Full wwPDB NMR Structure Validation Report (i)

Mar 6, 2026 – 04:03 AM UTC

PDB ID	:	8SG2 / pdb_00008sg2
BMRB ID	:	31080
Title	:	BIVALENT INTERACTIONS OF PIN1 WITH THE C-TERMINAL TAIL OF PKC
Authors	:	Dixit, K.; Yang, Y.; Chen, X.R.; Igumenova, T.I.
Deposited on	:	2023-04-11

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

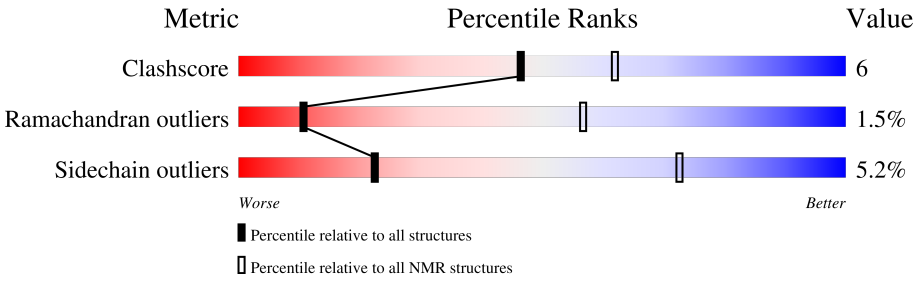
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance

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

The overall completeness of chemical shifts assignment is 80%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	163	80% 7% 12%
2	B	25	40% 32% 28%

2 Ensemble composition and analysis

This entry contains 20 models. Model 4 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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:7-A:37, A:52-A:163, B:639-B:640, B:642-B:646, B:650-B:659, B:661-B:661 (161)	1.07	4

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

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

The models can be grouped into 1 clusters and 10 single-model clusters were found.

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2902 atoms, of which 1420 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	163	2526	786	1244	239	251	6	0

- Molecule 2 is a protein called Protein kinase C beta type.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
2	B	25	376	122	176	30	46	2	1

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	638	ACE	-	acetylation	UNP P05771
B	662	NH2	-	amidation	UNP P05771

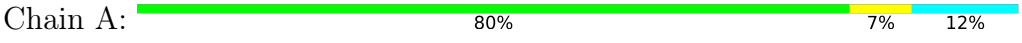
4 Residue-property plots

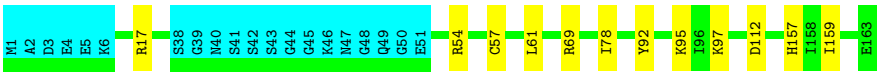
4.1 Average score per residue in the NMR ensemble

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: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1

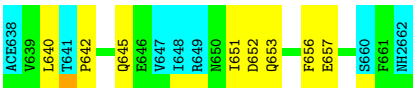
Chain A:





• Molecule 2: Protein kinase C beta type

Chain B:



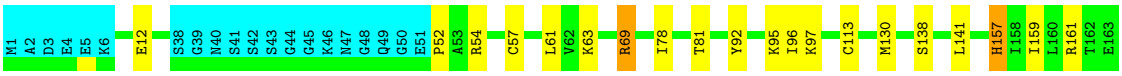
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

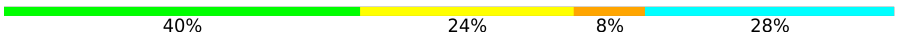
• Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1

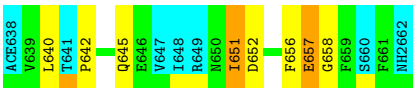
Chain A:



• Molecule 2: Protein kinase C beta type

Chain B:

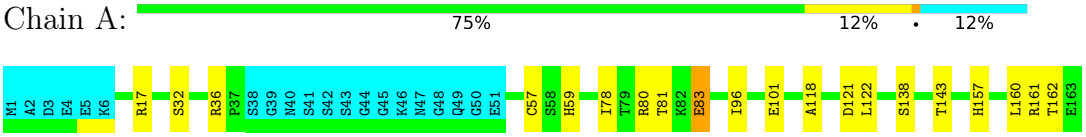




4.2.2 Score per residue for model 2

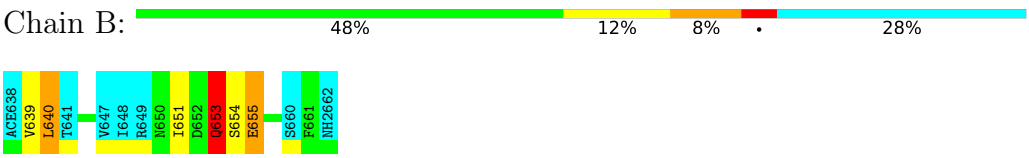
• Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1

Chain A:



• Molecule 2: Protein kinase C beta type

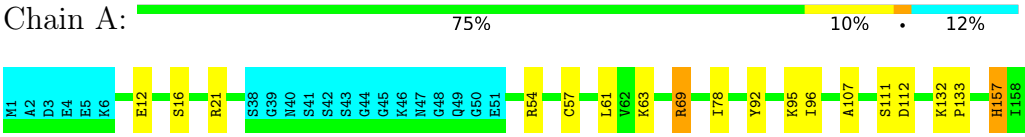
Chain B:



4.2.3 Score per residue for model 3

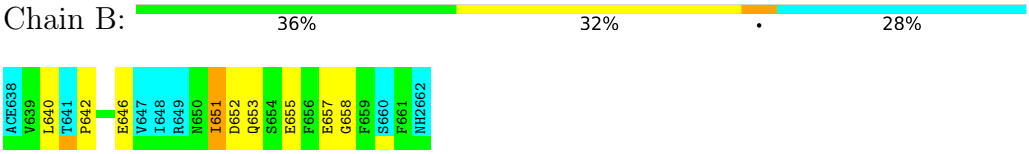
• Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1

Chain A:



• Molecule 2: Protein kinase C beta type

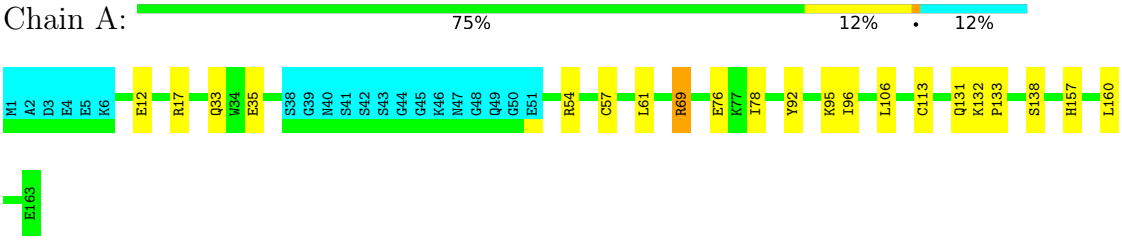
Chain B:



4.2.4 Score per residue for model 4 (medoid)

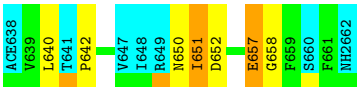
• Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1

Chain A:



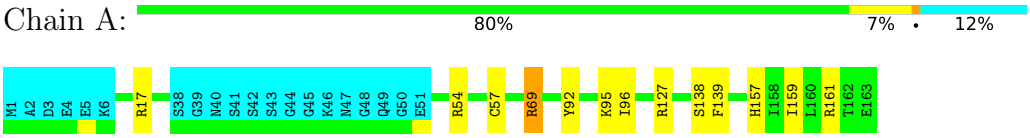
• Molecule 2: Protein kinase C beta type

Chain B:

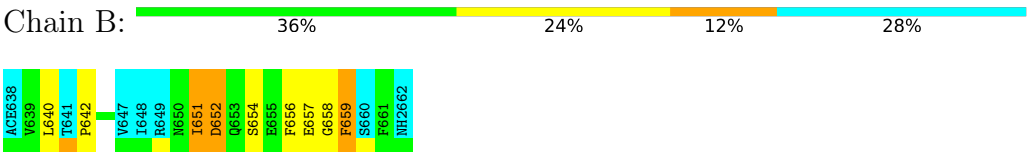


4.2.5 Score per residue for model 5

• Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1

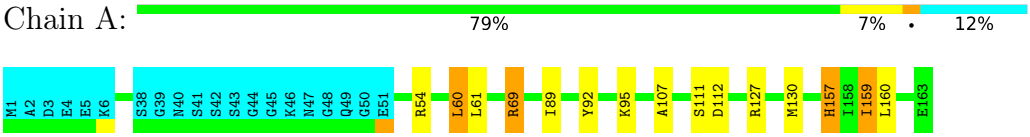


• Molecule 2: Protein kinase C beta type

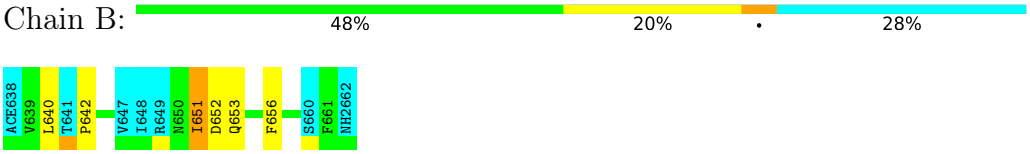


4.2.6 Score per residue for model 6

• Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1

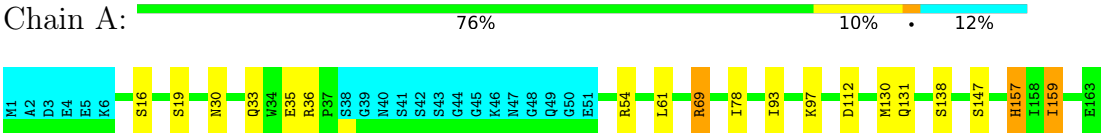


• Molecule 2: Protein kinase C beta type



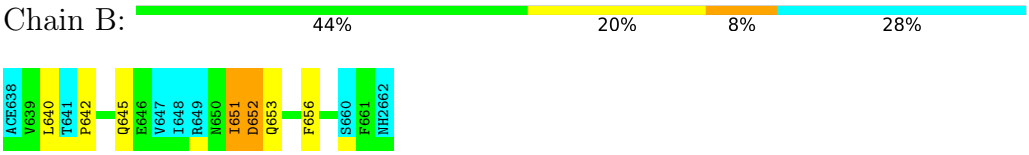
4.2.7 Score per residue for model 7

• Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1



• Molecule 2: Protein kinase C beta type

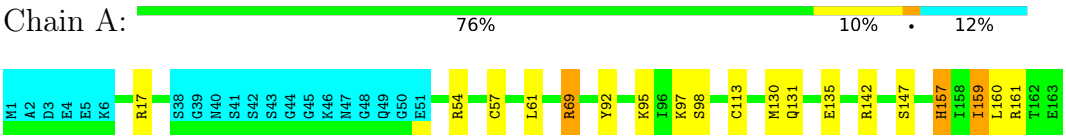
Chain B:



4.2.8 Score per residue for model 8

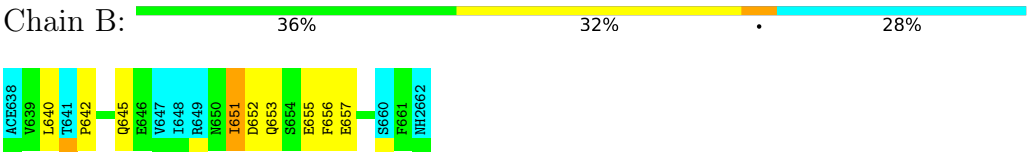
• Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1

Chain A:



• Molecule 2: Protein kinase C beta type

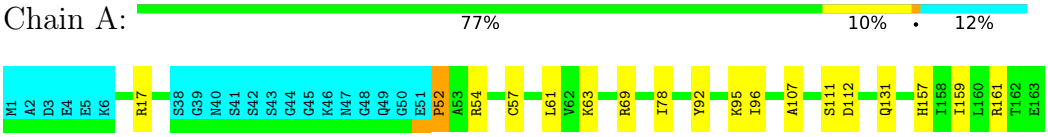
Chain B:



4.2.9 Score per residue for model 9

• Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1

Chain A:



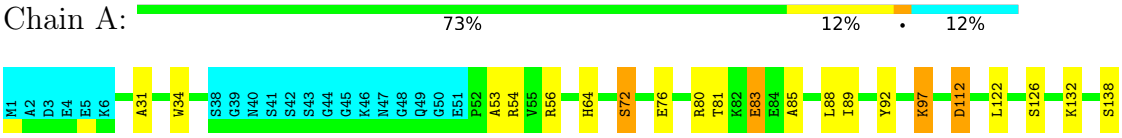
• Molecule 2: Protein kinase C beta type

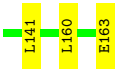
Chain B:

4.2.10 Score per residue for model 10

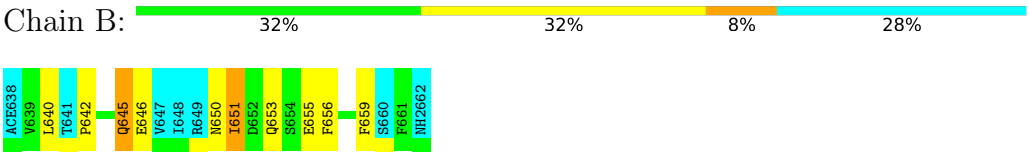
• Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1

Chain A:



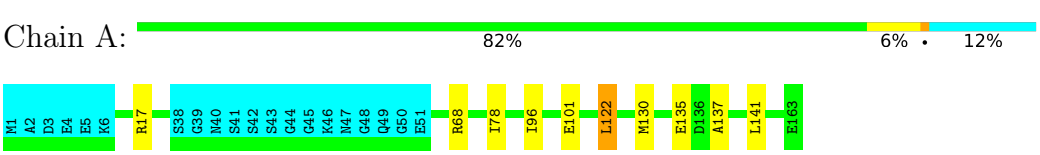


• Molecule 2: Protein kinase C beta type

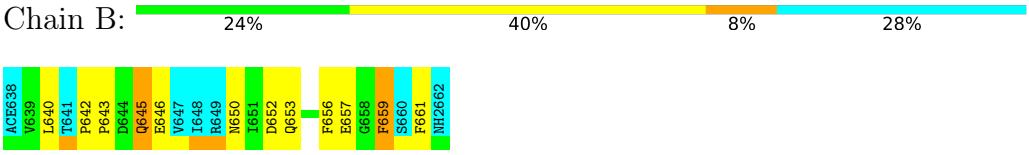


4.2.11 Score per residue for model 11

• Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1

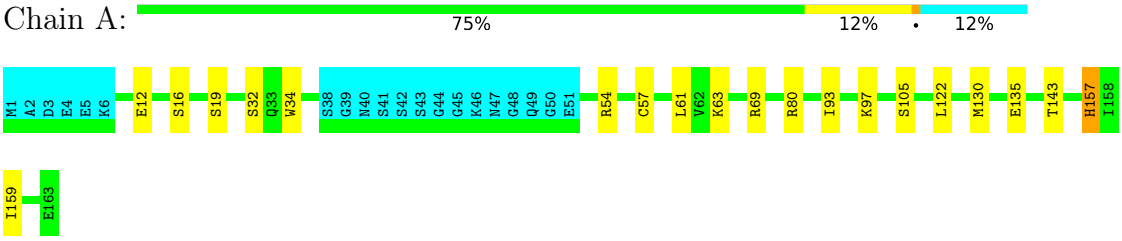


• Molecule 2: Protein kinase C beta type

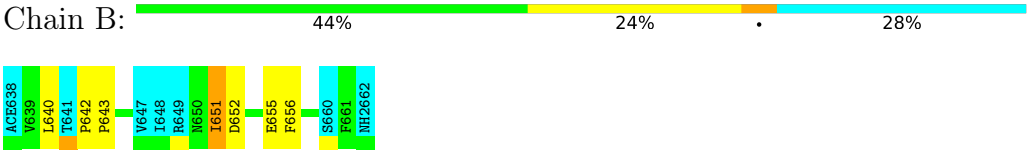


4.2.12 Score per residue for model 12

• Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1



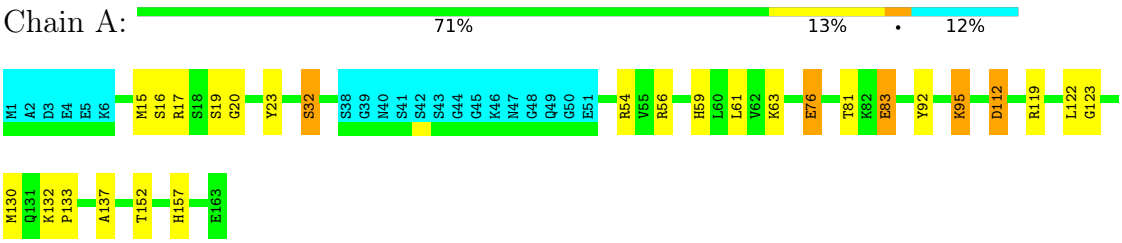
• Molecule 2: Protein kinase C beta type



4.2.13 Score per residue for model 13

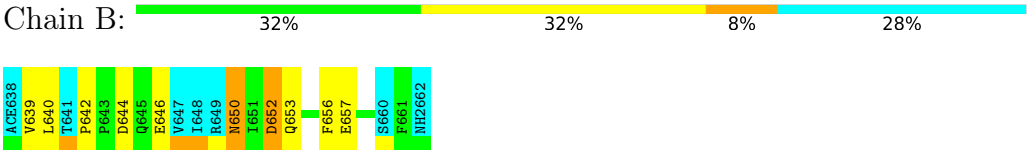
• Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1

Chain A:



• Molecule 2: Protein kinase C beta type

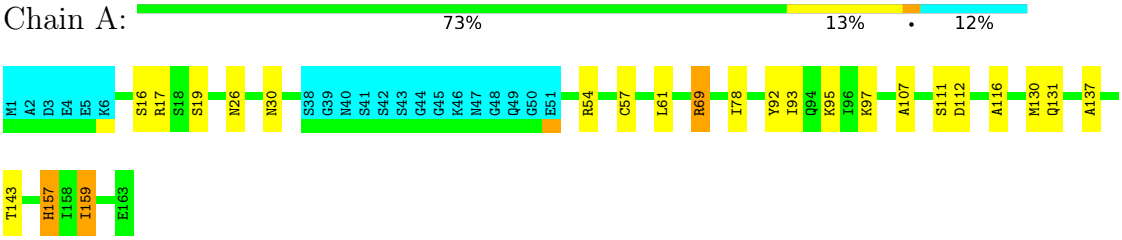
Chain B:



4.2.14 Score per residue for model 14

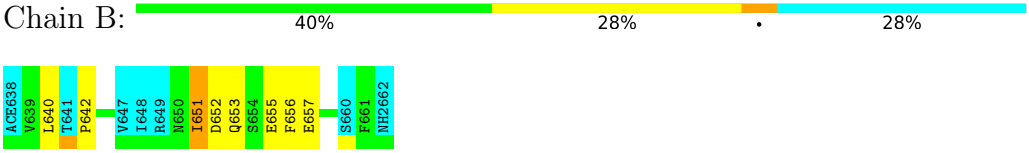
• Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1

Chain A:



• Molecule 2: Protein kinase C beta type

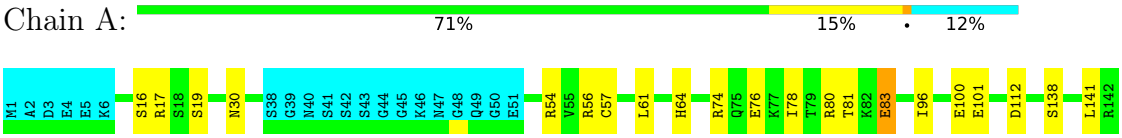
Chain B:

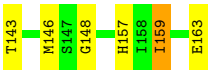


4.2.15 Score per residue for model 15

• Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1

Chain A:





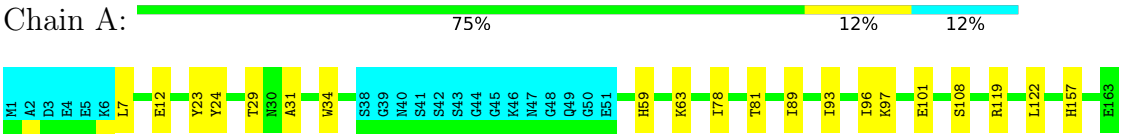
• Molecule 2: Protein kinase C beta type

Chain B:

4.2.16 Score per residue for model 16

• Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1

Chain A:



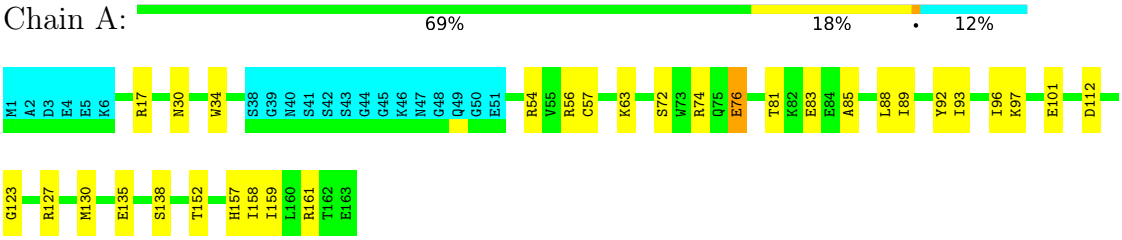
• Molecule 2: Protein kinase C beta type

Chain B:

4.2.17 Score per residue for model 17

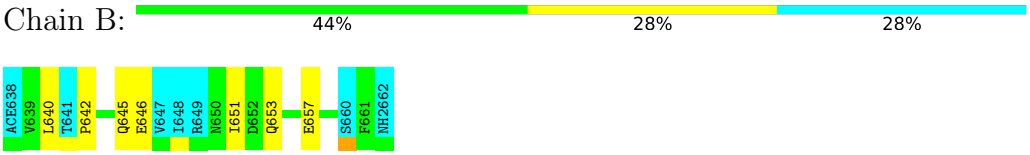
• Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1

Chain A:



• Molecule 2: Protein kinase C beta type

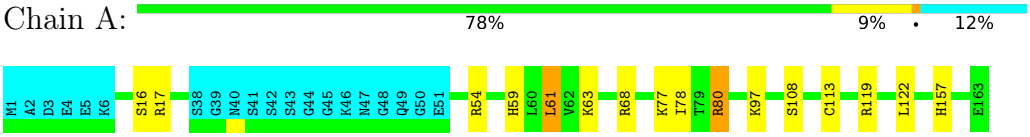
Chain B:



4.2.18 Score per residue for model 18

• Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1

Chain A:



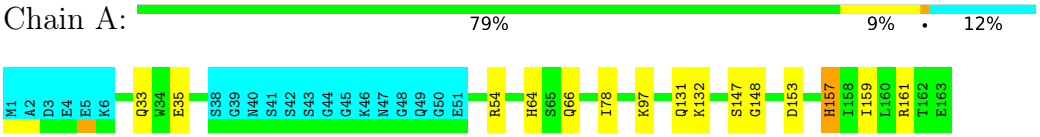
• Molecule 2: Protein kinase C beta type

Chain B:

4.2.19 Score per residue for model 19

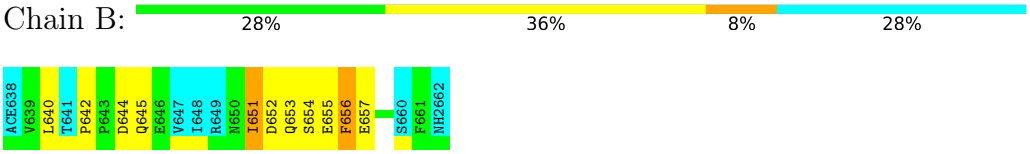
• Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1

Chain A:



• Molecule 2: Protein kinase C beta type

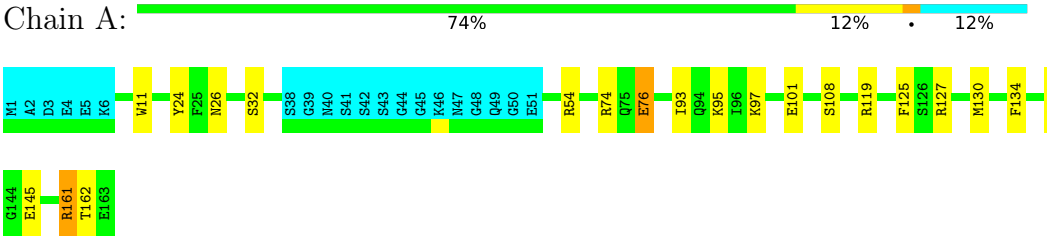
Chain B:



4.2.20 Score per residue for model 20

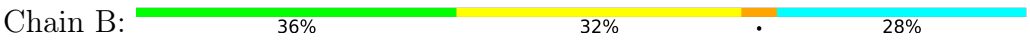
• Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1

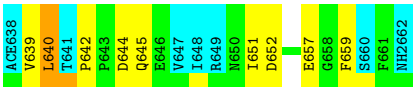
Chain A:



• Molecule 2: Protein kinase C beta type

Chain B:




ACE638
V639
L640
T641
P642
P643
D644
Q645
E646
V647
I648
R649
N650
I651
D652
E657
G658
F659
S660
F661
NH2662

5 Refinement protocol and experimental data overview

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

Of the 50 calculated structures, 20 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
X-PLOR NIH	refinement	
CYANA	structure calculation	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	2
Total number of shifts	1960
Number of shifts mapped to atoms	1960
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	80%

6 Model quality

6.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SEP, NH2, ACE, TPO

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	0.58±0.02	0±0/1173 (0.0± 0.0%)	0.71±0.01	0±0/1573 (0.0± 0.0%)
2	B	0.62±0.05	0±0/151 (0.0± 0.0%)	0.72±0.07	0±0/200 (0.1± 0.2%)
All	All	0.59	0/26480 (0.0%)	0.71	2/35460 (0.0%)

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	656	PHE	N-CA-C	-5.67	106.29	113.43	16	2

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1147	1125	1121	12±3
2	B	149	128	128	7±2
All	All	25920	25060	24980	312

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 6.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:640:LEU:O	2:B:642:PRO:HD2	0.70	1.85	11	14
2:B:653:GLN:H	2:B:653:GLN:NE2	0.68	1.86	15	1
1:A:61:LEU:HG	1:A:113:CYS:SG	0.65	2.31	18	1
1:A:63:LYS:O	1:A:80:ARG:HD3	0.64	1.93	18	1
1:A:107:ALA:O	1:A:111:SER:HB2	0.62	1.95	14	4
1:A:69:ARG:N	1:A:69:ARG:HD3	0.62	2.09	7	3
1:A:31:ALA:HA	2:B:645:GLN:NE2	0.61	2.10	10	1
1:A:92:TYR:HB3	1:A:106:LEU:HD21	0.60	1.71	4	1
1:A:64:HIS:CE1	1:A:66:GLN:HB2	0.60	2.32	19	1
1:A:72:SER:HB3	1:A:112:ASP:OD1	0.59	1.97	10	1
1:A:69:ARG:HD3	1:A:69:ARG:N	0.59	2.11	5	7
1:A:159:ILE:HG23	2:B:653:GLN:NE2	0.59	2.12	3	4
1:A:57:CYS:SG	2:B:652:ASP:HB2	0.59	2.38	9	8
2:B:640:LEU:C	2:B:642:PRO:HD2	0.58	2.24	15	10
2:B:654:SER:HB3	2:B:659:PHE:CE2	0.58	2.33	5	1
2:B:652:ASP:HB3	2:B:656:PHE:CG	0.57	2.34	5	1
1:A:141:LEU:HG	2:B:650:ASN:O	0.57	1.99	10	1
2:B:652:ASP:HA	2:B:656:PHE:CD2	0.57	2.34	19	1
1:A:57:CYS:SG	2:B:651:ILE:HG12	0.57	2.39	2	1
1:A:57:CYS:SG	2:B:651:ILE:HG13	0.56	2.40	15	2
1:A:148:GLY:HA3	2:B:644:ASP:OD2	0.55	2.01	19	1
2:B:652:ASP:HB3	2:B:656:PHE:CD2	0.54	2.36	5	1
1:A:130:MET:HB2	2:B:656:PHE:O	0.54	2.03	13	1
2:B:655:GLU:H	2:B:655:GLU:CD	0.54	2.10	2	2
2:B:651:ILE:O	2:B:656:PHE:HB3	0.54	2.02	19	1
1:A:81:THR:HB	1:A:83:GLU:OE2	0.53	2.03	13	2
2:B:645:GLN:NE2	2:B:646:GLU:H	0.53	2.01	10	1
1:A:59:HIS:CG	1:A:122:LEU:HD21	0.53	2.37	16	1
1:A:134:PHE:CG	2:B:652:ASP:HB3	0.53	2.39	20	1
2:B:651:ILE:HG12	2:B:652:ASP:H	0.53	1.62	5	10
1:A:93:ILE:HG21	2:B:644:ASP:HB3	0.53	1.79	20	1
1:A:108:SER:OG	1:A:119:ARG:HA	0.53	2.04	18	2
1:A:69:ARG:H	1:A:69:ARG:HD3	0.53	1.63	12	2
1:A:63:LYS:HB2	1:A:78:ILE:HD13	0.52	1.80	16	1
1:A:130:MET:SD	1:A:135:GLU:HA	0.52	2.45	11	3
1:A:34:TRP:CZ2	1:A:97:LYS:HE2	0.52	2.40	12	1
1:A:69:ARG:HD3	1:A:69:ARG:H	0.51	1.64	3	7
1:A:130:MET:HG3	2:B:656:PHE:O	0.51	2.05	6	2
1:A:17:ARG:NH2	2:B:639:VAL:HG21	0.51	2.21	18	1
1:A:132:LYS:HA	1:A:132:LYS:HE2	0.51	1.83	19	1
1:A:92:TYR:O	1:A:95:LYS:HG2	0.51	2.07	9	8
1:A:59:HIS:CD2	1:A:122:LEU:HD21	0.51	2.40	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:127:ARG:HB2	1:A:135:GLU:OE2	0.51	2.06	17	1
1:A:59:HIS:HB3	2:B:653:GLN:CD	0.50	2.31	18	1
1:A:138:SER:HA	2:B:651:ILE:HG13	0.50	1.84	2	1
1:A:74:ARG:HB2	1:A:112:ASP:OD2	0.50	2.06	17	1
1:A:54:ARG:O	1:A:54:ARG:HD2	0.50	2.05	4	2
2:B:651:ILE:HG23	2:B:652:ASP:N	0.50	2.22	12	9
1:A:138:SER:O	2:B:651:ILE:HG13	0.50	2.06	7	1
1:A:72:SER:HB2	1:A:112:ASP:OD1	0.50	2.06	17	1
1:A:143:THR:HG23	1:A:162:THR:O	0.50	2.06	20	2
1:A:131:GLN:CG	2:B:655:GLU:HB3	0.50	2.37	19	1
1:A:61:LEU:O	1:A:112:ASP:HB3	0.50	2.07	7	5
1:A:138:SER:HB3	2:B:651:ILE:HD13	0.50	1.83	17	2
1:A:53:ALA:O	1:A:126:SER:HA	0.49	2.07	10	1
1:A:61:LEU:HD23	1:A:157:HIS:ND1	0.49	2.22	8	3
1:A:157:HIS:CE1	2:B:653:GLN:HG3	0.49	2.42	7	2
1:A:64:HIS:HB2	1:A:80:ARG:O	0.49	2.08	15	2
1:A:30:ASN:O	2:B:645:GLN:HB3	0.49	2.08	15	2
2:B:640:LEU:O	2:B:642:PRO:HD3	0.48	2.08	19	3
1:A:159:ILE:HD12	2:B:651:ILE:HG22	0.48	1.83	7	1
1:A:132:LYS:HA	1:A:132:LYS:CE	0.48	2.38	19	1
1:A:93:ILE:O	1:A:97:LYS:HG3	0.48	2.08	14	3
2:B:657:GLU:CD	2:B:658:GLY:H	0.48	2.17	3	4
1:A:148:GLY:HA3	2:B:644:ASP:CG	0.48	2.33	15	1
1:A:127:ARG:HA	1:A:130:MET:SD	0.48	2.49	6	1
1:A:132:LYS:C	1:A:132:LYS:HD3	0.48	2.34	13	1
1:A:83:GLU:H	1:A:83:GLU:CD	0.47	2.17	10	3
2:B:643:PRO:HB2	2:B:645:GLN:OE1	0.47	2.08	11	1
1:A:118:ALA:HB3	1:A:121:ASP:O	0.47	2.09	2	1
1:A:63:LYS:O	1:A:80:ARG:HD2	0.47	2.10	12	1
1:A:61:LEU:HB3	1:A:113:CYS:SG	0.47	2.49	8	3
1:A:61:LEU:HA	1:A:157:HIS:HB3	0.47	1.85	7	4
1:A:127:ARG:HB3	1:A:139:PHE:CE1	0.47	2.44	5	1
1:A:137:ALA:O	2:B:650:ASN:HA	0.47	2.10	11	1
1:A:125:PHE:CZ	2:B:657:GLU:HG3	0.47	2.45	20	1
1:A:96:ILE:HA	1:A:101:GLU:O	0.46	2.09	11	5
1:A:85:ALA:O	1:A:88:LEU:HG	0.46	2.10	10	2
1:A:158:ILE:C	1:A:159:ILE:HD12	0.46	2.35	17	1
1:A:138:SER:HA	2:B:651:ILE:C	0.46	2.36	1	1
1:A:159:ILE:HG12	2:B:653:GLN:NE2	0.46	2.26	19	2
1:A:95:LYS:HD3	1:A:101:GLU:OE2	0.46	2.10	20	1
1:A:92:TYR:O	1:A:96:ILE:HG13	0.46	2.11	3	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:130:MET:HA	2:B:656:PHE:O	0.46	2.10	7	4
1:A:33:GLN:HG3	1:A:35:GLU:O	0.46	2.10	19	3
1:A:76:GLU:H	1:A:76:GLU:CD	0.46	2.19	13	1
1:A:56:ARG:HD3	1:A:163:GLU:OE2	0.46	2.11	15	1
1:A:63:LYS:HZ2	1:A:112:ASP:CG	0.45	2.19	13	1
1:A:23:TYR:HB3	1:A:34:TRP:CZ3	0.45	2.46	16	1
1:A:147:SER:CB	1:A:159:ILE:HG13	0.45	2.42	7	1
2:B:651:ILE:HG12	2:B:652:ASP:N	0.45	2.26	19	1
1:A:63:LYS:CD	1:A:69:ARG:HG2	0.45	2.42	9	1
1:A:57:CYS:SG	1:A:161:ARG:HG2	0.45	2.51	17	2
1:A:32:SER:O	2:B:643:PRO:HA	0.45	2.12	12	1
1:A:54:ARG:HD2	1:A:54:ARG:C	0.45	2.37	9	2
1:A:138:SER:HA	2:B:651:ILE:HA	0.45	1.89	1	5
1:A:16:SER:HB2	1:A:19:SER:OG	0.45	2.12	14	1
1:A:31:ALA:HA	2:B:644:ASP:O	0.45	2.12	16	1
1:A:132:LYS:N	1:A:133:PRO:HD2	0.44	2.27	3	3
2:B:640:LEU:HD11	2:B:644:ASP:HB2	0.44	1.89	16	1
1:A:60:LEU:HD23	1:A:61:LEU:H	0.44	1.72	6	1
1:A:89:ILE:CD1	1:A:157:HIS:HA	0.44	2.42	6	1
2:B:639:VAL:HG22	2:B:640:LEU:H	0.44	1.72	18	1
1:A:36:ARG:N	1:A:36:ARG:HD2	0.44	2.27	2	1
1:A:147:SER:HB3	1:A:159:ILE:HG13	0.44	1.88	7	1
1:A:24:TYR:O	1:A:32:SER:HA	0.44	2.13	20	1
1:A:34:TRP:CE3	1:A:97:LYS:HE2	0.44	2.48	10	1
1:A:122:LEU:HD22	2:B:656:PHE:CE2	0.44	2.48	12	1
1:A:16:SER:OG	1:A:19:SER:HB3	0.44	2.13	13	2
1:A:23:TYR:CE1	2:B:640:LEU:HB3	0.44	2.48	13	1
1:A:161:ARG:HB2	2:B:651:ILE:CD1	0.43	2.43	1	2
1:A:69:ARG:N	1:A:69:ARG:CD	0.43	2.81	9	2
1:A:122:LEU:HG	2:B:657:GLU:OE2	0.43	2.12	11	1
2:B:657:GLU:HG3	2:B:659:PHE:HB3	0.43	1.90	11	1
1:A:137:ALA:HB1	2:B:650:ASN:O	0.43	2.13	13	1
1:A:142:ARG:HA	1:A:161:ARG:NH1	0.43	2.29	8	1
1:A:56:ARG:HA	1:A:123:GLY:O	0.43	2.13	13	2
2:B:651:ILE:HG23	2:B:652:ASP:H	0.43	1.73	19	1
1:A:97:LYS:HD2	1:A:98:SER:N	0.43	2.29	8	1
1:A:89:ILE:HA	1:A:92:TYR:CD1	0.43	2.49	10	2
1:A:159:ILE:HG12	2:B:653:GLN:HE21	0.43	1.74	7	1
1:A:57:CYS:CB	1:A:161:ARG:HA	0.43	2.44	9	1
1:A:111:SER:HB3	1:A:116:ALA:HB2	0.43	1.91	14	1
1:A:93:ILE:HD11	1:A:158:ILE:HG21	0.43	1.90	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:652:ASP:O	2:B:653:GLN:HB2	0.43	2.13	11	1
1:A:76:GLU:CD	1:A:76:GLU:H	0.43	2.21	17	2
1:A:134:PHE:HA	1:A:137:ALA:HB3	0.43	1.90	20	1
1:A:32:SER:OG	2:B:640:LEU:HD21	0.43	2.14	2	1
1:A:138:SER:HA	2:B:652:ASP:N	0.42	2.28	5	1
1:A:17:ARG:O	1:A:17:ARG:HG3	0.42	2.13	5	1
1:A:159:ILE:CD1	2:B:651:ILE:HG22	0.42	2.44	7	1
1:A:157:HIS:NE2	2:B:652:ASP:OD2	0.42	2.52	13	1
1:A:159:ILE:HG12	2:B:651:ILE:O	0.42	2.14	15	1
1:A:157:HIS:NE2	2:B:653:GLN:HB3	0.42	2.29	19	1
1:A:16:SER:OG	1:A:21:ARG:HB2	0.42	2.14	3	1
1:A:159:ILE:HD13	2:B:651:ILE:HG22	0.42	1.92	19	1
1:A:161:ARG:HD3	1:A:161:ARG:C	0.42	2.40	20	2
1:A:142:ARG:HD2	1:A:145:GLU:OE2	0.42	2.14	20	1
1:A:32:SER:HB3	2:B:640:LEU:HD22	0.42	1.91	13	1
2:B:657:GLU:CG	2:B:659:PHE:HB3	0.42	2.44	11	1
1:A:63:LYS:HD2	1:A:69:ARG:O	0.42	2.15	3	1
1:A:152:THR:OG1	1:A:157:HIS:HE1	0.42	1.97	17	2
1:A:127:ARG:HA	1:A:130:MET:HE3	0.42	1.91	20	1
1:A:59:HIS:CG	2:B:653:GLN:HE21	0.41	2.33	16	1
1:A:130:MET:N	1:A:130:MET:SD	0.41	2.93	17	1
1:A:157:HIS:N	1:A:157:HIS:CD2	0.41	2.87	12	3
1:A:15:MET:SD	1:A:20:GLY:HA2	0.41	2.55	13	1
1:A:97:LYS:HD2	1:A:97:LYS:C	0.41	2.39	7	1
1:A:26:ASN:O	1:A:30:ASN:HA	0.41	2.16	14	1
1:A:131:GLN:HG2	2:B:655:GLU:HB3	0.41	1.92	19	1
1:A:74:ARG:HD3	1:A:112:ASP:HA	0.41	1.91	15	1
1:A:89:ILE:O	1:A:93:ILE:HG13	0.41	2.16	16	1
1:A:34:TRP:CD2	1:A:97:LYS:HE2	0.41	2.50	17	1
1:A:108:SER:HB2	1:A:119:ARG:HA	0.41	1.93	20	1
1:A:157:HIS:HE1	2:B:654:SER:OG	0.41	1.99	2	1
1:A:56:ARG:H	1:A:163:GLU:C	0.41	2.24	10	1
2:B:653:GLN:HA	2:B:656:PHE:CD2	0.41	2.51	13	1
1:A:157:HIS:CD2	2:B:653:GLN:HB2	0.41	2.51	18	1
1:A:63:LYS:HD3	1:A:69:ARG:NE	0.41	2.31	1	1
1:A:7:LEU:HD21	1:A:24:TYR:CD2	0.41	2.50	16	1
1:A:59:HIS:CD2	1:A:122:LEU:HD11	0.41	2.51	2	1
2:B:653:GLN:H	2:B:653:GLN:CD	0.41	2.23	15	1
1:A:11:TRP:CD2	1:A:26:ASN:HB2	0.41	2.51	20	1
1:A:137:ALA:O	2:B:651:ILE:HA	0.41	2.16	14	1
1:A:16:SER:HB2	1:A:19:SER:HB3	0.40	1.93	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:16:SER:HB2	1:A:19:SER:HB2	0.40	1.93	12	1
1:A:147:SER:HB3	1:A:159:ILE:HD12	0.40	1.92	19	1
1:A:34:TRP:NE1	2:B:643:PRO:HG3	0.40	2.32	16	1
1:A:157:HIS:NE2	2:B:653:GLN:HB2	0.40	2.32	18	1
1:A:59:HIS:HB3	2:B:653:GLN:NE2	0.40	2.32	2	1
1:A:61:LEU:HD22	1:A:157:HIS:ND1	0.40	2.32	3	1
2:B:640:LEU:HD23	2:B:640:LEU:H	0.40	1.77	11	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	142/163 (87%)	135±2 (95±1%)	6±2 (4±1%)	1±1 (1±0%)	26 74
2	B	18/25 (72%)	11±2 (62±10%)	5±1 (29±8%)	2±1 (9±5%)	1 11
All	All	3200/3760 (85%)	2927 (91%)	226 (7%)	47 (1%)	11 57

All 14 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	651	ILE	14
1	A	78	ILE	11
2	B	652	ASP	4
2	B	639	VAL	3
1	A	52	PRO	2
1	A	17	ARG	2
2	B	640	LEU	2
2	B	653	GLN	2
2	B	661	PHE	2
2	B	644	ASP	1
2	B	655	GLU	1
2	B	657	GLU	1
2	B	645	GLN	1
2	B	654	SER	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	124/138 (90%)	118±2 (95±2%)	6±2 (5±2%)	25 76
2	B	17/20 (85%)	15±1 (90±6%)	2±1 (10±6%)	10 55
All	All	2820/3160 (89%)	2673 (95%)	147 (5%)	22 72

All 42 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	54	ARG	13
1	A	157	HIS	13
1	A	159	ILE	10
2	B	657	GLU	9
1	A	69	ARG	8
1	A	97	LYS	6
1	A	160	LEU	6
1	A	76	GLU	6
1	A	12	GLU	5
1	A	81	THR	5
1	A	83	GLU	5
2	B	655	GLU	5
1	A	131	GLN	5
2	B	656	PHE	5
2	B	659	PHE	4
2	B	653	GLN	3
1	A	122	LEU	3
2	B	645	GLN	3
1	A	143	THR	3
1	A	61	LEU	3
1	A	80	ARG	2
2	B	646	GLU	2
1	A	95	LYS	2
1	A	112	ASP	2
1	A	141	LEU	2
1	A	60	LEU	1
1	A	30	ASN	1
1	A	72	SER	1

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Mol	Chain	Res	Type	Models (Total)
1	A	132	LYS	1
1	A	68	ARG	1
1	A	105	SER	1
1	A	32	SER	1
1	A	119	ARG	1
2	B	650	ASN	1
1	A	100	GLU	1
1	A	146	MET	1
1	A	77	LYS	1
2	B	654	SER	1
1	A	153	ASP	1
1	A	74	ARG	1
1	A	142	ARG	1
1	A	161	ARG	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)

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	TPO	B	641	2	8,10,11	1.63±0.09	1±0 (15±5%)
2	SEP	B	660	2	8,9,10	1.04±0.05	0±0 (0±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of

the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	TPO	B	641	2	10,14,16	1.75±0.03	4±1 (43±8%)
2	SEP	B	660	2	7,12,14	2.22±0.09	2±0 (28±0%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SEP	B	660	2	-	0±0,6,8,10	-
2	TPO	B	641	2	-	0±0,9,11,13	-

All unique bond 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(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	641	TPO	P-O1P	3.94	1.62	1.50	18	20
2	B	641	TPO	P-O3P	2.18	1.62	1.54	4	5

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(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	660	SEP	OG-P-O1P	4.25	117.92	106.44	7	20
2	B	660	SEP	OG-CB-CA	3.54	111.59	108.14	2	20
2	B	641	TPO	O2P-P-OG1	3.02	117.60	105.85	19	20
2	B	641	TPO	O-C-CA	2.64	117.98	124.77	13	20
2	B	641	TPO	O3P-P-O1P	2.50	101.08	110.83	16	20
2	B	641	TPO	O3P-P-O2P	2.31	116.47	107.80	2	15
2	B	641	TPO	OG1-P-O1P	2.20	101.48	109.33	11	12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6.5 Carbohydrates

There are no oligosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 80% for the well-defined parts and 79% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chemical_shifts_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	1776
Number of shifts mapped to atoms	1776
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	10

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	161	-0.25 ± 0.09	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	143	-0.14 ± 0.11	None needed (< 0.5 ppm)
$^{13}C'$	160	-0.03 ± 0.03	None needed (< 0.5 ppm)
^{15}N	153	0.08 ± 0.28	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 74%, i.e. 1623 atoms were assigned a chemical shift out of a possible 2206. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	701/798 (88%)	283/324 (87%)	283/322 (88%)	135/152 (89%)
Sidechain	817/1213 (67%)	534/778 (69%)	258/372 (69%)	25/63 (40%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	105/195 (54%)	59/96 (61%)	43/88 (49%)	3/11 (27%)
Overall	1623/2206 (74%)	876/1198 (73%)	584/782 (75%)	163/226 (72%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 72%, i.e. 1776 atoms were assigned a chemical shift out of a possible 2468. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	794/918 (86%)	320/375 (85%)	321/368 (87%)	153/175 (87%)
Sidechain	877/1355 (65%)	570/867 (66%)	281/417 (67%)	26/71 (37%)
Aromatic	105/195 (54%)	59/96 (61%)	43/88 (49%)	3/11 (27%)
Overall	1776/2468 (72%)	949/1338 (71%)	645/873 (74%)	182/257 (71%)

7.1.4 Statistically unusual chemical shifts (i)

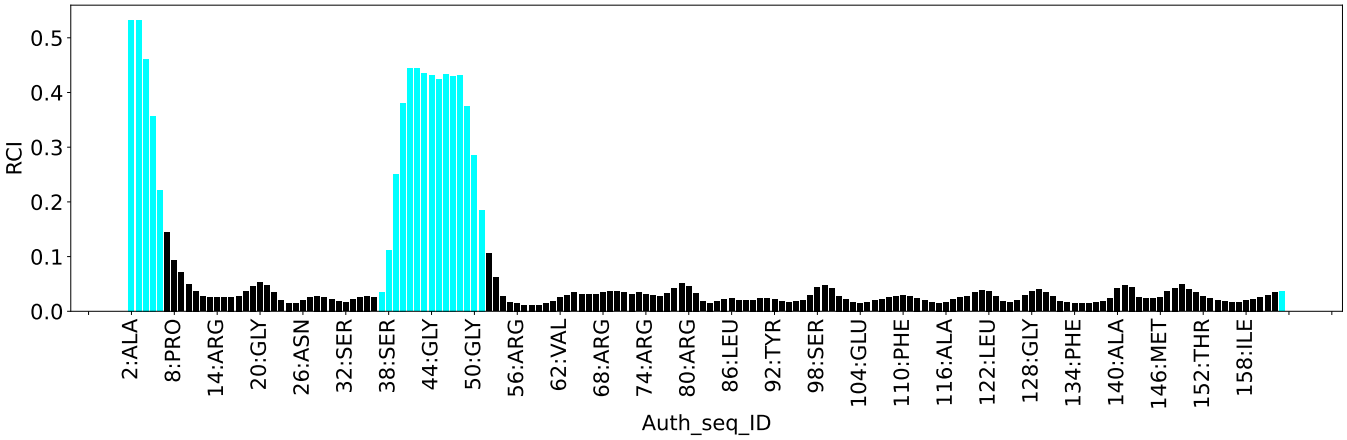
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	26	ASN	HB2	-0.66	1.27 – 4.34	-11.3
1	A	74	ARG	HG3	-0.55	0.15 – 2.94	-7.5
1	A	37	PRO	HG2	-0.03	0.41 – 3.45	-6.4
1	A	14	ARG	HB3	0.08	0.43 – 3.11	-6.3
1	A	26	ASN	HD22	4.24	4.69 – 9.61	-5.9
1	A	74	ARG	HG2	0.03	0.26 – 2.87	-5.9
1	A	109	GLN	HB2	0.77	0.80 – 3.29	-5.1
1	A	55	VAL	HG21	-0.58	-0.58 – 2.19	-5.0
1	A	55	VAL	HG22	-0.58	-0.58 – 2.19	-5.0
1	A	55	VAL	HG23	-0.58	-0.58 – 2.19	-5.0

7.1.5 Random Coil Index (RCI) plots (i)

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

Random coil index (RCI) for chain A:



7.2 Chemical shift list 2

File name: working_cs.cif

Chemical shift list name: *assigned_chemical_shifts_2*

7.2.1 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	184
Number of shifts mapped to atoms	184
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.2.2 Chemical shift referencing

No chemical shift referencing corrections were calculated (not enough data).

7.2.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 6%, i.e. 137 atoms were assigned a chemical shift out of a possible 2206. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	41/798 (5%)	33/324 (10%)	5/322 (2%)	3/152 (2%)

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	Total	^{1}H	^{13}C	^{15}N
Sidechain	76/1213 (6%)	67/778 (9%)	9/372 (2%)	0/63 (0%)
Aromatic	20/195 (10%)	10/96 (10%)	10/88 (11%)	0/11 (0%)
Overall	137/2206 (6%)	110/1198 (9%)	24/782 (3%)	3/226 (1%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 7%, i.e. 176 atoms were assigned a chemical shift out of a possible 2468. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	51/918 (6%)	39/375 (10%)	7/368 (2%)	5/175 (3%)
Sidechain	105/1355 (8%)	89/867 (10%)	16/417 (4%)	0/71 (0%)
Aromatic	20/195 (10%)	10/96 (10%)	10/88 (11%)	0/11 (0%)
Overall	176/2468 (7%)	138/1338 (10%)	33/873 (4%)	5/257 (2%)

7.2.4 Statistically unusual chemical shifts (i)

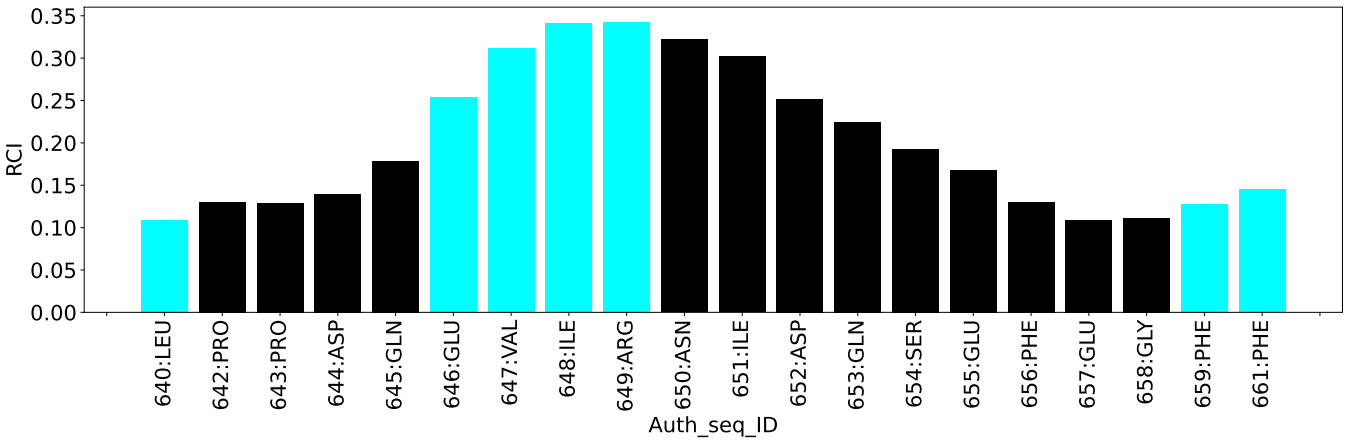
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
2	B	642	PRO	HG3	0.15	0.33 – 3.48	-5.6

7.2.5 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 B:


RCI
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
640:LEU
642:PRO
643:PRO
644:ASP
645:GLN
646:GLU
647:VAL
648:ILE
649:ARG
650:ASN
651:ILE
652:ASP
653:GLN
654:SER
655:GLU
656:PHE
657:GLU
658:GLY
659:PHE
661:PHE
Auth_seq_ID

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	5666
Intra-residue (|i-j|=0)	2179
Sequential (|i-j|=1)	1277
Medium range (|i-j|>1 and |i-j|<5)	732
Long range (|i-j|≥5)	1284
Inter-chain	111
Hydrogen bond restraints	83
Disulfide bond restraints	0
Total dihedral-angle restraints	244
Number of unmapped restraints	0
Number of restraints per residue	31.4
Number of long range restraints per residue[1]	7.0

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	58.7	0.2
0.2-0.5 (Medium)	130.8	0.5
>0.5 (Large)	75.0	12.07

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)	10.6	5.69
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis (i)

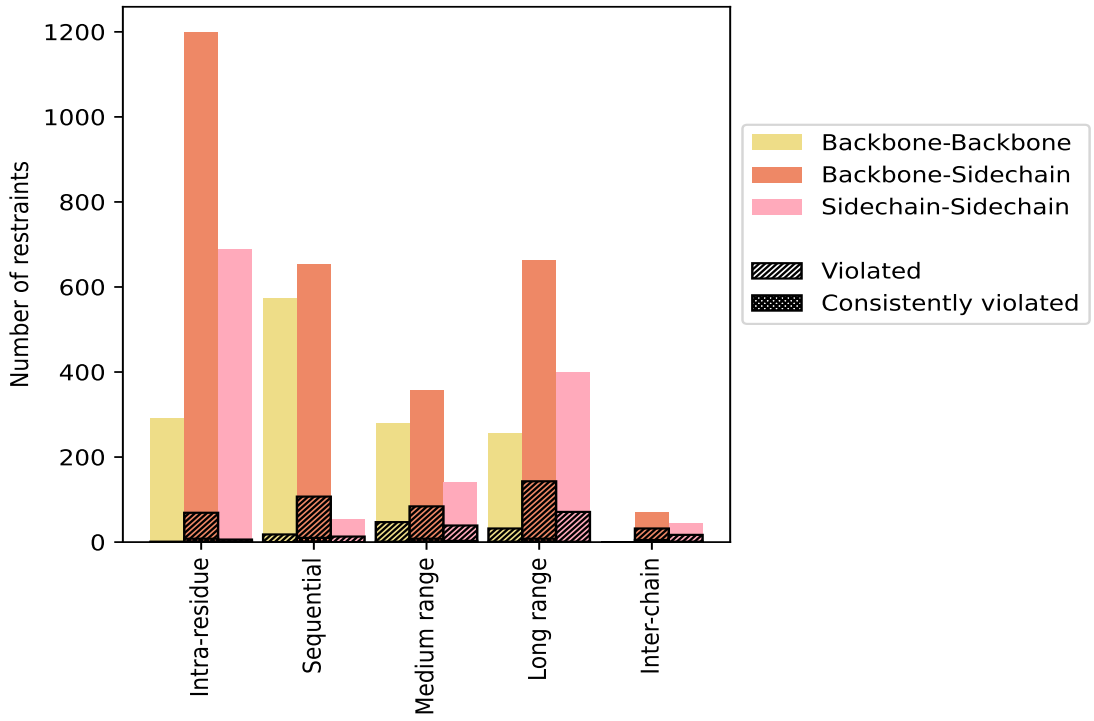
9.1 Summary of distance violations (i)

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

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	2179	38.5	76	3.5	1.3	10	0.5	0.2
Backbone-Backbone	292	5.2	1	0.3	0.0	0	0.0	0.0
Backbone-Sidechain	1199	21.2	69	5.8	1.2	8	0.7	0.1
Sidechain-Sidechain	688	12.1	6	0.9	0.1	2	0.3	0.0
Sequential (|i-j|=1)	1277	22.5	138	10.8	2.4	10	0.8	0.2
Backbone-Backbone	572	10.1	18	3.1	0.3	0	0.0	0.0
Backbone-Sidechain	652	11.5	107	16.4	1.9	10	1.5	0.2
Sidechain-Sidechain	53	0.9	13	24.5	0.2	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	732	12.9	154	21.0	2.7	11	1.5	0.2
Backbone-Backbone	280	4.9	47	16.8	0.8	1	0.4	0.0
Backbone-Sidechain	311	5.5	68	21.9	1.2	7	2.3	0.1
Sidechain-Sidechain	141	2.5	39	27.7	0.7	3	2.1	0.1
Long range (|i-j|≥5)	1284	22.7	238	18.5	4.2	10	0.8	0.2
Backbone-Backbone	256	4.5	32	12.5	0.6	1	0.4	0.0
Backbone-Sidechain	629	11.1	135	21.5	2.4	8	1.3	0.1
Sidechain-Sidechain	399	7.0	71	17.8	1.3	1	0.3	0.0
Inter-chain	111	2.0	49	44.1	0.9	6	5.4	0.1
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	69	1.2	32	46.4	0.6	5	7.2	0.1
Sidechain-Sidechain	42	0.7	17	40.5	0.3	1	2.4	0.0
Hydrogen bond	83	1.5	24	28.9	0.4	1	1.2	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	5666	100.0	679	12.0	12.0	48	0.8	0.8
Backbone-Backbone	1400	24.7	98	7.0	1.7	2	0.1	0.0
Backbone-Sidechain	2940	51.9	435	14.8	7.7	39	1.3	0.7
Sidechain-Sidechain	1326	23.4	146	11.0	2.6	7	0.5	0.1

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

9.1.1 Bar chart : Distribution of distance restraints and violations



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

9.2 Distance violation statistics for each model

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	37	52	69	93	24	275	0.47	10.81	0.92	0.37
2	34	52	64	85	23	258	0.46	9.46	0.78	0.38
3	30	56	60	103	26	275	0.47	11.07	0.93	0.37
4	34	49	65	89	24	261	0.47	11.49	0.98	0.37
5	32	61	68	94	25	280	0.46	10.54	0.89	0.37
6	32	50	70	95	28	275	0.47	9.95	0.89	0.4
7	31	59	68	85	20	263	0.46	10.86	0.94	0.36
8	31	58	57	93	24	263	0.47	11.25	0.94	0.36
9	30	53	55	92	27	257	0.49	11.6	0.97	0.37
10	32	47	62	95	26	262	0.47	8.4	0.74	0.4

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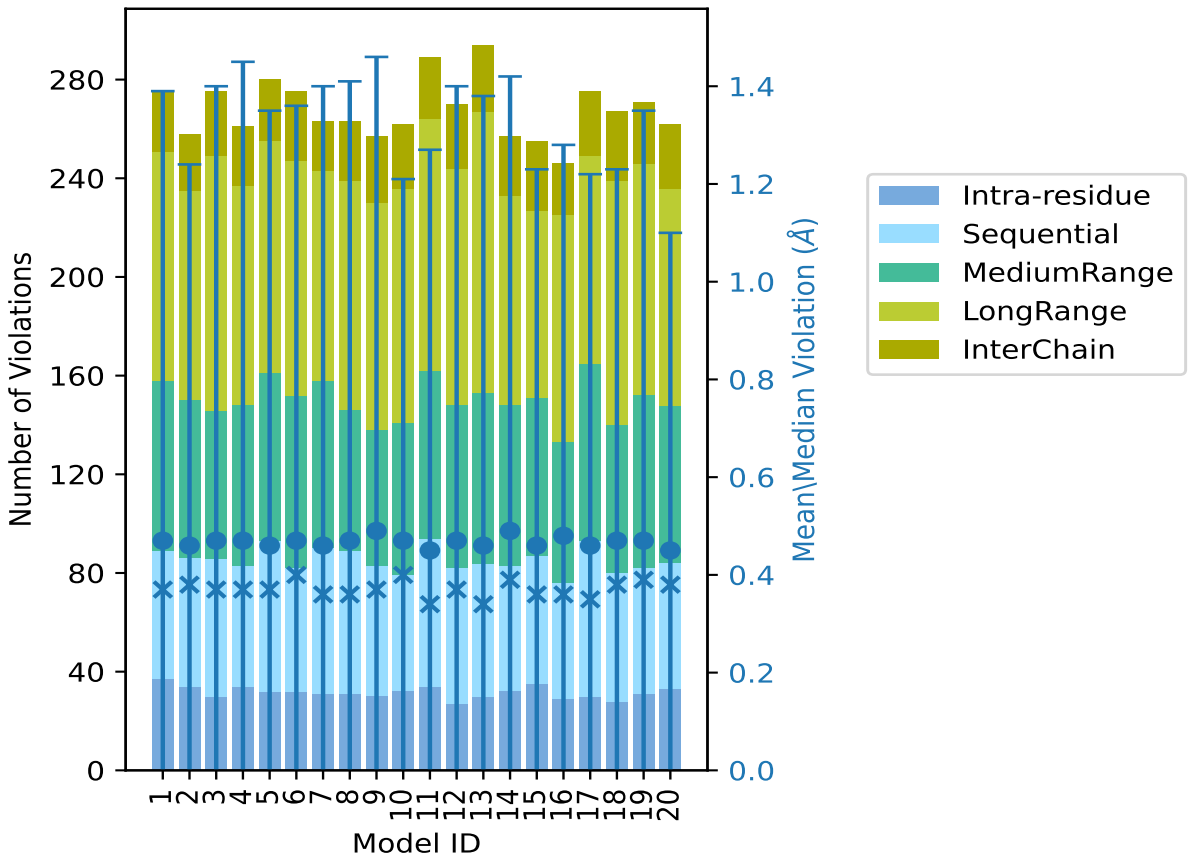
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
11	34	60	68	102	25	289	0.45	9.85	0.82	0.34
12	27	55	66	96	26	270	0.47	11.26	0.93	0.37
13	30	54	69	114	27	294	0.46	12.07	0.92	0.34
14	32	51	65	85	24	257	0.49	10.51	0.93	0.39
15	35	52	64	76	28	255	0.46	8.88	0.77	0.36
16	29	47	57	92	21	246	0.48	9.24	0.8	0.36
17	30	63	72	84	26	275	0.46	8.86	0.76	0.35
18	28	52	60	99	28	267	0.47	8.25	0.76	0.38
19	31	51	70	94	25	271	0.47	10.5	0.88	0.39
20	33	51	64	88	26	262	0.45	7.35	0.65	0.38

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

9.2.1 Bar graph : Distance Violation statistics for each model



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

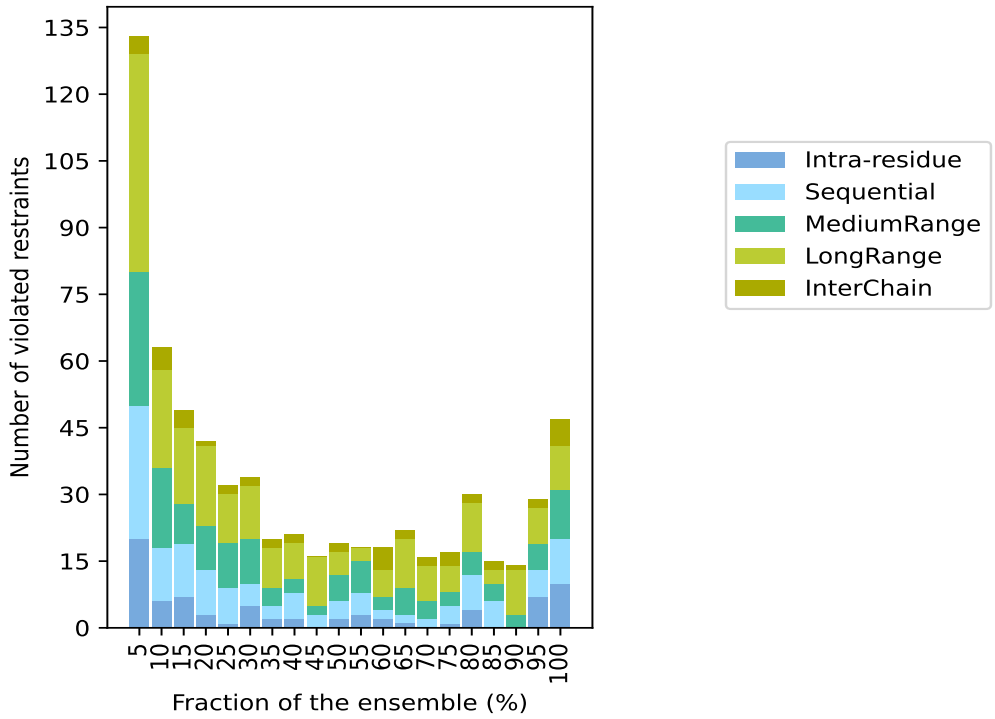
9.3 Distance violation statistics for the ensemble (i)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 4928(IR:2103, SQ:1139, MR:578, LR:1046, IC:62) 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]	%
20	30	30	49	4	133	1	5.0
6	12	18	22	5	63	2	10.0
7	12	9	17	4	49	3	15.0
3	10	10	18	1	42	4	20.0
1	8	10	11	2	32	5	25.0
5	5	10	12	2	34	6	30.0
2	3	4	9	2	20	7	35.0
2	6	3	8	2	21	8	40.0
0	3	2	11	0	16	9	45.0
2	4	6	5	2	19	10	50.0
3	5	7	3	0	18	11	55.0
2	2	3	6	5	18	12	60.0
1	2	6	11	2	22	13	65.0
0	2	4	8	2	16	14	70.0
1	4	3	6	3	17	15	75.0
4	8	5	11	2	30	16	80.0
0	6	4	3	2	15	17	85.0
0	0	3	10	1	14	18	90.0
7	6	6	8	2	29	19	95.0
10	10	11	10	6	47	20	100.0

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

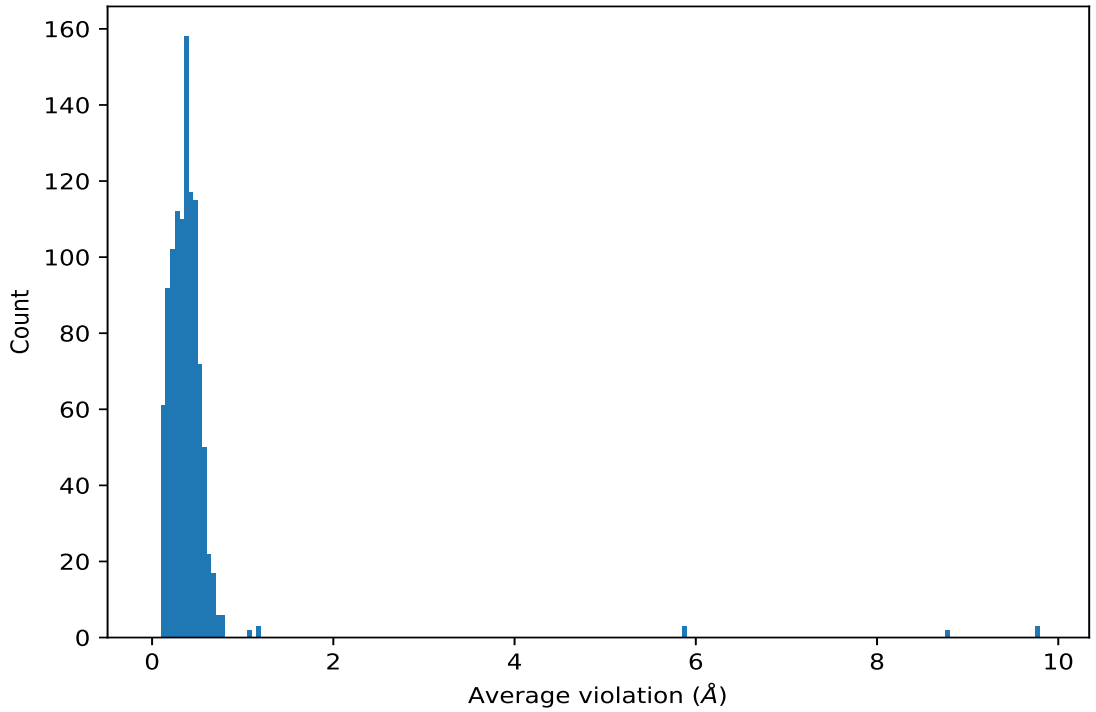
9.3.1 Bar graph : Distance violation statistics for the ensemble



9.4 Most violated distance restraints in the ensemble

9.4.1 Histogram : Distribution of mean distance violations

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



9.4.2 Table: Most violated distance restraints

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

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG21	20	9.76	1.66	10.5
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG22	20	9.76	1.66	10.5
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG23	20	9.76	1.66	10.5
(1,2595)	1:131:A:GLN:HG2	2:652:B:ASP:HA	20	8.75	0.86	9.09
(1,2595)	1:131:A:GLN:HG3	2:652:B:ASP:HA	20	8.75	0.86	9.09
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD11	20	5.87	0.88	6.39
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD12	20	5.87	0.88	6.39
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD13	20	5.87	0.88	6.39
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG21	20	1.19	0.42	1.18
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG22	20	1.19	0.42	1.18
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG23	20	1.19	0.42	1.18
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG21	20	0.75	0.08	0.75
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG22	20	0.75	0.08	0.75
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG23	20	0.75	0.08	0.75
(2,44)	1:131:A:GLN:HE21	1:153:A:ASP:H	20	0.71	0.11	0.72
(1,1227)	1:89:A:ILE:HG12	1:150:A:VAL:H	20	0.68	0.04	0.68

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,689)	1:86:A:LEU:HG	1:90:A:ASN:HD21	20	0.64	0.09	0.64
(2,45)	1:131:A:GLN:HE21	1:152:A:THR:HB	20	0.62	0.11	0.66
(2,103)	1:137:A:ALA:H	2:656:B:PHE:HB2	20	0.62	0.22	0.65
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD1	20	0.56	0.04	0.57
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD2	20	0.56	0.04	0.57
(1,816)	1:95:A:LYS:HD2	1:96:A:ILE:H	20	0.55	0.12	0.58
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD21	20	0.55	0.03	0.55
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD22	20	0.55	0.03	0.55
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD23	20	0.55	0.03	0.55
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD21	20	0.54	0.04	0.54
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD22	20	0.54	0.04	0.54
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD23	20	0.54	0.04	0.54
(1,1033)	1:108:A:SER:H	1:119:A:ARG:HB2	20	0.54	0.09	0.56
(1,2161)	1:119:A:ARG:H	1:119:A:ARG:HD3	20	0.52	0.1	0.55
(1,910)	1:102:A:ASP:H	1:106:A:LEU:HB3	20	0.51	0.05	0.52
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD11	20	0.51	0.04	0.5
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD12	20	0.51	0.04	0.5
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD13	20	0.51	0.04	0.5
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD21	20	0.5	0.02	0.5
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD22	20	0.5	0.02	0.5
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD23	20	0.5	0.02	0.5
(1,14)	1:6:A:LYS:HG2	1:7:A:LEU:H	20	0.5	0.14	0.46
(1,886)	1:103:A:PHE:HE1	1:107:A:ALA:H	20	0.5	0.06	0.5
(1,886)	1:103:A:PHE:HE2	1:107:A:ALA:H	20	0.5	0.06	0.5
(2,106)	1:139:A:PHE:H	2:656:B:PHE:HB2	20	0.49	0.12	0.52
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD11	20	0.48	0.11	0.51
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD12	20	0.48	0.11	0.51
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD13	20	0.48	0.11	0.51
(1,295)	1:27:A:HIS:H	1:29:A:THR:H	20	0.48	0.05	0.49
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG21	20	0.48	0.05	0.49
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG22	20	0.48	0.05	0.49
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG23	20	0.48	0.05	0.49
(1,287)	1:26:A:ASN:H	1:32:A:SER:HB2	20	0.48	0.12	0.51
(1,214)	1:11:A:TRP:HB2	1:25:A:PHE:H	20	0.46	0.09	0.48
(1,261)	1:25:A:PHE:HE1	1:26:A:ASN:H	20	0.45	0.04	0.44
(1,261)	1:25:A:PHE:HE2	1:26:A:ASN:H	20	0.45	0.04	0.44
(1,742)	1:89:A:ILE:HD11	1:90:A:ASN:H	20	0.43	0.11	0.49
(1,742)	1:89:A:ILE:HD12	1:90:A:ASN:H	20	0.43	0.11	0.49
(1,742)	1:89:A:ILE:HD13	1:90:A:ASN:H	20	0.43	0.11	0.49
(1,871)	1:96:A:ILE:HB	1:103:A:PHE:H	20	0.43	0.15	0.51
(1,213)	1:11:A:TRP:HA	1:25:A:PHE:H	20	0.42	0.07	0.44
(1,753)	1:90:A:ASN:HD22	1:91:A:GLY:H	20	0.42	0.08	0.42

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,12)	1:5:A:GLU:HB2	1:6:A:LYS:H	20	0.37	0.09	0.38
(1,369)	1:33:A:GLN:HG2	1:34:A:TRP:H	20	0.36	0.08	0.38
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB1	20	0.34	0.05	0.34
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB2	20	0.34	0.05	0.34
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB3	20	0.34	0.05	0.34
(2,25)	1:88:A:LEU:HG	1:92:A:TYR:H	20	0.32	0.08	0.29
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD11	20	0.31	0.05	0.32
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD12	20	0.31	0.05	0.32
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD13	20	0.31	0.05	0.32
(1,1750)	1:56:A:ARG:HA	1:56:A:ARG:HE	20	0.31	0.07	0.3
(1,311)	1:27:A:HIS:HB2	1:29:A:THR:H	20	0.31	0.07	0.33
(1,347)	1:31:A:ALA:HB1	1:33:A:GLN:H	20	0.3	0.08	0.32
(1,347)	1:31:A:ALA:HB2	1:33:A:GLN:H	20	0.3	0.08	0.32
(1,347)	1:31:A:ALA:HB3	1:33:A:GLN:H	20	0.3	0.08	0.32
(3,43)	1:72:A:SER:O	1:75:A:GLN:N	20	0.28	0.09	0.3
(1,1455)	1:6:A:LYS:H	1:6:A:LYS:HB3	20	0.26	0.06	0.29
(1,941)	1:106:A:LEU:HD11	1:107:A:ALA:H	20	0.26	0.09	0.26
(1,941)	1:106:A:LEU:HD12	1:107:A:ALA:H	20	0.26	0.09	0.26
(1,941)	1:106:A:LEU:HD13	1:107:A:ALA:H	20	0.26	0.09	0.26
(1,2103)	1:109:A:GLN:HG2	1:109:A:GLN:HE22	20	0.25	0.01	0.25
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD11	20	0.23	0.07	0.2
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD12	20	0.23	0.07	0.2
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD13	20	0.23	0.07	0.2
(1,1694)	1:35:A:GLU:H	1:35:A:GLU:HG3	20	0.2	0.04	0.2
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG21	20	0.19	0.02	0.18
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG22	20	0.19	0.02	0.18
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG23	20	0.19	0.02	0.18
(1,1485)	1:11:A:TRP:HD1	1:11:A:TRP:HE3	20	0.11	0.0	0.11
(1,296)	1:27:A:HIS:HA	1:30:A:ASN:HD21	19	0.68	0.17	0.74
(2,89)	1:55:A:VAL:H	2:651:B:ILE:HG12	19	0.62	0.14	0.62
(2,89)	1:55:A:VAL:H	2:651:B:ILE:HG13	19	0.62	0.14	0.62
(2,98)	1:124:A:ALA:H	2:656:B:PHE:HE1	19	0.61	0.11	0.62
(2,98)	1:124:A:ALA:H	2:656:B:PHE:HE2	19	0.61	0.11	0.62
(2,38)	1:126:A:SER:H	1:129:A:GLN:HB2	19	0.59	0.13	0.63
(1,1217)	1:145:A:GLU:HB3	1:147:A:SER:H	19	0.55	0.09	0.56
(1,86)	1:13:A:LYS:HE2	1:14:A:ARG:H	19	0.55	0.08	0.56
(1,397)	1:54:A:ARG:HG2	1:126:A:SER:H	19	0.52	0.11	0.55
(1,190)	1:13:A:LYS:HB3	1:24:A:TYR:HA	19	0.49	0.09	0.54
(1,64)	1:12:A:GLU:H	1:24:A:TYR:HD1	19	0.47	0.13	0.52
(1,64)	1:12:A:GLU:H	1:24:A:TYR:HD2	19	0.47	0.13	0.52
(1,134)	1:20:A:GLY:H	1:21:A:ARG:HA	19	0.46	0.1	0.49
(1,93)	1:14:A:ARG:H	1:22:A:VAL:HA	19	0.44	0.08	0.46

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1507)	1:13:A:LYS:H	1:13:A:LYS:HG3	19	0.44	0.06	0.44
(1,2158)	1:119:A:ARG:H	1:119:A:ARG:HD2	19	0.41	0.13	0.39
(1,465)	1:60:A:LEU:HB2	1:158:A:ILE:H	19	0.41	0.04	0.41
(1,366)	1:32:A:SER:H	1:33:A:GLN:HE22	19	0.41	0.06	0.41
(1,366)	1:32:A:SER:H	1:33:A:GLN:HE21	19	0.41	0.06	0.41
(1,66)	1:12:A:GLU:H	1:25:A:PHE:HE1	19	0.41	0.12	0.43
(1,66)	1:12:A:GLU:H	1:25:A:PHE:HE2	19	0.41	0.12	0.43
(1,1625)	1:27:A:HIS:H	1:27:A:HIS:HD1	19	0.39	0.08	0.39
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE1	19	0.39	0.08	0.42
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE2	19	0.39	0.08	0.42
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE3	19	0.39	0.08	0.42
(1,913)	1:103:A:PHE:H	1:106:A:LEU:HB3	19	0.38	0.1	0.37
(1,496)	1:62:A:VAL:HG11	1:88:A:LEU:H	19	0.37	0.09	0.38
(1,496)	1:62:A:VAL:HG12	1:88:A:LEU:H	19	0.37	0.09	0.38
(1,496)	1:62:A:VAL:HG13	1:88:A:LEU:H	19	0.37	0.09	0.38
(1,355)	1:25:A:PHE:HE1	1:32:A:SER:HB2	19	0.37	0.09	0.38
(1,355)	1:25:A:PHE:HE2	1:32:A:SER:HB2	19	0.37	0.09	0.38
(1,1206)	1:145:A:GLU:HB3	1:146:A:MET:HB2	19	0.35	0.12	0.34
(1,2033)	1:95:A:LYS:H	1:95:A:LYS:HD2	19	0.34	0.13	0.34
(1,1012)	1:116:A:ALA:H	1:119:A:ARG:H	19	0.32	0.1	0.33
(1,551)	1:70:A:PRO:HB3	1:71:A:SER:H	19	0.28	0.06	0.28
(1,1747)	1:56:A:ARG:H	1:56:A:ARG:HD2	19	0.27	0.11	0.3
(1,970)	1:108:A:SER:H	1:110:A:PHE:H	19	0.23	0.08	0.22
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB1	19	0.18	0.03	0.18
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB2	19	0.18	0.03	0.18
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB3	19	0.18	0.03	0.18
(1,1751)	1:56:A:ARG:H	1:56:A:ARG:HG3	19	0.18	0.04	0.19
(1,672)	1:64:A:HIS:HD2	1:85:A:ALA:H	18	0.61	0.07	0.62
(1,1109)	1:126:A:SER:HA	1:139:A:PHE:HD1	18	0.56	0.11	0.59
(1,1109)	1:126:A:SER:HA	1:139:A:PHE:HD2	18	0.56	0.11	0.59
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG11	18	0.55	0.19	0.55
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG12	18	0.55	0.19	0.55
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG13	18	0.55	0.19	0.55
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG21	18	0.55	0.19	0.55
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG22	18	0.55	0.19	0.55
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG23	18	0.55	0.19	0.55
(1,1130)	1:131:A:GLN:HE21	1:153:A:ASP:HB2	18	0.5	0.17	0.57
(1,1130)	1:131:A:GLN:HE21	1:153:A:ASP:HB3	18	0.5	0.17	0.57
(1,1032)	1:107:A:ALA:HB1	1:119:A:ARG:H	18	0.48	0.11	0.52
(1,1032)	1:107:A:ALA:HB2	1:119:A:ARG:H	18	0.48	0.11	0.52
(1,1032)	1:107:A:ALA:HB3	1:119:A:ARG:H	18	0.48	0.11	0.52
(1,27)	1:7:A:LEU:HD21	1:13:A:LYS:H	18	0.47	0.09	0.49

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,27)	1:7:A:LEU:HD22	1:13:A:LYS:H	18	0.47	0.09	0.49
(1,27)	1:7:A:LEU:HD23	1:13:A:LYS:H	18	0.47	0.09	0.49
(1,868)	1:60:A:LEU:HD21	1:103:A:PHE:HE1	18	0.45	0.15	0.51
(1,868)	1:60:A:LEU:HD21	1:103:A:PHE:HE2	18	0.45	0.15	0.51
(1,868)	1:60:A:LEU:HD22	1:103:A:PHE:HE1	18	0.45	0.15	0.51
(1,868)	1:60:A:LEU:HD22	1:103:A:PHE:HE2	18	0.45	0.15	0.51
(1,868)	1:60:A:LEU:HD23	1:103:A:PHE:HE1	18	0.45	0.15	0.51
(1,868)	1:60:A:LEU:HD23	1:103:A:PHE:HE2	18	0.45	0.15	0.51
(1,320)	1:25:A:PHE:HE1	1:30:A:ASN:H	18	0.4	0.1	0.44
(1,320)	1:25:A:PHE:HE2	1:30:A:ASN:H	18	0.4	0.1	0.44
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD11	18	0.38	0.16	0.34
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD12	18	0.38	0.16	0.34
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD13	18	0.38	0.16	0.34
(1,958)	1:108:A:SER:HA	1:110:A:PHE:H	18	0.37	0.07	0.38
(1,377)	1:33:A:GLN:HG2	1:35:A:GLU:H	18	0.33	0.13	0.4
(1,75)	1:13:A:LYS:HA	1:23:A:TYR:H	18	0.32	0.09	0.32
(1,321)	1:25:A:PHE:HZ	1:30:A:ASN:H	18	0.32	0.13	0.28
(1,1038)	1:119:A:ARG:HA	1:121:A:ASP:H	18	0.18	0.04	0.19
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG21	17	0.63	0.44	0.49
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG22	17	0.63	0.44	0.49
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG23	17	0.63	0.44	0.49
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG11	17	0.59	0.19	0.66
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG12	17	0.59	0.19	0.66
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG13	17	0.59	0.19	0.66
(1,1024)	1:118:A:ALA:HA	1:119:A:ARG:HE	17	0.53	0.04	0.54
(1,133)	1:20:A:GLY:H	1:21:A:ARG:HB2	17	0.47	0.04	0.47
(1,1434)	1:161:A:ARG:HD2	1:163:A:GLU:H	17	0.47	0.08	0.5
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD11	17	0.46	0.13	0.5
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD12	17	0.46	0.13	0.5
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD13	17	0.46	0.13	0.5
(1,1015)	1:116:A:ALA:HB1	1:120:A:GLY:H	17	0.35	0.11	0.36
(1,1015)	1:116:A:ALA:HB2	1:120:A:GLY:H	17	0.35	0.11	0.36
(1,1015)	1:116:A:ALA:HB3	1:120:A:GLY:H	17	0.35	0.11	0.36
(1,862)	1:101:A:GLU:HG2	1:102:A:ASP:H	17	0.35	0.11	0.39
(1,302)	1:27:A:HIS:HD2	1:28:A:ILE:H	17	0.32	0.12	0.33
(1,959)	1:108:A:SER:HA	1:111:A:SER:H	17	0.31	0.1	0.31
(1,1011)	1:116:A:ALA:HB1	1:119:A:ARG:H	17	0.27	0.06	0.27
(1,1011)	1:116:A:ALA:HB2	1:119:A:ARG:H	17	0.27	0.06	0.27
(1,1011)	1:116:A:ALA:HB3	1:119:A:ARG:H	17	0.27	0.06	0.27
(1,364)	1:24:A:TYR:HD1	1:33:A:GLN:H	17	0.26	0.1	0.25
(1,364)	1:24:A:TYR:HD2	1:33:A:GLN:H	17	0.26	0.1	0.25
(1,663)	1:82:A:LYS:HB3	1:83:A:GLU:H	17	0.24	0.06	0.24

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG21	17	0.22	0.06	0.2
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG22	17	0.22	0.06	0.2
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG23	17	0.22	0.06	0.2
(1,1259)	1:151:A:PHE:HB2	1:152:A:THR:H	17	0.16	0.04	0.15
(1,752)	1:89:A:ILE:HB	1:91:A:GLY:H	16	0.58	0.03	0.58
(1,148)	1:15:A:MET:HE1	1:22:A:VAL:HA	16	0.56	0.04	0.57
(1,148)	1:15:A:MET:HE2	1:22:A:VAL:HA	16	0.56	0.04	0.57
(1,148)	1:15:A:MET:HE3	1:22:A:VAL:HA	16	0.56	0.04	0.57
(1,637)	1:80:A:ARG:HE	1:85:A:ALA:H	16	0.55	0.13	0.61
(2,113)	1:162:A:THR:H	2:651:B:ILE:HG12	16	0.54	0.17	0.61
(2,113)	1:162:A:THR:H	2:651:B:ILE:HG13	16	0.54	0.17	0.61
(1,785)	1:89:A:ILE:HG21	1:93:A:ILE:H	16	0.54	0.06	0.54
(1,785)	1:89:A:ILE:HG22	1:93:A:ILE:H	16	0.54	0.06	0.54
(1,785)	1:89:A:ILE:HG23	1:93:A:ILE:H	16	0.54	0.06	0.54
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG11	16	0.53	0.17	0.6
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG12	16	0.53	0.17	0.6
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG13	16	0.53	0.17	0.6
(1,1326)	1:89:A:ILE:HG21	1:158:A:ILE:HB	16	0.53	0.06	0.54
(1,1326)	1:89:A:ILE:HG22	1:158:A:ILE:HB	16	0.53	0.06	0.54
(1,1326)	1:89:A:ILE:HG23	1:158:A:ILE:HB	16	0.53	0.06	0.54
(1,204)	1:24:A:TYR:HB2	1:33:A:GLN:HE21	16	0.52	0.13	0.56
(1,1977)	1:89:A:ILE:H	1:89:A:ILE:HG12	16	0.49	0.01	0.49
(1,592)	1:75:A:GLN:HB2	1:77:A:LYS:H	16	0.46	0.12	0.43
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG21	16	0.46	0.16	0.49
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG22	16	0.46	0.16	0.49
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG23	16	0.46	0.16	0.49
(1,591)	1:74:A:ARG:HE	1:75:A:GLN:H	16	0.44	0.15	0.48
(1,1192)	1:141:A:LEU:HD21	1:146:A:MET:H	16	0.4	0.11	0.44
(1,1192)	1:141:A:LEU:HD22	1:146:A:MET:H	16	0.4	0.11	0.44
(1,1192)	1:141:A:LEU:HD23	1:146:A:MET:H	16	0.4	0.11	0.44
(1,648)	1:66:A:GLN:HE22	1:82:A:LYS:HG3	16	0.39	0.14	0.36
(1,176)	1:23:A:TYR:HB3	1:24:A:TYR:HD1	16	0.39	0.14	0.42
(1,176)	1:23:A:TYR:HB3	1:24:A:TYR:HD2	16	0.39	0.14	0.42
(1,11)	1:4:A:GLU:H	1:6:A:LYS:H	16	0.36	0.09	0.36
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG21	16	0.36	0.14	0.41
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG22	16	0.36	0.14	0.41
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG23	16	0.36	0.14	0.41
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG11	16	0.36	0.12	0.4
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG12	16	0.36	0.12	0.4
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG13	16	0.36	0.12	0.4
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG11	16	0.36	0.12	0.4
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG12	16	0.36	0.12	0.4

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG13	16	0.36	0.12	0.4
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG11	16	0.36	0.12	0.4
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG12	16	0.36	0.12	0.4
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG13	16	0.36	0.12	0.4
(1,457)	1:60:A:LEU:HD11	1:108:A:SER:H	16	0.33	0.13	0.3
(1,457)	1:60:A:LEU:HD12	1:108:A:SER:H	16	0.33	0.13	0.3
(1,457)	1:60:A:LEU:HD13	1:108:A:SER:H	16	0.33	0.13	0.3
(1,554)	1:70:A:PRO:HG3	1:71:A:SER:H	16	0.32	0.16	0.34
(1,1913)	1:82:A:LYS:H	1:82:A:LYS:HD2	16	0.28	0.16	0.22
(1,743)	1:89:A:ILE:HG13	1:90:A:ASN:H	16	0.27	0.04	0.26
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB1	16	0.26	0.08	0.26
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB2	16	0.26	0.08	0.26
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB3	16	0.26	0.08	0.26
(1,2056)	1:101:A:GLU:H	1:101:A:GLU:HG2	16	0.25	0.12	0.23
(1,262)	1:25:A:PHE:HE1	1:26:A:ASN:HA	16	0.25	0.1	0.23
(1,262)	1:25:A:PHE:HE2	1:26:A:ASN:HA	16	0.25	0.1	0.23
(1,1382)	1:159:A:ILE:HG12	1:160:A:LEU:H	16	0.23	0.07	0.19
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG21	16	0.22	0.08	0.21
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG22	16	0.22	0.08	0.21
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG23	16	0.22	0.08	0.21
(1,7)	1:3:A:ASP:HA	1:4:A:GLU:H	16	0.22	0.08	0.2
(1,1200)	1:143:A:THR:H	1:144:A:GLY:H	16	0.19	0.05	0.19
(1,1660)	1:32:A:SER:H	1:32:A:SER:HB3	16	0.14	0.01	0.14
(1,834)	1:94:A:GLN:HE21	1:97:A:LYS:HD2	15	0.59	0.09	0.58
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD11	15	0.59	0.18	0.65
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD12	15	0.59	0.18	0.65
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD13	15	0.59	0.18	0.65
(1,2524)	2:647:B:VAL:HG11	2:650:B:ASN:HD22	15	0.56	0.19	0.61
(1,2524)	2:647:B:VAL:HG12	2:650:B:ASN:HD22	15	0.56	0.19	0.61
(1,2524)	2:647:B:VAL:HG13	2:650:B:ASN:HD22	15	0.56	0.19	0.61
(2,97)	1:94:A:GLN:HE21	2:640:B:LEU:HG	15	0.51	0.18	0.51
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB1	15	0.5	0.08	0.53
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB2	15	0.5	0.08	0.53
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB3	15	0.5	0.08	0.53
(2,4)	1:21:A:ARG:HE	1:22:A:VAL:H	15	0.5	0.14	0.49
(1,1193)	1:141:A:LEU:HD11	1:148:A:GLY:H	15	0.48	0.14	0.55
(1,1193)	1:141:A:LEU:HD12	1:148:A:GLY:H	15	0.48	0.14	0.55
(1,1193)	1:141:A:LEU:HD13	1:148:A:GLY:H	15	0.48	0.14	0.55
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE1	15	0.47	0.15	0.53
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE2	15	0.47	0.15	0.53
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE3	15	0.47	0.15	0.53
(1,2591)	1:123:A:GLY:H	2:656:B:PHE:HE1	15	0.42	0.17	0.42

