	2:462:B:LEU:N	2:462:B:LEU:CA	2:462:B:LEU:C	2:463:B:PRO:N	15	1.09
(1,236)	2:459:B:ILE:N	2:459:B:ILE:CA	2:459:B:ILE:C	2:460:B:SER:N	22	1.09
(1,223)	2:475:B:TYR:C	2:476:B:PRO:N	2:476:B:PRO:CA	2:476:B:PRO:C	10	1.09
(1,72)	1:115:A:HIS:C	1:116:A:THR:N	1:116:A:THR:CA	1:116:A:THR:C	8	1.09
(1,263)	2:454:B:PHE:N	2:454:B:PHE:CA	2:454:B:PHE:C	2:455:B:TYR:N	4	1.08
(1,263)	2:454:B:PHE:N	2:454:B:PHE:CA	2:454:B:PHE:C	2:455:B:TYR:N	23	1.08
(1,78)	1:127:A:ASN:C	1:128:A:PHE:N	1:128:A:PHE:CA	1:128:A:PHE:C	24	1.08
(1,72)	1:115:A:HIS:C	1:116:A:THR:N	1:116:A:THR:CA	1:116:A:THR:C	17	1.08
(1,55)	1:92:A:ALA:C	1:93:A:GLY:N	1:93:A:GLY:CA	1:93:A:GLY:C	22	1.08
(1,28)	1:55:A:LEU:C	1:56:A:ALA:N	1:56:A:ALA:CA	1:56:A:ALA:C	18	1.08
(1,305)	1:85:A:ILE:H	1:85:A:ILE:N	2:479:B:LEU:N	2:479:B:LEU:H	7	1.07
(1,285)	1:60:A:GLY:H	1:60:A:GLY:N	1:93:A:GLY:N	1:93:A:GLY:H	20	1.07
(1,281)	1:52:A:GLN:H	1:52:A:GLN:N	1:75:A:VAL:N	1:75:A:VAL:H	15	1.07
(1,264)	2:454:B:PHE:C	2:455:B:TYR:N	2:455:B:TYR:CA	2:455:B:TYR:C	23	1.07
(1,221)	2:473:B:LYS:C	2:474:B:SER:N	2:474:B:SER:CA	2:474:B:SER:C	13	1.07
(1,206)	2:457:B:HIS:C	2:458:B:PRO:N	2:458:B:PRO:CA	2:458:B:PRO:C	24	1.07
(1,202)	2:449:B:GLU:C	2:450:B:TRP:N	2:450:B:TRP:CA	2:450:B:TRP:C	24	1.07
(1,125)	1:57:A:LEU:N	1:57:A:LEU:CA	1:57:A:LEU:C	1:58:A:PRO:N	8	1.07
(1,125)	1:57:A:LEU:N	1:57:A:LEU:CA	1:57:A:LEU:C	1:58:A:PRO:N	23	1.07
(1,79)	1:128:A:PHE:C	1:129:A:ALA:N	1:129:A:ALA:CA	1:129:A:ALA:C	10	1.07
(1,72)	1:115:A:HIS:C	1:116:A:THR:N	1:116:A:THR:CA	1:116:A:THR:C	6	1.07
(1,25)	1:50:A:VAL:C	1:51:A:VAL:N	1:51:A:VAL:CA	1:51:A:VAL:C	7	1.07

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,24)	1:47:A:ALA:C	1:48:A:THR:N	1:48:A:THR:CA	1:48:A:THR:C	15	1.07
(1,273)	1:60:A:GLY:H	1:60:A:GLY:N	1:89:A:GLY:N	1:89:A:GLY:H	19	1.06
(1,263)	2:454:B:PHE:N	2:454:B:PHE:CA	2:454:B:PHE:C	2:455:B:TYR:N	6	1.06
(1,261)	2:453:B:ARG:N	2:453:B:ARG:CA	2:453:B:ARG:C	2:454:B:PHE:N	1	1.06
(1,249)	2:473:B:LYS:N	2:473:B:LYS:CA	2:473:B:LYS:C	2:474:B:SER:N	17	1.06
(1,244)	2:467:B:PRO:N	2:467:B:PRO:CA	2:467:B:PRO:C	2:468:B:TYR:N	5	1.06
(1,207)	2:458:B:PRO:C	2:459:B:ILE:N	2:459:B:ILE:CA	2:459:B:ILE:C	18	1.06