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2591)	1:123:A:GLY:H	2:656:B:PHE:HE2	15	0.42	0.17	0.42
(1,985)	1:61:A:LEU:HD21	1:113:A:CYS:HA	15	0.41	0.14	0.37
(1,985)	1:61:A:LEU:HD22	1:113:A:CYS:HA	15	0.41	0.14	0.37
(1,985)	1:61:A:LEU:HD23	1:113:A:CYS:HA	15	0.41	0.14	0.37
(1,35)	1:9:A:PRO:HG2	1:10:A:GLY:H	15	0.36	0.21	0.5
(3,44)	1:72:A:SER:O	1:75:A:GLN:H	15	0.33	0.08	0.34
(1,888)	1:103:A:PHE:HE1	1:120:A:GLY:H	15	0.33	0.15	0.33
(1,888)	1:103:A:PHE:HE2	1:120:A:GLY:H	15	0.33	0.15	0.33
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG21	15	0.28	0.11	0.29
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG22	15	0.28	0.11	0.29
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG23	15	0.28	0.11	0.29
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB1	15	0.25	0.09	0.24
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB2	15	0.25	0.09	0.24
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB3	15	0.25	0.09	0.24
(1,388)	1:35:A:GLU:HG2	1:36:A:ARG:H	15	0.22	0.08	0.19
(1,1568)	1:21:A:ARG:HB2	1:21:A:ARG:HE	15	0.2	0.08	0.17
(1,318)	1:29:A:THR:H	1:30:A:ASN:HB3	15	0.16	0.05	0.15
(2,110)	1:152:A:THR:HG21	2:661:B:PHE:HB2	14	0.69	0.37	0.64
(2,110)	1:152:A:THR:HG21	2:661:B:PHE:HB3	14	0.69	0.37	0.64
(2,110)	1:152:A:THR:HG22	2:661:B:PHE:HB2	14	0.69	0.37	0.64
(2,110)	1:152:A:THR:HG22	2:661:B:PHE:HB3	14	0.69	0.37	0.64
(2,110)	1:152:A:THR:HG23	2:661:B:PHE:HB2	14	0.69	0.37	0.64
(2,110)	1:152:A:THR:HG23	2:661:B:PHE:HB3	14	0.69	0.37	0.64
(1,2507)	2:643:B:PRO:HA	2:645:B:GLN:H	14	0.6	0.13	0.6
(1,841)	1:97:A:LYS:HB3	1:98:A:SER:H	14	0.51	0.16	0.58
(2,92)	1:58:A:SER:H	2:651:B:ILE:HG12	14	0.45	0.18	0.44
(2,92)	1:58:A:SER:H	2:651:B:ILE:HG13	14	0.45	0.18	0.44
(1,1107)	1:54:A:ARG:HD2	1:126:A:SER:HA	14	0.44	0.13	0.5
(1,541)	1:67:A:SER:HB3	1:70:A:PRO:HA	14	0.41	0.1	0.46
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB1	14	0.41	0.15	0.45
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB2	14	0.41	0.15	0.45
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB3	14	0.41	0.15	0.45
(1,1212)	1:146:A:MET:HG2	1:160:A:LEU:HG	14	0.37	0.15	0.32
(1,1311)	1:152:A:THR:HG21	1:157:A:HIS:H	14	0.36	0.17	0.36
(1,1311)	1:152:A:THR:HG22	1:157:A:HIS:H	14	0.36	0.17	0.36
(1,1311)	1:152:A:THR:HG23	1:157:A:HIS:H	14	0.36	0.17	0.36
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG21	14	0.36	0.13	0.32
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG22	14	0.36	0.13	0.32
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG23	14	0.36	0.13	0.32
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG21	14	0.36	0.13	0.32
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG22	14	0.36	0.13	0.32
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG23	14	0.36	0.13	0.32

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG21	14	0.36	0.13	0.32
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG22	14	0.36	0.13	0.32
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG23	14	0.36	0.13	0.32
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG21	14	0.34	0.11	0.38
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG22	14	0.34	0.11	0.38
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG23	14	0.34	0.11	0.38
(1,1423)	1:55:A:VAL:HB	1:163:A:GLU:H	14	0.34	0.11	0.32
(1,940)	1:106:A:LEU:HG	1:107:A:ALA:H	14	0.3	0.1	0.3
(1,1262)	1:151:A:PHE:H	1:156:A:ILE:HA	14	0.27	0.13	0.22
(1,659)	1:81:A:THR:HA	1:83:A:GLU:H	14	0.24	0.12	0.22
(1,644)	1:81:A:THR:HA	1:84:A:GLU:H	14	0.21	0.12	0.16
(1,2588)	1:122:A:LEU:H	2:656:B:PHE:HE1	13	0.52	0.14	0.57
(1,2588)	1:122:A:LEU:H	2:656:B:PHE:HE2	13	0.52	0.14	0.57
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG21	13	0.49	0.2	0.47
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG22	13	0.49	0.2	0.47
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG23	13	0.49	0.2	0.47
(2,58)	1:152:A:THR:HG21	1:157:A:HIS:HB3	13	0.47	0.15	0.46
(2,58)	1:152:A:THR:HG22	1:157:A:HIS:HB3	13	0.47	0.15	0.46
(2,58)	1:152:A:THR:HG23	1:157:A:HIS:HB3	13	0.47	0.15	0.46
(1,995)	1:108:A:SER:HA	1:116:A:ALA:H	13	0.43	0.14	0.51
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD11	13	0.42	0.13	0.49
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD12	13	0.42	0.13	0.49
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD13	13	0.42	0.13	0.49
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD11	13	0.42	0.13	0.49
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD12	13	0.42	0.13	0.49
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD13	13	0.42	0.13	0.49
(1,564)	1:72:A:SER:H	1:78:A:ILE:HG12	13	0.38	0.13	0.42
(1,2551)	2:652:B:ASP:H	2:654:B:SER:H	13	0.38	0.22	0.37
(1,194)	1:13:A:LYS:HG2	1:24:A:TYR:HA	13	0.36	0.11	0.34
(1,1156)	1:136:A:ASP:HB2	1:137:A:ALA:H	13	0.36	0.08	0.38
(1,1161)	1:136:A:ASP:HB2	1:138:A:SER:H	13	0.34	0.12	0.34
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB1	13	0.34	0.07	0.35
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB2	13	0.34	0.07	0.35
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB3	13	0.34	0.07	0.35
(1,521)	1:64:A:HIS:H	1:66:A:GLN:H	13	0.33	0.08	0.35
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE1	13	0.33	0.14	0.34
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE2	13	0.33	0.14	0.34
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE3	13	0.33	0.14	0.34
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE1	13	0.33	0.14	0.34
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE2	13	0.33	0.14	0.34
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE3	13	0.33	0.14	0.34
(1,52)	1:11:A:TRP:HE1	1:26:A:ASN:HB2	13	0.33	0.11	0.32

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,52)	1:11:A:TRP:HE1	1:26:A:ASN:HB3	13	0.33	0.11	0.32
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD11	13	0.32	0.18	0.34
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD12	13	0.32	0.18	0.34
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD13	13	0.32	0.18	0.34
(1,647)	1:65:A:SER:H	1:82:A:LYS:H	13	0.32	0.15	0.3
(1,1047)	1:119:A:ARG:HD2	1:121:A:ASP:H	13	0.31	0.14	0.28
(1,961)	1:108:A:SER:H	1:119:A:ARG:HG2	13	0.31	0.12	0.33
(1,914)	1:104:A:GLU:H	1:106:A:LEU:HB3	13	0.22	0.07	0.22
(1,189)	1:13:A:LYS:H	1:24:A:TYR:HA	13	0.19	0.06	0.2
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG21	13	0.19	0.07	0.16
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG22	13	0.19	0.07	0.16
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG23	13	0.19	0.07	0.16
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG21	13	0.19	0.07	0.16
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG22	13	0.19	0.07	0.16
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG23	13	0.19	0.07	0.16
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG21	13	0.19	0.07	0.16
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG22	13	0.19	0.07	0.16
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG23	13	0.19	0.07	0.16
(1,1450)	1:4:A:GLU:HA	1:4:A:GLU:HG2	13	0.15	0.04	0.14
(2,71)	2:651:B:ILE:HG21	2:656:B:PHE:H	12	0.69	0.12	0.68
(2,71)	2:651:B:ILE:HG22	2:656:B:PHE:H	12	0.69	0.12	0.68
(2,71)	2:651:B:ILE:HG23	2:656:B:PHE:H	12	0.69	0.12	0.68
(1,593)	1:71:A:SER:HB3	1:77:A:LYS:HA	12	0.52	0.09	0.56
(1,2586)	1:115:A:SER:H	2:659:B:PHE:HE1	12	0.48	0.1	0.5
(1,2586)	1:115:A:SER:H	2:659:B:PHE:HE2	12	0.48	0.1	0.5
(1,2587)	1:115:A:SER:H	2:659:B:PHE:HD1	12	0.47	0.11	0.49
(1,2587)	1:115:A:SER:H	2:659:B:PHE:HD2	12	0.47	0.11	0.49
(2,20)	1:68:A:ARG:H	1:153:A:ASP:HB2	12	0.46	0.16	0.42
(2,20)	1:68:A:ARG:H	1:153:A:ASP:HB3	12	0.46	0.16	0.42
(1,2533)	2:647:B:VAL:H	2:649:B:ARG:H	12	0.45	0.11	0.44
(2,9)	1:53:A:ALA:H	1:54:A:ARG:HD2	12	0.44	0.15	0.46
(1,2584)	1:114:A:SER:H	2:659:B:PHE:HD1	12	0.44	0.12	0.5
(1,2584)	1:114:A:SER:H	2:659:B:PHE:HD2	12	0.44	0.12	0.5
(1,69)	1:7:A:LEU:HD21	1:13:A:LYS:HE2	12	0.39	0.08	0.43
(1,69)	1:7:A:LEU:HD22	1:13:A:LYS:HE2	12	0.39	0.08	0.43
(1,69)	1:7:A:LEU:HD23	1:13:A:LYS:HE2	12	0.39	0.08	0.43
(1,69)	1:7:A:LEU:HD11	1:13:A:LYS:HE2	12	0.39	0.08	0.43
(1,69)	1:7:A:LEU:HD12	1:13:A:LYS:HE2	12	0.39	0.08	0.43
(1,69)	1:7:A:LEU:HD13	1:13:A:LYS:HE2	12	0.39	0.08	0.43
(2,93)	1:93:A:ILE:HD11	2:643:B:PRO:HA	12	0.37	0.2	0.32
(2,93)	1:93:A:ILE:HD12	2:643:B:PRO:HA	12	0.37	0.2	0.32
(2,93)	1:93:A:ILE:HD13	2:643:B:PRO:HA	12	0.37	0.2	0.32

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2582)	1:34:A:TRP:HE1	2:642:B:PRO:HB2	12	0.36	0.15	0.38
(1,2582)	1:34:A:TRP:HE1	2:642:B:PRO:HB3	12	0.36	0.15	0.38
(1,527)	1:66:A:GLN:HG2	1:81:A:THR:HG21	12	0.35	0.14	0.32
(1,527)	1:66:A:GLN:HG2	1:81:A:THR:HG22	12	0.35	0.14	0.32
(1,527)	1:66:A:GLN:HG2	1:81:A:THR:HG23	12	0.35	0.14	0.32
(1,723)	1:86:A:LEU:HD21	1:89:A:ILE:HB	12	0.35	0.11	0.38
(1,723)	1:86:A:LEU:HD22	1:89:A:ILE:HB	12	0.35	0.11	0.38
(1,723)	1:86:A:LEU:HD23	1:89:A:ILE:HB	12	0.35	0.11	0.38
(3,79)	1:105:A:SER:O	1:109:A:GLN:N	12	0.33	0.07	0.34
(1,538)	1:66:A:GLN:HG2	1:67:A:SER:H	12	0.26	0.15	0.25
(1,2046)	1:97:A:LYS:H	1:97:A:LYS:HB2	12	0.26	0.02	0.26
(1,669)	1:84:A:GLU:H	1:87:A:GLU:H	12	0.21	0.07	0.2
(1,108)	1:15:A:MET:H	1:22:A:VAL:HA	12	0.18	0.05	0.18
(1,1453)	1:5:A:GLU:H	1:5:A:GLU:HA	12	0.11	0.01	0.11
(1,1112)	1:126:A:SER:H	1:129:A:GLN:HE21	11	0.52	0.06	0.52
(2,74)	2:656:B:PHE:HB2	2:659:B:PHE:HD1	11	0.46	0.2	0.52
(2,74)	2:656:B:PHE:HB2	2:659:B:PHE:HD2	11	0.46	0.2	0.52
(2,74)	2:656:B:PHE:HB3	2:659:B:PHE:HD1	11	0.46	0.2	0.52
(2,74)	2:656:B:PHE:HB3	2:659:B:PHE:HD2	11	0.46	0.2	0.52
(1,1349)	1:158:A:ILE:H	1:159:A:ILE:HD11	11	0.45	0.1	0.46
(1,1349)	1:158:A:ILE:H	1:159:A:ILE:HD12	11	0.45	0.1	0.46
(1,1349)	1:158:A:ILE:H	1:159:A:ILE:HD13	11	0.45	0.1	0.46
(1,2384)	1:163:A:GLU:H	1:163:A:GLU:HG3	11	0.41	0.05	0.41
(1,1869)	1:75:A:GLN:H	1:75:A:GLN:HE22	11	0.39	0.21	0.38
(1,2526)	2:646:B:GLU:HB2	2:648:B:ILE:H	11	0.38	0.19	0.29
(2,39)	1:55:A:VAL:HG11	1:127:A:ARG:H	11	0.36	0.13	0.38
(2,39)	1:55:A:VAL:HG12	1:127:A:ARG:H	11	0.36	0.13	0.38
(2,39)	1:55:A:VAL:HG13	1:127:A:ARG:H	11	0.36	0.13	0.38
(1,618)	1:78:A:ILE:HA	1:80:A:ARG:H	11	0.35	0.08	0.38
(1,1177)	1:137:A:ALA:HB1	1:141:A:LEU:H	11	0.35	0.14	0.33
(1,1177)	1:137:A:ALA:HB2	1:141:A:LEU:H	11	0.35	0.14	0.33
(1,1177)	1:137:A:ALA:HB3	1:141:A:LEU:H	11	0.35	0.14	0.33
(1,569)	1:73:A:TRP:HE1	1:74:A:ARG:HB2	11	0.34	0.11	0.37
(2,52)	1:141:A:LEU:HD21	1:148:A:GLY:H	11	0.32	0.17	0.26
(2,52)	1:141:A:LEU:HD22	1:148:A:GLY:H	11	0.32	0.17	0.26
(2,52)	1:141:A:LEU:HD23	1:148:A:GLY:H	11	0.32	0.17	0.26
(1,1457)	1:6:A:LYS:H	1:6:A:LYS:HG2	11	0.3	0.07	0.27
(1,436)	1:58:A:SER:H	1:160:A:LEU:HG	11	0.23	0.12	0.22
(1,920)	1:106:A:LEU:HB3	1:108:A:SER:H	11	0.2	0.05	0.18
(2,1)	1:10:A:GLY:H	1:11:A:TRP:HB3	11	0.18	0.11	0.14
(1,277)	1:26:A:ASN:H	1:30:A:ASN:H	11	0.17	0.07	0.13
(1,89)	1:14:A:ARG:H	1:15:A:MET:HA	11	0.17	0.05	0.14

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,199)	1:23:A:TYR:H	1:24:A:TYR:H	11	0.11	0.01	0.11
(1,2045)	1:97:A:LYS:H	1:97:A:LYS:HD2	10	1.08	0.31	1.21
(2,79)	2:659:B:PHE:HE1	2:661:B:PHE:H	10	0.76	0.37	0.62
(2,79)	2:659:B:PHE:HE2	2:661:B:PHE:H	10	0.76	0.37	0.62
(2,75)	2:656:B:PHE:HB2	2:659:B:PHE:HE1	10	0.73	0.17	0.78
(2,75)	2:656:B:PHE:HB2	2:659:B:PHE:HE2	10	0.73	0.17	0.78
(2,75)	2:656:B:PHE:HB3	2:659:B:PHE:HE1	10	0.73	0.17	0.78
(2,75)	2:656:B:PHE:HB3	2:659:B:PHE:HE2	10	0.73	0.17	0.78
(1,830)	1:93:A:ILE:HG21	1:97:A:LYS:HD2	10	0.62	0.06	0.64
(1,830)	1:93:A:ILE:HG22	1:97:A:LYS:HD2	10	0.62	0.06	0.64
(1,830)	1:93:A:ILE:HG23	1:97:A:LYS:HD2	10	0.62	0.06	0.64
(1,572)	1:73:A:TRP:HE1	1:111:A:SER:HB2	10	0.57	0.05	0.58
(1,2520)	2:646:B:GLU:HG3	2:647:B:VAL:H	10	0.49	0.19	0.49
(1,845)	1:97:A:LYS:HD2	1:98:A:SER:H	10	0.48	0.17	0.55
(1,218)	1:12:A:GLU:HB2	1:25:A:PHE:H	10	0.46	0.12	0.5
(1,111)	1:15:A:MET:H	1:23:A:TYR:HD1	10	0.41	0.13	0.42
(1,111)	1:15:A:MET:H	1:23:A:TYR:HD2	10	0.41	0.13	0.42
(1,1051)	1:57:A:CYS:H	1:122:A:LEU:HD21	10	0.4	0.15	0.45
(1,1051)	1:57:A:CYS:H	1:122:A:LEU:HD22	10	0.4	0.15	0.45
(1,1051)	1:57:A:CYS:H	1:122:A:LEU:HD23	10	0.4	0.15	0.45
(1,2598)	1:146:A:MET:HE1	2:642:B:PRO:HB2	10	0.37	0.1	0.38
(1,2598)	1:146:A:MET:HE1	2:642:B:PRO:HB3	10	0.37	0.1	0.38
(1,2598)	1:146:A:MET:HE2	2:642:B:PRO:HB2	10	0.37	0.1	0.38
(1,2598)	1:146:A:MET:HE2	2:642:B:PRO:HB3	10	0.37	0.1	0.38
(1,2598)	1:146:A:MET:HE3	2:642:B:PRO:HB2	10	0.37	0.1	0.38
(1,2598)	1:146:A:MET:HE3	2:642:B:PRO:HB3	10	0.37	0.1	0.38
(2,111)	1:160:A:LEU:H	2:651:B:ILE:HG12	10	0.33	0.17	0.28
(2,111)	1:160:A:LEU:H	2:651:B:ILE:HG13	10	0.33	0.17	0.28
(1,764)	1:88:A:LEU:HA	1:92:A:TYR:H	10	0.28	0.09	0.26
(1,811)	1:94:A:GLN:H	1:96:A:ILE:H	10	0.27	0.08	0.29
(1,735)	1:89:A:ILE:HB	1:158:A:ILE:HD11	10	0.25	0.07	0.22
(1,735)	1:89:A:ILE:HB	1:158:A:ILE:HD12	10	0.25	0.07	0.22
(1,735)	1:89:A:ILE:HB	1:158:A:ILE:HD13	10	0.25	0.07	0.22
(1,1020)	1:116:A:ALA:HA	1:118:A:ALA:H	10	0.22	0.1	0.18
(1,424)	1:56:A:ARG:HE	1:57:A:CYS:H	10	0.2	0.05	0.19
(1,387)	1:35:A:GLU:HB2	1:36:A:ARG:H	10	0.13	0.04	0.12
(1,1611)	1:25:A:PHE:H	1:25:A:PHE:HD1	10	0.12	0.02	0.12
(1,1611)	1:25:A:PHE:H	1:25:A:PHE:HD2	10	0.12	0.02	0.12
(2,70)	2:651:B:ILE:HG21	2:656:B:PHE:HE1	9	0.49	0.23	0.59
(2,70)	2:651:B:ILE:HG21	2:656:B:PHE:HE2	9	0.49	0.23	0.59
(2,70)	2:651:B:ILE:HG22	2:656:B:PHE:HE1	9	0.49	0.23	0.59
(2,70)	2:651:B:ILE:HG22	2:656:B:PHE:HE2	9	0.49	0.23	0.59

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,70)	2:651:B:ILE:HG23	2:656:B:PHE:HE1	9	0.49	0.23	0.59
(2,70)	2:651:B:ILE:HG23	2:656:B:PHE:HE2	9	0.49	0.23	0.59
(1,1306)	1:89:A:ILE:HD11	1:157:A:HIS:HD2	9	0.41	0.16	0.41
(1,1306)	1:89:A:ILE:HD12	1:157:A:HIS:HD2	9	0.41	0.16	0.41
(1,1306)	1:89:A:ILE:HD13	1:157:A:HIS:HD2	9	0.41	0.16	0.41
(1,589)	1:74:A:ARG:H	1:112:A:ASP:HA	9	0.4	0.15	0.51
(1,422)	1:56:A:ARG:HG2	1:162:A:THR:HB	9	0.39	0.16	0.48
(2,82)	2:660:B:SEP:HA	2:661:B:PHE:HD1	9	0.39	0.09	0.38
(2,82)	2:660:B:SEP:HA	2:661:B:PHE:HD2	9	0.39	0.09	0.38
(1,1363)	1:96:A:ILE:HG21	1:160:A:LEU:HD11	9	0.35	0.15	0.38
(1,1363)	1:96:A:ILE:HG21	1:160:A:LEU:HD12	9	0.35	0.15	0.38
(1,1363)	1:96:A:ILE:HG21	1:160:A:LEU:HD13	9	0.35	0.15	0.38
(1,1363)	1:96:A:ILE:HG22	1:160:A:LEU:HD11	9	0.35	0.15	0.38
(1,1363)	1:96:A:ILE:HG22	1:160:A:LEU:HD12	9	0.35	0.15	0.38
(1,1363)	1:96:A:ILE:HG22	1:160:A:LEU:HD13	9	0.35	0.15	0.38
(1,1363)	1:96:A:ILE:HG23	1:160:A:LEU:HD11	9	0.35	0.15	0.38
(1,1363)	1:96:A:ILE:HG23	1:160:A:LEU:HD12	9	0.35	0.15	0.38
(1,1363)	1:96:A:ILE:HG23	1:160:A:LEU:HD13	9	0.35	0.15	0.38
(1,244)	1:11:A:TRP:H	1:26:A:ASN:HB2	9	0.35	0.09	0.33
(1,1348)	1:157:A:HIS:HB2	1:159:A:ILE:HD11	9	0.34	0.16	0.3
(1,1348)	1:157:A:HIS:HB2	1:159:A:ILE:HD12	9	0.34	0.16	0.3
(1,1348)	1:157:A:HIS:HB2	1:159:A:ILE:HD13	9	0.34	0.16	0.3
(1,1348)	1:157:A:HIS:HB3	1:159:A:ILE:HD11	9	0.34	0.16	0.3
(1,1348)	1:157:A:HIS:HB3	1:159:A:ILE:HD12	9	0.34	0.16	0.3
(1,1348)	1:157:A:HIS:HB3	1:159:A:ILE:HD13	9	0.34	0.16	0.3
(1,2523)	2:647:B:VAL:HA	2:649:B:ARG:H	9	0.34	0.11	0.38
(1,1353)	1:57:A:CYS:HB3	1:160:A:LEU:H	9	0.33	0.14	0.3
(1,515)	1:63:A:LYS:H	1:156:A:ILE:H	9	0.33	0.16	0.28
(1,61)	1:11:A:TRP:HA	1:12:A:GLU:HB3	9	0.33	0.08	0.33
(1,1369)	1:104:A:GLU:H	1:160:A:LEU:HD11	9	0.31	0.16	0.25
(1,1369)	1:104:A:GLU:H	1:160:A:LEU:HD12	9	0.31	0.16	0.25
(1,1369)	1:104:A:GLU:H	1:160:A:LEU:HD13	9	0.31	0.16	0.25
(1,2557)	2:654:B:SER:H	2:655:B:GLU:H	9	0.31	0.06	0.33
(1,98)	1:14:A:ARG:H	1:24:A:TYR:H	9	0.22	0.07	0.24
(1,208)	1:24:A:TYR:H	1:34:A:TRP:HB3	9	0.22	0.08	0.19
(3,71)	1:94:A:GLN:O	1:98:A:SER:N	9	0.21	0.07	0.19
(2,86)	1:29:A:THR:HG21	2:647:B:VAL:HA	8	0.63	0.18	0.64
(2,86)	1:29:A:THR:HG22	2:647:B:VAL:HA	8	0.63	0.18	0.64
(2,86)	1:29:A:THR:HG23	2:647:B:VAL:HA	8	0.63	0.18	0.64
(1,2578)	1:29:A:THR:HG21	2:646:B:GLU:HA	8	0.56	0.15	0.58
(1,2578)	1:29:A:THR:HG22	2:646:B:GLU:HA	8	0.56	0.15	0.58
(1,2578)	1:29:A:THR:HG23	2:646:B:GLU:HA	8	0.56	0.15	0.58

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,70)	1:12:A:GLU:HG2	1:13:A:LYS:H	8	0.55	0.02	0.55
(1,2568)	2:658:B:GLY:H	2:659:B:PHE:HD1	8	0.55	0.14	0.52
(1,2568)	2:658:B:GLY:H	2:659:B:PHE:HD2	8	0.55	0.14	0.52
(2,26)	1:94:A:GLN:HE21	1:97:A:LYS:HB3	8	0.52	0.16	0.58
(1,256)	1:23:A:TYR:HE1	1:26:A:ASN:H	8	0.48	0.14	0.51
(1,256)	1:23:A:TYR:HE2	1:26:A:ASN:H	8	0.48	0.14	0.51
(1,747)	1:90:A:ASN:HA	1:158:A:ILE:HD11	8	0.43	0.12	0.42
(1,747)	1:90:A:ASN:HA	1:158:A:ILE:HD12	8	0.43	0.12	0.42
(1,747)	1:90:A:ASN:HA	1:158:A:ILE:HD13	8	0.43	0.12	0.42
(1,1335)	1:57:A:CYS:HA	1:159:A:ILE:HG21	8	0.43	0.15	0.45
(1,1335)	1:57:A:CYS:HA	1:159:A:ILE:HG22	8	0.43	0.15	0.45
(1,1335)	1:57:A:CYS:HA	1:159:A:ILE:HG23	8	0.43	0.15	0.45
(1,671)	1:64:A:HIS:HB2	1:85:A:ALA:H	8	0.38	0.13	0.33
(1,925)	1:60:A:LEU:HG	1:107:A:ALA:H	8	0.37	0.13	0.42
(1,180)	1:23:A:TYR:HD1	1:33:A:GLN:HA	8	0.35	0.14	0.38
(1,180)	1:23:A:TYR:HD2	1:33:A:GLN:HA	8	0.35	0.14	0.38
(1,435)	1:58:A:SER:HA	1:122:A:LEU:HG	8	0.32	0.14	0.26
(1,1052)	1:58:A:SER:HB2	1:122:A:LEU:H	8	0.31	0.13	0.26
(1,363)	1:11:A:TRP:HE3	1:33:A:GLN:H	8	0.26	0.14	0.2
(1,1199)	1:142:A:ARG:HG2	1:143:A:THR:H	8	0.24	0.11	0.22
(1,674)	1:81:A:THR:H	1:85:A:ALA:H	8	0.21	0.08	0.19
(1,2530)	2:648:B:ILE:HD11	2:649:B:ARG:H	8	0.19	0.06	0.2
(1,2530)	2:648:B:ILE:HD12	2:649:B:ARG:H	8	0.19	0.06	0.2
(1,2530)	2:648:B:ILE:HD13	2:649:B:ARG:H	8	0.19	0.06	0.2
(1,2036)	1:96:A:ILE:H	1:96:A:ILE:HD11	8	0.17	0.04	0.18
(1,2036)	1:96:A:ILE:H	1:96:A:ILE:HD12	8	0.17	0.04	0.18
(1,2036)	1:96:A:ILE:H	1:96:A:ILE:HD13	8	0.17	0.04	0.18
(1,391)	1:35:A:GLU:HB3	1:36:A:ARG:H	8	0.15	0.03	0.15
(1,1036)	1:118:A:ALA:HB1	1:119:A:ARG:H	8	0.14	0.03	0.13
(1,1036)	1:118:A:ALA:HB2	1:119:A:ARG:H	8	0.14	0.03	0.13
(1,1036)	1:118:A:ALA:HB3	1:119:A:ARG:H	8	0.14	0.03	0.13
(1,2488)	2:656:B:PHE:HA	2:656:B:PHE:HE1	8	0.12	0.02	0.12
(1,2488)	2:656:B:PHE:HA	2:656:B:PHE:HE2	8	0.12	0.02	0.12
(2,88)	1:34:A:TRP:HE1	2:641:B:TPO:H	7	1.05	0.76	0.68
(2,76)	2:656:B:PHE:HE1	2:659:B:PHE:HE1	7	0.58	0.16	0.63
(2,76)	2:656:B:PHE:HE1	2:659:B:PHE:HE2	7	0.58	0.16	0.63
(2,76)	2:656:B:PHE:HE2	2:659:B:PHE:HE1	7	0.58	0.16	0.63
(2,76)	2:656:B:PHE:HE2	2:659:B:PHE:HE2	7	0.58	0.16	0.63
(1,1057)	1:59:A:HIS:H	1:122:A:LEU:HG	7	0.53	0.04	0.54
(1,138)	1:21:A:ARG:HE	1:34:A:TRP:HH2	7	0.5	0.1	0.52
(1,1303)	1:156:A:ILE:HG21	1:157:A:HIS:HD2	7	0.49	0.12	0.54
(1,1303)	1:156:A:ILE:HG22	1:157:A:HIS:HD2	7	0.49	0.12	0.54

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1303)	1:156:A:ILE:HG23	1:157:A:HIS:HD2	7	0.49	0.12	0.54
(1,1560)	1:18:A:SER:H	1:18:A:SER:HB3	7	0.44	0.02	0.43
(2,102)	1:135:A:GLU:H	2:656:B:PHE:HB2	7	0.42	0.22	0.38
(1,571)	1:73:A:TRP:HE1	1:74:A:ARG:HB3	7	0.39	0.16	0.42
(1,889)	1:103:A:PHE:HE1	1:146:A:MET:HE1	7	0.38	0.19	0.51
(1,889)	1:103:A:PHE:HE1	1:146:A:MET:HE2	7	0.38	0.19	0.51
(1,889)	1:103:A:PHE:HE1	1:146:A:MET:HE3	7	0.38	0.19	0.51
(1,889)	1:103:A:PHE:HE2	1:146:A:MET:HE1	7	0.38	0.19	0.51
(1,889)	1:103:A:PHE:HE2	1:146:A:MET:HE2	7	0.38	0.19	0.51
(1,889)	1:103:A:PHE:HE2	1:146:A:MET:HE3	7	0.38	0.19	0.51
(2,34)	1:59:A:HIS:H	1:122:A:LEU:HB2	7	0.37	0.19	0.42
(2,42)	1:130:A:MET:HB2	1:134:A:PHE:HD1	7	0.37	0.12	0.37
(2,42)	1:130:A:MET:HB2	1:134:A:PHE:HD2	7	0.37	0.12	0.37
(1,1441)	1:162:A:THR:HG21	1:163:A:GLU:HG3	7	0.36	0.19	0.32
(1,1441)	1:162:A:THR:HG22	1:163:A:GLU:HG3	7	0.36	0.19	0.32
(1,1441)	1:162:A:THR:HG23	1:163:A:GLU:HG3	7	0.36	0.19	0.32
(3,9)	1:16:A:SER:O	1:19:A:SER:N	7	0.33	0.09	0.37
(1,129)	1:16:A:SER:HB2	1:21:A:ARG:H	7	0.32	0.12	0.36
(1,1402)	1:143:A:THR:HG21	1:161:A:ARG:HD2	7	0.29	0.16	0.26
(1,1402)	1:143:A:THR:HG22	1:161:A:ARG:HD2	7	0.29	0.16	0.26
(1,1402)	1:143:A:THR:HG23	1:161:A:ARG:HD2	7	0.29	0.16	0.26
(1,1346)	1:148:A:GLY:H	1:159:A:ILE:H	7	0.26	0.1	0.25
(1,28)	1:7:A:LEU:HD21	1:13:A:LYS:HG3	7	0.25	0.11	0.2
(1,28)	1:7:A:LEU:HD22	1:13:A:LYS:HG3	7	0.25	0.11	0.2
(1,28)	1:7:A:LEU:HD23	1:13:A:LYS:HG3	7	0.25	0.11	0.2
(1,654)	1:82:A:LYS:HG2	1:84:A:GLU:H	7	0.22	0.08	0.21
(1,654)	1:82:A:LYS:HG3	1:84:A:GLU:H	7	0.22	0.08	0.21
(1,1703)	1:36:A:ARG:H	1:36:A:ARG:HD2	7	0.19	0.06	0.18
(1,96)	1:14:A:ARG:H	1:23:A:TYR:HD1	7	0.19	0.06	0.18
(1,96)	1:14:A:ARG:H	1:23:A:TYR:HD2	7	0.19	0.06	0.18
(1,619)	1:78:A:ILE:HB	1:80:A:ARG:H	7	0.17	0.05	0.15
(2,94)	1:93:A:ILE:HG21	2:643:B:PRO:HB3	6	0.49	0.16	0.53
(2,94)	1:93:A:ILE:HG22	2:643:B:PRO:HB3	6	0.49	0.16	0.53
(2,94)	1:93:A:ILE:HG23	2:643:B:PRO:HB3	6	0.49	0.16	0.53
(1,2514)	2:646:B:GLU:HA	2:649:B:ARG:H	6	0.48	0.18	0.48
(1,1410)	1:161:A:ARG:HE	1:163:A:GLU:HG2	6	0.43	0.19	0.5
(1,44)	1:8:A:PRO:HB2	1:11:A:TRP:HE1	6	0.42	0.11	0.47
(1,56)	1:11:A:TRP:HE1	1:31:A:ALA:HB1	6	0.42	0.16	0.38
(1,56)	1:11:A:TRP:HE1	1:31:A:ALA:HB2	6	0.42	0.16	0.38
(1,56)	1:11:A:TRP:HE1	1:31:A:ALA:HB3	6	0.42	0.16	0.38
(1,1282)	1:82:A:LYS:HE2	1:156:A:ILE:HD11	6	0.42	0.17	0.49
(1,1282)	1:82:A:LYS:HE2	1:156:A:ILE:HD12	6	0.42	0.17	0.49

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1282)	1:82:A:LYS:HE2	1:156:A:ILE:HD13	6	0.42	0.17	0.49
(1,1208)	1:103:A:PHE:HD1	1:146:A:MET:HB2	6	0.42	0.15	0.49
(1,1208)	1:103:A:PHE:HD2	1:146:A:MET:HB2	6	0.42	0.15	0.49
(1,1299)	1:152:A:THR:H	1:156:A:ILE:HG21	6	0.41	0.11	0.43
(1,1299)	1:152:A:THR:H	1:156:A:ILE:HG22	6	0.41	0.11	0.43
(1,1299)	1:152:A:THR:H	1:156:A:ILE:HG23	6	0.41	0.11	0.43
(1,123)	1:15:A:MET:HE1	1:20:A:GLY:H	6	0.4	0.1	0.45
(1,123)	1:15:A:MET:HE2	1:20:A:GLY:H	6	0.4	0.1	0.45
(1,123)	1:15:A:MET:HE3	1:20:A:GLY:H	6	0.4	0.1	0.45
(1,531)	1:64:A:HIS:HE1	1:67:A:SER:HB2	6	0.4	0.17	0.5
(1,401)	1:54:A:ARG:HD2	1:55:A:VAL:HA	6	0.38	0.15	0.32
(1,2209)	1:131:A:GLN:HA	1:131:A:GLN:HE22	6	0.35	0.06	0.34
(1,1276)	1:63:A:LYS:HA	1:155:A:GLY:HA2	6	0.34	0.14	0.3
(3,35)	1:62:A:VAL:N	1:156:A:ILE:O	6	0.33	0.03	0.34
(1,334)	1:27:A:HIS:HA	1:31:A:ALA:H	6	0.32	0.14	0.32
(1,178)	1:23:A:TYR:HE1	1:33:A:GLN:H	6	0.31	0.17	0.21
(1,178)	1:23:A:TYR:HE2	1:33:A:GLN:H	6	0.31	0.17	0.21
(1,1001)	1:113:A:CYS:H	1:116:A:ALA:HB1	6	0.3	0.14	0.3
(1,1001)	1:113:A:CYS:H	1:116:A:ALA:HB2	6	0.3	0.14	0.3
(1,1001)	1:113:A:CYS:H	1:116:A:ALA:HB3	6	0.3	0.14	0.3
(1,695)	1:86:A:LEU:HD21	1:149:A:PRO:HD3	6	0.29	0.14	0.22
(1,695)	1:86:A:LEU:HD22	1:149:A:PRO:HD3	6	0.29	0.14	0.22
(1,695)	1:86:A:LEU:HD23	1:149:A:PRO:HD3	6	0.29	0.14	0.22
(1,1085)	1:56:A:ARG:HE	1:124:A:ALA:H	6	0.28	0.16	0.3
(1,748)	1:87:A:GLU:HA	1:91:A:GLY:H	6	0.27	0.08	0.26
(1,2597)	1:138:A:SER:H	2:656:B:PHE:HB2	6	0.27	0.12	0.25
(1,1456)	1:6:A:LYS:H	1:6:A:LYS:HE2	6	0.26	0.15	0.18
(1,333)	1:25:A:PHE:HA	1:31:A:ALA:H	6	0.24	0.11	0.21
(1,393)	1:53:A:ALA:HB1	1:54:A:ARG:H	6	0.24	0.07	0.23
(1,393)	1:53:A:ALA:HB2	1:54:A:ARG:H	6	0.24	0.07	0.23
(1,393)	1:53:A:ALA:HB3	1:54:A:ARG:H	6	0.24	0.07	0.23
(1,2496)	2:659:B:PHE:H	2:659:B:PHE:HE1	6	0.22	0.05	0.2
(1,2496)	2:659:B:PHE:H	2:659:B:PHE:HE2	6	0.22	0.05	0.2
(1,242)	1:10:A:GLY:H	1:26:A:ASN:HD21	6	0.22	0.08	0.2
(1,681)	1:85:A:ALA:H	1:88:A:LEU:HD11	6	0.22	0.09	0.23
(1,681)	1:85:A:ALA:H	1:88:A:LEU:HD12	6	0.22	0.09	0.23
(1,681)	1:85:A:ALA:H	1:88:A:LEU:HD13	6	0.22	0.09	0.23
(1,772)	1:92:A:TYR:H	1:93:A:ILE:HB	6	0.21	0.06	0.23
(1,1906)	1:81:A:THR:H	1:81:A:THR:HG21	6	0.21	0.04	0.2
(1,1906)	1:81:A:THR:H	1:81:A:THR:HG22	6	0.21	0.04	0.2
(1,1906)	1:81:A:THR:H	1:81:A:THR:HG23	6	0.21	0.04	0.2
(1,649)	1:66:A:GLN:HE21	1:82:A:LYS:HB2	6	0.2	0.07	0.18

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(3,63)	1:90:A:ASN:O	1:94:A:GLN:N	6	0.2	0.07	0.19
(1,130)	1:16:A:SER:H	1:21:A:ARG:HA	6	0.19	0.05	0.19
(1,854)	1:98:A:SER:H	1:101:A:GLU:H	6	0.19	0.07	0.16
(1,1571)	1:21:A:ARG:H	1:21:A:ARG:HD2	6	0.18	0.1	0.11
(1,843)	1:97:A:LYS:HB2	1:98:A:SER:H	6	0.13	0.03	0.12
(1,469)	1:60:A:LEU:HB2	1:61:A:LEU:H	6	0.13	0.02	0.12
(1,2529)	2:648:B:ILE:HG21	2:649:B:ARG:HD2	5	0.62	0.08	0.61
(1,2529)	2:648:B:ILE:HG22	2:649:B:ARG:HD2	5	0.62	0.08	0.61
(1,2529)	2:648:B:ILE:HG23	2:649:B:ARG:HD2	5	0.62	0.08	0.61
(2,66)	2:645:B:GLN:H	2:648:B:ILE:H	5	0.6	0.17	0.56
(2,5)	1:23:A:TYR:H	1:34:A:TRP:HZ3	5	0.55	0.13	0.61
(2,90)	1:56:A:ARG:H	2:651:B:ILE:HG12	5	0.54	0.14	0.59
(2,90)	1:56:A:ARG:H	2:651:B:ILE:HG13	5	0.54	0.14	0.59
(1,1504)	1:13:A:LYS:H	1:13:A:LYS:HE2	5	0.51	0.03	0.52
(1,1313)	1:156:A:ILE:HA	1:157:A:HIS:HD2	5	0.51	0.06	0.51
(1,1054)	1:59:A:HIS:HD2	1:122:A:LEU:H	5	0.49	0.18	0.59
(1,2513)	2:646:B:GLU:HA	2:649:B:ARG:HD2	5	0.47	0.25	0.5
(1,1184)	1:140:A:ALA:H	1:141:A:LEU:HG	5	0.45	0.24	0.6
(1,1280)	1:64:A:HIS:HD2	1:156:A:ILE:HG12	5	0.43	0.12	0.45
(1,728)	1:89:A:ILE:HD11	1:92:A:TYR:HE1	5	0.4	0.16	0.43
(1,728)	1:89:A:ILE:HD11	1:92:A:TYR:HE2	5	0.4	0.16	0.43
(1,728)	1:89:A:ILE:HD12	1:92:A:TYR:HE1	5	0.4	0.16	0.43
(1,728)	1:89:A:ILE:HD12	1:92:A:TYR:HE2	5	0.4	0.16	0.43
(1,728)	1:89:A:ILE:HD13	1:92:A:TYR:HE1	5	0.4	0.16	0.43
(1,728)	1:89:A:ILE:HD13	1:92:A:TYR:HE2	5	0.4	0.16	0.43
(1,641)	1:65:A:SER:HB2	1:81:A:THR:HG21	5	0.35	0.14	0.3
(1,641)	1:65:A:SER:HB2	1:81:A:THR:HG22	5	0.35	0.14	0.3
(1,641)	1:65:A:SER:HB2	1:81:A:THR:HG23	5	0.35	0.14	0.3
(1,1399)	1:143:A:THR:H	1:161:A:ARG:HD2	5	0.35	0.09	0.37
(1,514)	1:63:A:LYS:HB2	1:70:A:PRO:HA	5	0.29	0.12	0.27
(1,1242)	1:150:A:VAL:HG11	1:157:A:HIS:H	5	0.27	0.11	0.23
(1,1242)	1:150:A:VAL:HG12	1:157:A:HIS:H	5	0.27	0.11	0.23
(1,1242)	1:150:A:VAL:HG13	1:157:A:HIS:H	5	0.27	0.11	0.23
(1,116)	1:16:A:SER:H	1:20:A:GLY:HA2	5	0.27	0.14	0.22
(1,2506)	2:644:B:ASP:H	2:645:B:GLN:HA	5	0.26	0.08	0.3
(1,1141)	1:130:A:MET:HB2	1:134:A:PHE:H	5	0.25	0.1	0.22
(1,2561)	2:655:B:GLU:H	2:656:B:PHE:HD1	5	0.25	0.11	0.19
(1,2561)	2:655:B:GLU:H	2:656:B:PHE:HD2	5	0.25	0.11	0.19
(1,828)	1:96:A:ILE:H	1:146:A:MET:HE1	5	0.24	0.1	0.25
(1,828)	1:96:A:ILE:H	1:146:A:MET:HE2	5	0.24	0.1	0.25
(1,828)	1:96:A:ILE:H	1:146:A:MET:HE3	5	0.24	0.1	0.25
(1,1331)	1:146:A:MET:HG2	1:158:A:ILE:HG21	5	0.23	0.13	0.2

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1331)	1:146:A:MET:HG2	1:158:A:ILE:HG22	5	0.23	0.13	0.2
(1,1331)	1:146:A:MET:HG2	1:158:A:ILE:HG23	5	0.23	0.13	0.2
(1,2517)	2:646:B:GLU:HG2	2:647:B:VAL:H	5	0.21	0.06	0.17
(1,373)	1:34:A:TRP:HD1	1:35:A:GLU:H	5	0.21	0.1	0.16
(3,10)	1:16:A:SER:O	1:19:A:SER:H	5	0.2	0.08	0.21
(1,2572)	1:16:A:SER:HB2	2:641:B:TPO:HG21	5	0.2	0.06	0.18
(1,2572)	1:16:A:SER:HB2	2:641:B:TPO:HG22	5	0.2	0.06	0.18
(1,2572)	1:16:A:SER:HB2	2:641:B:TPO:HG23	5	0.2	0.06	0.18
(1,1178)	1:137:A:ALA:HA	1:141:A:LEU:H	5	0.19	0.05	0.18
(1,799)	1:93:A:ILE:HB	1:146:A:MET:HE1	5	0.19	0.06	0.16
(1,799)	1:93:A:ILE:HB	1:146:A:MET:HE2	5	0.19	0.06	0.16
(1,799)	1:93:A:ILE:HB	1:146:A:MET:HE3	5	0.19	0.06	0.16
(1,278)	1:26:A:ASN:HB2	1:30:A:ASN:H	5	0.19	0.08	0.18
(1,205)	1:24:A:TYR:H	1:33:A:GLN:HG2	5	0.17	0.04	0.15
(1,921)	1:106:A:LEU:H	1:109:A:GLN:H	5	0.17	0.05	0.16
(1,750)	1:88:A:LEU:H	1:91:A:GLY:H	5	0.16	0.03	0.17
(1,378)	1:33:A:GLN:H	1:35:A:GLU:H	5	0.13	0.03	0.13
(1,878)	1:102:A:ASP:H	1:103:A:PHE:H	5	0.12	0.01	0.12
(3,27)	1:56:A:ARG:N	1:163:A:GLU:O	4	0.78	0.42	0.77
(1,833)	1:94:A:GLN:HE21	1:97:A:LYS:HG2	4	0.66	0.02	0.65
(1,1337)	1:59:A:HIS:H	1:159:A:ILE:HG21	4	0.56	0.13	0.62
(1,1337)	1:59:A:HIS:H	1:159:A:ILE:HG22	4	0.56	0.13	0.62
(1,1337)	1:59:A:HIS:H	1:159:A:ILE:HG23	4	0.56	0.13	0.62
(1,2525)	2:645:B:GLN:HE22	2:648:B:ILE:HD11	4	0.55	0.05	0.54
(1,2525)	2:645:B:GLN:HE22	2:648:B:ILE:HD12	4	0.55	0.05	0.54
(1,2525)	2:645:B:GLN:HE22	2:648:B:ILE:HD13	4	0.55	0.05	0.54
(1,840)	1:97:A:LYS:HG2	1:146:A:MET:HE1	4	0.54	0.01	0.54
(1,840)	1:97:A:LYS:HG2	1:146:A:MET:HE2	4	0.54	0.01	0.54
(1,840)	1:97:A:LYS:HG2	1:146:A:MET:HE3	4	0.54	0.01	0.54
(1,814)	1:94:A:GLN:HG2	1:95:A:LYS:H	4	0.53	0.04	0.53
(1,1328)	1:89:A:ILE:HG12	1:158:A:ILE:HB	4	0.52	0.01	0.52
(1,639)	1:65:A:SER:HB3	1:81:A:THR:HG21	4	0.51	0.22	0.58
(1,639)	1:65:A:SER:HB3	1:81:A:THR:HG22	4	0.51	0.22	0.58
(1,639)	1:65:A:SER:HB3	1:81:A:THR:HG23	4	0.51	0.22	0.58
(1,693)	1:86:A:LEU:HD21	1:149:A:PRO:HD2	4	0.47	0.02	0.48
(1,693)	1:86:A:LEU:HD22	1:149:A:PRO:HD2	4	0.47	0.02	0.48
(1,693)	1:86:A:LEU:HD23	1:149:A:PRO:HD2	4	0.47	0.02	0.48
(1,1244)	1:150:A:VAL:HG21	1:157:A:HIS:HB2	4	0.46	0.16	0.5
(1,1244)	1:150:A:VAL:HG21	1:157:A:HIS:HB3	4	0.46	0.16	0.5
(1,1244)	1:150:A:VAL:HG22	1:157:A:HIS:HB2	4	0.46	0.16	0.5
(1,1244)	1:150:A:VAL:HG22	1:157:A:HIS:HB3	4	0.46	0.16	0.5
(1,1244)	1:150:A:VAL:HG23	1:157:A:HIS:HB2	4	0.46	0.16	0.5

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1244)	1:150:A:VAL:HG23	1:157:A:HIS:HB3	4	0.46	0.16	0.5
(1,440)	1:59:A:HIS:H	1:115:A:SER:HB3	4	0.46	0.17	0.53
(1,640)	1:65:A:SER:HB3	1:81:A:THR:HA	4	0.45	0.14	0.43
(1,2593)	1:129:A:GLN:HE21	2:656:B:PHE:HE1	4	0.42	0.19	0.49
(1,2593)	1:129:A:GLN:HE21	2:656:B:PHE:HE2	4	0.42	0.19	0.49
(2,72)	2:653:B:GLN:HA	2:656:B:PHE:HE1	4	0.42	0.21	0.44
(2,72)	2:653:B:GLN:HA	2:656:B:PHE:HE2	4	0.42	0.21	0.44
(1,2022)	1:94:A:GLN:H	1:94:A:GLN:HG2	4	0.4	0.05	0.39
(1,1027)	1:118:A:ALA:HA	1:119:A:ARG:HG2	4	0.4	0.09	0.36
(1,1231)	1:149:A:PRO:HG2	1:150:A:VAL:H	4	0.39	0.16	0.48
(1,1429)	1:143:A:THR:HG21	1:163:A:GLU:HB2	4	0.38	0.09	0.36
(1,1429)	1:143:A:THR:HG22	1:163:A:GLU:HB2	4	0.38	0.09	0.36
(1,1429)	1:143:A:THR:HG23	1:163:A:GLU:HB2	4	0.38	0.09	0.36
(1,2532)	2:648:B:ILE:HG21	2:650:B:ASN:H	4	0.37	0.2	0.37
(1,2532)	2:648:B:ILE:HG22	2:650:B:ASN:H	4	0.37	0.2	0.37
(1,2532)	2:648:B:ILE:HG23	2:650:B:ASN:H	4	0.37	0.2	0.37
(1,1263)	1:151:A:PHE:H	1:156:A:ILE:HG21	4	0.37	0.07	0.39
(1,1263)	1:151:A:PHE:H	1:156:A:ILE:HG22	4	0.37	0.07	0.39
(1,1263)	1:151:A:PHE:H	1:156:A:ILE:HG23	4	0.37	0.07	0.39
(1,181)	1:23:A:TYR:HB2	1:34:A:TRP:HE3	4	0.33	0.16	0.35
(1,1406)	1:147:A:SER:H	1:161:A:ARG:H	4	0.32	0.17	0.3
(1,549)	1:70:A:PRO:HG2	1:71:A:SER:H	4	0.32	0.13	0.32
(1,520)	1:64:A:HIS:HE1	1:66:A:GLN:HG2	4	0.31	0.16	0.28
(1,2510)	2:645:B:GLN:H	2:647:B:VAL:H	4	0.3	0.1	0.28
(1,1428)	1:143:A:THR:HG21	1:163:A:GLU:H	4	0.28	0.14	0.26
(1,1428)	1:143:A:THR:HG22	1:163:A:GLU:H	4	0.28	0.14	0.26
(1,1428)	1:143:A:THR:HG23	1:163:A:GLU:H	4	0.28	0.14	0.26
(1,79)	1:13:A:LYS:H	1:24:A:TYR:HD1	4	0.28	0.13	0.24
(1,79)	1:13:A:LYS:H	1:24:A:TYR:HD2	4	0.28	0.13	0.24
(1,1368)	1:103:A:PHE:HB3	1:160:A:LEU:HD21	4	0.27	0.12	0.24
(1,1368)	1:103:A:PHE:HB3	1:160:A:LEU:HD22	4	0.27	0.12	0.24
(1,1368)	1:103:A:PHE:HB3	1:160:A:LEU:HD23	4	0.27	0.12	0.24
(3,65)	1:91:A:GLY:O	1:95:A:LYS:N	4	0.26	0.06	0.27
(1,103)	1:14:A:ARG:HG2	1:15:A:MET:H	4	0.26	0.03	0.26
(1,1078)	1:122:A:LEU:HG	1:123:A:GLY:H	4	0.25	0.12	0.18
(1,1031)	1:118:A:ALA:HB1	1:121:A:ASP:HB2	4	0.24	0.11	0.18
(1,1031)	1:118:A:ALA:HB2	1:121:A:ASP:HB2	4	0.24	0.11	0.18
(1,1031)	1:118:A:ALA:HB3	1:121:A:ASP:HB2	4	0.24	0.11	0.18
(1,1424)	1:55:A:VAL:HG21	1:163:A:GLU:H	4	0.24	0.04	0.23
(1,1424)	1:55:A:VAL:HG22	1:163:A:GLU:H	4	0.24	0.04	0.23
(1,1424)	1:55:A:VAL:HG23	1:163:A:GLU:H	4	0.24	0.04	0.23
(1,1424)	1:55:A:VAL:HG11	1:163:A:GLU:H	4	0.24	0.04	0.23

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1424)	1:55:A:VAL:HG12	1:163:A:GLU:H	4	0.24	0.04	0.23
(1,1424)	1:55:A:VAL:HG13	1:163:A:GLU:H	4	0.24	0.04	0.23
(1,740)	1:89:A:ILE:HG12	1:90:A:ASN:H	4	0.23	0.03	0.22
(3,45)	1:70:A:PRO:O	1:78:A:ILE:N	4	0.22	0.08	0.2
(3,47)	1:81:A:THR:O	1:85:A:ALA:N	4	0.2	0.04	0.2
(1,121)	1:17:A:ARG:HB2	1:18:A:SER:H	4	0.2	0.14	0.12
(1,978)	1:107:A:ALA:HB1	1:111:A:SER:HA	4	0.2	0.07	0.16
(1,978)	1:107:A:ALA:HB2	1:111:A:SER:HA	4	0.2	0.07	0.16
(1,978)	1:107:A:ALA:HB3	1:111:A:SER:HA	4	0.2	0.07	0.16
(1,737)	1:86:A:LEU:HB3	1:90:A:ASN:H	4	0.19	0.06	0.16
(1,2481)	2:656:B:PHE:H	2:656:B:PHE:HE1	4	0.18	0.02	0.18
(1,2481)	2:656:B:PHE:H	2:656:B:PHE:HE2	4	0.18	0.02	0.18
(1,510)	1:62:A:VAL:HG11	1:156:A:ILE:H	4	0.18	0.05	0.16
(1,510)	1:62:A:VAL:HG12	1:156:A:ILE:H	4	0.18	0.05	0.16
(1,510)	1:62:A:VAL:HG13	1:156:A:ILE:H	4	0.18	0.05	0.16
(1,2383)	1:163:A:GLU:H	1:163:A:GLU:HB2	4	0.15	0.02	0.15
(1,20)	1:7:A:LEU:HD11	1:11:A:TRP:H	4	0.14	0.02	0.13
(1,20)	1:7:A:LEU:HD12	1:11:A:TRP:H	4	0.14	0.02	0.13
(1,20)	1:7:A:LEU:HD13	1:11:A:TRP:H	4	0.14	0.02	0.13
(1,110)	1:15:A:MET:H	1:23:A:TYR:HE1	4	0.12	0.03	0.11
(1,110)	1:15:A:MET:H	1:23:A:TYR:HE2	4	0.12	0.03	0.11
(1,265)	1:26:A:ASN:H	1:27:A:HIS:H	4	0.12	0.02	0.12
(1,165)	1:22:A:VAL:H	1:23:A:TYR:H	4	0.12	0.02	0.11
(1,88)	1:12:A:GLU:HB2	1:14:A:ARG:HE	3	0.66	0.05	0.69
(1,88)	1:12:A:GLU:HB3	1:14:A:ARG:HE	3	0.66	0.05	0.69
(1,606)	1:75:A:GLN:HE22	1:78:A:ILE:HA	3	0.53	0.2	0.62
(1,1392)	1:160:A:LEU:HD11	1:162:A:THR:HG21	3	0.53	0.03	0.51
(1,1392)	1:160:A:LEU:HD11	1:162:A:THR:HG22	3	0.53	0.03	0.51
(1,1392)	1:160:A:LEU:HD11	1:162:A:THR:HG23	3	0.53	0.03	0.51
(1,1392)	1:160:A:LEU:HD12	1:162:A:THR:HG21	3	0.53	0.03	0.51
(1,1392)	1:160:A:LEU:HD12	1:162:A:THR:HG22	3	0.53	0.03	0.51
(1,1392)	1:160:A:LEU:HD12	1:162:A:THR:HG23	3	0.53	0.03	0.51
(1,1392)	1:160:A:LEU:HD13	1:162:A:THR:HG21	3	0.53	0.03	0.51
(1,1392)	1:160:A:LEU:HD13	1:162:A:THR:HG22	3	0.53	0.03	0.51
(1,1392)	1:160:A:LEU:HD13	1:162:A:THR:HG23	3	0.53	0.03	0.51
(1,2596)	1:137:A:ALA:HB1	2:651:B:ILE:HG12	3	0.5	0.18	0.54
(1,2596)	1:137:A:ALA:HB1	2:651:B:ILE:HG13	3	0.5	0.18	0.54
(1,2596)	1:137:A:ALA:HB2	2:651:B:ILE:HG12	3	0.5	0.18	0.54
(1,2596)	1:137:A:ALA:HB2	2:651:B:ILE:HG13	3	0.5	0.18	0.54
(1,2596)	1:137:A:ALA:HB3	2:651:B:ILE:HG12	3	0.5	0.18	0.54
(1,2596)	1:137:A:ALA:HB3	2:651:B:ILE:HG13	3	0.5	0.18	0.54
(3,28)	1:56:A:ARG:H	1:163:A:GLU:O	3	0.49	0.23	0.4

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,224)	1:14:A:ARG:HE	1:25:A:PHE:HB3	3	0.43	0.11	0.39
(1,480)	1:61:A:LEU:HD21	1:156:A:ILE:H	3	0.42	0.15	0.44
(1,480)	1:61:A:LEU:HD22	1:156:A:ILE:H	3	0.42	0.15	0.44
(1,480)	1:61:A:LEU:HD23	1:156:A:ILE:H	3	0.42	0.15	0.44
(1,384)	1:7:A:LEU:HD21	1:36:A:ARG:HA	3	0.41	0.21	0.55
(1,384)	1:7:A:LEU:HD22	1:36:A:ARG:HA	3	0.41	0.21	0.55
(1,384)	1:7:A:LEU:HD23	1:36:A:ARG:HA	3	0.41	0.21	0.55
(1,16)	1:6:A:LYS:HE2	1:7:A:LEU:H	3	0.41	0.14	0.45
(1,471)	1:61:A:LEU:HD21	1:63:A:LYS:HA	3	0.4	0.1	0.45
(1,471)	1:61:A:LEU:HD22	1:63:A:LYS:HA	3	0.4	0.1	0.45
(1,471)	1:61:A:LEU:HD23	1:63:A:LYS:HA	3	0.4	0.1	0.45
(1,479)	1:61:A:LEU:HD21	1:155:A:GLY:H	3	0.39	0.16	0.3
(1,479)	1:61:A:LEU:HD22	1:155:A:GLY:H	3	0.39	0.16	0.3
(1,479)	1:61:A:LEU:HD23	1:155:A:GLY:H	3	0.39	0.16	0.3
(2,55)	1:150:A:VAL:HG21	1:158:A:ILE:HA	3	0.38	0.17	0.31
(2,55)	1:150:A:VAL:HG22	1:158:A:ILE:HA	3	0.38	0.17	0.31
(2,55)	1:150:A:VAL:HG23	1:158:A:ILE:HA	3	0.38	0.17	0.31
(1,844)	1:97:A:LYS:HG2	1:98:A:SER:H	3	0.37	0.16	0.47
(2,68)	2:649:B:ARG:HD2	2:650:B:ASN:H	3	0.37	0.09	0.41
(2,108)	1:140:A:ALA:HB1	2:649:B:ARG:HA	3	0.36	0.2	0.3
(2,108)	1:140:A:ALA:HB2	2:649:B:ARG:HA	3	0.36	0.2	0.3
(2,108)	1:140:A:ALA:HB3	2:649:B:ARG:HA	3	0.36	0.2	0.3
(1,917)	1:105:A:SER:HB2	1:106:A:LEU:H	3	0.34	0.06	0.32
(1,385)	1:24:A:TYR:HD1	1:36:A:ARG:H	3	0.33	0.06	0.32
(1,385)	1:24:A:TYR:HD2	1:36:A:ARG:H	3	0.33	0.06	0.32
(1,1143)	1:130:A:MET:HB2	1:135:A:GLU:H	3	0.33	0.12	0.31
(2,107)	1:140:A:ALA:HB1	2:651:B:ILE:HA	3	0.32	0.24	0.2
(2,107)	1:140:A:ALA:HB2	2:651:B:ILE:HA	3	0.32	0.24	0.2
(2,107)	1:140:A:ALA:HB3	2:651:B:ILE:HA	3	0.32	0.24	0.2
(1,87)	1:13:A:LYS:HG3	1:14:A:ARG:H	3	0.32	0.21	0.21
(3,25)	1:55:A:VAL:N	1:125:A:PHE:O	3	0.3	0.05	0.31
(1,211)	1:24:A:TYR:HE1	1:36:A:ARG:HD2	3	0.29	0.09	0.32
(1,211)	1:24:A:TYR:HE2	1:36:A:ARG:HD2	3	0.29	0.09	0.32
(1,576)	1:73:A:TRP:HE1	1:115:A:SER:H	3	0.29	0.07	0.28
(1,1910)	1:82:A:LYS:H	1:82:A:LYS:HE2	3	0.27	0.12	0.2
(1,1152)	1:135:A:GLU:HG2	1:136:A:ASP:H	3	0.27	0.06	0.23
(1,2589)	1:122:A:LEU:HD21	2:656:B:PHE:HE1	3	0.27	0.11	0.29
(1,2589)	1:122:A:LEU:HD21	2:656:B:PHE:HE2	3	0.27	0.11	0.29
(1,2589)	1:122:A:LEU:HD22	2:656:B:PHE:HE1	3	0.27	0.11	0.29
(1,2589)	1:122:A:LEU:HD22	2:656:B:PHE:HE2	3	0.27	0.11	0.29
(1,2589)	1:122:A:LEU:HD23	2:656:B:PHE:HE1	3	0.27	0.11	0.29
(1,2589)	1:122:A:LEU:HD23	2:656:B:PHE:HE2	3	0.27	0.11	0.29

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,362)	1:11:A:TRP:HH2	1:33:A:GLN:HE21	3	0.27	0.1	0.22
(1,923)	1:106:A:LEU:HA	1:110:A:PHE:H	3	0.25	0.13	0.2
(1,1330)	1:92:A:TYR:HD1	1:158:A:ILE:HG21	3	0.25	0.07	0.29
(1,1330)	1:92:A:TYR:HD1	1:158:A:ILE:HG22	3	0.25	0.07	0.29
(1,1330)	1:92:A:TYR:HD1	1:158:A:ILE:HG23	3	0.25	0.07	0.29
(1,1330)	1:92:A:TYR:HD2	1:158:A:ILE:HG21	3	0.25	0.07	0.29
(1,1330)	1:92:A:TYR:HD2	1:158:A:ILE:HG22	3	0.25	0.07	0.29
(1,1330)	1:92:A:TYR:HD2	1:158:A:ILE:HG23	3	0.25	0.07	0.29
(1,2527)	2:646:B:GLU:H	2:648:B:ILE:H	3	0.24	0.12	0.21
(1,354)	1:24:A:TYR:H	1:32:A:SER:HB3	3	0.24	0.1	0.29
(1,634)	1:80:A:ARG:HB2	1:81:A:THR:H	3	0.23	0.07	0.21
(1,17)	1:6:A:LYS:HB3	1:7:A:LEU:H	3	0.23	0.05	0.2
(1,1700)	1:36:A:ARG:H	1:36:A:ARG:HG2	3	0.22	0.06	0.18
(1,751)	1:89:A:ILE:HG21	1:91:A:GLY:H	3	0.19	0.03	0.17
(1,751)	1:89:A:ILE:HG22	1:91:A:GLY:H	3	0.19	0.03	0.17
(1,751)	1:89:A:ILE:HG23	1:91:A:GLY:H	3	0.19	0.03	0.17
(1,998)	1:111:A:SER:H	1:116:A:ALA:HB1	3	0.19	0.09	0.14
(1,998)	1:111:A:SER:H	1:116:A:ALA:HB2	3	0.19	0.09	0.14
(1,998)	1:111:A:SER:H	1:116:A:ALA:HB3	3	0.19	0.09	0.14
(1,692)	1:86:A:LEU:HG	1:90:A:ASN:HD22	3	0.18	0.04	0.16
(1,1384)	1:159:A:ILE:HD11	1:160:A:LEU:H	3	0.17	0.0	0.17
(1,1384)	1:159:A:ILE:HD12	1:160:A:LEU:H	3	0.17	0.0	0.17
(1,1384)	1:159:A:ILE:HD13	1:160:A:LEU:H	3	0.17	0.0	0.17
(1,143)	1:15:A:MET:HA	1:22:A:VAL:H	3	0.16	0.03	0.18
(1,523)	1:64:A:HIS:HE1	1:66:A:GLN:H	3	0.16	0.05	0.13
(1,2386)	1:163:A:GLU:H	1:163:A:GLU:HG2	3	0.16	0.05	0.15
(1,383)	1:34:A:TRP:H	1:35:A:GLU:HB3	3	0.16	0.02	0.16
(1,367)	1:24:A:TYR:HD1	1:34:A:TRP:H	3	0.15	0.03	0.16
(1,367)	1:24:A:TYR:HD2	1:34:A:TRP:H	3	0.15	0.03	0.16
(1,805)	1:93:A:ILE:HG21	1:94:A:GLN:H	3	0.14	0.03	0.15
(1,805)	1:93:A:ILE:HG22	1:94:A:GLN:H	3	0.14	0.03	0.15
(1,805)	1:93:A:ILE:HG23	1:94:A:GLN:H	3	0.14	0.03	0.15
(1,2074)	1:104:A:GLU:H	1:104:A:GLU:HG2	3	0.14	0.05	0.11
(1,1324)	1:89:A:ILE:HA	1:158:A:ILE:HG21	3	0.13	0.02	0.13
(1,1324)	1:89:A:ILE:HA	1:158:A:ILE:HG22	3	0.13	0.02	0.13
(1,1324)	1:89:A:ILE:HA	1:158:A:ILE:HG23	3	0.13	0.02	0.13
(1,2466)	2:651:B:ILE:H	2:651:B:ILE:HD11	3	0.13	0.03	0.12
(1,2466)	2:651:B:ILE:H	2:651:B:ILE:HD12	3	0.13	0.03	0.12
(1,2466)	2:651:B:ILE:H	2:651:B:ILE:HD13	3	0.13	0.03	0.12
(1,926)	1:60:A:LEU:HD11	1:107:A:ALA:H	3	0.13	0.02	0.11
(1,926)	1:60:A:LEU:HD12	1:107:A:ALA:H	3	0.13	0.02	0.11
(1,926)	1:60:A:LEU:HD13	1:107:A:ALA:H	3	0.13	0.02	0.11

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1547)	1:15:A:MET:H	1:15:A:MET:HB2	3	0.12	0.02	0.12
(1,586)	1:73:A:TRP:HB3	1:74:A:ARG:H	3	0.12	0.01	0.11
(4,1958)	1:75:A:GLN:HB2	1:75:A:GLN:HE21	3	0.11	0.0	0.11
(4,1958)	1:75:A:GLN:HB2	1:75:A:GLN:HE22	3	0.11	0.0	0.11
(1,897)	1:104:A:GLU:HG2	1:108:A:SER:H	2	0.72	0.0	0.72
(1,2580)	1:34:A:TRP:HE1	2:641:B:TPO:HG21	2	0.68	0.44	0.68
(1,2580)	1:34:A:TRP:HE1	2:641:B:TPO:HG22	2	0.68	0.44	0.68
(1,2580)	1:34:A:TRP:HE1	2:641:B:TPO:HG23	2	0.68	0.44	0.68
(1,1376)	1:146:A:MET:HE1	1:160:A:LEU:HD21	2	0.48	0.01	0.48
(1,1376)	1:146:A:MET:HE1	1:160:A:LEU:HD22	2	0.48	0.01	0.48
(1,1376)	1:146:A:MET:HE1	1:160:A:LEU:HD23	2	0.48	0.01	0.48
(1,1376)	1:146:A:MET:HE2	1:160:A:LEU:HD21	2	0.48	0.01	0.48
(1,1376)	1:146:A:MET:HE2	1:160:A:LEU:HD22	2	0.48	0.01	0.48
(1,1376)	1:146:A:MET:HE2	1:160:A:LEU:HD23	2	0.48	0.01	0.48
(1,1376)	1:146:A:MET:HE3	1:160:A:LEU:HD21	2	0.48	0.01	0.48
(1,1376)	1:146:A:MET:HE3	1:160:A:LEU:HD22	2	0.48	0.01	0.48
(1,1376)	1:146:A:MET:HE3	1:160:A:LEU:HD23	2	0.48	0.01	0.48
(1,1370)	1:144:A:GLY:H	1:160:A:LEU:HD21	2	0.48	0.01	0.48
(1,1370)	1:144:A:GLY:H	1:160:A:LEU:HD22	2	0.48	0.01	0.48
(1,1370)	1:144:A:GLY:H	1:160:A:LEU:HD23	2	0.48	0.01	0.48
(1,608)	1:75:A:GLN:HE22	1:78:A:ILE:HD11	2	0.45	0.12	0.45
(1,608)	1:75:A:GLN:HE22	1:78:A:ILE:HD12	2	0.45	0.12	0.45
(1,608)	1:75:A:GLN:HE22	1:78:A:ILE:HD13	2	0.45	0.12	0.45
(1,612)	1:75:A:GLN:HE21	1:78:A:ILE:HA	2	0.45	0.14	0.45
(1,646)	1:81:A:THR:HG21	1:84:A:GLU:HB2	2	0.43	0.1	0.43
(1,646)	1:81:A:THR:HG22	1:84:A:GLU:HB2	2	0.43	0.1	0.43
(1,646)	1:81:A:THR:HG23	1:84:A:GLU:HB2	2	0.43	0.1	0.43
(1,2553)	2:651:B:ILE:HG21	2:653:B:GLN:HE21	2	0.43	0.15	0.43
(1,2553)	2:651:B:ILE:HG21	2:653:B:GLN:HE22	2	0.43	0.15	0.43
(1,2553)	2:651:B:ILE:HG22	2:653:B:GLN:HE21	2	0.43	0.15	0.43
(1,2553)	2:651:B:ILE:HG22	2:653:B:GLN:HE22	2	0.43	0.15	0.43
(1,2553)	2:651:B:ILE:HG23	2:653:B:GLN:HE21	2	0.43	0.15	0.43
(1,2553)	2:651:B:ILE:HG23	2:653:B:GLN:HE22	2	0.43	0.15	0.43
(1,1080)	1:54:A:ARG:HE	1:124:A:ALA:HB1	2	0.42	0.13	0.42
(1,1080)	1:54:A:ARG:HE	1:124:A:ALA:HB2	2	0.42	0.13	0.42
(1,1080)	1:54:A:ARG:HE	1:124:A:ALA:HB3	2	0.42	0.13	0.42
(1,2538)	2:649:B:ARG:H	2:650:B:ASN:HD21	2	0.41	0.19	0.41
(2,101)	1:129:A:GLN:HE21	2:657:B:GLU:HB2	2	0.4	0.24	0.4
(2,101)	1:129:A:GLN:HE21	2:657:B:GLU:HB3	2	0.4	0.24	0.4
(1,414)	1:56:A:ARG:H	1:124:A:ALA:HB1	2	0.4	0.04	0.4
(1,414)	1:56:A:ARG:H	1:124:A:ALA:HB2	2	0.4	0.04	0.4
(1,414)	1:56:A:ARG:H	1:124:A:ALA:HB3	2	0.4	0.04	0.4

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2590)	1:122:A:LEU:HD21	2:656:B:PHE:HD1	2	0.38	0.04	0.38
(1,2590)	1:122:A:LEU:HD21	2:656:B:PHE:HD2	2	0.38	0.04	0.38
(1,2590)	1:122:A:LEU:HD22	2:656:B:PHE:HD1	2	0.38	0.04	0.38
(1,2590)	1:122:A:LEU:HD22	2:656:B:PHE:HD2	2	0.38	0.04	0.38
(1,2590)	1:122:A:LEU:HD23	2:656:B:PHE:HD1	2	0.38	0.04	0.38
(1,2590)	1:122:A:LEU:HD23	2:656:B:PHE:HD2	2	0.38	0.04	0.38
(3,33)	1:60:A:LEU:N	1:158:A:ILE:O	2	0.38	0.01	0.38
(1,1378)	1:147:A:SER:H	1:160:A:LEU:H	2	0.38	0.19	0.38
(1,305)	1:27:A:HIS:HD2	1:28:A:ILE:HD11	2	0.36	0.12	0.36
(1,305)	1:27:A:HIS:HD2	1:28:A:ILE:HD12	2	0.36	0.12	0.36
(1,305)	1:27:A:HIS:HD2	1:28:A:ILE:HD13	2	0.36	0.12	0.36
(1,1355)	1:57:A:CYS:HB2	1:160:A:LEU:H	2	0.36	0.16	0.36
(2,91)	1:57:A:CYS:H	2:651:B:ILE:HG12	2	0.36	0.26	0.36
(2,91)	1:57:A:CYS:H	2:651:B:ILE:HG13	2	0.36	0.26	0.36
(1,125)	1:15:A:MET:HA	1:21:A:ARG:H	2	0.34	0.22	0.34
(1,2251)	1:141:A:LEU:H	1:141:A:LEU:HG	2	0.32	0.01	0.32
(1,188)	1:13:A:LYS:HG2	1:24:A:TYR:HE1	2	0.32	0.14	0.32
(1,188)	1:13:A:LYS:HG2	1:24:A:TYR:HE2	2	0.32	0.14	0.32
(1,1412)	1:56:A:ARG:HB2	1:162:A:THR:HG21	2	0.32	0.22	0.32
(1,1412)	1:56:A:ARG:HB2	1:162:A:THR:HG22	2	0.32	0.22	0.32
(1,1412)	1:56:A:ARG:HB2	1:162:A:THR:HG23	2	0.32	0.22	0.32
(1,901)	1:103:A:PHE:H	1:105:A:SER:H	2	0.3	0.01	0.3
(1,1435)	1:161:A:ARG:HG3	1:163:A:GLU:H	2	0.3	0.2	0.3
(1,1403)	1:144:A:GLY:H	1:161:A:ARG:HG2	2	0.3	0.1	0.3
(1,1525)	1:14:A:ARG:H	1:14:A:ARG:HE	2	0.3	0.1	0.3
(1,1309)	1:150:A:VAL:HB	1:157:A:HIS:H	2	0.3	0.15	0.3
(1,1000)	1:113:A:CYS:H	1:116:A:ALA:H	2	0.29	0.07	0.29
(1,475)	1:61:A:LEU:HD11	1:113:A:CYS:H	2	0.29	0.11	0.29
(1,475)	1:61:A:LEU:HD12	1:113:A:CYS:H	2	0.29	0.11	0.29
(1,475)	1:61:A:LEU:HD13	1:113:A:CYS:H	2	0.29	0.11	0.29
(1,475)	1:61:A:LEU:HD21	1:113:A:CYS:H	2	0.29	0.11	0.29
(1,475)	1:61:A:LEU:HD22	1:113:A:CYS:H	2	0.29	0.11	0.29
(1,475)	1:61:A:LEU:HD23	1:113:A:CYS:H	2	0.29	0.11	0.29
(1,2250)	1:141:A:LEU:H	1:141:A:LEU:HD21	2	0.29	0.0	0.29
(1,2250)	1:141:A:LEU:H	1:141:A:LEU:HD22	2	0.29	0.0	0.29
(1,2250)	1:141:A:LEU:H	1:141:A:LEU:HD23	2	0.29	0.0	0.29
(1,2250)	1:141:A:LEU:H	1:141:A:LEU:HD11	2	0.29	0.0	0.29
(1,2250)	1:141:A:LEU:H	1:141:A:LEU:HD12	2	0.29	0.0	0.29
(1,2250)	1:141:A:LEU:H	1:141:A:LEU:HD13	2	0.29	0.0	0.29
(2,105)	1:138:A:SER:H	2:656:B:PHE:HD1	2	0.28	0.08	0.28
(2,105)	1:138:A:SER:H	2:656:B:PHE:HD2	2	0.28	0.08	0.28
(1,81)	1:12:A:GLU:H	1:14:A:ARG:H	2	0.26	0.14	0.26

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,21)	1:73:A:TRP:HE1	1:74:A:ARG:HG3	2	0.26	0.05	0.26
(1,1066)	1:122:A:LEU:HD21	1:125:A:PHE:HD1	2	0.26	0.06	0.26
(1,1066)	1:122:A:LEU:HD21	1:125:A:PHE:HD2	2	0.26	0.06	0.26
(1,1066)	1:122:A:LEU:HD22	1:125:A:PHE:HD1	2	0.26	0.06	0.26
(1,1066)	1:122:A:LEU:HD22	1:125:A:PHE:HD2	2	0.26	0.06	0.26
(1,1066)	1:122:A:LEU:HD23	1:125:A:PHE:HD1	2	0.26	0.06	0.26
(1,1066)	1:122:A:LEU:HD23	1:125:A:PHE:HD2	2	0.26	0.06	0.26
(1,1187)	1:140:A:ALA:HB1	1:141:A:LEU:HD21	2	0.24	0.06	0.24
(1,1187)	1:140:A:ALA:HB1	1:141:A:LEU:HD22	2	0.24	0.06	0.24
(1,1187)	1:140:A:ALA:HB1	1:141:A:LEU:HD23	2	0.24	0.06	0.24
(1,1187)	1:140:A:ALA:HB2	1:141:A:LEU:HD21	2	0.24	0.06	0.24
(1,1187)	1:140:A:ALA:HB2	1:141:A:LEU:HD22	2	0.24	0.06	0.24
(1,1187)	1:140:A:ALA:HB2	1:141:A:LEU:HD23	2	0.24	0.06	0.24
(1,1187)	1:140:A:ALA:HB3	1:141:A:LEU:HD21	2	0.24	0.06	0.24
(1,1187)	1:140:A:ALA:HB3	1:141:A:LEU:HD22	2	0.24	0.06	0.24
(1,1187)	1:140:A:ALA:HB3	1:141:A:LEU:HD23	2	0.24	0.06	0.24
(1,223)	1:14:A:ARG:HB2	1:25:A:PHE:H	2	0.24	0.12	0.24
(1,599)	1:70:A:PRO:HB2	1:78:A:ILE:H	2	0.24	0.12	0.24
(3,39)	1:64:A:HIS:O	1:67:A:SER:N	2	0.23	0.05	0.23
(1,540)	1:67:A:SER:HA	1:69:A:ARG:H	2	0.22	0.06	0.22
(3,49)	1:82:A:LYS:O	1:86:A:LEU:N	2	0.22	0.0	0.22
(1,825)	1:96:A:ILE:HD11	1:106:A:LEU:HG	2	0.22	0.04	0.22
(1,825)	1:96:A:ILE:HD12	1:106:A:LEU:HG	2	0.22	0.04	0.22
(1,825)	1:96:A:ILE:HD13	1:106:A:LEU:HG	2	0.22	0.04	0.22
(1,1500)	1:12:A:GLU:H	1:12:A:GLU:HB2	2	0.22	0.02	0.22
(1,2302)	1:151:A:PHE:H	1:151:A:PHE:HE1	2	0.2	0.03	0.2
(1,2302)	1:151:A:PHE:H	1:151:A:PHE:HE2	2	0.2	0.03	0.2
(1,84)	1:13:A:LYS:HG2	1:14:A:ARG:H	2	0.2	0.09	0.2
(1,1029)	1:118:A:ALA:H	1:121:A:ASP:H	2	0.2	0.04	0.2
(1,885)	1:103:A:PHE:HA	1:106:A:LEU:HD11	2	0.19	0.07	0.19
(1,885)	1:103:A:PHE:HA	1:106:A:LEU:HD12	2	0.19	0.07	0.19
(1,885)	1:103:A:PHE:HA	1:106:A:LEU:HD13	2	0.19	0.07	0.19
(1,934)	1:104:A:GLU:HA	1:107:A:ALA:H	2	0.18	0.04	0.18
(3,34)	1:60:A:LEU:H	1:158:A:ILE:O	2	0.18	0.01	0.18
(1,157)	1:16:A:SER:H	1:22:A:VAL:HG11	2	0.18	0.04	0.18
(1,157)	1:16:A:SER:H	1:22:A:VAL:HG12	2	0.18	0.04	0.18
(1,157)	1:16:A:SER:H	1:22:A:VAL:HG13	2	0.18	0.04	0.18
(1,170)	1:16:A:SER:H	1:23:A:TYR:H	2	0.18	0.03	0.18
(1,402)	1:55:A:VAL:HA	1:125:A:PHE:H	2	0.18	0.02	0.18
(1,1190)	1:141:A:LEU:HD21	1:142:A:ARG:HB2	2	0.18	0.03	0.18
(1,1190)	1:141:A:LEU:HD22	1:142:A:ARG:HB2	2	0.18	0.03	0.18
(1,1190)	1:141:A:LEU:HD23	1:142:A:ARG:HB2	2	0.18	0.03	0.18

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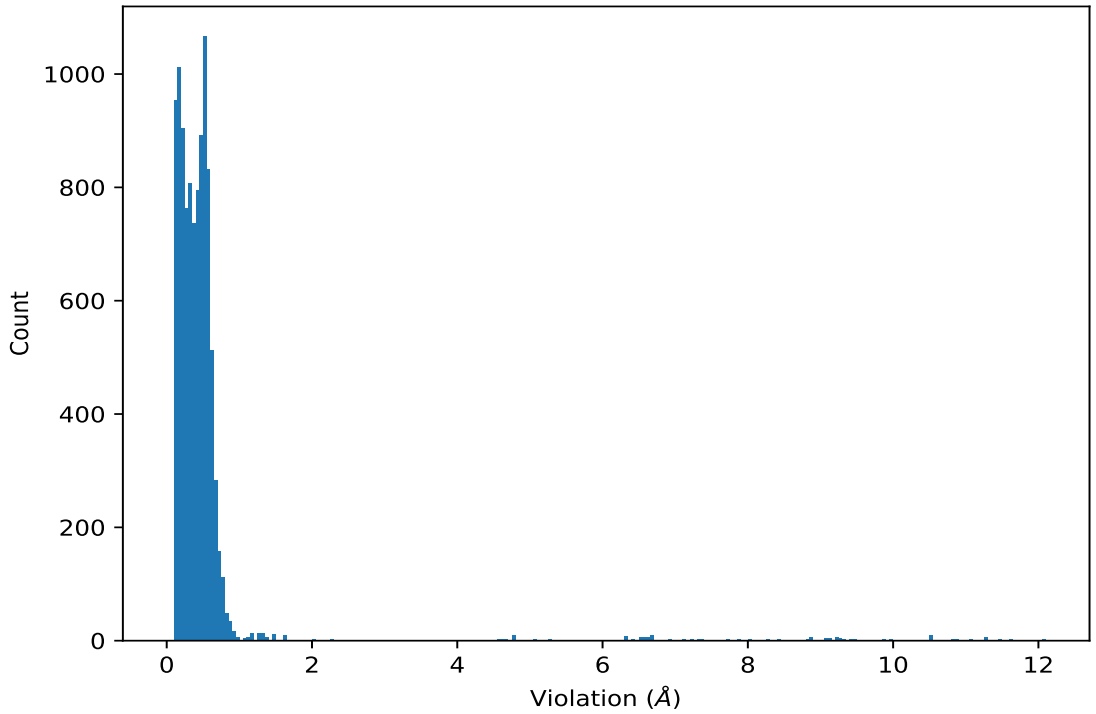
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1431)	1:161:A:ARG:HA	1:163:A:GLU:H	2	0.18	0.06	0.18
(1,857)	1:101:A:GLU:HG2	1:106:A:LEU:HD11	2	0.16	0.04	0.16
(1,857)	1:101:A:GLU:HG2	1:106:A:LEU:HD12	2	0.16	0.04	0.16
(1,857)	1:101:A:GLU:HG2	1:106:A:LEU:HD13	2	0.16	0.04	0.16
(3,46)	1:70:A:PRO:O	1:78:A:ILE:H	2	0.16	0.01	0.16
(1,698)	1:86:A:LEU:HD11	1:87:A:GLU:H	2	0.15	0.02	0.15
(1,698)	1:86:A:LEU:HD12	1:87:A:GLU:H	2	0.15	0.02	0.15
(1,698)	1:86:A:LEU:HD13	1:87:A:GLU:H	2	0.15	0.02	0.15
(3,80)	1:105:A:SER:O	1:109:A:GLN:H	2	0.14	0.0	0.14
(1,2)	1:2:A:ALA:HA	1:3:A:ASP:H	2	0.14	0.02	0.14
(4,2774)	1:26:A:ASN:H	1:31:A:ALA:O	2	0.14	0.02	0.14
(1,807)	1:93:A:ILE:HD11	1:94:A:GLN:H	2	0.13	0.01	0.13
(1,807)	1:93:A:ILE:HD12	1:94:A:GLN:H	2	0.13	0.01	0.13
(1,807)	1:93:A:ILE:HD13	1:94:A:GLN:H	2	0.13	0.01	0.13
(1,317)	1:28:A:ILE:HG12	1:29:A:THR:H	2	0.12	0.01	0.12
(1,1072)	1:121:A:ASP:HB2	1:123:A:GLY:H	2	0.12	0.01	0.12
(1,1235)	1:150:A:VAL:H	1:152:A:THR:HG21	2	0.12	0.02	0.12
(1,1235)	1:150:A:VAL:H	1:152:A:THR:HG22	2	0.12	0.02	0.12
(1,1235)	1:150:A:VAL:H	1:152:A:THR:HG23	2	0.12	0.02	0.12
(1,1026)	1:118:A:ALA:H	1:119:A:ARG:HA	2	0.12	0.0	0.12
(2,67)	2:646:B:GLU:HA	2:647:B:VAL:HG11	2	0.11	0.0	0.11
(2,67)	2:646:B:GLU:HA	2:647:B:VAL:HG12	2	0.11	0.0	0.11
(2,67)	2:646:B:GLU:HA	2:647:B:VAL:HG13	2	0.11	0.0	0.11
(4,2798)	1:72:A:SER:H	1:75:A:GLN:O	2	0.11	0.0	0.11
(1,236)	1:25:A:PHE:HA	1:31:A:ALA:HB1	2	0.11	0.0	0.11
(1,236)	1:25:A:PHE:HA	1:31:A:ALA:HB2	2	0.11	0.0	0.11
(1,236)	1:25:A:PHE:HA	1:31:A:ALA:HB3	2	0.11	0.0	0.11
(1,2083)	1:106:A:LEU:H	1:106:A:LEU:HG	2	0.1	0.0	0.1
(4,2764)	1:16:A:SER:H	1:21:A:ARG:O	2	0.1	0.0	0.1