(1,151)	1:97:A:TRP:N	1:97:A:TRP:CA	1:97:A:TRP:C	1:98:A:GLU:N	11	1.06
(1,125)	1:57:A:LEU:N	1:57:A:LEU:CA	1:57:A:LEU:C	1:58:A:PRO:N	11	1.06
(1,79)	1:128:A:PHE:C	1:129:A:ALA:N	1:129:A:ALA:CA	1:129:A:ALA:C	1	1.06
(1,59)	1:98:A:GLU:C	1:99:A:GLN:N	1:99:A:GLN:CA	1:99:A:GLN:C	12	1.06
(1,37)	1:67:A:GLU:C	1:68:A:HIS:N	1:68:A:HIS:CA	1:68:A:HIS:C	1	1.06
(1,28)	1:55:A:LEU:C	1:56:A:ALA:N	1:56:A:ALA:CA	1:56:A:ALA:C	15	1.06
(1,22)	1:45:A:THR:C	1:46:A:LEU:N	1:46:A:LEU:CA	1:46:A:LEU:C	1	1.06
(1,305)	1:85:A:ILE:H	1:85:A:ILE:N	2:479:B:LEU:N	2:479:B:LEU:H	9	1.05
(1,288)	1:75:A:VAL:H	1:75:A:VAL:N	1:127:A:ASN:N	1:127:A:ASN:H	11	1.05
(1,264)	2:454:B:PHE:C	2:455:B:TYR:N	2:455:B:TYR:CA	2:455:B:TYR:C	2	1.05
(1,206)	2:457:B:HIS:C	2:458:B:PRO:N	2:458:B:PRO:CA	2:458:B:PRO:C	12	1.05
(1,153)	1:101:A:LEU:N	1:101:A:LEU:CA	1:101:A:LEU:C	1:102:A:TYR:N	1	1.05
(1,145)	1:86:A:ARG:N	1:86:A:ARG:CA	1:86:A:ARG:C	1:87:A:LEU:N	5	1.05
(1,129)	1:63:A:HIS:N	1:63:A:HIS:CA	1:63:A:HIS:C	1:64:A:TRP:N	4	1.05
(1,81)	1:130:A:ASP:C	1:131:A:GLU:N	1:131:A:GLU:CA	1:131:A:GLU:C	22	1.05
(1,268)	2:469:B:VAL:C	2:470:B:GLN:N	2:470:B:GLN:CA	2:470:B:GLN:C	19	1.04
(1,261)	2:453:B:ARG:N	2:453:B:ARG:CA	2:453:B:ARG:C	2:454:B:PHE:N	18	1.04
(1,221)	2:473:B:LYS:C	2:474:B:SER:N	2:474:B:SER:CA	2:474:B:SER:C	23	1.04
(1,206)	2:457:B:HIS:C	2:458:B:PRO:N	2:458:B:PRO:CA	2:458:B:PRO:C	21	1.04
(1,156)	1:105:A:LEU:N	1:105:A:LEU:CA	1:105:A:LEU:C	1:106:A:VAL:N	18	1.04
(1,156)	1:105:A:LEU:N	1:105:A:LEU:CA	1:105:A:LEU:C	1:106:A:VAL:N	20	1.04
(1,125)	1:57:A:LEU:N	1:57:A:LEU:CA	1:57:A:LEU:C	1:58:A:PRO:N	22	1.04
(1,120)	1:47:A:ALA:N	1:47:A:ALA:CA	1:47:A:ALA:C	1:48:A:THR:N	9	1.04
(1,55)	1:92:A:ALA:C	1:93:A:GLY:N	1:93:A:GLY:CA	1:93:A:GLY:C	7	1.04
(1,55)	1:92:A:ALA:C	1:93:A:GLY:N	1:93:A:GLY:CA	1:93:A:GLY:C	24	1.04
(1,34)	1:63:A:HIS:C	1:64:A:TRP:N	1:64:A:TRP:CA	1:64:A:TRP:C	17	1.04
(1,305)	1:85:A:ILE:H	1:85:A:ILE:N	2:479:B:LEU:N	2:479:B:LEU:H	5	1.03
(1,268)	2:469:B:VAL:C	2:470:B:GLN:N	2:470:B:GLN:CA	2:470:B:GLN:C	11	1.03
(1,264)	2:454:B:PHE:C	2:455:B:TYR:N	2:455:B:TYR:CA	2:455:B:TYR:C	22	1.03
(1,261)	2:453:B:ARG:N	2:453:B:ARG:CA	2:453:B:ARG:C	2:454:B:PHE:N	4	1.03