[1]Number of violated models, [2]Standard deviation

9.5 All violated distance restraints (i)

9.5.1 Histogram : Distribution of distance violations (i)

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



9.5.2 Table : All distance violations (i)

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG21	13	12.07
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG22	13	12.07
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG23	13	12.07
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG21	9	11.6
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG22	9	11.6
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG23	9	11.6
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG21	4	11.49
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG22	4	11.49
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG23	4	11.49
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG21	12	11.26
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG22	12	11.26
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG23	12	11.26
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG21	8	11.25
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG22	8	11.25
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG23	8	11.25
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG21	3	11.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG22	3	11.07
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG23	3	11.07
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG21	7	10.86
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG22	7	10.86
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG23	7	10.86
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG21	1	10.81
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG22	1	10.81
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG23	1	10.81
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG21	5	10.54
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG22	5	10.54
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG23	5	10.54
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG21	14	10.51
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG22	14	10.51
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG23	14	10.51
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG21	19	10.5
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG22	19	10.5
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG23	19	10.5
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG21	6	9.95
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG22	6	9.95
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG23	6	9.95
(1,2595)	1:131:A:GLN:HG2	2:652:B:ASP:HA	11	9.85
(1,2595)	1:131:A:GLN:HG3	2:652:B:ASP:HA	11	9.85
(1,2595)	1:131:A:GLN:HG2	2:652:B:ASP:HA	2	9.46
(1,2595)	1:131:A:GLN:HG3	2:652:B:ASP:HA	2	9.46
(1,2595)	1:131:A:GLN:HG2	2:652:B:ASP:HA	13	9.42
(1,2595)	1:131:A:GLN:HG3	2:652:B:ASP:HA	13	9.42
(1,2595)	1:131:A:GLN:HG2	2:652:B:ASP:HA	3	9.33
(1,2595)	1:131:A:GLN:HG3	2:652:B:ASP:HA	3	9.33
(1,2595)	1:131:A:GLN:HG2	2:652:B:ASP:HA	4	9.26
(1,2595)	1:131:A:GLN:HG3	2:652:B:ASP:HA	4	9.26
(1,2595)	1:131:A:GLN:HG2	2:652:B:ASP:HA	6	9.25
(1,2595)	1:131:A:GLN:HG3	2:652:B:ASP:HA	6	9.25
(1,2595)	1:131:A:GLN:HG2	2:652:B:ASP:HA	1	9.24
(1,2595)	1:131:A:GLN:HG3	2:652:B:ASP:HA	1	9.24
(1,2595)	1:131:A:GLN:HG2	2:652:B:ASP:HA	16	9.24
(1,2595)	1:131:A:GLN:HG3	2:652:B:ASP:HA	16	9.24
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG21	11	9.2
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG22	11	9.2
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG23	11	9.2
(1,2595)	1:131:A:GLN:HG2	2:652:B:ASP:HA	9	9.14
(1,2595)	1:131:A:GLN:HG3	2:652:B:ASP:HA	9	9.14
(1,2595)	1:131:A:GLN:HG2	2:652:B:ASP:HA	7	9.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2595)	1:131:A:GLN:HG3	2:652:B:ASP:HA	7	9.1
(1,2595)	1:131:A:GLN:HG2	2:652:B:ASP:HA	14	9.07
(1,2595)	1:131:A:GLN:HG3	2:652:B:ASP:HA	14	9.07
(1,2595)	1:131:A:GLN:HG2	2:652:B:ASP:HA	5	9.05
(1,2595)	1:131:A:GLN:HG3	2:652:B:ASP:HA	5	9.05
(1,2595)	1:131:A:GLN:HG2	2:652:B:ASP:HA	15	8.88
(1,2595)	1:131:A:GLN:HG3	2:652:B:ASP:HA	15	8.88
(1,2595)	1:131:A:GLN:HG2	2:652:B:ASP:HA	12	8.87
(1,2595)	1:131:A:GLN:HG3	2:652:B:ASP:HA	12	8.87
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG21	17	8.86
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG22	17	8.86
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG23	17	8.86
(1,2595)	1:131:A:GLN:HG2	2:652:B:ASP:HA	8	8.84
(1,2595)	1:131:A:GLN:HG3	2:652:B:ASP:HA	8	8.84
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG21	10	8.4
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG22	10	8.4
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG23	10	8.4
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG21	18	8.25
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG22	18	8.25
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG23	18	8.25
(1,2595)	1:131:A:GLN:HG2	2:652:B:ASP:HA	19	8.0
(1,2595)	1:131:A:GLN:HG3	2:652:B:ASP:HA	19	8.0
(1,2595)	1:131:A:GLN:HG2	2:652:B:ASP:HA	17	7.85
(1,2595)	1:131:A:GLN:HG3	2:652:B:ASP:HA	17	7.85
(1,2595)	1:131:A:GLN:HG2	2:652:B:ASP:HA	10	7.74
(1,2595)	1:131:A:GLN:HG3	2:652:B:ASP:HA	10	7.74
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG21	20	7.35
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG22	20	7.35
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG23	20	7.35
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG21	2	7.34
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG22	2	7.34
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG23	2	7.34
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG21	15	7.21
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG22	15	7.21
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG23	15	7.21
(1,2595)	1:131:A:GLN:HG2	2:652:B:ASP:HA	18	7.12
(1,2595)	1:131:A:GLN:HG3	2:652:B:ASP:HA	18	7.12
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD11	4	6.92
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD12	4	6.92
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD13	4	6.92
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG21	16	6.69
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG22	16	6.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG23	16	6.69
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD11	1	6.69
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD12	1	6.69
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD13	1	6.69
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD11	3	6.66
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD12	3	6.66
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD13	3	6.66
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD11	14	6.62
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD12	14	6.62
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD13	14	6.62
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD11	19	6.62
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD12	19	6.62
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD13	19	6.62
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD11	6	6.59
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD12	6	6.59
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD13	6	6.59
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD11	7	6.55
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD12	7	6.55
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD13	7	6.55
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD11	5	6.54
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD12	5	6.54
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD13	5	6.54
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD11	12	6.54
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD12	12	6.54
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD13	12	6.54
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD11	8	6.44
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD12	8	6.44
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD13	8	6.44
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD11	9	6.34
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD12	9	6.34
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD13	9	6.34
(1,2595)	1:131:A:GLN:HG2	2:652:B:ASP:HA	20	6.32
(1,2595)	1:131:A:GLN:HG3	2:652:B:ASP:HA	20	6.32
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD11	18	6.3
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD12	18	6.3
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD13	18	6.3
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD11	15	5.28
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD12	15	5.28
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD13	15	5.28
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD11	16	5.07
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD12	16	5.07
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD13	16	5.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD11	2	4.78
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD12	2	4.78
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD13	2	4.78
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD11	10	4.75
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD12	10	4.75
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD13	10	4.75
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD11	13	4.75
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD12	13	4.75
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD13	13	4.75
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD11	17	4.68
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD12	17	4.68
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD13	17	4.68
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD11	20	4.61
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD12	20	4.61
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD13	20	4.61
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD11	11	4.59
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD12	11	4.59
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD13	11	4.59
(2,88)	1:34:A:TRP:HE1	2:641:B:TPO:H	16	2.68
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG21	18	2.26
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG22	18	2.26
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG23	18	2.26
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG21	16	2.0
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG22	16	2.0
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG23	16	2.0
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG21	19	1.63
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG22	19	1.63
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG23	19	1.63
(2,88)	1:34:A:TRP:HE1	2:641:B:TPO:H	12	1.61
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG21	16	1.61
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG22	16	1.61
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG23	16	1.61
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG21	18	1.61
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG22	18	1.61
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG23	18	1.61
(2,110)	1:152:A:THR:HG21	2:661:B:PHE:HB2	9	1.48
(2,110)	1:152:A:THR:HG21	2:661:B:PHE:HB3	9	1.48
(2,110)	1:152:A:THR:HG22	2:661:B:PHE:HB2	9	1.48
(2,110)	1:152:A:THR:HG22	2:661:B:PHE:HB3	9	1.48
(2,110)	1:152:A:THR:HG23	2:661:B:PHE:HB2	9	1.48
(2,110)	1:152:A:THR:HG23	2:661:B:PHE:HB3	9	1.48
(2,110)	1:152:A:THR:HG21	2:661:B:PHE:HB2	17	1.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,110)	1:152:A:THR:HG21	2:661:B:PHE:HB3	17	1.45
(2,110)	1:152:A:THR:HG22	2:661:B:PHE:HB2	17	1.45
(2,110)	1:152:A:THR:HG22	2:661:B:PHE:HB3	17	1.45
(2,110)	1:152:A:THR:HG23	2:661:B:PHE:HB2	17	1.45
(2,110)	1:152:A:THR:HG23	2:661:B:PHE:HB3	17	1.45
(1,2045)	1:97:A:LYS:H	1:97:A:LYS:HD2	15	1.39
(3,27)	1:56:A:ARG:N	1:163:A:GLU:O	13	1.38
(2,79)	2:659:B:PHE:HE1	2:661:B:PHE:H	15	1.38
(2,79)	2:659:B:PHE:HE2	2:661:B:PHE:H	15	1.38
(1,2045)	1:97:A:LYS:H	1:97:A:LYS:HD2	17	1.36
(1,2045)	1:97:A:LYS:H	1:97:A:LYS:HD2	13	1.35
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG21	6	1.33
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG22	6	1.33
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG23	6	1.33
(1,2045)	1:97:A:LYS:H	1:97:A:LYS:HD2	18	1.33
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG21	3	1.32
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG22	3	1.32
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG23	3	1.32
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG21	14	1.32
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG22	14	1.32
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG23	14	1.32
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG21	19	1.3
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG22	19	1.3
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG23	19	1.3
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG21	10	1.27
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG22	10	1.27
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG23	10	1.27
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG21	17	1.27
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG22	17	1.27
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG23	17	1.27
(2,79)	2:659:B:PHE:HE1	2:661:B:PHE:H	20	1.27
(2,79)	2:659:B:PHE:HE2	2:661:B:PHE:H	20	1.27
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG21	15	1.25
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG22	15	1.25
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG23	15	1.25
(2,79)	2:659:B:PHE:HE1	2:661:B:PHE:H	17	1.25
(2,79)	2:659:B:PHE:HE2	2:661:B:PHE:H	17	1.25
(1,2045)	1:97:A:LYS:H	1:97:A:LYS:HD2	16	1.24
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG21	8	1.19
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG22	8	1.19
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG23	8	1.19
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG21	4	1.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG22	4	1.18
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG23	4	1.18
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG21	11	1.18
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG22	11	1.18
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG23	11	1.18
(1,2045)	1:97:A:LYS:H	1:97:A:LYS:HD2	10	1.18
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG21	5	1.15
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG22	5	1.15
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG23	5	1.15
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG21	7	1.13
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG22	7	1.13
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG23	7	1.13
(1,2580)	1:34:A:TRP:HE1	2:641:B:TPO:HG21	16	1.13
(1,2580)	1:34:A:TRP:HE1	2:641:B:TPO:HG22	16	1.13
(1,2580)	1:34:A:TRP:HE1	2:641:B:TPO:HG23	16	1.13
(1,2045)	1:97:A:LYS:H	1:97:A:LYS:HD2	20	1.09
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG21	2	1.07
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG22	2	1.07
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG23	2	1.07
(2,71)	2:651:B:ILE:HG21	2:656:B:PHE:H	13	0.98
(2,71)	2:651:B:ILE:HG22	2:656:B:PHE:H	13	0.98
(2,71)	2:651:B:ILE:HG23	2:656:B:PHE:H	13	0.98
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG21	13	0.96
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG22	13	0.96
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG23	13	0.96
(2,110)	1:152:A:THR:HG21	2:661:B:PHE:HB2	12	0.94
(2,110)	1:152:A:THR:HG21	2:661:B:PHE:HB3	12	0.94
(2,110)	1:152:A:THR:HG22	2:661:B:PHE:HB2	12	0.94
(2,110)	1:152:A:THR:HG22	2:661:B:PHE:HB3	12	0.94
(2,110)	1:152:A:THR:HG23	2:661:B:PHE:HB2	12	0.94
(2,110)	1:152:A:THR:HG23	2:661:B:PHE:HB3	12	0.94
(2,75)	2:656:B:PHE:HB2	2:659:B:PHE:HE1	5	0.94
(2,75)	2:656:B:PHE:HB2	2:659:B:PHE:HE2	5	0.94
(2,75)	2:656:B:PHE:HB3	2:659:B:PHE:HE1	5	0.94
(2,75)	2:656:B:PHE:HB3	2:659:B:PHE:HE2	5	0.94
(2,103)	1:137:A:ALA:H	2:656:B:PHE:HB2	2	0.91
(2,103)	1:137:A:ALA:H	2:656:B:PHE:HB2	17	0.91
(2,89)	1:55:A:VAL:H	2:651:B:ILE:HG12	10	0.9
(2,89)	1:55:A:VAL:H	2:651:B:ILE:HG13	10	0.9
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG21	14	0.9
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG22	14	0.9
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG23	14	0.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG21	9	0.89
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG22	9	0.89
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG23	9	0.89
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG21	15	0.89
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG22	15	0.89
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG23	15	0.89
(1,2524)	2:647:B:VAL:HG11	2:650:B:ASN:HD22	13	0.88
(1,2524)	2:647:B:VAL:HG12	2:650:B:ASN:HD22	13	0.88
(1,2524)	2:647:B:VAL:HG13	2:650:B:ASN:HD22	13	0.88
(3,27)	1:56:A:ARG:N	1:163:A:GLU:O	17	0.87
(2,103)	1:137:A:ALA:H	2:656:B:PHE:HB2	15	0.87
(2,86)	1:29:A:THR:HG21	2:647:B:VAL:HA	17	0.87
(2,86)	1:29:A:THR:HG22	2:647:B:VAL:HA	17	0.87
(2,86)	1:29:A:THR:HG23	2:647:B:VAL:HA	17	0.87
(1,2513)	2:646:B:GLU:HA	2:649:B:ARG:HD2	20	0.87
(2,103)	1:137:A:ALA:H	2:656:B:PHE:HB2	20	0.86
(2,86)	1:29:A:THR:HG21	2:647:B:VAL:HA	10	0.86
(2,86)	1:29:A:THR:HG22	2:647:B:VAL:HA	10	0.86
(2,86)	1:29:A:THR:HG23	2:647:B:VAL:HA	10	0.86
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG21	3	0.86
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG22	3	0.86
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG23	3	0.86
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG11	18	0.86
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG12	18	0.86
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG13	18	0.86
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG21	18	0.86
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG22	18	0.86
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG23	18	0.86
(1,443)	1:59:A:HIS:HB2	1:158:A:ILE:H	16	0.86
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG21	8	0.85
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG22	8	0.85
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG23	8	0.85
(2,44)	1:131:A:GLN:HE21	1:153:A:ASP:H	1	0.85
(2,44)	1:131:A:GLN:HE21	1:153:A:ASP:H	7	0.85
(2,103)	1:137:A:ALA:H	2:656:B:PHE:HB2	11	0.84
(2,89)	1:55:A:VAL:H	2:651:B:ILE:HG12	5	0.84
(2,89)	1:55:A:VAL:H	2:651:B:ILE:HG13	5	0.84
(2,88)	1:34:A:TRP:HE1	2:641:B:TPO:H	18	0.84
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG11	20	0.84
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG12	20	0.84
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG13	20	0.84
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG21	20	0.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG22	20	0.84
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG23	20	0.84
(1,296)	1:27:A:HIS:HA	1:30:A:ASN:HD21	16	0.84
(2,66)	2:645:B:GLN:H	2:648:B:ILE:H	20	0.83
(2,44)	1:131:A:GLN:HE21	1:153:A:ASP:H	16	0.83
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG21	5	0.82
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG22	5	0.82
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG23	5	0.82
(2,44)	1:131:A:GLN:HE21	1:153:A:ASP:H	8	0.82
(2,44)	1:131:A:GLN:HE21	1:153:A:ASP:H	14	0.82
(1,2507)	2:643:B:PRO:HA	2:645:B:GLN:H	8	0.82
(1,2033)	1:95:A:LYS:H	1:95:A:LYS:HD2	7	0.82
(1,689)	1:86:A:LEU:HG	1:90:A:ASN:HD21	17	0.82
(3,28)	1:56:A:ARG:H	1:163:A:GLU:O	13	0.81
(2,103)	1:137:A:ALA:H	2:656:B:PHE:HB2	19	0.81
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG11	2	0.81
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG12	2	0.81
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG13	2	0.81
(2,75)	2:656:B:PHE:HB2	2:659:B:PHE:HE1	4	0.81
(2,75)	2:656:B:PHE:HB2	2:659:B:PHE:HE2	4	0.81
(2,75)	2:656:B:PHE:HB3	2:659:B:PHE:HE1	4	0.81
(2,75)	2:656:B:PHE:HB3	2:659:B:PHE:HE2	4	0.81
(1,2568)	2:658:B:GLY:H	2:659:B:PHE:HD1	1	0.81
(1,2568)	2:658:B:GLY:H	2:659:B:PHE:HD2	1	0.81
(1,834)	1:94:A:GLN:HE21	1:97:A:LYS:HD2	12	0.81
(2,97)	1:94:A:GLN:HE21	2:640:B:LEU:HG	10	0.8
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG21	1	0.8
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG22	1	0.8
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG23	1	0.8
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG21	7	0.8
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG22	7	0.8
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG23	7	0.8
(2,79)	2:659:B:PHE:HE1	2:661:B:PHE:H	18	0.8
(2,79)	2:659:B:PHE:HE2	2:661:B:PHE:H	18	0.8
(2,75)	2:656:B:PHE:HB2	2:659:B:PHE:HE1	3	0.8
(2,75)	2:656:B:PHE:HB2	2:659:B:PHE:HE2	3	0.8
(2,75)	2:656:B:PHE:HB3	2:659:B:PHE:HE1	3	0.8
(2,75)	2:656:B:PHE:HB3	2:659:B:PHE:HE2	3	0.8
(1,2520)	2:646:B:GLU:HG3	2:647:B:VAL:H	17	0.8
(1,2507)	2:643:B:PRO:HA	2:645:B:GLN:H	16	0.8
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG21	2	0.79
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG22	2	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG23	2	0.79
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG21	6	0.79
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG22	6	0.79
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG23	6	0.79
(2,75)	2:656:B:PHE:HB2	2:659:B:PHE:HE1	1	0.79
(2,75)	2:656:B:PHE:HB2	2:659:B:PHE:HE2	1	0.79
(2,75)	2:656:B:PHE:HB3	2:659:B:PHE:HE1	1	0.79
(2,75)	2:656:B:PHE:HB3	2:659:B:PHE:HE2	1	0.79
(2,75)	2:656:B:PHE:HB2	2:659:B:PHE:HE1	6	0.79
(2,75)	2:656:B:PHE:HB2	2:659:B:PHE:HE2	6	0.79
(2,75)	2:656:B:PHE:HB3	2:659:B:PHE:HE1	6	0.79
(2,75)	2:656:B:PHE:HB3	2:659:B:PHE:HE2	6	0.79
(2,71)	2:651:B:ILE:HG21	2:656:B:PHE:H	7	0.79
(2,71)	2:651:B:ILE:HG22	2:656:B:PHE:H	7	0.79
(2,71)	2:651:B:ILE:HG23	2:656:B:PHE:H	7	0.79
(2,70)	2:651:B:ILE:HG21	2:656:B:PHE:HE1	13	0.79
(2,70)	2:651:B:ILE:HG21	2:656:B:PHE:HE2	13	0.79
(2,70)	2:651:B:ILE:HG22	2:656:B:PHE:HE1	13	0.79
(2,70)	2:651:B:ILE:HG22	2:656:B:PHE:HE2	13	0.79
(2,70)	2:651:B:ILE:HG23	2:656:B:PHE:HE1	13	0.79
(2,70)	2:651:B:ILE:HG23	2:656:B:PHE:HE2	13	0.79
(2,44)	1:131:A:GLN:HE21	1:153:A:ASP:H	3	0.79
(1,2507)	2:643:B:PRO:HA	2:645:B:GLN:H	19	0.79
(2,113)	1:162:A:THR:H	2:651:B:ILE:HG12	19	0.78
(2,113)	1:162:A:THR:H	2:651:B:ILE:HG13	19	0.78
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG21	4	0.78
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG22	4	0.78
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG23	4	0.78
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG21	17	0.78
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG22	17	0.78
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG23	17	0.78
(2,75)	2:656:B:PHE:HB2	2:659:B:PHE:HE1	8	0.78
(2,75)	2:656:B:PHE:HB2	2:659:B:PHE:HE2	8	0.78
(2,75)	2:656:B:PHE:HB3	2:659:B:PHE:HE1	8	0.78
(2,75)	2:656:B:PHE:HB3	2:659:B:PHE:HE2	8	0.78
(2,71)	2:651:B:ILE:HG21	2:656:B:PHE:H	9	0.78
(2,71)	2:651:B:ILE:HG22	2:656:B:PHE:H	9	0.78
(2,71)	2:651:B:ILE:HG23	2:656:B:PHE:H	9	0.78
(1,296)	1:27:A:HIS:HA	1:30:A:ASN:HD21	6	0.78
(1,296)	1:27:A:HIS:HA	1:30:A:ASN:HD21	18	0.78
(2,110)	1:152:A:THR:HG21	2:661:B:PHE:HB2	3	0.77
(2,110)	1:152:A:THR:HG21	2:661:B:PHE:HB3	3	0.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,110)	1:152:A:THR:HG22	2:661:B:PHE:HB2	3	0.77
(2,110)	1:152:A:THR:HG22	2:661:B:PHE:HB3	3	0.77
(2,110)	1:152:A:THR:HG23	2:661:B:PHE:HB2	3	0.77
(2,110)	1:152:A:THR:HG23	2:661:B:PHE:HB3	3	0.77
(2,103)	1:137:A:ALA:H	2:656:B:PHE:HB2	10	0.77
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD11	13	0.77
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD12	13	0.77
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD13	13	0.77
(2,44)	1:131:A:GLN:HE21	1:153:A:ASP:H	9	0.77
(2,44)	1:131:A:GLN:HE21	1:153:A:ASP:H	11	0.77
(1,296)	1:27:A:HIS:HA	1:30:A:ASN:HD21	3	0.77
(1,296)	1:27:A:HIS:HA	1:30:A:ASN:HD21	5	0.77
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG11	11	0.76
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG12	11	0.76
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG13	11	0.76
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG11	9	0.76
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG12	9	0.76
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG13	9	0.76
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG21	9	0.76
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG22	9	0.76
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG23	9	0.76
(2,76)	2:656:B:PHE:HE1	2:659:B:PHE:HE1	15	0.76
(2,76)	2:656:B:PHE:HE1	2:659:B:PHE:HE2	15	0.76
(2,76)	2:656:B:PHE:HE2	2:659:B:PHE:HE1	15	0.76
(2,76)	2:656:B:PHE:HE2	2:659:B:PHE:HE2	15	0.76
(2,74)	2:656:B:PHE:HB2	2:659:B:PHE:HD1	19	0.76
(2,74)	2:656:B:PHE:HB2	2:659:B:PHE:HD2	19	0.76
(2,74)	2:656:B:PHE:HB3	2:659:B:PHE:HD1	19	0.76
(2,74)	2:656:B:PHE:HB3	2:659:B:PHE:HD2	19	0.76
(2,66)	2:645:B:GLN:H	2:648:B:ILE:H	13	0.76
(1,2578)	1:29:A:THR:HG21	2:646:B:GLU:HA	16	0.76
(1,2578)	1:29:A:THR:HG22	2:646:B:GLU:HA	16	0.76
(1,2578)	1:29:A:THR:HG23	2:646:B:GLU:HA	16	0.76
(1,2516)	2:646:B:GLU:HA	2:647:B:VAL:HG21	13	0.76
(1,2516)	2:646:B:GLU:HA	2:647:B:VAL:HG22	13	0.76
(1,2516)	2:646:B:GLU:HA	2:647:B:VAL:HG23	13	0.76
(1,2514)	2:646:B:GLU:HA	2:649:B:ARG:H	17	0.76
(1,1426)	1:56:A:ARG:HA	1:163:A:GLU:H	11	0.76
(1,296)	1:27:A:HIS:HA	1:30:A:ASN:HD21	12	0.76
(2,110)	1:152:A:THR:HG21	2:661:B:PHE:HB2	4	0.75
(2,110)	1:152:A:THR:HG21	2:661:B:PHE:HB3	4	0.75
(2,110)	1:152:A:THR:HG22	2:661:B:PHE:HB2	4	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,110)	1:152:A:THR:HG22	2:661:B:PHE:HB3	4	0.75
(2,110)	1:152:A:THR:HG23	2:661:B:PHE:HB2	4	0.75
(2,110)	1:152:A:THR:HG23	2:661:B:PHE:HB3	4	0.75
(2,98)	1:124:A:ALA:H	2:656:B:PHE:HE1	8	0.75
(2,98)	1:124:A:ALA:H	2:656:B:PHE:HE2	8	0.75
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG11	20	0.75
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG12	20	0.75
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG13	20	0.75
(2,89)	1:55:A:VAL:H	2:651:B:ILE:HG12	17	0.75
(2,89)	1:55:A:VAL:H	2:651:B:ILE:HG13	17	0.75
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG21	11	0.75
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG22	11	0.75
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG23	11	0.75
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG21	18	0.75
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG22	18	0.75
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG23	18	0.75
(2,44)	1:131:A:GLN:HE21	1:153:A:ASP:H	13	0.75
(1,2529)	2:648:B:ILE:HG21	2:649:B:ARG:HD2	18	0.75
(1,2529)	2:648:B:ILE:HG22	2:649:B:ARG:HD2	18	0.75
(1,2529)	2:648:B:ILE:HG23	2:649:B:ARG:HD2	18	0.75
(1,2524)	2:647:B:VAL:HG11	2:650:B:ASN:HD22	11	0.75
(1,2524)	2:647:B:VAL:HG12	2:650:B:ASN:HD22	11	0.75
(1,2524)	2:647:B:VAL:HG13	2:650:B:ASN:HD22	11	0.75
(1,296)	1:27:A:HIS:HA	1:30:A:ASN:HD21	2	0.75
(1,296)	1:27:A:HIS:HA	1:30:A:ASN:HD21	4	0.75
(1,296)	1:27:A:HIS:HA	1:30:A:ASN:HD21	15	0.75
(2,103)	1:137:A:ALA:H	2:656:B:PHE:HB2	18	0.74
(2,102)	1:135:A:GLU:H	2:656:B:PHE:HB2	20	0.74
(2,98)	1:124:A:ALA:H	2:656:B:PHE:HE1	17	0.74
(2,98)	1:124:A:ALA:H	2:656:B:PHE:HE2	17	0.74
(2,89)	1:55:A:VAL:H	2:651:B:ILE:HG12	15	0.74
(2,89)	1:55:A:VAL:H	2:651:B:ILE:HG13	15	0.74
(2,86)	1:29:A:THR:HG21	2:647:B:VAL:HA	2	0.74
(2,86)	1:29:A:THR:HG22	2:647:B:VAL:HA	2	0.74
(2,86)	1:29:A:THR:HG23	2:647:B:VAL:HA	2	0.74
(2,76)	2:656:B:PHE:HE1	2:659:B:PHE:HE1	11	0.74
(2,76)	2:656:B:PHE:HE1	2:659:B:PHE:HE2	11	0.74
(2,76)	2:656:B:PHE:HE2	2:659:B:PHE:HE1	11	0.74
(2,76)	2:656:B:PHE:HE2	2:659:B:PHE:HE2	11	0.74
(2,75)	2:656:B:PHE:HB2	2:659:B:PHE:HE1	14	0.74
(2,75)	2:656:B:PHE:HB2	2:659:B:PHE:HE2	14	0.74
(2,75)	2:656:B:PHE:HB3	2:659:B:PHE:HE1	14	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,75)	2:656:B:PHE:HB3	2:659:B:PHE:HE2	14	0.74
(2,45)	1:131:A:GLN:HE21	1:152:A:THR:HB	6	0.74
(2,45)	1:131:A:GLN:HE21	1:152:A:THR:HB	9	0.74
(1,1869)	1:75:A:GLN:H	1:75:A:GLN:HE22	13	0.74
(1,1227)	1:89:A:ILE:HG12	1:150:A:VAL:H	4	0.74
(1,1227)	1:89:A:ILE:HG12	1:150:A:VAL:H	11	0.74
(1,1227)	1:89:A:ILE:HG12	1:150:A:VAL:H	16	0.74
(1,296)	1:27:A:HIS:HA	1:30:A:ASN:HD21	10	0.74
(1,204)	1:24:A:TYR:HB2	1:33:A:GLN:HE21	13	0.74
(1,14)	1:6:A:LYS:HG2	1:7:A:LEU:H	18	0.74
(2,113)	1:162:A:THR:H	2:651:B:ILE:HG12	8	0.73
(2,113)	1:162:A:THR:H	2:651:B:ILE:HG13	8	0.73
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD11	9	0.73
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD12	9	0.73
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD13	9	0.73
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD11	15	0.73
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD12	15	0.73
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD13	15	0.73
(2,45)	1:131:A:GLN:HE21	1:152:A:THR:HB	1	0.73
(1,2578)	1:29:A:THR:HG21	2:646:B:GLU:HA	18	0.73
(1,2578)	1:29:A:THR:HG22	2:646:B:GLU:HA	18	0.73
(1,2578)	1:29:A:THR:HG23	2:646:B:GLU:HA	18	0.73
(1,2568)	2:658:B:GLY:H	2:659:B:PHE:HD1	4	0.73
(1,2568)	2:658:B:GLY:H	2:659:B:PHE:HD2	4	0.73
(1,2518)	2:646:B:GLU:H	2:647:B:VAL:HG21	13	0.73
(1,2518)	2:646:B:GLU:H	2:647:B:VAL:HG22	13	0.73
(1,2518)	2:646:B:GLU:H	2:647:B:VAL:HG23	13	0.73
(1,1227)	1:89:A:ILE:HG12	1:150:A:VAL:H	17	0.73
(1,1130)	1:131:A:GLN:HE21	1:153:A:ASP:HB2	18	0.73
(1,1130)	1:131:A:GLN:HE21	1:153:A:ASP:HB3	18	0.73
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG21	15	0.73
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG22	15	0.73
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG23	15	0.73
(1,86)	1:13:A:LYS:HE2	1:14:A:ARG:H	15	0.73
(2,110)	1:152:A:THR:HG21	2:661:B:PHE:HB2	18	0.72
(2,110)	1:152:A:THR:HG21	2:661:B:PHE:HB3	18	0.72
(2,110)	1:152:A:THR:HG22	2:661:B:PHE:HB2	18	0.72
(2,110)	1:152:A:THR:HG22	2:661:B:PHE:HB3	18	0.72
(2,110)	1:152:A:THR:HG23	2:661:B:PHE:HB2	18	0.72
(2,110)	1:152:A:THR:HG23	2:661:B:PHE:HB3	18	0.72
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG21	1	0.72
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG22	1	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG23	1	0.72
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG21	9	0.72
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG22	9	0.72
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG23	9	0.72
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG21	20	0.72
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG22	20	0.72
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG23	20	0.72
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG11	1	0.72
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG12	1	0.72
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG13	1	0.72
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG21	1	0.72
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG22	1	0.72
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG23	1	0.72
(2,75)	2:656:B:PHE:HB2	2:659:B:PHE:HE1	7	0.72
(2,75)	2:656:B:PHE:HB2	2:659:B:PHE:HE2	7	0.72
(2,75)	2:656:B:PHE:HB3	2:659:B:PHE:HE1	7	0.72
(2,75)	2:656:B:PHE:HB3	2:659:B:PHE:HE2	7	0.72
(2,44)	1:131:A:GLN:HE21	1:153:A:ASP:H	17	0.72
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG21	8	0.72
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG22	8	0.72
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG23	8	0.72
(1,2520)	2:646:B:GLU:HG3	2:647:B:VAL:H	11	0.72
(1,2507)	2:643:B:PRO:HA	2:645:B:GLN:H	4	0.72
(1,897)	1:104:A:GLU:HG2	1:108:A:SER:H	10	0.72
(1,897)	1:104:A:GLU:HG2	1:108:A:SER:H	18	0.72
(1,639)	1:65:A:SER:HB3	1:81:A:THR:HG21	20	0.72
(1,639)	1:65:A:SER:HB3	1:81:A:THR:HG22	20	0.72
(1,639)	1:65:A:SER:HB3	1:81:A:THR:HG23	20	0.72
(1,606)	1:75:A:GLN:HE22	1:78:A:ILE:HA	2	0.72
(1,296)	1:27:A:HIS:HA	1:30:A:ASN:HD21	14	0.72
(2,103)	1:137:A:ALA:H	2:656:B:PHE:HB2	5	0.71
(2,98)	1:124:A:ALA:H	2:656:B:PHE:HE1	11	0.71
(2,98)	1:124:A:ALA:H	2:656:B:PHE:HE2	11	0.71
(2,97)	1:94:A:GLN:HE21	2:640:B:LEU:HG	17	0.71
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG11	15	0.71
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG12	15	0.71
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG13	15	0.71
(2,92)	1:58:A:SER:H	2:651:B:ILE:HG12	10	0.71
(2,92)	1:58:A:SER:H	2:651:B:ILE:HG13	10	0.71
(2,89)	1:55:A:VAL:H	2:651:B:ILE:HG12	13	0.71
(2,89)	1:55:A:VAL:H	2:651:B:ILE:HG13	13	0.71
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD11	4	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD12	4	0.71
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD13	4	0.71
(2,71)	2:651:B:ILE:HG21	2:656:B:PHE:H	6	0.71
(2,71)	2:651:B:ILE:HG22	2:656:B:PHE:H	6	0.71
(2,71)	2:651:B:ILE:HG23	2:656:B:PHE:H	6	0.71
(2,45)	1:131:A:GLN:HE21	1:152:A:THR:HB	3	0.71
(2,45)	1:131:A:GLN:HE21	1:152:A:THR:HB	4	0.71
(2,44)	1:131:A:GLN:HE21	1:153:A:ASP:H	4	0.71
(2,44)	1:131:A:GLN:HE21	1:153:A:ASP:H	15	0.71
(2,20)	1:68:A:ARG:H	1:153:A:ASP:HB2	4	0.71
(2,20)	1:68:A:ARG:H	1:153:A:ASP:HB3	4	0.71
(1,2551)	2:652:B:ASP:H	2:654:B:SER:H	9	0.71
(1,1227)	1:89:A:ILE:HG12	1:150:A:VAL:H	18	0.71
(1,1184)	1:140:A:ALA:H	1:141:A:LEU:HG	11	0.71
(1,830)	1:93:A:ILE:HG21	1:97:A:LYS:HD2	8	0.71
(1,830)	1:93:A:ILE:HG22	1:97:A:LYS:HD2	8	0.71
(1,830)	1:93:A:ILE:HG23	1:97:A:LYS:HD2	8	0.71
(1,689)	1:86:A:LEU:HG	1:90:A:ASN:HD21	11	0.71
(1,296)	1:27:A:HIS:HA	1:30:A:ASN:HD21	19	0.71
(1,88)	1:12:A:GLU:HB2	1:14:A:ARG:HE	10	0.71
(1,88)	1:12:A:GLU:HB3	1:14:A:ARG:HE	10	0.71
(1,14)	1:6:A:LYS:HG2	1:7:A:LEU:H	8	0.71
(2,113)	1:162:A:THR:H	2:651:B:ILE:HG12	6	0.7
(2,113)	1:162:A:THR:H	2:651:B:ILE:HG13	6	0.7
(2,106)	1:139:A:PHE:H	2:656:B:PHE:HB2	3	0.7
(2,103)	1:137:A:ALA:H	2:656:B:PHE:HB2	16	0.7
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG11	10	0.7
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG12	10	0.7
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG13	10	0.7
(2,93)	1:93:A:ILE:HD11	2:643:B:PRO:HA	19	0.7
(2,93)	1:93:A:ILE:HD12	2:643:B:PRO:HA	19	0.7
(2,93)	1:93:A:ILE:HD13	2:643:B:PRO:HA	19	0.7
(2,76)	2:656:B:PHE:HE1	2:659:B:PHE:HE1	10	0.7
(2,76)	2:656:B:PHE:HE1	2:659:B:PHE:HE2	10	0.7
(2,76)	2:656:B:PHE:HE2	2:659:B:PHE:HE1	10	0.7
(2,76)	2:656:B:PHE:HE2	2:659:B:PHE:HE2	10	0.7
(2,71)	2:651:B:ILE:HG21	2:656:B:PHE:H	1	0.7
(2,71)	2:651:B:ILE:HG22	2:656:B:PHE:H	1	0.7
(2,71)	2:651:B:ILE:HG23	2:656:B:PHE:H	1	0.7
(2,71)	2:651:B:ILE:HG21	2:656:B:PHE:H	4	0.7
(2,71)	2:651:B:ILE:HG22	2:656:B:PHE:H	4	0.7
(2,71)	2:651:B:ILE:HG23	2:656:B:PHE:H	4	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,45)	1:131:A:GLN:HE21	1:152:A:THR:HB	2	0.7
(2,45)	1:131:A:GLN:HE21	1:152:A:THR:HB	10	0.7
(2,38)	1:126:A:SER:H	1:129:A:GLN:HB2	13	0.7
(1,2588)	1:122:A:LEU:H	2:656:B:PHE:HE1	8	0.7
(1,2588)	1:122:A:LEU:H	2:656:B:PHE:HE2	8	0.7
(1,2526)	2:646:B:GLU:HB2	2:648:B:ILE:H	8	0.7
(1,2045)	1:97:A:LYS:H	1:97:A:LYS:HD2	11	0.7
(1,1227)	1:89:A:ILE:HG12	1:150:A:VAL:H	12	0.7
(1,1227)	1:89:A:ILE:HG12	1:150:A:VAL:H	19	0.7
(1,1109)	1:126:A:SER:HA	1:139:A:PHE:HD1	10	0.7
(1,1109)	1:126:A:SER:HA	1:139:A:PHE:HD2	10	0.7
(1,689)	1:86:A:LEU:HG	1:90:A:ASN:HD21	12	0.7
(1,538)	1:66:A:GLN:HG2	1:67:A:SER:H	19	0.7
(1,296)	1:27:A:HIS:HA	1:30:A:ASN:HD21	1	0.7
(1,287)	1:26:A:ASN:H	1:32:A:SER:HB2	11	0.7
(1,14)	1:6:A:LYS:HG2	1:7:A:LEU:H	2	0.7
(2,110)	1:152:A:THR:HG21	2:661:B:PHE:HB2	5	0.69
(2,110)	1:152:A:THR:HG21	2:661:B:PHE:HB3	5	0.69
(2,110)	1:152:A:THR:HG22	2:661:B:PHE:HB2	5	0.69
(2,110)	1:152:A:THR:HG22	2:661:B:PHE:HB3	5	0.69
(2,110)	1:152:A:THR:HG23	2:661:B:PHE:HB2	5	0.69
(2,110)	1:152:A:THR:HG23	2:661:B:PHE:HB3	5	0.69
(2,98)	1:124:A:ALA:H	2:656:B:PHE:HE1	9	0.69
(2,98)	1:124:A:ALA:H	2:656:B:PHE:HE2	9	0.69
(2,98)	1:124:A:ALA:H	2:656:B:PHE:HE1	13	0.69
(2,98)	1:124:A:ALA:H	2:656:B:PHE:HE2	13	0.69
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG11	3	0.69
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG12	3	0.69
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG13	3	0.69
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG11	6	0.69
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG12	6	0.69
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG13	6	0.69
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG11	16	0.69
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG12	16	0.69
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG13	16	0.69
(2,94)	1:93:A:ILE:HG21	2:643:B:PRO:HB3	20	0.69
(2,94)	1:93:A:ILE:HG22	2:643:B:PRO:HB3	20	0.69
(2,94)	1:93:A:ILE:HG23	2:643:B:PRO:HB3	20	0.69
(2,89)	1:55:A:VAL:H	2:651:B:ILE:HG12	20	0.69
(2,89)	1:55:A:VAL:H	2:651:B:ILE:HG13	20	0.69
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD11	16	0.69
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD12	16	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD13	16	0.69
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG21	16	0.69
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG22	16	0.69
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG23	16	0.69
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG11	15	0.69
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG12	15	0.69
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG13	15	0.69
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG21	15	0.69
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG22	15	0.69
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG23	15	0.69
(2,75)	2:656:B:PHE:HB2	2:659:B:PHE:HE1	11	0.69
(2,75)	2:656:B:PHE:HB2	2:659:B:PHE:HE2	11	0.69
(2,75)	2:656:B:PHE:HB3	2:659:B:PHE:HE1	11	0.69
(2,75)	2:656:B:PHE:HB3	2:659:B:PHE:HE2	11	0.69
(2,44)	1:131:A:GLN:HE21	1:153:A:ASP:H	2	0.69
(2,38)	1:126:A:SER:H	1:129:A:GLN:HB2	7	0.69
(2,38)	1:126:A:SER:H	1:129:A:GLN:HB2	12	0.69
(2,38)	1:126:A:SER:H	1:129:A:GLN:HB2	16	0.69
(1,2596)	1:137:A:ALA:HB1	2:651:B:ILE:HG12	17	0.69
(1,2596)	1:137:A:ALA:HB1	2:651:B:ILE:HG13	17	0.69
(1,2596)	1:137:A:ALA:HB2	2:651:B:ILE:HG12	17	0.69
(1,2596)	1:137:A:ALA:HB2	2:651:B:ILE:HG13	17	0.69
(1,2596)	1:137:A:ALA:HB3	2:651:B:ILE:HG12	17	0.69
(1,2596)	1:137:A:ALA:HB3	2:651:B:ILE:HG13	17	0.69
(1,2524)	2:647:B:VAL:HG11	2:650:B:ASN:HD22	19	0.69
(1,2524)	2:647:B:VAL:HG12	2:650:B:ASN:HD22	19	0.69
(1,2524)	2:647:B:VAL:HG13	2:650:B:ASN:HD22	19	0.69
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG11	19	0.69
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG12	19	0.69
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG13	19	0.69
(1,1227)	1:89:A:ILE:HG12	1:150:A:VAL:H	8	0.69
(1,1227)	1:89:A:ILE:HG12	1:150:A:VAL:H	15	0.69
(1,1227)	1:89:A:ILE:HG12	1:150:A:VAL:H	20	0.69
(1,1217)	1:145:A:GLU:HB3	1:147:A:SER:H	20	0.69
(1,1060)	1:121:A:ASP:H	1:122:A:LEU:HD11	9	0.69
(1,1060)	1:121:A:ASP:H	1:122:A:LEU:HD12	9	0.69
(1,1060)	1:121:A:ASP:H	1:122:A:LEU:HD13	9	0.69
(1,834)	1:94:A:GLN:HE21	1:97:A:LYS:HD2	18	0.69
(1,834)	1:94:A:GLN:HE21	1:97:A:LYS:HD2	19	0.69
(1,816)	1:95:A:LYS:HD2	1:96:A:ILE:H	2	0.69
(1,639)	1:65:A:SER:HB3	1:81:A:THR:HG21	1	0.69
(1,639)	1:65:A:SER:HB3	1:81:A:THR:HG22	1	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,639)	1:65:A:SER:HB3	1:81:A:THR:HG23	1	0.69
(1,397)	1:54:A:ARG:HG2	1:126:A:SER:H	9	0.69
(1,296)	1:27:A:HIS:HA	1:30:A:ASN:HD21	20	0.69
(1,88)	1:12:A:GLU:HB2	1:14:A:ARG:HE	20	0.69
(1,88)	1:12:A:GLU:HB3	1:14:A:ARG:HE	20	0.69
(1,56)	1:11:A:TRP:HE1	1:31:A:ALA:HB1	11	0.69
(1,56)	1:11:A:TRP:HE1	1:31:A:ALA:HB2	11	0.69
(1,56)	1:11:A:TRP:HE1	1:31:A:ALA:HB3	11	0.69
(1,14)	1:6:A:LYS:HG2	1:7:A:LEU:H	17	0.69
(2,106)	1:139:A:PHE:H	2:656:B:PHE:HB2	5	0.68
(2,102)	1:135:A:GLU:H	2:656:B:PHE:HB2	16	0.68
(2,98)	1:124:A:ALA:H	2:656:B:PHE:HE1	20	0.68
(2,98)	1:124:A:ALA:H	2:656:B:PHE:HE2	20	0.68
(2,88)	1:34:A:TRP:HE1	2:641:B:TPO:H	7	0.68
(2,45)	1:131:A:GLN:HE21	1:152:A:THR:HB	8	0.68
(2,45)	1:131:A:GLN:HE21	1:152:A:THR:HB	12	0.68
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG11	2	0.68
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG12	2	0.68
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG13	2	0.68
(1,1227)	1:89:A:ILE:HG12	1:150:A:VAL:H	1	0.68
(1,1217)	1:145:A:GLU:HB3	1:147:A:SER:H	7	0.68
(1,1054)	1:59:A:HIS:HD2	1:122:A:LEU:H	19	0.68
(1,833)	1:94:A:GLN:HE21	1:97:A:LYS:HG2	13	0.68
(1,830)	1:93:A:ILE:HG21	1:97:A:LYS:HD2	3	0.68
(1,830)	1:93:A:ILE:HG22	1:97:A:LYS:HD2	3	0.68
(1,830)	1:93:A:ILE:HG23	1:97:A:LYS:HD2	3	0.68
(1,785)	1:89:A:ILE:HG21	1:93:A:ILE:H	17	0.68
(1,785)	1:89:A:ILE:HG22	1:93:A:ILE:H	17	0.68
(1,785)	1:89:A:ILE:HG23	1:93:A:ILE:H	17	0.68
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD11	3	0.68
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD12	3	0.68
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD13	3	0.68
(1,689)	1:86:A:LEU:HG	1:90:A:ASN:HD21	3	0.68
(1,689)	1:86:A:LEU:HG	1:90:A:ASN:HD21	5	0.68
(1,689)	1:86:A:LEU:HG	1:90:A:ASN:HD21	8	0.68
(1,689)	1:86:A:LEU:HG	1:90:A:ASN:HD21	15	0.68
(1,592)	1:75:A:GLN:HB2	1:77:A:LYS:H	3	0.68
(3,27)	1:56:A:ARG:N	1:163:A:GLU:O	16	0.67
(2,93)	1:93:A:ILE:HD11	2:643:B:PRO:HA	20	0.67
(2,93)	1:93:A:ILE:HD12	2:643:B:PRO:HA	20	0.67
(2,93)	1:93:A:ILE:HD13	2:643:B:PRO:HA	20	0.67
(2,90)	1:56:A:ARG:H	2:651:B:ILE:HG12	10	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,90)	1:56:A:ARG:H	2:651:B:ILE:HG13	10	0.67
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG21	2	0.67
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG22	2	0.67
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG23	2	0.67
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG21	10	0.67
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG22	10	0.67
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG23	10	0.67
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG21	19	0.67
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG22	19	0.67
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG23	19	0.67
(2,71)	2:651:B:ILE:HG21	2:656:B:PHE:H	5	0.67
(2,71)	2:651:B:ILE:HG22	2:656:B:PHE:H	5	0.67
(2,71)	2:651:B:ILE:HG23	2:656:B:PHE:H	5	0.67
(2,71)	2:651:B:ILE:HG21	2:656:B:PHE:H	14	0.67
(2,71)	2:651:B:ILE:HG22	2:656:B:PHE:H	14	0.67
(2,71)	2:651:B:ILE:HG23	2:656:B:PHE:H	14	0.67
(2,38)	1:126:A:SER:H	1:129:A:GLN:HB2	6	0.67
(2,38)	1:126:A:SER:H	1:129:A:GLN:HB2	9	0.67
(2,26)	1:94:A:GLN:HE21	1:97:A:LYS:HB3	10	0.67
(2,26)	1:94:A:GLN:HE21	1:97:A:LYS:HB3	17	0.67
(2,20)	1:68:A:ARG:H	1:153:A:ASP:HB2	12	0.67
(2,20)	1:68:A:ARG:H	1:153:A:ASP:HB3	12	0.67
(1,2551)	2:652:B:ASP:H	2:654:B:SER:H	7	0.67
(1,1227)	1:89:A:ILE:HG12	1:150:A:VAL:H	5	0.67
(1,1109)	1:126:A:SER:HA	1:139:A:PHE:HD1	13	0.67
(1,1109)	1:126:A:SER:HA	1:139:A:PHE:HD2	13	0.67
(1,845)	1:97:A:LYS:HD2	1:98:A:SER:H	20	0.67
(1,830)	1:93:A:ILE:HG21	1:97:A:LYS:HD2	4	0.67
(1,830)	1:93:A:ILE:HG22	1:97:A:LYS:HD2	4	0.67
(1,830)	1:93:A:ILE:HG23	1:97:A:LYS:HD2	4	0.67
(1,816)	1:95:A:LYS:HD2	1:96:A:ILE:H	1	0.67
(1,672)	1:64:A:HIS:HD2	1:85:A:ALA:H	10	0.67
(1,672)	1:64:A:HIS:HD2	1:85:A:ALA:H	16	0.67
(1,637)	1:80:A:ARG:HE	1:85:A:ALA:H	4	0.67
(1,256)	1:23:A:TYR:HE1	1:26:A:ASN:H	13	0.67
(1,256)	1:23:A:TYR:HE2	1:26:A:ASN:H	13	0.67
(2,113)	1:162:A:THR:H	2:651:B:ILE:HG12	10	0.66
(2,113)	1:162:A:THR:H	2:651:B:ILE:HG13	10	0.66
(2,107)	1:140:A:ALA:HB1	2:651:B:ILE:HA	17	0.66
(2,107)	1:140:A:ALA:HB2	2:651:B:ILE:HA	17	0.66
(2,107)	1:140:A:ALA:HB3	2:651:B:ILE:HA	17	0.66
(2,98)	1:124:A:ALA:H	2:656:B:PHE:HE1	18	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,98)	1:124:A:ALA:H	2:656:B:PHE:HE2	18	0.66
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG11	12	0.66
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG12	12	0.66
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG13	12	0.66
(2,89)	1:55:A:VAL:H	2:651:B:ILE:HG12	6	0.66
(2,89)	1:55:A:VAL:H	2:651:B:ILE:HG13	6	0.66
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD11	5	0.66
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD12	5	0.66
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD13	5	0.66
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD11	14	0.66
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD12	14	0.66
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD13	14	0.66
(2,79)	2:659:B:PHE:HE1	2:661:B:PHE:H	9	0.66
(2,79)	2:659:B:PHE:HE2	2:661:B:PHE:H	9	0.66
(2,74)	2:656:B:PHE:HB2	2:659:B:PHE:HD1	12	0.66
(2,74)	2:656:B:PHE:HB2	2:659:B:PHE:HD2	12	0.66
(2,74)	2:656:B:PHE:HB3	2:659:B:PHE:HD1	12	0.66
(2,74)	2:656:B:PHE:HB3	2:659:B:PHE:HD2	12	0.66
(2,70)	2:651:B:ILE:HG21	2:656:B:PHE:HE1	1	0.66
(2,70)	2:651:B:ILE:HG21	2:656:B:PHE:HE2	1	0.66
(2,70)	2:651:B:ILE:HG22	2:656:B:PHE:HE1	1	0.66
(2,70)	2:651:B:ILE:HG22	2:656:B:PHE:HE2	1	0.66
(2,70)	2:651:B:ILE:HG23	2:656:B:PHE:HE1	1	0.66
(2,70)	2:651:B:ILE:HG23	2:656:B:PHE:HE2	1	0.66
(2,45)	1:131:A:GLN:HE21	1:152:A:THR:HB	13	0.66
(2,26)	1:94:A:GLN:HE21	1:97:A:LYS:HB3	1	0.66
(2,4)	1:21:A:ARG:HE	1:22:A:VAL:H	8	0.66
(2,4)	1:21:A:ARG:HE	1:22:A:VAL:H	9	0.66
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG21	6	0.66
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG22	6	0.66
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG23	6	0.66
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG21	14	0.66
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG22	14	0.66
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG23	14	0.66
(1,2158)	1:119:A:ARG:H	1:119:A:ARG:HD2	10	0.66
(1,2158)	1:119:A:ARG:H	1:119:A:ARG:HD2	15	0.66
(1,1337)	1:59:A:HIS:H	1:159:A:ILE:HG21	19	0.66
(1,1337)	1:59:A:HIS:H	1:159:A:ILE:HG22	19	0.66
(1,1337)	1:59:A:HIS:H	1:159:A:ILE:HG23	19	0.66
(1,1227)	1:89:A:ILE:HG12	1:150:A:VAL:H	10	0.66
(1,1033)	1:108:A:SER:H	1:119:A:ARG:HB2	10	0.66
(1,985)	1:61:A:LEU:HD21	1:113:A:CYS:HA	15	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,985)	1:61:A:LEU:HD22	1:113:A:CYS:HA	15	0.66
(1,985)	1:61:A:LEU:HD23	1:113:A:CYS:HA	15	0.66
(1,985)	1:61:A:LEU:HD21	1:113:A:CYS:HA	18	0.66
(1,985)	1:61:A:LEU:HD22	1:113:A:CYS:HA	18	0.66
(1,985)	1:61:A:LEU:HD23	1:113:A:CYS:HA	18	0.66
(1,833)	1:94:A:GLN:HE21	1:97:A:LYS:HG2	15	0.66
(1,830)	1:93:A:ILE:HG21	1:97:A:LYS:HD2	14	0.66
(1,830)	1:93:A:ILE:HG22	1:97:A:LYS:HD2	14	0.66
(1,830)	1:93:A:ILE:HG23	1:97:A:LYS:HD2	14	0.66
(1,637)	1:80:A:ARG:HE	1:85:A:ALA:H	8	0.66
(1,592)	1:75:A:GLN:HB2	1:77:A:LYS:H	8	0.66
(1,397)	1:54:A:ARG:HG2	1:126:A:SER:H	12	0.66
(1,296)	1:27:A:HIS:HA	1:30:A:ASN:HD21	9	0.66
(1,296)	1:27:A:HIS:HA	1:30:A:ASN:HD21	17	0.66
(1,204)	1:24:A:TYR:HB2	1:33:A:GLN:HE21	5	0.66
(2,113)	1:162:A:THR:H	2:651:B:ILE:HG12	9	0.65
(2,113)	1:162:A:THR:H	2:651:B:ILE:HG13	9	0.65
(2,109)	1:150:A:VAL:HG21	2:649:B:ARG:HA	13	0.65
(2,109)	1:150:A:VAL:HG22	2:649:B:ARG:HA	13	0.65
(2,109)	1:150:A:VAL:HG23	2:649:B:ARG:HA	13	0.65
(2,101)	1:129:A:GLN:HE21	2:657:B:GLU:HB2	17	0.65
(2,101)	1:129:A:GLN:HE21	2:657:B:GLU:HB3	17	0.65
(2,98)	1:124:A:ALA:H	2:656:B:PHE:HE1	1	0.65
(2,98)	1:124:A:ALA:H	2:656:B:PHE:HE2	1	0.65
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG11	4	0.65
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG12	4	0.65
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG13	4	0.65
(2,89)	1:55:A:VAL:H	2:651:B:ILE:HG12	2	0.65
(2,89)	1:55:A:VAL:H	2:651:B:ILE:HG13	2	0.65
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD11	12	0.65
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD12	12	0.65
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD13	12	0.65
(2,86)	1:29:A:THR:HG21	2:647:B:VAL:HA	14	0.65
(2,86)	1:29:A:THR:HG22	2:647:B:VAL:HA	14	0.65
(2,86)	1:29:A:THR:HG23	2:647:B:VAL:HA	14	0.65
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG11	2	0.65
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG12	2	0.65
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG13	2	0.65
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG21	2	0.65
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG22	2	0.65
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG23	2	0.65
(2,71)	2:651:B:ILE:HG21	2:656:B:PHE:H	8	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,71)	2:651:B:ILE:HG22	2:656:B:PHE:H	8	0.65
(2,71)	2:651:B:ILE:HG23	2:656:B:PHE:H	8	0.65
(2,70)	2:651:B:ILE:HG21	2:656:B:PHE:HE1	4	0.65
(2,70)	2:651:B:ILE:HG21	2:656:B:PHE:HE2	4	0.65
(2,70)	2:651:B:ILE:HG22	2:656:B:PHE:HE1	4	0.65
(2,70)	2:651:B:ILE:HG22	2:656:B:PHE:HE2	4	0.65
(2,70)	2:651:B:ILE:HG23	2:656:B:PHE:HE1	4	0.65
(2,70)	2:651:B:ILE:HG23	2:656:B:PHE:HE2	4	0.65
(2,45)	1:131:A:GLN:HE21	1:152:A:THR:HB	14	0.65
(2,44)	1:131:A:GLN:HE21	1:153:A:ASP:H	19	0.65
(2,38)	1:126:A:SER:H	1:129:A:GLN:HB2	20	0.65
(2,34)	1:59:A:HIS:H	1:122:A:LEU:HB2	11	0.65
(2,5)	1:23:A:TYR:H	1:34:A:TRP:HZ3	19	0.65
(2,4)	1:21:A:ARG:HE	1:22:A:VAL:H	6	0.65
(2,4)	1:21:A:ARG:HE	1:22:A:VAL:H	16	0.65
(1,2591)	1:123:A:GLY:H	2:656:B:PHE:HE1	11	0.65
(1,2591)	1:123:A:GLY:H	2:656:B:PHE:HE2	11	0.65
(1,2587)	1:115:A:SER:H	2:659:B:PHE:HD1	18	0.65
(1,2587)	1:115:A:SER:H	2:659:B:PHE:HD2	18	0.65
(1,2582)	1:34:A:TRP:HE1	2:642:B:PRO:HB2	13	0.65
(1,2582)	1:34:A:TRP:HE1	2:642:B:PRO:HB3	13	0.65
(1,2158)	1:119:A:ARG:H	1:119:A:ARG:HD2	17	0.65
(1,1410)	1:161:A:ARG:HE	1:163:A:GLU:HG2	2	0.65
(1,1311)	1:152:A:THR:HG21	1:157:A:HIS:H	16	0.65
(1,1311)	1:152:A:THR:HG22	1:157:A:HIS:H	16	0.65
(1,1311)	1:152:A:THR:HG23	1:157:A:HIS:H	16	0.65
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG11	4	0.65
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG12	4	0.65
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG13	4	0.65
(1,1227)	1:89:A:ILE:HG12	1:150:A:VAL:H	9	0.65
(1,1130)	1:131:A:GLN:HE21	1:153:A:ASP:HB2	20	0.65
(1,1130)	1:131:A:GLN:HE21	1:153:A:ASP:HB3	20	0.65
(1,1109)	1:126:A:SER:HA	1:139:A:PHE:HD1	2	0.65
(1,1109)	1:126:A:SER:HA	1:139:A:PHE:HD2	2	0.65
(1,1033)	1:108:A:SER:H	1:119:A:ARG:HB2	9	0.65
(1,1033)	1:108:A:SER:H	1:119:A:ARG:HB2	15	0.65
(1,1033)	1:108:A:SER:H	1:119:A:ARG:HB2	18	0.65
(1,830)	1:93:A:ILE:HG21	1:97:A:LYS:HD2	7	0.65
(1,830)	1:93:A:ILE:HG22	1:97:A:LYS:HD2	7	0.65
(1,830)	1:93:A:ILE:HG23	1:97:A:LYS:HD2	7	0.65
(1,689)	1:86:A:LEU:HG	1:90:A:ASN:HD21	2	0.65
(1,689)	1:86:A:LEU:HG	1:90:A:ASN:HD21	13	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,672)	1:64:A:HIS:HD2	1:85:A:ALA:H	11	0.65
(1,637)	1:80:A:ARG:HE	1:85:A:ALA:H	7	0.65
(1,515)	1:63:A:LYS:H	1:156:A:ILE:H	12	0.65
(1,275)	1:26:A:ASN:H	1:29:A:THR:HG21	20	0.65
(1,275)	1:26:A:ASN:H	1:29:A:THR:HG22	20	0.65
(1,275)	1:26:A:ASN:H	1:29:A:THR:HG23	20	0.65
(2,106)	1:139:A:PHE:H	2:656:B:PHE:HB2	20	0.64
(2,98)	1:124:A:ALA:H	2:656:B:PHE:HE1	3	0.64
(2,98)	1:124:A:ALA:H	2:656:B:PHE:HE2	3	0.64
(2,97)	1:94:A:GLN:HE21	2:640:B:LEU:HG	4	0.64
(2,97)	1:94:A:GLN:HE21	2:640:B:LEU:HG	14	0.64
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG11	18	0.64
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG12	18	0.64
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG13	18	0.64
(2,90)	1:56:A:ARG:H	2:651:B:ILE:HG12	13	0.64
(2,90)	1:56:A:ARG:H	2:651:B:ILE:HG13	13	0.64
(2,89)	1:55:A:VAL:H	2:651:B:ILE:HG12	11	0.64
(2,89)	1:55:A:VAL:H	2:651:B:ILE:HG13	11	0.64
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD11	11	0.64
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD12	11	0.64
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD13	11	0.64
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG11	4	0.64
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG12	4	0.64
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG13	4	0.64
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG21	4	0.64
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG22	4	0.64
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG23	4	0.64
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG11	14	0.64
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG12	14	0.64
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG13	14	0.64
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG21	14	0.64
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG22	14	0.64
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG23	14	0.64
(2,58)	1:152:A:THR:HG21	1:157:A:HIS:HB3	16	0.64
(2,58)	1:152:A:THR:HG22	1:157:A:HIS:HB3	16	0.64
(2,58)	1:152:A:THR:HG23	1:157:A:HIS:HB3	16	0.64
(2,45)	1:131:A:GLN:HE21	1:152:A:THR:HB	15	0.64
(2,38)	1:126:A:SER:H	1:129:A:GLN:HB2	3	0.64
(2,38)	1:126:A:SER:H	1:129:A:GLN:HB2	14	0.64
(2,20)	1:68:A:ARG:H	1:153:A:ASP:HB2	7	0.64
(2,20)	1:68:A:ARG:H	1:153:A:ASP:HB3	7	0.64
(2,9)	1:53:A:ALA:H	1:54:A:ARG:HD2	19	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,5)	1:23:A:TYR:H	1:34:A:TRP:HZ3	15	0.64
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG21	8	0.64
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG22	8	0.64
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG23	8	0.64
(1,2529)	2:648:B:ILE:HG21	2:649:B:ARG:HD2	1	0.64
(1,2529)	2:648:B:ILE:HG22	2:649:B:ARG:HD2	1	0.64
(1,2529)	2:648:B:ILE:HG23	2:649:B:ARG:HD2	1	0.64
(1,1337)	1:59:A:HIS:H	1:159:A:ILE:HG21	18	0.64
(1,1337)	1:59:A:HIS:H	1:159:A:ILE:HG22	18	0.64
(1,1337)	1:59:A:HIS:H	1:159:A:ILE:HG23	18	0.64
(1,1306)	1:89:A:ILE:HD11	1:157:A:HIS:HD2	10	0.64
(1,1306)	1:89:A:ILE:HD12	1:157:A:HIS:HD2	10	0.64
(1,1306)	1:89:A:ILE:HD13	1:157:A:HIS:HD2	10	0.64
(1,1227)	1:89:A:ILE:HG12	1:150:A:VAL:H	2	0.64
(1,1227)	1:89:A:ILE:HG12	1:150:A:VAL:H	13	0.64
(1,1184)	1:140:A:ALA:H	1:141:A:LEU:HG	15	0.64
(1,841)	1:97:A:LYS:HB3	1:98:A:SER:H	5	0.64
(1,834)	1:94:A:GLN:HE21	1:97:A:LYS:HD2	16	0.64
(1,833)	1:94:A:GLN:HE21	1:97:A:LYS:HG2	2	0.64
(1,833)	1:94:A:GLN:HE21	1:97:A:LYS:HG2	11	0.64
(1,816)	1:95:A:LYS:HD2	1:96:A:ILE:H	11	0.64
(1,752)	1:89:A:ILE:HB	1:91:A:GLY:H	17	0.64
(1,689)	1:86:A:LEU:HG	1:90:A:ASN:HD21	4	0.64
(1,637)	1:80:A:ARG:HE	1:85:A:ALA:H	9	0.64
(1,572)	1:73:A:TRP:HE1	1:111:A:SER:HB2	2	0.64
(1,572)	1:73:A:TRP:HE1	1:111:A:SER:HB2	17	0.64
(1,138)	1:21:A:ARG:HE	1:34:A:TRP:HH2	17	0.64
(1,86)	1:13:A:LYS:HE2	1:14:A:ARG:H	17	0.64
(1,14)	1:6:A:LYS:HG2	1:7:A:LEU:H	16	0.64
(2,97)	1:94:A:GLN:HE21	2:640:B:LEU:HG	11	0.63
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG11	5	0.63
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG12	5	0.63
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG13	5	0.63
(2,92)	1:58:A:SER:H	2:651:B:ILE:HG12	8	0.63
(2,92)	1:58:A:SER:H	2:651:B:ILE:HG13	8	0.63
(2,92)	1:58:A:SER:H	2:651:B:ILE:HG12	13	0.63
(2,92)	1:58:A:SER:H	2:651:B:ILE:HG13	13	0.63
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD11	1	0.63
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD12	1	0.63
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD13	1	0.63
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG21	12	0.63
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG22	12	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG23	12	0.63
(2,76)	2:656:B:PHE:HE1	2:659:B:PHE:HE1	2	0.63
(2,76)	2:656:B:PHE:HE1	2:659:B:PHE:HE2	2	0.63
(2,76)	2:656:B:PHE:HE2	2:659:B:PHE:HE1	2	0.63
(2,76)	2:656:B:PHE:HE2	2:659:B:PHE:HE2	2	0.63
(2,71)	2:651:B:ILE:HG21	2:656:B:PHE:H	12	0.63
(2,71)	2:651:B:ILE:HG22	2:656:B:PHE:H	12	0.63
(2,71)	2:651:B:ILE:HG23	2:656:B:PHE:H	12	0.63
(2,52)	1:141:A:LEU:HD21	1:148:A:GLY:H	2	0.63
(2,52)	1:141:A:LEU:HD22	1:148:A:GLY:H	2	0.63
(2,52)	1:141:A:LEU:HD23	1:148:A:GLY:H	2	0.63
(2,44)	1:131:A:GLN:HE21	1:153:A:ASP:H	5	0.63
(2,38)	1:126:A:SER:H	1:129:A:GLN:HB2	4	0.63
(2,20)	1:68:A:ARG:H	1:153:A:ASP:HB2	18	0.63
(2,20)	1:68:A:ARG:H	1:153:A:ASP:HB3	18	0.63
(1,2588)	1:122:A:LEU:H	2:656:B:PHE:HE1	14	0.63
(1,2588)	1:122:A:LEU:H	2:656:B:PHE:HE2	14	0.63
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG21	10	0.63
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG22	10	0.63
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG23	10	0.63
(1,2551)	2:652:B:ASP:H	2:654:B:SER:H	2	0.63
(1,2533)	2:647:B:VAL:H	2:649:B:ARG:H	10	0.63
(1,2525)	2:645:B:GLN:HE22	2:648:B:ILE:HD11	18	0.63
(1,2525)	2:645:B:GLN:HE22	2:648:B:ILE:HD12	18	0.63
(1,2525)	2:645:B:GLN:HE22	2:648:B:ILE:HD13	18	0.63
(1,2524)	2:647:B:VAL:HG11	2:650:B:ASN:HD22	3	0.63
(1,2524)	2:647:B:VAL:HG12	2:650:B:ASN:HD22	3	0.63
(1,2524)	2:647:B:VAL:HG13	2:650:B:ASN:HD22	3	0.63
(1,2524)	2:647:B:VAL:HG11	2:650:B:ASN:HD22	8	0.63
(1,2524)	2:647:B:VAL:HG12	2:650:B:ASN:HD22	8	0.63
(1,2524)	2:647:B:VAL:HG13	2:650:B:ASN:HD22	8	0.63
(1,2507)	2:643:B:PRO:HA	2:645:B:GLN:H	6	0.63
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD21	16	0.63
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD22	16	0.63
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD23	16	0.63
(1,1625)	1:27:A:HIS:H	1:27:A:HIS:HD1	20	0.63
(1,1441)	1:162:A:THR:HG21	1:163:A:GLU:HG3	11	0.63
(1,1441)	1:162:A:THR:HG22	1:163:A:GLU:HG3	11	0.63
(1,1441)	1:162:A:THR:HG23	1:163:A:GLU:HG3	11	0.63
(1,1244)	1:150:A:VAL:HG21	1:157:A:HIS:HB2	11	0.63
(1,1244)	1:150:A:VAL:HG21	1:157:A:HIS:HB3	11	0.63
(1,1244)	1:150:A:VAL:HG22	1:157:A:HIS:HB2	11	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1244)	1:150:A:VAL:HG22	1:157:A:HIS:HB3	11	0.63
(1,1244)	1:150:A:VAL:HG23	1:157:A:HIS:HB2	11	0.63
(1,1244)	1:150:A:VAL:HG23	1:157:A:HIS:HB3	11	0.63
(1,1227)	1:89:A:ILE:HG12	1:150:A:VAL:H	6	0.63
(1,1227)	1:89:A:ILE:HG12	1:150:A:VAL:H	7	0.63
(1,1217)	1:145:A:GLU:HB3	1:147:A:SER:H	14	0.63
(1,1212)	1:146:A:MET:HG2	1:160:A:LEU:HG	20	0.63
(1,1193)	1:141:A:LEU:HD11	1:148:A:GLY:H	19	0.63
(1,1193)	1:141:A:LEU:HD12	1:148:A:GLY:H	19	0.63
(1,1193)	1:141:A:LEU:HD13	1:148:A:GLY:H	19	0.63
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB1	14	0.63
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB2	14	0.63
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB3	14	0.63
(1,871)	1:96:A:ILE:HB	1:103:A:PHE:H	18	0.63
(1,845)	1:97:A:LYS:HD2	1:98:A:SER:H	11	0.63
(1,830)	1:93:A:ILE:HG21	1:97:A:LYS:HD2	9	0.63
(1,830)	1:93:A:ILE:HG22	1:97:A:LYS:HD2	9	0.63
(1,830)	1:93:A:ILE:HG23	1:97:A:LYS:HD2	9	0.63
(1,689)	1:86:A:LEU:HG	1:90:A:ASN:HD21	1	0.63
(1,689)	1:86:A:LEU:HG	1:90:A:ASN:HD21	20	0.63
(1,672)	1:64:A:HIS:HD2	1:85:A:ALA:H	3	0.63
(1,672)	1:64:A:HIS:HD2	1:85:A:ALA:H	4	0.63
(1,672)	1:64:A:HIS:HD2	1:85:A:ALA:H	8	0.63
(1,672)	1:64:A:HIS:HD2	1:85:A:ALA:H	9	0.63
(1,672)	1:64:A:HIS:HD2	1:85:A:ALA:H	14	0.63
(1,672)	1:64:A:HIS:HD2	1:85:A:ALA:H	18	0.63
(1,671)	1:64:A:HIS:HB2	1:85:A:ALA:H	2	0.63
(1,640)	1:65:A:SER:HB3	1:81:A:THR:HA	15	0.63
(1,637)	1:80:A:ARG:HE	1:85:A:ALA:H	3	0.63
(1,637)	1:80:A:ARG:HE	1:85:A:ALA:H	14	0.63
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG21	13	0.63
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG22	13	0.63
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG23	13	0.63
(1,591)	1:74:A:ARG:HE	1:75:A:GLN:H	13	0.63
(1,204)	1:24:A:TYR:HB2	1:33:A:GLN:HE21	16	0.63
(1,148)	1:15:A:MET:HE1	1:22:A:VAL:HA	12	0.63
(1,148)	1:15:A:MET:HE2	1:22:A:VAL:HA	12	0.63
(1,148)	1:15:A:MET:HE3	1:22:A:VAL:HA	12	0.63
(1,86)	1:13:A:LYS:HE2	1:14:A:ARG:H	1	0.63
(2,113)	1:162:A:THR:H	2:651:B:ILE:HG12	12	0.62
(2,113)	1:162:A:THR:H	2:651:B:ILE:HG13	12	0.62
(2,111)	1:160:A:LEU:H	2:651:B:ILE:HG12	13	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,111)	1:160:A:LEU:H	2:651:B:ILE:HG13	13	0.62
(2,108)	1:140:A:ALA:HB1	2:649:B:ARG:HA	20	0.62
(2,108)	1:140:A:ALA:HB2	2:649:B:ARG:HA	20	0.62
(2,108)	1:140:A:ALA:HB3	2:649:B:ARG:HA	20	0.62
(2,98)	1:124:A:ALA:H	2:656:B:PHE:HE1	12	0.62
(2,98)	1:124:A:ALA:H	2:656:B:PHE:HE2	12	0.62
(2,97)	1:94:A:GLN:HE21	2:640:B:LEU:HG	2	0.62
(2,92)	1:58:A:SER:H	2:651:B:ILE:HG12	3	0.62
(2,92)	1:58:A:SER:H	2:651:B:ILE:HG13	3	0.62
(2,92)	1:58:A:SER:H	2:651:B:ILE:HG12	12	0.62
(2,92)	1:58:A:SER:H	2:651:B:ILE:HG13	12	0.62
(2,91)	1:57:A:CYS:H	2:651:B:ILE:HG12	10	0.62
(2,91)	1:57:A:CYS:H	2:651:B:ILE:HG13	10	0.62
(2,89)	1:55:A:VAL:H	2:651:B:ILE:HG12	19	0.62
(2,89)	1:55:A:VAL:H	2:651:B:ILE:HG13	19	0.62
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD11	3	0.62
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD12	3	0.62
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD13	3	0.62
(2,86)	1:29:A:THR:HG21	2:647:B:VAL:HA	15	0.62
(2,86)	1:29:A:THR:HG22	2:647:B:VAL:HA	15	0.62
(2,86)	1:29:A:THR:HG23	2:647:B:VAL:HA	15	0.62
(2,74)	2:656:B:PHE:HB2	2:659:B:PHE:HD1	9	0.62
(2,74)	2:656:B:PHE:HB2	2:659:B:PHE:HD2	9	0.62
(2,74)	2:656:B:PHE:HB3	2:659:B:PHE:HD1	9	0.62
(2,74)	2:656:B:PHE:HB3	2:659:B:PHE:HD2	9	0.62
(2,72)	2:653:B:GLN:HA	2:656:B:PHE:HE1	1	0.62
(2,72)	2:653:B:GLN:HA	2:656:B:PHE:HE2	1	0.62
(2,72)	2:653:B:GLN:HA	2:656:B:PHE:HE1	4	0.62
(2,72)	2:653:B:GLN:HA	2:656:B:PHE:HE2	4	0.62
(2,58)	1:152:A:THR:HG21	1:157:A:HIS:HB3	3	0.62
(2,58)	1:152:A:THR:HG22	1:157:A:HIS:HB3	3	0.62
(2,58)	1:152:A:THR:HG23	1:157:A:HIS:HB3	3	0.62
(2,58)	1:152:A:THR:HG21	1:157:A:HIS:HB3	8	0.62
(2,58)	1:152:A:THR:HG22	1:157:A:HIS:HB3	8	0.62
(2,58)	1:152:A:THR:HG23	1:157:A:HIS:HB3	8	0.62
(2,58)	1:152:A:THR:HG21	1:157:A:HIS:HB3	9	0.62
(2,58)	1:152:A:THR:HG22	1:157:A:HIS:HB3	9	0.62
(2,58)	1:152:A:THR:HG23	1:157:A:HIS:HB3	9	0.62
(2,55)	1:150:A:VAL:HG21	1:158:A:ILE:HA	11	0.62
(2,55)	1:150:A:VAL:HG22	1:158:A:ILE:HA	11	0.62
(2,55)	1:150:A:VAL:HG23	1:158:A:ILE:HA	11	0.62
(2,45)	1:131:A:GLN:HE21	1:152:A:THR:HB	19	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,44)	1:131:A:GLN:HE21	1:153:A:ASP:H	6	0.62
(2,44)	1:131:A:GLN:HE21	1:153:A:ASP:H	10	0.62
(2,44)	1:131:A:GLN:HE21	1:153:A:ASP:H	12	0.62
(2,38)	1:126:A:SER:H	1:129:A:GLN:HB2	1	0.62
(1,2586)	1:115:A:SER:H	2:659:B:PHE:HE1	2	0.62
(1,2586)	1:115:A:SER:H	2:659:B:PHE:HE2	2	0.62
(1,1913)	1:82:A:LYS:H	1:82:A:LYS:HD2	2	0.62
(1,1913)	1:82:A:LYS:H	1:82:A:LYS:HD2	13	0.62
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD11	10	0.62
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD12	10	0.62
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD13	10	0.62
(1,1335)	1:57:A:CYS:HA	1:159:A:ILE:HG21	4	0.62
(1,1335)	1:57:A:CYS:HA	1:159:A:ILE:HG22	4	0.62
(1,1335)	1:57:A:CYS:HA	1:159:A:ILE:HG23	4	0.62
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG11	14	0.62
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG12	14	0.62
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG13	14	0.62
(1,1217)	1:145:A:GLU:HB3	1:147:A:SER:H	6	0.62
(1,1193)	1:141:A:LEU:HD11	1:148:A:GLY:H	12	0.62
(1,1193)	1:141:A:LEU:HD12	1:148:A:GLY:H	12	0.62
(1,1193)	1:141:A:LEU:HD13	1:148:A:GLY:H	12	0.62
(1,1130)	1:131:A:GLN:HE21	1:153:A:ASP:HB2	15	0.62
(1,1130)	1:131:A:GLN:HE21	1:153:A:ASP:HB3	15	0.62
(1,1109)	1:126:A:SER:HA	1:139:A:PHE:HD1	3	0.62
(1,1109)	1:126:A:SER:HA	1:139:A:PHE:HD2	3	0.62
(1,1109)	1:126:A:SER:HA	1:139:A:PHE:HD1	11	0.62
(1,1109)	1:126:A:SER:HA	1:139:A:PHE:HD2	11	0.62
(1,1109)	1:126:A:SER:HA	1:139:A:PHE:HD1	16	0.62
(1,1109)	1:126:A:SER:HA	1:139:A:PHE:HD2	16	0.62
(1,1054)	1:59:A:HIS:HD2	1:122:A:LEU:H	16	0.62
(1,841)	1:97:A:LYS:HB3	1:98:A:SER:H	6	0.62
(1,834)	1:94:A:GLN:HE21	1:97:A:LYS:HD2	14	0.62
(1,816)	1:95:A:LYS:HD2	1:96:A:ILE:H	19	0.62
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD1	17	0.62
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD2	17	0.62
(1,689)	1:86:A:LEU:HG	1:90:A:ASN:HD21	6	0.62
(1,689)	1:86:A:LEU:HG	1:90:A:ASN:HD21	7	0.62
(1,689)	1:86:A:LEU:HG	1:90:A:ASN:HD21	19	0.62
(1,672)	1:64:A:HIS:HD2	1:85:A:ALA:H	5	0.62
(1,672)	1:64:A:HIS:HD2	1:85:A:ALA:H	7	0.62
(1,637)	1:80:A:ARG:HE	1:85:A:ALA:H	13	0.62
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG21	19	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG22	19	0.62
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG23	19	0.62
(1,606)	1:75:A:GLN:HE22	1:78:A:ILE:HA	18	0.62
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD11	15	0.62
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD12	15	0.62
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD13	15	0.62
(1,479)	1:61:A:LEU:HD21	1:155:A:GLY:H	3	0.62
(1,479)	1:61:A:LEU:HD22	1:155:A:GLY:H	3	0.62
(1,479)	1:61:A:LEU:HD23	1:155:A:GLY:H	3	0.62
(1,397)	1:54:A:ARG:HG2	1:126:A:SER:H	1	0.62
(1,287)	1:26:A:ASN:H	1:32:A:SER:HB2	5	0.62
(1,204)	1:24:A:TYR:HB2	1:33:A:GLN:HE21	1	0.62
(1,204)	1:24:A:TYR:HB2	1:33:A:GLN:HE21	12	0.62
(1,148)	1:15:A:MET:HE1	1:22:A:VAL:HA	14	0.62
(1,148)	1:15:A:MET:HE2	1:22:A:VAL:HA	14	0.62
(1,148)	1:15:A:MET:HE3	1:22:A:VAL:HA	14	0.62
(1,87)	1:13:A:LYS:HG3	1:14:A:ARG:H	15	0.62
(1,64)	1:12:A:GLU:H	1:24:A:TYR:HD1	1	0.62
(1,64)	1:12:A:GLU:H	1:24:A:TYR:HD2	1	0.62
(1,14)	1:6:A:LYS:HG2	1:7:A:LEU:H	13	0.62
(2,113)	1:162:A:THR:H	2:651:B:ILE:HG12	3	0.61
(2,113)	1:162:A:THR:H	2:651:B:ILE:HG13	3	0.61
(2,113)	1:162:A:THR:H	2:651:B:ILE:HG12	14	0.61
(2,113)	1:162:A:THR:H	2:651:B:ILE:HG13	14	0.61
(2,113)	1:162:A:THR:H	2:651:B:ILE:HG12	18	0.61
(2,113)	1:162:A:THR:H	2:651:B:ILE:HG13	18	0.61
(2,111)	1:160:A:LEU:H	2:651:B:ILE:HG12	10	0.61
(2,111)	1:160:A:LEU:H	2:651:B:ILE:HG13	10	0.61
(2,98)	1:124:A:ALA:H	2:656:B:PHE:HE1	14	0.61
(2,98)	1:124:A:ALA:H	2:656:B:PHE:HE2	14	0.61
(2,97)	1:94:A:GLN:HE21	2:640:B:LEU:HG	6	0.61
(2,89)	1:55:A:VAL:H	2:651:B:ILE:HG12	14	0.61
(2,89)	1:55:A:VAL:H	2:651:B:ILE:HG13	14	0.61
(2,89)	1:55:A:VAL:H	2:651:B:ILE:HG12	18	0.61
(2,89)	1:55:A:VAL:H	2:651:B:ILE:HG13	18	0.61
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG21	13	0.61
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG22	13	0.61
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG23	13	0.61
(2,74)	2:656:B:PHE:HB2	2:659:B:PHE:HD1	2	0.61
(2,74)	2:656:B:PHE:HB2	2:659:B:PHE:HD2	2	0.61
(2,74)	2:656:B:PHE:HB3	2:659:B:PHE:HD1	2	0.61
(2,74)	2:656:B:PHE:HB3	2:659:B:PHE:HD2	2	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,70)	2:651:B:ILE:HG21	2:656:B:PHE:HE1	7	0.61
(2,70)	2:651:B:ILE:HG21	2:656:B:PHE:HE2	7	0.61
(2,70)	2:651:B:ILE:HG22	2:656:B:PHE:HE1	7	0.61
(2,70)	2:651:B:ILE:HG22	2:656:B:PHE:HE2	7	0.61
(2,70)	2:651:B:ILE:HG23	2:656:B:PHE:HE1	7	0.61
(2,70)	2:651:B:ILE:HG23	2:656:B:PHE:HE2	7	0.61
(2,39)	1:55:A:VAL:HG11	1:127:A:ARG:H	4	0.61
(2,39)	1:55:A:VAL:HG12	1:127:A:ARG:H	4	0.61
(2,39)	1:55:A:VAL:HG13	1:127:A:ARG:H	4	0.61
(2,38)	1:126:A:SER:H	1:129:A:GLN:HB2	2	0.61
(2,38)	1:126:A:SER:H	1:129:A:GLN:HB2	18	0.61
(2,26)	1:94:A:GLN:HE21	1:97:A:LYS:HB3	12	0.61
(2,9)	1:53:A:ALA:H	1:54:A:ARG:HD2	3	0.61
(2,9)	1:53:A:ALA:H	1:54:A:ARG:HD2	7	0.61
(2,5)	1:23:A:TYR:H	1:34:A:TRP:HZ3	11	0.61
(2,4)	1:21:A:ARG:HE	1:22:A:VAL:H	17	0.61
(1,2588)	1:122:A:LEU:H	2:656:B:PHE:HE1	3	0.61
(1,2588)	1:122:A:LEU:H	2:656:B:PHE:HE2	3	0.61
(1,2588)	1:122:A:LEU:H	2:656:B:PHE:HE1	9	0.61
(1,2588)	1:122:A:LEU:H	2:656:B:PHE:HE2	9	0.61
(1,2588)	1:122:A:LEU:H	2:656:B:PHE:HE1	12	0.61
(1,2588)	1:122:A:LEU:H	2:656:B:PHE:HE2	12	0.61
(1,2551)	2:652:B:ASP:H	2:654:B:SER:H	10	0.61
(1,2529)	2:648:B:ILE:HG21	2:649:B:ARG:HD2	11	0.61
(1,2529)	2:648:B:ILE:HG22	2:649:B:ARG:HD2	11	0.61
(1,2529)	2:648:B:ILE:HG23	2:649:B:ARG:HD2	11	0.61
(1,2524)	2:647:B:VAL:HG11	2:650:B:ASN:HD22	6	0.61
(1,2524)	2:647:B:VAL:HG12	2:650:B:ASN:HD22	6	0.61
(1,2524)	2:647:B:VAL:HG13	2:650:B:ASN:HD22	6	0.61
(1,2524)	2:647:B:VAL:HG11	2:650:B:ASN:HD22	14	0.61
(1,2524)	2:647:B:VAL:HG12	2:650:B:ASN:HD22	14	0.61
(1,2524)	2:647:B:VAL:HG13	2:650:B:ASN:HD22	14	0.61
(1,2524)	2:647:B:VAL:HG11	2:650:B:ASN:HD22	16	0.61
(1,2524)	2:647:B:VAL:HG12	2:650:B:ASN:HD22	16	0.61
(1,2524)	2:647:B:VAL:HG13	2:650:B:ASN:HD22	16	0.61
(1,2520)	2:646:B:GLU:HG3	2:647:B:VAL:H	8	0.61
(1,2507)	2:643:B:PRO:HA	2:645:B:GLN:H	14	0.61
(1,2045)	1:97:A:LYS:H	1:97:A:LYS:HD2	2	0.61
(1,1869)	1:75:A:GLN:H	1:75:A:GLN:HE22	3	0.61
(1,1434)	1:161:A:ARG:HD2	1:163:A:GLU:H	20	0.61
(1,1326)	1:89:A:ILE:HG21	1:158:A:ILE:HB	18	0.61
(1,1326)	1:89:A:ILE:HG22	1:158:A:ILE:HB	18	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1326)	1:89:A:ILE:HG23	1:158:A:ILE:HB	18	0.61
(1,1303)	1:156:A:ILE:HG21	1:157:A:HIS:HD2	11	0.61
(1,1303)	1:156:A:ILE:HG22	1:157:A:HIS:HD2	11	0.61
(1,1303)	1:156:A:ILE:HG23	1:157:A:HIS:HD2	11	0.61
(1,1282)	1:82:A:LYS:HE2	1:156:A:ILE:HD11	2	0.61
(1,1282)	1:82:A:LYS:HE2	1:156:A:ILE:HD12	2	0.61
(1,1282)	1:82:A:LYS:HE2	1:156:A:ILE:HD13	2	0.61
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG11	1	0.61
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG12	1	0.61
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG13	1	0.61
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG11	5	0.61
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG12	5	0.61
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG13	5	0.61
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG11	10	0.61
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG12	10	0.61
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG13	10	0.61
(1,1130)	1:131:A:GLN:HE21	1:153:A:ASP:HB2	11	0.61
(1,1130)	1:131:A:GLN:HE21	1:153:A:ASP:HB3	11	0.61
(1,1112)	1:126:A:SER:H	1:129:A:GLN:HE21	3	0.61
(1,1033)	1:108:A:SER:H	1:119:A:ARG:HB2	3	0.61
(1,1033)	1:108:A:SER:H	1:119:A:ARG:HB2	16	0.61
(1,1032)	1:107:A:ALA:HB1	1:119:A:ARG:H	13	0.61
(1,1032)	1:107:A:ALA:HB2	1:119:A:ARG:H	13	0.61
(1,1032)	1:107:A:ALA:HB3	1:119:A:ARG:H	13	0.61
(1,888)	1:103:A:PHE:HE1	1:120:A:GLY:H	13	0.61
(1,888)	1:103:A:PHE:HE2	1:120:A:GLY:H	13	0.61
(1,841)	1:97:A:LYS:HB3	1:98:A:SER:H	3	0.61
(1,841)	1:97:A:LYS:HB3	1:98:A:SER:H	9	0.61
(1,834)	1:94:A:GLN:HE21	1:97:A:LYS:HD2	7	0.61
(1,830)	1:93:A:ILE:HG21	1:97:A:LYS:HD2	5	0.61
(1,830)	1:93:A:ILE:HG22	1:97:A:LYS:HD2	5	0.61
(1,830)	1:93:A:ILE:HG23	1:97:A:LYS:HD2	5	0.61
(1,830)	1:93:A:ILE:HG21	1:97:A:LYS:HD2	6	0.61
(1,830)	1:93:A:ILE:HG22	1:97:A:LYS:HD2	6	0.61
(1,830)	1:93:A:ILE:HG23	1:97:A:LYS:HD2	6	0.61
(1,816)	1:95:A:LYS:HD2	1:96:A:ILE:H	5	0.61
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE1	14	0.61
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE2	14	0.61
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE3	14	0.61
(1,785)	1:89:A:ILE:HG21	1:93:A:ILE:H	4	0.61
(1,785)	1:89:A:ILE:HG22	1:93:A:ILE:H	4	0.61
(1,785)	1:89:A:ILE:HG23	1:93:A:ILE:H	4	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD11	2	0.61
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD12	2	0.61
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD13	2	0.61
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD1	18	0.61
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD2	18	0.61
(1,689)	1:86:A:LEU:HG	1:90:A:ASN:HD21	10	0.61
(1,689)	1:86:A:LEU:HG	1:90:A:ASN:HD21	16	0.61
(1,637)	1:80:A:ARG:HE	1:85:A:ALA:H	12	0.61
(1,637)	1:80:A:ARG:HE	1:85:A:ALA:H	18	0.61
(1,592)	1:75:A:GLN:HB2	1:77:A:LYS:H	7	0.61
(1,592)	1:75:A:GLN:HB2	1:77:A:LYS:H	9	0.61
(1,572)	1:73:A:TRP:HE1	1:111:A:SER:HB2	13	0.61
(1,527)	1:66:A:GLN:HG2	1:81:A:THR:HG21	19	0.61
(1,527)	1:66:A:GLN:HG2	1:81:A:THR:HG22	19	0.61
(1,527)	1:66:A:GLN:HG2	1:81:A:THR:HG23	19	0.61
(1,397)	1:54:A:ARG:HG2	1:126:A:SER:H	7	0.61
(1,218)	1:12:A:GLU:HB2	1:25:A:PHE:H	18	0.61
(1,148)	1:15:A:MET:HE1	1:22:A:VAL:HA	19	0.61
(1,148)	1:15:A:MET:HE2	1:22:A:VAL:HA	19	0.61
(1,148)	1:15:A:MET:HE3	1:22:A:VAL:HA	19	0.61
(1,86)	1:13:A:LYS:HE2	1:14:A:ARG:H	9	0.61
(1,35)	1:9:A:PRO:HG2	1:10:A:GLY:H	15	0.61
(2,106)	1:139:A:PHE:H	2:656:B:PHE:HB2	6	0.6
(2,103)	1:137:A:ALA:H	2:656:B:PHE:HB2	1	0.6
(2,98)	1:124:A:ALA:H	2:656:B:PHE:HE1	7	0.6
(2,98)	1:124:A:ALA:H	2:656:B:PHE:HE2	7	0.6
(2,98)	1:124:A:ALA:H	2:656:B:PHE:HE1	15	0.6
(2,98)	1:124:A:ALA:H	2:656:B:PHE:HE2	15	0.6
(2,92)	1:58:A:SER:H	2:651:B:ILE:HG12	9	0.6
(2,92)	1:58:A:SER:H	2:651:B:ILE:HG13	9	0.6
(2,89)	1:55:A:VAL:H	2:651:B:ILE:HG12	3	0.6
(2,89)	1:55:A:VAL:H	2:651:B:ILE:HG13	3	0.6
(2,89)	1:55:A:VAL:H	2:651:B:ILE:HG12	8	0.6
(2,89)	1:55:A:VAL:H	2:651:B:ILE:HG13	8	0.6
(2,74)	2:656:B:PHE:HB2	2:659:B:PHE:HD1	13	0.6
(2,74)	2:656:B:PHE:HB2	2:659:B:PHE:HD2	13	0.6
(2,74)	2:656:B:PHE:HB3	2:659:B:PHE:HD1	13	0.6
(2,74)	2:656:B:PHE:HB3	2:659:B:PHE:HD2	13	0.6
(2,58)	1:152:A:THR:HG21	1:157:A:HIS:HB3	11	0.6
(2,58)	1:152:A:THR:HG22	1:157:A:HIS:HB3	11	0.6
(2,58)	1:152:A:THR:HG23	1:157:A:HIS:HB3	11	0.6
(2,45)	1:131:A:GLN:HE21	1:152:A:THR:HB	7	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2593)	1:129:A:GLN:HE21	2:656:B:PHE:HE1	17	0.6
(1,2593)	1:129:A:GLN:HE21	2:656:B:PHE:HE2	17	0.6
(1,2591)	1:123:A:GLY:H	2:656:B:PHE:HE1	6	0.6
(1,2591)	1:123:A:GLY:H	2:656:B:PHE:HE2	6	0.6
(1,2586)	1:115:A:SER:H	2:659:B:PHE:HE1	15	0.6
(1,2586)	1:115:A:SER:H	2:659:B:PHE:HE2	15	0.6
(1,2578)	1:29:A:THR:HG21	2:646:B:GLU:HA	15	0.6
(1,2578)	1:29:A:THR:HG22	2:646:B:GLU:HA	15	0.6
(1,2578)	1:29:A:THR:HG23	2:646:B:GLU:HA	15	0.6
(1,2538)	2:649:B:ARG:H	2:650:B:ASN:HD21	19	0.6
(1,2514)	2:646:B:GLU:HA	2:649:B:ARG:H	2	0.6
(1,2507)	2:643:B:PRO:HA	2:645:B:GLN:H	12	0.6
(1,1349)	1:158:A:ILE:H	1:159:A:ILE:HD11	3	0.6
(1,1349)	1:158:A:ILE:H	1:159:A:ILE:HD12	3	0.6
(1,1349)	1:158:A:ILE:H	1:159:A:ILE:HD13	3	0.6
(1,1348)	1:157:A:HIS:HB2	1:159:A:ILE:HD11	5	0.6
(1,1348)	1:157:A:HIS:HB2	1:159:A:ILE:HD12	5	0.6
(1,1348)	1:157:A:HIS:HB2	1:159:A:ILE:HD13	5	0.6
(1,1348)	1:157:A:HIS:HB3	1:159:A:ILE:HD11	5	0.6
(1,1348)	1:157:A:HIS:HB3	1:159:A:ILE:HD12	5	0.6
(1,1348)	1:157:A:HIS:HB3	1:159:A:ILE:HD13	5	0.6
(1,1337)	1:59:A:HIS:H	1:159:A:ILE:HG21	16	0.6
(1,1337)	1:59:A:HIS:H	1:159:A:ILE:HG22	16	0.6
(1,1337)	1:59:A:HIS:H	1:159:A:ILE:HG23	16	0.6
(1,1326)	1:89:A:ILE:HG21	1:158:A:ILE:HB	10	0.6
(1,1326)	1:89:A:ILE:HG22	1:158:A:ILE:HB	10	0.6
(1,1326)	1:89:A:ILE:HG23	1:158:A:ILE:HB	10	0.6
(1,1303)	1:156:A:ILE:HG21	1:157:A:HIS:HD2	17	0.6
(1,1303)	1:156:A:ILE:HG22	1:157:A:HIS:HD2	17	0.6
(1,1303)	1:156:A:ILE:HG23	1:157:A:HIS:HD2	17	0.6
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD11	15	0.6
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD12	15	0.6
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD13	15	0.6
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG11	12	0.6
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG12	12	0.6
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG13	12	0.6
(1,1227)	1:89:A:ILE:HG12	1:150:A:VAL:H	14	0.6
(1,1217)	1:145:A:GLU:HB3	1:147:A:SER:H	2	0.6
(1,1217)	1:145:A:GLU:HB3	1:147:A:SER:H	16	0.6
(1,1184)	1:140:A:ALA:H	1:141:A:LEU:HG	7	0.6
(1,1130)	1:131:A:GLN:HE21	1:153:A:ASP:HB2	19	0.6
(1,1130)	1:131:A:GLN:HE21	1:153:A:ASP:HB3	19	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1109)	1:126:A:SER:HA	1:139:A:PHE:HD1	8	0.6
(1,1109)	1:126:A:SER:HA	1:139:A:PHE:HD2	8	0.6
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE1	20	0.6
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE2	20	0.6
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE3	20	0.6
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE1	20	0.6
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE2	20	0.6
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE3	20	0.6
(1,1032)	1:107:A:ALA:HB1	1:119:A:ARG:H	17	0.6
(1,1032)	1:107:A:ALA:HB2	1:119:A:ARG:H	17	0.6
(1,1032)	1:107:A:ALA:HB3	1:119:A:ARG:H	17	0.6
(1,868)	1:60:A:LEU:HD21	1:103:A:PHE:HE1	7	0.6
(1,868)	1:60:A:LEU:HD21	1:103:A:PHE:HE2	7	0.6
(1,868)	1:60:A:LEU:HD22	1:103:A:PHE:HE1	7	0.6
(1,868)	1:60:A:LEU:HD22	1:103:A:PHE:HE2	7	0.6
(1,868)	1:60:A:LEU:HD23	1:103:A:PHE:HE1	7	0.6
(1,868)	1:60:A:LEU:HD23	1:103:A:PHE:HE2	7	0.6
(1,845)	1:97:A:LYS:HD2	1:98:A:SER:H	16	0.6
(1,841)	1:97:A:LYS:HB3	1:98:A:SER:H	8	0.6
(1,841)	1:97:A:LYS:HB3	1:98:A:SER:H	12	0.6
(1,834)	1:94:A:GLN:HE21	1:97:A:LYS:HD2	4	0.6
(1,816)	1:95:A:LYS:HD2	1:96:A:ILE:H	3	0.6
(1,816)	1:95:A:LYS:HD2	1:96:A:ILE:H	9	0.6
(1,785)	1:89:A:ILE:HG21	1:93:A:ILE:H	1	0.6
(1,785)	1:89:A:ILE:HG22	1:93:A:ILE:H	1	0.6
(1,785)	1:89:A:ILE:HG23	1:93:A:ILE:H	1	0.6
(1,752)	1:89:A:ILE:HB	1:91:A:GLY:H	4	0.6
(1,752)	1:89:A:ILE:HB	1:91:A:GLY:H	18	0.6
(1,752)	1:89:A:ILE:HB	1:91:A:GLY:H	20	0.6
(1,747)	1:90:A:ASN:HA	1:158:A:ILE:HD11	8	0.6
(1,747)	1:90:A:ASN:HA	1:158:A:ILE:HD12	8	0.6
(1,747)	1:90:A:ASN:HA	1:158:A:ILE:HD13	8	0.6
(1,689)	1:86:A:LEU:HG	1:90:A:ASN:HD21	9	0.6
(1,672)	1:64:A:HIS:HD2	1:85:A:ALA:H	1	0.6
(1,672)	1:64:A:HIS:HD2	1:85:A:ALA:H	6	0.6
(1,672)	1:64:A:HIS:HD2	1:85:A:ALA:H	12	0.6
(1,672)	1:64:A:HIS:HD2	1:85:A:ALA:H	20	0.6
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG21	17	0.6
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG22	17	0.6
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG23	17	0.6
(1,593)	1:71:A:SER:HB3	1:77:A:LYS:HA	20	0.6
(1,591)	1:74:A:ARG:HE	1:75:A:GLN:H	3	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB1	3	0.6
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB2	3	0.6
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB3	3	0.6
(1,440)	1:59:A:HIS:H	1:115:A:SER:HB3	19	0.6
(1,401)	1:54:A:ARG:HD2	1:55:A:VAL:HA	19	0.6
(1,397)	1:54:A:ARG:HG2	1:126:A:SER:H	6	0.6
(1,296)	1:27:A:HIS:HA	1:30:A:ASN:HD21	11	0.6
(1,204)	1:24:A:TYR:HB2	1:33:A:GLN:HE21	9	0.6
(1,148)	1:15:A:MET:HE1	1:22:A:VAL:HA	18	0.6
(1,148)	1:15:A:MET:HE2	1:22:A:VAL:HA	18	0.6
(1,148)	1:15:A:MET:HE3	1:22:A:VAL:HA	18	0.6
(1,86)	1:13:A:LYS:HE2	1:14:A:ARG:H	5	0.6
(1,86)	1:13:A:LYS:HE2	1:14:A:ARG:H	14	0.6
(1,66)	1:12:A:GLU:H	1:25:A:PHE:HE1	10	0.6
(1,66)	1:12:A:GLU:H	1:25:A:PHE:HE2	10	0.6
(2,98)	1:124:A:ALA:H	2:656:B:PHE:HE1	5	0.59
(2,98)	1:124:A:ALA:H	2:656:B:PHE:HE2	5	0.59
(2,94)	1:93:A:ILE:HG21	2:643:B:PRO:HB3	19	0.59
(2,94)	1:93:A:ILE:HG22	2:643:B:PRO:HB3	19	0.59
(2,94)	1:93:A:ILE:HG23	2:643:B:PRO:HB3	19	0.59
(2,93)	1:93:A:ILE:HD11	2:643:B:PRO:HA	10	0.59
(2,93)	1:93:A:ILE:HD12	2:643:B:PRO:HA	10	0.59
(2,93)	1:93:A:ILE:HD13	2:643:B:PRO:HA	10	0.59
(2,90)	1:56:A:ARG:H	2:651:B:ILE:HG12	20	0.59
(2,90)	1:56:A:ARG:H	2:651:B:ILE:HG13	20	0.59
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD11	19	0.59
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD12	19	0.59
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD13	19	0.59
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG21	20	0.59
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG22	20	0.59
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG23	20	0.59
(2,70)	2:651:B:ILE:HG21	2:656:B:PHE:HE1	6	0.59
(2,70)	2:651:B:ILE:HG21	2:656:B:PHE:HE2	6	0.59
(2,70)	2:651:B:ILE:HG22	2:656:B:PHE:HE1	6	0.59
(2,70)	2:651:B:ILE:HG22	2:656:B:PHE:HE2	6	0.59
(2,70)	2:651:B:ILE:HG23	2:656:B:PHE:HE1	6	0.59
(2,70)	2:651:B:ILE:HG23	2:656:B:PHE:HE2	6	0.59
(2,44)	1:131:A:GLN:HE21	1:153:A:ASP:H	18	0.59
(2,4)	1:21:A:ARG:HE	1:22:A:VAL:H	7	0.59
(1,2591)	1:123:A:GLY:H	2:656:B:PHE:HE1	3	0.59
(1,2591)	1:123:A:GLY:H	2:656:B:PHE:HE2	3	0.59
(1,2588)	1:122:A:LEU:H	2:656:B:PHE:HE1	6	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2588)	1:122:A:LEU:H	2:656:B:PHE:HE2	6	0.59
(1,2578)	1:29:A:THR:HG21	2:646:B:GLU:HA	20	0.59
(1,2578)	1:29:A:THR:HG22	2:646:B:GLU:HA	20	0.59
(1,2578)	1:29:A:THR:HG23	2:646:B:GLU:HA	20	0.59
(1,2533)	2:647:B:VAL:H	2:649:B:ARG:H	14	0.59
(1,2532)	2:648:B:ILE:HG21	2:650:B:ASN:H	15	0.59
(1,2532)	2:648:B:ILE:HG22	2:650:B:ASN:H	15	0.59
(1,2532)	2:648:B:ILE:HG23	2:650:B:ASN:H	15	0.59
(1,2507)	2:643:B:PRO:HA	2:645:B:GLN:H	1	0.59
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD21	20	0.59
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD22	20	0.59
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD23	20	0.59
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD11	2	0.59
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD12	2	0.59
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD13	2	0.59
(1,1326)	1:89:A:ILE:HG21	1:158:A:ILE:HB	2	0.59
(1,1326)	1:89:A:ILE:HG22	1:158:A:ILE:HB	2	0.59
(1,1326)	1:89:A:ILE:HG23	1:158:A:ILE:HB	2	0.59
(1,1326)	1:89:A:ILE:HG21	1:158:A:ILE:HB	11	0.59
(1,1326)	1:89:A:ILE:HG22	1:158:A:ILE:HB	11	0.59
(1,1326)	1:89:A:ILE:HG23	1:158:A:ILE:HB	11	0.59
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD11	6	0.59
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD12	6	0.59
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD13	6	0.59
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD11	12	0.59
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD12	12	0.59
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD13	12	0.59
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG11	13	0.59
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG12	13	0.59
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG13	13	0.59
(1,1227)	1:89:A:ILE:HG12	1:150:A:VAL:H	3	0.59
(1,1217)	1:145:A:GLU:HB3	1:147:A:SER:H	9	0.59
(1,1217)	1:145:A:GLU:HB3	1:147:A:SER:H	10	0.59
(1,1217)	1:145:A:GLU:HB3	1:147:A:SER:H	11	0.59
(1,1215)	1:141:A:LEU:HD21	1:147:A:SER:HB2	13	0.59
(1,1215)	1:141:A:LEU:HD22	1:147:A:SER:HB2	13	0.59
(1,1215)	1:141:A:LEU:HD23	1:147:A:SER:HB2	13	0.59
(1,1130)	1:131:A:GLN:HE21	1:153:A:ASP:HB2	2	0.59
(1,1130)	1:131:A:GLN:HE21	1:153:A:ASP:HB3	2	0.59
(1,1109)	1:126:A:SER:HA	1:139:A:PHE:HD1	5	0.59
(1,1109)	1:126:A:SER:HA	1:139:A:PHE:HD2	5	0.59
(1,1109)	1:126:A:SER:HA	1:139:A:PHE:HD1	6	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1109)	1:126:A:SER:HA	1:139:A:PHE:HD2	6	0.59
(1,1109)	1:126:A:SER:HA	1:139:A:PHE:HD1	20	0.59
(1,1109)	1:126:A:SER:HA	1:139:A:PHE:HD2	20	0.59
(1,1107)	1:54:A:ARG:HD2	1:126:A:SER:HA	13	0.59
(1,1107)	1:54:A:ARG:HD2	1:126:A:SER:HA	15	0.59
(1,1054)	1:59:A:HIS:HD2	1:122:A:LEU:H	18	0.59
(1,995)	1:108:A:SER:HA	1:116:A:ALA:H	10	0.59
(1,889)	1:103:A:PHE:HE1	1:146:A:MET:HE1	19	0.59
(1,889)	1:103:A:PHE:HE1	1:146:A:MET:HE2	19	0.59
(1,889)	1:103:A:PHE:HE1	1:146:A:MET:HE3	19	0.59
(1,889)	1:103:A:PHE:HE2	1:146:A:MET:HE1	19	0.59
(1,889)	1:103:A:PHE:HE2	1:146:A:MET:HE2	19	0.59
(1,889)	1:103:A:PHE:HE2	1:146:A:MET:HE3	19	0.59
(1,888)	1:103:A:PHE:HE1	1:120:A:GLY:H	14	0.59
(1,888)	1:103:A:PHE:HE2	1:120:A:GLY:H	14	0.59
(1,841)	1:97:A:LYS:HB3	1:98:A:SER:H	1	0.59
(1,816)	1:95:A:LYS:HD2	1:96:A:ILE:H	12	0.59
(1,816)	1:95:A:LYS:HD2	1:96:A:ILE:H	17	0.59
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD11	15	0.59
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD12	15	0.59
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD13	15	0.59
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE1	8	0.59
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE2	8	0.59
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE3	8	0.59
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD1	1	0.59
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD2	1	0.59
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD1	2	0.59
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD2	2	0.59
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD1	3	0.59
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD2	3	0.59
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD1	10	0.59
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD2	10	0.59
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD1	11	0.59
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD2	11	0.59
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD1	15	0.59
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD2	15	0.59
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD1	19	0.59
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD2	19	0.59
(1,753)	1:90:A:ASN:HD22	1:91:A:GLY:H	2	0.59
(1,752)	1:89:A:ILE:HB	1:91:A:GLY:H	9	0.59
(1,752)	1:89:A:ILE:HB	1:91:A:GLY:H	14	0.59
(1,752)	1:89:A:ILE:HB	1:91:A:GLY:H	16	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,689)	1:86:A:LEU:HG	1:90:A:ASN:HD21	18	0.59
(1,648)	1:66:A:GLN:HE22	1:82:A:LYS:HG3	4	0.59
(1,612)	1:75:A:GLN:HE21	1:78:A:ILE:HA	17	0.59
(1,572)	1:73:A:TRP:HE1	1:111:A:SER:HB2	16	0.59
(1,572)	1:73:A:TRP:HE1	1:111:A:SER:HB2	18	0.59
(1,554)	1:70:A:PRO:HG3	1:71:A:SER:H	20	0.59
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD21	2	0.59
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD22	2	0.59
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD23	2	0.59
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD21	9	0.59
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD22	9	0.59
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD23	9	0.59
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD21	15	0.59
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD22	15	0.59
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD23	15	0.59
(1,480)	1:61:A:LEU:HD21	1:156:A:ILE:H	13	0.59
(1,480)	1:61:A:LEU:HD22	1:156:A:ILE:H	13	0.59
(1,480)	1:61:A:LEU:HD23	1:156:A:ILE:H	13	0.59
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG21	20	0.59
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG22	20	0.59
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG23	20	0.59
(1,190)	1:13:A:LYS:HB3	1:24:A:TYR:HA	17	0.59
(1,148)	1:15:A:MET:HE1	1:22:A:VAL:HA	8	0.59
(1,148)	1:15:A:MET:HE2	1:22:A:VAL:HA	8	0.59
(1,148)	1:15:A:MET:HE3	1:22:A:VAL:HA	8	0.59
(1,148)	1:15:A:MET:HE1	1:22:A:VAL:HA	9	0.59
(1,148)	1:15:A:MET:HE2	1:22:A:VAL:HA	9	0.59
(1,148)	1:15:A:MET:HE3	1:22:A:VAL:HA	9	0.59
(1,134)	1:20:A:GLY:H	1:21:A:ARG:HA	2	0.59
(1,88)	1:12:A:GLU:HB2	1:14:A:ARG:HE	13	0.59
(1,88)	1:12:A:GLU:HB3	1:14:A:ARG:HE	13	0.59
(1,86)	1:13:A:LYS:HE2	1:14:A:ARG:H	8	0.59
(1,70)	1:12:A:GLU:HG2	1:13:A:LYS:H	5	0.59
(1,70)	1:12:A:GLU:HG2	1:13:A:LYS:H	10	0.59
(1,66)	1:12:A:GLU:H	1:25:A:PHE:HE1	16	0.59
(1,66)	1:12:A:GLU:H	1:25:A:PHE:HE2	16	0.59
(1,56)	1:11:A:TRP:HE1	1:31:A:ALA:HB1	17	0.59
(1,56)	1:11:A:TRP:HE1	1:31:A:ALA:HB2	17	0.59
(1,56)	1:11:A:TRP:HE1	1:31:A:ALA:HB3	17	0.59
(1,35)	1:9:A:PRO:HG2	1:10:A:GLY:H	8	0.59
(2,110)	1:152:A:THR:HG21	2:661:B:PHE:HB2	1	0.58
(2,110)	1:152:A:THR:HG21	2:661:B:PHE:HB3	1	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,110)	1:152:A:THR:HG22	2:661:B:PHE:HB2	1	0.58
(2,110)	1:152:A:THR:HG22	2:661:B:PHE:HB3	1	0.58
(2,110)	1:152:A:THR:HG23	2:661:B:PHE:HB2	1	0.58
(2,110)	1:152:A:THR:HG23	2:661:B:PHE:HB3	1	0.58
(2,106)	1:139:A:PHE:H	2:656:B:PHE:HB2	4	0.58
(2,103)	1:137:A:ALA:H	2:656:B:PHE:HB2	6	0.58
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG11	10	0.58
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG12	10	0.58
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG13	10	0.58
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG21	10	0.58
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG22	10	0.58
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG23	10	0.58
(2,38)	1:126:A:SER:H	1:129:A:GLN:HB2	10	0.58
(1,2587)	1:115:A:SER:H	2:659:B:PHE:HD1	19	0.58
(1,2587)	1:115:A:SER:H	2:659:B:PHE:HD2	19	0.58
(1,2578)	1:29:A:THR:HG21	2:646:B:GLU:HA	5	0.58
(1,2578)	1:29:A:THR:HG22	2:646:B:GLU:HA	5	0.58
(1,2578)	1:29:A:THR:HG23	2:646:B:GLU:HA	5	0.58
(1,2578)	1:29:A:THR:HG21	2:646:B:GLU:HA	6	0.58
(1,2578)	1:29:A:THR:HG22	2:646:B:GLU:HA	6	0.58
(1,2578)	1:29:A:THR:HG23	2:646:B:GLU:HA	6	0.58
(1,2553)	2:651:B:ILE:HG21	2:653:B:GLN:HE21	17	0.58
(1,2553)	2:651:B:ILE:HG21	2:653:B:GLN:HE22	17	0.58
(1,2553)	2:651:B:ILE:HG22	2:653:B:GLN:HE21	17	0.58
(1,2553)	2:651:B:ILE:HG22	2:653:B:GLN:HE22	17	0.58
(1,2553)	2:651:B:ILE:HG23	2:653:B:GLN:HE21	17	0.58
(1,2553)	2:651:B:ILE:HG23	2:653:B:GLN:HE22	17	0.58
(1,2529)	2:648:B:ILE:HG21	2:649:B:ARG:HD2	14	0.58
(1,2529)	2:648:B:ILE:HG22	2:649:B:ARG:HD2	14	0.58
(1,2529)	2:648:B:ILE:HG23	2:649:B:ARG:HD2	14	0.58
(1,2526)	2:646:B:GLU:HB2	2:648:B:ILE:H	6	0.58
(1,2526)	2:646:B:GLU:HB2	2:648:B:ILE:H	7	0.58
(1,2161)	1:119:A:ARG:H	1:119:A:ARG:HD3	12	0.58
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD21	14	0.58
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD22	14	0.58
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD23	14	0.58
(1,1869)	1:75:A:GLN:H	1:75:A:GLN:HE22	7	0.58
(1,1392)	1:160:A:LEU:HD11	1:162:A:THR:HG21	8	0.58
(1,1392)	1:160:A:LEU:HD11	1:162:A:THR:HG22	8	0.58
(1,1392)	1:160:A:LEU:HD11	1:162:A:THR:HG23	8	0.58
(1,1392)	1:160:A:LEU:HD12	1:162:A:THR:HG21	8	0.58
(1,1392)	1:160:A:LEU:HD12	1:162:A:THR:HG22	8	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1392)	1:160:A:LEU:HD12	1:162:A:THR:HG23	8	0.58
(1,1392)	1:160:A:LEU:HD13	1:162:A:THR:HG21	8	0.58
(1,1392)	1:160:A:LEU:HD13	1:162:A:THR:HG22	8	0.58
(1,1392)	1:160:A:LEU:HD13	1:162:A:THR:HG23	8	0.58
(1,1363)	1:96:A:ILE:HG21	1:160:A:LEU:HD11	12	0.58
(1,1363)	1:96:A:ILE:HG21	1:160:A:LEU:HD12	12	0.58
(1,1363)	1:96:A:ILE:HG21	1:160:A:LEU:HD13	12	0.58
(1,1363)	1:96:A:ILE:HG22	1:160:A:LEU:HD11	12	0.58
(1,1363)	1:96:A:ILE:HG22	1:160:A:LEU:HD12	12	0.58
(1,1363)	1:96:A:ILE:HG22	1:160:A:LEU:HD13	12	0.58
(1,1363)	1:96:A:ILE:HG23	1:160:A:LEU:HD11	12	0.58
(1,1363)	1:96:A:ILE:HG23	1:160:A:LEU:HD12	12	0.58
(1,1363)	1:96:A:ILE:HG23	1:160:A:LEU:HD13	12	0.58
(1,1349)	1:158:A:ILE:H	1:159:A:ILE:HD11	4	0.58
(1,1349)	1:158:A:ILE:H	1:159:A:ILE:HD12	4	0.58
(1,1349)	1:158:A:ILE:H	1:159:A:ILE:HD13	4	0.58
(1,1335)	1:57:A:CYS:HA	1:159:A:ILE:HG21	6	0.58
(1,1335)	1:57:A:CYS:HA	1:159:A:ILE:HG22	6	0.58
(1,1335)	1:57:A:CYS:HA	1:159:A:ILE:HG23	6	0.58
(1,1326)	1:89:A:ILE:HG21	1:158:A:ILE:HB	16	0.58
(1,1326)	1:89:A:ILE:HG22	1:158:A:ILE:HB	16	0.58
(1,1326)	1:89:A:ILE:HG23	1:158:A:ILE:HB	16	0.58
(1,1313)	1:156:A:ILE:HA	1:157:A:HIS:HD2	17	0.58
(1,1244)	1:150:A:VAL:HG21	1:157:A:HIS:HB2	16	0.58
(1,1244)	1:150:A:VAL:HG21	1:157:A:HIS:HB3	16	0.58
(1,1244)	1:150:A:VAL:HG22	1:157:A:HIS:HB2	16	0.58
(1,1244)	1:150:A:VAL:HG22	1:157:A:HIS:HB3	16	0.58
(1,1244)	1:150:A:VAL:HG23	1:157:A:HIS:HB2	16	0.58
(1,1244)	1:150:A:VAL:HG23	1:157:A:HIS:HB3	16	0.58
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG11	6	0.58
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG12	6	0.58
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG13	6	0.58
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG11	9	0.58
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG12	9	0.58
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG13	9	0.58
(1,1212)	1:146:A:MET:HG2	1:160:A:LEU:HG	5	0.58
(1,1193)	1:141:A:LEU:HD11	1:148:A:GLY:H	1	0.58
(1,1193)	1:141:A:LEU:HD12	1:148:A:GLY:H	1	0.58
(1,1193)	1:141:A:LEU:HD13	1:148:A:GLY:H	1	0.58
(1,1193)	1:141:A:LEU:HD11	1:148:A:GLY:H	17	0.58
(1,1193)	1:141:A:LEU:HD12	1:148:A:GLY:H	17	0.58
(1,1193)	1:141:A:LEU:HD13	1:148:A:GLY:H	17	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1177)	1:137:A:ALA:HB1	1:141:A:LEU:H	11	0.58
(1,1177)	1:137:A:ALA:HB2	1:141:A:LEU:H	11	0.58
(1,1177)	1:137:A:ALA:HB3	1:141:A:LEU:H	11	0.58
(1,1130)	1:131:A:GLN:HE21	1:153:A:ASP:HB2	10	0.58
(1,1130)	1:131:A:GLN:HE21	1:153:A:ASP:HB3	10	0.58
(1,1122)	1:126:A:SER:H	1:129:A:GLN:HG2	17	0.58
(1,1112)	1:126:A:SER:H	1:129:A:GLN:HE21	1	0.58
(1,1109)	1:126:A:SER:HA	1:139:A:PHE:HD1	12	0.58
(1,1109)	1:126:A:SER:HA	1:139:A:PHE:HD2	12	0.58
(1,1109)	1:126:A:SER:HA	1:139:A:PHE:HD1	18	0.58
(1,1109)	1:126:A:SER:HA	1:139:A:PHE:HD2	18	0.58
(1,1057)	1:59:A:HIS:H	1:122:A:LEU:HG	2	0.58
(1,1052)	1:58:A:SER:HB2	1:122:A:LEU:H	6	0.58
(1,1024)	1:118:A:ALA:HA	1:119:A:ARG:HE	4	0.58
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB1	2	0.58
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB2	2	0.58
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB3	2	0.58
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB1	17	0.58
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB2	17	0.58
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB3	17	0.58
(1,910)	1:102:A:ASP:H	1:106:A:LEU:HB3	7	0.58
(1,871)	1:96:A:ILE:HB	1:103:A:PHE:H	4	0.58
(1,868)	1:60:A:LEU:HD21	1:103:A:PHE:HE1	3	0.58
(1,868)	1:60:A:LEU:HD21	1:103:A:PHE:HE2	3	0.58
(1,868)	1:60:A:LEU:HD22	1:103:A:PHE:HE1	3	0.58
(1,868)	1:60:A:LEU:HD22	1:103:A:PHE:HE2	3	0.58
(1,868)	1:60:A:LEU:HD23	1:103:A:PHE:HE1	3	0.58
(1,868)	1:60:A:LEU:HD23	1:103:A:PHE:HE2	3	0.58
(1,841)	1:97:A:LYS:HB3	1:98:A:SER:H	4	0.58
(1,834)	1:94:A:GLN:HE21	1:97:A:LYS:HD2	9	0.58
(1,816)	1:95:A:LYS:HD2	1:96:A:ILE:H	14	0.58
(1,816)	1:95:A:LYS:HD2	1:96:A:ILE:H	15	0.58
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD1	5	0.58
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD2	5	0.58
(1,752)	1:89:A:ILE:HB	1:91:A:GLY:H	2	0.58
(1,752)	1:89:A:ILE:HB	1:91:A:GLY:H	7	0.58
(1,672)	1:64:A:HIS:HD2	1:85:A:ALA:H	17	0.58
(1,672)	1:64:A:HIS:HD2	1:85:A:ALA:H	19	0.58
(1,648)	1:66:A:GLN:HE22	1:82:A:LYS:HG3	1	0.58
(1,637)	1:80:A:ARG:HE	1:85:A:ALA:H	6	0.58
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG21	5	0.58
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG22	5	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG23	5	0.58
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG21	11	0.58
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG22	11	0.58
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG23	11	0.58
(1,593)	1:71:A:SER:HB3	1:77:A:LYS:HA	4	0.58
(1,593)	1:71:A:SER:HB3	1:77:A:LYS:HA	5	0.58
(1,593)	1:71:A:SER:HB3	1:77:A:LYS:HA	14	0.58
(1,592)	1:75:A:GLN:HB2	1:77:A:LYS:H	13	0.58
(1,571)	1:73:A:TRP:HE1	1:74:A:ARG:HB3	15	0.58
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD21	3	0.58
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD22	3	0.58
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD23	3	0.58
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD21	4	0.58
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD22	4	0.58
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD23	4	0.58
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD21	16	0.58
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD22	16	0.58
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD23	16	0.58
(1,397)	1:54:A:ARG:HG2	1:126:A:SER:H	3	0.58
(1,350)	1:23:A:TYR:HE1	1:32:A:SER:HB2	13	0.58
(1,350)	1:23:A:TYR:HE2	1:32:A:SER:HB2	13	0.58
(1,224)	1:14:A:ARG:HE	1:25:A:PHE:HB3	1	0.58
(1,214)	1:11:A:TRP:HB2	1:25:A:PHE:H	15	0.58
(1,204)	1:24:A:TYR:HB2	1:33:A:GLN:HE21	7	0.58
(1,190)	1:13:A:LYS:HB3	1:24:A:TYR:HA	5	0.58
(1,190)	1:13:A:LYS:HB3	1:24:A:TYR:HA	11	0.58
(1,138)	1:21:A:ARG:HE	1:34:A:TRP:HH2	18	0.58
(1,66)	1:12:A:GLU:H	1:25:A:PHE:HE1	18	0.58
(1,66)	1:12:A:GLU:H	1:25:A:PHE:HE2	18	0.58
(1,64)	1:12:A:GLU:H	1:24:A:TYR:HD1	6	0.58
(1,64)	1:12:A:GLU:H	1:24:A:TYR:HD2	6	0.58
(1,35)	1:9:A:PRO:HG2	1:10:A:GLY:H	13	0.58
(2,106)	1:139:A:PHE:H	2:656:B:PHE:HB2	14	0.57
(2,103)	1:137:A:ALA:H	2:656:B:PHE:HB2	3	0.57
(2,103)	1:137:A:ALA:H	2:656:B:PHE:HB2	9	0.57
(2,94)	1:93:A:ILE:HG21	2:643:B:PRO:HB3	2	0.57
(2,94)	1:93:A:ILE:HG22	2:643:B:PRO:HB3	2	0.57
(2,94)	1:93:A:ILE:HG23	2:643:B:PRO:HB3	2	0.57
(2,82)	2:660:B:SEP:HA	2:661:B:PHE:HD1	2	0.57
(2,82)	2:660:B:SEP:HA	2:661:B:PHE:HD2	2	0.57
(2,79)	2:659:B:PHE:HE1	2:661:B:PHE:H	11	0.57
(2,79)	2:659:B:PHE:HE2	2:661:B:PHE:H	11	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,52)	1:141:A:LEU:HD21	1:148:A:GLY:H	8	0.57
(2,52)	1:141:A:LEU:HD22	1:148:A:GLY:H	8	0.57
(2,52)	1:141:A:LEU:HD23	1:148:A:GLY:H	8	0.57
(2,42)	1:130:A:MET:HB2	1:134:A:PHE:HD1	8	0.57
(2,42)	1:130:A:MET:HB2	1:134:A:PHE:HD2	8	0.57
(2,9)	1:53:A:ALA:H	1:54:A:ARG:HD2	14	0.57
(1,2588)	1:122:A:LEU:H	2:656:B:PHE:HE1	7	0.57
(1,2588)	1:122:A:LEU:H	2:656:B:PHE:HE2	7	0.57
(1,2587)	1:115:A:SER:H	2:659:B:PHE:HD1	8	0.57
(1,2587)	1:115:A:SER:H	2:659:B:PHE:HD2	8	0.57
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG21	9	0.57
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG22	9	0.57
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG23	9	0.57
(1,2568)	2:658:B:GLY:H	2:659:B:PHE:HD1	14	0.57
(1,2568)	2:658:B:GLY:H	2:659:B:PHE:HD2	14	0.57
(1,2533)	2:647:B:VAL:H	2:649:B:ARG:H	12	0.57
(1,2524)	2:647:B:VAL:HG11	2:650:B:ASN:HD22	5	0.57
(1,2524)	2:647:B:VAL:HG12	2:650:B:ASN:HD22	5	0.57
(1,2524)	2:647:B:VAL:HG13	2:650:B:ASN:HD22	5	0.57
(1,2524)	2:647:B:VAL:HG11	2:650:B:ASN:HD22	12	0.57
(1,2524)	2:647:B:VAL:HG12	2:650:B:ASN:HD22	12	0.57
(1,2524)	2:647:B:VAL:HG13	2:650:B:ASN:HD22	12	0.57
(1,2161)	1:119:A:ARG:H	1:119:A:ARG:HD3	2	0.57
(1,2161)	1:119:A:ARG:H	1:119:A:ARG:HD3	8	0.57
(1,2161)	1:119:A:ARG:H	1:119:A:ARG:HD3	9	0.57
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD21	3	0.57
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD22	3	0.57
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD23	3	0.57
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD21	10	0.57
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD22	10	0.57
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD23	10	0.57
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD21	15	0.57
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD22	15	0.57
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD23	15	0.57
(1,1869)	1:75:A:GLN:H	1:75:A:GLN:HE22	8	0.57
(1,1434)	1:161:A:ARG:HD2	1:163:A:GLU:H	13	0.57
(1,1410)	1:161:A:ARG:HE	1:163:A:GLU:HG2	11	0.57
(1,1410)	1:161:A:ARG:HE	1:163:A:GLU:HG2	18	0.57
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD11	18	0.57
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD12	18	0.57
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD13	18	0.57
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG11	8	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG12	8	0.57
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG13	8	0.57
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG11	15	0.57
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG12	15	0.57
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG13	15	0.57
(1,1130)	1:131:A:GLN:HE21	1:153:A:ASP:HB2	3	0.57
(1,1130)	1:131:A:GLN:HE21	1:153:A:ASP:HB3	3	0.57
(1,1130)	1:131:A:GLN:HE21	1:153:A:ASP:HB2	13	0.57
(1,1130)	1:131:A:GLN:HE21	1:153:A:ASP:HB3	13	0.57
(1,1130)	1:131:A:GLN:HE21	1:153:A:ASP:HB2	17	0.57
(1,1130)	1:131:A:GLN:HE21	1:153:A:ASP:HB3	17	0.57
(1,1112)	1:126:A:SER:H	1:129:A:GLN:HE21	6	0.57
(1,1051)	1:57:A:CYS:H	1:122:A:LEU:HD21	8	0.57
(1,1051)	1:57:A:CYS:H	1:122:A:LEU:HD22	8	0.57
(1,1051)	1:57:A:CYS:H	1:122:A:LEU:HD23	8	0.57
(1,1033)	1:108:A:SER:H	1:119:A:ARG:HB2	17	0.57
(1,1033)	1:108:A:SER:H	1:119:A:ARG:HB2	19	0.57
(1,1032)	1:107:A:ALA:HB1	1:119:A:ARG:H	20	0.57
(1,1032)	1:107:A:ALA:HB2	1:119:A:ARG:H	20	0.57
(1,1032)	1:107:A:ALA:HB3	1:119:A:ARG:H	20	0.57
(1,1024)	1:118:A:ALA:HA	1:119:A:ARG:HE	1	0.57
(1,1024)	1:118:A:ALA:HA	1:119:A:ARG:HE	6	0.57
(1,1024)	1:118:A:ALA:HA	1:119:A:ARG:HE	8	0.57
(1,1024)	1:118:A:ALA:HA	1:119:A:ARG:HE	19	0.57
(1,985)	1:61:A:LEU:HD21	1:113:A:CYS:HA	11	0.57
(1,985)	1:61:A:LEU:HD22	1:113:A:CYS:HA	11	0.57
(1,985)	1:61:A:LEU:HD23	1:113:A:CYS:HA	11	0.57
(1,868)	1:60:A:LEU:HD21	1:103:A:PHE:HE1	1	0.57
(1,868)	1:60:A:LEU:HD21	1:103:A:PHE:HE2	1	0.57
(1,868)	1:60:A:LEU:HD22	1:103:A:PHE:HE1	1	0.57
(1,868)	1:60:A:LEU:HD22	1:103:A:PHE:HE2	1	0.57
(1,868)	1:60:A:LEU:HD23	1:103:A:PHE:HE1	1	0.57
(1,868)	1:60:A:LEU:HD23	1:103:A:PHE:HE2	1	0.57
(1,841)	1:97:A:LYS:HB3	1:98:A:SER:H	7	0.57
(1,841)	1:97:A:LYS:HB3	1:98:A:SER:H	14	0.57
(1,834)	1:94:A:GLN:HE21	1:97:A:LYS:HD2	20	0.57
(1,814)	1:94:A:GLN:HG2	1:95:A:LYS:H	2	0.57
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD11	20	0.57
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD12	20	0.57
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD13	20	0.57
(1,785)	1:89:A:ILE:HG21	1:93:A:ILE:H	9	0.57
(1,785)	1:89:A:ILE:HG22	1:93:A:ILE:H	9	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,785)	1:89:A:ILE:HG23	1:93:A:ILE:H	9	0.57
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD11	20	0.57
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD12	20	0.57
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD13	20	0.57
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD11	20	0.57
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD12	20	0.57
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD13	20	0.57
(1,752)	1:89:A:ILE:HB	1:91:A:GLY:H	10	0.57
(1,647)	1:65:A:SER:H	1:82:A:LYS:H	15	0.57
(1,637)	1:80:A:ARG:HE	1:85:A:ALA:H	1	0.57
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG21	20	0.57
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG22	20	0.57
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG23	20	0.57
(1,608)	1:75:A:GLN:HE22	1:78:A:ILE:HD11	20	0.57
(1,608)	1:75:A:GLN:HE22	1:78:A:ILE:HD12	20	0.57
(1,608)	1:75:A:GLN:HE22	1:78:A:ILE:HD13	20	0.57
(1,593)	1:71:A:SER:HB3	1:77:A:LYS:HA	1	0.57
(1,591)	1:74:A:ARG:HE	1:75:A:GLN:H	16	0.57
(1,572)	1:73:A:TRP:HE1	1:111:A:SER:HB2	10	0.57
(1,571)	1:73:A:TRP:HE1	1:74:A:ARG:HB3	10	0.57
(1,564)	1:72:A:SER:H	1:78:A:ILE:HG12	17	0.57
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD21	1	0.57
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD22	1	0.57
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD23	1	0.57
(1,401)	1:54:A:ARG:HD2	1:55:A:VAL:HA	5	0.57
(1,397)	1:54:A:ARG:HG2	1:126:A:SER:H	17	0.57
(1,397)	1:54:A:ARG:HG2	1:126:A:SER:H	18	0.57
(1,384)	1:7:A:LEU:HD21	1:36:A:ARG:HA	13	0.57
(1,384)	1:7:A:LEU:HD22	1:36:A:ARG:HA	13	0.57
(1,384)	1:7:A:LEU:HD23	1:36:A:ARG:HA	13	0.57
(1,366)	1:32:A:SER:H	1:33:A:GLN:HE22	5	0.57
(1,366)	1:32:A:SER:H	1:33:A:GLN:HE21	5	0.57
(1,287)	1:26:A:ASN:H	1:32:A:SER:HB2	12	0.57
(1,256)	1:23:A:TYR:HE1	1:26:A:ASN:H	10	0.57
(1,256)	1:23:A:TYR:HE2	1:26:A:ASN:H	10	0.57
(1,256)	1:23:A:TYR:HE1	1:26:A:ASN:H	15	0.57
(1,256)	1:23:A:TYR:HE2	1:26:A:ASN:H	15	0.57
(1,214)	1:11:A:TRP:HB2	1:25:A:PHE:H	4	0.57
(1,214)	1:11:A:TRP:HB2	1:25:A:PHE:H	6	0.57
(1,204)	1:24:A:TYR:HB2	1:33:A:GLN:HE21	6	0.57
(1,190)	1:13:A:LYS:HB3	1:24:A:TYR:HA	1	0.57
(1,190)	1:13:A:LYS:HB3	1:24:A:TYR:HA	14	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,148)	1:15:A:MET:HE1	1:22:A:VAL:HA	1	0.57
(1,148)	1:15:A:MET:HE2	1:22:A:VAL:HA	1	0.57
(1,148)	1:15:A:MET:HE3	1:22:A:VAL:HA	1	0.57
(1,148)	1:15:A:MET:HE1	1:22:A:VAL:HA	2	0.57
(1,148)	1:15:A:MET:HE2	1:22:A:VAL:HA	2	0.57
(1,148)	1:15:A:MET:HE3	1:22:A:VAL:HA	2	0.57
(1,148)	1:15:A:MET:HE1	1:22:A:VAL:HA	5	0.57
(1,148)	1:15:A:MET:HE2	1:22:A:VAL:HA	5	0.57
(1,148)	1:15:A:MET:HE3	1:22:A:VAL:HA	5	0.57
(1,86)	1:13:A:LYS:HE2	1:14:A:ARG:H	6	0.57
(1,86)	1:13:A:LYS:HE2	1:14:A:ARG:H	11	0.57
(1,70)	1:12:A:GLU:HG2	1:13:A:LYS:H	14	0.57
(1,64)	1:12:A:GLU:H	1:24:A:TYR:HD1	5	0.57
(1,64)	1:12:A:GLU:H	1:24:A:TYR:HD2	5	0.57
(2,106)	1:139:A:PHE:H	2:656:B:PHE:HB2	7	0.56
(2,106)	1:139:A:PHE:H	2:656:B:PHE:HB2	8	0.56
(2,106)	1:139:A:PHE:H	2:656:B:PHE:HB2	12	0.56
(2,98)	1:124:A:ALA:H	2:656:B:PHE:HE1	6	0.56
(2,98)	1:124:A:ALA:H	2:656:B:PHE:HE2	6	0.56
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG11	1	0.56
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG12	1	0.56
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG13	1	0.56
(2,66)	2:645:B:GLN:H	2:648:B:ILE:H	17	0.56
(2,45)	1:131:A:GLN:HE21	1:152:A:THR:HB	11	0.56
(2,38)	1:126:A:SER:H	1:129:A:GLN:HB2	19	0.56
(2,26)	1:94:A:GLN:HE21	1:97:A:LYS:HB3	5	0.56
(1,2591)	1:123:A:GLY:H	2:656:B:PHE:HE1	12	0.56
(1,2591)	1:123:A:GLY:H	2:656:B:PHE:HE2	12	0.56
(1,2584)	1:114:A:SER:H	2:659:B:PHE:HD1	9	0.56
(1,2584)	1:114:A:SER:H	2:659:B:PHE:HD2	9	0.56
(1,2524)	2:647:B:VAL:HG11	2:650:B:ASN:HD22	4	0.56
(1,2524)	2:647:B:VAL:HG12	2:650:B:ASN:HD22	4	0.56
(1,2524)	2:647:B:VAL:HG13	2:650:B:ASN:HD22	4	0.56
(1,2514)	2:646:B:GLU:HA	2:649:B:ARG:H	14	0.56
(1,2161)	1:119:A:ARG:H	1:119:A:ARG:HD3	14	0.56
(1,2161)	1:119:A:ARG:H	1:119:A:ARG:HD3	18	0.56
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD21	2	0.56
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD22	2	0.56
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD23	2	0.56
(1,1406)	1:147:A:SER:H	1:161:A:ARG:H	3	0.56
(1,1378)	1:147:A:SER:H	1:160:A:LEU:H	3	0.56
(1,1349)	1:158:A:ILE:H	1:159:A:ILE:HD11	19	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1349)	1:158:A:ILE:H	1:159:A:ILE:HD12	19	0.56
(1,1349)	1:158:A:ILE:H	1:159:A:ILE:HD13	19	0.56
(1,1306)	1:89:A:ILE:HD11	1:157:A:HIS:HD2	17	0.56
(1,1306)	1:89:A:ILE:HD12	1:157:A:HIS:HD2	17	0.56
(1,1306)	1:89:A:ILE:HD13	1:157:A:HIS:HD2	17	0.56
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD11	11	0.56
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD12	11	0.56
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD13	11	0.56
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD11	17	0.56
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD12	17	0.56
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD13	17	0.56
(1,1282)	1:82:A:LYS:HE2	1:156:A:ILE:HD11	10	0.56
(1,1282)	1:82:A:LYS:HE2	1:156:A:ILE:HD12	10	0.56
(1,1282)	1:82:A:LYS:HE2	1:156:A:ILE:HD13	10	0.56
(1,1217)	1:145:A:GLU:HB3	1:147:A:SER:H	8	0.56
(1,1130)	1:131:A:GLN:HE21	1:153:A:ASP:HB2	7	0.56
(1,1130)	1:131:A:GLN:HE21	1:153:A:ASP:HB3	7	0.56
(1,1109)	1:126:A:SER:HA	1:139:A:PHE:HD1	14	0.56
(1,1109)	1:126:A:SER:HA	1:139:A:PHE:HD2	14	0.56
(1,1107)	1:54:A:ARG:HD2	1:126:A:SER:HA	19	0.56
(1,1051)	1:57:A:CYS:H	1:122:A:LEU:HD21	5	0.56
(1,1051)	1:57:A:CYS:H	1:122:A:LEU:HD22	5	0.56
(1,1051)	1:57:A:CYS:H	1:122:A:LEU:HD23	5	0.56
(1,1051)	1:57:A:CYS:H	1:122:A:LEU:HD21	9	0.56
(1,1051)	1:57:A:CYS:H	1:122:A:LEU:HD22	9	0.56
(1,1051)	1:57:A:CYS:H	1:122:A:LEU:HD23	9	0.56
(1,1033)	1:108:A:SER:H	1:119:A:ARG:HB2	11	0.56
(1,1033)	1:108:A:SER:H	1:119:A:ARG:HB2	13	0.56
(1,1032)	1:107:A:ALA:HB1	1:119:A:ARG:H	7	0.56
(1,1032)	1:107:A:ALA:HB2	1:119:A:ARG:H	7	0.56
(1,1032)	1:107:A:ALA:HB3	1:119:A:ARG:H	7	0.56
(1,1024)	1:118:A:ALA:HA	1:119:A:ARG:HE	7	0.56
(1,1024)	1:118:A:ALA:HA	1:119:A:ARG:HE	9	0.56
(1,1024)	1:118:A:ALA:HA	1:119:A:ARG:HE	11	0.56
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB1	3	0.56
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB2	3	0.56
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB3	3	0.56
(1,995)	1:108:A:SER:HA	1:116:A:ALA:H	2	0.56
(1,910)	1:102:A:ASP:H	1:106:A:LEU:HB3	18	0.56
(1,886)	1:103:A:PHE:HE1	1:107:A:ALA:H	14	0.56
(1,886)	1:103:A:PHE:HE2	1:107:A:ALA:H	14	0.56
(1,868)	1:60:A:LEU:HD21	1:103:A:PHE:HE1	6	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,868)	1:60:A:LEU:HD21	1:103:A:PHE:HE2	6	0.56
(1,868)	1:60:A:LEU:HD22	1:103:A:PHE:HE1	6	0.56
(1,868)	1:60:A:LEU:HD22	1:103:A:PHE:HE2	6	0.56
(1,868)	1:60:A:LEU:HD23	1:103:A:PHE:HE1	6	0.56
(1,868)	1:60:A:LEU:HD23	1:103:A:PHE:HE2	6	0.56
(1,868)	1:60:A:LEU:HD21	1:103:A:PHE:HE1	17	0.56
(1,868)	1:60:A:LEU:HD21	1:103:A:PHE:HE2	17	0.56
(1,868)	1:60:A:LEU:HD22	1:103:A:PHE:HE1	17	0.56
(1,868)	1:60:A:LEU:HD22	1:103:A:PHE:HE2	17	0.56
(1,868)	1:60:A:LEU:HD23	1:103:A:PHE:HE1	17	0.56
(1,868)	1:60:A:LEU:HD23	1:103:A:PHE:HE2	17	0.56
(1,845)	1:97:A:LYS:HD2	1:98:A:SER:H	2	0.56
(1,845)	1:97:A:LYS:HD2	1:98:A:SER:H	18	0.56
(1,834)	1:94:A:GLN:HE21	1:97:A:LYS:HD2	6	0.56
(1,816)	1:95:A:LYS:HD2	1:96:A:ILE:H	16	0.56
(1,816)	1:95:A:LYS:HD2	1:96:A:ILE:H	18	0.56
(1,814)	1:94:A:GLN:HG2	1:95:A:LYS:H	11	0.56
(1,785)	1:89:A:ILE:HG21	1:93:A:ILE:H	19	0.56
(1,785)	1:89:A:ILE:HG22	1:93:A:ILE:H	19	0.56
(1,785)	1:89:A:ILE:HG23	1:93:A:ILE:H	19	0.56
(1,785)	1:89:A:ILE:HG21	1:93:A:ILE:H	20	0.56
(1,785)	1:89:A:ILE:HG22	1:93:A:ILE:H	20	0.56
(1,785)	1:89:A:ILE:HG23	1:93:A:ILE:H	20	0.56
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD1	4	0.56
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD2	4	0.56
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD1	7	0.56
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD2	7	0.56
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD1	8	0.56
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD2	8	0.56
(1,752)	1:89:A:ILE:HB	1:91:A:GLY:H	3	0.56
(1,752)	1:89:A:ILE:HB	1:91:A:GLY:H	15	0.56
(1,747)	1:90:A:ASN:HA	1:158:A:ILE:HD11	5	0.56
(1,747)	1:90:A:ASN:HA	1:158:A:ILE:HD12	5	0.56
(1,747)	1:90:A:ASN:HA	1:158:A:ILE:HD13	5	0.56
(1,728)	1:89:A:ILE:HD11	1:92:A:TYR:HE1	13	0.56
(1,728)	1:89:A:ILE:HD11	1:92:A:TYR:HE2	13	0.56
(1,728)	1:89:A:ILE:HD12	1:92:A:TYR:HE1	13	0.56
(1,728)	1:89:A:ILE:HD12	1:92:A:TYR:HE2	13	0.56
(1,728)	1:89:A:ILE:HD13	1:92:A:TYR:HE1	13	0.56
(1,728)	1:89:A:ILE:HD13	1:92:A:TYR:HE2	13	0.56
(1,648)	1:66:A:GLN:HE22	1:82:A:LYS:HG3	18	0.56
(1,593)	1:71:A:SER:HB3	1:77:A:LYS:HA	8	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,591)	1:74:A:ARG:HE	1:75:A:GLN:H	2	0.56
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB1	4	0.56
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB2	4	0.56
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB3	4	0.56
(1,572)	1:73:A:TRP:HE1	1:111:A:SER:HB2	6	0.56
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD21	19	0.56
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD22	19	0.56
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD23	19	0.56
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD21	20	0.56
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD22	20	0.56
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD23	20	0.56
(1,435)	1:58:A:SER:HA	1:122:A:LEU:HG	11	0.56
(1,214)	1:11:A:TRP:HB2	1:25:A:PHE:H	13	0.56
(1,204)	1:24:A:TYR:HB2	1:33:A:GLN:HE21	3	0.56
(1,204)	1:24:A:TYR:HB2	1:33:A:GLN:HE21	8	0.56
(1,178)	1:23:A:TYR:HE1	1:33:A:GLN:H	13	0.56
(1,178)	1:23:A:TYR:HE2	1:33:A:GLN:H	13	0.56
(1,176)	1:23:A:TYR:HB3	1:24:A:TYR:HD1	4	0.56
(1,176)	1:23:A:TYR:HB3	1:24:A:TYR:HD2	4	0.56
(1,176)	1:23:A:TYR:HB3	1:24:A:TYR:HD1	20	0.56
(1,176)	1:23:A:TYR:HB3	1:24:A:TYR:HD2	20	0.56
(1,148)	1:15:A:MET:HE1	1:22:A:VAL:HA	4	0.56
(1,148)	1:15:A:MET:HE2	1:22:A:VAL:HA	4	0.56
(1,148)	1:15:A:MET:HE3	1:22:A:VAL:HA	4	0.56
(1,148)	1:15:A:MET:HE1	1:22:A:VAL:HA	6	0.56
(1,148)	1:15:A:MET:HE2	1:22:A:VAL:HA	6	0.56
(1,148)	1:15:A:MET:HE3	1:22:A:VAL:HA	6	0.56
(1,148)	1:15:A:MET:HE1	1:22:A:VAL:HA	7	0.56
(1,148)	1:15:A:MET:HE2	1:22:A:VAL:HA	7	0.56
(1,148)	1:15:A:MET:HE3	1:22:A:VAL:HA	7	0.56
(1,138)	1:21:A:ARG:HE	1:34:A:TRP:HH2	7	0.56
(1,86)	1:13:A:LYS:HE2	1:14:A:ARG:H	7	0.56
(1,86)	1:13:A:LYS:HE2	1:14:A:ARG:H	19	0.56
(1,70)	1:12:A:GLU:HG2	1:13:A:LYS:H	7	0.56
(1,64)	1:12:A:GLU:H	1:24:A:TYR:HD1	20	0.56
(1,64)	1:12:A:GLU:H	1:24:A:TYR:HD2	20	0.56
(1,14)	1:6:A:LYS:HG2	1:7:A:LEU:H	15	0.56
(2,110)	1:152:A:THR:HG21	2:661:B:PHE:HB2	6	0.55
(2,110)	1:152:A:THR:HG21	2:661:B:PHE:HB3	6	0.55
(2,110)	1:152:A:THR:HG22	2:661:B:PHE:HB2	6	0.55
(2,110)	1:152:A:THR:HG22	2:661:B:PHE:HB3	6	0.55
(2,110)	1:152:A:THR:HG23	2:661:B:PHE:HB2	6	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,110)	1:152:A:THR:HG23	2:661:B:PHE:HB3	6	0.55
(2,98)	1:124:A:ALA:H	2:656:B:PHE:HE1	4	0.55
(2,98)	1:124:A:ALA:H	2:656:B:PHE:HE2	4	0.55
(2,34)	1:59:A:HIS:H	1:122:A:LEU:HB2	10	0.55
(1,2591)	1:123:A:GLY:H	2:656:B:PHE:HE1	9	0.55
(1,2591)	1:123:A:GLY:H	2:656:B:PHE:HE2	9	0.55
(1,2588)	1:122:A:LEU:H	2:656:B:PHE:HE1	17	0.55
(1,2588)	1:122:A:LEU:H	2:656:B:PHE:HE2	17	0.55
(1,2586)	1:115:A:SER:H	2:659:B:PHE:HE1	16	0.55
(1,2586)	1:115:A:SER:H	2:659:B:PHE:HE2	16	0.55
(1,2584)	1:114:A:SER:H	2:659:B:PHE:HD1	14	0.55
(1,2584)	1:114:A:SER:H	2:659:B:PHE:HD2	14	0.55
(1,2533)	2:647:B:VAL:H	2:649:B:ARG:H	6	0.55
(1,2532)	2:648:B:ILE:HG21	2:650:B:ASN:H	18	0.55
(1,2532)	2:648:B:ILE:HG22	2:650:B:ASN:H	18	0.55
(1,2532)	2:648:B:ILE:HG23	2:650:B:ASN:H	18	0.55
(1,2526)	2:646:B:GLU:HB2	2:648:B:ILE:H	4	0.55
(1,2525)	2:645:B:GLN:HE22	2:648:B:ILE:HD11	10	0.55
(1,2525)	2:645:B:GLN:HE22	2:648:B:ILE:HD12	10	0.55
(1,2525)	2:645:B:GLN:HE22	2:648:B:ILE:HD13	10	0.55
(1,2524)	2:647:B:VAL:HG11	2:650:B:ASN:HD22	7	0.55
(1,2524)	2:647:B:VAL:HG12	2:650:B:ASN:HD22	7	0.55
(1,2524)	2:647:B:VAL:HG13	2:650:B:ASN:HD22	7	0.55
(1,2507)	2:643:B:PRO:HA	2:645:B:GLN:H	3	0.55
(1,2161)	1:119:A:ARG:H	1:119:A:ARG:HD3	1	0.55
(1,2161)	1:119:A:ARG:H	1:119:A:ARG:HD3	3	0.55
(1,2161)	1:119:A:ARG:H	1:119:A:ARG:HD3	5	0.55
(1,2161)	1:119:A:ARG:H	1:119:A:ARG:HD3	6	0.55
(1,2161)	1:119:A:ARG:H	1:119:A:ARG:HD3	7	0.55
(1,2161)	1:119:A:ARG:H	1:119:A:ARG:HD3	20	0.55
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD21	5	0.55
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD22	5	0.55
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD23	5	0.55
(1,2056)	1:101:A:GLU:H	1:101:A:GLU:HG2	16	0.55
(1,2045)	1:97:A:LYS:H	1:97:A:LYS:HD2	1	0.55
(1,1504)	1:13:A:LYS:H	1:13:A:LYS:HE2	11	0.55
(1,1456)	1:6:A:LYS:H	1:6:A:LYS:HE2	2	0.55
(1,1441)	1:162:A:THR:HG21	1:163:A:GLU:HG3	19	0.55
(1,1441)	1:162:A:THR:HG22	1:163:A:GLU:HG3	19	0.55
(1,1441)	1:162:A:THR:HG23	1:163:A:GLU:HG3	19	0.55
(1,1423)	1:55:A:VAL:HB	1:163:A:GLU:H	18	0.55
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD11	13	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD12	13	0.55
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD13	13	0.55
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD11	19	0.55
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD12	19	0.55
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD13	19	0.55
(1,1348)	1:157:A:HIS:HB2	1:159:A:ILE:HD11	6	0.55
(1,1348)	1:157:A:HIS:HB2	1:159:A:ILE:HD12	6	0.55
(1,1348)	1:157:A:HIS:HB2	1:159:A:ILE:HD13	6	0.55
(1,1348)	1:157:A:HIS:HB3	1:159:A:ILE:HD11	6	0.55
(1,1348)	1:157:A:HIS:HB3	1:159:A:ILE:HD12	6	0.55
(1,1348)	1:157:A:HIS:HB3	1:159:A:ILE:HD13	6	0.55
(1,1326)	1:89:A:ILE:HG21	1:158:A:ILE:HB	14	0.55
(1,1326)	1:89:A:ILE:HG22	1:158:A:ILE:HB	14	0.55
(1,1326)	1:89:A:ILE:HG23	1:158:A:ILE:HB	14	0.55
(1,1326)	1:89:A:ILE:HG21	1:158:A:ILE:HB	20	0.55
(1,1326)	1:89:A:ILE:HG22	1:158:A:ILE:HB	20	0.55
(1,1326)	1:89:A:ILE:HG23	1:158:A:ILE:HB	20	0.55
(1,1303)	1:156:A:ILE:HG21	1:157:A:HIS:HD2	18	0.55
(1,1303)	1:156:A:ILE:HG22	1:157:A:HIS:HD2	18	0.55
(1,1303)	1:156:A:ILE:HG23	1:157:A:HIS:HD2	18	0.55
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG21	13	0.55
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG22	13	0.55
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG23	13	0.55
(1,1280)	1:64:A:HIS:HD2	1:156:A:ILE:HG12	6	0.55
(1,1217)	1:145:A:GLU:HB3	1:147:A:SER:H	12	0.55
(1,1217)	1:145:A:GLU:HB3	1:147:A:SER:H	15	0.55
(1,1208)	1:103:A:PHE:HD1	1:146:A:MET:HB2	13	0.55
(1,1208)	1:103:A:PHE:HD2	1:146:A:MET:HB2	13	0.55
(1,1206)	1:145:A:GLU:HB3	1:146:A:MET:HB2	6	0.55
(1,1193)	1:141:A:LEU:HD11	1:148:A:GLY:H	5	0.55
(1,1193)	1:141:A:LEU:HD12	1:148:A:GLY:H	5	0.55
(1,1193)	1:141:A:LEU:HD13	1:148:A:GLY:H	5	0.55
(1,1193)	1:141:A:LEU:HD11	1:148:A:GLY:H	8	0.55
(1,1193)	1:141:A:LEU:HD12	1:148:A:GLY:H	8	0.55
(1,1193)	1:141:A:LEU:HD13	1:148:A:GLY:H	8	0.55
(1,1193)	1:141:A:LEU:HD11	1:148:A:GLY:H	14	0.55
(1,1193)	1:141:A:LEU:HD12	1:148:A:GLY:H	14	0.55
(1,1193)	1:141:A:LEU:HD13	1:148:A:GLY:H	14	0.55
(1,1193)	1:141:A:LEU:HD11	1:148:A:GLY:H	15	0.55
(1,1193)	1:141:A:LEU:HD12	1:148:A:GLY:H	15	0.55
(1,1193)	1:141:A:LEU:HD13	1:148:A:GLY:H	15	0.55
(1,1130)	1:131:A:GLN:HE21	1:153:A:ASP:HB2	16	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1130)	1:131:A:GLN:HE21	1:153:A:ASP:HB3	16	0.55
(1,1080)	1:54:A:ARG:HE	1:124:A:ALA:HB1	4	0.55
(1,1080)	1:54:A:ARG:HE	1:124:A:ALA:HB2	4	0.55
(1,1080)	1:54:A:ARG:HE	1:124:A:ALA:HB3	4	0.55
(1,1057)	1:59:A:HIS:H	1:122:A:LEU:HG	19	0.55
(1,1057)	1:59:A:HIS:H	1:122:A:LEU:HG	20	0.55
(1,1033)	1:108:A:SER:H	1:119:A:ARG:HB2	20	0.55
(1,1032)	1:107:A:ALA:HB1	1:119:A:ARG:H	2	0.55
(1,1032)	1:107:A:ALA:HB2	1:119:A:ARG:H	2	0.55
(1,1032)	1:107:A:ALA:HB3	1:119:A:ARG:H	2	0.55
(1,1032)	1:107:A:ALA:HB1	1:119:A:ARG:H	6	0.55
(1,1032)	1:107:A:ALA:HB2	1:119:A:ARG:H	6	0.55
(1,1032)	1:107:A:ALA:HB3	1:119:A:ARG:H	6	0.55
(1,1032)	1:107:A:ALA:HB1	1:119:A:ARG:H	14	0.55
(1,1032)	1:107:A:ALA:HB2	1:119:A:ARG:H	14	0.55
(1,1032)	1:107:A:ALA:HB3	1:119:A:ARG:H	14	0.55
(1,1032)	1:107:A:ALA:HB1	1:119:A:ARG:H	19	0.55
(1,1032)	1:107:A:ALA:HB2	1:119:A:ARG:H	19	0.55
(1,1032)	1:107:A:ALA:HB3	1:119:A:ARG:H	19	0.55
(1,995)	1:108:A:SER:HA	1:116:A:ALA:H	7	0.55
(1,995)	1:108:A:SER:HA	1:116:A:ALA:H	17	0.55
(1,910)	1:102:A:ASP:H	1:106:A:LEU:HB3	1	0.55
(1,910)	1:102:A:ASP:H	1:106:A:LEU:HB3	5	0.55
(1,910)	1:102:A:ASP:H	1:106:A:LEU:HB3	10	0.55
(1,910)	1:102:A:ASP:H	1:106:A:LEU:HB3	16	0.55
(1,886)	1:103:A:PHE:HE1	1:107:A:ALA:H	1	0.55
(1,886)	1:103:A:PHE:HE2	1:107:A:ALA:H	1	0.55
(1,886)	1:103:A:PHE:HE1	1:107:A:ALA:H	9	0.55
(1,886)	1:103:A:PHE:HE2	1:107:A:ALA:H	9	0.55
(1,871)	1:96:A:ILE:HB	1:103:A:PHE:H	8	0.55
(1,871)	1:96:A:ILE:HB	1:103:A:PHE:H	12	0.55
(1,871)	1:96:A:ILE:HB	1:103:A:PHE:H	14	0.55
(1,868)	1:60:A:LEU:HD21	1:103:A:PHE:HE1	14	0.55
(1,868)	1:60:A:LEU:HD21	1:103:A:PHE:HE2	14	0.55
(1,868)	1:60:A:LEU:HD22	1:103:A:PHE:HE1	14	0.55
(1,868)	1:60:A:LEU:HD22	1:103:A:PHE:HE2	14	0.55
(1,868)	1:60:A:LEU:HD23	1:103:A:PHE:HE1	14	0.55
(1,868)	1:60:A:LEU:HD23	1:103:A:PHE:HE2	14	0.55
(1,840)	1:97:A:LYS:HG2	1:146:A:MET:HE1	18	0.55
(1,840)	1:97:A:LYS:HG2	1:146:A:MET:HE2	18	0.55
(1,840)	1:97:A:LYS:HG2	1:146:A:MET:HE3	18	0.55
(1,816)	1:95:A:LYS:HD2	1:96:A:ILE:H	6	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD11	13	0.55
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD12	13	0.55
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD13	13	0.55
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD11	17	0.55
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD12	17	0.55
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD13	17	0.55
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE1	9	0.55
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE2	9	0.55
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE3	9	0.55
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE1	19	0.55
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE2	19	0.55
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE3	19	0.55
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD11	18	0.55
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD12	18	0.55
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD13	18	0.55
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD11	18	0.55
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD12	18	0.55
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD13	18	0.55
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD11	10	0.55
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD12	10	0.55
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD13	10	0.55
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD1	9	0.55
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD2	9	0.55
(1,752)	1:89:A:ILE:HB	1:91:A:GLY:H	1	0.55
(1,752)	1:89:A:ILE:HB	1:91:A:GLY:H	6	0.55
(1,752)	1:89:A:ILE:HB	1:91:A:GLY:H	19	0.55
(1,648)	1:66:A:GLN:HE22	1:82:A:LYS:HG3	9	0.55
(1,644)	1:81:A:THR:HA	1:84:A:GLU:H	17	0.55
(1,593)	1:71:A:SER:HB3	1:77:A:LYS:HA	9	0.55
(1,591)	1:74:A:ARG:HE	1:75:A:GLN:H	7	0.55
(1,591)	1:74:A:ARG:HE	1:75:A:GLN:H	19	0.55
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB1	19	0.55
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB2	19	0.55
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB3	19	0.55
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD21	6	0.55
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD22	6	0.55
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD23	6	0.55
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD21	10	0.55
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD22	10	0.55
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD23	10	0.55
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD11	11	0.55
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD12	11	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD13	11	0.55
(1,422)	1:56:A:ARG:HG2	1:162:A:THR:HB	17	0.55
(1,397)	1:54:A:ARG:HG2	1:126:A:SER:H	8	0.55
(1,397)	1:54:A:ARG:HG2	1:126:A:SER:H	14	0.55
(1,397)	1:54:A:ARG:HG2	1:126:A:SER:H	15	0.55
(1,384)	1:7:A:LEU:HD21	1:36:A:ARG:HA	8	0.55
(1,384)	1:7:A:LEU:HD22	1:36:A:ARG:HA	8	0.55
(1,384)	1:7:A:LEU:HD23	1:36:A:ARG:HA	8	0.55
(1,295)	1:27:A:HIS:H	1:29:A:THR:H	18	0.55
(1,287)	1:26:A:ASN:H	1:32:A:SER:HB2	15	0.55
(1,274)	1:26:A:ASN:HD21	1:29:A:THR:HG21	20	0.55
(1,274)	1:26:A:ASN:HD21	1:29:A:THR:HG22	20	0.55
(1,274)	1:26:A:ASN:HD21	1:29:A:THR:HG23	20	0.55
(1,256)	1:23:A:TYR:HE1	1:26:A:ASN:H	5	0.55
(1,256)	1:23:A:TYR:HE2	1:26:A:ASN:H	5	0.55
(1,218)	1:12:A:GLU:HB2	1:25:A:PHE:H	10	0.55
(1,218)	1:12:A:GLU:HB2	1:25:A:PHE:H	20	0.55
(1,213)	1:11:A:TRP:HA	1:25:A:PHE:H	11	0.55
(1,190)	1:13:A:LYS:HB3	1:24:A:TYR:HA	9	0.55
(1,190)	1:13:A:LYS:HB3	1:24:A:TYR:HA	13	0.55
(1,180)	1:23:A:TYR:HD1	1:33:A:GLN:HA	13	0.55
(1,180)	1:23:A:TYR:HD2	1:33:A:GLN:HA	13	0.55
(1,178)	1:23:A:TYR:HE1	1:33:A:GLN:H	20	0.55
(1,178)	1:23:A:TYR:HE2	1:33:A:GLN:H	20	0.55
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG11	4	0.55
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG12	4	0.55
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG13	4	0.55
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG11	4	0.55
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG12	4	0.55
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG13	4	0.55
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG11	4	0.55
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG12	4	0.55
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG13	4	0.55
(1,134)	1:20:A:GLY:H	1:21:A:ARG:HA	16	0.55
(1,133)	1:20:A:GLY:H	1:21:A:ARG:HB2	8	0.55
(1,125)	1:15:A:MET:HA	1:21:A:ARG:H	10	0.55
(1,111)	1:15:A:MET:H	1:23:A:TYR:HD1	10	0.55
(1,111)	1:15:A:MET:H	1:23:A:TYR:HD2	10	0.55
(1,111)	1:15:A:MET:H	1:23:A:TYR:HD1	13	0.55
(1,111)	1:15:A:MET:H	1:23:A:TYR:HD2	13	0.55
(1,64)	1:12:A:GLU:H	1:24:A:TYR:HD1	3	0.55
(1,64)	1:12:A:GLU:H	1:24:A:TYR:HD2	3	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,64)	1:12:A:GLU:H	1:24:A:TYR:HD1	7	0.55
(1,64)	1:12:A:GLU:H	1:24:A:TYR:HD2	7	0.55
(1,35)	1:9:A:PRO:HG2	1:10:A:GLY:H	14	0.55
(1,27)	1:7:A:LEU:HD21	1:13:A:LYS:H	14	0.55
(1,27)	1:7:A:LEU:HD22	1:13:A:LYS:H	14	0.55
(1,27)	1:7:A:LEU:HD23	1:13:A:LYS:H	14	0.55
(1,16)	1:6:A:LYS:HE2	1:7:A:LEU:H	13	0.55
(2,93)	1:93:A:ILE:HD11	2:643:B:PRO:HA	15	0.54
(2,93)	1:93:A:ILE:HD12	2:643:B:PRO:HA	15	0.54
(2,93)	1:93:A:ILE:HD13	2:643:B:PRO:HA	15	0.54
(2,90)	1:56:A:ARG:H	2:651:B:ILE:HG12	19	0.54
(2,90)	1:56:A:ARG:H	2:651:B:ILE:HG13	19	0.54
(2,88)	1:34:A:TRP:HE1	2:641:B:TPO:H	6	0.54
(2,79)	2:659:B:PHE:HE1	2:661:B:PHE:H	14	0.54
(2,79)	2:659:B:PHE:HE2	2:661:B:PHE:H	14	0.54
(2,58)	1:152:A:THR:HG21	1:157:A:HIS:HB3	6	0.54
(2,58)	1:152:A:THR:HG22	1:157:A:HIS:HB3	6	0.54
(2,58)	1:152:A:THR:HG23	1:157:A:HIS:HB3	6	0.54
(2,45)	1:131:A:GLN:HE21	1:152:A:THR:HB	16	0.54
(1,2596)	1:137:A:ALA:HB1	2:651:B:ILE:HG12	15	0.54
(1,2596)	1:137:A:ALA:HB1	2:651:B:ILE:HG13	15	0.54
(1,2596)	1:137:A:ALA:HB2	2:651:B:ILE:HG12	15	0.54
(1,2596)	1:137:A:ALA:HB2	2:651:B:ILE:HG13	15	0.54
(1,2596)	1:137:A:ALA:HB3	2:651:B:ILE:HG12	15	0.54
(1,2596)	1:137:A:ALA:HB3	2:651:B:ILE:HG13	15	0.54
(1,2593)	1:129:A:GLN:HE21	2:656:B:PHE:HE1	18	0.54
(1,2593)	1:129:A:GLN:HE21	2:656:B:PHE:HE2	18	0.54
(1,2587)	1:115:A:SER:H	2:659:B:PHE:HD1	6	0.54
(1,2587)	1:115:A:SER:H	2:659:B:PHE:HD2	6	0.54
(1,2587)	1:115:A:SER:H	2:659:B:PHE:HD1	12	0.54
(1,2587)	1:115:A:SER:H	2:659:B:PHE:HD2	12	0.54
(1,2586)	1:115:A:SER:H	2:659:B:PHE:HE1	10	0.54
(1,2586)	1:115:A:SER:H	2:659:B:PHE:HE2	10	0.54
(1,2551)	2:652:B:ASP:H	2:654:B:SER:H	14	0.54
(1,2513)	2:646:B:GLU:HA	2:649:B:ARG:HD2	10	0.54
(1,2507)	2:643:B:PRO:HA	2:645:B:GLN:H	5	0.54
(1,2161)	1:119:A:ARG:H	1:119:A:ARG:HD3	4	0.54
(1,2161)	1:119:A:ARG:H	1:119:A:ARG:HD3	11	0.54
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD21	4	0.54
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD22	4	0.54
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD23	4	0.54
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD21	11	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD22	11	0.54
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD23	11	0.54
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD21	13	0.54
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD22	13	0.54
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD23	13	0.54
(1,1504)	1:13:A:LYS:H	1:13:A:LYS:HE2	13	0.54
(1,1434)	1:161:A:ARG:HD2	1:163:A:GLU:H	18	0.54
(1,1412)	1:56:A:ARG:HB2	1:162:A:THR:HG21	20	0.54
(1,1412)	1:56:A:ARG:HB2	1:162:A:THR:HG22	20	0.54
(1,1412)	1:56:A:ARG:HB2	1:162:A:THR:HG23	20	0.54
(1,1402)	1:143:A:THR:HG21	1:161:A:ARG:HD2	5	0.54
(1,1402)	1:143:A:THR:HG22	1:161:A:ARG:HD2	5	0.54
(1,1402)	1:143:A:THR:HG23	1:161:A:ARG:HD2	5	0.54
(1,1369)	1:104:A:GLU:H	1:160:A:LEU:HD11	2	0.54
(1,1369)	1:104:A:GLU:H	1:160:A:LEU:HD12	2	0.54
(1,1369)	1:104:A:GLU:H	1:160:A:LEU:HD13	2	0.54
(1,1328)	1:89:A:ILE:HG12	1:158:A:ILE:HB	5	0.54
(1,1326)	1:89:A:ILE:HG21	1:158:A:ILE:HB	15	0.54
(1,1326)	1:89:A:ILE:HG22	1:158:A:ILE:HB	15	0.54
(1,1326)	1:89:A:ILE:HG23	1:158:A:ILE:HB	15	0.54
(1,1311)	1:152:A:THR:HG21	1:157:A:HIS:H	9	0.54
(1,1311)	1:152:A:THR:HG22	1:157:A:HIS:H	9	0.54
(1,1311)	1:152:A:THR:HG23	1:157:A:HIS:H	9	0.54
(1,1311)	1:152:A:THR:HG21	1:157:A:HIS:H	11	0.54
(1,1311)	1:152:A:THR:HG22	1:157:A:HIS:H	11	0.54
(1,1311)	1:152:A:THR:HG23	1:157:A:HIS:H	11	0.54
(1,1303)	1:156:A:ILE:HG21	1:157:A:HIS:HD2	13	0.54
(1,1303)	1:156:A:ILE:HG22	1:157:A:HIS:HD2	13	0.54
(1,1303)	1:156:A:ILE:HG23	1:157:A:HIS:HD2	13	0.54
(1,1299)	1:152:A:THR:H	1:156:A:ILE:HG21	4	0.54
(1,1299)	1:152:A:THR:H	1:156:A:ILE:HG22	4	0.54
(1,1299)	1:152:A:THR:H	1:156:A:ILE:HG23	4	0.54
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD11	10	0.54
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD12	10	0.54
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD13	10	0.54
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD11	13	0.54
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD12	13	0.54
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD13	13	0.54
(1,1217)	1:145:A:GLU:HB3	1:147:A:SER:H	4	0.54
(1,1217)	1:145:A:GLU:HB3	1:147:A:SER:H	5	0.54
(1,1217)	1:145:A:GLU:HB3	1:147:A:SER:H	18	0.54
(1,1212)	1:146:A:MET:HG2	1:160:A:LEU:HG	12	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1208)	1:103:A:PHE:HD1	1:146:A:MET:HB2	2	0.54
(1,1208)	1:103:A:PHE:HD2	1:146:A:MET:HB2	2	0.54
(1,1208)	1:103:A:PHE:HD1	1:146:A:MET:HB2	10	0.54
(1,1208)	1:103:A:PHE:HD2	1:146:A:MET:HB2	10	0.54
(1,1193)	1:141:A:LEU:HD11	1:148:A:GLY:H	10	0.54
(1,1193)	1:141:A:LEU:HD12	1:148:A:GLY:H	10	0.54
(1,1193)	1:141:A:LEU:HD13	1:148:A:GLY:H	10	0.54
(1,1112)	1:126:A:SER:H	1:129:A:GLN:HE21	5	0.54
(1,1109)	1:126:A:SER:HA	1:139:A:PHE:HD1	7	0.54
(1,1109)	1:126:A:SER:HA	1:139:A:PHE:HD2	7	0.54
(1,1107)	1:54:A:ARG:HD2	1:126:A:SER:HA	4	0.54
(1,1107)	1:54:A:ARG:HD2	1:126:A:SER:HA	12	0.54
(1,1058)	1:59:A:HIS:HD2	1:122:A:LEU:HD11	16	0.54
(1,1058)	1:59:A:HIS:HD2	1:122:A:LEU:HD12	16	0.54
(1,1058)	1:59:A:HIS:HD2	1:122:A:LEU:HD13	16	0.54
(1,1057)	1:59:A:HIS:H	1:122:A:LEU:HG	11	0.54
(1,1027)	1:118:A:ALA:HA	1:119:A:ARG:HG2	15	0.54
(1,1024)	1:118:A:ALA:HA	1:119:A:ARG:HE	12	0.54
(1,995)	1:108:A:SER:HA	1:116:A:ALA:H	8	0.54
(1,985)	1:61:A:LEU:HD21	1:113:A:CYS:HA	10	0.54
(1,985)	1:61:A:LEU:HD22	1:113:A:CYS:HA	10	0.54
(1,985)	1:61:A:LEU:HD23	1:113:A:CYS:HA	10	0.54
(1,913)	1:103:A:PHE:H	1:106:A:LEU:HB3	20	0.54
(1,910)	1:102:A:ASP:H	1:106:A:LEU:HB3	6	0.54
(1,910)	1:102:A:ASP:H	1:106:A:LEU:HB3	9	0.54
(1,889)	1:103:A:PHE:HE1	1:146:A:MET:HE1	10	0.54
(1,889)	1:103:A:PHE:HE1	1:146:A:MET:HE2	10	0.54
(1,889)	1:103:A:PHE:HE1	1:146:A:MET:HE3	10	0.54
(1,889)	1:103:A:PHE:HE2	1:146:A:MET:HE1	10	0.54
(1,889)	1:103:A:PHE:HE2	1:146:A:MET:HE2	10	0.54
(1,889)	1:103:A:PHE:HE2	1:146:A:MET:HE3	10	0.54
(1,889)	1:103:A:PHE:HE1	1:146:A:MET:HE1	18	0.54
(1,889)	1:103:A:PHE:HE1	1:146:A:MET:HE2	18	0.54
(1,889)	1:103:A:PHE:HE1	1:146:A:MET:HE3	18	0.54
(1,889)	1:103:A:PHE:HE2	1:146:A:MET:HE1	18	0.54
(1,889)	1:103:A:PHE:HE2	1:146:A:MET:HE2	18	0.54
(1,889)	1:103:A:PHE:HE2	1:146:A:MET:HE3	18	0.54
(1,886)	1:103:A:PHE:HE1	1:107:A:ALA:H	7	0.54
(1,886)	1:103:A:PHE:HE2	1:107:A:ALA:H	7	0.54
(1,871)	1:96:A:ILE:HB	1:103:A:PHE:H	5	0.54
(1,868)	1:60:A:LEU:HD21	1:103:A:PHE:HE1	4	0.54
(1,868)	1:60:A:LEU:HD21	1:103:A:PHE:HE2	4	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,868)	1:60:A:LEU:HD22	1:103:A:PHE:HE1	4	0.54
(1,868)	1:60:A:LEU:HD22	1:103:A:PHE:HE2	4	0.54
(1,868)	1:60:A:LEU:HD23	1:103:A:PHE:HE1	4	0.54
(1,868)	1:60:A:LEU:HD23	1:103:A:PHE:HE2	4	0.54
(1,840)	1:97:A:LYS:HG2	1:146:A:MET:HE1	13	0.54
(1,840)	1:97:A:LYS:HG2	1:146:A:MET:HE2	13	0.54
(1,840)	1:97:A:LYS:HG2	1:146:A:MET:HE3	13	0.54
(1,834)	1:94:A:GLN:HE21	1:97:A:LYS:HD2	3	0.54
(1,834)	1:94:A:GLN:HE21	1:97:A:LYS:HD2	8	0.54
(1,816)	1:95:A:LYS:HD2	1:96:A:ILE:H	8	0.54
(1,816)	1:95:A:LYS:HD2	1:96:A:ILE:H	13	0.54
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD11	18	0.54
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD12	18	0.54
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD13	18	0.54
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE1	1	0.54
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE2	1	0.54
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE3	1	0.54
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE1	7	0.54
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE2	7	0.54
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE3	7	0.54
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE1	12	0.54
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE2	12	0.54
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE3	12	0.54
(1,785)	1:89:A:ILE:HG21	1:93:A:ILE:H	2	0.54
(1,785)	1:89:A:ILE:HG22	1:93:A:ILE:H	2	0.54
(1,785)	1:89:A:ILE:HG23	1:93:A:ILE:H	2	0.54
(1,785)	1:89:A:ILE:HG21	1:93:A:ILE:H	11	0.54
(1,785)	1:89:A:ILE:HG22	1:93:A:ILE:H	11	0.54
(1,785)	1:89:A:ILE:HG23	1:93:A:ILE:H	11	0.54
(1,785)	1:89:A:ILE:HG21	1:93:A:ILE:H	16	0.54
(1,785)	1:89:A:ILE:HG22	1:93:A:ILE:H	16	0.54
(1,785)	1:89:A:ILE:HG23	1:93:A:ILE:H	16	0.54
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD1	20	0.54
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD2	20	0.54
(1,752)	1:89:A:ILE:HB	1:91:A:GLY:H	11	0.54
(1,695)	1:86:A:LEU:HD21	1:149:A:PRO:HD3	20	0.54
(1,695)	1:86:A:LEU:HD22	1:149:A:PRO:HD3	20	0.54
(1,695)	1:86:A:LEU:HD23	1:149:A:PRO:HD3	20	0.54
(1,647)	1:65:A:SER:H	1:82:A:LYS:H	6	0.54
(1,640)	1:65:A:SER:HB3	1:81:A:THR:HA	13	0.54
(1,637)	1:80:A:ARG:HE	1:85:A:ALA:H	5	0.54
(1,589)	1:74:A:ARG:H	1:112:A:ASP:HA	1	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,589)	1:74:A:ARG:H	1:112:A:ASP:HA	9	0.54
(1,589)	1:74:A:ARG:H	1:112:A:ASP:HA	15	0.54
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB1	1	0.54
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB2	1	0.54
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB3	1	0.54
(1,569)	1:73:A:TRP:HE1	1:74:A:ARG:HB2	8	0.54
(1,541)	1:67:A:SER:HB3	1:70:A:PRO:HA	10	0.54
(1,520)	1:64:A:HIS:HE1	1:66:A:GLN:HG2	19	0.54
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD21	7	0.54
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD22	7	0.54
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD23	7	0.54
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD21	11	0.54
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD22	11	0.54
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD23	11	0.54
(1,457)	1:60:A:LEU:HD11	1:108:A:SER:H	6	0.54
(1,457)	1:60:A:LEU:HD12	1:108:A:SER:H	6	0.54
(1,457)	1:60:A:LEU:HD13	1:108:A:SER:H	6	0.54
(1,422)	1:56:A:ARG:HG2	1:162:A:THR:HB	6	0.54
(1,422)	1:56:A:ARG:HG2	1:162:A:THR:HB	8	0.54
(1,397)	1:54:A:ARG:HG2	1:126:A:SER:H	11	0.54
(1,287)	1:26:A:ASN:H	1:32:A:SER:HB2	9	0.54
(1,287)	1:26:A:ASN:H	1:32:A:SER:HB2	20	0.54
(1,190)	1:13:A:LYS:HB3	1:24:A:TYR:HA	2	0.54
(1,190)	1:13:A:LYS:HB3	1:24:A:TYR:HA	7	0.54
(1,190)	1:13:A:LYS:HB3	1:24:A:TYR:HA	20	0.54
(1,176)	1:23:A:TYR:HB3	1:24:A:TYR:HD1	3	0.54
(1,176)	1:23:A:TYR:HB3	1:24:A:TYR:HD2	3	0.54
(1,134)	1:20:A:GLY:H	1:21:A:ARG:HA	10	0.54
(1,93)	1:14:A:ARG:H	1:22:A:VAL:HA	18	0.54
(1,86)	1:13:A:LYS:HE2	1:14:A:ARG:H	18	0.54
(1,86)	1:13:A:LYS:HE2	1:14:A:ARG:H	20	0.54
(1,70)	1:12:A:GLU:HG2	1:13:A:LYS:H	6	0.54
(1,70)	1:12:A:GLU:HG2	1:13:A:LYS:H	20	0.54
(1,35)	1:9:A:PRO:HG2	1:10:A:GLY:H	2	0.54
(1,35)	1:9:A:PRO:HG2	1:10:A:GLY:H	9	0.54
(1,27)	1:7:A:LEU:HD21	1:13:A:LYS:H	20	0.54
(1,27)	1:7:A:LEU:HD22	1:13:A:LYS:H	20	0.54
(1,27)	1:7:A:LEU:HD23	1:13:A:LYS:H	20	0.54
(2,106)	1:139:A:PHE:H	2:656:B:PHE:HB2	9	0.53
(2,88)	1:34:A:TRP:HE1	2:641:B:TPO:H	5	0.53
(2,86)	1:29:A:THR:HG21	2:647:B:VAL:HA	9	0.53
(2,86)	1:29:A:THR:HG22	2:647:B:VAL:HA	9	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,86)	1:29:A:THR:HG23	2:647:B:VAL:HA	9	0.53
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG11	12	0.53
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG12	12	0.53
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG13	12	0.53
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG21	12	0.53
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG22	12	0.53
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG23	12	0.53
(2,71)	2:651:B:ILE:HG21	2:656:B:PHE:H	19	0.53
(2,71)	2:651:B:ILE:HG22	2:656:B:PHE:H	19	0.53
(2,71)	2:651:B:ILE:HG23	2:656:B:PHE:H	19	0.53
(2,70)	2:651:B:ILE:HG21	2:656:B:PHE:HE1	14	0.53
(2,70)	2:651:B:ILE:HG21	2:656:B:PHE:HE2	14	0.53
(2,70)	2:651:B:ILE:HG22	2:656:B:PHE:HE1	14	0.53
(2,70)	2:651:B:ILE:HG22	2:656:B:PHE:HE2	14	0.53
(2,70)	2:651:B:ILE:HG23	2:656:B:PHE:HE1	14	0.53
(2,70)	2:651:B:ILE:HG23	2:656:B:PHE:HE2	14	0.53
(2,25)	1:88:A:LEU:HG	1:92:A:TYR:H	18	0.53
(1,2587)	1:115:A:SER:H	2:659:B:PHE:HD1	14	0.53
(1,2587)	1:115:A:SER:H	2:659:B:PHE:HD2	14	0.53
(1,2525)	2:645:B:GLN:HE22	2:648:B:ILE:HD11	19	0.53
(1,2525)	2:645:B:GLN:HE22	2:648:B:ILE:HD12	19	0.53
(1,2525)	2:645:B:GLN:HE22	2:648:B:ILE:HD13	19	0.53
(1,2520)	2:646:B:GLU:HG3	2:647:B:VAL:H	7	0.53
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE1	15	0.53
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE2	15	0.53
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE3	15	0.53
(1,2161)	1:119:A:ARG:H	1:119:A:ARG:HD3	16	0.53
(1,2161)	1:119:A:ARG:H	1:119:A:ARG:HD3	19	0.53
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD21	8	0.53