(1,254)	2:479:B:LEU:N	2:479:B:LEU:CA	2:479:B:LEU:C	2:480:B:ALA:N	24	1.03
(1,207)	2:458:B:PRO:C	2:459:B:ILE:N	2:459:B:ILE:CA	2:459:B:ILE:C	23	1.03
(1,153)	1:101:A:LEU:N	1:101:A:LEU:CA	1:101:A:LEU:C	1:102:A:TYR:N	7	1.03
(1,129)	1:63:A:HIS:N	1:63:A:HIS:CA	1:63:A:HIS:C	1:64:A:TRP:N	19	1.03
(1,55)	1:92:A:ALA:C	1:93:A:GLY:N	1:93:A:GLY:CA	1:93:A:GLY:C	11	1.03
(1,275)	1:63:A:HIS:H	1:63:A:HIS:N	1:75:A:VAL:N	1:75:A:VAL:H	18	1.02
(1,264)	2:454:B:PHE:C	2:455:B:TYR:N	2:455:B:TYR:CA	2:455:B:TYR:C	6	1.02
(1,151)	1:97:A:TRP:N	1:97:A:TRP:CA	1:97:A:TRP:C	1:98:A:GLU:N	4	1.02
(1,139)	1:80:A:GLN:N	1:80:A:GLN:CA	1:80:A:GLN:C	1:81:A:LYS:N	8	1.02
(1,139)	1:80:A:GLN:N	1:80:A:GLN:CA	1:80:A:GLN:C	1:81:A:LYS:N	13	1.02
(1,129)	1:63:A:HIS:N	1:63:A:HIS:CA	1:63:A:HIS:C	1:64:A:TRP:N	3	1.02
(1,125)	1:57:A:LEU:N	1:57:A:LEU:CA	1:57:A:LEU:C	1:58:A:PRO:N	7	1.02
(1,70)	1:113:A:PHE:C	1:114:A:PHE:N	1:114:A:PHE:CA	1:114:A:PHE:C	8	1.02
(1,61)	1:100:A:GLU:C	1:101:A:LEU:N	1:101:A:LEU:CA	1:101:A:LEU:C	24	1.02

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,302)	1:51:A:VAL:H	1:51:A:VAL:N	2:470:B:GLN:N	2:470:B:GLN:H	5	1.01
(1,285)	1:60:A:GLY:H	1:60:A:GLY:N	1:93:A:GLY:N	1:93:A:GLY:H	19	1.01
(1,263)	2:454:B:PHE:N	2:454:B:PHE:CA	2:454:B:PHE:C	2:455:B:TYR:N	16	1.01
(1,261)	2:453:B:ARG:N	2:453:B:ARG:CA	2:453:B:ARG:C	2:454:B:PHE:N	8	1.01
(1,212)	2:463:B:PRO:C	2:464:B:PRO:N	2:464:B:PRO:CA	2:464:B:PRO:C	18	1.01
(1,208)	2:459:B:ILE:C	2:460:B:SER:N	2:460:B:SER:CA	2:460:B:SER:C	1	1.01
(1,120)	1:47:A:ALA:N	1:47:A:ALA:CA	1:47:A:ALA:C	1:48:A:THR:N	10	1.01
(1,119)	1:46:A:LEU:N	1:46:A:LEU:CA	1:46:A:LEU:C	1:47:A:ALA:N	14	1.01
(1,72)	1:115:A:HIS:C	1:116:A:THR:N	1:116:A:THR:CA	1:116:A:THR:C	9	1.01
(1,51)	1:86:A:ARG:C	1:87:A:LEU:N	1:87:A:LEU:CA	1:87:A:LEU:C	15	1.01
(1,47)	1:82:A:SER:C	1:83:A:TYR:N	1:83:A:TYR:CA	1:83:A:TYR:C	11	1.01
(1,254)	2:479:B:LEU:N	2:479:B:LEU:CA	2:479:B:LEU:C	2:480:B:ALA:N	11	1.0
(1,131)	1:66:A:LYS:N	1:66:A:LYS:CA	1:66:A:LYS:C	1:67:A:GLU:N	22	1.0
(1,120)	1:47:A:ALA:N	1:47:A:ALA:CA	1:47:A:ALA:C	1:48:A:THR:N	12	1.0
(1,46)	1:81:A:LYS:C	1:82:A:SER:N	1:82:A:SER:CA	1:82:A:SER:C	7	1.0