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD22	8	0.53
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD23	8	0.53
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD21	9	0.53
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD22	9	0.53
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD23	9	0.53
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD21	19	0.53
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD22	19	0.53
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD23	19	0.53
(1,1507)	1:13:A:LYS:H	1:13:A:LYS:HG3	8	0.53
(1,1434)	1:161:A:ARG:HD2	1:163:A:GLU:H	9	0.53
(1,1434)	1:161:A:ARG:HD2	1:163:A:GLU:H	14	0.53
(1,1434)	1:161:A:ARG:HD2	1:163:A:GLU:H	16	0.53
(1,1429)	1:143:A:THR:HG21	1:163:A:GLU:HB2	20	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1429)	1:143:A:THR:HG22	1:163:A:GLU:HB2	20	0.53
(1,1429)	1:143:A:THR:HG23	1:163:A:GLU:HB2	20	0.53
(1,1402)	1:143:A:THR:HG21	1:161:A:ARG:HD2	6	0.53
(1,1402)	1:143:A:THR:HG22	1:161:A:ARG:HD2	6	0.53
(1,1402)	1:143:A:THR:HG23	1:161:A:ARG:HD2	6	0.53
(1,1328)	1:89:A:ILE:HG12	1:158:A:ILE:HB	8	0.53
(1,1326)	1:89:A:ILE:HG21	1:158:A:ILE:HB	1	0.53
(1,1326)	1:89:A:ILE:HG22	1:158:A:ILE:HB	1	0.53
(1,1326)	1:89:A:ILE:HG23	1:158:A:ILE:HB	1	0.53
(1,1313)	1:156:A:ILE:HA	1:157:A:HIS:HD2	20	0.53
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD11	5	0.53
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD12	5	0.53
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD13	5	0.53
(1,1276)	1:63:A:LYS:HA	1:155:A:GLY:HA2	3	0.53
(1,1212)	1:146:A:MET:HG2	1:160:A:LEU:HG	19	0.53
(1,1177)	1:137:A:ALA:HB1	1:141:A:LEU:H	17	0.53
(1,1177)	1:137:A:ALA:HB2	1:141:A:LEU:H	17	0.53
(1,1177)	1:137:A:ALA:HB3	1:141:A:LEU:H	17	0.53
(1,1112)	1:126:A:SER:H	1:129:A:GLN:HE21	19	0.53
(1,1107)	1:54:A:ARG:HD2	1:126:A:SER:HA	16	0.53
(1,1057)	1:59:A:HIS:H	1:122:A:LEU:HG	13	0.53
(1,1024)	1:118:A:ALA:HA	1:119:A:ARG:HE	3	0.53
(1,995)	1:108:A:SER:HA	1:116:A:ALA:H	14	0.53
(1,886)	1:103:A:PHE:HE1	1:107:A:ALA:H	8	0.53
(1,886)	1:103:A:PHE:HE2	1:107:A:ALA:H	8	0.53
(1,886)	1:103:A:PHE:HE1	1:107:A:ALA:H	13	0.53
(1,886)	1:103:A:PHE:HE2	1:107:A:ALA:H	13	0.53
(1,871)	1:96:A:ILE:HB	1:103:A:PHE:H	6	0.53
(1,868)	1:60:A:LEU:HD21	1:103:A:PHE:HE1	15	0.53
(1,868)	1:60:A:LEU:HD21	1:103:A:PHE:HE2	15	0.53
(1,868)	1:60:A:LEU:HD22	1:103:A:PHE:HE1	15	0.53
(1,868)	1:60:A:LEU:HD22	1:103:A:PHE:HE2	15	0.53
(1,868)	1:60:A:LEU:HD23	1:103:A:PHE:HE1	15	0.53
(1,868)	1:60:A:LEU:HD23	1:103:A:PHE:HE2	15	0.53
(1,845)	1:97:A:LYS:HD2	1:98:A:SER:H	15	0.53
(1,840)	1:97:A:LYS:HG2	1:146:A:MET:HE1	16	0.53
(1,840)	1:97:A:LYS:HG2	1:146:A:MET:HE2	16	0.53
(1,840)	1:97:A:LYS:HG2	1:146:A:MET:HE3	16	0.53
(1,830)	1:93:A:ILE:HG21	1:97:A:LYS:HD2	12	0.53
(1,830)	1:93:A:ILE:HG22	1:97:A:LYS:HD2	12	0.53
(1,830)	1:93:A:ILE:HG23	1:97:A:LYS:HD2	12	0.53
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD11	2	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD12	2	0.53
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD13	2	0.53
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD11	14	0.53
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD12	14	0.53
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD13	14	0.53
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE1	6	0.53
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE2	6	0.53
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE3	6	0.53
(1,785)	1:89:A:ILE:HG21	1:93:A:ILE:H	10	0.53
(1,785)	1:89:A:ILE:HG22	1:93:A:ILE:H	10	0.53
(1,785)	1:89:A:ILE:HG23	1:93:A:ILE:H	10	0.53
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD11	8	0.53
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD12	8	0.53
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD13	8	0.53
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD1	6	0.53
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD2	6	0.53
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD1	13	0.53
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD2	13	0.53
(1,753)	1:90:A:ASN:HD22	1:91:A:GLY:H	11	0.53
(1,747)	1:90:A:ASN:HA	1:158:A:ILE:HD11	12	0.53
(1,747)	1:90:A:ASN:HA	1:158:A:ILE:HD12	12	0.53
(1,747)	1:90:A:ASN:HA	1:158:A:ILE:HD13	12	0.53
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD21	3	0.53
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD22	3	0.53
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD23	3	0.53
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD21	6	0.53
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD22	6	0.53
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD23	6	0.53
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD21	12	0.53
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD22	12	0.53
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD23	12	0.53
(1,659)	1:81:A:THR:HA	1:83:A:GLU:H	10	0.53
(1,648)	1:66:A:GLN:HE22	1:82:A:LYS:HG3	5	0.53
(1,648)	1:66:A:GLN:HE22	1:82:A:LYS:HG3	7	0.53
(1,646)	1:81:A:THR:HG21	1:84:A:GLU:HB2	17	0.53
(1,646)	1:81:A:THR:HG22	1:84:A:GLU:HB2	17	0.53
(1,646)	1:81:A:THR:HG23	1:84:A:GLU:HB2	17	0.53
(1,641)	1:65:A:SER:HB2	1:81:A:THR:HG21	6	0.53
(1,641)	1:65:A:SER:HB2	1:81:A:THR:HG22	6	0.53
(1,641)	1:65:A:SER:HB2	1:81:A:THR:HG23	6	0.53
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB1	5	0.53
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB2	5	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB3	5	0.53
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB1	8	0.53
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB2	8	0.53
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB3	8	0.53
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB1	12	0.53
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB2	12	0.53
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB3	12	0.53
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB1	14	0.53
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB2	14	0.53
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB3	14	0.53
(1,554)	1:70:A:PRO:HG3	1:71:A:SER:H	19	0.53
(1,531)	1:64:A:HIS:HE1	1:67:A:SER:HB2	10	0.53
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD21	8	0.53
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD22	8	0.53
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD23	8	0.53
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD21	13	0.53
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD22	13	0.53
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD23	13	0.53
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD21	18	0.53
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD22	18	0.53
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD23	18	0.53
(1,496)	1:62:A:VAL:HG11	1:88:A:LEU:H	5	0.53
(1,496)	1:62:A:VAL:HG12	1:88:A:LEU:H	5	0.53
(1,496)	1:62:A:VAL:HG13	1:88:A:LEU:H	5	0.53
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD11	2	0.53
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD12	2	0.53
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD13	2	0.53
(1,457)	1:60:A:LEU:HD11	1:108:A:SER:H	18	0.53
(1,457)	1:60:A:LEU:HD12	1:108:A:SER:H	18	0.53
(1,457)	1:60:A:LEU:HD13	1:108:A:SER:H	18	0.53
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG21	10	0.53
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG22	10	0.53
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG23	10	0.53
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG21	10	0.53
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG22	10	0.53
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG23	10	0.53
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG21	10	0.53
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG22	10	0.53
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG23	10	0.53
(1,440)	1:59:A:HIS:H	1:115:A:SER:HB3	15	0.53
(1,440)	1:59:A:HIS:H	1:115:A:SER:HB3	17	0.53
(1,320)	1:25:A:PHE:HE1	1:30:A:ASN:H	15	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,320)	1:25:A:PHE:HE2	1:30:A:ASN:H	15	0.53
(1,295)	1:27:A:HIS:H	1:29:A:THR:H	16	0.53
(1,295)	1:27:A:HIS:H	1:29:A:THR:H	17	0.53
(1,287)	1:26:A:ASN:H	1:32:A:SER:HB2	3	0.53
(1,287)	1:26:A:ASN:H	1:32:A:SER:HB2	7	0.53
(1,218)	1:12:A:GLU:HB2	1:25:A:PHE:H	2	0.53
(1,218)	1:12:A:GLU:HB2	1:25:A:PHE:H	19	0.53
(1,214)	1:11:A:TRP:HB2	1:25:A:PHE:H	1	0.53
(1,214)	1:11:A:TRP:HB2	1:25:A:PHE:H	8	0.53
(1,214)	1:11:A:TRP:HB2	1:25:A:PHE:H	14	0.53
(1,194)	1:13:A:LYS:HG2	1:24:A:TYR:HA	14	0.53
(1,148)	1:15:A:MET:HE1	1:22:A:VAL:HA	17	0.53
(1,148)	1:15:A:MET:HE2	1:22:A:VAL:HA	17	0.53
(1,148)	1:15:A:MET:HE3	1:22:A:VAL:HA	17	0.53
(1,133)	1:20:A:GLY:H	1:21:A:ARG:HB2	2	0.53
(1,116)	1:16:A:SER:H	1:20:A:GLY:HA2	2	0.53
(1,93)	1:14:A:ARG:H	1:22:A:VAL:HA	9	0.53
(1,86)	1:13:A:LYS:HE2	1:14:A:ARG:H	16	0.53
(1,70)	1:12:A:GLU:HG2	1:13:A:LYS:H	9	0.53
(1,64)	1:12:A:GLU:H	1:24:A:TYR:HD1	14	0.53
(1,64)	1:12:A:GLU:H	1:24:A:TYR:HD2	14	0.53
(1,64)	1:12:A:GLU:H	1:24:A:TYR:HD1	16	0.53
(1,64)	1:12:A:GLU:H	1:24:A:TYR:HD2	16	0.53
(1,27)	1:7:A:LEU:HD21	1:13:A:LYS:H	10	0.53
(1,27)	1:7:A:LEU:HD22	1:13:A:LYS:H	10	0.53
(1,27)	1:7:A:LEU:HD23	1:13:A:LYS:H	10	0.53
(1,27)	1:7:A:LEU:HD21	1:13:A:LYS:H	15	0.53
(1,27)	1:7:A:LEU:HD22	1:13:A:LYS:H	15	0.53
(1,27)	1:7:A:LEU:HD23	1:13:A:LYS:H	15	0.53
(1,27)	1:7:A:LEU:HD21	1:13:A:LYS:H	17	0.53
(1,27)	1:7:A:LEU:HD22	1:13:A:LYS:H	17	0.53
(1,27)	1:7:A:LEU:HD23	1:13:A:LYS:H	17	0.53
(2,113)	1:162:A:THR:H	2:651:B:ILE:HG12	7	0.52
(2,113)	1:162:A:THR:H	2:651:B:ILE:HG13	7	0.52
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG11	3	0.52
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG12	3	0.52
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG13	3	0.52
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG21	3	0.52
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG22	3	0.52
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG23	3	0.52
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG11	13	0.52
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG12	13	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG13	13	0.52
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG21	13	0.52
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG22	13	0.52
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG23	13	0.52
(2,74)	2:656:B:PHE:HB2	2:659:B:PHE:HD1	18	0.52
(2,74)	2:656:B:PHE:HB2	2:659:B:PHE:HD2	18	0.52
(2,74)	2:656:B:PHE:HB3	2:659:B:PHE:HD1	18	0.52
(2,74)	2:656:B:PHE:HB3	2:659:B:PHE:HD2	18	0.52
(2,71)	2:651:B:ILE:HG21	2:656:B:PHE:H	3	0.52
(2,71)	2:651:B:ILE:HG22	2:656:B:PHE:H	3	0.52
(2,71)	2:651:B:ILE:HG23	2:656:B:PHE:H	3	0.52
(2,39)	1:55:A:VAL:HG11	1:127:A:ARG:H	11	0.52
(2,39)	1:55:A:VAL:HG12	1:127:A:ARG:H	11	0.52
(2,39)	1:55:A:VAL:HG13	1:127:A:ARG:H	11	0.52
(2,38)	1:126:A:SER:H	1:129:A:GLN:HB2	8	0.52
(2,5)	1:23:A:TYR:H	1:34:A:TRP:HZ3	3	0.52
(1,2591)	1:123:A:GLY:H	2:656:B:PHE:HE1	8	0.52
(1,2591)	1:123:A:GLY:H	2:656:B:PHE:HE2	8	0.52
(1,2584)	1:114:A:SER:H	2:659:B:PHE:HD1	7	0.52
(1,2584)	1:114:A:SER:H	2:659:B:PHE:HD2	7	0.52
(1,2568)	2:658:B:GLY:H	2:659:B:PHE:HD1	6	0.52
(1,2568)	2:658:B:GLY:H	2:659:B:PHE:HD2	6	0.52
(1,2568)	2:658:B:GLY:H	2:659:B:PHE:HD1	7	0.52
(1,2568)	2:658:B:GLY:H	2:659:B:PHE:HD2	7	0.52
(1,2523)	2:647:B:VAL:HA	2:649:B:ARG:H	6	0.52
(1,2384)	1:163:A:GLU:H	1:163:A:GLU:HG3	12	0.52
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD21	17	0.52
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD22	17	0.52
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD23	17	0.52
(1,1504)	1:13:A:LYS:H	1:13:A:LYS:HE2	17	0.52
(1,1369)	1:104:A:GLU:H	1:160:A:LEU:HD11	10	0.52
(1,1369)	1:104:A:GLU:H	1:160:A:LEU:HD12	10	0.52
(1,1369)	1:104:A:GLU:H	1:160:A:LEU:HD13	10	0.52
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD11	7	0.52
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD12	7	0.52
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD13	7	0.52
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD11	20	0.52
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD12	20	0.52
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD13	20	0.52
(1,1355)	1:57:A:CYS:HB2	1:160:A:LEU:H	19	0.52
(1,1353)	1:57:A:CYS:HB3	1:160:A:LEU:H	19	0.52
(1,1326)	1:89:A:ILE:HG21	1:158:A:ILE:HB	4	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1326)	1:89:A:ILE:HG22	1:158:A:ILE:HB	4	0.52
(1,1326)	1:89:A:ILE:HG23	1:158:A:ILE:HB	4	0.52
(1,1311)	1:152:A:THR:HG21	1:157:A:HIS:H	1	0.52
(1,1311)	1:152:A:THR:HG22	1:157:A:HIS:H	1	0.52
(1,1311)	1:152:A:THR:HG23	1:157:A:HIS:H	1	0.52
(1,1311)	1:152:A:THR:HG21	1:157:A:HIS:H	4	0.52
(1,1311)	1:152:A:THR:HG22	1:157:A:HIS:H	4	0.52
(1,1311)	1:152:A:THR:HG23	1:157:A:HIS:H	4	0.52
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD11	8	0.52
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD12	8	0.52
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD13	8	0.52
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD11	19	0.52
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD12	19	0.52
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD13	19	0.52
(1,1206)	1:145:A:GLU:HB3	1:146:A:MET:HB2	9	0.52
(1,1206)	1:145:A:GLU:HB3	1:146:A:MET:HB2	16	0.52
(1,1193)	1:141:A:LEU:HD11	1:148:A:GLY:H	4	0.52
(1,1193)	1:141:A:LEU:HD12	1:148:A:GLY:H	4	0.52
(1,1193)	1:141:A:LEU:HD13	1:148:A:GLY:H	4	0.52
(1,1125)	1:129:A:GLN:HG2	1:130:A:MET:H	17	0.52
(1,1112)	1:126:A:SER:H	1:129:A:GLN:HE21	4	0.52
(1,1112)	1:126:A:SER:H	1:129:A:GLN:HE21	14	0.52
(1,1057)	1:59:A:HIS:H	1:122:A:LEU:HG	10	0.52
(1,1047)	1:119:A:ARG:HD2	1:121:A:ASP:H	15	0.52
(1,1033)	1:108:A:SER:H	1:119:A:ARG:HB2	14	0.52
(1,1032)	1:107:A:ALA:HB1	1:119:A:ARG:H	5	0.52
(1,1032)	1:107:A:ALA:HB2	1:119:A:ARG:H	5	0.52
(1,1032)	1:107:A:ALA:HB3	1:119:A:ARG:H	5	0.52
(1,1032)	1:107:A:ALA:HB1	1:119:A:ARG:H	12	0.52
(1,1032)	1:107:A:ALA:HB2	1:119:A:ARG:H	12	0.52
(1,1032)	1:107:A:ALA:HB3	1:119:A:ARG:H	12	0.52
(1,910)	1:102:A:ASP:H	1:106:A:LEU:HB3	3	0.52
(1,910)	1:102:A:ASP:H	1:106:A:LEU:HB3	8	0.52
(1,910)	1:102:A:ASP:H	1:106:A:LEU:HB3	11	0.52
(1,910)	1:102:A:ASP:H	1:106:A:LEU:HB3	12	0.52
(1,910)	1:102:A:ASP:H	1:106:A:LEU:HB3	20	0.52
(1,886)	1:103:A:PHE:HE1	1:107:A:ALA:H	17	0.52
(1,886)	1:103:A:PHE:HE2	1:107:A:ALA:H	17	0.52
(1,871)	1:96:A:ILE:HB	1:103:A:PHE:H	10	0.52
(1,840)	1:97:A:LYS:HG2	1:146:A:MET:HE1	20	0.52
(1,840)	1:97:A:LYS:HG2	1:146:A:MET:HE2	20	0.52
(1,840)	1:97:A:LYS:HG2	1:146:A:MET:HE3	20	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,834)	1:94:A:GLN:HE21	1:97:A:LYS:HD2	5	0.52
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD11	10	0.52
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD12	10	0.52
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD13	10	0.52
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE1	3	0.52
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE2	3	0.52
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE3	3	0.52
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE1	4	0.52
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE2	4	0.52
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE3	4	0.52
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD11	16	0.52
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD12	16	0.52
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD13	16	0.52
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD11	16	0.52
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD12	16	0.52
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD13	16	0.52
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD11	5	0.52
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD12	5	0.52
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD13	5	0.52
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD1	16	0.52
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD2	16	0.52
(1,753)	1:90:A:ASN:HD22	1:91:A:GLY:H	17	0.52
(1,728)	1:89:A:ILE:HD11	1:92:A:TYR:HE1	12	0.52
(1,728)	1:89:A:ILE:HD11	1:92:A:TYR:HE2	12	0.52
(1,728)	1:89:A:ILE:HD12	1:92:A:TYR:HE1	12	0.52
(1,728)	1:89:A:ILE:HD12	1:92:A:TYR:HE2	12	0.52
(1,728)	1:89:A:ILE:HD13	1:92:A:TYR:HE1	12	0.52
(1,728)	1:89:A:ILE:HD13	1:92:A:TYR:HE2	12	0.52
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD21	2	0.52
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD22	2	0.52
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD23	2	0.52
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD21	9	0.52
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD22	9	0.52
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD23	9	0.52
(1,671)	1:64:A:HIS:HB2	1:85:A:ALA:H	11	0.52
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG21	14	0.52
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG22	14	0.52
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG23	14	0.52
(1,591)	1:74:A:ARG:HE	1:75:A:GLN:H	8	0.52
(1,589)	1:74:A:ARG:H	1:112:A:ASP:HA	5	0.52
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB1	13	0.52
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB2	13	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB3	13	0.52
(1,554)	1:70:A:PRO:HG3	1:71:A:SER:H	16	0.52
(1,531)	1:64:A:HIS:HE1	1:67:A:SER:HB2	15	0.52
(1,531)	1:64:A:HIS:HE1	1:67:A:SER:HB2	19	0.52
(1,530)	1:64:A:HIS:HE1	1:67:A:SER:HA	19	0.52
(1,527)	1:66:A:GLN:HG2	1:81:A:THR:HG21	1	0.52
(1,527)	1:66:A:GLN:HG2	1:81:A:THR:HG22	1	0.52
(1,527)	1:66:A:GLN:HG2	1:81:A:THR:HG23	1	0.52
(1,515)	1:63:A:LYS:H	1:156:A:ILE:H	8	0.52
(1,514)	1:63:A:LYS:HB2	1:70:A:PRO:HA	18	0.52
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD21	14	0.52
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD22	14	0.52
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD23	14	0.52
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD21	17	0.52
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD22	17	0.52
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD23	17	0.52
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD11	18	0.52
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD12	18	0.52
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD13	18	0.52
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG21	11	0.52
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG22	11	0.52
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG23	11	0.52
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG21	11	0.52
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG22	11	0.52
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG23	11	0.52
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG21	11	0.52
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG22	11	0.52
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG23	11	0.52
(1,397)	1:54:A:ARG:HG2	1:126:A:SER:H	4	0.52
(1,366)	1:32:A:SER:H	1:33:A:GLN:HE22	13	0.52
(1,366)	1:32:A:SER:H	1:33:A:GLN:HE21	13	0.52
(1,363)	1:11:A:TRP:HE3	1:33:A:GLN:H	12	0.52
(1,321)	1:25:A:PHE:HZ	1:30:A:ASN:H	17	0.52
(1,295)	1:27:A:HIS:H	1:29:A:THR:H	2	0.52
(1,295)	1:27:A:HIS:H	1:29:A:THR:H	15	0.52
(1,287)	1:26:A:ASN:H	1:32:A:SER:HB2	10	0.52
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG21	1	0.52
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG22	1	0.52
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG23	1	0.52
(1,267)	1:26:A:ASN:HD21	1:28:A:ILE:HG12	20	0.52
(1,261)	1:25:A:PHE:HE1	1:26:A:ASN:H	1	0.52
(1,261)	1:25:A:PHE:HE2	1:26:A:ASN:H	1	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,261)	1:25:A:PHE:HE1	1:26:A:ASN:H	5	0.52
(1,261)	1:25:A:PHE:HE2	1:26:A:ASN:H	5	0.52
(1,194)	1:13:A:LYS:HG2	1:24:A:TYR:HA	20	0.52
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG11	1	0.52
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG12	1	0.52
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG13	1	0.52
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG11	1	0.52
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG12	1	0.52
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG13	1	0.52
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG11	1	0.52
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG12	1	0.52
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG13	1	0.52
(1,138)	1:21:A:ARG:HE	1:34:A:TRP:HH2	5	0.52
(1,138)	1:21:A:ARG:HE	1:34:A:TRP:HH2	12	0.52
(1,133)	1:20:A:GLY:H	1:21:A:ARG:HB2	17	0.52
(1,111)	1:15:A:MET:H	1:23:A:TYR:HD1	16	0.52
(1,111)	1:15:A:MET:H	1:23:A:TYR:HD2	16	0.52
(1,93)	1:14:A:ARG:H	1:22:A:VAL:HA	20	0.52
(1,70)	1:12:A:GLU:HG2	1:13:A:LYS:H	8	0.52
(1,64)	1:12:A:GLU:H	1:24:A:TYR:HD1	9	0.52
(1,64)	1:12:A:GLU:H	1:24:A:TYR:HD2	9	0.52
(1,64)	1:12:A:GLU:H	1:24:A:TYR:HD1	18	0.52
(1,64)	1:12:A:GLU:H	1:24:A:TYR:HD2	18	0.52
(1,11)	1:4:A:GLU:H	1:6:A:LYS:H	12	0.52
(1,11)	1:4:A:GLU:H	1:6:A:LYS:H	17	0.52
(2,111)	1:160:A:LEU:H	2:651:B:ILE:HG12	12	0.51
(2,111)	1:160:A:LEU:H	2:651:B:ILE:HG13	12	0.51
(2,106)	1:139:A:PHE:H	2:656:B:PHE:HB2	16	0.51
(2,97)	1:94:A:GLN:HE21	2:640:B:LEU:HG	5	0.51
(2,86)	1:29:A:THR:HG21	2:647:B:VAL:HA	19	0.51
(2,86)	1:29:A:THR:HG22	2:647:B:VAL:HA	19	0.51
(2,86)	1:29:A:THR:HG23	2:647:B:VAL:HA	19	0.51
(2,9)	1:53:A:ALA:H	1:54:A:ARG:HD2	5	0.51
(2,1)	1:10:A:GLY:H	1:11:A:TRP:HB3	20	0.51
(1,2586)	1:115:A:SER:H	2:659:B:PHE:HE1	19	0.51
(1,2586)	1:115:A:SER:H	2:659:B:PHE:HE2	19	0.51
(1,2586)	1:115:A:SER:H	2:659:B:PHE:HE1	20	0.51
(1,2586)	1:115:A:SER:H	2:659:B:PHE:HE2	20	0.51
(1,2584)	1:114:A:SER:H	2:659:B:PHE:HD1	12	0.51
(1,2584)	1:114:A:SER:H	2:659:B:PHE:HD2	12	0.51
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG21	14	0.51
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG22	14	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG23	14	0.51
(1,2529)	2:648:B:ILE:HG21	2:649:B:ARG:HD2	19	0.51
(1,2529)	2:648:B:ILE:HG22	2:649:B:ARG:HD2	19	0.51
(1,2529)	2:648:B:ILE:HG23	2:649:B:ARG:HD2	19	0.51
(1,2520)	2:646:B:GLU:HG3	2:647:B:VAL:H	4	0.51
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD21	1	0.51
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD22	1	0.51
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD23	1	0.51
(1,1869)	1:75:A:GLN:H	1:75:A:GLN:HE22	9	0.51
(1,1441)	1:162:A:THR:HG21	1:163:A:GLU:HG3	12	0.51
(1,1441)	1:162:A:THR:HG22	1:163:A:GLU:HG3	12	0.51
(1,1441)	1:162:A:THR:HG23	1:163:A:GLU:HG3	12	0.51
(1,1423)	1:55:A:VAL:HB	1:163:A:GLU:H	9	0.51
(1,1392)	1:160:A:LEU:HD11	1:162:A:THR:HG21	11	0.51
(1,1392)	1:160:A:LEU:HD11	1:162:A:THR:HG22	11	0.51
(1,1392)	1:160:A:LEU:HD11	1:162:A:THR:HG23	11	0.51
(1,1392)	1:160:A:LEU:HD12	1:162:A:THR:HG21	11	0.51
(1,1392)	1:160:A:LEU:HD12	1:162:A:THR:HG22	11	0.51
(1,1392)	1:160:A:LEU:HD12	1:162:A:THR:HG23	11	0.51
(1,1392)	1:160:A:LEU:HD13	1:162:A:THR:HG21	11	0.51
(1,1392)	1:160:A:LEU:HD13	1:162:A:THR:HG22	11	0.51
(1,1392)	1:160:A:LEU:HD13	1:162:A:THR:HG23	11	0.51
(1,1392)	1:160:A:LEU:HD11	1:162:A:THR:HG21	17	0.51
(1,1392)	1:160:A:LEU:HD11	1:162:A:THR:HG22	17	0.51
(1,1392)	1:160:A:LEU:HD11	1:162:A:THR:HG23	17	0.51
(1,1392)	1:160:A:LEU:HD12	1:162:A:THR:HG21	17	0.51
(1,1392)	1:160:A:LEU:HD12	1:162:A:THR:HG22	17	0.51
(1,1392)	1:160:A:LEU:HD12	1:162:A:THR:HG23	17	0.51
(1,1392)	1:160:A:LEU:HD13	1:162:A:THR:HG21	17	0.51
(1,1392)	1:160:A:LEU:HD13	1:162:A:THR:HG22	17	0.51
(1,1392)	1:160:A:LEU:HD13	1:162:A:THR:HG23	17	0.51
(1,1369)	1:104:A:GLU:H	1:160:A:LEU:HD11	18	0.51
(1,1369)	1:104:A:GLU:H	1:160:A:LEU:HD12	18	0.51
(1,1369)	1:104:A:GLU:H	1:160:A:LEU:HD13	18	0.51
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD11	3	0.51
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD12	3	0.51
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD13	3	0.51
(1,1328)	1:89:A:ILE:HG12	1:158:A:ILE:HB	12	0.51
(1,1328)	1:89:A:ILE:HG12	1:158:A:ILE:HB	13	0.51
(1,1326)	1:89:A:ILE:HG21	1:158:A:ILE:HB	3	0.51
(1,1326)	1:89:A:ILE:HG22	1:158:A:ILE:HB	3	0.51
(1,1326)	1:89:A:ILE:HG23	1:158:A:ILE:HB	3	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1326)	1:89:A:ILE:HG21	1:158:A:ILE:HB	7	0.51
(1,1326)	1:89:A:ILE:HG22	1:158:A:ILE:HB	7	0.51
(1,1326)	1:89:A:ILE:HG23	1:158:A:ILE:HB	7	0.51
(1,1313)	1:156:A:ILE:HA	1:157:A:HIS:HD2	11	0.51
(1,1313)	1:156:A:ILE:HA	1:157:A:HIS:HD2	18	0.51
(1,1306)	1:89:A:ILE:HD11	1:157:A:HIS:HD2	20	0.51
(1,1306)	1:89:A:ILE:HD12	1:157:A:HIS:HD2	20	0.51
(1,1306)	1:89:A:ILE:HD13	1:157:A:HIS:HD2	20	0.51
(1,1299)	1:152:A:THR:H	1:156:A:ILE:HG21	16	0.51
(1,1299)	1:152:A:THR:H	1:156:A:ILE:HG22	16	0.51
(1,1299)	1:152:A:THR:H	1:156:A:ILE:HG23	16	0.51
(1,1262)	1:151:A:PHE:H	1:156:A:ILE:HA	1	0.51
(1,1109)	1:126:A:SER:HA	1:139:A:PHE:HD1	19	0.51
(1,1109)	1:126:A:SER:HA	1:139:A:PHE:HD2	19	0.51
(1,1107)	1:54:A:ARG:HD2	1:126:A:SER:HA	18	0.51
(1,1033)	1:108:A:SER:H	1:119:A:ARG:HB2	6	0.51
(1,1032)	1:107:A:ALA:HB1	1:119:A:ARG:H	10	0.51
(1,1032)	1:107:A:ALA:HB2	1:119:A:ARG:H	10	0.51
(1,1032)	1:107:A:ALA:HB3	1:119:A:ARG:H	10	0.51
(1,1024)	1:118:A:ALA:HA	1:119:A:ARG:HE	16	0.51
(1,1024)	1:118:A:ALA:HA	1:119:A:ARG:HE	20	0.51
(1,995)	1:108:A:SER:HA	1:116:A:ALA:H	11	0.51
(1,985)	1:61:A:LEU:HD21	1:113:A:CYS:HA	13	0.51
(1,985)	1:61:A:LEU:HD22	1:113:A:CYS:HA	13	0.51
(1,985)	1:61:A:LEU:HD23	1:113:A:CYS:HA	13	0.51
(1,913)	1:103:A:PHE:H	1:106:A:LEU:HB3	17	0.51
(1,910)	1:102:A:ASP:H	1:106:A:LEU:HB3	15	0.51
(1,889)	1:103:A:PHE:HE1	1:146:A:MET:HE1	2	0.51
(1,889)	1:103:A:PHE:HE1	1:146:A:MET:HE2	2	0.51
(1,889)	1:103:A:PHE:HE1	1:146:A:MET:HE3	2	0.51
(1,889)	1:103:A:PHE:HE2	1:146:A:MET:HE1	2	0.51
(1,889)	1:103:A:PHE:HE2	1:146:A:MET:HE2	2	0.51
(1,889)	1:103:A:PHE:HE2	1:146:A:MET:HE3	2	0.51
(1,886)	1:103:A:PHE:HE1	1:107:A:ALA:H	5	0.51
(1,886)	1:103:A:PHE:HE2	1:107:A:ALA:H	5	0.51
(1,886)	1:103:A:PHE:HE1	1:107:A:ALA:H	6	0.51
(1,886)	1:103:A:PHE:HE2	1:107:A:ALA:H	6	0.51
(1,886)	1:103:A:PHE:HE1	1:107:A:ALA:H	12	0.51
(1,886)	1:103:A:PHE:HE2	1:107:A:ALA:H	12	0.51
(1,871)	1:96:A:ILE:HB	1:103:A:PHE:H	1	0.51
(1,871)	1:96:A:ILE:HB	1:103:A:PHE:H	3	0.51
(1,871)	1:96:A:ILE:HB	1:103:A:PHE:H	7	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,868)	1:60:A:LEU:HD21	1:103:A:PHE:HE1	9	0.51
(1,868)	1:60:A:LEU:HD21	1:103:A:PHE:HE2	9	0.51
(1,868)	1:60:A:LEU:HD22	1:103:A:PHE:HE1	9	0.51
(1,868)	1:60:A:LEU:HD22	1:103:A:PHE:HE2	9	0.51
(1,868)	1:60:A:LEU:HD23	1:103:A:PHE:HE1	9	0.51
(1,868)	1:60:A:LEU:HD23	1:103:A:PHE:HE2	9	0.51
(1,868)	1:60:A:LEU:HD21	1:103:A:PHE:HE1	11	0.51
(1,868)	1:60:A:LEU:HD21	1:103:A:PHE:HE2	11	0.51
(1,868)	1:60:A:LEU:HD22	1:103:A:PHE:HE1	11	0.51
(1,868)	1:60:A:LEU:HD22	1:103:A:PHE:HE2	11	0.51
(1,868)	1:60:A:LEU:HD23	1:103:A:PHE:HE1	11	0.51
(1,868)	1:60:A:LEU:HD23	1:103:A:PHE:HE2	11	0.51
(1,868)	1:60:A:LEU:HD21	1:103:A:PHE:HE1	12	0.51
(1,868)	1:60:A:LEU:HD21	1:103:A:PHE:HE2	12	0.51
(1,868)	1:60:A:LEU:HD22	1:103:A:PHE:HE1	12	0.51
(1,868)	1:60:A:LEU:HD22	1:103:A:PHE:HE2	12	0.51
(1,868)	1:60:A:LEU:HD23	1:103:A:PHE:HE1	12	0.51
(1,868)	1:60:A:LEU:HD23	1:103:A:PHE:HE2	12	0.51
(1,845)	1:97:A:LYS:HD2	1:98:A:SER:H	13	0.51
(1,816)	1:95:A:LYS:HD2	1:96:A:ILE:H	10	0.51
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE1	18	0.51
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE2	18	0.51
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE3	18	0.51
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD11	2	0.51
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD12	2	0.51
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD13	2	0.51
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD11	2	0.51
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD12	2	0.51
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD13	2	0.51
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD11	4	0.51
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD12	4	0.51
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD13	4	0.51
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD11	4	0.51
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD12	4	0.51
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD13	4	0.51
(1,742)	1:89:A:ILE:HD11	1:90:A:ASN:H	7	0.51
(1,742)	1:89:A:ILE:HD12	1:90:A:ASN:H	7	0.51
(1,742)	1:89:A:ILE:HD13	1:90:A:ASN:H	7	0.51
(1,742)	1:89:A:ILE:HD11	1:90:A:ASN:H	10	0.51
(1,742)	1:89:A:ILE:HD12	1:90:A:ASN:H	10	0.51
(1,742)	1:89:A:ILE:HD13	1:90:A:ASN:H	10	0.51
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD21	1	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD22	1	0.51
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD23	1	0.51
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD21	14	0.51
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD22	14	0.51
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD23	14	0.51
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD21	19	0.51
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD22	19	0.51
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD23	19	0.51
(1,647)	1:65:A:SER:H	1:82:A:LYS:H	19	0.51
(1,593)	1:71:A:SER:HB3	1:77:A:LYS:HA	6	0.51
(1,593)	1:71:A:SER:HB3	1:77:A:LYS:HA	12	0.51
(1,589)	1:74:A:ARG:H	1:112:A:ASP:HA	11	0.51
(1,572)	1:73:A:TRP:HE1	1:111:A:SER:HB2	3	0.51
(1,572)	1:73:A:TRP:HE1	1:111:A:SER:HB2	14	0.51
(1,541)	1:67:A:SER:HB3	1:70:A:PRO:HA	6	0.51
(1,521)	1:64:A:HIS:H	1:66:A:GLN:H	7	0.51
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD21	5	0.51
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD22	5	0.51
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD23	5	0.51
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD21	12	0.51
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD22	12	0.51
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD23	12	0.51
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG21	3	0.51
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG22	3	0.51
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG23	3	0.51
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG21	3	0.51
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG22	3	0.51
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG23	3	0.51
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG21	3	0.51
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG22	3	0.51
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG23	3	0.51
(1,435)	1:58:A:SER:HA	1:122:A:LEU:HG	13	0.51
(1,422)	1:56:A:ARG:HG2	1:162:A:THR:HB	12	0.51
(1,397)	1:54:A:ARG:HG2	1:126:A:SER:H	19	0.51
(1,366)	1:32:A:SER:H	1:33:A:GLN:HE22	7	0.51
(1,366)	1:32:A:SER:H	1:33:A:GLN:HE21	7	0.51
(1,355)	1:25:A:PHE:HE1	1:32:A:SER:HB2	20	0.51
(1,355)	1:25:A:PHE:HE2	1:32:A:SER:HB2	20	0.51
(1,334)	1:27:A:HIS:HA	1:31:A:ALA:H	8	0.51
(1,295)	1:27:A:HIS:H	1:29:A:THR:H	6	0.51
(1,295)	1:27:A:HIS:H	1:29:A:THR:H	7	0.51
(1,287)	1:26:A:ASN:H	1:32:A:SER:HB2	6	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,287)	1:26:A:ASN:H	1:32:A:SER:HB2	17	0.51
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG21	8	0.51
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG22	8	0.51
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG23	8	0.51
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG21	18	0.51
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG22	18	0.51
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG23	18	0.51
(1,194)	1:13:A:LYS:HG2	1:24:A:TYR:HA	1	0.51
(1,181)	1:23:A:TYR:HB2	1:34:A:TRP:HE3	11	0.51
(1,148)	1:15:A:MET:HE1	1:22:A:VAL:HA	16	0.51
(1,148)	1:15:A:MET:HE2	1:22:A:VAL:HA	16	0.51
(1,148)	1:15:A:MET:HE3	1:22:A:VAL:HA	16	0.51
(1,148)	1:15:A:MET:HE1	1:22:A:VAL:HA	20	0.51
(1,148)	1:15:A:MET:HE2	1:22:A:VAL:HA	20	0.51
(1,148)	1:15:A:MET:HE3	1:22:A:VAL:HA	20	0.51
(1,134)	1:20:A:GLY:H	1:21:A:ARG:HA	7	0.51
(1,134)	1:20:A:GLY:H	1:21:A:ARG:HA	14	0.51
(1,134)	1:20:A:GLY:H	1:21:A:ARG:HA	17	0.51
(1,133)	1:20:A:GLY:H	1:21:A:ARG:HB2	5	0.51
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG21	3	0.51
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG22	3	0.51
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG23	3	0.51
(1,66)	1:12:A:GLU:H	1:25:A:PHE:HE1	15	0.51
(1,66)	1:12:A:GLU:H	1:25:A:PHE:HE2	15	0.51
(1,64)	1:12:A:GLU:H	1:24:A:TYR:HD1	2	0.51
(1,64)	1:12:A:GLU:H	1:24:A:TYR:HD2	2	0.51
(1,64)	1:12:A:GLU:H	1:24:A:TYR:HD1	4	0.51
(1,64)	1:12:A:GLU:H	1:24:A:TYR:HD2	4	0.51
(1,64)	1:12:A:GLU:H	1:24:A:TYR:HD1	17	0.51
(1,64)	1:12:A:GLU:H	1:24:A:TYR:HD2	17	0.51
(1,44)	1:8:A:PRO:HB2	1:11:A:TRP:HE1	3	0.51
(1,35)	1:9:A:PRO:HG2	1:10:A:GLY:H	16	0.51
(1,14)	1:6:A:LYS:HG2	1:7:A:LEU:H	6	0.51
(1,14)	1:6:A:LYS:HG2	1:7:A:LEU:H	14	0.51
(2,102)	1:135:A:GLU:H	2:656:B:PHE:HB2	11	0.5
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG11	14	0.5
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG12	14	0.5
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG13	14	0.5
(2,45)	1:131:A:GLN:HE21	1:152:A:THR:HB	18	0.5
(2,4)	1:21:A:ARG:HE	1:22:A:VAL:H	15	0.5
(1,2598)	1:146:A:MET:HE1	2:642:B:PRO:HB2	20	0.5
(1,2598)	1:146:A:MET:HE1	2:642:B:PRO:HB3	20	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2598)	1:146:A:MET:HE2	2:642:B:PRO:HB2	20	0.5
(1,2598)	1:146:A:MET:HE2	2:642:B:PRO:HB3	20	0.5
(1,2598)	1:146:A:MET:HE3	2:642:B:PRO:HB2	20	0.5
(1,2598)	1:146:A:MET:HE3	2:642:B:PRO:HB3	20	0.5
(1,2586)	1:115:A:SER:H	2:659:B:PHE:HE1	11	0.5
(1,2586)	1:115:A:SER:H	2:659:B:PHE:HE2	11	0.5
(1,2584)	1:114:A:SER:H	2:659:B:PHE:HD1	1	0.5
(1,2584)	1:114:A:SER:H	2:659:B:PHE:HD2	1	0.5
(1,2584)	1:114:A:SER:H	2:659:B:PHE:HD1	4	0.5
(1,2584)	1:114:A:SER:H	2:659:B:PHE:HD2	4	0.5
(1,2584)	1:114:A:SER:H	2:659:B:PHE:HD1	8	0.5
(1,2584)	1:114:A:SER:H	2:659:B:PHE:HD2	8	0.5
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG21	1	0.5
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG22	1	0.5
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG23	1	0.5
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG21	4	0.5
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG22	4	0.5
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG23	4	0.5
(1,2533)	2:647:B:VAL:H	2:649:B:ARG:H	1	0.5
(1,2526)	2:646:B:GLU:HB2	2:648:B:ILE:H	3	0.5
(1,2525)	2:645:B:GLN:HE22	2:648:B:ILE:HD11	16	0.5
(1,2525)	2:645:B:GLN:HE22	2:648:B:ILE:HD12	16	0.5
(1,2525)	2:645:B:GLN:HE22	2:648:B:ILE:HD13	16	0.5
(1,2513)	2:646:B:GLU:HA	2:649:B:ARG:HD2	13	0.5
(1,2507)	2:643:B:PRO:HA	2:645:B:GLN:H	9	0.5
(1,2161)	1:119:A:ARG:H	1:119:A:ARG:HD3	10	0.5
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD21	7	0.5
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD22	7	0.5
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD23	7	0.5
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD21	12	0.5
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD22	12	0.5
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD23	12	0.5
(1,1977)	1:89:A:ILE:H	1:89:A:ILE:HG12	11	0.5
(1,1977)	1:89:A:ILE:H	1:89:A:ILE:HG12	16	0.5
(1,1977)	1:89:A:ILE:H	1:89:A:ILE:HG12	20	0.5
(1,1435)	1:161:A:ARG:HG3	1:163:A:GLU:H	20	0.5
(1,1434)	1:161:A:ARG:HD2	1:163:A:GLU:H	5	0.5
(1,1434)	1:161:A:ARG:HD2	1:163:A:GLU:H	10	0.5
(1,1434)	1:161:A:ARG:HD2	1:163:A:GLU:H	15	0.5
(1,1428)	1:143:A:THR:HG21	1:163:A:GLU:H	10	0.5
(1,1428)	1:143:A:THR:HG22	1:163:A:GLU:H	10	0.5
(1,1428)	1:143:A:THR:HG23	1:163:A:GLU:H	10	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1423)	1:55:A:VAL:HB	1:163:A:GLU:H	6	0.5
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD11	12	0.5
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD12	12	0.5
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD13	12	0.5
(1,1326)	1:89:A:ILE:HG21	1:158:A:ILE:HB	17	0.5
(1,1326)	1:89:A:ILE:HG22	1:158:A:ILE:HB	17	0.5
(1,1326)	1:89:A:ILE:HG23	1:158:A:ILE:HB	17	0.5
(1,1306)	1:89:A:ILE:HD11	1:157:A:HIS:HD2	13	0.5
(1,1306)	1:89:A:ILE:HD12	1:157:A:HIS:HD2	13	0.5
(1,1306)	1:89:A:ILE:HD13	1:157:A:HIS:HD2	13	0.5
(1,1299)	1:152:A:THR:H	1:156:A:ILE:HG21	1	0.5
(1,1299)	1:152:A:THR:H	1:156:A:ILE:HG22	1	0.5
(1,1299)	1:152:A:THR:H	1:156:A:ILE:HG23	1	0.5
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG21	12	0.5
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG22	12	0.5
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG23	12	0.5
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD11	9	0.5
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD12	9	0.5
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD13	9	0.5
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD11	14	0.5
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD12	14	0.5
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD13	14	0.5
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD11	16	0.5
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD12	16	0.5
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD13	16	0.5
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD11	20	0.5
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD12	20	0.5
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD13	20	0.5
(1,1282)	1:82:A:LYS:HE2	1:156:A:ILE:HD11	19	0.5
(1,1282)	1:82:A:LYS:HE2	1:156:A:ILE:HD12	19	0.5
(1,1282)	1:82:A:LYS:HE2	1:156:A:ILE:HD13	19	0.5
(1,1276)	1:63:A:LYS:HA	1:155:A:GLY:HA2	12	0.5
(1,1177)	1:137:A:ALA:HB1	1:141:A:LEU:H	15	0.5
(1,1177)	1:137:A:ALA:HB2	1:141:A:LEU:H	15	0.5
(1,1177)	1:137:A:ALA:HB3	1:141:A:LEU:H	15	0.5
(1,1112)	1:126:A:SER:H	1:129:A:GLN:HE21	7	0.5
(1,1112)	1:126:A:SER:H	1:129:A:GLN:HE21	9	0.5
(1,1051)	1:57:A:CYS:H	1:122:A:LEU:HD21	14	0.5
(1,1051)	1:57:A:CYS:H	1:122:A:LEU:HD22	14	0.5
(1,1051)	1:57:A:CYS:H	1:122:A:LEU:HD23	14	0.5
(1,1015)	1:116:A:ALA:HB1	1:120:A:GLY:H	15	0.5
(1,1015)	1:116:A:ALA:HB2	1:120:A:GLY:H	15	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1015)	1:116:A:ALA:HB3	1:120:A:GLY:H	15	0.5
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB1	6	0.5
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB2	6	0.5
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB3	6	0.5
(1,913)	1:103:A:PHE:H	1:106:A:LEU:HB3	13	0.5
(1,913)	1:103:A:PHE:H	1:106:A:LEU:HB3	14	0.5
(1,910)	1:102:A:ASP:H	1:106:A:LEU:HB3	19	0.5
(1,886)	1:103:A:PHE:HE1	1:107:A:ALA:H	18	0.5
(1,886)	1:103:A:PHE:HE2	1:107:A:ALA:H	18	0.5
(1,886)	1:103:A:PHE:HE1	1:107:A:ALA:H	20	0.5
(1,886)	1:103:A:PHE:HE2	1:107:A:ALA:H	20	0.5
(1,844)	1:97:A:LYS:HG2	1:98:A:SER:H	2	0.5
(1,830)	1:93:A:ILE:HG21	1:97:A:LYS:HD2	1	0.5
(1,830)	1:93:A:ILE:HG22	1:97:A:LYS:HD2	1	0.5
(1,830)	1:93:A:ILE:HG23	1:97:A:LYS:HD2	1	0.5
(1,814)	1:94:A:GLN:HG2	1:95:A:LYS:H	17	0.5
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD11	6	0.5
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD12	6	0.5
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD13	6	0.5
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD11	7	0.5
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD12	7	0.5
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD13	7	0.5
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD11	8	0.5
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD12	8	0.5
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD13	8	0.5
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD11	16	0.5
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD12	16	0.5
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD13	16	0.5
(1,785)	1:89:A:ILE:HG21	1:93:A:ILE:H	7	0.5
(1,785)	1:89:A:ILE:HG22	1:93:A:ILE:H	7	0.5
(1,785)	1:89:A:ILE:HG23	1:93:A:ILE:H	7	0.5
(1,785)	1:89:A:ILE:HG21	1:93:A:ILE:H	14	0.5
(1,785)	1:89:A:ILE:HG22	1:93:A:ILE:H	14	0.5
(1,785)	1:89:A:ILE:HG23	1:93:A:ILE:H	14	0.5
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD11	1	0.5
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD12	1	0.5
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD13	1	0.5
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD11	1	0.5
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD12	1	0.5
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD13	1	0.5
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD11	13	0.5
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD12	13	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD13	13	0.5
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD1	14	0.5
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD2	14	0.5
(1,742)	1:89:A:ILE:HD11	1:90:A:ASN:H	2	0.5
(1,742)	1:89:A:ILE:HD12	1:90:A:ASN:H	2	0.5
(1,742)	1:89:A:ILE:HD13	1:90:A:ASN:H	2	0.5
(1,742)	1:89:A:ILE:HD11	1:90:A:ASN:H	3	0.5
(1,742)	1:89:A:ILE:HD12	1:90:A:ASN:H	3	0.5
(1,742)	1:89:A:ILE:HD13	1:90:A:ASN:H	3	0.5
(1,742)	1:89:A:ILE:HD11	1:90:A:ASN:H	4	0.5
(1,742)	1:89:A:ILE:HD12	1:90:A:ASN:H	4	0.5
(1,742)	1:89:A:ILE:HD13	1:90:A:ASN:H	4	0.5
(1,742)	1:89:A:ILE:HD11	1:90:A:ASN:H	6	0.5
(1,742)	1:89:A:ILE:HD12	1:90:A:ASN:H	6	0.5
(1,742)	1:89:A:ILE:HD13	1:90:A:ASN:H	6	0.5
(1,742)	1:89:A:ILE:HD11	1:90:A:ASN:H	11	0.5
(1,742)	1:89:A:ILE:HD12	1:90:A:ASN:H	11	0.5
(1,742)	1:89:A:ILE:HD13	1:90:A:ASN:H	11	0.5
(1,742)	1:89:A:ILE:HD11	1:90:A:ASN:H	15	0.5
(1,742)	1:89:A:ILE:HD12	1:90:A:ASN:H	15	0.5
(1,742)	1:89:A:ILE:HD13	1:90:A:ASN:H	15	0.5
(1,742)	1:89:A:ILE:HD11	1:90:A:ASN:H	16	0.5
(1,742)	1:89:A:ILE:HD12	1:90:A:ASN:H	16	0.5
(1,742)	1:89:A:ILE:HD13	1:90:A:ASN:H	16	0.5
(1,742)	1:89:A:ILE:HD11	1:90:A:ASN:H	18	0.5
(1,742)	1:89:A:ILE:HD12	1:90:A:ASN:H	18	0.5
(1,742)	1:89:A:ILE:HD13	1:90:A:ASN:H	18	0.5
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD21	4	0.5
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD22	4	0.5
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD23	4	0.5
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD21	5	0.5
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD22	5	0.5
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD23	5	0.5
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD21	8	0.5
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD22	8	0.5
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD23	8	0.5
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD21	16	0.5
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD22	16	0.5
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD23	16	0.5
(1,641)	1:65:A:SER:HB2	1:81:A:THR:HG21	4	0.5
(1,641)	1:65:A:SER:HB2	1:81:A:THR:HG22	4	0.5
(1,641)	1:65:A:SER:HB2	1:81:A:THR:HG23	4	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,593)	1:71:A:SER:HB3	1:77:A:LYS:HA	3	0.5
(1,591)	1:74:A:ARG:HE	1:75:A:GLN:H	17	0.5
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB1	6	0.5
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB2	6	0.5
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB3	6	0.5
(1,572)	1:73:A:TRP:HE1	1:111:A:SER:HB2	9	0.5
(1,571)	1:73:A:TRP:HE1	1:74:A:ARG:HB3	17	0.5
(1,541)	1:67:A:SER:HB3	1:70:A:PRO:HA	4	0.5
(1,541)	1:67:A:SER:HB3	1:70:A:PRO:HA	9	0.5
(1,471)	1:61:A:LEU:HD21	1:63:A:LYS:HA	18	0.5
(1,471)	1:61:A:LEU:HD22	1:63:A:LYS:HA	18	0.5
(1,471)	1:61:A:LEU:HD23	1:63:A:LYS:HA	18	0.5
(1,465)	1:60:A:LEU:HB2	1:158:A:ILE:H	5	0.5
(1,457)	1:60:A:LEU:HD11	1:108:A:SER:H	9	0.5
(1,457)	1:60:A:LEU:HD12	1:108:A:SER:H	9	0.5
(1,457)	1:60:A:LEU:HD13	1:108:A:SER:H	9	0.5
(1,377)	1:33:A:GLN:HG2	1:35:A:GLU:H	18	0.5
(1,355)	1:25:A:PHE:HE1	1:32:A:SER:HB2	16	0.5
(1,355)	1:25:A:PHE:HE2	1:32:A:SER:HB2	16	0.5
(1,321)	1:25:A:PHE:HZ	1:30:A:ASN:H	6	0.5
(1,320)	1:25:A:PHE:HE1	1:30:A:ASN:H	17	0.5
(1,320)	1:25:A:PHE:HE2	1:30:A:ASN:H	17	0.5
(1,295)	1:27:A:HIS:H	1:29:A:THR:H	9	0.5
(1,295)	1:27:A:HIS:H	1:29:A:THR:H	10	0.5
(1,287)	1:26:A:ASN:H	1:32:A:SER:HB2	4	0.5
(1,287)	1:26:A:ASN:H	1:32:A:SER:HB2	14	0.5
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG21	4	0.5
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG22	4	0.5
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG23	4	0.5
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG21	5	0.5
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG22	5	0.5
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG23	5	0.5
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG21	10	0.5
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG22	10	0.5
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG23	10	0.5
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG21	14	0.5
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG22	14	0.5
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG23	14	0.5
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG21	19	0.5
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG22	19	0.5
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG23	19	0.5
(1,214)	1:11:A:TRP:HB2	1:25:A:PHE:H	3	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,214)	1:11:A:TRP:HB2	1:25:A:PHE:H	5	0.5
(1,213)	1:11:A:TRP:HA	1:25:A:PHE:H	1	0.5
(1,134)	1:20:A:GLY:H	1:21:A:ARG:HA	8	0.5
(1,134)	1:20:A:GLY:H	1:21:A:ARG:HA	12	0.5
(1,111)	1:15:A:MET:H	1:23:A:TYR:HD1	19	0.5
(1,111)	1:15:A:MET:H	1:23:A:TYR:HD2	19	0.5
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG21	4	0.5
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG22	4	0.5
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG23	4	0.5
(1,79)	1:13:A:LYS:H	1:24:A:TYR:HD1	12	0.5
(1,79)	1:13:A:LYS:H	1:24:A:TYR:HD2	12	0.5
(1,66)	1:12:A:GLU:H	1:25:A:PHE:HE1	8	0.5
(1,66)	1:12:A:GLU:H	1:25:A:PHE:HE2	8	0.5
(1,35)	1:9:A:PRO:HG2	1:10:A:GLY:H	20	0.5
(1,27)	1:7:A:LEU:HD21	1:13:A:LYS:H	6	0.5
(1,27)	1:7:A:LEU:HD22	1:13:A:LYS:H	6	0.5
(1,27)	1:7:A:LEU:HD23	1:13:A:LYS:H	6	0.5
(1,27)	1:7:A:LEU:HD21	1:13:A:LYS:H	7	0.5
(1,27)	1:7:A:LEU:HD22	1:13:A:LYS:H	7	0.5
(1,27)	1:7:A:LEU:HD23	1:13:A:LYS:H	7	0.5
(1,27)	1:7:A:LEU:HD21	1:13:A:LYS:H	9	0.5
(1,27)	1:7:A:LEU:HD22	1:13:A:LYS:H	9	0.5
(1,27)	1:7:A:LEU:HD23	1:13:A:LYS:H	9	0.5
(2,113)	1:162:A:THR:H	2:651:B:ILE:HG12	5	0.49
(2,113)	1:162:A:THR:H	2:651:B:ILE:HG13	5	0.49
(2,110)	1:152:A:THR:HG21	2:661:B:PHE:HB2	13	0.49
(2,110)	1:152:A:THR:HG21	2:661:B:PHE:HB3	13	0.49
(2,110)	1:152:A:THR:HG22	2:661:B:PHE:HB2	13	0.49
(2,110)	1:152:A:THR:HG22	2:661:B:PHE:HB3	13	0.49
(2,110)	1:152:A:THR:HG23	2:661:B:PHE:HB2	13	0.49
(2,110)	1:152:A:THR:HG23	2:661:B:PHE:HB3	13	0.49
(2,94)	1:93:A:ILE:HG21	2:643:B:PRO:HB3	13	0.49
(2,94)	1:93:A:ILE:HG22	2:643:B:PRO:HB3	13	0.49
(2,94)	1:93:A:ILE:HG23	2:643:B:PRO:HB3	13	0.49
(2,89)	1:55:A:VAL:H	2:651:B:ILE:HG12	12	0.49
(2,89)	1:55:A:VAL:H	2:651:B:ILE:HG13	12	0.49
(2,79)	2:659:B:PHE:HE1	2:661:B:PHE:H	13	0.49
(2,79)	2:659:B:PHE:HE2	2:661:B:PHE:H	13	0.49
(2,76)	2:656:B:PHE:HE1	2:659:B:PHE:HE1	18	0.49
(2,76)	2:656:B:PHE:HE1	2:659:B:PHE:HE2	18	0.49
(2,76)	2:656:B:PHE:HE2	2:659:B:PHE:HE1	18	0.49
(2,76)	2:656:B:PHE:HE2	2:659:B:PHE:HE2	18	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,45)	1:131:A:GLN:HE21	1:152:A:THR:HB	17	0.49
(2,42)	1:130:A:MET:HB2	1:134:A:PHE:HD1	7	0.49
(2,42)	1:130:A:MET:HB2	1:134:A:PHE:HD2	7	0.49
(2,34)	1:59:A:HIS:H	1:122:A:LEU:HB2	18	0.49
(2,4)	1:21:A:ARG:HE	1:22:A:VAL:H	5	0.49
(1,2582)	1:34:A:TRP:HE1	2:642:B:PRO:HB2	15	0.49
(1,2582)	1:34:A:TRP:HE1	2:642:B:PRO:HB3	15	0.49
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG21	3	0.49
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG22	3	0.49
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG23	3	0.49
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG21	17	0.49
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG22	17	0.49
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG23	17	0.49
(1,2384)	1:163:A:GLU:H	1:163:A:GLU:HG3	14	0.49
(1,2158)	1:119:A:ARG:H	1:119:A:ARG:HD2	5	0.49
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD21	6	0.49
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD22	6	0.49
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD23	6	0.49
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD21	18	0.49
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD22	18	0.49
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD23	18	0.49
(1,2022)	1:94:A:GLN:H	1:94:A:GLN:HG2	20	0.49
(1,1977)	1:89:A:ILE:H	1:89:A:ILE:HG12	1	0.49
(1,1977)	1:89:A:ILE:H	1:89:A:ILE:HG12	4	0.49
(1,1977)	1:89:A:ILE:H	1:89:A:ILE:HG12	6	0.49
(1,1977)	1:89:A:ILE:H	1:89:A:ILE:HG12	7	0.49
(1,1977)	1:89:A:ILE:H	1:89:A:ILE:HG12	15	0.49
(1,1977)	1:89:A:ILE:H	1:89:A:ILE:HG12	18	0.49
(1,1977)	1:89:A:ILE:H	1:89:A:ILE:HG12	19	0.49
(1,1747)	1:56:A:ARG:H	1:56:A:ARG:HD2	9	0.49
(1,1376)	1:146:A:MET:HE1	1:160:A:LEU:HD21	11	0.49
(1,1376)	1:146:A:MET:HE1	1:160:A:LEU:HD22	11	0.49
(1,1376)	1:146:A:MET:HE1	1:160:A:LEU:HD23	11	0.49
(1,1376)	1:146:A:MET:HE2	1:160:A:LEU:HD21	11	0.49
(1,1376)	1:146:A:MET:HE2	1:160:A:LEU:HD22	11	0.49
(1,1376)	1:146:A:MET:HE2	1:160:A:LEU:HD23	11	0.49
(1,1376)	1:146:A:MET:HE3	1:160:A:LEU:HD21	11	0.49
(1,1376)	1:146:A:MET:HE3	1:160:A:LEU:HD22	11	0.49
(1,1376)	1:146:A:MET:HE3	1:160:A:LEU:HD23	11	0.49
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD11	1	0.49
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD12	1	0.49
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD13	1	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD11	5	0.49
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD12	5	0.49
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD13	5	0.49
(1,1363)	1:96:A:ILE:HG21	1:160:A:LEU:HD11	5	0.49
(1,1363)	1:96:A:ILE:HG21	1:160:A:LEU:HD12	5	0.49
(1,1363)	1:96:A:ILE:HG21	1:160:A:LEU:HD13	5	0.49
(1,1363)	1:96:A:ILE:HG22	1:160:A:LEU:HD11	5	0.49
(1,1363)	1:96:A:ILE:HG22	1:160:A:LEU:HD12	5	0.49
(1,1363)	1:96:A:ILE:HG22	1:160:A:LEU:HD13	5	0.49
(1,1363)	1:96:A:ILE:HG23	1:160:A:LEU:HD11	5	0.49
(1,1363)	1:96:A:ILE:HG23	1:160:A:LEU:HD12	5	0.49
(1,1363)	1:96:A:ILE:HG23	1:160:A:LEU:HD13	5	0.49
(1,1363)	1:96:A:ILE:HG21	1:160:A:LEU:HD11	6	0.49
(1,1363)	1:96:A:ILE:HG21	1:160:A:LEU:HD12	6	0.49
(1,1363)	1:96:A:ILE:HG21	1:160:A:LEU:HD13	6	0.49
(1,1363)	1:96:A:ILE:HG22	1:160:A:LEU:HD11	6	0.49
(1,1363)	1:96:A:ILE:HG22	1:160:A:LEU:HD12	6	0.49
(1,1363)	1:96:A:ILE:HG22	1:160:A:LEU:HD13	6	0.49
(1,1363)	1:96:A:ILE:HG23	1:160:A:LEU:HD11	6	0.49
(1,1363)	1:96:A:ILE:HG23	1:160:A:LEU:HD12	6	0.49
(1,1363)	1:96:A:ILE:HG23	1:160:A:LEU:HD13	6	0.49
(1,1353)	1:57:A:CYS:HB3	1:160:A:LEU:H	5	0.49
(1,1335)	1:57:A:CYS:HA	1:159:A:ILE:HG21	3	0.49
(1,1335)	1:57:A:CYS:HA	1:159:A:ILE:HG22	3	0.49
(1,1335)	1:57:A:CYS:HA	1:159:A:ILE:HG23	3	0.49
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG21	8	0.49
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG22	8	0.49
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG23	8	0.49
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG21	18	0.49
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG22	18	0.49
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG23	18	0.49
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG21	20	0.49
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG22	20	0.49
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG23	20	0.49
(1,1280)	1:64:A:HIS:HD2	1:156:A:ILE:HG12	9	0.49
(1,1240)	1:150:A:VAL:H	1:157:A:HIS:HD2	10	0.49
(1,1231)	1:149:A:PRO:HG2	1:150:A:VAL:H	8	0.49
(1,1231)	1:149:A:PRO:HG2	1:150:A:VAL:H	12	0.49
(1,1217)	1:145:A:GLU:HB3	1:147:A:SER:H	1	0.49
(1,1206)	1:145:A:GLU:HB3	1:146:A:MET:HB2	1	0.49
(1,1192)	1:141:A:LEU:HD21	1:146:A:MET:H	2	0.49
(1,1192)	1:141:A:LEU:HD22	1:146:A:MET:H	2	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1192)	1:141:A:LEU:HD23	1:146:A:MET:H	2	0.49
(1,1192)	1:141:A:LEU:HD21	1:146:A:MET:H	3	0.49
(1,1192)	1:141:A:LEU:HD22	1:146:A:MET:H	3	0.49
(1,1192)	1:141:A:LEU:HD23	1:146:A:MET:H	3	0.49
(1,1161)	1:136:A:ASP:HB2	1:138:A:SER:H	4	0.49
(1,1161)	1:136:A:ASP:HB2	1:138:A:SER:H	5	0.49
(1,1143)	1:130:A:MET:HB2	1:135:A:GLU:H	13	0.49
(1,1047)	1:119:A:ARG:HD2	1:121:A:ASP:H	10	0.49
(1,1047)	1:119:A:ARG:HD2	1:121:A:ASP:H	17	0.49
(1,1032)	1:107:A:ALA:HB1	1:119:A:ARG:H	11	0.49
(1,1032)	1:107:A:ALA:HB2	1:119:A:ARG:H	11	0.49
(1,1032)	1:107:A:ALA:HB3	1:119:A:ARG:H	11	0.49
(1,1024)	1:118:A:ALA:HA	1:119:A:ARG:HE	14	0.49
(1,1015)	1:116:A:ALA:HB1	1:120:A:GLY:H	6	0.49
(1,1015)	1:116:A:ALA:HB2	1:120:A:GLY:H	6	0.49
(1,1015)	1:116:A:ALA:HB3	1:120:A:GLY:H	6	0.49
(1,1001)	1:113:A:CYS:H	1:116:A:ALA:HB1	11	0.49
(1,1001)	1:113:A:CYS:H	1:116:A:ALA:HB2	11	0.49
(1,1001)	1:113:A:CYS:H	1:116:A:ALA:HB3	11	0.49
(1,940)	1:106:A:LEU:HG	1:107:A:ALA:H	16	0.49
(1,925)	1:60:A:LEU:HG	1:107:A:ALA:H	12	0.49
(1,925)	1:60:A:LEU:HG	1:107:A:ALA:H	15	0.49
(1,886)	1:103:A:PHE:HE1	1:107:A:ALA:H	3	0.49
(1,886)	1:103:A:PHE:HE2	1:107:A:ALA:H	3	0.49
(1,886)	1:103:A:PHE:HE1	1:107:A:ALA:H	4	0.49
(1,886)	1:103:A:PHE:HE2	1:107:A:ALA:H	4	0.49
(1,886)	1:103:A:PHE:HE1	1:107:A:ALA:H	16	0.49
(1,886)	1:103:A:PHE:HE2	1:107:A:ALA:H	16	0.49
(1,871)	1:96:A:ILE:HB	1:103:A:PHE:H	9	0.49
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD11	12	0.49
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD12	12	0.49
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD13	12	0.49
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD11	6	0.49
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD12	6	0.49
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD13	6	0.49
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD11	6	0.49
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD12	6	0.49
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD13	6	0.49
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD11	4	0.49
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD12	4	0.49
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD13	4	0.49
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD21	7	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD22	7	0.49
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD23	7	0.49
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD21	11	0.49
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD22	11	0.49
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD23	11	0.49
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD21	13	0.49
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD22	13	0.49
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD23	13	0.49
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD21	15	0.49
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD22	15	0.49
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD23	15	0.49
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD21	20	0.49
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD22	20	0.49
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD23	20	0.49
(1,693)	1:86:A:LEU:HD21	1:149:A:PRO:HD2	9	0.49
(1,693)	1:86:A:LEU:HD22	1:149:A:PRO:HD2	9	0.49
(1,693)	1:86:A:LEU:HD23	1:149:A:PRO:HD2	9	0.49
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB1	7	0.49
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB2	7	0.49
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB3	7	0.49
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB1	11	0.49
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB2	11	0.49
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB3	11	0.49
(1,564)	1:72:A:SER:H	1:78:A:ILE:HG12	6	0.49
(1,496)	1:62:A:VAL:HG11	1:88:A:LEU:H	6	0.49
(1,496)	1:62:A:VAL:HG12	1:88:A:LEU:H	6	0.49
(1,496)	1:62:A:VAL:HG13	1:88:A:LEU:H	6	0.49
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG21	2	0.49
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG22	2	0.49
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG23	2	0.49
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG21	2	0.49
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG22	2	0.49
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG23	2	0.49
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG21	2	0.49
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG22	2	0.49
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG23	2	0.49
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG21	16	0.49
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG22	16	0.49
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG23	16	0.49
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG21	16	0.49
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG22	16	0.49
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG23	16	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG21	16	0.49
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG22	16	0.49
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG23	16	0.49
(1,436)	1:58:A:SER:H	1:160:A:LEU:HG	8	0.49
(1,375)	1:33:A:GLN:HE21	1:35:A:GLU:H	11	0.49
(1,321)	1:25:A:PHE:HZ	1:30:A:ASN:H	12	0.49
(1,321)	1:25:A:PHE:HZ	1:30:A:ASN:H	13	0.49
(1,320)	1:25:A:PHE:HE1	1:30:A:ASN:H	6	0.49
(1,320)	1:25:A:PHE:HE2	1:30:A:ASN:H	6	0.49
(1,320)	1:25:A:PHE:HE1	1:30:A:ASN:H	12	0.49
(1,320)	1:25:A:PHE:HE2	1:30:A:ASN:H	12	0.49
(1,305)	1:27:A:HIS:HD2	1:28:A:ILE:HD11	18	0.49
(1,305)	1:27:A:HIS:HD2	1:28:A:ILE:HD12	18	0.49
(1,305)	1:27:A:HIS:HD2	1:28:A:ILE:HD13	18	0.49
(1,295)	1:27:A:HIS:H	1:29:A:THR:H	1	0.49
(1,295)	1:27:A:HIS:H	1:29:A:THR:H	3	0.49
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG21	11	0.49
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG22	11	0.49
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG23	11	0.49
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG21	16	0.49
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG22	16	0.49
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG23	16	0.49
(1,261)	1:25:A:PHE:HE1	1:26:A:ASN:H	14	0.49
(1,261)	1:25:A:PHE:HE2	1:26:A:ASN:H	14	0.49
(1,213)	1:11:A:TRP:HA	1:25:A:PHE:H	3	0.49
(1,176)	1:23:A:TYR:HB3	1:24:A:TYR:HD1	18	0.49
(1,176)	1:23:A:TYR:HB3	1:24:A:TYR:HD2	18	0.49
(1,134)	1:20:A:GLY:H	1:21:A:ARG:HA	4	0.49
(1,134)	1:20:A:GLY:H	1:21:A:ARG:HA	5	0.49
(1,133)	1:20:A:GLY:H	1:21:A:ARG:HB2	7	0.49
(1,133)	1:20:A:GLY:H	1:21:A:ARG:HB2	12	0.49
(1,93)	1:14:A:ARG:H	1:22:A:VAL:HA	1	0.49
(1,44)	1:8:A:PRO:HB2	1:11:A:TRP:HE1	11	0.49
(1,28)	1:7:A:LEU:HD21	1:13:A:LYS:HG3	4	0.49
(1,28)	1:7:A:LEU:HD22	1:13:A:LYS:HG3	4	0.49
(1,28)	1:7:A:LEU:HD23	1:13:A:LYS:HG3	4	0.49
(1,27)	1:7:A:LEU:HD21	1:13:A:LYS:H	1	0.49
(1,27)	1:7:A:LEU:HD22	1:13:A:LYS:H	1	0.49
(1,27)	1:7:A:LEU:HD23	1:13:A:LYS:H	1	0.49
(1,27)	1:7:A:LEU:HD21	1:13:A:LYS:H	5	0.49
(1,27)	1:7:A:LEU:HD22	1:13:A:LYS:H	5	0.49
(1,27)	1:7:A:LEU:HD23	1:13:A:LYS:H	5	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,106)	1:139:A:PHE:H	2:656:B:PHE:HB2	1	0.48
(2,103)	1:137:A:ALA:H	2:656:B:PHE:HB2	13	0.48
(2,66)	2:645:B:GLN:H	2:648:B:ILE:H	16	0.48
(2,20)	1:68:A:ARG:H	1:153:A:ASP:HB2	1	0.48
(2,20)	1:68:A:ARG:H	1:153:A:ASP:HB3	1	0.48
(1,2598)	1:146:A:MET:HE1	2:642:B:PRO:HB2	10	0.48
(1,2598)	1:146:A:MET:HE1	2:642:B:PRO:HB3	10	0.48
(1,2598)	1:146:A:MET:HE2	2:642:B:PRO:HB2	10	0.48
(1,2598)	1:146:A:MET:HE2	2:642:B:PRO:HB3	10	0.48
(1,2598)	1:146:A:MET:HE3	2:642:B:PRO:HB2	10	0.48
(1,2598)	1:146:A:MET:HE3	2:642:B:PRO:HB3	10	0.48
(1,2591)	1:123:A:GLY:H	2:656:B:PHE:HE1	19	0.48
(1,2591)	1:123:A:GLY:H	2:656:B:PHE:HE2	19	0.48
(1,2584)	1:114:A:SER:H	2:659:B:PHE:HD1	6	0.48
(1,2584)	1:114:A:SER:H	2:659:B:PHE:HD2	6	0.48
(1,2507)	2:643:B:PRO:HA	2:645:B:GLN:H	7	0.48
(1,2158)	1:119:A:ARG:H	1:119:A:ARG:HD2	16	0.48
(1,1977)	1:89:A:ILE:H	1:89:A:ILE:HG12	9	0.48
(1,1977)	1:89:A:ILE:H	1:89:A:ILE:HG12	10	0.48
(1,1977)	1:89:A:ILE:H	1:89:A:ILE:HG12	14	0.48
(1,1507)	1:13:A:LYS:H	1:13:A:LYS:HG3	14	0.48
(1,1504)	1:13:A:LYS:H	1:13:A:LYS:HE2	2	0.48
(1,1504)	1:13:A:LYS:H	1:13:A:LYS:HE2	10	0.48
(1,1370)	1:144:A:GLY:H	1:160:A:LEU:HD21	10	0.48
(1,1370)	1:144:A:GLY:H	1:160:A:LEU:HD22	10	0.48
(1,1370)	1:144:A:GLY:H	1:160:A:LEU:HD23	10	0.48
(1,1353)	1:57:A:CYS:HB3	1:160:A:LEU:H	10	0.48
(1,1349)	1:158:A:ILE:H	1:159:A:ILE:HD11	18	0.48
(1,1349)	1:158:A:ILE:H	1:159:A:ILE:HD12	18	0.48
(1,1349)	1:158:A:ILE:H	1:159:A:ILE:HD13	18	0.48
(1,1335)	1:57:A:CYS:HA	1:159:A:ILE:HG21	1	0.48
(1,1335)	1:57:A:CYS:HA	1:159:A:ILE:HG22	1	0.48
(1,1335)	1:57:A:CYS:HA	1:159:A:ILE:HG23	1	0.48
(1,1331)	1:146:A:MET:HG2	1:158:A:ILE:HG21	15	0.48
(1,1331)	1:146:A:MET:HG2	1:158:A:ILE:HG22	15	0.48
(1,1331)	1:146:A:MET:HG2	1:158:A:ILE:HG23	15	0.48
(1,1326)	1:89:A:ILE:HG21	1:158:A:ILE:HB	19	0.48
(1,1326)	1:89:A:ILE:HG22	1:158:A:ILE:HB	19	0.48
(1,1326)	1:89:A:ILE:HG23	1:158:A:ILE:HB	19	0.48
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD11	2	0.48
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD12	2	0.48
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD13	2	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1282)	1:82:A:LYS:HE2	1:156:A:ILE:HD11	13	0.48
(1,1282)	1:82:A:LYS:HE2	1:156:A:ILE:HD12	13	0.48
(1,1282)	1:82:A:LYS:HE2	1:156:A:ILE:HD13	13	0.48
(1,1242)	1:150:A:VAL:HG11	1:157:A:HIS:H	4	0.48
(1,1242)	1:150:A:VAL:HG12	1:157:A:HIS:H	4	0.48
(1,1242)	1:150:A:VAL:HG13	1:157:A:HIS:H	4	0.48
(1,1217)	1:145:A:GLU:HB3	1:147:A:SER:H	17	0.48
(1,1212)	1:146:A:MET:HG2	1:160:A:LEU:HG	13	0.48
(1,1199)	1:142:A:ARG:HG2	1:143:A:THR:H	2	0.48
(1,1161)	1:136:A:ASP:HB2	1:138:A:SER:H	17	0.48
(1,1112)	1:126:A:SER:H	1:129:A:GLN:HE21	8	0.48
(1,1107)	1:54:A:ARG:HD2	1:126:A:SER:HA	8	0.48
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE1	17	0.48
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE2	17	0.48
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE3	17	0.48
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE1	17	0.48
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE2	17	0.48
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE3	17	0.48
(1,1033)	1:108:A:SER:H	1:119:A:ARG:HB2	8	0.48
(1,1033)	1:108:A:SER:H	1:119:A:ARG:HB2	12	0.48
(1,1024)	1:118:A:ALA:HA	1:119:A:ARG:HE	2	0.48
(1,1024)	1:118:A:ALA:HA	1:119:A:ARG:HE	5	0.48
(1,1024)	1:118:A:ALA:HA	1:119:A:ARG:HE	18	0.48
(1,1015)	1:116:A:ALA:HB1	1:120:A:GLY:H	5	0.48
(1,1015)	1:116:A:ALA:HB2	1:120:A:GLY:H	5	0.48
(1,1015)	1:116:A:ALA:HB3	1:120:A:GLY:H	5	0.48
(1,958)	1:108:A:SER:HA	1:110:A:PHE:H	16	0.48
(1,913)	1:103:A:PHE:H	1:106:A:LEU:HB3	11	0.48
(1,913)	1:103:A:PHE:H	1:106:A:LEU:HB3	12	0.48
(1,910)	1:102:A:ASP:H	1:106:A:LEU:HB3	2	0.48
(1,910)	1:102:A:ASP:H	1:106:A:LEU:HB3	14	0.48
(1,886)	1:103:A:PHE:HE1	1:107:A:ALA:H	11	0.48
(1,886)	1:103:A:PHE:HE2	1:107:A:ALA:H	11	0.48
(1,886)	1:103:A:PHE:HE1	1:107:A:ALA:H	19	0.48
(1,886)	1:103:A:PHE:HE2	1:107:A:ALA:H	19	0.48
(1,862)	1:101:A:GLU:HG2	1:102:A:ASP:H	19	0.48
(1,816)	1:95:A:LYS:HD2	1:96:A:ILE:H	20	0.48
(1,814)	1:94:A:GLN:HG2	1:95:A:LYS:H	20	0.48
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD11	11	0.48
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD12	11	0.48
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD13	11	0.48
(1,785)	1:89:A:ILE:HG21	1:93:A:ILE:H	6	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,785)	1:89:A:ILE:HG22	1:93:A:ILE:H	6	0.48
(1,785)	1:89:A:ILE:HG23	1:93:A:ILE:H	6	0.48
(1,753)	1:90:A:ASN:HD22	1:91:A:GLY:H	16	0.48
(1,742)	1:89:A:ILE:HD11	1:90:A:ASN:H	9	0.48
(1,742)	1:89:A:ILE:HD12	1:90:A:ASN:H	9	0.48
(1,742)	1:89:A:ILE:HD13	1:90:A:ASN:H	9	0.48
(1,723)	1:86:A:LEU:HD21	1:89:A:ILE:HB	6	0.48
(1,723)	1:86:A:LEU:HD22	1:89:A:ILE:HB	6	0.48
(1,723)	1:86:A:LEU:HD23	1:89:A:ILE:HB	6	0.48
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD21	18	0.48
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD22	18	0.48
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD23	18	0.48
(1,693)	1:86:A:LEU:HD21	1:149:A:PRO:HD2	13	0.48
(1,693)	1:86:A:LEU:HD22	1:149:A:PRO:HD2	13	0.48
(1,693)	1:86:A:LEU:HD23	1:149:A:PRO:HD2	13	0.48
(1,693)	1:86:A:LEU:HD21	1:149:A:PRO:HD2	20	0.48
(1,693)	1:86:A:LEU:HD22	1:149:A:PRO:HD2	20	0.48
(1,693)	1:86:A:LEU:HD23	1:149:A:PRO:HD2	20	0.48
(1,639)	1:65:A:SER:HB3	1:81:A:THR:HG21	15	0.48
(1,639)	1:65:A:SER:HB3	1:81:A:THR:HG22	15	0.48
(1,639)	1:65:A:SER:HB3	1:81:A:THR:HG23	15	0.48
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB1	9	0.48
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB2	9	0.48
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB3	9	0.48
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB1	15	0.48
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB2	15	0.48
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB3	15	0.48
(1,564)	1:72:A:SER:H	1:78:A:ILE:HG12	10	0.48
(1,554)	1:70:A:PRO:HG3	1:71:A:SER:H	14	0.48
(1,527)	1:66:A:GLN:HG2	1:81:A:THR:HG21	15	0.48
(1,527)	1:66:A:GLN:HG2	1:81:A:THR:HG22	15	0.48
(1,527)	1:66:A:GLN:HG2	1:81:A:THR:HG23	15	0.48
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG21	15	0.48
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG22	15	0.48
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG23	15	0.48
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG21	15	0.48
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG22	15	0.48
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG23	15	0.48
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG21	15	0.48
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG22	15	0.48
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG23	15	0.48
(1,422)	1:56:A:ARG:HG2	1:162:A:THR:HB	7	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,320)	1:25:A:PHE:HE1	1:30:A:ASN:H	10	0.48
(1,320)	1:25:A:PHE:HE2	1:30:A:ASN:H	10	0.48
(1,302)	1:27:A:HIS:HD2	1:28:A:ILE:H	11	0.48
(1,295)	1:27:A:HIS:H	1:29:A:THR:H	14	0.48
(1,287)	1:26:A:ASN:H	1:32:A:SER:HB2	1	0.48
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG21	2	0.48
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG22	2	0.48
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG23	2	0.48
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG21	13	0.48
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG22	13	0.48
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG23	13	0.48
(1,261)	1:25:A:PHE:HE1	1:26:A:ASN:H	18	0.48
(1,261)	1:25:A:PHE:HE2	1:26:A:ASN:H	18	0.48
(1,244)	1:11:A:TRP:H	1:26:A:ASN:HB2	9	0.48
(1,214)	1:11:A:TRP:HB2	1:25:A:PHE:H	7	0.48
(1,214)	1:11:A:TRP:HB2	1:25:A:PHE:H	9	0.48
(1,213)	1:11:A:TRP:HA	1:25:A:PHE:H	9	0.48
(1,190)	1:13:A:LYS:HB3	1:24:A:TYR:HA	19	0.48
(1,176)	1:23:A:TYR:HB3	1:24:A:TYR:HD1	1	0.48
(1,176)	1:23:A:TYR:HB3	1:24:A:TYR:HD2	1	0.48
(1,133)	1:20:A:GLY:H	1:21:A:ARG:HB2	9	0.48
(1,123)	1:15:A:MET:HE1	1:20:A:GLY:H	10	0.48
(1,123)	1:15:A:MET:HE2	1:20:A:GLY:H	10	0.48
(1,123)	1:15:A:MET:HE3	1:20:A:GLY:H	10	0.48
(1,93)	1:14:A:ARG:H	1:22:A:VAL:HA	2	0.48
(1,86)	1:13:A:LYS:HE2	1:14:A:ARG:H	2	0.48
(1,86)	1:13:A:LYS:HE2	1:14:A:ARG:H	12	0.48
(1,44)	1:8:A:PRO:HB2	1:11:A:TRP:HE1	4	0.48
(1,27)	1:7:A:LEU:HD21	1:13:A:LYS:H	12	0.48
(1,27)	1:7:A:LEU:HD22	1:13:A:LYS:H	12	0.48
(1,27)	1:7:A:LEU:HD23	1:13:A:LYS:H	12	0.48
(1,27)	1:7:A:LEU:HD21	1:13:A:LYS:H	16	0.48
(1,27)	1:7:A:LEU:HD22	1:13:A:LYS:H	16	0.48
(1,27)	1:7:A:LEU:HD23	1:13:A:LYS:H	16	0.48
(1,12)	1:5:A:GLU:HB2	1:6:A:LYS:H	1	0.48
(3,79)	1:105:A:SER:O	1:109:A:GLN:N	20	0.47
(2,113)	1:162:A:THR:H	2:651:B:ILE:HG12	4	0.47
(2,113)	1:162:A:THR:H	2:651:B:ILE:HG13	4	0.47
(2,113)	1:162:A:THR:H	2:651:B:ILE:HG12	16	0.47
(2,113)	1:162:A:THR:H	2:651:B:ILE:HG13	16	0.47
(2,38)	1:126:A:SER:H	1:129:A:GLN:HB2	11	0.47
(2,25)	1:88:A:LEU:HG	1:92:A:TYR:H	6	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,9)	1:53:A:ALA:H	1:54:A:ARG:HD2	18	0.47
(2,4)	1:21:A:ARG:HE	1:22:A:VAL:H	11	0.47
(1,2597)	1:138:A:SER:H	2:656:B:PHE:HB2	20	0.47
(1,2586)	1:115:A:SER:H	2:659:B:PHE:HE1	9	0.47
(1,2586)	1:115:A:SER:H	2:659:B:PHE:HE2	9	0.47
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG21	17	0.47
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG22	17	0.47
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG23	17	0.47
(1,2568)	2:658:B:GLY:H	2:659:B:PHE:HD1	3	0.47
(1,2568)	2:658:B:GLY:H	2:659:B:PHE:HD2	3	0.47
(1,2533)	2:647:B:VAL:H	2:649:B:ARG:H	7	0.47
(1,2520)	2:646:B:GLU:HG3	2:647:B:VAL:H	5	0.47
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE1	14	0.47
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE2	14	0.47
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE3	14	0.47
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE1	19	0.47
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE2	19	0.47
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE3	19	0.47
(1,2158)	1:119:A:ARG:H	1:119:A:ARG:HD2	19	0.47
(1,1977)	1:89:A:ILE:H	1:89:A:ILE:HG12	2	0.47
(1,1977)	1:89:A:ILE:H	1:89:A:ILE:HG12	17	0.47
(1,1625)	1:27:A:HIS:H	1:27:A:HIS:HD1	1	0.47
(1,1560)	1:18:A:SER:H	1:18:A:SER:HB3	11	0.47
(1,1507)	1:13:A:LYS:H	1:13:A:LYS:HG3	5	0.47
(1,1507)	1:13:A:LYS:H	1:13:A:LYS:HG3	7	0.47
(1,1399)	1:143:A:THR:H	1:161:A:ARG:HD2	16	0.47
(1,1376)	1:146:A:MET:HE1	1:160:A:LEU:HD21	8	0.47
(1,1376)	1:146:A:MET:HE1	1:160:A:LEU:HD22	8	0.47
(1,1376)	1:146:A:MET:HE1	1:160:A:LEU:HD23	8	0.47
(1,1376)	1:146:A:MET:HE2	1:160:A:LEU:HD21	8	0.47
(1,1376)	1:146:A:MET:HE2	1:160:A:LEU:HD22	8	0.47
(1,1376)	1:146:A:MET:HE2	1:160:A:LEU:HD23	8	0.47
(1,1376)	1:146:A:MET:HE3	1:160:A:LEU:HD21	8	0.47
(1,1376)	1:146:A:MET:HE3	1:160:A:LEU:HD22	8	0.47
(1,1376)	1:146:A:MET:HE3	1:160:A:LEU:HD23	8	0.47
(1,1370)	1:144:A:GLY:H	1:160:A:LEU:HD21	19	0.47
(1,1370)	1:144:A:GLY:H	1:160:A:LEU:HD22	19	0.47
(1,1370)	1:144:A:GLY:H	1:160:A:LEU:HD23	19	0.47
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD11	16	0.47
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD12	16	0.47
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD13	16	0.47
(1,1349)	1:158:A:ILE:H	1:159:A:ILE:HD11	5	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1349)	1:158:A:ILE:H	1:159:A:ILE:HD12	5	0.47
(1,1349)	1:158:A:ILE:H	1:159:A:ILE:HD13	5	0.47
(1,1303)	1:156:A:ILE:HG21	1:157:A:HIS:HD2	20	0.47
(1,1303)	1:156:A:ILE:HG22	1:157:A:HIS:HD2	20	0.47
(1,1303)	1:156:A:ILE:HG23	1:157:A:HIS:HD2	20	0.47
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG21	2	0.47
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG22	2	0.47
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG23	2	0.47
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD11	18	0.47
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD12	18	0.47
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD13	18	0.47
(1,1262)	1:151:A:PHE:H	1:156:A:ILE:HA	4	0.47
(1,1231)	1:149:A:PRO:HG2	1:150:A:VAL:H	7	0.47
(1,1192)	1:141:A:LEU:HD21	1:146:A:MET:H	13	0.47
(1,1192)	1:141:A:LEU:HD22	1:146:A:MET:H	13	0.47
(1,1192)	1:141:A:LEU:HD23	1:146:A:MET:H	13	0.47
(1,1192)	1:141:A:LEU:HD21	1:146:A:MET:H	19	0.47
(1,1192)	1:141:A:LEU:HD22	1:146:A:MET:H	19	0.47
(1,1192)	1:141:A:LEU:HD23	1:146:A:MET:H	19	0.47
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB1	14	0.47
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB2	14	0.47
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB3	14	0.47
(1,1085)	1:56:A:ARG:HE	1:124:A:ALA:H	20	0.47
(1,1033)	1:108:A:SER:H	1:119:A:ARG:HB2	7	0.47
(1,1015)	1:116:A:ALA:HB1	1:120:A:GLY:H	12	0.47
(1,1015)	1:116:A:ALA:HB2	1:120:A:GLY:H	12	0.47
(1,1015)	1:116:A:ALA:HB3	1:120:A:GLY:H	12	0.47
(1,1012)	1:116:A:ALA:H	1:119:A:ARG:H	2	0.47
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB1	7	0.47
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB2	7	0.47
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB3	7	0.47
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB1	19	0.47
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB2	19	0.47
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB3	19	0.47
(1,961)	1:108:A:SER:H	1:119:A:ARG:HG2	13	0.47
(1,940)	1:106:A:LEU:HG	1:107:A:ALA:H	20	0.47
(1,925)	1:60:A:LEU:HG	1:107:A:ALA:H	7	0.47
(1,910)	1:102:A:ASP:H	1:106:A:LEU:HB3	4	0.47
(1,862)	1:101:A:GLU:HG2	1:102:A:ASP:H	2	0.47
(1,844)	1:97:A:LYS:HG2	1:98:A:SER:H	11	0.47
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD11	1	0.47
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD12	1	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD13	1	0.47
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD11	3	0.47
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD12	3	0.47
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD13	3	0.47
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD11	9	0.47
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD12	9	0.47
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD13	9	0.47
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD11	19	0.47
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD12	19	0.47
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD13	19	0.47
(1,785)	1:89:A:ILE:HG21	1:93:A:ILE:H	18	0.47
(1,785)	1:89:A:ILE:HG22	1:93:A:ILE:H	18	0.47
(1,785)	1:89:A:ILE:HG23	1:93:A:ILE:H	18	0.47
(1,753)	1:90:A:ASN:HD22	1:91:A:GLY:H	15	0.47
(1,742)	1:89:A:ILE:HD11	1:90:A:ASN:H	1	0.47
(1,742)	1:89:A:ILE:HD12	1:90:A:ASN:H	1	0.47
(1,742)	1:89:A:ILE:HD13	1:90:A:ASN:H	1	0.47
(1,742)	1:89:A:ILE:HD11	1:90:A:ASN:H	14	0.47
(1,742)	1:89:A:ILE:HD12	1:90:A:ASN:H	14	0.47
(1,742)	1:89:A:ILE:HD13	1:90:A:ASN:H	14	0.47
(1,742)	1:89:A:ILE:HD11	1:90:A:ASN:H	19	0.47
(1,742)	1:89:A:ILE:HD12	1:90:A:ASN:H	19	0.47
(1,742)	1:89:A:ILE:HD13	1:90:A:ASN:H	19	0.47
(1,723)	1:86:A:LEU:HD21	1:89:A:ILE:HB	1	0.47
(1,723)	1:86:A:LEU:HD22	1:89:A:ILE:HB	1	0.47
(1,723)	1:86:A:LEU:HD23	1:89:A:ILE:HB	1	0.47
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD21	17	0.47
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD22	17	0.47
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD23	17	0.47
(1,541)	1:67:A:SER:HB3	1:70:A:PRO:HA	5	0.47
(1,541)	1:67:A:SER:HB3	1:70:A:PRO:HA	11	0.47
(1,531)	1:64:A:HIS:HE1	1:67:A:SER:HB2	17	0.47
(1,496)	1:62:A:VAL:HG11	1:88:A:LEU:H	16	0.47
(1,496)	1:62:A:VAL:HG12	1:88:A:LEU:H	16	0.47
(1,496)	1:62:A:VAL:HG13	1:88:A:LEU:H	16	0.47
(1,377)	1:33:A:GLN:HG2	1:35:A:GLU:H	14	0.47
(1,369)	1:33:A:GLN:HG2	1:34:A:TRP:H	8	0.47
(1,364)	1:24:A:TYR:HD1	1:33:A:GLN:H	13	0.47
(1,364)	1:24:A:TYR:HD2	1:33:A:GLN:H	13	0.47
(1,333)	1:25:A:PHE:HA	1:31:A:ALA:H	8	0.47
(1,320)	1:25:A:PHE:HE1	1:30:A:ASN:H	16	0.47
(1,320)	1:25:A:PHE:HE2	1:30:A:ASN:H	16	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,302)	1:27:A:HIS:HD2	1:28:A:ILE:H	3	0.47
(1,302)	1:27:A:HIS:HD2	1:28:A:ILE:H	18	0.47
(1,295)	1:27:A:HIS:H	1:29:A:THR:H	4	0.47
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG21	3	0.47
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG22	3	0.47
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG23	3	0.47
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG21	9	0.47
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG22	9	0.47
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG23	9	0.47
(1,261)	1:25:A:PHE:HE1	1:26:A:ASN:H	2	0.47
(1,261)	1:25:A:PHE:HE2	1:26:A:ASN:H	2	0.47
(1,261)	1:25:A:PHE:HE1	1:26:A:ASN:H	3	0.47
(1,261)	1:25:A:PHE:HE2	1:26:A:ASN:H	3	0.47
(1,256)	1:23:A:TYR:HE1	1:26:A:ASN:H	6	0.47
(1,256)	1:23:A:TYR:HE2	1:26:A:ASN:H	6	0.47
(1,244)	1:11:A:TRP:H	1:26:A:ASN:HB2	11	0.47
(1,213)	1:11:A:TRP:HA	1:25:A:PHE:H	5	0.47
(1,213)	1:11:A:TRP:HA	1:25:A:PHE:H	10	0.47
(1,204)	1:24:A:TYR:HB2	1:33:A:GLN:HE21	17	0.47
(1,188)	1:13:A:LYS:HG2	1:24:A:TYR:HE1	8	0.47
(1,188)	1:13:A:LYS:HG2	1:24:A:TYR:HE2	8	0.47
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG11	6	0.47
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG12	6	0.47
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG13	6	0.47
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG11	6	0.47
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG12	6	0.47
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG13	6	0.47
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG11	6	0.47
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG12	6	0.47
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG13	6	0.47
(1,134)	1:20:A:GLY:H	1:21:A:ARG:HA	1	0.47
(1,134)	1:20:A:GLY:H	1:21:A:ARG:HA	3	0.47
(1,134)	1:20:A:GLY:H	1:21:A:ARG:HA	6	0.47
(1,133)	1:20:A:GLY:H	1:21:A:ARG:HB2	3	0.47
(1,133)	1:20:A:GLY:H	1:21:A:ARG:HB2	6	0.47
(1,129)	1:16:A:SER:HB2	1:21:A:ARG:H	2	0.47
(1,123)	1:15:A:MET:HE1	1:20:A:GLY:H	18	0.47
(1,123)	1:15:A:MET:HE2	1:20:A:GLY:H	18	0.47
(1,123)	1:15:A:MET:HE3	1:20:A:GLY:H	18	0.47
(1,93)	1:14:A:ARG:H	1:22:A:VAL:HA	7	0.47
(1,93)	1:14:A:ARG:H	1:22:A:VAL:HA	11	0.47
(1,75)	1:13:A:LYS:HA	1:23:A:TYR:H	7	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,69)	1:7:A:LEU:HD21	1:13:A:LYS:HE2	3	0.47
(1,69)	1:7:A:LEU:HD22	1:13:A:LYS:HE2	3	0.47
(1,69)	1:7:A:LEU:HD23	1:13:A:LYS:HE2	3	0.47
(1,69)	1:7:A:LEU:HD11	1:13:A:LYS:HE2	3	0.47
(1,69)	1:7:A:LEU:HD12	1:13:A:LYS:HE2	3	0.47
(1,69)	1:7:A:LEU:HD13	1:13:A:LYS:HE2	3	0.47
(1,27)	1:7:A:LEU:HD21	1:13:A:LYS:H	11	0.47
(1,27)	1:7:A:LEU:HD22	1:13:A:LYS:H	11	0.47
(1,27)	1:7:A:LEU:HD23	1:13:A:LYS:H	11	0.47
(3,44)	1:72:A:SER:O	1:75:A:GLN:H	10	0.46
(2,98)	1:124:A:ALA:H	2:656:B:PHE:HE1	19	0.46
(2,98)	1:124:A:ALA:H	2:656:B:PHE:HE2	19	0.46
(2,97)	1:94:A:GLN:HE21	2:640:B:LEU:HG	3	0.46
(2,97)	1:94:A:GLN:HE21	2:640:B:LEU:HG	12	0.46
(2,89)	1:55:A:VAL:H	2:651:B:ILE:HG12	4	0.46
(2,89)	1:55:A:VAL:H	2:651:B:ILE:HG13	4	0.46
(2,68)	2:649:B:ARG:HD2	2:650:B:ASN:H	20	0.46
(2,58)	1:152:A:THR:HG21	1:157:A:HIS:HB3	4	0.46
(2,58)	1:152:A:THR:HG22	1:157:A:HIS:HB3	4	0.46
(2,58)	1:152:A:THR:HG23	1:157:A:HIS:HB3	4	0.46
(2,9)	1:53:A:ALA:H	1:54:A:ARG:HD2	1	0.46
(2,4)	1:21:A:ARG:HE	1:22:A:VAL:H	13	0.46
(1,2598)	1:146:A:MET:HE1	2:642:B:PRO:HB2	18	0.46
(1,2598)	1:146:A:MET:HE1	2:642:B:PRO:HB3	18	0.46
(1,2598)	1:146:A:MET:HE2	2:642:B:PRO:HB2	18	0.46
(1,2598)	1:146:A:MET:HE2	2:642:B:PRO:HB3	18	0.46
(1,2598)	1:146:A:MET:HE3	2:642:B:PRO:HB2	18	0.46
(1,2598)	1:146:A:MET:HE3	2:642:B:PRO:HB3	18	0.46
(1,2588)	1:122:A:LEU:H	2:656:B:PHE:HE1	1	0.46
(1,2588)	1:122:A:LEU:H	2:656:B:PHE:HE2	1	0.46
(1,2582)	1:34:A:TRP:HE1	2:642:B:PRO:HB2	11	0.46
(1,2582)	1:34:A:TRP:HE1	2:642:B:PRO:HB3	11	0.46
(1,2577)	1:23:A:TYR:HD1	2:641:B:TPO:HG21	18	0.46
(1,2577)	1:23:A:TYR:HD1	2:641:B:TPO:HG22	18	0.46
(1,2577)	1:23:A:TYR:HD1	2:641:B:TPO:HG23	18	0.46
(1,2577)	1:23:A:TYR:HD2	2:641:B:TPO:HG21	18	0.46
(1,2577)	1:23:A:TYR:HD2	2:641:B:TPO:HG22	18	0.46
(1,2577)	1:23:A:TYR:HD2	2:641:B:TPO:HG23	18	0.46
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG21	15	0.46
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG22	15	0.46
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG23	15	0.46
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG21	6	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG22	6	0.46
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG23	6	0.46
(1,2520)	2:646:B:GLU:HG3	2:647:B:VAL:H	6	0.46
(1,2510)	2:645:B:GLN:H	2:647:B:VAL:H	9	0.46
(1,2161)	1:119:A:ARG:H	1:119:A:ARG:HD3	15	0.46
(1,2158)	1:119:A:ARG:H	1:119:A:ARG:HD2	14	0.46
(1,2135)	1:117:A:LYS:H	1:117:A:LYS:HD2	19	0.46
(1,1977)	1:89:A:ILE:H	1:89:A:ILE:HG12	3	0.46
(1,1747)	1:56:A:ARG:H	1:56:A:ARG:HD2	1	0.46
(1,1507)	1:13:A:LYS:H	1:13:A:LYS:HG3	3	0.46
(1,1507)	1:13:A:LYS:H	1:13:A:LYS:HG3	4	0.46
(1,1434)	1:161:A:ARG:HD2	1:163:A:GLU:H	3	0.46
(1,1400)	1:143:A:THR:HG21	1:161:A:ARG:HE	2	0.46
(1,1400)	1:143:A:THR:HG22	1:161:A:ARG:HE	2	0.46
(1,1400)	1:143:A:THR:HG23	1:161:A:ARG:HE	2	0.46
(1,1349)	1:158:A:ILE:H	1:159:A:ILE:HD11	6	0.46
(1,1349)	1:158:A:ILE:H	1:159:A:ILE:HD12	6	0.46
(1,1349)	1:158:A:ILE:H	1:159:A:ILE:HD13	6	0.46
(1,1192)	1:141:A:LEU:HD21	1:146:A:MET:H	9	0.46
(1,1192)	1:141:A:LEU:HD22	1:146:A:MET:H	9	0.46
(1,1192)	1:141:A:LEU:HD23	1:146:A:MET:H	9	0.46
(1,1177)	1:137:A:ALA:HB1	1:141:A:LEU:H	1	0.46
(1,1177)	1:137:A:ALA:HB2	1:141:A:LEU:H	1	0.46
(1,1177)	1:137:A:ALA:HB3	1:141:A:LEU:H	1	0.46
(1,1078)	1:122:A:LEU:HG	1:123:A:GLY:H	19	0.46
(1,1051)	1:57:A:CYS:H	1:122:A:LEU:HD21	6	0.46
(1,1051)	1:57:A:CYS:H	1:122:A:LEU:HD22	6	0.46
(1,1051)	1:57:A:CYS:H	1:122:A:LEU:HD23	6	0.46
(1,1033)	1:108:A:SER:H	1:119:A:ARG:HB2	5	0.46
(1,1012)	1:116:A:ALA:H	1:119:A:ARG:H	9	0.46
(1,1012)	1:116:A:ALA:H	1:119:A:ARG:H	17	0.46
(1,985)	1:61:A:LEU:HD21	1:113:A:CYS:HA	17	0.46
(1,985)	1:61:A:LEU:HD22	1:113:A:CYS:HA	17	0.46
(1,985)	1:61:A:LEU:HD23	1:113:A:CYS:HA	17	0.46
(1,961)	1:108:A:SER:H	1:119:A:ARG:HG2	16	0.46
(1,959)	1:108:A:SER:HA	1:111:A:SER:H	20	0.46
(1,958)	1:108:A:SER:HA	1:110:A:PHE:H	5	0.46
(1,958)	1:108:A:SER:HA	1:110:A:PHE:H	9	0.46
(1,913)	1:103:A:PHE:H	1:106:A:LEU:HB3	7	0.46
(1,888)	1:103:A:PHE:HE1	1:120:A:GLY:H	5	0.46
(1,888)	1:103:A:PHE:HE2	1:120:A:GLY:H	5	0.46
(1,888)	1:103:A:PHE:HE1	1:120:A:GLY:H	6	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,888)	1:103:A:PHE:HE2	1:120:A:GLY:H	6	0.46
(1,886)	1:103:A:PHE:HE1	1:107:A:ALA:H	10	0.46
(1,886)	1:103:A:PHE:HE2	1:107:A:ALA:H	10	0.46
(1,862)	1:101:A:GLU:HG2	1:102:A:ASP:H	5	0.46
(1,834)	1:94:A:GLN:HE21	1:97:A:LYS:HD2	17	0.46
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD11	5	0.46
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD12	5	0.46
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD13	5	0.46
(1,785)	1:89:A:ILE:HG21	1:93:A:ILE:H	15	0.46
(1,785)	1:89:A:ILE:HG22	1:93:A:ILE:H	15	0.46
(1,785)	1:89:A:ILE:HG23	1:93:A:ILE:H	15	0.46
(1,723)	1:86:A:LEU:HD21	1:89:A:ILE:HB	3	0.46
(1,723)	1:86:A:LEU:HD22	1:89:A:ILE:HB	3	0.46
(1,723)	1:86:A:LEU:HD23	1:89:A:ILE:HB	3	0.46
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD21	10	0.46
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD22	10	0.46
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD23	10	0.46
(1,637)	1:80:A:ARG:HE	1:85:A:ALA:H	2	0.46
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG21	12	0.46
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG22	12	0.46
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG23	12	0.46
(1,592)	1:75:A:GLN:HB2	1:77:A:LYS:H	11	0.46
(1,591)	1:74:A:ARG:HE	1:75:A:GLN:H	18	0.46
(1,564)	1:72:A:SER:H	1:78:A:ILE:HG12	5	0.46
(1,564)	1:72:A:SER:H	1:78:A:ILE:HG12	11	0.46
(1,549)	1:70:A:PRO:HG2	1:71:A:SER:H	7	0.46
(1,541)	1:67:A:SER:HB3	1:70:A:PRO:HA	12	0.46
(1,541)	1:67:A:SER:HB3	1:70:A:PRO:HA	15	0.46
(1,496)	1:62:A:VAL:HG11	1:88:A:LEU:H	15	0.46
(1,496)	1:62:A:VAL:HG12	1:88:A:LEU:H	15	0.46
(1,496)	1:62:A:VAL:HG13	1:88:A:LEU:H	15	0.46
(1,457)	1:60:A:LEU:HD11	1:108:A:SER:H	1	0.46
(1,457)	1:60:A:LEU:HD12	1:108:A:SER:H	1	0.46
(1,457)	1:60:A:LEU:HD13	1:108:A:SER:H	1	0.46
(1,397)	1:54:A:ARG:HG2	1:126:A:SER:H	2	0.46
(1,397)	1:54:A:ARG:HG2	1:126:A:SER:H	10	0.46
(1,363)	1:11:A:TRP:HE3	1:33:A:GLN:H	5	0.46
(1,352)	1:23:A:TYR:HE1	1:32:A:SER:HA	13	0.46
(1,352)	1:23:A:TYR:HE2	1:32:A:SER:HA	13	0.46
(1,347)	1:31:A:ALA:HB1	1:33:A:GLN:H	2	0.46
(1,347)	1:31:A:ALA:HB2	1:33:A:GLN:H	2	0.46
(1,347)	1:31:A:ALA:HB3	1:33:A:GLN:H	2	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,320)	1:25:A:PHE:HE1	1:30:A:ASN:H	3	0.46
(1,320)	1:25:A:PHE:HE2	1:30:A:ASN:H	3	0.46
(1,320)	1:25:A:PHE:HE1	1:30:A:ASN:H	19	0.46
(1,320)	1:25:A:PHE:HE2	1:30:A:ASN:H	19	0.46
(1,295)	1:27:A:HIS:H	1:29:A:THR:H	8	0.46
(1,295)	1:27:A:HIS:H	1:29:A:THR:H	11	0.46
(1,295)	1:27:A:HIS:H	1:29:A:THR:H	12	0.46
(1,295)	1:27:A:HIS:H	1:29:A:THR:H	13	0.46
(1,295)	1:27:A:HIS:H	1:29:A:THR:H	19	0.46
(1,261)	1:25:A:PHE:HE1	1:26:A:ASN:H	7	0.46
(1,261)	1:25:A:PHE:HE2	1:26:A:ASN:H	7	0.46
(1,261)	1:25:A:PHE:HE1	1:26:A:ASN:H	16	0.46
(1,261)	1:25:A:PHE:HE2	1:26:A:ASN:H	16	0.46
(1,261)	1:25:A:PHE:HE1	1:26:A:ASN:H	20	0.46
(1,261)	1:25:A:PHE:HE2	1:26:A:ASN:H	20	0.46
(1,218)	1:12:A:GLU:HB2	1:25:A:PHE:H	12	0.46
(1,214)	1:11:A:TRP:HB2	1:25:A:PHE:H	10	0.46
(1,214)	1:11:A:TRP:HB2	1:25:A:PHE:H	17	0.46
(1,190)	1:13:A:LYS:HB3	1:24:A:TYR:HA	10	0.46
(1,180)	1:23:A:TYR:HD1	1:33:A:GLN:HA	20	0.46
(1,180)	1:23:A:TYR:HD2	1:33:A:GLN:HA	20	0.46
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG11	12	0.46
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG12	12	0.46
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG13	12	0.46
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG11	12	0.46
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG12	12	0.46
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG13	12	0.46
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG11	12	0.46
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG12	12	0.46
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG13	12	0.46
(1,134)	1:20:A:GLY:H	1:21:A:ARG:HA	11	0.46
(1,123)	1:15:A:MET:HE1	1:20:A:GLY:H	19	0.46
(1,123)	1:15:A:MET:HE2	1:20:A:GLY:H	19	0.46
(1,123)	1:15:A:MET:HE3	1:20:A:GLY:H	19	0.46
(1,93)	1:14:A:ARG:H	1:22:A:VAL:HA	6	0.46
(1,93)	1:14:A:ARG:H	1:22:A:VAL:HA	10	0.46
(1,93)	1:14:A:ARG:H	1:22:A:VAL:HA	12	0.46
(1,93)	1:14:A:ARG:H	1:22:A:VAL:HA	13	0.46
(1,93)	1:14:A:ARG:H	1:22:A:VAL:HA	19	0.46
(1,66)	1:12:A:GLU:H	1:25:A:PHE:HE1	1	0.46
(1,66)	1:12:A:GLU:H	1:25:A:PHE:HE2	1	0.46
(1,66)	1:12:A:GLU:H	1:25:A:PHE:HE1	4	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,66)	1:12:A:GLU:H	1:25:A:PHE:HE2	4	0.46
(1,52)	1:11:A:TRP:HE1	1:26:A:ASN:HB2	5	0.46
(1,52)	1:11:A:TRP:HE1	1:26:A:ASN:HB3	5	0.46
(1,44)	1:8:A:PRO:HB2	1:11:A:TRP:HE1	20	0.46
(1,14)	1:6:A:LYS:HG2	1:7:A:LEU:H	19	0.46
(1,12)	1:5:A:GLU:HB2	1:6:A:LYS:H	2	0.46
(1,12)	1:5:A:GLU:HB2	1:6:A:LYS:H	5	0.46
(2,106)	1:139:A:PHE:H	2:656:B:PHE:HB2	2	0.45
(2,92)	1:58:A:SER:H	2:651:B:ILE:HG12	14	0.45
(2,92)	1:58:A:SER:H	2:651:B:ILE:HG13	14	0.45
(2,88)	1:34:A:TRP:HE1	2:641:B:TPO:H	20	0.45
(2,52)	1:141:A:LEU:HD21	1:148:A:GLY:H	4	0.45
(2,52)	1:141:A:LEU:HD22	1:148:A:GLY:H	4	0.45
(2,52)	1:141:A:LEU:HD23	1:148:A:GLY:H	4	0.45
(2,4)	1:21:A:ARG:HE	1:22:A:VAL:H	12	0.45
(1,2588)	1:122:A:LEU:H	2:656:B:PHE:HE1	13	0.45
(1,2588)	1:122:A:LEU:H	2:656:B:PHE:HE2	13	0.45
(1,2587)	1:115:A:SER:H	2:659:B:PHE:HD1	1	0.45
(1,2587)	1:115:A:SER:H	2:659:B:PHE:HD2	1	0.45
(1,2586)	1:115:A:SER:H	2:659:B:PHE:HE1	12	0.45
(1,2586)	1:115:A:SER:H	2:659:B:PHE:HE2	12	0.45
(1,2582)	1:34:A:TRP:HE1	2:642:B:PRO:HB2	2	0.45
(1,2582)	1:34:A:TRP:HE1	2:642:B:PRO:HB3	2	0.45
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG21	5	0.45
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG22	5	0.45
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG23	5	0.45
(1,2561)	2:655:B:GLU:H	2:656:B:PHE:HD1	17	0.45
(1,2561)	2:655:B:GLU:H	2:656:B:PHE:HD2	17	0.45
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE1	8	0.45
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE2	8	0.45
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE3	8	0.45
(1,2209)	1:131:A:GLN:HA	1:131:A:GLN:HE22	2	0.45
(1,1913)	1:82:A:LYS:H	1:82:A:LYS:HD2	10	0.45
(1,1645)	1:29:A:THR:H	1:29:A:THR:HG21	20	0.45
(1,1645)	1:29:A:THR:H	1:29:A:THR:HG22	20	0.45
(1,1645)	1:29:A:THR:H	1:29:A:THR:HG23	20	0.45
(1,1625)	1:27:A:HIS:H	1:27:A:HIS:HD1	5	0.45
(1,1560)	1:18:A:SER:H	1:18:A:SER:HB3	16	0.45
(1,1507)	1:13:A:LYS:H	1:13:A:LYS:HG3	16	0.45
(1,1507)	1:13:A:LYS:H	1:13:A:LYS:HG3	18	0.45
(1,1507)	1:13:A:LYS:H	1:13:A:LYS:HG3	20	0.45
(1,1434)	1:161:A:ARG:HD2	1:163:A:GLU:H	6	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1368)	1:103:A:PHE:HB3	1:160:A:LEU:HD21	3	0.45
(1,1368)	1:103:A:PHE:HB3	1:160:A:LEU:HD22	3	0.45
(1,1368)	1:103:A:PHE:HB3	1:160:A:LEU:HD23	3	0.45
(1,1348)	1:157:A:HIS:HB2	1:159:A:ILE:HD11	12	0.45
(1,1348)	1:157:A:HIS:HB2	1:159:A:ILE:HD12	12	0.45
(1,1348)	1:157:A:HIS:HB2	1:159:A:ILE:HD13	12	0.45
(1,1348)	1:157:A:HIS:HB3	1:159:A:ILE:HD11	12	0.45
(1,1348)	1:157:A:HIS:HB3	1:159:A:ILE:HD12	12	0.45
(1,1348)	1:157:A:HIS:HB3	1:159:A:ILE:HD13	12	0.45
(1,1311)	1:152:A:THR:HG21	1:157:A:HIS:H	17	0.45
(1,1311)	1:152:A:THR:HG22	1:157:A:HIS:H	17	0.45
(1,1311)	1:152:A:THR:HG23	1:157:A:HIS:H	17	0.45
(1,1280)	1:64:A:HIS:HD2	1:156:A:ILE:HG12	3	0.45
(1,1262)	1:151:A:PHE:H	1:156:A:ILE:HA	16	0.45
(1,1206)	1:145:A:GLU:HB3	1:146:A:MET:HB2	3	0.45
(1,1193)	1:141:A:LEU:HD11	1:148:A:GLY:H	18	0.45
(1,1193)	1:141:A:LEU:HD12	1:148:A:GLY:H	18	0.45
(1,1193)	1:141:A:LEU:HD13	1:148:A:GLY:H	18	0.45
(1,1192)	1:141:A:LEU:HD21	1:146:A:MET:H	11	0.45
(1,1192)	1:141:A:LEU:HD22	1:146:A:MET:H	11	0.45
(1,1192)	1:141:A:LEU:HD23	1:146:A:MET:H	11	0.45
(1,1192)	1:141:A:LEU:HD21	1:146:A:MET:H	16	0.45
(1,1192)	1:141:A:LEU:HD22	1:146:A:MET:H	16	0.45
(1,1192)	1:141:A:LEU:HD23	1:146:A:MET:H	16	0.45
(1,1156)	1:136:A:ASP:HB2	1:137:A:ALA:H	5	0.45
(1,1047)	1:119:A:ARG:HD2	1:121:A:ASP:H	4	0.45
(1,1047)	1:119:A:ARG:HD2	1:121:A:ASP:H	19	0.45
(1,1032)	1:107:A:ALA:HB1	1:119:A:ARG:H	3	0.45
(1,1032)	1:107:A:ALA:HB2	1:119:A:ARG:H	3	0.45
(1,1032)	1:107:A:ALA:HB3	1:119:A:ARG:H	3	0.45
(1,1015)	1:116:A:ALA:HB1	1:120:A:GLY:H	3	0.45
(1,1015)	1:116:A:ALA:HB2	1:120:A:GLY:H	3	0.45
(1,1015)	1:116:A:ALA:HB3	1:120:A:GLY:H	3	0.45
(1,1012)	1:116:A:ALA:H	1:119:A:ARG:H	10	0.45
(1,961)	1:108:A:SER:H	1:119:A:ARG:HG2	14	0.45
(1,959)	1:108:A:SER:HA	1:111:A:SER:H	16	0.45
(1,958)	1:108:A:SER:HA	1:110:A:PHE:H	15	0.45
(1,910)	1:102:A:ASP:H	1:106:A:LEU:HB3	13	0.45
(1,841)	1:97:A:LYS:HB3	1:98:A:SER:H	10	0.45
(1,785)	1:89:A:ILE:HG21	1:93:A:ILE:H	3	0.45
(1,785)	1:89:A:ILE:HG22	1:93:A:ILE:H	3	0.45
(1,785)	1:89:A:ILE:HG23	1:93:A:ILE:H	3	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD11	19	0.45
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD12	19	0.45
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD13	19	0.45
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD11	19	0.45
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD12	19	0.45
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD13	19	0.45
(1,753)	1:90:A:ASN:HD22	1:91:A:GLY:H	18	0.45
(1,742)	1:89:A:ILE:HD11	1:90:A:ASN:H	20	0.45
(1,742)	1:89:A:ILE:HD12	1:90:A:ASN:H	20	0.45
(1,742)	1:89:A:ILE:HD13	1:90:A:ASN:H	20	0.45
(1,671)	1:64:A:HIS:HB2	1:85:A:ALA:H	1	0.45
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG21	8	0.45
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG22	8	0.45
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG23	8	0.45
(1,618)	1:78:A:ILE:HA	1:80:A:ARG:H	11	0.45
(1,618)	1:78:A:ILE:HA	1:80:A:ARG:H	15	0.45
(1,591)	1:74:A:ARG:HE	1:75:A:GLN:H	5	0.45
(1,564)	1:72:A:SER:H	1:78:A:ILE:HG12	16	0.45
(1,549)	1:70:A:PRO:HG2	1:71:A:SER:H	17	0.45
(1,496)	1:62:A:VAL:HG11	1:88:A:LEU:H	12	0.45
(1,496)	1:62:A:VAL:HG12	1:88:A:LEU:H	12	0.45
(1,496)	1:62:A:VAL:HG13	1:88:A:LEU:H	12	0.45
(1,471)	1:61:A:LEU:HD21	1:63:A:LYS:HA	15	0.45
(1,471)	1:61:A:LEU:HD22	1:63:A:LYS:HA	15	0.45
(1,471)	1:61:A:LEU:HD23	1:63:A:LYS:HA	15	0.45
(1,465)	1:60:A:LEU:HB2	1:158:A:ILE:H	8	0.45
(1,369)	1:33:A:GLN:HG2	1:34:A:TRP:H	11	0.45
(1,369)	1:33:A:GLN:HG2	1:34:A:TRP:H	19	0.45
(1,355)	1:25:A:PHE:HE1	1:32:A:SER:HB2	5	0.45
(1,355)	1:25:A:PHE:HE2	1:32:A:SER:HB2	5	0.45
(1,355)	1:25:A:PHE:HE1	1:32:A:SER:HB2	14	0.45
(1,355)	1:25:A:PHE:HE2	1:32:A:SER:HB2	14	0.45
(1,334)	1:27:A:HIS:HA	1:31:A:ALA:H	13	0.45
(1,321)	1:25:A:PHE:HZ	1:30:A:ASN:H	1	0.45
(1,320)	1:25:A:PHE:HE1	1:30:A:ASN:H	14	0.45
(1,320)	1:25:A:PHE:HE2	1:30:A:ASN:H	14	0.45
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG21	15	0.45
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG22	15	0.45
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG23	15	0.45
(1,262)	1:25:A:PHE:HE1	1:26:A:ASN:HA	18	0.45
(1,262)	1:25:A:PHE:HE2	1:26:A:ASN:HA	18	0.45
(1,261)	1:25:A:PHE:HE1	1:26:A:ASN:H	8	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,261)	1:25:A:PHE:HE2	1:26:A:ASN:H	8	0.45
(1,213)	1:11:A:TRP:HA	1:25:A:PHE:H	2	0.45
(1,213)	1:11:A:TRP:HA	1:25:A:PHE:H	12	0.45
(1,181)	1:23:A:TYR:HB2	1:34:A:TRP:HE3	15	0.45
(1,180)	1:23:A:TYR:HD1	1:33:A:GLN:HA	10	0.45
(1,180)	1:23:A:TYR:HD2	1:33:A:GLN:HA	10	0.45
(1,176)	1:23:A:TYR:HB3	1:24:A:TYR:HD1	16	0.45
(1,176)	1:23:A:TYR:HB3	1:24:A:TYR:HD2	16	0.45
(1,148)	1:15:A:MET:HE1	1:22:A:VAL:HA	3	0.45
(1,148)	1:15:A:MET:HE2	1:22:A:VAL:HA	3	0.45
(1,148)	1:15:A:MET:HE3	1:22:A:VAL:HA	3	0.45
(1,134)	1:20:A:GLY:H	1:21:A:ARG:HA	9	0.45
(1,133)	1:20:A:GLY:H	1:21:A:ARG:HB2	1	0.45
(1,133)	1:20:A:GLY:H	1:21:A:ARG:HB2	4	0.45
(1,133)	1:20:A:GLY:H	1:21:A:ARG:HB2	10	0.45
(1,93)	1:14:A:ARG:H	1:22:A:VAL:HA	14	0.45
(1,75)	1:13:A:LYS:HA	1:23:A:TYR:H	10	0.45
(1,69)	1:7:A:LEU:HD21	1:13:A:LYS:HE2	7	0.45
(1,69)	1:7:A:LEU:HD22	1:13:A:LYS:HE2	7	0.45
(1,69)	1:7:A:LEU:HD23	1:13:A:LYS:HE2	7	0.45
(1,69)	1:7:A:LEU:HD11	1:13:A:LYS:HE2	7	0.45
(1,69)	1:7:A:LEU:HD12	1:13:A:LYS:HE2	7	0.45
(1,69)	1:7:A:LEU:HD13	1:13:A:LYS:HE2	7	0.45
(1,66)	1:12:A:GLU:H	1:25:A:PHE:HE1	20	0.45
(1,66)	1:12:A:GLU:H	1:25:A:PHE:HE2	20	0.45
(1,52)	1:11:A:TRP:HE1	1:26:A:ASN:HB2	3	0.45
(1,52)	1:11:A:TRP:HE1	1:26:A:ASN:HB3	3	0.45
(1,27)	1:7:A:LEU:HD21	1:13:A:LYS:H	3	0.45
(1,27)	1:7:A:LEU:HD22	1:13:A:LYS:H	3	0.45
(1,27)	1:7:A:LEU:HD23	1:13:A:LYS:H	3	0.45
(1,16)	1:6:A:LYS:HE2	1:7:A:LEU:H	15	0.45
(1,14)	1:6:A:LYS:HG2	1:7:A:LEU:H	3	0.45
(1,11)	1:4:A:GLU:H	1:6:A:LYS:H	6	0.45
(3,44)	1:72:A:SER:O	1:75:A:GLN:H	17	0.44
(2,98)	1:124:A:ALA:H	2:656:B:PHE:HE1	16	0.44
(2,98)	1:124:A:ALA:H	2:656:B:PHE:HE2	16	0.44
(2,94)	1:93:A:ILE:HG21	2:643:B:PRO:HB3	10	0.44
(2,94)	1:93:A:ILE:HG22	2:643:B:PRO:HB3	10	0.44
(2,94)	1:93:A:ILE:HG23	2:643:B:PRO:HB3	10	0.44
(2,92)	1:58:A:SER:H	2:651:B:ILE:HG12	6	0.44
(2,92)	1:58:A:SER:H	2:651:B:ILE:HG13	6	0.44
(2,39)	1:55:A:VAL:HG11	1:127:A:ARG:H	9	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,39)	1:55:A:VAL:HG12	1:127:A:ARG:H	9	0.44
(2,39)	1:55:A:VAL:HG13	1:127:A:ARG:H	9	0.44
(2,20)	1:68:A:ARG:H	1:153:A:ASP:HB2	6	0.44
(2,20)	1:68:A:ARG:H	1:153:A:ASP:HB3	6	0.44
(1,2593)	1:129:A:GLN:HE21	2:656:B:PHE:HE1	11	0.44
(1,2593)	1:129:A:GLN:HE21	2:656:B:PHE:HE2	11	0.44
(1,2588)	1:122:A:LEU:H	2:656:B:PHE:HE1	11	0.44
(1,2588)	1:122:A:LEU:H	2:656:B:PHE:HE2	11	0.44
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG21	4	0.44
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG22	4	0.44
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG23	4	0.44
(1,2568)	2:658:B:GLY:H	2:659:B:PHE:HD1	8	0.44
(1,2568)	2:658:B:GLY:H	2:659:B:PHE:HD2	8	0.44
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE1	10	0.44
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE2	10	0.44
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE3	10	0.44
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE1	12	0.44
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE2	12	0.44
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE3	12	0.44
(1,1910)	1:82:A:LYS:H	1:82:A:LYS:HE2	20	0.44
(1,1565)	1:21:A:ARG:H	1:21:A:ARG:HG2	2	0.44
(1,1560)	1:18:A:SER:H	1:18:A:SER:HB3	4	0.44
(1,1507)	1:13:A:LYS:H	1:13:A:LYS:HG3	9	0.44
(1,1507)	1:13:A:LYS:H	1:13:A:LYS:HG3	11	0.44
(1,1507)	1:13:A:LYS:H	1:13:A:LYS:HG3	12	0.44
(1,1507)	1:13:A:LYS:H	1:13:A:LYS:HG3	13	0.44
(1,1457)	1:6:A:LYS:H	1:6:A:LYS:HG2	10	0.44
(1,1440)	1:162:A:THR:HG21	1:163:A:GLU:HB3	11	0.44
(1,1440)	1:162:A:THR:HG22	1:163:A:GLU:HB3	11	0.44
(1,1440)	1:162:A:THR:HG23	1:163:A:GLU:HB3	11	0.44
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD11	14	0.44
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD12	14	0.44
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD13	14	0.44
(1,1309)	1:150:A:VAL:HB	1:157:A:HIS:H	16	0.44
(1,1263)	1:151:A:PHE:H	1:156:A:ILE:HG21	4	0.44
(1,1263)	1:151:A:PHE:H	1:156:A:ILE:HG22	4	0.44
(1,1263)	1:151:A:PHE:H	1:156:A:ILE:HG23	4	0.44
(1,1208)	1:103:A:PHE:HD1	1:146:A:MET:HB2	19	0.44
(1,1208)	1:103:A:PHE:HD2	1:146:A:MET:HB2	19	0.44
(1,1192)	1:141:A:LEU:HD21	1:146:A:MET:H	5	0.44
(1,1192)	1:141:A:LEU:HD22	1:146:A:MET:H	5	0.44
(1,1192)	1:141:A:LEU:HD23	1:146:A:MET:H	5	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1156)	1:136:A:ASP:HB2	1:137:A:ALA:H	17	0.44
(1,1130)	1:131:A:GLN:HE21	1:153:A:ASP:HB2	5	0.44
(1,1130)	1:131:A:GLN:HE21	1:153:A:ASP:HB3	5	0.44
(1,1085)	1:56:A:ARG:HE	1:124:A:ALA:H	10	0.44
(1,1051)	1:57:A:CYS:H	1:122:A:LEU:HD21	12	0.44
(1,1051)	1:57:A:CYS:H	1:122:A:LEU:HD22	12	0.44
(1,1051)	1:57:A:CYS:H	1:122:A:LEU:HD23	12	0.44
(1,1033)	1:108:A:SER:H	1:119:A:ARG:HB2	1	0.44
(1,1031)	1:118:A:ALA:HB1	1:121:A:ASP:HB2	10	0.44
(1,1031)	1:118:A:ALA:HB2	1:121:A:ASP:HB2	10	0.44
(1,1031)	1:118:A:ALA:HB3	1:121:A:ASP:HB2	10	0.44
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB1	8	0.44
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB2	8	0.44
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB3	8	0.44
(1,925)	1:60:A:LEU:HG	1:107:A:ALA:H	9	0.44
(1,886)	1:103:A:PHE:HE1	1:107:A:ALA:H	2	0.44
(1,886)	1:103:A:PHE:HE2	1:107:A:ALA:H	2	0.44
(1,862)	1:101:A:GLU:HG2	1:102:A:ASP:H	11	0.44
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE1	17	0.44
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE2	17	0.44
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE3	17	0.44
(1,764)	1:88:A:LEU:HA	1:92:A:TYR:H	6	0.44
(1,753)	1:90:A:ASN:HD22	1:91:A:GLY:H	1	0.44
(1,753)	1:90:A:ASN:HD22	1:91:A:GLY:H	3	0.44
(1,753)	1:90:A:ASN:HD22	1:91:A:GLY:H	10	0.44
(1,753)	1:90:A:ASN:HD22	1:91:A:GLY:H	13	0.44
(1,747)	1:90:A:ASN:HA	1:158:A:ILE:HD11	2	0.44
(1,747)	1:90:A:ASN:HA	1:158:A:ILE:HD12	2	0.44
(1,747)	1:90:A:ASN:HA	1:158:A:ILE:HD13	2	0.44
(1,735)	1:89:A:ILE:HB	1:158:A:ILE:HD11	2	0.44
(1,735)	1:89:A:ILE:HB	1:158:A:ILE:HD12	2	0.44
(1,735)	1:89:A:ILE:HB	1:158:A:ILE:HD13	2	0.44
(1,693)	1:86:A:LEU:HD21	1:149:A:PRO:HD2	14	0.44
(1,693)	1:86:A:LEU:HD22	1:149:A:PRO:HD2	14	0.44
(1,693)	1:86:A:LEU:HD23	1:149:A:PRO:HD2	14	0.44
(1,591)	1:74:A:ARG:HE	1:75:A:GLN:H	9	0.44
(1,569)	1:73:A:TRP:HE1	1:74:A:ARG:HB2	4	0.44
(1,569)	1:73:A:TRP:HE1	1:74:A:ARG:HB2	14	0.44
(1,527)	1:66:A:GLN:HG2	1:81:A:THR:HG21	3	0.44
(1,527)	1:66:A:GLN:HG2	1:81:A:THR:HG22	3	0.44
(1,527)	1:66:A:GLN:HG2	1:81:A:THR:HG23	3	0.44
(1,496)	1:62:A:VAL:HG11	1:88:A:LEU:H	9	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,496)	1:62:A:VAL:HG12	1:88:A:LEU:H	9	0.44
(1,496)	1:62:A:VAL:HG13	1:88:A:LEU:H	9	0.44
(1,480)	1:61:A:LEU:HD21	1:156:A:ILE:H	3	0.44
(1,480)	1:61:A:LEU:HD22	1:156:A:ILE:H	3	0.44
(1,480)	1:61:A:LEU:HD23	1:156:A:ILE:H	3	0.44
(1,465)	1:60:A:LEU:HB2	1:158:A:ILE:H	16	0.44
(1,414)	1:56:A:ARG:H	1:124:A:ALA:HB1	20	0.44
(1,414)	1:56:A:ARG:H	1:124:A:ALA:HB2	20	0.44
(1,414)	1:56:A:ARG:H	1:124:A:ALA:HB3	20	0.44
(1,377)	1:33:A:GLN:HG2	1:35:A:GLU:H	19	0.44
(1,366)	1:32:A:SER:H	1:33:A:GLN:HE22	9	0.44
(1,366)	1:32:A:SER:H	1:33:A:GLN:HE21	9	0.44
(1,355)	1:25:A:PHE:HE1	1:32:A:SER:HB2	2	0.44
(1,355)	1:25:A:PHE:HE2	1:32:A:SER:HB2	2	0.44
(1,302)	1:27:A:HIS:HD2	1:28:A:ILE:H	15	0.44
(1,261)	1:25:A:PHE:HE1	1:26:A:ASN:H	4	0.44
(1,261)	1:25:A:PHE:HE2	1:26:A:ASN:H	4	0.44
(1,261)	1:25:A:PHE:HE1	1:26:A:ASN:H	13	0.44
(1,261)	1:25:A:PHE:HE2	1:26:A:ASN:H	13	0.44
(1,218)	1:12:A:GLU:HB2	1:25:A:PHE:H	16	0.44
(1,213)	1:11:A:TRP:HA	1:25:A:PHE:H	7	0.44
(1,213)	1:11:A:TRP:HA	1:25:A:PHE:H	8	0.44
(1,213)	1:11:A:TRP:HA	1:25:A:PHE:H	13	0.44
(1,190)	1:13:A:LYS:HB3	1:24:A:TYR:HA	6	0.44
(1,190)	1:13:A:LYS:HB3	1:24:A:TYR:HA	16	0.44
(1,176)	1:23:A:TYR:HB3	1:24:A:TYR:HD1	7	0.44
(1,176)	1:23:A:TYR:HB3	1:24:A:TYR:HD2	7	0.44
(1,133)	1:20:A:GLY:H	1:21:A:ARG:HB2	14	0.44
(1,123)	1:15:A:MET:HE1	1:20:A:GLY:H	13	0.44
(1,123)	1:15:A:MET:HE2	1:20:A:GLY:H	13	0.44
(1,123)	1:15:A:MET:HE3	1:20:A:GLY:H	13	0.44
(1,121)	1:17:A:ARG:HB2	1:18:A:SER:H	2	0.44
(1,93)	1:14:A:ARG:H	1:22:A:VAL:HA	5	0.44
(1,86)	1:13:A:LYS:HE2	1:14:A:ARG:H	4	0.44
(1,75)	1:13:A:LYS:HA	1:23:A:TYR:H	16	0.44
(1,69)	1:7:A:LEU:HD21	1:13:A:LYS:HE2	1	0.44
(1,69)	1:7:A:LEU:HD22	1:13:A:LYS:HE2	1	0.44
(1,69)	1:7:A:LEU:HD23	1:13:A:LYS:HE2	1	0.44
(1,69)	1:7:A:LEU:HD11	1:13:A:LYS:HE2	1	0.44
(1,69)	1:7:A:LEU:HD12	1:13:A:LYS:HE2	1	0.44
(1,69)	1:7:A:LEU:HD13	1:13:A:LYS:HE2	1	0.44
(1,69)	1:7:A:LEU:HD21	1:13:A:LYS:HE2	4	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,69)	1:7:A:LEU:HD22	1:13:A:LYS:HE2	4	0.44
(1,69)	1:7:A:LEU:HD23	1:13:A:LYS:HE2	4	0.44
(1,69)	1:7:A:LEU:HD11	1:13:A:LYS:HE2	4	0.44
(1,69)	1:7:A:LEU:HD12	1:13:A:LYS:HE2	4	0.44
(1,69)	1:7:A:LEU:HD13	1:13:A:LYS:HE2	4	0.44
(1,69)	1:7:A:LEU:HD21	1:13:A:LYS:HE2	9	0.44
(1,69)	1:7:A:LEU:HD22	1:13:A:LYS:HE2	9	0.44
(1,69)	1:7:A:LEU:HD23	1:13:A:LYS:HE2	9	0.44
(1,69)	1:7:A:LEU:HD11	1:13:A:LYS:HE2	9	0.44
(1,69)	1:7:A:LEU:HD12	1:13:A:LYS:HE2	9	0.44
(1,69)	1:7:A:LEU:HD13	1:13:A:LYS:HE2	9	0.44
(1,69)	1:7:A:LEU:HD21	1:13:A:LYS:HE2	16	0.44
(1,69)	1:7:A:LEU:HD22	1:13:A:LYS:HE2	16	0.44
(1,69)	1:7:A:LEU:HD23	1:13:A:LYS:HE2	16	0.44
(1,69)	1:7:A:LEU:HD11	1:13:A:LYS:HE2	16	0.44
(1,69)	1:7:A:LEU:HD12	1:13:A:LYS:HE2	16	0.44
(1,69)	1:7:A:LEU:HD13	1:13:A:LYS:HE2	16	0.44
(1,66)	1:12:A:GLU:H	1:25:A:PHE:HE1	2	0.44
(1,66)	1:12:A:GLU:H	1:25:A:PHE:HE2	2	0.44
(1,64)	1:12:A:GLU:H	1:24:A:TYR:HD1	10	0.44
(1,64)	1:12:A:GLU:H	1:24:A:TYR:HD2	10	0.44
(1,27)	1:7:A:LEU:HD21	1:13:A:LYS:H	4	0.44
(1,27)	1:7:A:LEU:HD22	1:13:A:LYS:H	4	0.44
(1,27)	1:7:A:LEU:HD23	1:13:A:LYS:H	4	0.44
(1,14)	1:6:A:LYS:HG2	1:7:A:LEU:H	4	0.44
(3,43)	1:72:A:SER:O	1:75:A:GLN:N	11	0.43
(2,106)	1:139:A:PHE:H	2:656:B:PHE:HB2	19	0.43
(2,97)	1:94:A:GLN:HE21	2:640:B:LEU:HG	18	0.43
(2,82)	2:660:B:SEP:HA	2:661:B:PHE:HD1	10	0.43
(2,82)	2:660:B:SEP:HA	2:661:B:PHE:HD2	10	0.43
(2,39)	1:55:A:VAL:HG11	1:127:A:ARG:H	7	0.43
(2,39)	1:55:A:VAL:HG12	1:127:A:ARG:H	7	0.43
(2,39)	1:55:A:VAL:HG13	1:127:A:ARG:H	7	0.43
(2,26)	1:94:A:GLN:HE21	1:97:A:LYS:HB3	3	0.43
(1,2590)	1:122:A:LEU:HD21	2:656:B:PHE:HD1	19	0.43
(1,2590)	1:122:A:LEU:HD21	2:656:B:PHE:HD2	19	0.43
(1,2590)	1:122:A:LEU:HD22	2:656:B:PHE:HD1	19	0.43
(1,2590)	1:122:A:LEU:HD22	2:656:B:PHE:HD2	19	0.43
(1,2590)	1:122:A:LEU:HD23	2:656:B:PHE:HD1	19	0.43
(1,2590)	1:122:A:LEU:HD23	2:656:B:PHE:HD2	19	0.43
(1,2587)	1:115:A:SER:H	2:659:B:PHE:HD1	4	0.43
(1,2587)	1:115:A:SER:H	2:659:B:PHE:HD2	4	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2586)	1:115:A:SER:H	2:659:B:PHE:HE1	5	0.43
(1,2586)	1:115:A:SER:H	2:659:B:PHE:HE2	5	0.43
(1,2582)	1:34:A:TRP:HE1	2:642:B:PRO:HB2	3	0.43
(1,2582)	1:34:A:TRP:HE1	2:642:B:PRO:HB3	3	0.43
(1,2523)	2:647:B:VAL:HA	2:649:B:ARG:H	19	0.43
(1,2384)	1:163:A:GLU:H	1:163:A:GLU:HG3	3	0.43
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE1	2	0.43
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE2	2	0.43
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE3	2	0.43
(1,1750)	1:56:A:ARG:HA	1:56:A:ARG:HE	13	0.43
(1,1560)	1:18:A:SER:H	1:18:A:SER:HB3	6	0.43
(1,1560)	1:18:A:SER:H	1:18:A:SER:HB3	7	0.43
(1,1507)	1:13:A:LYS:H	1:13:A:LYS:HG3	1	0.43
(1,1507)	1:13:A:LYS:H	1:13:A:LYS:HG3	6	0.43
(1,1507)	1:13:A:LYS:H	1:13:A:LYS:HG3	19	0.43
(1,1363)	1:96:A:ILE:HG21	1:160:A:LEU:HD11	9	0.43
(1,1363)	1:96:A:ILE:HG21	1:160:A:LEU:HD12	9	0.43
(1,1363)	1:96:A:ILE:HG21	1:160:A:LEU:HD13	9	0.43
(1,1363)	1:96:A:ILE:HG22	1:160:A:LEU:HD11	9	0.43
(1,1363)	1:96:A:ILE:HG22	1:160:A:LEU:HD12	9	0.43
(1,1363)	1:96:A:ILE:HG22	1:160:A:LEU:HD13	9	0.43
(1,1363)	1:96:A:ILE:HG23	1:160:A:LEU:HD11	9	0.43
(1,1363)	1:96:A:ILE:HG23	1:160:A:LEU:HD12	9	0.43
(1,1363)	1:96:A:ILE:HG23	1:160:A:LEU:HD13	9	0.43
(1,1326)	1:89:A:ILE:HG21	1:158:A:ILE:HB	6	0.43
(1,1326)	1:89:A:ILE:HG22	1:158:A:ILE:HB	6	0.43
(1,1326)	1:89:A:ILE:HG23	1:158:A:ILE:HB	6	0.43
(1,1280)	1:64:A:HIS:HD2	1:156:A:ILE:HG12	12	0.43
(1,1192)	1:141:A:LEU:HD21	1:146:A:MET:H	4	0.43
(1,1192)	1:141:A:LEU:HD22	1:146:A:MET:H	4	0.43
(1,1192)	1:141:A:LEU:HD23	1:146:A:MET:H	4	0.43
(1,1192)	1:141:A:LEU:HD21	1:146:A:MET:H	8	0.43
(1,1192)	1:141:A:LEU:HD22	1:146:A:MET:H	8	0.43
(1,1192)	1:141:A:LEU:HD23	1:146:A:MET:H	8	0.43
(1,1192)	1:141:A:LEU:HD21	1:146:A:MET:H	12	0.43
(1,1192)	1:141:A:LEU:HD22	1:146:A:MET:H	12	0.43
(1,1192)	1:141:A:LEU:HD23	1:146:A:MET:H	12	0.43
(1,1192)	1:141:A:LEU:HD21	1:146:A:MET:H	17	0.43
(1,1192)	1:141:A:LEU:HD22	1:146:A:MET:H	17	0.43
(1,1192)	1:141:A:LEU:HD23	1:146:A:MET:H	17	0.43
(1,1161)	1:136:A:ASP:HB2	1:138:A:SER:H	6	0.43
(1,1161)	1:136:A:ASP:HB2	1:138:A:SER:H	14	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1156)	1:136:A:ASP:HB2	1:137:A:ALA:H	2	0.43
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB1	6	0.43
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB2	6	0.43
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB3	6	0.43
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE1	2	0.43
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE2	2	0.43
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE3	2	0.43
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE1	2	0.43
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE2	2	0.43
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE3	2	0.43
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE1	19	0.43
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE2	19	0.43
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE3	19	0.43
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE1	19	0.43
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE2	19	0.43
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE3	19	0.43
(1,1085)	1:56:A:ARG:HE	1:124:A:ALA:H	13	0.43
(1,1057)	1:59:A:HIS:H	1:122:A:LEU:HG	18	0.43
(1,958)	1:108:A:SER:HA	1:110:A:PHE:H	14	0.43
(1,923)	1:106:A:LEU:HA	1:110:A:PHE:H	2	0.43
(1,834)	1:94:A:GLN:HE21	1:97:A:LYS:HD2	10	0.43
(1,816)	1:95:A:LYS:HD2	1:96:A:ILE:H	7	0.43
(1,764)	1:88:A:LEU:HA	1:92:A:TYR:H	18	0.43
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD1	12	0.43
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD2	12	0.43
(1,742)	1:89:A:ILE:HD11	1:90:A:ASN:H	17	0.43
(1,742)	1:89:A:ILE:HD12	1:90:A:ASN:H	17	0.43
(1,742)	1:89:A:ILE:HD13	1:90:A:ASN:H	17	0.43
(1,728)	1:89:A:ILE:HD11	1:92:A:TYR:HE1	20	0.43
(1,728)	1:89:A:ILE:HD11	1:92:A:TYR:HE2	20	0.43
(1,728)	1:89:A:ILE:HD12	1:92:A:TYR:HE1	20	0.43
(1,728)	1:89:A:ILE:HD12	1:92:A:TYR:HE2	20	0.43
(1,728)	1:89:A:ILE:HD13	1:92:A:TYR:HE1	20	0.43
(1,728)	1:89:A:ILE:HD13	1:92:A:TYR:HE2	20	0.43
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB1	16	0.43
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB2	16	0.43
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB3	16	0.43
(1,647)	1:65:A:SER:H	1:82:A:LYS:H	2	0.43
(1,618)	1:78:A:ILE:HA	1:80:A:ARG:H	10	0.43
(1,592)	1:75:A:GLN:HB2	1:77:A:LYS:H	1	0.43
(1,592)	1:75:A:GLN:HB2	1:77:A:LYS:H	14	0.43
(1,592)	1:75:A:GLN:HB2	1:77:A:LYS:H	17	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,557)	1:71:A:SER:H	1:78:A:ILE:HD11	6	0.43
(1,557)	1:71:A:SER:H	1:78:A:ILE:HD12	6	0.43
(1,557)	1:71:A:SER:H	1:78:A:ILE:HD13	6	0.43
(1,465)	1:60:A:LEU:HB2	1:158:A:ILE:H	15	0.43
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB1	6	0.43
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB2	6	0.43
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB3	6	0.43
(1,377)	1:33:A:GLN:HG2	1:35:A:GLU:H	20	0.43
(1,355)	1:25:A:PHE:HE1	1:32:A:SER:HB2	4	0.43
(1,355)	1:25:A:PHE:HE2	1:32:A:SER:HB2	4	0.43
(1,355)	1:25:A:PHE:HE1	1:32:A:SER:HB2	6	0.43
(1,355)	1:25:A:PHE:HE2	1:32:A:SER:HB2	6	0.43
(1,320)	1:25:A:PHE:HE1	1:30:A:ASN:H	9	0.43
(1,320)	1:25:A:PHE:HE2	1:30:A:ASN:H	9	0.43
(1,320)	1:25:A:PHE:HE1	1:30:A:ASN:H	13	0.43
(1,320)	1:25:A:PHE:HE2	1:30:A:ASN:H	13	0.43
(1,295)	1:27:A:HIS:H	1:29:A:THR:H	5	0.43
(1,287)	1:26:A:ASN:H	1:32:A:SER:HB2	18	0.43
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG21	17	0.43
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG22	17	0.43
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG23	17	0.43
(1,261)	1:25:A:PHE:HE1	1:26:A:ASN:H	9	0.43
(1,261)	1:25:A:PHE:HE2	1:26:A:ASN:H	9	0.43
(1,261)	1:25:A:PHE:HE1	1:26:A:ASN:H	19	0.43
(1,261)	1:25:A:PHE:HE2	1:26:A:ASN:H	19	0.43
(1,213)	1:11:A:TRP:HA	1:25:A:PHE:H	17	0.43
(1,194)	1:13:A:LYS:HG2	1:24:A:TYR:HA	5	0.43
(1,190)	1:13:A:LYS:HB3	1:24:A:TYR:HA	4	0.43
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG11	8	0.43
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG12	8	0.43
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG13	8	0.43
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG11	8	0.43
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG12	8	0.43
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG13	8	0.43
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG11	8	0.43
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG12	8	0.43
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG13	8	0.43
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG11	16	0.43
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG12	16	0.43
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG13	16	0.43
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG11	16	0.43
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG12	16	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG13	16	0.43
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG11	16	0.43
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG12	16	0.43
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG13	16	0.43
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG11	19	0.43
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG12	19	0.43
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG13	19	0.43
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG11	19	0.43
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG12	19	0.43
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG13	19	0.43
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG11	19	0.43
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG12	19	0.43
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG13	19	0.43
(1,134)	1:20:A:GLY:H	1:21:A:ARG:HA	18	0.43
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG21	11	0.43
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG22	11	0.43
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG23	11	0.43
(1,86)	1:13:A:LYS:HE2	1:14:A:ARG:H	13	0.43
(1,66)	1:12:A:GLU:H	1:25:A:PHE:HE1	19	0.43
(1,66)	1:12:A:GLU:H	1:25:A:PHE:HE2	19	0.43
(1,52)	1:11:A:TRP:HE1	1:26:A:ASN:HB2	9	0.43
(1,52)	1:11:A:TRP:HE1	1:26:A:ASN:HB3	9	0.43
(1,27)	1:7:A:LEU:HD21	1:13:A:LYS:H	2	0.43
(1,27)	1:7:A:LEU:HD22	1:13:A:LYS:H	2	0.43
(1,27)	1:7:A:LEU:HD23	1:13:A:LYS:H	2	0.43
(1,14)	1:6:A:LYS:HG2	1:7:A:LEU:H	5	0.43
(1,12)	1:5:A:GLU:HB2	1:6:A:LYS:H	16	0.43
(3,44)	1:72:A:SER:O	1:75:A:GLN:H	2	0.42
(2,106)	1:139:A:PHE:H	2:656:B:PHE:HB2	18	0.42
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG11	8	0.42
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG12	8	0.42
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG13	8	0.42
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG21	8	0.42
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG22	8	0.42
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG23	8	0.42
(2,52)	1:141:A:LEU:HD21	1:148:A:GLY:H	5	0.42
(2,52)	1:141:A:LEU:HD22	1:148:A:GLY:H	5	0.42
(2,52)	1:141:A:LEU:HD23	1:148:A:GLY:H	5	0.42
(2,39)	1:55:A:VAL:HG11	1:127:A:ARG:H	1	0.42
(2,39)	1:55:A:VAL:HG12	1:127:A:ARG:H	1	0.42
(2,39)	1:55:A:VAL:HG13	1:127:A:ARG:H	1	0.42
(2,34)	1:59:A:HIS:H	1:122:A:LEU:HB2	8	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2591)	1:123:A:GLY:H	2:656:B:PHE:HE1	1	0.42
(1,2591)	1:123:A:GLY:H	2:656:B:PHE:HE2	1	0.42
(1,2591)	1:123:A:GLY:H	2:656:B:PHE:HE1	7	0.42
(1,2591)	1:123:A:GLY:H	2:656:B:PHE:HE2	7	0.42
(1,2584)	1:114:A:SER:H	2:659:B:PHE:HD1	19	0.42
(1,2584)	1:114:A:SER:H	2:659:B:PHE:HD2	19	0.42
(1,2582)	1:34:A:TRP:HE1	2:642:B:PRO:HB2	8	0.42
(1,2582)	1:34:A:TRP:HE1	2:642:B:PRO:HB3	8	0.42
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG21	5	0.42
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG22	5	0.42
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG23	5	0.42
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG21	7	0.42
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG22	7	0.42
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG23	7	0.42
(1,2533)	2:647:B:VAL:H	2:649:B:ARG:H	3	0.42
(1,2507)	2:643:B:PRO:HA	2:645:B:GLN:H	15	0.42
(1,2384)	1:163:A:GLU:H	1:163:A:GLU:HG3	1	0.42
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE1	1	0.42
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE2	1	0.42
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE3	1	0.42
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE1	5	0.42
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE2	5	0.42
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE3	5	0.42
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE1	18	0.42
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE2	18	0.42
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE3	18	0.42
(1,2056)	1:101:A:GLU:H	1:101:A:GLU:HG2	13	0.42
(1,1750)	1:56:A:ARG:HA	1:56:A:ARG:HE	15	0.42
(1,1625)	1:27:A:HIS:H	1:27:A:HIS:HD1	13	0.42
(1,1625)	1:27:A:HIS:H	1:27:A:HIS:HD1	14	0.42
(1,1625)	1:27:A:HIS:H	1:27:A:HIS:HD1	19	0.42
(1,1560)	1:18:A:SER:H	1:18:A:SER:HB3	8	0.42
(1,1410)	1:161:A:ARG:HE	1:163:A:GLU:HG2	13	0.42
(1,1349)	1:158:A:ILE:H	1:159:A:ILE:HD11	1	0.42
(1,1349)	1:158:A:ILE:H	1:159:A:ILE:HD12	1	0.42
(1,1349)	1:158:A:ILE:H	1:159:A:ILE:HD13	1	0.42
(1,1335)	1:57:A:CYS:HA	1:159:A:ILE:HG21	5	0.42
(1,1335)	1:57:A:CYS:HA	1:159:A:ILE:HG22	5	0.42
(1,1335)	1:57:A:CYS:HA	1:159:A:ILE:HG23	5	0.42
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG21	13	0.42
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG22	13	0.42
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG23	13	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG21	6	0.42
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG22	6	0.42
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG23	6	0.42
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG21	15	0.42
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG22	15	0.42
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG23	15	0.42
(1,1263)	1:151:A:PHE:H	1:156:A:ILE:HG21	1	0.42
(1,1263)	1:151:A:PHE:H	1:156:A:ILE:HG22	1	0.42
(1,1263)	1:151:A:PHE:H	1:156:A:ILE:HG23	1	0.42
(1,1244)	1:150:A:VAL:HG21	1:157:A:HIS:HB2	18	0.42
(1,1244)	1:150:A:VAL:HG21	1:157:A:HIS:HB3	18	0.42
(1,1244)	1:150:A:VAL:HG22	1:157:A:HIS:HB2	18	0.42
(1,1244)	1:150:A:VAL:HG22	1:157:A:HIS:HB3	18	0.42
(1,1244)	1:150:A:VAL:HG23	1:157:A:HIS:HB2	18	0.42
(1,1244)	1:150:A:VAL:HG23	1:157:A:HIS:HB3	18	0.42
(1,1206)	1:145:A:GLU:HB3	1:146:A:MET:HB2	4	0.42
(1,1206)	1:145:A:GLU:HB3	1:146:A:MET:HB2	17	0.42
(1,1206)	1:145:A:GLU:HB3	1:146:A:MET:HB2	18	0.42
(1,1107)	1:54:A:ARG:HD2	1:126:A:SER:HA	10	0.42
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE1	10	0.42
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE2	10	0.42
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE3	10	0.42
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE1	10	0.42
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE2	10	0.42
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE3	10	0.42
(1,1024)	1:118:A:ALA:HA	1:119:A:ARG:HE	13	0.42
(1,1015)	1:116:A:ALA:HB1	1:120:A:GLY:H	14	0.42
(1,1015)	1:116:A:ALA:HB2	1:120:A:GLY:H	14	0.42
(1,1015)	1:116:A:ALA:HB3	1:120:A:GLY:H	14	0.42
(1,995)	1:108:A:SER:HA	1:116:A:ALA:H	19	0.42
(1,970)	1:108:A:SER:H	1:110:A:PHE:H	16	0.42
(1,961)	1:108:A:SER:H	1:119:A:ARG:HG2	5	0.42
(1,959)	1:108:A:SER:HA	1:111:A:SER:H	15	0.42
(1,917)	1:105:A:SER:HB2	1:106:A:LEU:H	19	0.42
(1,868)	1:60:A:LEU:HD21	1:103:A:PHE:HE1	5	0.42
(1,868)	1:60:A:LEU:HD21	1:103:A:PHE:HE2	5	0.42
(1,868)	1:60:A:LEU:HD22	1:103:A:PHE:HE1	5	0.42
(1,868)	1:60:A:LEU:HD22	1:103:A:PHE:HE2	5	0.42
(1,868)	1:60:A:LEU:HD23	1:103:A:PHE:HE1	5	0.42
(1,868)	1:60:A:LEU:HD23	1:103:A:PHE:HE2	5	0.42
(1,868)	1:60:A:LEU:HD21	1:103:A:PHE:HE1	8	0.42
(1,868)	1:60:A:LEU:HD21	1:103:A:PHE:HE2	8	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,868)	1:60:A:LEU:HD22	1:103:A:PHE:HE1	8	0.42
(1,868)	1:60:A:LEU:HD22	1:103:A:PHE:HE2	8	0.42
(1,868)	1:60:A:LEU:HD23	1:103:A:PHE:HE1	8	0.42
(1,868)	1:60:A:LEU:HD23	1:103:A:PHE:HE2	8	0.42
(1,862)	1:101:A:GLU:HG2	1:102:A:ASP:H	9	0.42
(1,862)	1:101:A:GLU:HG2	1:102:A:ASP:H	10	0.42
(1,862)	1:101:A:GLU:HG2	1:102:A:ASP:H	18	0.42
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD11	4	0.42
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD12	4	0.42
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD13	4	0.42
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB1	19	0.42
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB2	19	0.42
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB3	19	0.42
(1,618)	1:78:A:ILE:HA	1:80:A:ARG:H	20	0.42
(1,571)	1:73:A:TRP:HE1	1:74:A:ARG:HB3	18	0.42
(1,564)	1:72:A:SER:H	1:78:A:ILE:HG12	1	0.42
(1,541)	1:67:A:SER:HB3	1:70:A:PRO:HA	3	0.42
(1,521)	1:64:A:HIS:H	1:66:A:GLN:H	8	0.42
(1,496)	1:62:A:VAL:HG11	1:88:A:LEU:H	8	0.42
(1,496)	1:62:A:VAL:HG12	1:88:A:LEU:H	8	0.42
(1,496)	1:62:A:VAL:HG13	1:88:A:LEU:H	8	0.42
(1,465)	1:60:A:LEU:HB2	1:158:A:ILE:H	1	0.42
(1,465)	1:60:A:LEU:HB2	1:158:A:ILE:H	7	0.42
(1,465)	1:60:A:LEU:HB2	1:158:A:ILE:H	11	0.42
(1,465)	1:60:A:LEU:HB2	1:158:A:ILE:H	12	0.42
(1,465)	1:60:A:LEU:HB2	1:158:A:ILE:H	20	0.42
(1,377)	1:33:A:GLN:HG2	1:35:A:GLU:H	3	0.42
(1,377)	1:33:A:GLN:HG2	1:35:A:GLU:H	11	0.42
(1,369)	1:33:A:GLN:HG2	1:34:A:TRP:H	2	0.42
(1,369)	1:33:A:GLN:HG2	1:34:A:TRP:H	7	0.42
(1,366)	1:32:A:SER:H	1:33:A:GLN:HE22	1	0.42
(1,366)	1:32:A:SER:H	1:33:A:GLN:HE21	1	0.42
(1,366)	1:32:A:SER:H	1:33:A:GLN:HE22	3	0.42
(1,366)	1:32:A:SER:H	1:33:A:GLN:HE21	3	0.42
(1,366)	1:32:A:SER:H	1:33:A:GLN:HE22	8	0.42
(1,366)	1:32:A:SER:H	1:33:A:GLN:HE21	8	0.42
(1,355)	1:25:A:PHE:HE1	1:32:A:SER:HB2	3	0.42
(1,355)	1:25:A:PHE:HE2	1:32:A:SER:HB2	3	0.42
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB1	20	0.42
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB2	20	0.42
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB3	20	0.42
(1,334)	1:27:A:HIS:HA	1:31:A:ALA:H	1	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,302)	1:27:A:HIS:HD2	1:28:A:ILE:H	13	0.42
(1,214)	1:11:A:TRP:HB2	1:25:A:PHE:H	11	0.42
(1,213)	1:11:A:TRP:HA	1:25:A:PHE:H	16	0.42
(1,213)	1:11:A:TRP:HA	1:25:A:PHE:H	20	0.42
(1,194)	1:13:A:LYS:HG2	1:24:A:TYR:HA	19	0.42
(1,176)	1:23:A:TYR:HB3	1:24:A:TYR:HD1	10	0.42
(1,176)	1:23:A:TYR:HB3	1:24:A:TYR:HD2	10	0.42
(1,133)	1:20:A:GLY:H	1:21:A:ARG:HB2	15	0.42
(1,133)	1:20:A:GLY:H	1:21:A:ARG:HB2	18	0.42
(1,129)	1:16:A:SER:HB2	1:21:A:ARG:H	15	0.42
(1,111)	1:15:A:MET:H	1:23:A:TYR:HD1	2	0.42
(1,111)	1:15:A:MET:H	1:23:A:TYR:HD2	2	0.42
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG21	18	0.42
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG22	18	0.42
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG23	18	0.42
(1,75)	1:13:A:LYS:HA	1:23:A:TYR:H	12	0.42
(1,69)	1:7:A:LEU:HD21	1:13:A:LYS:HE2	6	0.42
(1,69)	1:7:A:LEU:HD22	1:13:A:LYS:HE2	6	0.42
(1,69)	1:7:A:LEU:HD23	1:13:A:LYS:HE2	6	0.42
(1,69)	1:7:A:LEU:HD11	1:13:A:LYS:HE2	6	0.42
(1,69)	1:7:A:LEU:HD12	1:13:A:LYS:HE2	6	0.42
(1,69)	1:7:A:LEU:HD13	1:13:A:LYS:HE2	6	0.42
(1,64)	1:12:A:GLU:H	1:24:A:TYR:HD1	12	0.42
(1,64)	1:12:A:GLU:H	1:24:A:TYR:HD2	12	0.42
(1,52)	1:11:A:TRP:HE1	1:26:A:ASN:HB2	1	0.42
(1,52)	1:11:A:TRP:HE1	1:26:A:ASN:HB3	1	0.42
(1,52)	1:11:A:TRP:HE1	1:26:A:ASN:HB2	10	0.42
(1,52)	1:11:A:TRP:HE1	1:26:A:ASN:HB3	10	0.42
(1,14)	1:6:A:LYS:HG2	1:7:A:LEU:H	9	0.42
(1,12)	1:5:A:GLU:HB2	1:6:A:LYS:H	9	0.42
(1,12)	1:5:A:GLU:HB2	1:6:A:LYS:H	14	0.42
(1,11)	1:4:A:GLU:H	1:6:A:LYS:H	7	0.42
(3,9)	1:16:A:SER:O	1:19:A:SER:N	19	0.41
(2,110)	1:152:A:THR:HG21	2:661:B:PHE:HB2	8	0.41
(2,110)	1:152:A:THR:HG21	2:661:B:PHE:HB3	8	0.41
(2,110)	1:152:A:THR:HG22	2:661:B:PHE:HB2	8	0.41
(2,110)	1:152:A:THR:HG22	2:661:B:PHE:HB3	8	0.41
(2,110)	1:152:A:THR:HG23	2:661:B:PHE:HB2	8	0.41
(2,110)	1:152:A:THR:HG23	2:661:B:PHE:HB3	8	0.41
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG11	6	0.41
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG12	6	0.41
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG13	6	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG21	6	0.41
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG22	6	0.41
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG23	6	0.41
(2,68)	2:649:B:ARG:HD2	2:650:B:ASN:H	18	0.41
(2,58)	1:152:A:THR:HG21	1:157:A:HIS:HB3	1	0.41
(2,58)	1:152:A:THR:HG22	1:157:A:HIS:HB3	1	0.41
(2,58)	1:152:A:THR:HG23	1:157:A:HIS:HB3	1	0.41
(2,58)	1:152:A:THR:HG21	1:157:A:HIS:HB3	12	0.41
(2,58)	1:152:A:THR:HG22	1:157:A:HIS:HB3	12	0.41
(2,58)	1:152:A:THR:HG23	1:157:A:HIS:HB3	12	0.41
(2,44)	1:131:A:GLN:HE21	1:153:A:ASP:H	20	0.41
(2,20)	1:68:A:ARG:H	1:153:A:ASP:HB2	8	0.41
(2,20)	1:68:A:ARG:H	1:153:A:ASP:HB3	8	0.41
(2,9)	1:53:A:ALA:H	1:54:A:ARG:HD2	6	0.41
(1,2591)	1:123:A:GLY:H	2:656:B:PHE:HE1	14	0.41
(1,2591)	1:123:A:GLY:H	2:656:B:PHE:HE2	14	0.41
(1,2591)	1:123:A:GLY:H	2:656:B:PHE:HE1	18	0.41
(1,2591)	1:123:A:GLY:H	2:656:B:PHE:HE2	18	0.41
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG21	18	0.41
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG22	18	0.41
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG23	18	0.41
(1,2527)	2:646:B:GLU:H	2:648:B:ILE:H	20	0.41
(1,2384)	1:163:A:GLU:H	1:163:A:GLU:HG3	9	0.41
(1,2384)	1:163:A:GLU:H	1:163:A:GLU:HG3	19	0.41
(1,2158)	1:119:A:ARG:H	1:119:A:ARG:HD2	6	0.41
(1,2158)	1:119:A:ARG:H	1:119:A:ARG:HD2	9	0.41
(1,2056)	1:101:A:GLU:H	1:101:A:GLU:HG2	10	0.41
(1,1750)	1:56:A:ARG:HA	1:56:A:ARG:HE	10	0.41
(1,1625)	1:27:A:HIS:H	1:27:A:HIS:HD1	7	0.41
(1,1625)	1:27:A:HIS:H	1:27:A:HIS:HD1	8	0.41
(1,1568)	1:21:A:ARG:HB2	1:21:A:ARG:HE	6	0.41
(1,1560)	1:18:A:SER:H	1:18:A:SER:HB3	14	0.41
(1,1406)	1:147:A:SER:H	1:161:A:ARG:H	1	0.41
(1,1399)	1:143:A:THR:H	1:161:A:ARG:HD2	18	0.41
(1,1353)	1:57:A:CYS:HB3	1:160:A:LEU:H	20	0.41
(1,1335)	1:57:A:CYS:HA	1:159:A:ILE:HG21	12	0.41
(1,1335)	1:57:A:CYS:HA	1:159:A:ILE:HG22	12	0.41
(1,1335)	1:57:A:CYS:HA	1:159:A:ILE:HG23	12	0.41
(1,1311)	1:152:A:THR:HG21	1:157:A:HIS:H	7	0.41
(1,1311)	1:152:A:THR:HG22	1:157:A:HIS:H	7	0.41
(1,1311)	1:152:A:THR:HG23	1:157:A:HIS:H	7	0.41
(1,1306)	1:89:A:ILE:HD11	1:157:A:HIS:HD2	3	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1306)	1:89:A:ILE:HD12	1:157:A:HIS:HD2	3	0.41
(1,1306)	1:89:A:ILE:HD13	1:157:A:HIS:HD2	3	0.41
(1,1303)	1:156:A:ILE:HG21	1:157:A:HIS:HD2	3	0.41
(1,1303)	1:156:A:ILE:HG22	1:157:A:HIS:HD2	3	0.41
(1,1303)	1:156:A:ILE:HG23	1:157:A:HIS:HD2	3	0.41
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG21	12	0.41
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG22	12	0.41
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG23	12	0.41
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG21	15	0.41
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG22	15	0.41
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG23	15	0.41
(1,1217)	1:145:A:GLU:HB3	1:147:A:SER:H	13	0.41
(1,1193)	1:141:A:LEU:HD11	1:148:A:GLY:H	2	0.41
(1,1193)	1:141:A:LEU:HD12	1:148:A:GLY:H	2	0.41
(1,1193)	1:141:A:LEU:HD13	1:148:A:GLY:H	2	0.41
(1,1156)	1:136:A:ASP:HB2	1:137:A:ALA:H	15	0.41
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB1	8	0.41
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB2	8	0.41
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB3	8	0.41
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE1	12	0.41
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE2	12	0.41
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE3	12	0.41
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE1	12	0.41
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE2	12	0.41
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE3	12	0.41
(1,1027)	1:118:A:ALA:HA	1:119:A:ARG:HG2	17	0.41
(1,959)	1:108:A:SER:HA	1:111:A:SER:H	10	0.41
(1,925)	1:60:A:LEU:HG	1:107:A:ALA:H	1	0.41
(1,913)	1:103:A:PHE:H	1:106:A:LEU:HB3	15	0.41
(1,753)	1:90:A:ASN:HD22	1:91:A:GLY:H	4	0.41
(1,753)	1:90:A:ASN:HD22	1:91:A:GLY:H	19	0.41
(1,674)	1:81:A:THR:H	1:85:A:ALA:H	6	0.41
(1,637)	1:80:A:ARG:HE	1:85:A:ALA:H	19	0.41
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG21	3	0.41
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG22	3	0.41
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG23	3	0.41
(1,618)	1:78:A:ILE:HA	1:80:A:ARG:H	13	0.41
(1,593)	1:71:A:SER:HB3	1:77:A:LYS:HA	19	0.41
(1,569)	1:73:A:TRP:HE1	1:74:A:ARG:HB2	1	0.41
(1,554)	1:70:A:PRO:HG3	1:71:A:SER:H	9	0.41
(1,527)	1:66:A:GLN:HG2	1:81:A:THR:HG21	14	0.41
(1,527)	1:66:A:GLN:HG2	1:81:A:THR:HG22	14	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,527)	1:66:A:GLN:HG2	1:81:A:THR:HG23	14	0.41
(1,496)	1:62:A:VAL:HG11	1:88:A:LEU:H	3	0.41
(1,496)	1:62:A:VAL:HG12	1:88:A:LEU:H	3	0.41
(1,496)	1:62:A:VAL:HG13	1:88:A:LEU:H	3	0.41
(1,465)	1:60:A:LEU:HB2	1:158:A:ILE:H	2	0.41
(1,465)	1:60:A:LEU:HB2	1:158:A:ILE:H	3	0.41
(1,465)	1:60:A:LEU:HB2	1:158:A:ILE:H	4	0.41
(1,465)	1:60:A:LEU:HB2	1:158:A:ILE:H	13	0.41
(1,465)	1:60:A:LEU:HB2	1:158:A:ILE:H	19	0.41
(1,457)	1:60:A:LEU:HD11	1:108:A:SER:H	20	0.41
(1,457)	1:60:A:LEU:HD12	1:108:A:SER:H	20	0.41
(1,457)	1:60:A:LEU:HD13	1:108:A:SER:H	20	0.41
(1,385)	1:24:A:TYR:HD1	1:36:A:ARG:H	2	0.41
(1,385)	1:24:A:TYR:HD2	1:36:A:ARG:H	2	0.41
(1,377)	1:33:A:GLN:HG2	1:35:A:GLU:H	6	0.41
(1,369)	1:33:A:GLN:HG2	1:34:A:TRP:H	9	0.41
(1,369)	1:33:A:GLN:HG2	1:34:A:TRP:H	20	0.41
(1,366)	1:32:A:SER:H	1:33:A:GLN:HE22	12	0.41
(1,366)	1:32:A:SER:H	1:33:A:GLN:HE21	12	0.41
(1,366)	1:32:A:SER:H	1:33:A:GLN:HE22	14	0.41
(1,366)	1:32:A:SER:H	1:33:A:GLN:HE21	14	0.41
(1,366)	1:32:A:SER:H	1:33:A:GLN:HE22	15	0.41
(1,366)	1:32:A:SER:H	1:33:A:GLN:HE21	15	0.41
(1,362)	1:11:A:TRP:HH2	1:33:A:GLN:HE21	5	0.41
(1,311)	1:27:A:HIS:HB2	1:29:A:THR:H	14	0.41
(1,302)	1:27:A:HIS:HD2	1:28:A:ILE:H	4	0.41
(1,261)	1:25:A:PHE:HE1	1:26:A:ASN:H	6	0.41
(1,261)	1:25:A:PHE:HE2	1:26:A:ASN:H	6	0.41
(1,261)	1:25:A:PHE:HE1	1:26:A:ASN:H	10	0.41
(1,261)	1:25:A:PHE:HE2	1:26:A:ASN:H	10	0.41
(1,261)	1:25:A:PHE:HE1	1:26:A:ASN:H	15	0.41
(1,261)	1:25:A:PHE:HE2	1:26:A:ASN:H	15	0.41
(1,190)	1:13:A:LYS:HB3	1:24:A:TYR:HA	8	0.41
(1,176)	1:23:A:TYR:HB3	1:24:A:TYR:HD1	6	0.41
(1,176)	1:23:A:TYR:HB3	1:24:A:TYR:HD2	6	0.41
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG11	20	0.41
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG12	20	0.41
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG13	20	0.41
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG11	20	0.41
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG12	20	0.41
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG13	20	0.41
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG11	20	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG12	20	0.41
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG13	20	0.41
(1,133)	1:20:A:GLY:H	1:21:A:ARG:HB2	11	0.41
(1,129)	1:16:A:SER:HB2	1:21:A:ARG:H	17	0.41
(1,111)	1:15:A:MET:H	1:23:A:TYR:HD1	5	0.41
(1,111)	1:15:A:MET:H	1:23:A:TYR:HD2	5	0.41
(1,111)	1:15:A:MET:H	1:23:A:TYR:HD1	14	0.41
(1,111)	1:15:A:MET:H	1:23:A:TYR:HD2	14	0.41
(1,66)	1:12:A:GLU:H	1:25:A:PHE:HE1	14	0.41
(1,66)	1:12:A:GLU:H	1:25:A:PHE:HE2	14	0.41
(1,61)	1:11:A:TRP:HA	1:12:A:GLU:HB3	15	0.41
(1,44)	1:8:A:PRO:HB2	1:11:A:TRP:HE1	12	0.41
(1,12)	1:5:A:GLU:HB2	1:6:A:LYS:H	18	0.41
(1,12)	1:5:A:GLU:HB2	1:6:A:LYS:H	19	0.41
(3,79)	1:105:A:SER:O	1:109:A:GLN:N	13	0.4
(3,43)	1:72:A:SER:O	1:75:A:GLN:N	19	0.4
(3,28)	1:56:A:ARG:H	1:163:A:GLU:O	17	0.4
(3,9)	1:16:A:SER:O	1:19:A:SER:N	10	0.4
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG11	17	0.4
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG12	17	0.4
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG13	17	0.4
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG21	17	0.4
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG22	17	0.4
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG23	17	0.4
(2,82)	2:660:B:SEP:HA	2:661:B:PHE:HD1	17	0.4
(2,82)	2:660:B:SEP:HA	2:661:B:PHE:HD2	17	0.4
(2,25)	1:88:A:LEU:HG	1:92:A:TYR:H	11	0.4
(2,25)	1:88:A:LEU:HG	1:92:A:TYR:H	14	0.4
(2,20)	1:68:A:ARG:H	1:153:A:ASP:HB2	9	0.4
(2,20)	1:68:A:ARG:H	1:153:A:ASP:HB3	9	0.4
(1,2551)	2:652:B:ASP:H	2:654:B:SER:H	3	0.4
(1,2533)	2:647:B:VAL:H	2:649:B:ARG:H	8	0.4
(1,2523)	2:647:B:VAL:HA	2:649:B:ARG:H	7	0.4
(1,2514)	2:646:B:GLU:HA	2:649:B:ARG:H	10	0.4
(1,2384)	1:163:A:GLU:H	1:163:A:GLU:HG3	6	0.4
(1,2022)	1:94:A:GLN:H	1:94:A:GLN:HG2	11	0.4
(1,1750)	1:56:A:ARG:HA	1:56:A:ARG:HE	5	0.4
(1,1747)	1:56:A:ARG:H	1:56:A:ARG:HD2	8	0.4
(1,1625)	1:27:A:HIS:H	1:27:A:HIS:HD1	12	0.4
(1,1434)	1:161:A:ARG:HD2	1:163:A:GLU:H	7	0.4
(1,1313)	1:156:A:ILE:HA	1:157:A:HIS:HD2	13	0.4
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG21	5	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG22	5	0.4
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG23	5	0.4
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG21	18	0.4
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG22	18	0.4
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG23	18	0.4
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG21	5	0.4
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG22	5	0.4
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG23	5	0.4
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG21	17	0.4
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG22	17	0.4
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG23	17	0.4
(1,1212)	1:146:A:MET:HG2	1:160:A:LEU:HG	10	0.4
(1,1156)	1:136:A:ASP:HB2	1:137:A:ALA:H	7	0.4
(1,1156)	1:136:A:ASP:HB2	1:137:A:ALA:H	18	0.4
(1,1130)	1:131:A:GLN:HE21	1:153:A:ASP:HB2	8	0.4
(1,1130)	1:131:A:GLN:HE21	1:153:A:ASP:HB3	8	0.4
(1,1109)	1:126:A:SER:HA	1:139:A:PHE:HD1	1	0.4
(1,1109)	1:126:A:SER:HA	1:139:A:PHE:HD2	1	0.4
(1,1020)	1:116:A:ALA:HA	1:118:A:ALA:H	4	0.4
(1,1020)	1:116:A:ALA:HA	1:118:A:ALA:H	12	0.4
(1,1015)	1:116:A:ALA:HB1	1:120:A:GLY:H	7	0.4
(1,1015)	1:116:A:ALA:HB2	1:120:A:GLY:H	7	0.4
(1,1015)	1:116:A:ALA:HB3	1:120:A:GLY:H	7	0.4
(1,1012)	1:116:A:ALA:H	1:119:A:ARG:H	5	0.4
(1,1001)	1:113:A:CYS:H	1:116:A:ALA:HB1	5	0.4
(1,1001)	1:113:A:CYS:H	1:116:A:ALA:HB2	5	0.4
(1,1001)	1:113:A:CYS:H	1:116:A:ALA:HB3	5	0.4
(1,1001)	1:113:A:CYS:H	1:116:A:ALA:HB1	7	0.4
(1,1001)	1:113:A:CYS:H	1:116:A:ALA:HB2	7	0.4
(1,1001)	1:113:A:CYS:H	1:116:A:ALA:HB3	7	0.4
(1,958)	1:108:A:SER:HA	1:110:A:PHE:H	10	0.4
(1,941)	1:106:A:LEU:HD11	1:107:A:ALA:H	18	0.4
(1,941)	1:106:A:LEU:HD12	1:107:A:ALA:H	18	0.4
(1,941)	1:106:A:LEU:HD13	1:107:A:ALA:H	18	0.4
(1,888)	1:103:A:PHE:HE1	1:120:A:GLY:H	9	0.4
(1,888)	1:103:A:PHE:HE2	1:120:A:GLY:H	9	0.4
(1,871)	1:96:A:ILE:HB	1:103:A:PHE:H	2	0.4
(1,871)	1:96:A:ILE:HB	1:103:A:PHE:H	20	0.4
(1,862)	1:101:A:GLU:HG2	1:102:A:ASP:H	1	0.4
(1,753)	1:90:A:ASN:HD22	1:91:A:GLY:H	6	0.4
(1,748)	1:87:A:GLU:HA	1:91:A:GLY:H	18	0.4
(1,747)	1:90:A:ASN:HA	1:158:A:ILE:HD11	13	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,747)	1:90:A:ASN:HA	1:158:A:ILE:HD12	13	0.4
(1,747)	1:90:A:ASN:HA	1:158:A:ILE:HD13	13	0.4
(1,723)	1:86:A:LEU:HD21	1:89:A:ILE:HB	19	0.4
(1,723)	1:86:A:LEU:HD22	1:89:A:ILE:HB	19	0.4
(1,723)	1:86:A:LEU:HD23	1:89:A:ILE:HB	19	0.4
(1,695)	1:86:A:LEU:HD21	1:149:A:PRO:HD3	11	0.4
(1,695)	1:86:A:LEU:HD22	1:149:A:PRO:HD3	11	0.4
(1,695)	1:86:A:LEU:HD23	1:149:A:PRO:HD3	11	0.4
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB1	4	0.4
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB2	4	0.4
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB3	4	0.4
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB1	10	0.4
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB2	10	0.4
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB3	10	0.4
(1,647)	1:65:A:SER:H	1:82:A:LYS:H	10	0.4
(1,637)	1:80:A:ARG:HE	1:85:A:ALA:H	17	0.4
(1,592)	1:75:A:GLN:HB2	1:77:A:LYS:H	5	0.4
(1,592)	1:75:A:GLN:HB2	1:77:A:LYS:H	12	0.4
(1,592)	1:75:A:GLN:HB2	1:77:A:LYS:H	19	0.4
(1,521)	1:64:A:HIS:H	1:66:A:GLN:H	5	0.4
(1,465)	1:60:A:LEU:HB2	1:158:A:ILE:H	9	0.4
(1,465)	1:60:A:LEU:HB2	1:158:A:ILE:H	14	0.4
(1,377)	1:33:A:GLN:HG2	1:35:A:GLU:H	1	0.4
(1,377)	1:33:A:GLN:HG2	1:35:A:GLU:H	7	0.4
(1,369)	1:33:A:GLN:HG2	1:34:A:TRP:H	10	0.4
(1,355)	1:25:A:PHE:HE1	1:32:A:SER:HB2	7	0.4
(1,355)	1:25:A:PHE:HE2	1:32:A:SER:HB2	7	0.4
(1,347)	1:31:A:ALA:HB1	1:33:A:GLN:H	5	0.4
(1,347)	1:31:A:ALA:HB2	1:33:A:GLN:H	5	0.4
(1,347)	1:31:A:ALA:HB3	1:33:A:GLN:H	5	0.4
(1,320)	1:25:A:PHE:HE1	1:30:A:ASN:H	8	0.4
(1,320)	1:25:A:PHE:HE2	1:30:A:ASN:H	8	0.4
(1,287)	1:26:A:ASN:H	1:32:A:SER:HB2	8	0.4
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG21	6	0.4
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG22	6	0.4
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG23	6	0.4
(1,261)	1:25:A:PHE:HE1	1:26:A:ASN:H	11	0.4
(1,261)	1:25:A:PHE:HE2	1:26:A:ASN:H	11	0.4
(1,218)	1:12:A:GLU:HB2	1:25:A:PHE:H	11	0.4
(1,204)	1:24:A:TYR:HB2	1:33:A:GLN:HE21	11	0.4
(1,190)	1:13:A:LYS:HB3	1:24:A:TYR:HA	12	0.4
(1,180)	1:23:A:TYR:HD1	1:33:A:GLN:HA	16	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,180)	1:23:A:TYR:HD2	1:33:A:GLN:HA	16	0.4
(1,176)	1:23:A:TYR:HB3	1:24:A:TYR:HD1	9	0.4
(1,176)	1:23:A:TYR:HB3	1:24:A:TYR:HD2	9	0.4
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG11	9	0.4
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG12	9	0.4
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG13	9	0.4
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG11	9	0.4
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG12	9	0.4
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG13	9	0.4
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG11	9	0.4
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG12	9	0.4
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG13	9	0.4
(1,134)	1:20:A:GLY:H	1:21:A:ARG:HA	15	0.4
(1,133)	1:20:A:GLY:H	1:21:A:ARG:HB2	16	0.4
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG21	1	0.4
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG22	1	0.4
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG23	1	0.4
(1,93)	1:14:A:ARG:H	1:22:A:VAL:HA	16	0.4
(1,81)	1:12:A:GLU:H	1:14:A:ARG:H	15	0.4
(1,75)	1:13:A:LYS:HA	1:23:A:TYR:H	5	0.4
(1,69)	1:7:A:LEU:HD21	1:13:A:LYS:HE2	18	0.4
(1,69)	1:7:A:LEU:HD22	1:13:A:LYS:HE2	18	0.4
(1,69)	1:7:A:LEU:HD23	1:13:A:LYS:HE2	18	0.4
(1,69)	1:7:A:LEU:HD11	1:13:A:LYS:HE2	18	0.4
(1,69)	1:7:A:LEU:HD12	1:13:A:LYS:HE2	18	0.4
(1,69)	1:7:A:LEU:HD13	1:13:A:LYS:HE2	18	0.4
(1,61)	1:11:A:TRP:HA	1:12:A:GLU:HB3	13	0.4
(1,12)	1:5:A:GLU:HB2	1:6:A:LYS:H	4	0.4
(1,11)	1:4:A:GLU:H	1:6:A:LYS:H	11	0.4
(1,11)	1:4:A:GLU:H	1:6:A:LYS:H	14	0.4
(3,44)	1:72:A:SER:O	1:75:A:GLN:H	15	0.39
(3,44)	1:72:A:SER:O	1:75:A:GLN:H	19	0.39
(3,33)	1:60:A:LEU:N	1:158:A:ILE:O	19	0.39
(2,89)	1:55:A:VAL:H	2:651:B:ILE:HG12	1	0.39
(2,89)	1:55:A:VAL:H	2:651:B:ILE:HG13	1	0.39
(2,89)	1:55:A:VAL:H	2:651:B:ILE:HG12	9	0.39
(2,89)	1:55:A:VAL:H	2:651:B:ILE:HG13	9	0.39
(2,82)	2:660:B:SEP:HA	2:661:B:PHE:HD1	4	0.39
(2,82)	2:660:B:SEP:HA	2:661:B:PHE:HD2	4	0.39
(2,52)	1:141:A:LEU:HD21	1:148:A:GLY:H	1	0.39
(2,52)	1:141:A:LEU:HD22	1:148:A:GLY:H	1	0.39
(2,52)	1:141:A:LEU:HD23	1:148:A:GLY:H	1	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,25)	1:88:A:LEU:HG	1:92:A:TYR:H	15	0.39
(2,4)	1:21:A:ARG:HE	1:22:A:VAL:H	3	0.39
(1,2589)	1:122:A:LEU:HD21	2:656:B:PHE:HE1	13	0.39
(1,2589)	1:122:A:LEU:HD21	2:656:B:PHE:HE2	13	0.39
(1,2589)	1:122:A:LEU:HD22	2:656:B:PHE:HE1	13	0.39
(1,2589)	1:122:A:LEU:HD22	2:656:B:PHE:HE2	13	0.39
(1,2589)	1:122:A:LEU:HD23	2:656:B:PHE:HE1	13	0.39
(1,2589)	1:122:A:LEU:HD23	2:656:B:PHE:HE2	13	0.39
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG21	7	0.39
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG22	7	0.39
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG23	7	0.39
(1,2507)	2:643:B:PRO:HA	2:645:B:GLN:H	13	0.39
(1,2384)	1:163:A:GLU:H	1:163:A:GLU:HG3	7	0.39
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE1	13	0.39
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE2	13	0.39
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE3	13	0.39
(1,2209)	1:131:A:GLN:HA	1:131:A:GLN:HE22	15	0.39
(1,2158)	1:119:A:ARG:H	1:119:A:ARG:HD2	3	0.39
(1,2158)	1:119:A:ARG:H	1:119:A:ARG:HD2	4	0.39
(1,2033)	1:95:A:LYS:H	1:95:A:LYS:HD2	2	0.39
(1,1625)	1:27:A:HIS:H	1:27:A:HIS:HD1	6	0.39
(1,1525)	1:14:A:ARG:H	1:14:A:ARG:HE	1	0.39
(1,1507)	1:13:A:LYS:H	1:13:A:LYS:HG3	10	0.39
(1,1434)	1:161:A:ARG:HD2	1:163:A:GLU:H	4	0.39
(1,1403)	1:144:A:GLY:H	1:161:A:ARG:HG2	2	0.39
(1,1348)	1:157:A:HIS:HB2	1:159:A:ILE:HD11	4	0.39
(1,1348)	1:157:A:HIS:HB2	1:159:A:ILE:HD12	4	0.39
(1,1348)	1:157:A:HIS:HB2	1:159:A:ILE:HD13	4	0.39
(1,1348)	1:157:A:HIS:HB3	1:159:A:ILE:HD11	4	0.39
(1,1348)	1:157:A:HIS:HB3	1:159:A:ILE:HD12	4	0.39
(1,1348)	1:157:A:HIS:HB3	1:159:A:ILE:HD13	4	0.39
(1,1344)	1:147:A:SER:HA	1:159:A:ILE:H	3	0.39
(1,1306)	1:89:A:ILE:HD11	1:157:A:HIS:HD2	11	0.39
(1,1306)	1:89:A:ILE:HD12	1:157:A:HIS:HD2	11	0.39
(1,1306)	1:89:A:ILE:HD13	1:157:A:HIS:HD2	11	0.39
(1,1296)	1:89:A:ILE:HG13	1:156:A:ILE:HG21	6	0.39
(1,1296)	1:89:A:ILE:HG13	1:156:A:ILE:HG22	6	0.39
(1,1296)	1:89:A:ILE:HG13	1:156:A:ILE:HG23	6	0.39
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD11	3	0.39
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD12	3	0.39
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD13	3	0.39
(1,1192)	1:141:A:LEU:HD21	1:146:A:MET:H	6	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1192)	1:141:A:LEU:HD22	1:146:A:MET:H	6	0.39
(1,1192)	1:141:A:LEU:HD23	1:146:A:MET:H	6	0.39
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB1	12	0.39
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB2	12	0.39
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB3	12	0.39
(1,1141)	1:130:A:MET:HB2	1:134:A:PHE:H	18	0.39
(1,1052)	1:58:A:SER:HB2	1:122:A:LEU:H	3	0.39
(1,1033)	1:108:A:SER:H	1:119:A:ARG:HB2	4	0.39
(1,1032)	1:107:A:ALA:HB1	1:119:A:ARG:H	8	0.39
(1,1032)	1:107:A:ALA:HB2	1:119:A:ARG:H	8	0.39
(1,1032)	1:107:A:ALA:HB3	1:119:A:ARG:H	8	0.39
(1,985)	1:61:A:LEU:HD21	1:113:A:CYS:HA	2	0.39
(1,985)	1:61:A:LEU:HD22	1:113:A:CYS:HA	2	0.39
(1,985)	1:61:A:LEU:HD23	1:113:A:CYS:HA	2	0.39
(1,959)	1:108:A:SER:HA	1:111:A:SER:H	7	0.39
(1,958)	1:108:A:SER:HA	1:110:A:PHE:H	8	0.39
(1,862)	1:101:A:GLU:HG2	1:102:A:ASP:H	6	0.39
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD11	19	0.39
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD12	19	0.39
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD13	19	0.39
(1,753)	1:90:A:ASN:HD22	1:91:A:GLY:H	14	0.39
(1,648)	1:66:A:GLN:HE22	1:82:A:LYS:HG3	3	0.39
(1,648)	1:66:A:GLN:HE22	1:82:A:LYS:HG3	14	0.39
(1,592)	1:75:A:GLN:HB2	1:77:A:LYS:H	16	0.39
(1,569)	1:73:A:TRP:HE1	1:74:A:ARG:HB2	7	0.39
(1,564)	1:72:A:SER:H	1:78:A:ILE:HG12	2	0.39
(1,564)	1:72:A:SER:H	1:78:A:ILE:HG12	13	0.39
(1,475)	1:61:A:LEU:HD11	1:113:A:CYS:H	10	0.39
(1,475)	1:61:A:LEU:HD12	1:113:A:CYS:H	10	0.39
(1,475)	1:61:A:LEU:HD13	1:113:A:CYS:H	10	0.39
(1,475)	1:61:A:LEU:HD21	1:113:A:CYS:H	10	0.39
(1,475)	1:61:A:LEU:HD22	1:113:A:CYS:H	10	0.39
(1,475)	1:61:A:LEU:HD23	1:113:A:CYS:H	10	0.39
(1,377)	1:33:A:GLN:HG2	1:35:A:GLU:H	9	0.39
(1,369)	1:33:A:GLN:HG2	1:34:A:TRP:H	3	0.39
(1,366)	1:32:A:SER:H	1:33:A:GLN:HE22	16	0.39
(1,366)	1:32:A:SER:H	1:33:A:GLN:HE21	16	0.39
(1,347)	1:31:A:ALA:HB1	1:33:A:GLN:H	16	0.39
(1,347)	1:31:A:ALA:HB2	1:33:A:GLN:H	16	0.39
(1,347)	1:31:A:ALA:HB3	1:33:A:GLN:H	16	0.39
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB1	1	0.39
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB2	1	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB3	1	0.39
(1,321)	1:25:A:PHE:HZ	1:30:A:ASN:H	20	0.39
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG21	7	0.39
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG22	7	0.39
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG23	7	0.39
(1,262)	1:25:A:PHE:HE1	1:26:A:ASN:HA	1	0.39
(1,262)	1:25:A:PHE:HE2	1:26:A:ASN:HA	1	0.39
(1,261)	1:25:A:PHE:HE1	1:26:A:ASN:H	12	0.39
(1,261)	1:25:A:PHE:HE2	1:26:A:ASN:H	12	0.39
(1,261)	1:25:A:PHE:HE1	1:26:A:ASN:H	17	0.39
(1,261)	1:25:A:PHE:HE2	1:26:A:ASN:H	17	0.39
(1,256)	1:23:A:TYR:HE1	1:26:A:ASN:H	3	0.39
(1,256)	1:23:A:TYR:HE2	1:26:A:ASN:H	3	0.39
(1,224)	1:14:A:ARG:HE	1:25:A:PHE:HB3	5	0.39
(1,214)	1:11:A:TRP:HB2	1:25:A:PHE:H	19	0.39
(1,214)	1:11:A:TRP:HB2	1:25:A:PHE:H	20	0.39
(1,211)	1:24:A:TYR:HE1	1:36:A:ARG:HD2	14	0.39
(1,211)	1:24:A:TYR:HE2	1:36:A:ARG:HD2	14	0.39
(1,176)	1:23:A:TYR:HB3	1:24:A:TYR:HD1	14	0.39
(1,176)	1:23:A:TYR:HB3	1:24:A:TYR:HD2	14	0.39
(1,66)	1:12:A:GLU:H	1:25:A:PHE:HE1	5	0.39
(1,66)	1:12:A:GLU:H	1:25:A:PHE:HE2	5	0.39
(1,61)	1:11:A:TRP:HA	1:12:A:GLU:HB3	14	0.39
(1,7)	1:3:A:ASP:HA	1:4:A:GLU:H	11	0.39
(3,44)	1:72:A:SER:O	1:75:A:GLN:H	18	0.38
(3,43)	1:72:A:SER:O	1:75:A:GLN:N	1	0.38
(3,33)	1:60:A:LEU:N	1:158:A:ILE:O	18	0.38
(2,102)	1:135:A:GLU:H	2:656:B:PHE:HB2	17	0.38
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD11	10	0.38
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD12	10	0.38
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD13	10	0.38
(2,82)	2:660:B:SEP:HA	2:661:B:PHE:HD1	16	0.38
(2,82)	2:660:B:SEP:HA	2:661:B:PHE:HD2	16	0.38
(2,76)	2:656:B:PHE:HE1	2:659:B:PHE:HE1	16	0.38
(2,76)	2:656:B:PHE:HE1	2:659:B:PHE:HE2	16	0.38
(2,76)	2:656:B:PHE:HE2	2:659:B:PHE:HE1	16	0.38
(2,76)	2:656:B:PHE:HE2	2:659:B:PHE:HE2	16	0.38
(2,45)	1:131:A:GLN:HE21	1:152:A:THR:HB	5	0.38
(2,42)	1:130:A:MET:HB2	1:134:A:PHE:HD1	9	0.38
(2,42)	1:130:A:MET:HB2	1:134:A:PHE:HD2	9	0.38
(2,39)	1:55:A:VAL:HG11	1:127:A:ARG:H	3	0.38
(2,39)	1:55:A:VAL:HG12	1:127:A:ARG:H	3	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,39)	1:55:A:VAL:HG13	1:127:A:ARG:H	3	0.38
(1,2598)	1:146:A:MET:HE1	2:642:B:PRO:HB2	8	0.38
(1,2598)	1:146:A:MET:HE1	2:642:B:PRO:HB3	8	0.38
(1,2598)	1:146:A:MET:HE2	2:642:B:PRO:HB2	8	0.38
(1,2598)	1:146:A:MET:HE2	2:642:B:PRO:HB3	8	0.38
(1,2598)	1:146:A:MET:HE3	2:642:B:PRO:HB2	8	0.38
(1,2598)	1:146:A:MET:HE3	2:642:B:PRO:HB3	8	0.38
(1,2598)	1:146:A:MET:HE1	2:642:B:PRO:HB2	17	0.38
(1,2598)	1:146:A:MET:HE1	2:642:B:PRO:HB3	17	0.38
(1,2598)	1:146:A:MET:HE2	2:642:B:PRO:HB2	17	0.38
(1,2598)	1:146:A:MET:HE2	2:642:B:PRO:HB3	17	0.38
(1,2598)	1:146:A:MET:HE3	2:642:B:PRO:HB2	17	0.38
(1,2598)	1:146:A:MET:HE3	2:642:B:PRO:HB3	17	0.38
(1,2587)	1:115:A:SER:H	2:659:B:PHE:HD1	15	0.38
(1,2587)	1:115:A:SER:H	2:659:B:PHE:HD2	15	0.38
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG21	2	0.38
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG22	2	0.38
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG23	2	0.38
(1,2524)	2:647:B:VAL:HG11	2:650:B:ASN:HD22	15	0.38
(1,2524)	2:647:B:VAL:HG12	2:650:B:ASN:HD22	15	0.38
(1,2524)	2:647:B:VAL:HG13	2:650:B:ASN:HD22	15	0.38
(1,2523)	2:647:B:VAL:HA	2:649:B:ARG:H	5	0.38
(1,2523)	2:647:B:VAL:HA	2:649:B:ARG:H	12	0.38
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE1	6	0.38
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE2	6	0.38
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE3	6	0.38
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE1	7	0.38
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE2	7	0.38
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE3	7	0.38
(1,2022)	1:94:A:GLN:H	1:94:A:GLN:HG2	2	0.38
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD11	4	0.38
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD12	4	0.38
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD13	4	0.38
(1,1869)	1:75:A:GLN:H	1:75:A:GLN:HE22	6	0.38
(1,1750)	1:56:A:ARG:HA	1:56:A:ARG:HE	8	0.38
(1,1507)	1:13:A:LYS:H	1:13:A:LYS:HG3	17	0.38
(1,1457)	1:6:A:LYS:H	1:6:A:LYS:HG2	7	0.38
(1,1434)	1:161:A:ARG:HD2	1:163:A:GLU:H	1	0.38
(1,1434)	1:161:A:ARG:HD2	1:163:A:GLU:H	8	0.38
(1,1429)	1:143:A:THR:HG21	1:163:A:GLU:HB2	2	0.38
(1,1429)	1:143:A:THR:HG22	1:163:A:GLU:HB2	2	0.38
(1,1429)	1:143:A:THR:HG23	1:163:A:GLU:HB2	2	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1423)	1:55:A:VAL:HB	1:163:A:GLU:H	12	0.38
(1,1404)	1:144:A:GLY:HA2	1:161:A:ARG:H	7	0.38
(1,1391)	1:160:A:LEU:HD11	1:162:A:THR:HA	11	0.38
(1,1391)	1:160:A:LEU:HD12	1:162:A:THR:HA	11	0.38
(1,1391)	1:160:A:LEU:HD13	1:162:A:THR:HA	11	0.38
(1,1363)	1:96:A:ILE:HG21	1:160:A:LEU:HD11	1	0.38
(1,1363)	1:96:A:ILE:HG21	1:160:A:LEU:HD12	1	0.38
(1,1363)	1:96:A:ILE:HG21	1:160:A:LEU:HD13	1	0.38
(1,1363)	1:96:A:ILE:HG22	1:160:A:LEU:HD11	1	0.38
(1,1363)	1:96:A:ILE:HG22	1:160:A:LEU:HD12	1	0.38
(1,1363)	1:96:A:ILE:HG22	1:160:A:LEU:HD13	1	0.38
(1,1363)	1:96:A:ILE:HG23	1:160:A:LEU:HD11	1	0.38
(1,1363)	1:96:A:ILE:HG23	1:160:A:LEU:HD12	1	0.38
(1,1363)	1:96:A:ILE:HG23	1:160:A:LEU:HD13	1	0.38
(1,1349)	1:158:A:ILE:H	1:159:A:ILE:HD11	8	0.38
(1,1349)	1:158:A:ILE:H	1:159:A:ILE:HD12	8	0.38
(1,1349)	1:158:A:ILE:H	1:159:A:ILE:HD13	8	0.38
(1,1349)	1:158:A:ILE:H	1:159:A:ILE:HD11	12	0.38
(1,1349)	1:158:A:ILE:H	1:159:A:ILE:HD12	12	0.38
(1,1349)	1:158:A:ILE:H	1:159:A:ILE:HD13	12	0.38
(1,1346)	1:148:A:GLY:H	1:159:A:ILE:H	13	0.38
(1,1156)	1:136:A:ASP:HB2	1:137:A:ALA:H	14	0.38
(1,1130)	1:131:A:GLN:HE21	1:153:A:ASP:HB2	14	0.38
(1,1130)	1:131:A:GLN:HE21	1:153:A:ASP:HB3	14	0.38
(1,1107)	1:54:A:ARG:HD2	1:126:A:SER:HA	6	0.38
(1,1052)	1:58:A:SER:HB2	1:122:A:LEU:H	8	0.38
(1,1015)	1:116:A:ALA:HB1	1:120:A:GLY:H	9	0.38
(1,1015)	1:116:A:ALA:HB2	1:120:A:GLY:H	9	0.38
(1,1015)	1:116:A:ALA:HB3	1:120:A:GLY:H	9	0.38
(1,1012)	1:116:A:ALA:H	1:119:A:ARG:H	13	0.38
(1,958)	1:108:A:SER:HA	1:110:A:PHE:H	1	0.38
(1,958)	1:108:A:SER:HA	1:110:A:PHE:H	7	0.38
(1,941)	1:106:A:LEU:HD11	1:107:A:ALA:H	13	0.38
(1,941)	1:106:A:LEU:HD12	1:107:A:ALA:H	13	0.38
(1,941)	1:106:A:LEU:HD13	1:107:A:ALA:H	13	0.38
(1,940)	1:106:A:LEU:HG	1:107:A:ALA:H	11	0.38
(1,913)	1:103:A:PHE:H	1:106:A:LEU:HB3	3	0.38
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD11	20	0.38
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD12	20	0.38
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD13	20	0.38
(1,729)	1:89:A:ILE:HG12	1:93:A:ILE:HD11	5	0.38
(1,729)	1:89:A:ILE:HG12	1:93:A:ILE:HD12	5	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,729)	1:89:A:ILE:HG12	1:93:A:ILE:HD13	5	0.38
(1,723)	1:86:A:LEU:HD21	1:89:A:ILE:HB	2	0.38
(1,723)	1:86:A:LEU:HD22	1:89:A:ILE:HB	2	0.38
(1,723)	1:86:A:LEU:HD23	1:89:A:ILE:HB	2	0.38
(1,723)	1:86:A:LEU:HD21	1:89:A:ILE:HB	4	0.38
(1,723)	1:86:A:LEU:HD22	1:89:A:ILE:HB	4	0.38
(1,723)	1:86:A:LEU:HD23	1:89:A:ILE:HB	4	0.38
(1,723)	1:86:A:LEU:HD21	1:89:A:ILE:HB	9	0.38
(1,723)	1:86:A:LEU:HD22	1:89:A:ILE:HB	9	0.38
(1,723)	1:86:A:LEU:HD23	1:89:A:ILE:HB	9	0.38
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB1	8	0.38
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB2	8	0.38
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB3	8	0.38
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB1	14	0.38
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB2	14	0.38
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB3	14	0.38
(1,654)	1:82:A:LYS:HG2	1:84:A:GLU:H	17	0.38
(1,654)	1:82:A:LYS:HG3	1:84:A:GLU:H	17	0.38
(1,618)	1:78:A:ILE:HA	1:80:A:ARG:H	6	0.38
(1,592)	1:75:A:GLN:HB2	1:77:A:LYS:H	6	0.38
(1,576)	1:73:A:TRP:HE1	1:115:A:SER:H	20	0.38
(1,496)	1:62:A:VAL:HG11	1:88:A:LEU:H	1	0.38
(1,496)	1:62:A:VAL:HG12	1:88:A:LEU:H	1	0.38
(1,496)	1:62:A:VAL:HG13	1:88:A:LEU:H	1	0.38
(1,496)	1:62:A:VAL:HG11	1:88:A:LEU:H	4	0.38
(1,496)	1:62:A:VAL:HG12	1:88:A:LEU:H	4	0.38
(1,496)	1:62:A:VAL:HG13	1:88:A:LEU:H	4	0.38
(1,465)	1:60:A:LEU:HB2	1:158:A:ILE:H	10	0.38
(1,457)	1:60:A:LEU:HD11	1:108:A:SER:H	15	0.38
(1,457)	1:60:A:LEU:HD12	1:108:A:SER:H	15	0.38
(1,457)	1:60:A:LEU:HD13	1:108:A:SER:H	15	0.38
(1,388)	1:35:A:GLU:HG2	1:36:A:ARG:H	1	0.38
(1,388)	1:35:A:GLU:HG2	1:36:A:ARG:H	3	0.38
(1,369)	1:33:A:GLN:HG2	1:34:A:TRP:H	5	0.38
(1,366)	1:32:A:SER:H	1:33:A:GLN:HE22	2	0.38
(1,366)	1:32:A:SER:H	1:33:A:GLN:HE21	2	0.38
(1,366)	1:32:A:SER:H	1:33:A:GLN:HE22	4	0.38
(1,366)	1:32:A:SER:H	1:33:A:GLN:HE21	4	0.38
(1,366)	1:32:A:SER:H	1:33:A:GLN:HE22	20	0.38
(1,366)	1:32:A:SER:H	1:33:A:GLN:HE21	20	0.38
(1,355)	1:25:A:PHE:HE1	1:32:A:SER:HB2	17	0.38
(1,355)	1:25:A:PHE:HE2	1:32:A:SER:HB2	17	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,347)	1:31:A:ALA:HB1	1:33:A:GLN:H	19	0.38
(1,347)	1:31:A:ALA:HB2	1:33:A:GLN:H	19	0.38
(1,347)	1:31:A:ALA:HB3	1:33:A:GLN:H	19	0.38
(1,321)	1:25:A:PHE:HZ	1:30:A:ASN:H	14	0.38
(1,320)	1:25:A:PHE:HE1	1:30:A:ASN:H	18	0.38
(1,320)	1:25:A:PHE:HE2	1:30:A:ASN:H	18	0.38
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG21	12	0.38
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG22	12	0.38
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG23	12	0.38
(1,256)	1:23:A:TYR:HE1	1:26:A:ASN:H	20	0.38
(1,256)	1:23:A:TYR:HE2	1:26:A:ASN:H	20	0.38
(1,244)	1:11:A:TRP:H	1:26:A:ASN:HB2	3	0.38
(1,244)	1:11:A:TRP:H	1:26:A:ASN:HB2	7	0.38
(1,242)	1:10:A:GLY:H	1:26:A:ASN:HD21	20	0.38
(1,214)	1:11:A:TRP:HB2	1:25:A:PHE:H	12	0.38
(1,213)	1:11:A:TRP:HA	1:25:A:PHE:H	14	0.38
(1,204)	1:24:A:TYR:HB2	1:33:A:GLN:HE21	4	0.38
(1,204)	1:24:A:TYR:HB2	1:33:A:GLN:HE21	15	0.38
(1,139)	1:21:A:ARG:HD2	1:34:A:TRP:HZ3	18	0.38
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG21	6	0.38
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG22	6	0.38
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG23	6	0.38
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG21	12	0.38
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG22	12	0.38
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG23	12	0.38
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG21	20	0.38
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG22	20	0.38
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG23	20	0.38
(1,56)	1:11:A:TRP:HE1	1:31:A:ALA:HB1	12	0.38
(1,56)	1:11:A:TRP:HE1	1:31:A:ALA:HB2	12	0.38
(1,56)	1:11:A:TRP:HE1	1:31:A:ALA:HB3	12	0.38
(1,52)	1:11:A:TRP:HE1	1:26:A:ASN:HB2	4	0.38
(1,52)	1:11:A:TRP:HE1	1:26:A:ASN:HB3	4	0.38
(1,14)	1:6:A:LYS:HG2	1:7:A:LEU:H	20	0.38
(1,12)	1:5:A:GLU:HB2	1:6:A:LYS:H	3	0.38
(1,12)	1:5:A:GLU:HB2	1:6:A:LYS:H	6	0.38
(1,12)	1:5:A:GLU:HB2	1:6:A:LYS:H	12	0.38
(1,12)	1:5:A:GLU:HB2	1:6:A:LYS:H	15	0.38
(1,12)	1:5:A:GLU:HB2	1:6:A:LYS:H	20	0.38
(3,79)	1:105:A:SER:O	1:109:A:GLN:N	17	0.37
(3,43)	1:72:A:SER:O	1:75:A:GLN:N	6	0.37
(3,9)	1:16:A:SER:O	1:19:A:SER:N	13	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,9)	1:16:A:SER:O	1:19:A:SER:N	15	0.37
(2,93)	1:93:A:ILE:HD11	2:643:B:PRO:HA	13	0.37
(2,93)	1:93:A:ILE:HD12	2:643:B:PRO:HA	13	0.37
(2,93)	1:93:A:ILE:HD13	2:643:B:PRO:HA	13	0.37
(2,92)	1:58:A:SER:H	2:651:B:ILE:HG12	7	0.37
(2,92)	1:58:A:SER:H	2:651:B:ILE:HG13	7	0.37
(2,82)	2:660:B:SEP:HA	2:661:B:PHE:HD1	12	0.37
(2,82)	2:660:B:SEP:HA	2:661:B:PHE:HD2	12	0.37
(2,82)	2:660:B:SEP:HA	2:661:B:PHE:HD1	18	0.37
(2,82)	2:660:B:SEP:HA	2:661:B:PHE:HD2	18	0.37
(2,74)	2:656:B:PHE:HB2	2:659:B:PHE:HD1	10	0.37
(2,74)	2:656:B:PHE:HB2	2:659:B:PHE:HD2	10	0.37
(2,74)	2:656:B:PHE:HB3	2:659:B:PHE:HD1	10	0.37
(2,74)	2:656:B:PHE:HB3	2:659:B:PHE:HD2	10	0.37
(2,58)	1:152:A:THR:HG21	1:157:A:HIS:HB3	5	0.37
(2,58)	1:152:A:THR:HG22	1:157:A:HIS:HB3	5	0.37
(2,58)	1:152:A:THR:HG23	1:157:A:HIS:HB3	5	0.37
(2,58)	1:152:A:THR:HG21	1:157:A:HIS:HB3	7	0.37
(2,58)	1:152:A:THR:HG22	1:157:A:HIS:HB3	7	0.37
(2,58)	1:152:A:THR:HG23	1:157:A:HIS:HB3	7	0.37
(2,42)	1:130:A:MET:HB2	1:134:A:PHE:HD1	12	0.37
(2,42)	1:130:A:MET:HB2	1:134:A:PHE:HD2	12	0.37
(2,38)	1:126:A:SER:H	1:129:A:GLN:HB2	5	0.37
(2,25)	1:88:A:LEU:HG	1:92:A:TYR:H	4	0.37
(2,9)	1:53:A:ALA:H	1:54:A:ARG:HD2	12	0.37
(1,2598)	1:146:A:MET:HE1	2:642:B:PRO:HB2	2	0.37
(1,2598)	1:146:A:MET:HE1	2:642:B:PRO:HB3	2	0.37
(1,2598)	1:146:A:MET:HE2	2:642:B:PRO:HB2	2	0.37
(1,2598)	1:146:A:MET:HE2	2:642:B:PRO:HB3	2	0.37
(1,2598)	1:146:A:MET:HE3	2:642:B:PRO:HB2	2	0.37
(1,2598)	1:146:A:MET:HE3	2:642:B:PRO:HB3	2	0.37
(1,2598)	1:146:A:MET:HE1	2:642:B:PRO:HB2	6	0.37
(1,2598)	1:146:A:MET:HE1	2:642:B:PRO:HB3	6	0.37
(1,2598)	1:146:A:MET:HE2	2:642:B:PRO:HB2	6	0.37
(1,2598)	1:146:A:MET:HE2	2:642:B:PRO:HB3	6	0.37
(1,2598)	1:146:A:MET:HE3	2:642:B:PRO:HB2	6	0.37
(1,2598)	1:146:A:MET:HE3	2:642:B:PRO:HB3	6	0.37
(1,2578)	1:29:A:THR:HG21	2:646:B:GLU:HA	11	0.37
(1,2578)	1:29:A:THR:HG22	2:646:B:GLU:HA	11	0.37
(1,2578)	1:29:A:THR:HG23	2:646:B:GLU:HA	11	0.37
(1,2551)	2:652:B:ASP:H	2:654:B:SER:H	8	0.37
(1,2533)	2:647:B:VAL:H	2:649:B:ARG:H	9	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2384)	1:163:A:GLU:H	1:163:A:GLU:HG3	4	0.37
(1,2384)	1:163:A:GLU:H	1:163:A:GLU:HG3	8	0.37
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE1	9	0.37
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE2	9	0.37
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE3	9	0.37
(1,2158)	1:119:A:ARG:H	1:119:A:ARG:HD2	1	0.37
(1,2033)	1:95:A:LYS:H	1:95:A:LYS:HD2	10	0.37
(1,2033)	1:95:A:LYS:H	1:95:A:LYS:HD2	16	0.37
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD11	5	0.37
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD12	5	0.37
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD13	5	0.37
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD11	9	0.37
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD12	9	0.37
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD13	9	0.37
(1,1625)	1:27:A:HIS:H	1:27:A:HIS:HD1	9	0.37
(1,1457)	1:6:A:LYS:H	1:6:A:LYS:HG2	1	0.37
(1,1423)	1:55:A:VAL:HB	1:163:A:GLU:H	14	0.37
(1,1399)	1:143:A:THR:H	1:161:A:ARG:HD2	5	0.37
(1,1346)	1:148:A:GLY:H	1:159:A:ILE:H	12	0.37
(1,1326)	1:89:A:ILE:HG21	1:158:A:ILE:HB	9	0.37
(1,1326)	1:89:A:ILE:HG22	1:158:A:ILE:HB	9	0.37
(1,1326)	1:89:A:ILE:HG23	1:158:A:ILE:HB	9	0.37
(1,1156)	1:136:A:ASP:HB2	1:137:A:ALA:H	6	0.37
(1,1011)	1:116:A:ALA:HB1	1:119:A:ARG:H	18	0.37
(1,1011)	1:116:A:ALA:HB2	1:119:A:ARG:H	18	0.37
(1,1011)	1:116:A:ALA:HB3	1:119:A:ARG:H	18	0.37
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB1	12	0.37
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB2	12	0.37
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB3	12	0.37
(1,985)	1:61:A:LEU:HD21	1:113:A:CYS:HA	4	0.37
(1,985)	1:61:A:LEU:HD22	1:113:A:CYS:HA	4	0.37
(1,985)	1:61:A:LEU:HD23	1:113:A:CYS:HA	4	0.37
(1,961)	1:108:A:SER:H	1:119:A:ARG:HG2	3	0.37
(1,959)	1:108:A:SER:HA	1:111:A:SER:H	14	0.37
(1,958)	1:108:A:SER:HA	1:110:A:PHE:H	11	0.37
(1,941)	1:106:A:LEU:HD11	1:107:A:ALA:H	1	0.37
(1,941)	1:106:A:LEU:HD12	1:107:A:ALA:H	1	0.37
(1,941)	1:106:A:LEU:HD13	1:107:A:ALA:H	1	0.37
(1,913)	1:103:A:PHE:H	1:106:A:LEU:HB3	6	0.37
(1,913)	1:103:A:PHE:H	1:106:A:LEU:HB3	16	0.37
(1,888)	1:103:A:PHE:HE1	1:120:A:GLY:H	15	0.37
(1,888)	1:103:A:PHE:HE2	1:120:A:GLY:H	15	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,862)	1:101:A:GLU:HG2	1:102:A:ASP:H	15	0.37
(1,811)	1:94:A:GLN:H	1:96:A:ILE:H	17	0.37
(1,753)	1:90:A:ASN:HD22	1:91:A:GLY:H	7	0.37
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB1	1	0.37
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB2	1	0.37
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB3	1	0.37
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB1	2	0.37
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB2	2	0.37
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB3	2	0.37
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB1	6	0.37
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB2	6	0.37
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB3	6	0.37
(1,592)	1:75:A:GLN:HB2	1:77:A:LYS:H	10	0.37
(1,578)	1:73:A:TRP:HE1	1:116:A:ALA:HB1	16	0.37
(1,578)	1:73:A:TRP:HE1	1:116:A:ALA:HB2	16	0.37
(1,578)	1:73:A:TRP:HE1	1:116:A:ALA:HB3	16	0.37
(1,569)	1:73:A:TRP:HE1	1:74:A:ARG:HB2	9	0.37
(1,541)	1:67:A:SER:HB3	1:70:A:PRO:HA	14	0.37
(1,521)	1:64:A:HIS:H	1:66:A:GLN:H	4	0.37
(1,521)	1:64:A:HIS:H	1:66:A:GLN:H	12	0.37
(1,521)	1:64:A:HIS:H	1:66:A:GLN:H	20	0.37
(1,496)	1:62:A:VAL:HG11	1:88:A:LEU:H	7	0.37
(1,496)	1:62:A:VAL:HG12	1:88:A:LEU:H	7	0.37
(1,496)	1:62:A:VAL:HG13	1:88:A:LEU:H	7	0.37
(1,496)	1:62:A:VAL:HG11	1:88:A:LEU:H	13	0.37
(1,496)	1:62:A:VAL:HG12	1:88:A:LEU:H	13	0.37
(1,496)	1:62:A:VAL:HG13	1:88:A:LEU:H	13	0.37
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD11	4	0.37
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD12	4	0.37
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD13	4	0.37
(1,435)	1:58:A:SER:HA	1:122:A:LEU:HG	19	0.37
(1,397)	1:54:A:ARG:HG2	1:126:A:SER:H	5	0.37
(1,369)	1:33:A:GLN:HG2	1:34:A:TRP:H	17	0.37
(1,347)	1:31:A:ALA:HB1	1:33:A:GLN:H	3	0.37
(1,347)	1:31:A:ALA:HB2	1:33:A:GLN:H	3	0.37
(1,347)	1:31:A:ALA:HB3	1:33:A:GLN:H	3	0.37
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB1	14	0.37
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB2	14	0.37
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB3	14	0.37
(1,311)	1:27:A:HIS:HB2	1:29:A:THR:H	1	0.37
(1,311)	1:27:A:HIS:HB2	1:29:A:THR:H	6	0.37
(1,311)	1:27:A:HIS:HB2	1:29:A:THR:H	7	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,302)	1:27:A:HIS:HD2	1:28:A:ILE:H	2	0.37
(1,93)	1:14:A:ARG:H	1:22:A:VAL:HA	8	0.37
(1,75)	1:13:A:LYS:HA	1:23:A:TYR:H	4	0.37
(1,56)	1:11:A:TRP:HE1	1:31:A:ALA:HB1	3	0.37
(1,56)	1:11:A:TRP:HE1	1:31:A:ALA:HB2	3	0.37
(1,56)	1:11:A:TRP:HE1	1:31:A:ALA:HB3	3	0.37
(1,14)	1:6:A:LYS:HG2	1:7:A:LEU:H	7	0.37
(1,14)	1:6:A:LYS:HG2	1:7:A:LEU:H	10	0.37
(1,12)	1:5:A:GLU:HB2	1:6:A:LYS:H	11	0.37
(1,11)	1:4:A:GLU:H	1:6:A:LYS:H	1	0.37
(3,79)	1:105:A:SER:O	1:109:A:GLN:N	12	0.36
(3,43)	1:72:A:SER:O	1:75:A:GLN:N	15	0.36
(3,35)	1:62:A:VAL:N	1:156:A:ILE:O	6	0.36
(2,106)	1:139:A:PHE:H	2:656:B:PHE:HB2	15	0.36
(2,105)	1:138:A:SER:H	2:656:B:PHE:HD1	5	0.36
(2,105)	1:138:A:SER:H	2:656:B:PHE:HD2	5	0.36
(2,93)	1:93:A:ILE:HD11	2:643:B:PRO:HA	11	0.36
(2,93)	1:93:A:ILE:HD12	2:643:B:PRO:HA	11	0.36
(2,93)	1:93:A:ILE:HD13	2:643:B:PRO:HA	11	0.36
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG21	12	0.36
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG22	12	0.36
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG23	12	0.36
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG11	19	0.36
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG12	19	0.36
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG13	19	0.36
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG21	19	0.36
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG22	19	0.36
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG23	19	0.36
(2,79)	2:659:B:PHE:HE1	2:661:B:PHE:H	8	0.36
(2,79)	2:659:B:PHE:HE2	2:661:B:PHE:H	8	0.36
(2,76)	2:656:B:PHE:HE1	2:659:B:PHE:HE1	5	0.36
(2,76)	2:656:B:PHE:HE1	2:659:B:PHE:HE2	5	0.36
(2,76)	2:656:B:PHE:HE2	2:659:B:PHE:HE1	5	0.36
(2,76)	2:656:B:PHE:HE2	2:659:B:PHE:HE2	5	0.36
(2,66)	2:645:B:GLN:H	2:648:B:ILE:H	2	0.36
(2,25)	1:88:A:LEU:HG	1:92:A:TYR:H	9	0.36
(2,20)	1:68:A:ARG:H	1:153:A:ASP:HB2	14	0.36
(2,20)	1:68:A:ARG:H	1:153:A:ASP:HB3	14	0.36
(2,4)	1:21:A:ARG:HE	1:22:A:VAL:H	1	0.36
(1,2587)	1:115:A:SER:H	2:659:B:PHE:HD1	9	0.36
(1,2587)	1:115:A:SER:H	2:659:B:PHE:HD2	9	0.36
(1,2557)	2:654:B:SER:H	2:655:B:GLU:H	3	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2557)	2:654:B:SER:H	2:655:B:GLU:H	5	0.36
(1,2209)	1:131:A:GLN:HA	1:131:A:GLN:HE22	11	0.36
(1,2033)	1:95:A:LYS:H	1:95:A:LYS:HD2	9	0.36
(1,2033)	1:95:A:LYS:H	1:95:A:LYS:HD2	11	0.36
(1,2033)	1:95:A:LYS:H	1:95:A:LYS:HD2	20	0.36
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD11	20	0.36
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD12	20	0.36
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD13	20	0.36
(1,1750)	1:56:A:ARG:HA	1:56:A:ARG:HE	2	0.36
(1,1625)	1:27:A:HIS:H	1:27:A:HIS:HD1	15	0.36
(1,1571)	1:21:A:ARG:H	1:21:A:ARG:HD2	14	0.36
(1,1456)	1:6:A:LYS:H	1:6:A:LYS:HE2	15	0.36
(1,1434)	1:161:A:ARG:HD2	1:163:A:GLU:H	12	0.36
(1,1423)	1:55:A:VAL:HB	1:163:A:GLU:H	10	0.36
(1,1382)	1:159:A:ILE:HG12	1:160:A:LEU:H	20	0.36
(1,1369)	1:104:A:GLU:H	1:160:A:LEU:HD11	20	0.36
(1,1369)	1:104:A:GLU:H	1:160:A:LEU:HD12	20	0.36
(1,1369)	1:104:A:GLU:H	1:160:A:LEU:HD13	20	0.36
(1,1345)	1:147:A:SER:H	1:159:A:ILE:HB	3	0.36
(1,1299)	1:152:A:THR:H	1:156:A:ILE:HG21	9	0.36
(1,1299)	1:152:A:THR:H	1:156:A:ILE:HG22	9	0.36
(1,1299)	1:152:A:THR:H	1:156:A:ILE:HG23	9	0.36
(1,1263)	1:151:A:PHE:H	1:156:A:ILE:HG21	16	0.36
(1,1263)	1:151:A:PHE:H	1:156:A:ILE:HG22	16	0.36
(1,1263)	1:151:A:PHE:H	1:156:A:ILE:HG23	16	0.36
(1,1262)	1:151:A:PHE:H	1:156:A:ILE:HA	19	0.36
(1,1193)	1:141:A:LEU:HD11	1:148:A:GLY:H	11	0.36
(1,1193)	1:141:A:LEU:HD12	1:148:A:GLY:H	11	0.36
(1,1193)	1:141:A:LEU:HD13	1:148:A:GLY:H	11	0.36
(1,1177)	1:137:A:ALA:HB1	1:141:A:LEU:H	16	0.36
(1,1177)	1:137:A:ALA:HB2	1:141:A:LEU:H	16	0.36
(1,1177)	1:137:A:ALA:HB3	1:141:A:LEU:H	16	0.36
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB1	5	0.36
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB2	5	0.36
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB3	5	0.36
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB1	7	0.36
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB2	7	0.36
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB3	7	0.36
(1,1152)	1:135:A:GLU:HG2	1:136:A:ASP:H	19	0.36
(1,1109)	1:126:A:SER:HA	1:139:A:PHE:HD1	9	0.36
(1,1109)	1:126:A:SER:HA	1:139:A:PHE:HD2	9	0.36
(1,1015)	1:116:A:ALA:HB1	1:120:A:GLY:H	19	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1015)	1:116:A:ALA:HB2	1:120:A:GLY:H	19	0.36
(1,1015)	1:116:A:ALA:HB3	1:120:A:GLY:H	19	0.36
(1,1012)	1:116:A:ALA:H	1:119:A:ARG:H	18	0.36
(1,1000)	1:113:A:CYS:H	1:116:A:ALA:H	7	0.36
(1,995)	1:108:A:SER:HA	1:116:A:ALA:H	3	0.36
(1,970)	1:108:A:SER:H	1:110:A:PHE:H	10	0.36
(1,961)	1:108:A:SER:H	1:119:A:ARG:HG2	9	0.36
(1,941)	1:106:A:LEU:HD11	1:107:A:ALA:H	17	0.36
(1,941)	1:106:A:LEU:HD12	1:107:A:ALA:H	17	0.36
(1,941)	1:106:A:LEU:HD13	1:107:A:ALA:H	17	0.36
(1,910)	1:102:A:ASP:H	1:106:A:LEU:HB3	17	0.36
(1,888)	1:103:A:PHE:HE1	1:120:A:GLY:H	3	0.36
(1,888)	1:103:A:PHE:HE2	1:120:A:GLY:H	3	0.36
(1,841)	1:97:A:LYS:HB3	1:98:A:SER:H	17	0.36
(1,811)	1:94:A:GLN:H	1:96:A:ILE:H	20	0.36
(1,747)	1:90:A:ASN:HA	1:158:A:ILE:HD11	18	0.36
(1,747)	1:90:A:ASN:HA	1:158:A:ILE:HD12	18	0.36
(1,747)	1:90:A:ASN:HA	1:158:A:ILE:HD13	18	0.36
(1,728)	1:89:A:ILE:HD11	1:92:A:TYR:HE1	16	0.36
(1,728)	1:89:A:ILE:HD11	1:92:A:TYR:HE2	16	0.36
(1,728)	1:89:A:ILE:HD12	1:92:A:TYR:HE1	16	0.36
(1,728)	1:89:A:ILE:HD12	1:92:A:TYR:HE2	16	0.36
(1,728)	1:89:A:ILE:HD13	1:92:A:TYR:HE1	16	0.36
(1,728)	1:89:A:ILE:HD13	1:92:A:TYR:HE2	16	0.36
(1,723)	1:86:A:LEU:HD21	1:89:A:ILE:HB	17	0.36
(1,723)	1:86:A:LEU:HD22	1:89:A:ILE:HB	17	0.36
(1,723)	1:86:A:LEU:HD23	1:89:A:ILE:HB	17	0.36
(1,591)	1:74:A:ARG:HE	1:75:A:GLN:H	12	0.36
(1,554)	1:70:A:PRO:HG3	1:71:A:SER:H	7	0.36
(1,554)	1:70:A:PRO:HG3	1:71:A:SER:H	8	0.36
(1,538)	1:66:A:GLN:HG2	1:67:A:SER:H	17	0.36
(1,520)	1:64:A:HIS:HE1	1:66:A:GLN:HG2	7	0.36
(1,508)	1:62:A:VAL:H	1:156:A:ILE:HB	13	0.36
(1,496)	1:62:A:VAL:HG11	1:88:A:LEU:H	14	0.36
(1,496)	1:62:A:VAL:HG12	1:88:A:LEU:H	14	0.36
(1,496)	1:62:A:VAL:HG13	1:88:A:LEU:H	14	0.36
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD11	17	0.36
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD12	17	0.36
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD13	17	0.36
(1,465)	1:60:A:LEU:HB2	1:158:A:ILE:H	17	0.36
(1,414)	1:56:A:ARG:H	1:124:A:ALA:HB1	9	0.36
(1,414)	1:56:A:ARG:H	1:124:A:ALA:HB2	9	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,414)	1:56:A:ARG:H	1:124:A:ALA:HB3	9	0.36
(1,397)	1:54:A:ARG:HG2	1:126:A:SER:H	20	0.36
(1,366)	1:32:A:SER:H	1:33:A:GLN:HE22	6	0.36
(1,366)	1:32:A:SER:H	1:33:A:GLN:HE21	6	0.36
(1,366)	1:32:A:SER:H	1:33:A:GLN:HE22	17	0.36
(1,366)	1:32:A:SER:H	1:33:A:GLN:HE21	17	0.36
(1,366)	1:32:A:SER:H	1:33:A:GLN:HE22	19	0.36
(1,366)	1:32:A:SER:H	1:33:A:GLN:HE21	19	0.36
(1,364)	1:24:A:TYR:HD1	1:33:A:GLN:H	10	0.36
(1,364)	1:24:A:TYR:HD2	1:33:A:GLN:H	10	0.36
(1,347)	1:31:A:ALA:HB1	1:33:A:GLN:H	7	0.36
(1,347)	1:31:A:ALA:HB2	1:33:A:GLN:H	7	0.36
(1,347)	1:31:A:ALA:HB3	1:33:A:GLN:H	7	0.36
(1,347)	1:31:A:ALA:HB1	1:33:A:GLN:H	15	0.36
(1,347)	1:31:A:ALA:HB2	1:33:A:GLN:H	15	0.36
(1,347)	1:31:A:ALA:HB3	1:33:A:GLN:H	15	0.36
(1,311)	1:27:A:HIS:HB2	1:29:A:THR:H	15	0.36
(1,311)	1:27:A:HIS:HB2	1:29:A:THR:H	17	0.36
(1,262)	1:25:A:PHE:HE1	1:26:A:ASN:HA	2	0.36
(1,262)	1:25:A:PHE:HE2	1:26:A:ASN:HA	2	0.36
(1,213)	1:11:A:TRP:HA	1:25:A:PHE:H	4	0.36
(1,208)	1:24:A:TYR:H	1:34:A:TRP:HB3	16	0.36
(1,180)	1:23:A:TYR:HD1	1:33:A:GLN:HA	15	0.36
(1,180)	1:23:A:TYR:HD2	1:33:A:GLN:HA	15	0.36
(1,138)	1:21:A:ARG:HE	1:34:A:TRP:HH2	10	0.36
(1,129)	1:16:A:SER:HB2	1:21:A:ARG:H	16	0.36
(1,123)	1:15:A:MET:HE1	1:20:A:GLY:H	11	0.36
(1,123)	1:15:A:MET:HE2	1:20:A:GLY:H	11	0.36
(1,123)	1:15:A:MET:HE3	1:20:A:GLY:H	11	0.36
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG21	19	0.36
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG22	19	0.36
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG23	19	0.36
(1,93)	1:14:A:ARG:H	1:22:A:VAL:HA	3	0.36
(1,86)	1:13:A:LYS:HE2	1:14:A:ARG:H	3	0.36
(1,14)	1:6:A:LYS:HG2	1:7:A:LEU:H	11	0.36
(1,11)	1:4:A:GLU:H	1:6:A:LYS:H	13	0.36
(3,45)	1:70:A:PRO:O	1:78:A:ILE:N	11	0.35
(3,44)	1:72:A:SER:O	1:75:A:GLN:H	20	0.35
(3,35)	1:62:A:VAL:N	1:156:A:ILE:O	12	0.35
(3,35)	1:62:A:VAL:N	1:156:A:ILE:O	13	0.35
(3,25)	1:55:A:VAL:N	1:125:A:PHE:O	13	0.35
(2,97)	1:94:A:GLN:HE21	2:640:B:LEU:HG	7	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,89)	1:55:A:VAL:H	2:651:B:ILE:HG12	16	0.35
(2,89)	1:55:A:VAL:H	2:651:B:ILE:HG13	16	0.35
(2,74)	2:656:B:PHE:HB2	2:659:B:PHE:HD1	20	0.35
(2,74)	2:656:B:PHE:HB2	2:659:B:PHE:HD2	20	0.35
(2,74)	2:656:B:PHE:HB3	2:659:B:PHE:HD1	20	0.35
(2,74)	2:656:B:PHE:HB3	2:659:B:PHE:HD2	20	0.35
(2,26)	1:94:A:GLN:HE21	1:97:A:LYS:HB3	6	0.35
(1,2588)	1:122:A:LEU:H	2:656:B:PHE:HE1	4	0.35
(1,2588)	1:122:A:LEU:H	2:656:B:PHE:HE2	4	0.35
(1,2586)	1:115:A:SER:H	2:659:B:PHE:HE1	13	0.35
(1,2586)	1:115:A:SER:H	2:659:B:PHE:HE2	13	0.35
(1,2557)	2:654:B:SER:H	2:655:B:GLU:H	7	0.35
(1,2158)	1:119:A:ARG:H	1:119:A:ARG:HD2	8	0.35
(1,2033)	1:95:A:LYS:H	1:95:A:LYS:HD2	1	0.35
(1,2022)	1:94:A:GLN:H	1:94:A:GLN:HG2	17	0.35
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD11	7	0.35
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD12	7	0.35
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD13	7	0.35
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD11	17	0.35
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD12	17	0.35
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD13	17	0.35
(1,1913)	1:82:A:LYS:H	1:82:A:LYS:HD2	9	0.35
(1,1913)	1:82:A:LYS:H	1:82:A:LYS:HD2	18	0.35
(1,1869)	1:75:A:GLN:H	1:75:A:GLN:HE22	20	0.35
(1,1750)	1:56:A:ARG:HA	1:56:A:ARG:HE	14	0.35
(1,1747)	1:56:A:ARG:H	1:56:A:ARG:HD2	7	0.35
(1,1747)	1:56:A:ARG:H	1:56:A:ARG:HD2	14	0.35
(1,1625)	1:27:A:HIS:H	1:27:A:HIS:HD1	10	0.35
(1,1625)	1:27:A:HIS:H	1:27:A:HIS:HD1	11	0.35
(1,1457)	1:6:A:LYS:H	1:6:A:LYS:HG2	9	0.35
(1,1382)	1:159:A:ILE:HG12	1:160:A:LEU:H	2	0.35
(1,1346)	1:148:A:GLY:H	1:159:A:ILE:H	5	0.35
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG21	8	0.35
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG22	8	0.35
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG23	8	0.35
(1,1276)	1:63:A:LYS:HA	1:155:A:GLY:HA2	4	0.35
(1,1262)	1:151:A:PHE:H	1:156:A:ILE:HA	9	0.35
(1,1212)	1:146:A:MET:HG2	1:160:A:LEU:HG	14	0.35
(1,1206)	1:145:A:GLU:HB3	1:146:A:MET:HB2	8	0.35
(1,1161)	1:136:A:ASP:HB2	1:138:A:SER:H	12	0.35
(1,1156)	1:136:A:ASP:HB2	1:137:A:ALA:H	12	0.35
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB1	3	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB2	3	0.35
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB3	3	0.35
(1,1130)	1:131:A:GLN:HE21	1:153:A:ASP:HB2	1	0.35
(1,1130)	1:131:A:GLN:HE21	1:153:A:ASP:HB3	1	0.35
(1,1112)	1:126:A:SER:H	1:129:A:GLN:HE21	12	0.35
(1,1032)	1:107:A:ALA:HB1	1:119:A:ARG:H	4	0.35
(1,1032)	1:107:A:ALA:HB2	1:119:A:ARG:H	4	0.35
(1,1032)	1:107:A:ALA:HB3	1:119:A:ARG:H	4	0.35
(1,1015)	1:116:A:ALA:HB1	1:120:A:GLY:H	1	0.35
(1,1015)	1:116:A:ALA:HB2	1:120:A:GLY:H	1	0.35
(1,1015)	1:116:A:ALA:HB3	1:120:A:GLY:H	1	0.35
(1,1011)	1:116:A:ALA:HB1	1:119:A:ARG:H	3	0.35
(1,1011)	1:116:A:ALA:HB2	1:119:A:ARG:H	3	0.35
(1,1011)	1:116:A:ALA:HB3	1:119:A:ARG:H	3	0.35
(1,1011)	1:116:A:ALA:HB1	1:119:A:ARG:H	17	0.35
(1,1011)	1:116:A:ALA:HB2	1:119:A:ARG:H	17	0.35
(1,1011)	1:116:A:ALA:HB3	1:119:A:ARG:H	17	0.35
(1,995)	1:108:A:SER:HA	1:116:A:ALA:H	9	0.35
(1,985)	1:61:A:LEU:HD21	1:113:A:CYS:HA	5	0.35
(1,985)	1:61:A:LEU:HD22	1:113:A:CYS:HA	5	0.35
(1,985)	1:61:A:LEU:HD23	1:113:A:CYS:HA	5	0.35
(1,941)	1:106:A:LEU:HD11	1:107:A:ALA:H	9	0.35
(1,941)	1:106:A:LEU:HD12	1:107:A:ALA:H	9	0.35
(1,941)	1:106:A:LEU:HD13	1:107:A:ALA:H	9	0.35
(1,913)	1:103:A:PHE:H	1:106:A:LEU:HB3	18	0.35
(1,828)	1:96:A:ILE:H	1:146:A:MET:HE1	14	0.35
(1,828)	1:96:A:ILE:H	1:146:A:MET:HE2	14	0.35
(1,828)	1:96:A:ILE:H	1:146:A:MET:HE3	14	0.35
(1,753)	1:90:A:ASN:HD22	1:91:A:GLY:H	9	0.35
(1,747)	1:90:A:ASN:HA	1:158:A:ILE:HD11	3	0.35
(1,747)	1:90:A:ASN:HA	1:158:A:ILE:HD12	3	0.35
(1,747)	1:90:A:ASN:HA	1:158:A:ILE:HD13	3	0.35
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB1	15	0.35
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB2	15	0.35
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB3	15	0.35
(1,672)	1:64:A:HIS:HD2	1:85:A:ALA:H	15	0.35
(1,669)	1:84:A:GLU:H	1:87:A:GLU:H	17	0.35
(1,599)	1:70:A:PRO:HB2	1:78:A:ILE:H	18	0.35
(1,551)	1:70:A:PRO:HB3	1:71:A:SER:H	7	0.35
(1,541)	1:67:A:SER:HB3	1:70:A:PRO:HA	13	0.35
(1,527)	1:66:A:GLN:HG2	1:81:A:THR:HG21	11	0.35
(1,527)	1:66:A:GLN:HG2	1:81:A:THR:HG22	11	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,527)	1:66:A:GLN:HG2	1:81:A:THR:HG23	11	0.35
(1,521)	1:64:A:HIS:H	1:66:A:GLN:H	6	0.35
(1,521)	1:64:A:HIS:H	1:66:A:GLN:H	9	0.35
(1,515)	1:63:A:LYS:H	1:156:A:ILE:H	3	0.35
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB1	9	0.35
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB2	9	0.35
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB3	9	0.35
(1,373)	1:34:A:TRP:HD1	1:35:A:GLU:H	12	0.35
(1,369)	1:33:A:GLN:HG2	1:34:A:TRP:H	15	0.35
(1,364)	1:24:A:TYR:HD1	1:33:A:GLN:H	8	0.35
(1,364)	1:24:A:TYR:HD2	1:33:A:GLN:H	8	0.35
(1,355)	1:25:A:PHE:HE1	1:32:A:SER:HB2	1	0.35
(1,355)	1:25:A:PHE:HE2	1:32:A:SER:HB2	1	0.35
(1,355)	1:25:A:PHE:HE1	1:32:A:SER:HB2	9	0.35
(1,355)	1:25:A:PHE:HE2	1:32:A:SER:HB2	9	0.35
(1,347)	1:31:A:ALA:HB1	1:33:A:GLN:H	9	0.35
(1,347)	1:31:A:ALA:HB2	1:33:A:GLN:H	9	0.35
(1,347)	1:31:A:ALA:HB3	1:33:A:GLN:H	9	0.35
(1,347)	1:31:A:ALA:HB1	1:33:A:GLN:H	10	0.35
(1,347)	1:31:A:ALA:HB2	1:33:A:GLN:H	10	0.35
(1,347)	1:31:A:ALA:HB3	1:33:A:GLN:H	10	0.35
(1,311)	1:27:A:HIS:HB2	1:29:A:THR:H	18	0.35
(1,311)	1:27:A:HIS:HB2	1:29:A:THR:H	20	0.35
(1,287)	1:26:A:ASN:H	1:32:A:SER:HB2	19	0.35
(1,223)	1:14:A:ARG:HB2	1:25:A:PHE:H	13	0.35
(1,214)	1:11:A:TRP:HB2	1:25:A:PHE:H	16	0.35
(1,213)	1:11:A:TRP:HA	1:25:A:PHE:H	19	0.35
(1,198)	1:23:A:TYR:HE1	1:24:A:TYR:H	20	0.35
(1,198)	1:23:A:TYR:HE2	1:24:A:TYR:H	20	0.35
(1,194)	1:13:A:LYS:HG2	1:24:A:TYR:HA	4	0.35
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG11	5	0.35
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG12	5	0.35
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG13	5	0.35
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG11	5	0.35
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG12	5	0.35
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG13	5	0.35
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG11	5	0.35
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG12	5	0.35
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG13	5	0.35
(1,138)	1:21:A:ARG:HE	1:34:A:TRP:HH2	6	0.35
(1,111)	1:15:A:MET:H	1:23:A:TYR:HD1	8	0.35
(1,111)	1:15:A:MET:H	1:23:A:TYR:HD2	8	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,75)	1:13:A:LYS:HA	1:23:A:TYR:H	3	0.35
(1,69)	1:7:A:LEU:HD21	1:13:A:LYS:HE2	14	0.35
(1,69)	1:7:A:LEU:HD22	1:13:A:LYS:HE2	14	0.35
(1,69)	1:7:A:LEU:HD23	1:13:A:LYS:HE2	14	0.35
(1,69)	1:7:A:LEU:HD11	1:13:A:LYS:HE2	14	0.35
(1,69)	1:7:A:LEU:HD12	1:13:A:LYS:HE2	14	0.35
(1,69)	1:7:A:LEU:HD13	1:13:A:LYS:HE2	14	0.35
(1,12)	1:5:A:GLU:HB2	1:6:A:LYS:H	10	0.35
(1,11)	1:4:A:GLU:H	1:6:A:LYS:H	3	0.35
(1,11)	1:4:A:GLU:H	1:6:A:LYS:H	9	0.35
(1,7)	1:3:A:ASP:HA	1:4:A:GLU:H	1	0.35
(3,79)	1:105:A:SER:O	1:109:A:GLN:N	2	0.34
(3,79)	1:105:A:SER:O	1:109:A:GLN:N	7	0.34
(3,79)	1:105:A:SER:O	1:109:A:GLN:N	11	0.34
(3,71)	1:94:A:GLN:O	1:98:A:SER:N	14	0.34
(3,44)	1:72:A:SER:O	1:75:A:GLN:H	16	0.34
(3,43)	1:72:A:SER:O	1:75:A:GLN:N	4	0.34
(3,10)	1:16:A:SER:O	1:19:A:SER:H	19	0.34
(3,9)	1:16:A:SER:O	1:19:A:SER:N	5	0.34
(2,113)	1:162:A:THR:H	2:651:B:ILE:HG12	1	0.34
(2,113)	1:162:A:THR:H	2:651:B:ILE:HG13	1	0.34
(2,106)	1:139:A:PHE:H	2:656:B:PHE:HB2	13	0.34
(2,103)	1:137:A:ALA:H	2:656:B:PHE:HB2	7	0.34
(2,97)	1:94:A:GLN:HE21	2:640:B:LEU:HG	9	0.34
(2,82)	2:660:B:SEP:HA	2:661:B:PHE:HD1	5	0.34
(2,82)	2:660:B:SEP:HA	2:661:B:PHE:HD2	5	0.34
(2,45)	1:131:A:GLN:HE21	1:152:A:THR:HB	20	0.34
(2,25)	1:88:A:LEU:HG	1:92:A:TYR:H	7	0.34
(1,2597)	1:138:A:SER:H	2:656:B:PHE:HB2	2	0.34
(1,2590)	1:122:A:LEU:HD21	2:656:B:PHE:HD1	13	0.34
(1,2590)	1:122:A:LEU:HD21	2:656:B:PHE:HD2	13	0.34
(1,2590)	1:122:A:LEU:HD22	2:656:B:PHE:HD1	13	0.34
(1,2590)	1:122:A:LEU:HD22	2:656:B:PHE:HD2	13	0.34
(1,2590)	1:122:A:LEU:HD23	2:656:B:PHE:HD1	13	0.34
(1,2590)	1:122:A:LEU:HD23	2:656:B:PHE:HD2	13	0.34
(1,2582)	1:34:A:TRP:HE1	2:642:B:PRO:HB2	1	0.34
(1,2582)	1:34:A:TRP:HE1	2:642:B:PRO:HB3	1	0.34
(1,2575)	1:21:A:ARG:H	2:641:B:TPO:HG21	2	0.34
(1,2575)	1:21:A:ARG:H	2:641:B:TPO:HG22	2	0.34
(1,2575)	1:21:A:ARG:H	2:641:B:TPO:HG23	2	0.34
(1,2568)	2:658:B:GLY:H	2:659:B:PHE:HD1	5	0.34
(1,2568)	2:658:B:GLY:H	2:659:B:PHE:HD2	5	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2557)	2:654:B:SER:H	2:655:B:GLU:H	11	0.34
(1,2510)	2:645:B:GLN:H	2:647:B:VAL:H	1	0.34
(1,2384)	1:163:A:GLU:H	1:163:A:GLU:HG3	5	0.34
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE1	3	0.34
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE2	3	0.34
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE3	3	0.34
(1,2161)	1:119:A:ARG:H	1:119:A:ARG:HD3	17	0.34
(1,2158)	1:119:A:ARG:H	1:119:A:ARG:HD2	2	0.34
(1,2157)	1:119:A:ARG:H	1:119:A:ARG:HG2	13	0.34
(1,2033)	1:95:A:LYS:H	1:95:A:LYS:HD2	5	0.34
(1,2033)	1:95:A:LYS:H	1:95:A:LYS:HD2	14	0.34
(1,2033)	1:95:A:LYS:H	1:95:A:LYS:HD2	19	0.34
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD11	6	0.34
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD12	6	0.34
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD13	6	0.34
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD11	7	0.34
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD12	7	0.34
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD13	7	0.34
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD11	17	0.34
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD12	17	0.34
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD13	17	0.34
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD11	11	0.34
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD12	11	0.34
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD13	11	0.34
(1,1747)	1:56:A:ARG:H	1:56:A:ARG:HD2	12	0.34
(1,1625)	1:27:A:HIS:H	1:27:A:HIS:HD1	16	0.34
(1,1625)	1:27:A:HIS:H	1:27:A:HIS:HD1	17	0.34
(1,1455)	1:6:A:LYS:H	1:6:A:LYS:HB3	11	0.34
(1,1299)	1:152:A:THR:H	1:156:A:ILE:HG21	3	0.34
(1,1299)	1:152:A:THR:H	1:156:A:ILE:HG22	3	0.34
(1,1299)	1:152:A:THR:H	1:156:A:ILE:HG23	3	0.34
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG21	13	0.34
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG22	13	0.34
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG23	13	0.34
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG21	13	0.34
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG22	13	0.34
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG23	13	0.34
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG21	13	0.34
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG22	13	0.34
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG23	13	0.34
(1,1206)	1:145:A:GLU:HB3	1:146:A:MET:HB2	2	0.34
(1,1206)	1:145:A:GLU:HB3	1:146:A:MET:HB2	19	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1199)	1:142:A:ARG:HG2	1:143:A:THR:H	7	0.34
(1,1161)	1:136:A:ASP:HB2	1:138:A:SER:H	3	0.34
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE1	4	0.34
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE2	4	0.34
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE3	4	0.34
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE1	4	0.34
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE2	4	0.34
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE3	4	0.34
(1,1032)	1:107:A:ALA:HB1	1:119:A:ARG:H	9	0.34
(1,1032)	1:107:A:ALA:HB2	1:119:A:ARG:H	9	0.34
(1,1032)	1:107:A:ALA:HB3	1:119:A:ARG:H	9	0.34
(1,1015)	1:116:A:ALA:HB1	1:120:A:GLY:H	17	0.34
(1,1015)	1:116:A:ALA:HB2	1:120:A:GLY:H	17	0.34
(1,1015)	1:116:A:ALA:HB3	1:120:A:GLY:H	17	0.34
(1,1012)	1:116:A:ALA:H	1:119:A:ARG:H	8	0.34
(1,1011)	1:116:A:ALA:HB1	1:119:A:ARG:H	1	0.34
(1,1011)	1:116:A:ALA:HB2	1:119:A:ARG:H	1	0.34
(1,1011)	1:116:A:ALA:HB3	1:119:A:ARG:H	1	0.34
(1,970)	1:108:A:SER:H	1:110:A:PHE:H	3	0.34
(1,958)	1:108:A:SER:HA	1:110:A:PHE:H	13	0.34
(1,940)	1:106:A:LEU:HG	1:107:A:ALA:H	14	0.34
(1,868)	1:60:A:LEU:HD21	1:103:A:PHE:HE1	18	0.34
(1,868)	1:60:A:LEU:HD21	1:103:A:PHE:HE2	18	0.34
(1,868)	1:60:A:LEU:HD22	1:103:A:PHE:HE1	18	0.34
(1,868)	1:60:A:LEU:HD22	1:103:A:PHE:HE2	18	0.34
(1,868)	1:60:A:LEU:HD23	1:103:A:PHE:HE1	18	0.34
(1,868)	1:60:A:LEU:HD23	1:103:A:PHE:HE2	18	0.34
(1,828)	1:96:A:ILE:H	1:146:A:MET:HE1	1	0.34
(1,828)	1:96:A:ILE:H	1:146:A:MET:HE2	1	0.34
(1,828)	1:96:A:ILE:H	1:146:A:MET:HE3	1	0.34
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD11	11	0.34
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD12	11	0.34
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD13	11	0.34
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD11	11	0.34
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD12	11	0.34
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD13	11	0.34
(1,764)	1:88:A:LEU:HA	1:92:A:TYR:H	14	0.34
(1,753)	1:90:A:ASN:HD22	1:91:A:GLY:H	12	0.34
(1,743)	1:89:A:ILE:HG13	1:90:A:ASN:H	10	0.34
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB1	7	0.34
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB2	7	0.34
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB3	7	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB1	12	0.34
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB2	12	0.34
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB3	12	0.34
(1,663)	1:82:A:LYS:HB3	1:83:A:GLU:H	6	0.34
(1,663)	1:82:A:LYS:HB3	1:83:A:GLU:H	12	0.34
(1,659)	1:81:A:THR:HA	1:83:A:GLU:H	17	0.34
(1,554)	1:70:A:PRO:HG3	1:71:A:SER:H	17	0.34
(1,551)	1:70:A:PRO:HB3	1:71:A:SER:H	15	0.34
(1,551)	1:70:A:PRO:HB3	1:71:A:SER:H	17	0.34
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD11	1	0.34
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD12	1	0.34
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD13	1	0.34
(1,457)	1:60:A:LEU:HD11	1:108:A:SER:H	7	0.34
(1,457)	1:60:A:LEU:HD12	1:108:A:SER:H	7	0.34
(1,457)	1:60:A:LEU:HD13	1:108:A:SER:H	7	0.34
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG21	14	0.34
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG22	14	0.34
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG23	14	0.34
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG21	14	0.34
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG22	14	0.34
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG23	14	0.34
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG21	14	0.34
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG22	14	0.34
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG23	14	0.34
(1,369)	1:33:A:GLN:HG2	1:34:A:TRP:H	18	0.34
(1,366)	1:32:A:SER:H	1:33:A:GLN:HE22	18	0.34
(1,366)	1:32:A:SER:H	1:33:A:GLN:HE21	18	0.34
(1,364)	1:24:A:TYR:HD1	1:33:A:GLN:H	4	0.34
(1,364)	1:24:A:TYR:HD2	1:33:A:GLN:H	4	0.34
(1,355)	1:25:A:PHE:HE1	1:32:A:SER:HB2	12	0.34
(1,355)	1:25:A:PHE:HE2	1:32:A:SER:HB2	12	0.34
(1,355)	1:25:A:PHE:HE1	1:32:A:SER:HB2	19	0.34
(1,355)	1:25:A:PHE:HE2	1:32:A:SER:HB2	19	0.34
(1,321)	1:25:A:PHE:HZ	1:30:A:ASN:H	5	0.34
(1,320)	1:25:A:PHE:HE1	1:30:A:ASN:H	7	0.34
(1,320)	1:25:A:PHE:HE2	1:30:A:ASN:H	7	0.34
(1,320)	1:25:A:PHE:HE1	1:30:A:ASN:H	11	0.34
(1,320)	1:25:A:PHE:HE2	1:30:A:ASN:H	11	0.34
(1,302)	1:27:A:HIS:HD2	1:28:A:ILE:H	17	0.34
(1,213)	1:11:A:TRP:HA	1:25:A:PHE:H	6	0.34
(1,204)	1:24:A:TYR:HB2	1:33:A:GLN:HE21	20	0.34
(1,194)	1:13:A:LYS:HG2	1:24:A:TYR:HA	6	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,75)	1:13:A:LYS:HA	1:23:A:TYR:H	19	0.34
(1,61)	1:11:A:TRP:HA	1:12:A:GLU:HB3	6	0.34
(1,14)	1:6:A:LYS:HG2	1:7:A:LEU:H	12	0.34
(1,11)	1:4:A:GLU:H	1:6:A:LYS:H	2	0.34
(3,79)	1:105:A:SER:O	1:109:A:GLN:N	1	0.33
(3,79)	1:105:A:SER:O	1:109:A:GLN:N	6	0.33
(3,65)	1:91:A:GLY:O	1:95:A:LYS:N	4	0.33
(3,44)	1:72:A:SER:O	1:75:A:GLN:H	14	0.33
(3,43)	1:72:A:SER:O	1:75:A:GLN:N	5	0.33
(3,43)	1:72:A:SER:O	1:75:A:GLN:N	12	0.33
(3,43)	1:72:A:SER:O	1:75:A:GLN:N	14	0.33
(3,43)	1:72:A:SER:O	1:75:A:GLN:N	20	0.33
(3,9)	1:16:A:SER:O	1:19:A:SER:N	14	0.33
(2,113)	1:162:A:THR:H	2:651:B:ILE:HG12	13	0.33
(2,113)	1:162:A:THR:H	2:651:B:ILE:HG13	13	0.33
(2,92)	1:58:A:SER:H	2:651:B:ILE:HG12	5	0.33
(2,92)	1:58:A:SER:H	2:651:B:ILE:HG13	5	0.33
(2,79)	2:659:B:PHE:HE1	2:661:B:PHE:H	12	0.33
(2,79)	2:659:B:PHE:HE2	2:661:B:PHE:H	12	0.33
(2,42)	1:130:A:MET:HB2	1:134:A:PHE:HD1	4	0.33
(2,42)	1:130:A:MET:HB2	1:134:A:PHE:HD2	4	0.33
(1,2615)	1:49:A:GLN:H	1:49:A:GLN:HG2	18	0.33
(1,2598)	1:146:A:MET:HE1	2:642:B:PRO:HB2	15	0.33
(1,2598)	1:146:A:MET:HE1	2:642:B:PRO:HB3	15	0.33
(1,2598)	1:146:A:MET:HE2	2:642:B:PRO:HB2	15	0.33
(1,2598)	1:146:A:MET:HE2	2:642:B:PRO:HB3	15	0.33
(1,2598)	1:146:A:MET:HE3	2:642:B:PRO:HB2	15	0.33
(1,2598)	1:146:A:MET:HE3	2:642:B:PRO:HB3	15	0.33
(1,2557)	2:654:B:SER:H	2:655:B:GLU:H	14	0.33
(1,2515)	2:645:B:GLN:HA	2:647:B:VAL:H	10	0.33
(1,2506)	2:644:B:ASP:H	2:645:B:GLN:HA	18	0.33
(1,2251)	1:141:A:LEU:H	1:141:A:LEU:HG	15	0.33
(1,2158)	1:119:A:ARG:H	1:119:A:ARG:HD2	11	0.33
(1,2056)	1:101:A:GLU:H	1:101:A:GLU:HG2	7	0.33
(1,2033)	1:95:A:LYS:H	1:95:A:LYS:HD2	8	0.33
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD11	1	0.33
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD12	1	0.33
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD13	1	0.33
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD11	12	0.33
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD12	12	0.33
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD13	12	0.33
(1,1913)	1:82:A:LYS:H	1:82:A:LYS:HD2	15	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1750)	1:56:A:ARG:HA	1:56:A:ARG:HE	9	0.33
(1,1625)	1:27:A:HIS:H	1:27:A:HIS:HD1	2	0.33
(1,1625)	1:27:A:HIS:H	1:27:A:HIS:HD1	3	0.33
(1,1568)	1:21:A:ARG:HB2	1:21:A:ARG:HE	4	0.33
(1,1429)	1:143:A:THR:HG21	1:163:A:GLU:HB2	18	0.33
(1,1429)	1:143:A:THR:HG22	1:163:A:GLU:HB2	18	0.33
(1,1429)	1:143:A:THR:HG23	1:163:A:GLU:HB2	18	0.33
(1,1423)	1:55:A:VAL:HB	1:163:A:GLU:H	8	0.33
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD11	6	0.33
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD12	6	0.33
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD13	6	0.33
(1,1349)	1:158:A:ILE:H	1:159:A:ILE:HD11	14	0.33
(1,1349)	1:158:A:ILE:H	1:159:A:ILE:HD12	14	0.33
(1,1349)	1:158:A:ILE:H	1:159:A:ILE:HD13	14	0.33
(1,1337)	1:59:A:HIS:H	1:159:A:ILE:HG21	2	0.33
(1,1337)	1:59:A:HIS:H	1:159:A:ILE:HG22	2	0.33
(1,1337)	1:59:A:HIS:H	1:159:A:ILE:HG23	2	0.33
(1,1306)	1:89:A:ILE:HD11	1:157:A:HIS:HD2	18	0.33
(1,1306)	1:89:A:ILE:HD12	1:157:A:HIS:HD2	18	0.33
(1,1306)	1:89:A:ILE:HD13	1:157:A:HIS:HD2	18	0.33
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG11	7	0.33
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG12	7	0.33
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG13	7	0.33
(1,1208)	1:103:A:PHE:HD1	1:146:A:MET:HB2	18	0.33
(1,1208)	1:103:A:PHE:HD2	1:146:A:MET:HB2	18	0.33
(1,1206)	1:145:A:GLU:HB3	1:146:A:MET:HB2	11	0.33
(1,1177)	1:137:A:ALA:HB1	1:141:A:LEU:H	18	0.33
(1,1177)	1:137:A:ALA:HB2	1:141:A:LEU:H	18	0.33
(1,1177)	1:137:A:ALA:HB3	1:141:A:LEU:H	18	0.33
(1,1161)	1:136:A:ASP:HB2	1:138:A:SER:H	7	0.33
(1,1156)	1:136:A:ASP:HB2	1:137:A:ALA:H	3	0.33
(1,1141)	1:130:A:MET:HB2	1:134:A:PHE:H	11	0.33
(1,1012)	1:116:A:ALA:H	1:119:A:ARG:H	1	0.33
(1,1012)	1:116:A:ALA:H	1:119:A:ARG:H	15	0.33
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB1	5	0.33
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB2	5	0.33
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB3	5	0.33
(1,985)	1:61:A:LEU:HD21	1:113:A:CYS:HA	9	0.33
(1,985)	1:61:A:LEU:HD22	1:113:A:CYS:HA	9	0.33
(1,985)	1:61:A:LEU:HD23	1:113:A:CYS:HA	9	0.33
(1,961)	1:108:A:SER:H	1:119:A:ARG:HG2	2	0.33
(1,959)	1:108:A:SER:HA	1:111:A:SER:H	11	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,958)	1:108:A:SER:HA	1:110:A:PHE:H	3	0.33
(1,958)	1:108:A:SER:HA	1:110:A:PHE:H	6	0.33
(1,940)	1:106:A:LEU:HG	1:107:A:ALA:H	15	0.33
(1,940)	1:106:A:LEU:HG	1:107:A:ALA:H	17	0.33
(1,914)	1:104:A:GLU:H	1:106:A:LEU:HB3	17	0.33
(1,913)	1:103:A:PHE:H	1:106:A:LEU:HB3	1	0.33
(1,913)	1:103:A:PHE:H	1:106:A:LEU:HB3	2	0.33
(1,888)	1:103:A:PHE:HE1	1:120:A:GLY:H	4	0.33
(1,888)	1:103:A:PHE:HE2	1:120:A:GLY:H	4	0.33
(1,888)	1:103:A:PHE:HE1	1:120:A:GLY:H	17	0.33
(1,888)	1:103:A:PHE:HE2	1:120:A:GLY:H	17	0.33
(1,753)	1:90:A:ASN:HD22	1:91:A:GLY:H	20	0.33
(1,748)	1:87:A:GLU:HA	1:91:A:GLY:H	15	0.33
(1,681)	1:85:A:ALA:H	1:88:A:LEU:HD11	10	0.33
(1,681)	1:85:A:ALA:H	1:88:A:LEU:HD12	10	0.33
(1,681)	1:85:A:ALA:H	1:88:A:LEU:HD13	10	0.33
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB1	17	0.33
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB2	17	0.33
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB3	17	0.33
(1,671)	1:64:A:HIS:HB2	1:85:A:ALA:H	5	0.33
(1,671)	1:64:A:HIS:HB2	1:85:A:ALA:H	6	0.33
(1,669)	1:84:A:GLU:H	1:87:A:GLU:H	9	0.33
(1,648)	1:66:A:GLN:HE22	1:82:A:LYS:HG3	10	0.33
(1,646)	1:81:A:THR:HG21	1:84:A:GLU:HB2	16	0.33
(1,646)	1:81:A:THR:HG22	1:84:A:GLU:HB2	16	0.33
(1,646)	1:81:A:THR:HG23	1:84:A:GLU:HB2	16	0.33
(1,644)	1:81:A:THR:HA	1:84:A:GLU:H	16	0.33
(1,644)	1:81:A:THR:HA	1:84:A:GLU:H	19	0.33
(1,608)	1:75:A:GLN:HE22	1:78:A:ILE:HD11	13	0.33
(1,608)	1:75:A:GLN:HE22	1:78:A:ILE:HD12	13	0.33
(1,608)	1:75:A:GLN:HE22	1:78:A:ILE:HD13	13	0.33
(1,554)	1:70:A:PRO:HG3	1:71:A:SER:H	15	0.33
(1,551)	1:70:A:PRO:HB3	1:71:A:SER:H	14	0.33
(1,551)	1:70:A:PRO:HB3	1:71:A:SER:H	16	0.33
(1,515)	1:63:A:LYS:H	1:156:A:ILE:H	5	0.33
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB1	3	0.33
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB2	3	0.33
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB3	3	0.33
(1,436)	1:58:A:SER:H	1:160:A:LEU:HG	1	0.33
(1,422)	1:56:A:ARG:HG2	1:162:A:THR:HB	10	0.33
(1,401)	1:54:A:ARG:HD2	1:55:A:VAL:HA	10	0.33
(1,393)	1:53:A:ALA:HB1	1:54:A:ARG:H	16	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,393)	1:53:A:ALA:HB2	1:54:A:ARG:H	16	0.33
(1,393)	1:53:A:ALA:HB3	1:54:A:ARG:H	16	0.33
(1,388)	1:35:A:GLU:HG2	1:36:A:ARG:H	13	0.33
(1,377)	1:33:A:GLN:HG2	1:35:A:GLU:H	5	0.33
(1,369)	1:33:A:GLN:HG2	1:34:A:TRP:H	4	0.33
(1,369)	1:33:A:GLN:HG2	1:34:A:TRP:H	6	0.33
(1,364)	1:24:A:TYR:HD1	1:33:A:GLN:H	1	0.33
(1,364)	1:24:A:TYR:HD2	1:33:A:GLN:H	1	0.33
(1,311)	1:27:A:HIS:HB2	1:29:A:THR:H	9	0.33
(1,311)	1:27:A:HIS:HB2	1:29:A:THR:H	16	0.33
(1,311)	1:27:A:HIS:HB2	1:29:A:THR:H	19	0.33
(1,302)	1:27:A:HIS:HD2	1:28:A:ILE:H	10	0.33
(1,287)	1:26:A:ASN:H	1:32:A:SER:HB2	13	0.33
(1,278)	1:26:A:ASN:HB2	1:30:A:ASN:H	12	0.33
(1,262)	1:25:A:PHE:HE1	1:26:A:ASN:HA	14	0.33
(1,262)	1:25:A:PHE:HE2	1:26:A:ASN:HA	14	0.33
(1,244)	1:11:A:TRP:H	1:26:A:ASN:HB2	2	0.33
(1,244)	1:11:A:TRP:H	1:26:A:ASN:HB2	17	0.33
(1,208)	1:24:A:TYR:H	1:34:A:TRP:HB3	2	0.33
(1,190)	1:13:A:LYS:HB3	1:24:A:TYR:HA	18	0.33
(1,98)	1:14:A:ARG:H	1:24:A:TYR:H	8	0.33
(1,66)	1:12:A:GLU:H	1:25:A:PHE:HE1	6	0.33
(1,66)	1:12:A:GLU:H	1:25:A:PHE:HE2	6	0.33
(1,61)	1:11:A:TRP:HA	1:12:A:GLU:HB3	5	0.33
(1,61)	1:11:A:TRP:HA	1:12:A:GLU:HB3	9	0.33
(1,27)	1:7:A:LEU:HD21	1:13:A:LYS:H	19	0.33
(1,27)	1:7:A:LEU:HD22	1:13:A:LYS:H	19	0.33
(1,27)	1:7:A:LEU:HD23	1:13:A:LYS:H	19	0.33
(1,7)	1:3:A:ASP:HA	1:4:A:GLU:H	6	0.33
(3,65)	1:91:A:GLY:O	1:95:A:LYS:N	18	0.32
(3,44)	1:72:A:SER:O	1:75:A:GLN:H	13	0.32
(3,35)	1:62:A:VAL:N	1:156:A:ILE:O	8	0.32
(2,110)	1:152:A:THR:HG21	2:661:B:PHE:HB2	11	0.32
(2,110)	1:152:A:THR:HG21	2:661:B:PHE:HB3	11	0.32
(2,110)	1:152:A:THR:HG22	2:661:B:PHE:HB2	11	0.32
(2,110)	1:152:A:THR:HG22	2:661:B:PHE:HB3	11	0.32
(2,110)	1:152:A:THR:HG23	2:661:B:PHE:HB2	11	0.32
(2,110)	1:152:A:THR:HG23	2:661:B:PHE:HB3	11	0.32
(2,110)	1:152:A:THR:HG21	2:661:B:PHE:HB2	14	0.32
(2,110)	1:152:A:THR:HG21	2:661:B:PHE:HB3	14	0.32
(2,110)	1:152:A:THR:HG22	2:661:B:PHE:HB2	14	0.32
(2,110)	1:152:A:THR:HG22	2:661:B:PHE:HB3	14	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,110)	1:152:A:THR:HG23	2:661:B:PHE:HB2	14	0.32
(2,110)	1:152:A:THR:HG23	2:661:B:PHE:HB3	14	0.32
(2,102)	1:135:A:GLU:H	2:656:B:PHE:HB2	2	0.32
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG11	8	0.32
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG12	8	0.32
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG13	8	0.32
(1,2584)	1:114:A:SER:H	2:659:B:PHE:HD1	5	0.32
(1,2584)	1:114:A:SER:H	2:659:B:PHE:HD2	5	0.32
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG21	19	0.32
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG22	19	0.32
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG23	19	0.32
(1,2550)	2:652:B:ASP:H	2:653:B:GLN:H	16	0.32
(1,2523)	2:647:B:VAL:HA	2:649:B:ARG:H	8	0.32
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE1	4	0.32
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE2	4	0.32
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE3	4	0.32
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE1	17	0.32
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE2	17	0.32
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE3	17	0.32
(1,2251)	1:141:A:LEU:H	1:141:A:LEU:HG	11	0.32
(1,2209)	1:131:A:GLN:HA	1:131:A:GLN:HE22	16	0.32
(1,2158)	1:119:A:ARG:H	1:119:A:ARG:HD2	7	0.32
(1,2033)	1:95:A:LYS:H	1:95:A:LYS:HD2	15	0.32
(1,2033)	1:95:A:LYS:H	1:95:A:LYS:HD2	18	0.32
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD11	13	0.32
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD12	13	0.32
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD13	13	0.32
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD11	14	0.32
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD12	14	0.32
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD13	14	0.32
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD11	15	0.32
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD12	15	0.32
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD13	15	0.32
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD11	16	0.32
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD12	16	0.32
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD13	16	0.32
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD11	19	0.32
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD12	19	0.32
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD13	19	0.32
(1,1747)	1:56:A:ARG:H	1:56:A:ARG:HD2	6	0.32
(1,1455)	1:6:A:LYS:H	1:6:A:LYS:HB3	3	0.32
(1,1455)	1:6:A:LYS:H	1:6:A:LYS:HB3	7	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1455)	1:6:A:LYS:H	1:6:A:LYS:HB3	9	0.32
(1,1441)	1:162:A:THR:HG21	1:163:A:GLU:HG3	14	0.32
(1,1441)	1:162:A:THR:HG22	1:163:A:GLU:HG3	14	0.32
(1,1441)	1:162:A:THR:HG23	1:163:A:GLU:HG3	14	0.32
(1,1428)	1:143:A:THR:HG21	1:163:A:GLU:H	20	0.32
(1,1428)	1:143:A:THR:HG22	1:163:A:GLU:H	20	0.32
(1,1428)	1:143:A:THR:HG23	1:163:A:GLU:H	20	0.32
(1,1423)	1:55:A:VAL:HB	1:163:A:GLU:H	3	0.32
(1,1423)	1:55:A:VAL:HB	1:163:A:GLU:H	11	0.32
(1,1382)	1:159:A:ILE:HG12	1:160:A:LEU:H	11	0.32
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD11	9	0.32
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD12	9	0.32
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD13	9	0.32
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG21	7	0.32
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG22	7	0.32
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG23	7	0.32
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG21	16	0.32
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG22	16	0.32
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG23	16	0.32
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD11	7	0.32
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD12	7	0.32
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD13	7	0.32
(1,1200)	1:143:A:THR:H	1:144:A:GLY:H	11	0.32
(1,1156)	1:136:A:ASP:HB2	1:137:A:ALA:H	8	0.32
(1,1066)	1:122:A:LEU:HD21	1:125:A:PHE:HD1	13	0.32
(1,1066)	1:122:A:LEU:HD21	1:125:A:PHE:HD2	13	0.32
(1,1066)	1:122:A:LEU:HD22	1:125:A:PHE:HD1	13	0.32
(1,1066)	1:122:A:LEU:HD22	1:125:A:PHE:HD2	13	0.32
(1,1066)	1:122:A:LEU:HD23	1:125:A:PHE:HD1	13	0.32
(1,1066)	1:122:A:LEU:HD23	1:125:A:PHE:HD2	13	0.32
(1,1047)	1:119:A:ARG:HD2	1:121:A:ASP:H	3	0.32
(1,1027)	1:118:A:ALA:HA	1:119:A:ARG:HG2	10	0.32
(1,1027)	1:118:A:ALA:HA	1:119:A:ARG:HG2	13	0.32
(1,1012)	1:116:A:ALA:H	1:119:A:ARG:H	3	0.32
(1,1011)	1:116:A:ALA:HB1	1:119:A:ARG:H	12	0.32
(1,1011)	1:116:A:ALA:HB2	1:119:A:ARG:H	12	0.32
(1,1011)	1:116:A:ALA:HB3	1:119:A:ARG:H	12	0.32
(1,985)	1:61:A:LEU:HD21	1:113:A:CYS:HA	12	0.32
(1,985)	1:61:A:LEU:HD22	1:113:A:CYS:HA	12	0.32
(1,985)	1:61:A:LEU:HD23	1:113:A:CYS:HA	12	0.32
(1,978)	1:107:A:ALA:HB1	1:111:A:SER:HA	17	0.32
(1,978)	1:107:A:ALA:HB2	1:111:A:SER:HA	17	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,978)	1:107:A:ALA:HB3	1:111:A:SER:HA	17	0.32
(1,941)	1:106:A:LEU:HD11	1:107:A:ALA:H	11	0.32
(1,941)	1:106:A:LEU:HD12	1:107:A:ALA:H	11	0.32
(1,941)	1:106:A:LEU:HD13	1:107:A:ALA:H	11	0.32
(1,941)	1:106:A:LEU:HD11	1:107:A:ALA:H	14	0.32
(1,941)	1:106:A:LEU:HD12	1:107:A:ALA:H	14	0.32
(1,941)	1:106:A:LEU:HD13	1:107:A:ALA:H	14	0.32
(1,941)	1:106:A:LEU:HD11	1:107:A:ALA:H	20	0.32
(1,941)	1:106:A:LEU:HD12	1:107:A:ALA:H	20	0.32
(1,941)	1:106:A:LEU:HD13	1:107:A:ALA:H	20	0.32
(1,917)	1:105:A:SER:HB2	1:106:A:LEU:H	15	0.32
(1,871)	1:96:A:ILE:HB	1:103:A:PHE:H	13	0.32
(1,868)	1:60:A:LEU:HD21	1:103:A:PHE:HE1	19	0.32
(1,868)	1:60:A:LEU:HD21	1:103:A:PHE:HE2	19	0.32
(1,868)	1:60:A:LEU:HD22	1:103:A:PHE:HE1	19	0.32
(1,868)	1:60:A:LEU:HD22	1:103:A:PHE:HE2	19	0.32
(1,868)	1:60:A:LEU:HD23	1:103:A:PHE:HE1	19	0.32
(1,868)	1:60:A:LEU:HD23	1:103:A:PHE:HE2	19	0.32
(1,868)	1:60:A:LEU:HD21	1:103:A:PHE:HE1	20	0.32
(1,868)	1:60:A:LEU:HD21	1:103:A:PHE:HE2	20	0.32
(1,868)	1:60:A:LEU:HD22	1:103:A:PHE:HE1	20	0.32
(1,868)	1:60:A:LEU:HD22	1:103:A:PHE:HE2	20	0.32
(1,868)	1:60:A:LEU:HD23	1:103:A:PHE:HE1	20	0.32
(1,868)	1:60:A:LEU:HD23	1:103:A:PHE:HE2	20	0.32
(1,862)	1:101:A:GLU:HG2	1:102:A:ASP:H	12	0.32
(1,854)	1:98:A:SER:H	1:101:A:GLU:H	8	0.32
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD11	14	0.32
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD12	14	0.32
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD13	14	0.32
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD11	14	0.32
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD12	14	0.32
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD13	14	0.32
(1,743)	1:89:A:ILE:HG13	1:90:A:ASN:H	2	0.32
(1,743)	1:89:A:ILE:HG13	1:90:A:ASN:H	3	0.32
(1,681)	1:85:A:ALA:H	1:88:A:LEU:HD11	14	0.32
(1,681)	1:85:A:ALA:H	1:88:A:LEU:HD12	14	0.32
(1,681)	1:85:A:ALA:H	1:88:A:LEU:HD13	14	0.32
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB1	13	0.32
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB2	13	0.32
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB3	13	0.32
(1,659)	1:81:A:THR:HA	1:83:A:GLU:H	2	0.32
(1,659)	1:81:A:THR:HA	1:83:A:GLU:H	13	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,659)	1:81:A:THR:HA	1:83:A:GLU:H	14	0.32
(1,659)	1:81:A:THR:HA	1:83:A:GLU:H	19	0.32
(1,649)	1:66:A:GLN:HE21	1:82:A:LYS:HB2	7	0.32
(1,648)	1:66:A:GLN:HE22	1:82:A:LYS:HG3	16	0.32
(1,648)	1:66:A:GLN:HE22	1:82:A:LYS:HG3	20	0.32
(1,647)	1:65:A:SER:H	1:82:A:LYS:H	17	0.32
(1,640)	1:65:A:SER:HB3	1:81:A:THR:HA	1	0.32
(1,634)	1:80:A:ARG:HB2	1:81:A:THR:H	15	0.32
(1,618)	1:78:A:ILE:HA	1:80:A:ARG:H	1	0.32
(1,589)	1:74:A:ARG:H	1:112:A:ASP:HA	7	0.32
(1,569)	1:73:A:TRP:HE1	1:74:A:ARG:HB2	12	0.32
(1,551)	1:70:A:PRO:HB3	1:71:A:SER:H	9	0.32
(1,551)	1:70:A:PRO:HB3	1:71:A:SER:H	19	0.32
(1,551)	1:70:A:PRO:HB3	1:71:A:SER:H	20	0.32
(1,444)	1:59:A:HIS:HA	1:158:A:ILE:H	6	0.32
(1,401)	1:54:A:ARG:HD2	1:55:A:VAL:HA	12	0.32
(1,393)	1:53:A:ALA:HB1	1:54:A:ARG:H	2	0.32
(1,393)	1:53:A:ALA:HB2	1:54:A:ARG:H	2	0.32
(1,393)	1:53:A:ALA:HB3	1:54:A:ARG:H	2	0.32
(1,385)	1:24:A:TYR:HD1	1:36:A:ARG:H	15	0.32
(1,385)	1:24:A:TYR:HD2	1:36:A:ARG:H	15	0.32
(1,366)	1:32:A:SER:H	1:33:A:GLN:HE22	10	0.32
(1,366)	1:32:A:SER:H	1:33:A:GLN:HE21	10	0.32
(1,364)	1:24:A:TYR:HD1	1:33:A:GLN:H	9	0.32
(1,364)	1:24:A:TYR:HD2	1:33:A:GLN:H	9	0.32
(1,364)	1:24:A:TYR:HD1	1:33:A:GLN:H	11	0.32
(1,364)	1:24:A:TYR:HD2	1:33:A:GLN:H	11	0.32
(1,354)	1:24:A:TYR:H	1:32:A:SER:HB3	13	0.32
(1,347)	1:31:A:ALA:HB1	1:33:A:GLN:H	4	0.32
(1,347)	1:31:A:ALA:HB2	1:33:A:GLN:H	4	0.32
(1,347)	1:31:A:ALA:HB3	1:33:A:GLN:H	4	0.32
(1,262)	1:25:A:PHE:HE1	1:26:A:ASN:HA	16	0.32
(1,262)	1:25:A:PHE:HE2	1:26:A:ASN:HA	16	0.32
(1,224)	1:14:A:ARG:HE	1:25:A:PHE:HB3	12	0.32
(1,214)	1:11:A:TRP:HB2	1:25:A:PHE:H	2	0.32
(1,213)	1:11:A:TRP:HA	1:25:A:PHE:H	15	0.32
(1,211)	1:24:A:TYR:HE1	1:36:A:ARG:HD2	12	0.32
(1,211)	1:24:A:TYR:HE2	1:36:A:ARG:HD2	12	0.32
(1,189)	1:13:A:LYS:H	1:24:A:TYR:HA	12	0.32
(1,93)	1:14:A:ARG:H	1:22:A:VAL:HA	4	0.32
(1,75)	1:13:A:LYS:HA	1:23:A:TYR:H	14	0.32
(1,61)	1:11:A:TRP:HA	1:12:A:GLU:HB3	7	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,52)	1:11:A:TRP:HE1	1:26:A:ASN:HB2	2	0.32
(1,52)	1:11:A:TRP:HE1	1:26:A:ASN:HB3	2	0.32
(1,28)	1:7:A:LEU:HD21	1:13:A:LYS:HG3	19	0.32
(1,28)	1:7:A:LEU:HD22	1:13:A:LYS:HG3	19	0.32
(1,28)	1:7:A:LEU:HD23	1:13:A:LYS:HG3	19	0.32
(3,63)	1:90:A:ASN:O	1:94:A:GLN:N	2	0.31
(3,25)	1:55:A:VAL:N	1:125:A:PHE:O	10	0.31
(2,106)	1:139:A:PHE:H	2:656:B:PHE:HB2	10	0.31
(2,106)	1:139:A:PHE:H	2:656:B:PHE:HB2	11	0.31
(2,103)	1:137:A:ALA:H	2:656:B:PHE:HB2	12	0.31
(2,92)	1:58:A:SER:H	2:651:B:ILE:HG12	16	0.31
(2,92)	1:58:A:SER:H	2:651:B:ILE:HG13	16	0.31
(2,55)	1:150:A:VAL:HG21	1:158:A:ILE:HA	16	0.31
(2,55)	1:150:A:VAL:HG22	1:158:A:ILE:HA	16	0.31
(2,55)	1:150:A:VAL:HG23	1:158:A:ILE:HA	16	0.31
(2,39)	1:55:A:VAL:HG11	1:127:A:ARG:H	13	0.31
(2,39)	1:55:A:VAL:HG12	1:127:A:ARG:H	13	0.31
(2,39)	1:55:A:VAL:HG13	1:127:A:ARG:H	13	0.31
(2,21)	1:73:A:TRP:HE1	1:74:A:ARG:HG3	8	0.31
(2,5)	1:23:A:TYR:H	1:34:A:TRP:HZ3	8	0.31
(1,2597)	1:138:A:SER:H	2:656:B:PHE:HB2	15	0.31
(1,2578)	1:29:A:THR:HG21	2:646:B:GLU:HA	12	0.31
(1,2578)	1:29:A:THR:HG22	2:646:B:GLU:HA	12	0.31
(1,2578)	1:29:A:THR:HG23	2:646:B:GLU:HA	12	0.31
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG21	15	0.31
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG22	15	0.31
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG23	15	0.31
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG21	16	0.31
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG22	16	0.31
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG23	16	0.31
(1,2557)	2:654:B:SER:H	2:655:B:GLU:H	1	0.31
(1,2533)	2:647:B:VAL:H	2:649:B:ARG:H	4	0.31
(1,2533)	2:647:B:VAL:H	2:649:B:ARG:H	5	0.31
(1,2514)	2:646:B:GLU:HA	2:649:B:ARG:H	1	0.31
(1,2434)	2:648:B:ILE:H	2:648:B:ILE:HG12	13	0.31
(1,2403)	2:645:B:GLN:H	2:645:B:GLN:HG2	19	0.31
(1,2209)	1:131:A:GLN:HA	1:131:A:GLN:HE22	18	0.31
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD11	2	0.31
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD12	2	0.31
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD13	2	0.31
(1,1750)	1:56:A:ARG:HA	1:56:A:ARG:HE	16	0.31
(1,1747)	1:56:A:ARG:H	1:56:A:ARG:HD2	3	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1747)	1:56:A:ARG:H	1:56:A:ARG:HD2	4	0.31
(1,1700)	1:36:A:ARG:H	1:36:A:ARG:HG2	13	0.31
(1,1455)	1:6:A:LYS:H	1:6:A:LYS:HB3	4	0.31
(1,1455)	1:6:A:LYS:H	1:6:A:LYS:HB3	5	0.31
(1,1455)	1:6:A:LYS:H	1:6:A:LYS:HB3	12	0.31
(1,1455)	1:6:A:LYS:H	1:6:A:LYS:HB3	19	0.31
(1,1455)	1:6:A:LYS:H	1:6:A:LYS:HB3	20	0.31
(1,1439)	1:162:A:THR:HG21	1:163:A:GLU:H	11	0.31
(1,1439)	1:162:A:THR:HG22	1:163:A:GLU:H	11	0.31
(1,1439)	1:162:A:THR:HG23	1:163:A:GLU:H	11	0.31
(1,1424)	1:55:A:VAL:HG21	1:163:A:GLU:H	18	0.31
(1,1424)	1:55:A:VAL:HG22	1:163:A:GLU:H	18	0.31
(1,1424)	1:55:A:VAL:HG23	1:163:A:GLU:H	18	0.31
(1,1424)	1:55:A:VAL:HG11	1:163:A:GLU:H	18	0.31
(1,1424)	1:55:A:VAL:HG12	1:163:A:GLU:H	18	0.31
(1,1424)	1:55:A:VAL:HG13	1:163:A:GLU:H	18	0.31
(1,1382)	1:159:A:ILE:HG12	1:160:A:LEU:H	10	0.31
(1,1368)	1:103:A:PHE:HB3	1:160:A:LEU:HD21	15	0.31
(1,1368)	1:103:A:PHE:HB3	1:160:A:LEU:HD22	15	0.31
(1,1368)	1:103:A:PHE:HB3	1:160:A:LEU:HD23	15	0.31
(1,1311)	1:152:A:THR:HG21	1:157:A:HIS:H	3	0.31
(1,1311)	1:152:A:THR:HG22	1:157:A:HIS:H	3	0.31
(1,1311)	1:152:A:THR:HG23	1:157:A:HIS:H	3	0.31
(1,1311)	1:152:A:THR:HG21	1:157:A:HIS:H	8	0.31
(1,1311)	1:152:A:THR:HG22	1:157:A:HIS:H	8	0.31
(1,1311)	1:152:A:THR:HG23	1:157:A:HIS:H	8	0.31
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG21	2	0.31
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG22	2	0.31
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG23	2	0.31
(1,1206)	1:145:A:GLU:HB3	1:146:A:MET:HB2	7	0.31
(1,1192)	1:141:A:LEU:HD21	1:146:A:MET:H	10	0.31
(1,1192)	1:141:A:LEU:HD22	1:146:A:MET:H	10	0.31
(1,1192)	1:141:A:LEU:HD23	1:146:A:MET:H	10	0.31
(1,1187)	1:140:A:ALA:HB1	1:141:A:LEU:HD21	11	0.31
(1,1187)	1:140:A:ALA:HB1	1:141:A:LEU:HD22	11	0.31
(1,1187)	1:140:A:ALA:HB1	1:141:A:LEU:HD23	11	0.31
(1,1187)	1:140:A:ALA:HB2	1:141:A:LEU:HD21	11	0.31
(1,1187)	1:140:A:ALA:HB2	1:141:A:LEU:HD22	11	0.31
(1,1187)	1:140:A:ALA:HB2	1:141:A:LEU:HD23	11	0.31
(1,1187)	1:140:A:ALA:HB3	1:141:A:LEU:HD21	11	0.31
(1,1187)	1:140:A:ALA:HB3	1:141:A:LEU:HD22	11	0.31
(1,1187)	1:140:A:ALA:HB3	1:141:A:LEU:HD23	11	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB1	18	0.31
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB2	18	0.31
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB3	18	0.31
(1,1143)	1:130:A:MET:HB2	1:135:A:GLU:H	11	0.31
(1,1054)	1:59:A:HIS:HD2	1:122:A:LEU:H	2	0.31
(1,1033)	1:108:A:SER:H	1:119:A:ARG:HB2	2	0.31
(1,1012)	1:116:A:ALA:H	1:119:A:ARG:H	12	0.31
(1,1011)	1:116:A:ALA:HB1	1:119:A:ARG:H	9	0.31
(1,1011)	1:116:A:ALA:HB2	1:119:A:ARG:H	9	0.31
(1,1011)	1:116:A:ALA:HB3	1:119:A:ARG:H	9	0.31
(1,998)	1:111:A:SER:H	1:116:A:ALA:HB1	3	0.31
(1,998)	1:111:A:SER:H	1:116:A:ALA:HB2	3	0.31
(1,998)	1:111:A:SER:H	1:116:A:ALA:HB3	3	0.31
(1,970)	1:108:A:SER:H	1:110:A:PHE:H	9	0.31
(1,959)	1:108:A:SER:HA	1:111:A:SER:H	8	0.31
(1,959)	1:108:A:SER:HA	1:111:A:SER:H	13	0.31
(1,958)	1:108:A:SER:HA	1:110:A:PHE:H	12	0.31
(1,940)	1:106:A:LEU:HG	1:107:A:ALA:H	1	0.31
(1,920)	1:106:A:LEU:HB3	1:108:A:SER:H	17	0.31
(1,909)	1:102:A:ASP:HB2	1:106:A:LEU:H	2	0.31
(1,901)	1:103:A:PHE:H	1:105:A:SER:H	19	0.31
(1,862)	1:101:A:GLU:HG2	1:102:A:ASP:H	20	0.31
(1,845)	1:97:A:LYS:HD2	1:98:A:SER:H	10	0.31
(1,811)	1:94:A:GLN:H	1:96:A:ILE:H	2	0.31
(1,811)	1:94:A:GLN:H	1:96:A:ILE:H	10	0.31
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD11	17	0.31
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD12	17	0.31
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD13	17	0.31
(1,753)	1:90:A:ASN:HD22	1:91:A:GLY:H	8	0.31
(1,689)	1:86:A:LEU:HG	1:90:A:ASN:HD21	14	0.31
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB1	9	0.31
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB2	9	0.31
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB3	9	0.31
(1,671)	1:64:A:HIS:HB2	1:85:A:ALA:H	7	0.31
(1,671)	1:64:A:HIS:HB2	1:85:A:ALA:H	13	0.31
(1,663)	1:82:A:LYS:HB3	1:83:A:GLU:H	4	0.31
(1,663)	1:82:A:LYS:HB3	1:83:A:GLU:H	17	0.31
(1,612)	1:75:A:GLN:HE21	1:78:A:ILE:HA	11	0.31
(1,538)	1:66:A:GLN:HG2	1:67:A:SER:H	10	0.31
(1,465)	1:60:A:LEU:HB2	1:158:A:ILE:H	18	0.31
(1,457)	1:60:A:LEU:HD11	1:108:A:SER:H	11	0.31
(1,457)	1:60:A:LEU:HD12	1:108:A:SER:H	11	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,457)	1:60:A:LEU:HD13	1:108:A:SER:H	11	0.31
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB1	18	0.31
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB2	18	0.31
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB3	18	0.31
(1,436)	1:58:A:SER:H	1:160:A:LEU:HG	13	0.31
(1,364)	1:24:A:TYR:HD1	1:33:A:GLN:H	12	0.31
(1,364)	1:24:A:TYR:HD2	1:33:A:GLN:H	12	0.31
(1,355)	1:25:A:PHE:HE1	1:32:A:SER:HB2	15	0.31
(1,355)	1:25:A:PHE:HE2	1:32:A:SER:HB2	15	0.31
(1,347)	1:31:A:ALA:HB1	1:33:A:GLN:H	8	0.31
(1,347)	1:31:A:ALA:HB2	1:33:A:GLN:H	8	0.31
(1,347)	1:31:A:ALA:HB3	1:33:A:GLN:H	8	0.31
(1,347)	1:31:A:ALA:HB1	1:33:A:GLN:H	18	0.31
(1,347)	1:31:A:ALA:HB2	1:33:A:GLN:H	18	0.31
(1,347)	1:31:A:ALA:HB3	1:33:A:GLN:H	18	0.31
(1,302)	1:27:A:HIS:HD2	1:28:A:ILE:H	16	0.31
(1,208)	1:24:A:TYR:H	1:34:A:TRP:HB3	18	0.31
(1,194)	1:13:A:LYS:HG2	1:24:A:TYR:HA	8	0.31
(1,194)	1:13:A:LYS:HG2	1:24:A:TYR:HA	16	0.31
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG11	3	0.31
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG12	3	0.31
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG13	3	0.31
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG11	3	0.31
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG12	3	0.31
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG13	3	0.31
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG11	3	0.31
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG12	3	0.31
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG13	3	0.31
(1,75)	1:13:A:LYS:HA	1:23:A:TYR:H	9	0.31
(1,75)	1:13:A:LYS:HA	1:23:A:TYR:H	11	0.31
(1,69)	1:7:A:LEU:HD21	1:13:A:LYS:HE2	5	0.31
(1,69)	1:7:A:LEU:HD22	1:13:A:LYS:HE2	5	0.31
(1,69)	1:7:A:LEU:HD23	1:13:A:LYS:HE2	5	0.31
(1,69)	1:7:A:LEU:HD11	1:13:A:LYS:HE2	5	0.31
(1,69)	1:7:A:LEU:HD12	1:13:A:LYS:HE2	5	0.31
(1,69)	1:7:A:LEU:HD13	1:13:A:LYS:HE2	5	0.31
(1,66)	1:12:A:GLU:H	1:25:A:PHE:HE1	3	0.31
(1,66)	1:12:A:GLU:H	1:25:A:PHE:HE2	3	0.31
(1,56)	1:11:A:TRP:HE1	1:31:A:ALA:HB1	9	0.31
(1,56)	1:11:A:TRP:HE1	1:31:A:ALA:HB2	9	0.31
(1,56)	1:11:A:TRP:HE1	1:31:A:ALA:HB3	9	0.31
(1,12)	1:5:A:GLU:HB2	1:6:A:LYS:H	7	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,11)	1:4:A:GLU:H	1:6:A:LYS:H	4	0.31
(1,11)	1:4:A:GLU:H	1:6:A:LYS:H	20	0.31
(1,7)	1:3:A:ASP:HA	1:4:A:GLU:H	18	0.31
(3,71)	1:94:A:GLN:O	1:98:A:SER:N	12	0.3
(3,44)	1:72:A:SER:O	1:75:A:GLN:H	6	0.3
(3,35)	1:62:A:VAL:N	1:156:A:ILE:O	3	0.3
(2,111)	1:160:A:LEU:H	2:651:B:ILE:HG12	14	0.3
(2,111)	1:160:A:LEU:H	2:651:B:ILE:HG13	14	0.3
(2,108)	1:140:A:ALA:HB1	2:649:B:ARG:HA	18	0.3
(2,108)	1:140:A:ALA:HB2	2:649:B:ARG:HA	18	0.3
(2,108)	1:140:A:ALA:HB3	2:649:B:ARG:HA	18	0.3
(2,106)	1:139:A:PHE:H	2:656:B:PHE:HB2	17	0.3
(2,92)	1:58:A:SER:H	2:651:B:ILE:HG12	4	0.3
(2,92)	1:58:A:SER:H	2:651:B:ILE:HG13	4	0.3
(2,39)	1:55:A:VAL:HG11	1:127:A:ARG:H	8	0.3
(2,39)	1:55:A:VAL:HG12	1:127:A:ARG:H	8	0.3
(2,39)	1:55:A:VAL:HG13	1:127:A:ARG:H	8	0.3
(2,25)	1:88:A:LEU:HG	1:92:A:TYR:H	1	0.3
(2,20)	1:68:A:ARG:H	1:153:A:ASP:HB2	3	0.3
(2,20)	1:68:A:ARG:H	1:153:A:ASP:HB3	3	0.3
(1,2582)	1:34:A:TRP:HE1	2:642:B:PRO:HB2	10	0.3
(1,2582)	1:34:A:TRP:HE1	2:642:B:PRO:HB3	10	0.3
(1,2572)	1:16:A:SER:HB2	2:641:B:TPO:HG21	20	0.3
(1,2572)	1:16:A:SER:HB2	2:641:B:TPO:HG22	20	0.3
(1,2572)	1:16:A:SER:HB2	2:641:B:TPO:HG23	20	0.3
(1,2533)	2:647:B:VAL:H	2:649:B:ARG:H	19	0.3
(1,2506)	2:644:B:ASP:H	2:645:B:GLN:HA	3	0.3
(1,2506)	2:644:B:ASP:H	2:645:B:GLN:HA	20	0.3
(1,2496)	2:659:B:PHE:H	2:659:B:PHE:HE1	1	0.3
(1,2496)	2:659:B:PHE:H	2:659:B:PHE:HE2	1	0.3
(1,2056)	1:101:A:GLU:H	1:101:A:GLU:HG2	15	0.3
(1,1750)	1:56:A:ARG:HA	1:56:A:ARG:HE	1	0.3
(1,1750)	1:56:A:ARG:HA	1:56:A:ARG:HE	3	0.3
(1,1750)	1:56:A:ARG:HA	1:56:A:ARG:HE	6	0.3
(1,1747)	1:56:A:ARG:H	1:56:A:ARG:HD2	5	0.3
(1,1747)	1:56:A:ARG:H	1:56:A:ARG:HD2	15	0.3
(1,1434)	1:161:A:ARG:HD2	1:163:A:GLU:H	17	0.3
(1,1423)	1:55:A:VAL:HB	1:163:A:GLU:H	16	0.3
(1,1382)	1:159:A:ILE:HG12	1:160:A:LEU:H	5	0.3
(1,1353)	1:57:A:CYS:HB3	1:160:A:LEU:H	14	0.3
(1,1348)	1:157:A:HIS:HB2	1:159:A:ILE:HD11	8	0.3
(1,1348)	1:157:A:HIS:HB2	1:159:A:ILE:HD12	8	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1348)	1:157:A:HIS:HB2	1:159:A:ILE:HD13	8	0.3
(1,1348)	1:157:A:HIS:HB3	1:159:A:ILE:HD11	8	0.3
(1,1348)	1:157:A:HIS:HB3	1:159:A:ILE:HD12	8	0.3
(1,1348)	1:157:A:HIS:HB3	1:159:A:ILE:HD13	8	0.3
(1,1330)	1:92:A:TYR:HD1	1:158:A:ILE:HG21	20	0.3
(1,1330)	1:92:A:TYR:HD1	1:158:A:ILE:HG22	20	0.3
(1,1330)	1:92:A:TYR:HD1	1:158:A:ILE:HG23	20	0.3
(1,1330)	1:92:A:TYR:HD2	1:158:A:ILE:HG21	20	0.3
(1,1330)	1:92:A:TYR:HD2	1:158:A:ILE:HG22	20	0.3
(1,1330)	1:92:A:TYR:HD2	1:158:A:ILE:HG23	20	0.3
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG21	5	0.3
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG22	5	0.3
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG23	5	0.3
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG21	8	0.3
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG22	8	0.3
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG23	8	0.3
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD11	1	0.3
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD12	1	0.3
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD13	1	0.3
(1,1262)	1:151:A:PHE:H	1:156:A:ILE:HA	14	0.3
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG21	1	0.3
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG22	1	0.3
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG23	1	0.3
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG21	1	0.3
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG22	1	0.3
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG23	1	0.3
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG21	1	0.3
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG22	1	0.3
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG23	1	0.3
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB1	15	0.3
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB2	15	0.3
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB3	15	0.3
(1,1107)	1:54:A:ARG:HD2	1:126:A:SER:HA	20	0.3
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE1	16	0.3
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE2	16	0.3
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE3	16	0.3
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE1	16	0.3
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE2	16	0.3
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE3	16	0.3
(1,1051)	1:57:A:CYS:H	1:122:A:LEU:HD21	3	0.3
(1,1051)	1:57:A:CYS:H	1:122:A:LEU:HD22	3	0.3
(1,1051)	1:57:A:CYS:H	1:122:A:LEU:HD23	3	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1012)	1:116:A:ALA:H	1:119:A:ARG:H	14	0.3
(1,961)	1:108:A:SER:H	1:119:A:ARG:HG2	11	0.3
(1,961)	1:108:A:SER:H	1:119:A:ARG:HG2	18	0.3
(1,958)	1:108:A:SER:HA	1:110:A:PHE:H	19	0.3
(1,925)	1:60:A:LEU:HG	1:107:A:ALA:H	11	0.3
(1,914)	1:104:A:GLU:H	1:106:A:LEU:HB3	7	0.3
(1,914)	1:104:A:GLU:H	1:106:A:LEU:HB3	12	0.3
(1,914)	1:104:A:GLU:H	1:106:A:LEU:HB3	20	0.3
(1,901)	1:103:A:PHE:H	1:105:A:SER:H	18	0.3
(1,849)	1:98:A:SER:HB2	1:99:A:GLY:H	15	0.3
(1,799)	1:93:A:ILE:HB	1:146:A:MET:HE1	8	0.3
(1,799)	1:93:A:ILE:HB	1:146:A:MET:HE2	8	0.3
(1,799)	1:93:A:ILE:HB	1:146:A:MET:HE3	8	0.3
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD11	1	0.3
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD12	1	0.3
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD13	1	0.3
(1,764)	1:88:A:LEU:HA	1:92:A:TYR:H	11	0.3
(1,748)	1:87:A:GLU:HA	1:91:A:GLY:H	2	0.3
(1,743)	1:89:A:ILE:HG13	1:90:A:ASN:H	7	0.3
(1,743)	1:89:A:ILE:HG13	1:90:A:ASN:H	14	0.3
(1,647)	1:65:A:SER:H	1:82:A:LYS:H	5	0.3
(1,641)	1:65:A:SER:HB2	1:81:A:THR:HG21	10	0.3
(1,641)	1:65:A:SER:HB2	1:81:A:THR:HG22	10	0.3
(1,641)	1:65:A:SER:HB2	1:81:A:THR:HG23	10	0.3
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG21	4	0.3
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG22	4	0.3
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG23	4	0.3
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG21	18	0.3
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG22	18	0.3
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG23	18	0.3
(1,589)	1:74:A:ARG:H	1:112:A:ASP:HA	14	0.3
(1,479)	1:61:A:LEU:HD21	1:155:A:GLY:H	13	0.3
(1,479)	1:61:A:LEU:HD22	1:155:A:GLY:H	13	0.3
(1,479)	1:61:A:LEU:HD23	1:155:A:GLY:H	13	0.3
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG21	7	0.3
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG22	7	0.3
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG23	7	0.3
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG21	7	0.3
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG22	7	0.3
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG23	7	0.3
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG21	7	0.3
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG22	7	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG23	7	0.3
(1,436)	1:58:A:SER:H	1:160:A:LEU:HG	11	0.3
(1,435)	1:58:A:SER:HA	1:122:A:LEU:HG	16	0.3
(1,424)	1:56:A:ARG:HE	1:57:A:CYS:H	16	0.3
(1,373)	1:34:A:TRP:HD1	1:35:A:GLU:H	17	0.3
(1,369)	1:33:A:GLN:HG2	1:34:A:TRP:H	14	0.3
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB1	9	0.3
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB2	9	0.3
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB3	9	0.3
(1,318)	1:29:A:THR:H	1:30:A:ASN:HB3	20	0.3
(1,311)	1:27:A:HIS:HB2	1:29:A:THR:H	8	0.3
(1,311)	1:27:A:HIS:HB2	1:29:A:THR:H	10	0.3
(1,218)	1:12:A:GLU:HB2	1:25:A:PHE:H	3	0.3
(1,194)	1:13:A:LYS:HG2	1:24:A:TYR:HA	7	0.3
(1,75)	1:13:A:LYS:HA	1:23:A:TYR:H	6	0.3
(1,64)	1:12:A:GLU:H	1:24:A:TYR:HD1	13	0.3
(1,64)	1:12:A:GLU:H	1:24:A:TYR:HD2	13	0.3
(1,61)	1:11:A:TRP:HA	1:12:A:GLU:HB3	8	0.3
(1,52)	1:11:A:TRP:HE1	1:26:A:ASN:HB2	7	0.3
(1,52)	1:11:A:TRP:HE1	1:26:A:ASN:HB3	7	0.3
(1,17)	1:6:A:LYS:HB3	1:7:A:LEU:H	14	0.3
(3,44)	1:72:A:SER:O	1:75:A:GLN:H	1	0.29
(3,35)	1:62:A:VAL:N	1:156:A:ILE:O	5	0.29
(2,93)	1:93:A:ILE:HD11	2:643:B:PRO:HA	3	0.29
(2,93)	1:93:A:ILE:HD12	2:643:B:PRO:HA	3	0.29
(2,93)	1:93:A:ILE:HD13	2:643:B:PRO:HA	3	0.29
(2,42)	1:130:A:MET:HB2	1:134:A:PHE:HD1	1	0.29
(2,42)	1:130:A:MET:HB2	1:134:A:PHE:HD2	1	0.29
(2,25)	1:88:A:LEU:HG	1:92:A:TYR:H	13	0.29
(2,4)	1:21:A:ARG:HE	1:22:A:VAL:H	4	0.29
(1,2589)	1:122:A:LEU:HD21	2:656:B:PHE:HE1	19	0.29
(1,2589)	1:122:A:LEU:HD21	2:656:B:PHE:HE2	19	0.29
(1,2589)	1:122:A:LEU:HD22	2:656:B:PHE:HE1	19	0.29
(1,2589)	1:122:A:LEU:HD22	2:656:B:PHE:HE2	19	0.29
(1,2589)	1:122:A:LEU:HD23	2:656:B:PHE:HE1	19	0.29
(1,2589)	1:122:A:LEU:HD23	2:656:B:PHE:HE2	19	0.29
(1,2587)	1:115:A:SER:H	2:659:B:PHE:HD1	3	0.29
(1,2587)	1:115:A:SER:H	2:659:B:PHE:HD2	3	0.29
(1,2561)	2:655:B:GLU:H	2:656:B:PHE:HD1	15	0.29
(1,2561)	2:655:B:GLU:H	2:656:B:PHE:HD2	15	0.29
(1,2551)	2:652:B:ASP:H	2:654:B:SER:H	6	0.29
(1,2526)	2:646:B:GLU:HB2	2:648:B:ILE:H	14	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2520)	2:646:B:GLU:HG3	2:647:B:VAL:H	3	0.29
(1,2520)	2:646:B:GLU:HG3	2:647:B:VAL:H	12	0.29
(1,2517)	2:646:B:GLU:HG2	2:647:B:VAL:H	17	0.29
(1,2496)	2:659:B:PHE:H	2:659:B:PHE:HE1	7	0.29
(1,2496)	2:659:B:PHE:H	2:659:B:PHE:HE2	7	0.29
(1,2250)	1:141:A:LEU:H	1:141:A:LEU:HD21	15	0.29
(1,2250)	1:141:A:LEU:H	1:141:A:LEU:HD22	15	0.29
(1,2250)	1:141:A:LEU:H	1:141:A:LEU:HD23	15	0.29
(1,2250)	1:141:A:LEU:H	1:141:A:LEU:HD11	15	0.29
(1,2250)	1:141:A:LEU:H	1:141:A:LEU:HD12	15	0.29
(1,2250)	1:141:A:LEU:H	1:141:A:LEU:HD13	15	0.29
(1,2046)	1:97:A:LYS:H	1:97:A:LYS:HB2	12	0.29
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD11	10	0.29
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD12	10	0.29
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD13	10	0.29
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD11	18	0.29
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD12	18	0.29
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD13	18	0.29
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD11	10	0.29
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD12	10	0.29
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD13	10	0.29
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD11	19	0.29
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD12	19	0.29
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD13	19	0.29
(1,1750)	1:56:A:ARG:HA	1:56:A:ARG:HE	12	0.29
(1,1455)	1:6:A:LYS:H	1:6:A:LYS:HB3	17	0.29
(1,1429)	1:143:A:THR:HG21	1:163:A:GLU:HB2	10	0.29
(1,1429)	1:143:A:THR:HG22	1:163:A:GLU:HB2	10	0.29
(1,1429)	1:143:A:THR:HG23	1:163:A:GLU:HB2	10	0.29
(1,1399)	1:143:A:THR:H	1:161:A:ARG:HD2	14	0.29
(1,1353)	1:57:A:CYS:HB3	1:160:A:LEU:H	11	0.29
(1,1349)	1:158:A:ILE:H	1:159:A:ILE:HD11	7	0.29
(1,1349)	1:158:A:ILE:H	1:159:A:ILE:HD12	7	0.29
(1,1349)	1:158:A:ILE:H	1:159:A:ILE:HD13	7	0.29
(1,1348)	1:157:A:HIS:HB2	1:159:A:ILE:HD11	19	0.29
(1,1348)	1:157:A:HIS:HB2	1:159:A:ILE:HD12	19	0.29
(1,1348)	1:157:A:HIS:HB2	1:159:A:ILE:HD13	19	0.29
(1,1348)	1:157:A:HIS:HB3	1:159:A:ILE:HD11	19	0.29
(1,1348)	1:157:A:HIS:HB3	1:159:A:ILE:HD12	19	0.29
(1,1348)	1:157:A:HIS:HB3	1:159:A:ILE:HD13	19	0.29
(1,1330)	1:92:A:TYR:HD1	1:158:A:ILE:HG21	16	0.29
(1,1330)	1:92:A:TYR:HD1	1:158:A:ILE:HG22	16	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1330)	1:92:A:TYR:HD1	1:158:A:ILE:HG23	16	0.29
(1,1330)	1:92:A:TYR:HD2	1:158:A:ILE:HG21	16	0.29
(1,1330)	1:92:A:TYR:HD2	1:158:A:ILE:HG22	16	0.29
(1,1330)	1:92:A:TYR:HD2	1:158:A:ILE:HG23	16	0.29
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG21	6	0.29
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG22	6	0.29
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG23	6	0.29
(1,1242)	1:150:A:VAL:HG11	1:157:A:HIS:H	20	0.29
(1,1242)	1:150:A:VAL:HG12	1:157:A:HIS:H	20	0.29
(1,1242)	1:150:A:VAL:HG13	1:157:A:HIS:H	20	0.29
(1,1217)	1:145:A:GLU:HB3	1:147:A:SER:H	19	0.29
(1,1212)	1:146:A:MET:HG2	1:160:A:LEU:HG	2	0.29
(1,1177)	1:137:A:ALA:HB1	1:141:A:LEU:H	12	0.29
(1,1177)	1:137:A:ALA:HB2	1:141:A:LEU:H	12	0.29
(1,1177)	1:137:A:ALA:HB3	1:141:A:LEU:H	12	0.29
(1,1161)	1:136:A:ASP:HB2	1:138:A:SER:H	8	0.29
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB1	1	0.29
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB2	1	0.29
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB3	1	0.29
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB1	17	0.29
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB2	17	0.29
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB3	17	0.29
(1,1080)	1:54:A:ARG:HE	1:124:A:ALA:HB1	8	0.29
(1,1080)	1:54:A:ARG:HE	1:124:A:ALA:HB2	8	0.29
(1,1080)	1:54:A:ARG:HE	1:124:A:ALA:HB3	8	0.29
(1,1051)	1:57:A:CYS:H	1:122:A:LEU:HD21	7	0.29
(1,1051)	1:57:A:CYS:H	1:122:A:LEU:HD22	7	0.29
(1,1051)	1:57:A:CYS:H	1:122:A:LEU:HD23	7	0.29
(1,1032)	1:107:A:ALA:HB1	1:119:A:ARG:H	16	0.29
(1,1032)	1:107:A:ALA:HB2	1:119:A:ARG:H	16	0.29
(1,1032)	1:107:A:ALA:HB3	1:119:A:ARG:H	16	0.29
(1,1011)	1:116:A:ALA:HB1	1:119:A:ARG:H	10	0.29
(1,1011)	1:116:A:ALA:HB2	1:119:A:ARG:H	10	0.29
(1,1011)	1:116:A:ALA:HB3	1:119:A:ARG:H	10	0.29
(1,985)	1:61:A:LEU:HD21	1:113:A:CYS:HA	1	0.29
(1,985)	1:61:A:LEU:HD22	1:113:A:CYS:HA	1	0.29
(1,985)	1:61:A:LEU:HD23	1:113:A:CYS:HA	1	0.29
(1,985)	1:61:A:LEU:HD21	1:113:A:CYS:HA	14	0.29
(1,985)	1:61:A:LEU:HD22	1:113:A:CYS:HA	14	0.29
(1,985)	1:61:A:LEU:HD23	1:113:A:CYS:HA	14	0.29
(1,970)	1:108:A:SER:H	1:110:A:PHE:H	18	0.29
(1,959)	1:108:A:SER:HA	1:111:A:SER:H	9	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,958)	1:108:A:SER:HA	1:110:A:PHE:H	4	0.29
(1,958)	1:108:A:SER:HA	1:110:A:PHE:H	20	0.29
(1,941)	1:106:A:LEU:HD11	1:107:A:ALA:H	15	0.29
(1,941)	1:106:A:LEU:HD12	1:107:A:ALA:H	15	0.29
(1,941)	1:106:A:LEU:HD13	1:107:A:ALA:H	15	0.29
(1,914)	1:104:A:GLU:H	1:106:A:LEU:HB3	14	0.29
(1,871)	1:96:A:ILE:HB	1:103:A:PHE:H	15	0.29
(1,811)	1:94:A:GLN:H	1:96:A:ILE:H	15	0.29
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE1	16	0.29
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE2	16	0.29
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE3	16	0.29
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD11	14	0.29
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD12	14	0.29
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD13	14	0.29
(1,743)	1:89:A:ILE:HG13	1:90:A:ASN:H	15	0.29
(1,737)	1:86:A:LEU:HB3	1:90:A:ASN:H	1	0.29
(1,735)	1:89:A:ILE:HB	1:158:A:ILE:HD11	19	0.29
(1,735)	1:89:A:ILE:HB	1:158:A:ILE:HD12	19	0.29
(1,735)	1:89:A:ILE:HB	1:158:A:ILE:HD13	19	0.29
(1,681)	1:85:A:ALA:H	1:88:A:LEU:HD11	17	0.29
(1,681)	1:85:A:ALA:H	1:88:A:LEU:HD12	17	0.29
(1,681)	1:85:A:ALA:H	1:88:A:LEU:HD13	17	0.29
(1,640)	1:65:A:SER:HB3	1:81:A:THR:HA	20	0.29
(1,551)	1:70:A:PRO:HB3	1:71:A:SER:H	8	0.29
(1,541)	1:67:A:SER:HB3	1:70:A:PRO:HA	7	0.29
(1,527)	1:66:A:GLN:HG2	1:81:A:THR:HG21	13	0.29
(1,527)	1:66:A:GLN:HG2	1:81:A:THR:HG22	13	0.29
(1,527)	1:66:A:GLN:HG2	1:81:A:THR:HG23	13	0.29
(1,496)	1:62:A:VAL:HG11	1:88:A:LEU:H	19	0.29
(1,496)	1:62:A:VAL:HG12	1:88:A:LEU:H	19	0.29
(1,496)	1:62:A:VAL:HG13	1:88:A:LEU:H	19	0.29
(1,457)	1:60:A:LEU:HD11	1:108:A:SER:H	16	0.29
(1,457)	1:60:A:LEU:HD12	1:108:A:SER:H	16	0.29
(1,457)	1:60:A:LEU:HD13	1:108:A:SER:H	16	0.29
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB1	10	0.29
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB2	10	0.29
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB3	10	0.29
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB1	16	0.29
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB2	16	0.29
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB3	16	0.29
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG21	4	0.29
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG22	4	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG23	4	0.29
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG21	4	0.29
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG22	4	0.29
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG23	4	0.29
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG21	4	0.29
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG22	4	0.29
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG23	4	0.29
(1,369)	1:33:A:GLN:HG2	1:34:A:TRP:H	1	0.29
(1,355)	1:25:A:PHE:HE1	1:32:A:SER:HB2	10	0.29
(1,355)	1:25:A:PHE:HE2	1:32:A:SER:HB2	10	0.29
(1,354)	1:24:A:TYR:H	1:32:A:SER:HB3	16	0.29
(1,349)	1:23:A:TYR:HD1	1:32:A:SER:HB2	13	0.29
(1,349)	1:23:A:TYR:HD2	1:32:A:SER:HB2	13	0.29
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB1	7	0.29
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB2	7	0.29
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB3	7	0.29
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB1	17	0.29
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB2	17	0.29
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB3	17	0.29
(1,311)	1:27:A:HIS:HB2	1:29:A:THR:H	13	0.29
(1,277)	1:26:A:ASN:H	1:30:A:ASN:H	12	0.29
(1,176)	1:23:A:TYR:HB3	1:24:A:TYR:HD1	2	0.29
(1,176)	1:23:A:TYR:HB3	1:24:A:TYR:HD2	2	0.29
(1,103)	1:14:A:ARG:HG2	1:15:A:MET:H	10	0.29
(1,103)	1:14:A:ARG:HG2	1:15:A:MET:H	16	0.29
(1,98)	1:14:A:ARG:H	1:24:A:TYR:H	13	0.29
(1,66)	1:12:A:GLU:H	1:25:A:PHE:HE1	13	0.29
(1,66)	1:12:A:GLU:H	1:25:A:PHE:HE2	13	0.29
(1,11)	1:4:A:GLU:H	1:6:A:LYS:H	5	0.29
(3,39)	1:64:A:HIS:O	1:67:A:SER:N	1	0.28
(2,111)	1:160:A:LEU:H	2:651:B:ILE:HG12	3	0.28
(2,111)	1:160:A:LEU:H	2:651:B:ILE:HG13	3	0.28
(2,111)	1:160:A:LEU:H	2:651:B:ILE:HG12	8	0.28
(2,111)	1:160:A:LEU:H	2:651:B:ILE:HG13	8	0.28
(2,111)	1:160:A:LEU:H	2:651:B:ILE:HG12	9	0.28
(2,111)	1:160:A:LEU:H	2:651:B:ILE:HG13	9	0.28
(2,103)	1:137:A:ALA:H	2:656:B:PHE:HB2	14	0.28
(2,86)	1:29:A:THR:HG21	2:647:B:VAL:HA	13	0.28
(2,86)	1:29:A:THR:HG22	2:647:B:VAL:HA	13	0.28
(2,86)	1:29:A:THR:HG23	2:647:B:VAL:HA	13	0.28
(2,25)	1:88:A:LEU:HG	1:92:A:TYR:H	3	0.28
(2,25)	1:88:A:LEU:HG	1:92:A:TYR:H	8	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,20)	1:68:A:ARG:H	1:153:A:ASP:HB2	17	0.28
(2,20)	1:68:A:ARG:H	1:153:A:ASP:HB3	17	0.28
(1,2587)	1:115:A:SER:H	2:659:B:PHE:HD1	7	0.28
(1,2587)	1:115:A:SER:H	2:659:B:PHE:HD2	7	0.28
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG21	16	0.28
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG22	16	0.28
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG23	16	0.28
(1,2557)	2:654:B:SER:H	2:655:B:GLU:H	4	0.28
(1,2553)	2:651:B:ILE:HG21	2:653:B:GLN:HE21	13	0.28
(1,2553)	2:651:B:ILE:HG21	2:653:B:GLN:HE22	13	0.28
(1,2553)	2:651:B:ILE:HG22	2:653:B:GLN:HE21	13	0.28
(1,2553)	2:651:B:ILE:HG22	2:653:B:GLN:HE22	13	0.28
(1,2553)	2:651:B:ILE:HG23	2:653:B:GLN:HE21	13	0.28
(1,2553)	2:651:B:ILE:HG23	2:653:B:GLN:HE22	13	0.28
(1,2530)	2:648:B:ILE:HD11	2:649:B:ARG:H	17	0.28
(1,2530)	2:648:B:ILE:HD12	2:649:B:ARG:H	17	0.28
(1,2530)	2:648:B:ILE:HD13	2:649:B:ARG:H	17	0.28
(1,2517)	2:646:B:GLU:HG2	2:647:B:VAL:H	19	0.28
(1,2250)	1:141:A:LEU:H	1:141:A:LEU:HD21	11	0.28
(1,2250)	1:141:A:LEU:H	1:141:A:LEU:HD22	11	0.28
(1,2250)	1:141:A:LEU:H	1:141:A:LEU:HD23	11	0.28
(1,2250)	1:141:A:LEU:H	1:141:A:LEU:HD11	11	0.28
(1,2250)	1:141:A:LEU:H	1:141:A:LEU:HD12	11	0.28
(1,2250)	1:141:A:LEU:H	1:141:A:LEU:HD13	11	0.28
(1,2103)	1:109:A:GLN:HG2	1:109:A:GLN:HE22	3	0.28
(1,2103)	1:109:A:GLN:HG2	1:109:A:GLN:HE22	5	0.28
(1,2033)	1:95:A:LYS:H	1:95:A:LYS:HD2	3	0.28
(1,1703)	1:36:A:ARG:H	1:36:A:ARG:HD2	8	0.28
(1,1571)	1:21:A:ARG:H	1:21:A:ARG:HD2	3	0.28
(1,1457)	1:6:A:LYS:H	1:6:A:LYS:HG2	3	0.28
(1,1455)	1:6:A:LYS:H	1:6:A:LYS:HB3	2	0.28
(1,1363)	1:96:A:ILE:HG21	1:160:A:LEU:HD11	14	0.28
(1,1363)	1:96:A:ILE:HG21	1:160:A:LEU:HD12	14	0.28
(1,1363)	1:96:A:ILE:HG21	1:160:A:LEU:HD13	14	0.28
(1,1363)	1:96:A:ILE:HG22	1:160:A:LEU:HD11	14	0.28
(1,1363)	1:96:A:ILE:HG22	1:160:A:LEU:HD12	14	0.28
(1,1363)	1:96:A:ILE:HG22	1:160:A:LEU:HD13	14	0.28
(1,1363)	1:96:A:ILE:HG23	1:160:A:LEU:HD11	14	0.28
(1,1363)	1:96:A:ILE:HG23	1:160:A:LEU:HD12	14	0.28
(1,1363)	1:96:A:ILE:HG23	1:160:A:LEU:HD13	14	0.28
(1,1335)	1:57:A:CYS:HA	1:159:A:ILE:HG21	14	0.28
(1,1335)	1:57:A:CYS:HA	1:159:A:ILE:HG22	14	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1335)	1:57:A:CYS:HA	1:159:A:ILE:HG23	14	0.28
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG21	18	0.28
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG22	18	0.28
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG23	18	0.28
(1,1212)	1:146:A:MET:HG2	1:160:A:LEU:HG	18	0.28
(1,1206)	1:145:A:GLU:HB3	1:146:A:MET:HB2	12	0.28
(1,1178)	1:137:A:ALA:HA	1:141:A:LEU:H	1	0.28
(1,1161)	1:136:A:ASP:HB2	1:138:A:SER:H	1	0.28
(1,1047)	1:119:A:ARG:HD2	1:121:A:ASP:H	11	0.28
(1,1015)	1:116:A:ALA:HB1	1:120:A:GLY:H	16	0.28
(1,1015)	1:116:A:ALA:HB2	1:120:A:GLY:H	16	0.28
(1,1015)	1:116:A:ALA:HB3	1:120:A:GLY:H	16	0.28
(1,1011)	1:116:A:ALA:HB1	1:119:A:ARG:H	15	0.28
(1,1011)	1:116:A:ALA:HB2	1:119:A:ARG:H	15	0.28
(1,1011)	1:116:A:ALA:HB3	1:119:A:ARG:H	15	0.28
(1,959)	1:108:A:SER:HA	1:111:A:SER:H	19	0.28
(1,940)	1:106:A:LEU:HG	1:107:A:ALA:H	18	0.28
(1,917)	1:105:A:SER:HB2	1:106:A:LEU:H	17	0.28
(1,913)	1:103:A:PHE:H	1:106:A:LEU:HB3	4	0.28
(1,913)	1:103:A:PHE:H	1:106:A:LEU:HB3	9	0.28
(1,888)	1:103:A:PHE:HE1	1:120:A:GLY:H	8	0.28
(1,888)	1:103:A:PHE:HE2	1:120:A:GLY:H	8	0.28
(1,811)	1:94:A:GLN:H	1:96:A:ILE:H	11	0.28
(1,772)	1:92:A:TYR:H	1:93:A:ILE:HB	3	0.28
(1,764)	1:88:A:LEU:HA	1:92:A:TYR:H	7	0.28
(1,753)	1:90:A:ASN:HD22	1:91:A:GLY:H	5	0.28
(1,743)	1:89:A:ILE:HG13	1:90:A:ASN:H	6	0.28
(1,723)	1:86:A:LEU:HD21	1:89:A:ILE:HB	14	0.28
(1,723)	1:86:A:LEU:HD22	1:89:A:ILE:HB	14	0.28
(1,723)	1:86:A:LEU:HD23	1:89:A:ILE:HB	14	0.28
(1,723)	1:86:A:LEU:HD21	1:89:A:ILE:HB	20	0.28
(1,723)	1:86:A:LEU:HD22	1:89:A:ILE:HB	20	0.28
(1,723)	1:86:A:LEU:HD23	1:89:A:ILE:HB	20	0.28
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB1	3	0.28
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB2	3	0.28
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB3	3	0.28
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB1	20	0.28
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB2	20	0.28
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB3	20	0.28
(1,648)	1:66:A:GLN:HE22	1:82:A:LYS:HG3	2	0.28
(1,648)	1:66:A:GLN:HE22	1:82:A:LYS:HG3	8	0.28
(1,647)	1:65:A:SER:H	1:82:A:LYS:H	13	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG21	2	0.28
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG22	2	0.28
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG23	2	0.28
(1,618)	1:78:A:ILE:HA	1:80:A:ARG:H	5	0.28
(1,576)	1:73:A:TRP:HE1	1:115:A:SER:H	17	0.28
(1,551)	1:70:A:PRO:HB3	1:71:A:SER:H	12	0.28
(1,540)	1:67:A:SER:HA	1:69:A:ARG:H	17	0.28
(1,527)	1:66:A:GLN:HG2	1:81:A:THR:HG21	4	0.28
(1,527)	1:66:A:GLN:HG2	1:81:A:THR:HG22	4	0.28
(1,527)	1:66:A:GLN:HG2	1:81:A:THR:HG23	4	0.28
(1,515)	1:63:A:LYS:H	1:156:A:ILE:H	9	0.28
(1,457)	1:60:A:LEU:HD11	1:108:A:SER:H	10	0.28
(1,457)	1:60:A:LEU:HD12	1:108:A:SER:H	10	0.28
(1,457)	1:60:A:LEU:HD13	1:108:A:SER:H	10	0.28
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB1	11	0.28
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB2	11	0.28
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB3	11	0.28
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG21	17	0.28
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG22	17	0.28
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG23	17	0.28
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG21	17	0.28
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG22	17	0.28
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG23	17	0.28
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG21	17	0.28
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG22	17	0.28
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG23	17	0.28
(1,415)	1:56:A:ARG:HA	1:124:A:ALA:H	3	0.28
(1,377)	1:33:A:GLN:HG2	1:35:A:GLU:H	16	0.28
(1,321)	1:25:A:PHE:HZ	1:30:A:ASN:H	10	0.28
(1,321)	1:25:A:PHE:HZ	1:30:A:ASN:H	15	0.28
(1,320)	1:25:A:PHE:HE1	1:30:A:ASN:H	4	0.28
(1,320)	1:25:A:PHE:HE2	1:30:A:ASN:H	4	0.28
(1,295)	1:27:A:HIS:H	1:29:A:THR:H	20	0.28
(1,262)	1:25:A:PHE:HE1	1:26:A:ASN:HA	5	0.28
(1,262)	1:25:A:PHE:HE2	1:26:A:ASN:HA	5	0.28
(1,244)	1:11:A:TRP:H	1:26:A:ASN:HB2	8	0.28
(1,244)	1:11:A:TRP:H	1:26:A:ASN:HB2	12	0.28
(1,190)	1:13:A:LYS:HB3	1:24:A:TYR:HA	3	0.28
(1,108)	1:15:A:MET:H	1:22:A:VAL:HA	18	0.28
(1,84)	1:13:A:LYS:HG2	1:14:A:ARG:H	1	0.28
(1,75)	1:13:A:LYS:HA	1:23:A:TYR:H	13	0.28
(1,69)	1:7:A:LEU:HD21	1:13:A:LYS:HE2	20	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,69)	1:7:A:LEU:HD22	1:13:A:LYS:HE2	20	0.28
(1,69)	1:7:A:LEU:HD23	1:13:A:LYS:HE2	20	0.28
(1,69)	1:7:A:LEU:HD11	1:13:A:LYS:HE2	20	0.28
(1,69)	1:7:A:LEU:HD12	1:13:A:LYS:HE2	20	0.28
(1,69)	1:7:A:LEU:HD13	1:13:A:LYS:HE2	20	0.28
(1,66)	1:12:A:GLU:H	1:25:A:PHE:HE1	17	0.28
(1,66)	1:12:A:GLU:H	1:25:A:PHE:HE2	17	0.28
(1,52)	1:11:A:TRP:HE1	1:26:A:ASN:HB2	12	0.28
(1,52)	1:11:A:TRP:HE1	1:26:A:ASN:HB3	12	0.28
(1,52)	1:11:A:TRP:HE1	1:26:A:ASN:HB2	17	0.28
(1,52)	1:11:A:TRP:HE1	1:26:A:ASN:HB3	17	0.28
(1,14)	1:6:A:LYS:HG2	1:7:A:LEU:H	1	0.28
(3,43)	1:72:A:SER:O	1:75:A:GLN:N	10	0.27
(3,43)	1:72:A:SER:O	1:75:A:GLN:N	16	0.27
(3,28)	1:56:A:ARG:H	1:163:A:GLU:O	16	0.27
(2,98)	1:124:A:ALA:H	2:656:B:PHE:HE1	2	0.27
(2,98)	1:124:A:ALA:H	2:656:B:PHE:HE2	2	0.27
(2,90)	1:56:A:ARG:H	2:651:B:ILE:HG12	18	0.27
(2,90)	1:56:A:ARG:H	2:651:B:ILE:HG13	18	0.27
(2,25)	1:88:A:LEU:HG	1:92:A:TYR:H	2	0.27
(2,25)	1:88:A:LEU:HG	1:92:A:TYR:H	19	0.27
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG21	4	0.27
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG22	4	0.27
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG23	4	0.27
(1,2523)	2:647:B:VAL:HA	2:649:B:ARG:H	4	0.27
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE1	20	0.27
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE2	20	0.27
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE3	20	0.27
(1,2209)	1:131:A:GLN:HA	1:131:A:GLN:HE22	20	0.27
(1,2103)	1:109:A:GLN:HG2	1:109:A:GLN:HE22	1	0.27
(1,2046)	1:97:A:LYS:H	1:97:A:LYS:HB2	5	0.27
(1,2046)	1:97:A:LYS:H	1:97:A:LYS:HB2	6	0.27
(1,2046)	1:97:A:LYS:H	1:97:A:LYS:HB2	7	0.27
(1,2046)	1:97:A:LYS:H	1:97:A:LYS:HB2	8	0.27
(1,2046)	1:97:A:LYS:H	1:97:A:LYS:HB2	14	0.27
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD11	9	0.27
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD12	9	0.27
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD13	9	0.27
(1,1906)	1:81:A:THR:H	1:81:A:THR:HG21	20	0.27
(1,1906)	1:81:A:THR:H	1:81:A:THR:HG22	20	0.27
(1,1906)	1:81:A:THR:H	1:81:A:THR:HG23	20	0.27
(1,1750)	1:56:A:ARG:HA	1:56:A:ARG:HE	7	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1750)	1:56:A:ARG:HA	1:56:A:ARG:HE	18	0.27
(1,1694)	1:35:A:GLU:H	1:35:A:GLU:HG3	11	0.27
(1,1457)	1:6:A:LYS:H	1:6:A:LYS:HG2	12	0.27
(1,1457)	1:6:A:LYS:H	1:6:A:LYS:HG2	19	0.27
(1,1455)	1:6:A:LYS:H	1:6:A:LYS:HB3	1	0.27
(1,1423)	1:55:A:VAL:HB	1:163:A:GLU:H	19	0.27
(1,1413)	1:56:A:ARG:HD2	1:162:A:THR:HG21	20	0.27
(1,1413)	1:56:A:ARG:HD2	1:162:A:THR:HG22	20	0.27
(1,1413)	1:56:A:ARG:HD2	1:162:A:THR:HG23	20	0.27
(1,1382)	1:159:A:ILE:HG12	1:160:A:LEU:H	16	0.27
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG21	11	0.27
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG22	11	0.27
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG23	11	0.27
(1,1199)	1:142:A:ARG:HG2	1:143:A:THR:H	10	0.27
(1,1161)	1:136:A:ASP:HB2	1:138:A:SER:H	15	0.27
(1,1052)	1:58:A:SER:HB2	1:122:A:LEU:H	5	0.27
(1,1015)	1:116:A:ALA:HB1	1:120:A:GLY:H	8	0.27
(1,1015)	1:116:A:ALA:HB2	1:120:A:GLY:H	8	0.27
(1,1015)	1:116:A:ALA:HB3	1:120:A:GLY:H	8	0.27
(1,1015)	1:116:A:ALA:HB1	1:120:A:GLY:H	18	0.27
(1,1015)	1:116:A:ALA:HB2	1:120:A:GLY:H	18	0.27
(1,1015)	1:116:A:ALA:HB3	1:120:A:GLY:H	18	0.27
(1,1012)	1:116:A:ALA:H	1:119:A:ARG:H	4	0.27
(1,1011)	1:116:A:ALA:HB1	1:119:A:ARG:H	14	0.27
(1,1011)	1:116:A:ALA:HB2	1:119:A:ARG:H	14	0.27
(1,1011)	1:116:A:ALA:HB3	1:119:A:ARG:H	14	0.27
(1,985)	1:61:A:LEU:HD21	1:113:A:CYS:HA	16	0.27
(1,985)	1:61:A:LEU:HD22	1:113:A:CYS:HA	16	0.27
(1,985)	1:61:A:LEU:HD23	1:113:A:CYS:HA	16	0.27
(1,940)	1:106:A:LEU:HG	1:107:A:ALA:H	13	0.27
(1,913)	1:103:A:PHE:H	1:106:A:LEU:HB3	8	0.27
(1,886)	1:103:A:PHE:HE1	1:107:A:ALA:H	15	0.27
(1,886)	1:103:A:PHE:HE2	1:107:A:ALA:H	15	0.27
(1,862)	1:101:A:GLU:HG2	1:102:A:ASP:H	17	0.27
(1,811)	1:94:A:GLN:H	1:96:A:ILE:H	18	0.27
(1,743)	1:89:A:ILE:HG13	1:90:A:ASN:H	9	0.27
(1,740)	1:89:A:ILE:HG12	1:90:A:ASN:H	5	0.27
(1,721)	1:61:A:LEU:HA	1:89:A:ILE:HD11	13	0.27
(1,721)	1:61:A:LEU:HA	1:89:A:ILE:HD12	13	0.27
(1,721)	1:61:A:LEU:HA	1:89:A:ILE:HD13	13	0.27
(1,663)	1:82:A:LYS:HB3	1:83:A:GLU:H	3	0.27
(1,654)	1:82:A:LYS:HG2	1:84:A:GLU:H	6	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,654)	1:82:A:LYS:HG3	1:84:A:GLU:H	6	0.27
(1,648)	1:66:A:GLN:HE22	1:82:A:LYS:HG3	13	0.27
(1,618)	1:78:A:ILE:HA	1:80:A:ARG:H	7	0.27
(1,593)	1:71:A:SER:HB3	1:77:A:LYS:HA	18	0.27
(1,591)	1:74:A:ARG:HE	1:75:A:GLN:H	11	0.27
(1,591)	1:74:A:ARG:HE	1:75:A:GLN:H	15	0.27
(1,564)	1:72:A:SER:H	1:78:A:ILE:HG12	4	0.27
(1,554)	1:70:A:PRO:HG3	1:71:A:SER:H	3	0.27
(1,551)	1:70:A:PRO:HB3	1:71:A:SER:H	3	0.27
(1,538)	1:66:A:GLN:HG2	1:67:A:SER:H	7	0.27
(1,527)	1:66:A:GLN:HG2	1:81:A:THR:HG21	9	0.27
(1,527)	1:66:A:GLN:HG2	1:81:A:THR:HG22	9	0.27
(1,527)	1:66:A:GLN:HG2	1:81:A:THR:HG23	9	0.27
(1,527)	1:66:A:GLN:HG2	1:81:A:THR:HG21	18	0.27
(1,527)	1:66:A:GLN:HG2	1:81:A:THR:HG22	18	0.27
(1,527)	1:66:A:GLN:HG2	1:81:A:THR:HG23	18	0.27
(1,521)	1:64:A:HIS:H	1:66:A:GLN:H	3	0.27
(1,515)	1:63:A:LYS:H	1:156:A:ILE:H	6	0.27
(1,514)	1:63:A:LYS:HB2	1:70:A:PRO:HA	1	0.27
(1,514)	1:63:A:LYS:HB2	1:70:A:PRO:HA	2	0.27
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB1	7	0.27
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB2	7	0.27
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB3	7	0.27
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG21	19	0.27
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG22	19	0.27
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG23	19	0.27
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG21	19	0.27
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG22	19	0.27
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG23	19	0.27
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG21	19	0.27
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG22	19	0.27
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG23	19	0.27
(1,424)	1:56:A:ARG:HE	1:57:A:CYS:H	8	0.27
(1,393)	1:53:A:ALA:HB1	1:54:A:ARG:H	10	0.27
(1,393)	1:53:A:ALA:HB2	1:54:A:ARG:H	10	0.27
(1,393)	1:53:A:ALA:HB3	1:54:A:ARG:H	10	0.27
(1,388)	1:35:A:GLU:HG2	1:36:A:ARG:H	9	0.27
(1,333)	1:25:A:PHE:HA	1:31:A:ALA:H	13	0.27
(1,311)	1:27:A:HIS:HB2	1:29:A:THR:H	4	0.27
(1,277)	1:26:A:ASN:H	1:30:A:ASN:H	18	0.27
(1,262)	1:25:A:PHE:HE1	1:26:A:ASN:HA	4	0.27
(1,262)	1:25:A:PHE:HE2	1:26:A:ASN:HA	4	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,194)	1:13:A:LYS:HG2	1:24:A:TYR:HA	9	0.27
(1,189)	1:13:A:LYS:H	1:24:A:TYR:HA	11	0.27
(1,180)	1:23:A:TYR:HD1	1:33:A:GLN:HA	6	0.27
(1,180)	1:23:A:TYR:HD2	1:33:A:GLN:HA	6	0.27
(1,176)	1:23:A:TYR:HB3	1:24:A:TYR:HD1	11	0.27
(1,176)	1:23:A:TYR:HB3	1:24:A:TYR:HD2	11	0.27
(1,134)	1:20:A:GLY:H	1:21:A:ARG:HA	20	0.27
(1,116)	1:16:A:SER:H	1:20:A:GLY:HA2	14	0.27
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG21	15	0.27
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG22	15	0.27
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG23	15	0.27
(1,96)	1:14:A:ARG:H	1:23:A:TYR:HD1	8	0.27
(1,96)	1:14:A:ARG:H	1:23:A:TYR:HD2	8	0.27
(1,89)	1:14:A:ARG:H	1:15:A:MET:HA	9	0.27
(1,75)	1:13:A:LYS:HA	1:23:A:TYR:H	2	0.27
(1,66)	1:12:A:GLU:H	1:25:A:PHE:HE1	7	0.27
(1,66)	1:12:A:GLU:H	1:25:A:PHE:HE2	7	0.27
(1,12)	1:5:A:GLU:HB2	1:6:A:LYS:H	8	0.27
(3,79)	1:105:A:SER:O	1:109:A:GLN:N	16	0.26
(3,71)	1:94:A:GLN:O	1:98:A:SER:N	9	0.26
(3,47)	1:81:A:THR:O	1:85:A:ALA:N	6	0.26
(2,103)	1:137:A:ALA:H	2:656:B:PHE:HB2	4	0.26
(2,103)	1:137:A:ALA:H	2:656:B:PHE:HB2	8	0.26
(2,75)	2:656:B:PHE:HB2	2:659:B:PHE:HE1	18	0.26
(2,75)	2:656:B:PHE:HB2	2:659:B:PHE:HE2	18	0.26
(2,75)	2:656:B:PHE:HB3	2:659:B:PHE:HE1	18	0.26
(2,75)	2:656:B:PHE:HB3	2:659:B:PHE:HE2	18	0.26
(2,74)	2:656:B:PHE:HB2	2:659:B:PHE:HD1	17	0.26
(2,74)	2:656:B:PHE:HB2	2:659:B:PHE:HD2	17	0.26
(2,74)	2:656:B:PHE:HB3	2:659:B:PHE:HD1	17	0.26
(2,74)	2:656:B:PHE:HB3	2:659:B:PHE:HD2	17	0.26
(2,72)	2:653:B:GLN:HA	2:656:B:PHE:HE1	16	0.26
(2,72)	2:653:B:GLN:HA	2:656:B:PHE:HE2	16	0.26
(2,58)	1:152:A:THR:HG21	1:157:A:HIS:HB3	14	0.26
(2,58)	1:152:A:THR:HG22	1:157:A:HIS:HB3	14	0.26
(2,58)	1:152:A:THR:HG23	1:157:A:HIS:HB3	14	0.26
(2,52)	1:141:A:LEU:HD21	1:148:A:GLY:H	13	0.26
(2,52)	1:141:A:LEU:HD22	1:148:A:GLY:H	13	0.26
(2,52)	1:141:A:LEU:HD23	1:148:A:GLY:H	13	0.26
(2,25)	1:88:A:LEU:HG	1:92:A:TYR:H	5	0.26
(2,25)	1:88:A:LEU:HG	1:92:A:TYR:H	20	0.26
(1,2596)	1:137:A:ALA:HB1	2:651:B:ILE:HG12	11	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2596)	1:137:A:ALA:HB1	2:651:B:ILE:HG13	11	0.26
(1,2596)	1:137:A:ALA:HB2	2:651:B:ILE:HG12	11	0.26
(1,2596)	1:137:A:ALA:HB2	2:651:B:ILE:HG13	11	0.26
(1,2596)	1:137:A:ALA:HB3	2:651:B:ILE:HG12	11	0.26
(1,2596)	1:137:A:ALA:HB3	2:651:B:ILE:HG13	11	0.26
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG21	1	0.26
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG22	1	0.26
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG23	1	0.26
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG21	10	0.26
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG22	10	0.26
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG23	10	0.26
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG21	15	0.26
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG22	15	0.26
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG23	15	0.26
(1,2530)	2:648:B:ILE:HD11	2:649:B:ARG:H	9	0.26
(1,2530)	2:648:B:ILE:HD12	2:649:B:ARG:H	9	0.26
(1,2530)	2:648:B:ILE:HD13	2:649:B:ARG:H	9	0.26
(1,2526)	2:646:B:GLU:HB2	2:648:B:ILE:H	12	0.26
(1,2103)	1:109:A:GLN:HG2	1:109:A:GLN:HE22	8	0.26
(1,2103)	1:109:A:GLN:HG2	1:109:A:GLN:HE22	9	0.26
(1,2046)	1:97:A:LYS:H	1:97:A:LYS:HB2	3	0.26
(1,2046)	1:97:A:LYS:H	1:97:A:LYS:HB2	4	0.26
(1,2046)	1:97:A:LYS:H	1:97:A:LYS:HB2	9	0.26
(1,2033)	1:95:A:LYS:H	1:95:A:LYS:HD2	6	0.26
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD11	4	0.26
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD12	4	0.26
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD13	4	0.26
(1,1750)	1:56:A:ARG:HA	1:56:A:ARG:HE	19	0.26
(1,1703)	1:36:A:ARG:H	1:36:A:ARG:HD2	1	0.26
(1,1455)	1:6:A:LYS:H	1:6:A:LYS:HB3	8	0.26
(1,1450)	1:4:A:GLU:HA	1:4:A:GLU:HG2	11	0.26
(1,1402)	1:143:A:THR:HG21	1:161:A:ARG:HD2	8	0.26
(1,1402)	1:143:A:THR:HG22	1:161:A:ARG:HD2	8	0.26
(1,1402)	1:143:A:THR:HG23	1:161:A:ARG:HD2	8	0.26
(1,1402)	1:143:A:THR:HG21	1:161:A:ARG:HD2	9	0.26
(1,1402)	1:143:A:THR:HG22	1:161:A:ARG:HD2	9	0.26
(1,1402)	1:143:A:THR:HG23	1:161:A:ARG:HD2	9	0.26
(1,1342)	1:147:A:SER:H	1:159:A:ILE:HD11	17	0.26
(1,1342)	1:147:A:SER:H	1:159:A:ILE:HD12	17	0.26
(1,1342)	1:147:A:SER:H	1:159:A:ILE:HD13	17	0.26
(1,1276)	1:63:A:LYS:HA	1:155:A:GLY:HA2	9	0.26
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG21	7	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG22	7	0.26
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG23	7	0.26
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG21	7	0.26
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG22	7	0.26
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG23	7	0.26
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG21	7	0.26
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG22	7	0.26
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG23	7	0.26
(1,1212)	1:146:A:MET:HG2	1:160:A:LEU:HG	4	0.26
(1,1177)	1:137:A:ALA:HB1	1:141:A:LEU:H	5	0.26
(1,1177)	1:137:A:ALA:HB2	1:141:A:LEU:H	5	0.26
(1,1177)	1:137:A:ALA:HB3	1:141:A:LEU:H	5	0.26
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB1	11	0.26
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB2	11	0.26
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB3	11	0.26
(1,970)	1:108:A:SER:H	1:110:A:PHE:H	5	0.26
(1,941)	1:106:A:LEU:HD11	1:107:A:ALA:H	12	0.26
(1,941)	1:106:A:LEU:HD12	1:107:A:ALA:H	12	0.26
(1,941)	1:106:A:LEU:HD13	1:107:A:ALA:H	12	0.26
(1,920)	1:106:A:LEU:HB3	1:108:A:SER:H	18	0.26
(1,885)	1:103:A:PHE:HA	1:106:A:LEU:HD11	3	0.26
(1,885)	1:103:A:PHE:HA	1:106:A:LEU:HD12	3	0.26
(1,885)	1:103:A:PHE:HA	1:106:A:LEU:HD13	3	0.26
(1,841)	1:97:A:LYS:HB3	1:98:A:SER:H	2	0.26
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD11	9	0.26
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD12	9	0.26
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD13	9	0.26
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD11	9	0.26
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD12	9	0.26
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD13	9	0.26
(1,743)	1:89:A:ILE:HG13	1:90:A:ASN:H	18	0.26
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB1	5	0.26
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB2	5	0.26
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB3	5	0.26
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB1	11	0.26
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB2	11	0.26
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB3	11	0.26
(1,669)	1:84:A:GLU:H	1:87:A:GLU:H	1	0.26
(1,669)	1:84:A:GLU:H	1:87:A:GLU:H	11	0.26
(1,659)	1:81:A:THR:HA	1:83:A:GLU:H	5	0.26
(1,641)	1:65:A:SER:HB2	1:81:A:THR:HG21	3	0.26
(1,641)	1:65:A:SER:HB2	1:81:A:THR:HG22	3	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,641)	1:65:A:SER:HB2	1:81:A:THR:HG23	3	0.26
(1,619)	1:78:A:ILE:HB	1:80:A:ARG:H	1	0.26
(1,618)	1:78:A:ILE:HA	1:80:A:ARG:H	2	0.26
(1,606)	1:75:A:GLN:HE22	1:78:A:ILE:HA	17	0.26
(1,551)	1:70:A:PRO:HB3	1:71:A:SER:H	1	0.26
(1,541)	1:67:A:SER:HB3	1:70:A:PRO:HA	8	0.26
(1,538)	1:66:A:GLN:HG2	1:67:A:SER:H	6	0.26
(1,538)	1:66:A:GLN:HG2	1:67:A:SER:H	20	0.26
(1,521)	1:64:A:HIS:H	1:66:A:GLN:H	16	0.26
(1,496)	1:62:A:VAL:HG11	1:88:A:LEU:H	2	0.26
(1,496)	1:62:A:VAL:HG12	1:88:A:LEU:H	2	0.26
(1,496)	1:62:A:VAL:HG13	1:88:A:LEU:H	2	0.26
(1,496)	1:62:A:VAL:HG11	1:88:A:LEU:H	10	0.26
(1,496)	1:62:A:VAL:HG12	1:88:A:LEU:H	10	0.26
(1,496)	1:62:A:VAL:HG13	1:88:A:LEU:H	10	0.26
(1,471)	1:61:A:LEU:HD21	1:63:A:LYS:HA	13	0.26
(1,471)	1:61:A:LEU:HD22	1:63:A:LYS:HA	13	0.26
(1,471)	1:61:A:LEU:HD23	1:63:A:LYS:HA	13	0.26
(1,457)	1:60:A:LEU:HD11	1:108:A:SER:H	19	0.26
(1,457)	1:60:A:LEU:HD12	1:108:A:SER:H	19	0.26
(1,457)	1:60:A:LEU:HD13	1:108:A:SER:H	19	0.26
(1,436)	1:58:A:SER:H	1:160:A:LEU:HG	4	0.26
(1,422)	1:56:A:ARG:HG2	1:162:A:THR:HB	15	0.26
(1,401)	1:54:A:ARG:HD2	1:55:A:VAL:HA	17	0.26
(1,388)	1:35:A:GLU:HG2	1:36:A:ARG:H	5	0.26
(1,385)	1:24:A:TYR:HD1	1:36:A:ARG:H	20	0.26
(1,385)	1:24:A:TYR:HD2	1:36:A:ARG:H	20	0.26
(1,369)	1:33:A:GLN:HG2	1:34:A:TRP:H	16	0.26
(1,347)	1:31:A:ALA:HB1	1:33:A:GLN:H	6	0.26
(1,347)	1:31:A:ALA:HB2	1:33:A:GLN:H	6	0.26
(1,347)	1:31:A:ALA:HB3	1:33:A:GLN:H	6	0.26
(1,347)	1:31:A:ALA:HB1	1:33:A:GLN:H	13	0.26
(1,347)	1:31:A:ALA:HB2	1:33:A:GLN:H	13	0.26
(1,347)	1:31:A:ALA:HB3	1:33:A:GLN:H	13	0.26
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB1	3	0.26
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB2	3	0.26
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB3	3	0.26
(1,323)	1:25:A:PHE:HZ	1:30:A:ASN:HB2	13	0.26
(1,321)	1:25:A:PHE:HZ	1:30:A:ASN:H	9	0.26
(1,320)	1:25:A:PHE:HE1	1:30:A:ASN:H	20	0.26
(1,320)	1:25:A:PHE:HE2	1:30:A:ASN:H	20	0.26
(1,264)	1:26:A:ASN:HD21	1:27:A:HIS:H	20	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,242)	1:10:A:GLY:H	1:26:A:ASN:HD21	9	0.26
(1,214)	1:11:A:TRP:HB2	1:25:A:PHE:H	18	0.26
(1,130)	1:16:A:SER:H	1:21:A:ARG:HA	2	0.26
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG21	9	0.26
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG22	9	0.26
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG23	9	0.26
(1,98)	1:14:A:ARG:H	1:24:A:TYR:H	11	0.26
(1,89)	1:14:A:ARG:H	1:15:A:MET:HA	1	0.26
(1,19)	1:7:A:LEU:HD11	1:11:A:TRP:HE3	13	0.26
(1,19)	1:7:A:LEU:HD12	1:11:A:TRP:HE3	13	0.26
(1,19)	1:7:A:LEU:HD13	1:11:A:TRP:HE3	13	0.26
(3,79)	1:105:A:SER:O	1:109:A:GLN:N	18	0.25
(3,71)	1:94:A:GLN:O	1:98:A:SER:N	6	0.25
(3,63)	1:90:A:ASN:O	1:94:A:GLN:N	11	0.25
(3,43)	1:72:A:SER:O	1:75:A:GLN:N	13	0.25
(2,68)	2:649:B:ARG:HD2	2:650:B:ASN:H	13	0.25
(2,39)	1:55:A:VAL:HG11	1:127:A:ARG:H	12	0.25
(2,39)	1:55:A:VAL:HG12	1:127:A:ARG:H	12	0.25
(2,39)	1:55:A:VAL:HG13	1:127:A:ARG:H	12	0.25
(2,34)	1:59:A:HIS:H	1:122:A:LEU:HB2	5	0.25
(2,25)	1:88:A:LEU:HG	1:92:A:TYR:H	10	0.25
(2,25)	1:88:A:LEU:HG	1:92:A:TYR:H	17	0.25
(1,2598)	1:146:A:MET:HE1	2:642:B:PRO:HB2	3	0.25
(1,2598)	1:146:A:MET:HE1	2:642:B:PRO:HB3	3	0.25
(1,2598)	1:146:A:MET:HE2	2:642:B:PRO:HB2	3	0.25
(1,2598)	1:146:A:MET:HE2	2:642:B:PRO:HB3	3	0.25
(1,2598)	1:146:A:MET:HE3	2:642:B:PRO:HB2	3	0.25
(1,2598)	1:146:A:MET:HE3	2:642:B:PRO:HB3	3	0.25
(1,2591)	1:123:A:GLY:H	2:656:B:PHE:HE1	13	0.25
(1,2591)	1:123:A:GLY:H	2:656:B:PHE:HE2	13	0.25
(1,2584)	1:114:A:SER:H	2:659:B:PHE:HD1	11	0.25
(1,2584)	1:114:A:SER:H	2:659:B:PHE:HD2	11	0.25
(1,2513)	2:646:B:GLU:HA	2:649:B:ARG:HD2	17	0.25
(1,2506)	2:644:B:ASP:H	2:645:B:GLN:HA	15	0.25
(1,2407)	2:645:B:GLN:H	2:645:B:GLN:HE21	20	0.25
(1,2385)	1:163:A:GLU:H	1:163:A:GLU:HB3	11	0.25
(1,2158)	1:119:A:ARG:H	1:119:A:ARG:HD2	12	0.25
(1,2103)	1:109:A:GLN:HG2	1:109:A:GLN:HE22	6	0.25
(1,2103)	1:109:A:GLN:HG2	1:109:A:GLN:HE22	10	0.25
(1,2103)	1:109:A:GLN:HG2	1:109:A:GLN:HE22	12	0.25
(1,2103)	1:109:A:GLN:HG2	1:109:A:GLN:HE22	14	0.25
(1,2103)	1:109:A:GLN:HG2	1:109:A:GLN:HE22	15	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2103)	1:109:A:GLN:HG2	1:109:A:GLN:HE22	16	0.25
(1,2103)	1:109:A:GLN:HG2	1:109:A:GLN:HE22	18	0.25
(1,2103)	1:109:A:GLN:HG2	1:109:A:GLN:HE22	19	0.25
(1,2056)	1:101:A:GLU:H	1:101:A:GLU:HG2	3	0.25
(1,2046)	1:97:A:LYS:H	1:97:A:LYS:HB2	1	0.25
(1,1869)	1:75:A:GLN:H	1:75:A:GLN:HE22	4	0.25
(1,1747)	1:56:A:ARG:H	1:56:A:ARG:HD2	17	0.25
(1,1694)	1:35:A:GLU:H	1:35:A:GLU:HG3	15	0.25
(1,1694)	1:35:A:GLU:H	1:35:A:GLU:HG3	18	0.25
(1,1568)	1:21:A:ARG:HB2	1:21:A:ARG:HE	1	0.25
(1,1457)	1:6:A:LYS:H	1:6:A:LYS:HG2	5	0.25
(1,1455)	1:6:A:LYS:H	1:6:A:LYS:HB3	10	0.25
(1,1455)	1:6:A:LYS:H	1:6:A:LYS:HB3	16	0.25
(1,1369)	1:104:A:GLU:H	1:160:A:LEU:HD11	5	0.25
(1,1369)	1:104:A:GLU:H	1:160:A:LEU:HD12	5	0.25
(1,1369)	1:104:A:GLU:H	1:160:A:LEU:HD13	5	0.25
(1,1346)	1:148:A:GLY:H	1:159:A:ILE:H	1	0.25
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG21	10	0.25
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG22	10	0.25
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG23	10	0.25
(1,1263)	1:151:A:PHE:H	1:156:A:ILE:HG21	9	0.25
(1,1263)	1:151:A:PHE:H	1:156:A:ILE:HG22	9	0.25
(1,1263)	1:151:A:PHE:H	1:156:A:ILE:HG23	9	0.25
(1,1259)	1:151:A:PHE:HB2	1:152:A:THR:H	10	0.25
(1,1206)	1:145:A:GLU:HB3	1:146:A:MET:HB2	5	0.25
(1,1052)	1:58:A:SER:HB2	1:122:A:LEU:H	18	0.25
(1,1047)	1:119:A:ARG:HD2	1:121:A:ASP:H	8	0.25
(1,1038)	1:119:A:ARG:HA	1:121:A:ASP:H	2	0.25
(1,1038)	1:119:A:ARG:HA	1:121:A:ASP:H	10	0.25
(1,1011)	1:116:A:ALA:HB1	1:119:A:ARG:H	6	0.25
(1,1011)	1:116:A:ALA:HB2	1:119:A:ARG:H	6	0.25
(1,1011)	1:116:A:ALA:HB3	1:119:A:ARG:H	6	0.25
(1,1011)	1:116:A:ALA:HB1	1:119:A:ARG:H	8	0.25
(1,1011)	1:116:A:ALA:HB2	1:119:A:ARG:H	8	0.25
(1,1011)	1:116:A:ALA:HB3	1:119:A:ARG:H	8	0.25
(1,941)	1:106:A:LEU:HD11	1:107:A:ALA:H	7	0.25
(1,941)	1:106:A:LEU:HD12	1:107:A:ALA:H	7	0.25
(1,941)	1:106:A:LEU:HD13	1:107:A:ALA:H	7	0.25
(1,940)	1:106:A:LEU:HG	1:107:A:ALA:H	9	0.25
(1,921)	1:106:A:LEU:H	1:109:A:GLN:H	13	0.25
(1,914)	1:104:A:GLU:H	1:106:A:LEU:HB3	15	0.25
(1,907)	1:102:A:ASP:HB3	1:106:A:LEU:H	5	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,871)	1:96:A:ILE:HB	1:103:A:PHE:H	17	0.25
(1,828)	1:96:A:ILE:H	1:146:A:MET:HE1	13	0.25
(1,828)	1:96:A:ILE:H	1:146:A:MET:HE2	13	0.25
(1,828)	1:96:A:ILE:H	1:146:A:MET:HE3	13	0.25
(1,825)	1:96:A:ILE:HD11	1:106:A:LEU:HG	18	0.25
(1,825)	1:96:A:ILE:HD12	1:106:A:LEU:HG	18	0.25
(1,825)	1:96:A:ILE:HD13	1:106:A:LEU:HG	18	0.25
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD11	7	0.25
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD12	7	0.25
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD13	7	0.25
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD11	7	0.25
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD12	7	0.25
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD13	7	0.25
(1,772)	1:92:A:TYR:H	1:93:A:ILE:HB	2	0.25
(1,743)	1:89:A:ILE:HG13	1:90:A:ASN:H	11	0.25
(1,742)	1:89:A:ILE:HD11	1:90:A:ASN:H	5	0.25
(1,742)	1:89:A:ILE:HD12	1:90:A:ASN:H	5	0.25
(1,742)	1:89:A:ILE:HD13	1:90:A:ASN:H	5	0.25
(1,735)	1:89:A:ILE:HB	1:158:A:ILE:HD11	8	0.25
(1,735)	1:89:A:ILE:HB	1:158:A:ILE:HD12	8	0.25
(1,735)	1:89:A:ILE:HB	1:158:A:ILE:HD13	8	0.25
(1,735)	1:89:A:ILE:HB	1:158:A:ILE:HD11	11	0.25
(1,735)	1:89:A:ILE:HB	1:158:A:ILE:HD12	11	0.25
(1,735)	1:89:A:ILE:HB	1:158:A:ILE:HD13	11	0.25
(1,674)	1:81:A:THR:H	1:85:A:ALA:H	1	0.25
(1,649)	1:66:A:GLN:HE21	1:82:A:LYS:HB2	9	0.25
(1,644)	1:81:A:THR:HA	1:84:A:GLU:H	4	0.25
(1,571)	1:73:A:TRP:HE1	1:74:A:ARG:HB3	16	0.25
(1,551)	1:70:A:PRO:HB3	1:71:A:SER:H	5	0.25
(1,510)	1:62:A:VAL:HG11	1:156:A:ILE:H	12	0.25
(1,510)	1:62:A:VAL:HG12	1:156:A:ILE:H	12	0.25
(1,510)	1:62:A:VAL:HG13	1:156:A:ILE:H	12	0.25
(1,496)	1:62:A:VAL:HG11	1:88:A:LEU:H	18	0.25
(1,496)	1:62:A:VAL:HG12	1:88:A:LEU:H	18	0.25
(1,496)	1:62:A:VAL:HG13	1:88:A:LEU:H	18	0.25
(1,479)	1:61:A:LEU:HD21	1:155:A:GLY:H	15	0.25
(1,479)	1:61:A:LEU:HD22	1:155:A:GLY:H	15	0.25
(1,479)	1:61:A:LEU:HD23	1:155:A:GLY:H	15	0.25
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB1	1	0.25
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB2	1	0.25
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB3	1	0.25
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB1	5	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB2	5	0.25
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB3	5	0.25
(1,388)	1:35:A:GLU:HG2	1:36:A:ARG:H	7	0.25
(1,379)	1:33:A:GLN:HE21	1:35:A:GLU:HB3	11	0.25
(1,379)	1:33:A:GLN:HE22	1:35:A:GLU:HB3	11	0.25
(1,364)	1:24:A:TYR:HD1	1:33:A:GLN:H	3	0.25
(1,364)	1:24:A:TYR:HD2	1:33:A:GLN:H	3	0.25
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB1	13	0.25
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB2	13	0.25
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB3	13	0.25
(1,321)	1:25:A:PHE:HZ	1:30:A:ASN:H	16	0.25
(1,318)	1:29:A:THR:H	1:30:A:ASN:HB3	1	0.25
(1,311)	1:27:A:HIS:HB2	1:29:A:THR:H	2	0.25
(1,311)	1:27:A:HIS:HB2	1:29:A:THR:H	3	0.25
(1,302)	1:27:A:HIS:HD2	1:28:A:ILE:H	8	0.25
(1,296)	1:27:A:HIS:HA	1:30:A:ASN:HD21	7	0.25
(1,277)	1:26:A:ASN:H	1:30:A:ASN:H	6	0.25
(1,204)	1:24:A:TYR:HB2	1:33:A:GLN:HE21	14	0.25
(1,181)	1:23:A:TYR:HB2	1:34:A:TRP:HE3	20	0.25
(1,129)	1:16:A:SER:HB2	1:21:A:ARG:H	13	0.25
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG21	8	0.25
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG22	8	0.25
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG23	8	0.25
(1,108)	1:15:A:MET:H	1:22:A:VAL:HA	11	0.25
(1,98)	1:14:A:ARG:H	1:24:A:TYR:H	20	0.25
(1,96)	1:14:A:ARG:H	1:23:A:TYR:HD1	3	0.25
(1,96)	1:14:A:ARG:H	1:23:A:TYR:HD2	3	0.25
(1,79)	1:13:A:LYS:H	1:24:A:TYR:HD1	8	0.25
(1,79)	1:13:A:LYS:H	1:24:A:TYR:HD2	8	0.25
(3,44)	1:72:A:SER:O	1:75:A:GLN:H	11	0.24
(2,70)	2:651:B:ILE:HG21	2:656:B:PHE:HE1	3	0.24
(2,70)	2:651:B:ILE:HG21	2:656:B:PHE:HE2	3	0.24
(2,70)	2:651:B:ILE:HG22	2:656:B:PHE:HE1	3	0.24
(2,70)	2:651:B:ILE:HG22	2:656:B:PHE:HE2	3	0.24
(2,70)	2:651:B:ILE:HG23	2:656:B:PHE:HE1	3	0.24
(2,70)	2:651:B:ILE:HG23	2:656:B:PHE:HE2	3	0.24
(2,9)	1:53:A:ALA:H	1:54:A:ARG:HD2	10	0.24
(2,9)	1:53:A:ALA:H	1:54:A:ARG:HD2	13	0.24
(1,2586)	1:115:A:SER:H	2:659:B:PHE:HE1	18	0.24
(1,2586)	1:115:A:SER:H	2:659:B:PHE:HE2	18	0.24
(1,2582)	1:34:A:TRP:HE1	2:642:B:PRO:HB2	17	0.24
(1,2582)	1:34:A:TRP:HE1	2:642:B:PRO:HB3	17	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2580)	1:34:A:TRP:HE1	2:641:B:TPO:HG21	18	0.24
(1,2580)	1:34:A:TRP:HE1	2:641:B:TPO:HG22	18	0.24
(1,2580)	1:34:A:TRP:HE1	2:641:B:TPO:HG23	18	0.24
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG21	3	0.24
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG22	3	0.24
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG23	3	0.24
(1,2557)	2:654:B:SER:H	2:655:B:GLU:H	8	0.24
(1,2530)	2:648:B:ILE:HD11	2:649:B:ARG:H	5	0.24
(1,2530)	2:648:B:ILE:HD12	2:649:B:ARG:H	5	0.24
(1,2530)	2:648:B:ILE:HD13	2:649:B:ARG:H	5	0.24
(1,2103)	1:109:A:GLN:HG2	1:109:A:GLN:HE22	4	0.24
(1,2103)	1:109:A:GLN:HG2	1:109:A:GLN:HE22	7	0.24
(1,2103)	1:109:A:GLN:HG2	1:109:A:GLN:HE22	11	0.24
(1,2103)	1:109:A:GLN:HG2	1:109:A:GLN:HE22	13	0.24
(1,2103)	1:109:A:GLN:HG2	1:109:A:GLN:HE22	17	0.24
(1,2103)	1:109:A:GLN:HG2	1:109:A:GLN:HE22	20	0.24
(1,2056)	1:101:A:GLU:H	1:101:A:GLU:HG2	17	0.24
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD11	11	0.24
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD12	11	0.24
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD13	11	0.24
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD11	16	0.24
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD12	16	0.24
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD13	16	0.24
(1,1906)	1:81:A:THR:H	1:81:A:THR:HG21	10	0.24
(1,1906)	1:81:A:THR:H	1:81:A:THR:HG22	10	0.24
(1,1906)	1:81:A:THR:H	1:81:A:THR:HG23	10	0.24
(1,1694)	1:35:A:GLU:H	1:35:A:GLU:HG3	10	0.24
(1,1694)	1:35:A:GLU:H	1:35:A:GLU:HG3	12	0.24
(1,1694)	1:35:A:GLU:H	1:35:A:GLU:HG3	17	0.24
(1,1625)	1:27:A:HIS:H	1:27:A:HIS:HD1	4	0.24
(1,1507)	1:13:A:LYS:H	1:13:A:LYS:HG3	2	0.24
(1,1500)	1:12:A:GLU:H	1:12:A:GLU:HB2	10	0.24
(1,1424)	1:55:A:VAL:HG21	1:163:A:GLU:H	6	0.24
(1,1424)	1:55:A:VAL:HG22	1:163:A:GLU:H	6	0.24
(1,1424)	1:55:A:VAL:HG23	1:163:A:GLU:H	6	0.24
(1,1424)	1:55:A:VAL:HG11	1:163:A:GLU:H	6	0.24
(1,1424)	1:55:A:VAL:HG12	1:163:A:GLU:H	6	0.24
(1,1424)	1:55:A:VAL:HG13	1:163:A:GLU:H	6	0.24
(1,1303)	1:156:A:ILE:HG21	1:157:A:HIS:HD2	10	0.24
(1,1303)	1:156:A:ILE:HG22	1:157:A:HIS:HD2	10	0.24
(1,1303)	1:156:A:ILE:HG23	1:157:A:HIS:HD2	10	0.24
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG21	20	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG22	20	0.24
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG23	20	0.24
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG21	11	0.24
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG22	11	0.24
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG23	11	0.24
(1,1262)	1:151:A:PHE:H	1:156:A:ILE:HA	7	0.24
(1,1259)	1:151:A:PHE:HB2	1:152:A:THR:H	11	0.24
(1,1206)	1:145:A:GLU:HB3	1:146:A:MET:HB2	13	0.24
(1,1177)	1:137:A:ALA:HB1	1:141:A:LEU:H	13	0.24
(1,1177)	1:137:A:ALA:HB2	1:141:A:LEU:H	13	0.24
(1,1177)	1:137:A:ALA:HB3	1:141:A:LEU:H	13	0.24
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB1	2	0.24
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB2	2	0.24
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB3	2	0.24
(1,1109)	1:126:A:SER:HA	1:139:A:PHE:HD1	4	0.24
(1,1109)	1:126:A:SER:HA	1:139:A:PHE:HD2	4	0.24
(1,1108)	1:54:A:ARG:HG2	1:126:A:SER:HA	15	0.24
(1,1107)	1:54:A:ARG:HD2	1:126:A:SER:HA	14	0.24
(1,1047)	1:119:A:ARG:HD2	1:121:A:ASP:H	20	0.24
(1,1020)	1:116:A:ALA:HA	1:118:A:ALA:H	9	0.24
(1,1011)	1:116:A:ALA:HB1	1:119:A:ARG:H	4	0.24
(1,1011)	1:116:A:ALA:HB2	1:119:A:ARG:H	4	0.24
(1,1011)	1:116:A:ALA:HB3	1:119:A:ARG:H	4	0.24
(1,1011)	1:116:A:ALA:HB1	1:119:A:ARG:H	16	0.24
(1,1011)	1:116:A:ALA:HB2	1:119:A:ARG:H	16	0.24
(1,1011)	1:116:A:ALA:HB3	1:119:A:ARG:H	16	0.24
(1,995)	1:108:A:SER:HA	1:116:A:ALA:H	13	0.24
(1,970)	1:108:A:SER:H	1:110:A:PHE:H	1	0.24
(1,970)	1:108:A:SER:H	1:110:A:PHE:H	11	0.24
(1,959)	1:108:A:SER:HA	1:111:A:SER:H	5	0.24
(1,845)	1:97:A:LYS:HD2	1:98:A:SER:H	17	0.24
(1,772)	1:92:A:TYR:H	1:93:A:ILE:HB	8	0.24
(1,740)	1:89:A:ILE:HG12	1:90:A:ASN:H	8	0.24
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB1	18	0.24
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB2	18	0.24
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB3	18	0.24
(1,663)	1:82:A:LYS:HB3	1:83:A:GLU:H	7	0.24
(1,663)	1:82:A:LYS:HB3	1:83:A:GLU:H	9	0.24
(1,663)	1:82:A:LYS:HB3	1:83:A:GLU:H	14	0.24
(1,663)	1:82:A:LYS:HB3	1:83:A:GLU:H	16	0.24
(1,644)	1:81:A:THR:HA	1:84:A:GLU:H	6	0.24
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB1	10	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB2	10	0.24
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB3	10	0.24
(1,571)	1:73:A:TRP:HE1	1:74:A:ARG:HB3	2	0.24
(1,551)	1:70:A:PRO:HB3	1:71:A:SER:H	4	0.24
(1,551)	1:70:A:PRO:HB3	1:71:A:SER:H	18	0.24
(1,538)	1:66:A:GLN:HG2	1:67:A:SER:H	1	0.24
(1,523)	1:64:A:HIS:HE1	1:66:A:GLN:H	7	0.24
(1,515)	1:63:A:LYS:H	1:156:A:ILE:H	13	0.24
(1,457)	1:60:A:LEU:HD11	1:108:A:SER:H	13	0.24
(1,457)	1:60:A:LEU:HD12	1:108:A:SER:H	13	0.24
(1,457)	1:60:A:LEU:HD13	1:108:A:SER:H	13	0.24
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB1	6	0.24
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB2	6	0.24
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB3	6	0.24
(1,321)	1:25:A:PHE:HZ	1:30:A:ASN:H	3	0.24
(1,305)	1:27:A:HIS:HD2	1:28:A:ILE:HD11	3	0.24
(1,305)	1:27:A:HIS:HD2	1:28:A:ILE:HD12	3	0.24
(1,305)	1:27:A:HIS:HD2	1:28:A:ILE:HD13	3	0.24
(1,302)	1:27:A:HIS:HD2	1:28:A:ILE:H	9	0.24
(1,302)	1:27:A:HIS:HD2	1:28:A:ILE:H	12	0.24
(1,262)	1:25:A:PHE:HE1	1:26:A:ASN:HA	7	0.24
(1,262)	1:25:A:PHE:HE2	1:26:A:ASN:HA	7	0.24
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG11	14	0.24
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG12	14	0.24
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG13	14	0.24
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG11	14	0.24
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG12	14	0.24
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG13	14	0.24
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG11	14	0.24
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG12	14	0.24
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG13	14	0.24
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG11	17	0.24
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG12	17	0.24
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG13	17	0.24
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG11	17	0.24
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG12	17	0.24
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG13	17	0.24
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG11	17	0.24
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG12	17	0.24
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG13	17	0.24
(1,103)	1:14:A:ARG:HG2	1:15:A:MET:H	14	0.24
(1,98)	1:14:A:ARG:H	1:24:A:TYR:H	17	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,52)	1:11:A:TRP:HE1	1:26:A:ASN:HB2	8	0.24
(1,52)	1:11:A:TRP:HE1	1:26:A:ASN:HB3	8	0.24
(3,43)	1:72:A:SER:O	1:75:A:GLN:N	18	0.23
(3,25)	1:55:A:VAL:N	1:125:A:PHE:O	4	0.23
(3,10)	1:16:A:SER:O	1:19:A:SER:H	15	0.23
(2,110)	1:152:A:THR:HG21	2:661:B:PHE:HB2	15	0.23
(2,110)	1:152:A:THR:HG21	2:661:B:PHE:HB3	15	0.23
(2,110)	1:152:A:THR:HG22	2:661:B:PHE:HB2	15	0.23
(2,110)	1:152:A:THR:HG22	2:661:B:PHE:HB3	15	0.23
(2,110)	1:152:A:THR:HG23	2:661:B:PHE:HB2	15	0.23
(2,110)	1:152:A:THR:HG23	2:661:B:PHE:HB3	15	0.23
(2,93)	1:93:A:ILE:HD11	2:643:B:PRO:HA	17	0.23
(2,93)	1:93:A:ILE:HD12	2:643:B:PRO:HA	17	0.23
(2,93)	1:93:A:ILE:HD13	2:643:B:PRO:HA	17	0.23
(2,69)	2:651:B:ILE:HG21	2:656:B:PHE:HD1	13	0.23
(2,69)	2:651:B:ILE:HG21	2:656:B:PHE:HD2	13	0.23
(2,69)	2:651:B:ILE:HG22	2:656:B:PHE:HD1	13	0.23
(2,69)	2:651:B:ILE:HG22	2:656:B:PHE:HD2	13	0.23
(2,69)	2:651:B:ILE:HG23	2:656:B:PHE:HD1	13	0.23
(2,69)	2:651:B:ILE:HG23	2:656:B:PHE:HD2	13	0.23
(2,25)	1:88:A:LEU:HG	1:92:A:TYR:H	12	0.23
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG21	11	0.23
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG22	11	0.23
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG23	11	0.23
(1,2514)	2:646:B:GLU:HA	2:649:B:ARG:H	19	0.23
(1,2386)	1:163:A:GLU:H	1:163:A:GLU:HG2	19	0.23
(1,2302)	1:151:A:PHE:H	1:151:A:PHE:HE1	10	0.23
(1,2302)	1:151:A:PHE:H	1:151:A:PHE:HE2	10	0.23
(1,2103)	1:109:A:GLN:HG2	1:109:A:GLN:HE22	2	0.23
(1,2056)	1:101:A:GLU:H	1:101:A:GLU:HG2	14	0.23
(1,2056)	1:101:A:GLU:H	1:101:A:GLU:HG2	19	0.23
(1,2046)	1:97:A:LYS:H	1:97:A:LYS:HB2	10	0.23
(1,1906)	1:81:A:THR:H	1:81:A:THR:HG21	16	0.23
(1,1906)	1:81:A:THR:H	1:81:A:THR:HG22	16	0.23
(1,1906)	1:81:A:THR:H	1:81:A:THR:HG23	16	0.23
(1,1751)	1:56:A:ARG:H	1:56:A:ARG:HG3	1	0.23
(1,1751)	1:56:A:ARG:H	1:56:A:ARG:HG3	5	0.23
(1,1751)	1:56:A:ARG:H	1:56:A:ARG:HG3	9	0.23
(1,1750)	1:56:A:ARG:HA	1:56:A:ARG:HE	20	0.23
(1,1568)	1:21:A:ARG:HB2	1:21:A:ARG:HE	7	0.23
(1,1441)	1:162:A:THR:HG21	1:163:A:GLU:HG3	8	0.23
(1,1441)	1:162:A:THR:HG22	1:163:A:GLU:HG3	8	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1441)	1:162:A:THR:HG23	1:163:A:GLU:HG3	8	0.23
(1,1431)	1:161:A:ARG:HA	1:163:A:GLU:H	20	0.23
(1,1423)	1:55:A:VAL:HB	1:163:A:GLU:H	7	0.23
(1,1382)	1:159:A:ILE:HG12	1:160:A:LEU:H	13	0.23
(1,1348)	1:157:A:HIS:HB2	1:159:A:ILE:HD11	3	0.23
(1,1348)	1:157:A:HIS:HB2	1:159:A:ILE:HD12	3	0.23
(1,1348)	1:157:A:HIS:HB2	1:159:A:ILE:HD13	3	0.23
(1,1348)	1:157:A:HIS:HB3	1:159:A:ILE:HD11	3	0.23
(1,1348)	1:157:A:HIS:HB3	1:159:A:ILE:HD12	3	0.23
(1,1348)	1:157:A:HIS:HB3	1:159:A:ILE:HD13	3	0.23
(1,1331)	1:146:A:MET:HG2	1:158:A:ILE:HG21	7	0.23
(1,1331)	1:146:A:MET:HG2	1:158:A:ILE:HG22	7	0.23
(1,1331)	1:146:A:MET:HG2	1:158:A:ILE:HG23	7	0.23
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG21	2	0.23
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG22	2	0.23
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG23	2	0.23
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG21	12	0.23
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG22	12	0.23
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG23	12	0.23
(1,1311)	1:152:A:THR:HG21	1:157:A:HIS:H	13	0.23
(1,1311)	1:152:A:THR:HG22	1:157:A:HIS:H	13	0.23
(1,1311)	1:152:A:THR:HG23	1:157:A:HIS:H	13	0.23
(1,1299)	1:152:A:THR:H	1:156:A:ILE:HG21	7	0.23
(1,1299)	1:152:A:THR:H	1:156:A:ILE:HG22	7	0.23
(1,1299)	1:152:A:THR:H	1:156:A:ILE:HG23	7	0.23
(1,1282)	1:82:A:LYS:HE2	1:156:A:ILE:HD11	11	0.23
(1,1282)	1:82:A:LYS:HE2	1:156:A:ILE:HD12	11	0.23
(1,1282)	1:82:A:LYS:HE2	1:156:A:ILE:HD13	11	0.23
(1,1242)	1:150:A:VAL:HG11	1:157:A:HIS:H	9	0.23
(1,1242)	1:150:A:VAL:HG12	1:157:A:HIS:H	9	0.23
(1,1242)	1:150:A:VAL:HG13	1:157:A:HIS:H	9	0.23
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG21	5	0.23
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG22	5	0.23
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG23	5	0.23
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG21	5	0.23
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG22	5	0.23
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG23	5	0.23
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG21	5	0.23
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG22	5	0.23
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG23	5	0.23
(1,1212)	1:146:A:MET:HG2	1:160:A:LEU:HG	6	0.23
(1,1200)	1:143:A:THR:H	1:144:A:GLY:H	15	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1200)	1:143:A:THR:H	1:144:A:GLY:H	18	0.23
(1,1199)	1:142:A:ARG:HG2	1:143:A:THR:H	13	0.23
(1,1156)	1:136:A:ASP:HB2	1:137:A:ALA:H	4	0.23
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB1	4	0.23
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB2	4	0.23
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB3	4	0.23
(1,1152)	1:135:A:GLU:HG2	1:136:A:ASP:H	13	0.23
(1,1107)	1:54:A:ARG:HD2	1:126:A:SER:HA	2	0.23
(1,1107)	1:54:A:ARG:HD2	1:126:A:SER:HA	17	0.23
(1,1054)	1:59:A:HIS:HD2	1:122:A:LEU:H	11	0.23
(1,1052)	1:58:A:SER:HB2	1:122:A:LEU:H	12	0.23
(1,1052)	1:58:A:SER:HB2	1:122:A:LEU:H	15	0.23
(1,1038)	1:119:A:ARG:HA	1:121:A:ASP:H	7	0.23
(1,1029)	1:118:A:ALA:H	1:121:A:ASP:H	1	0.23
(1,958)	1:108:A:SER:HA	1:110:A:PHE:H	18	0.23
(1,941)	1:106:A:LEU:HD11	1:107:A:ALA:H	6	0.23
(1,941)	1:106:A:LEU:HD12	1:107:A:ALA:H	6	0.23
(1,941)	1:106:A:LEU:HD13	1:107:A:ALA:H	6	0.23
(1,925)	1:60:A:LEU:HG	1:107:A:ALA:H	19	0.23
(1,920)	1:106:A:LEU:HB3	1:108:A:SER:H	12	0.23
(1,913)	1:103:A:PHE:H	1:106:A:LEU:HB3	19	0.23
(1,862)	1:101:A:GLU:HG2	1:102:A:ASP:H	7	0.23
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD11	7	0.23
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD12	7	0.23
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD13	7	0.23
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD11	18	0.23
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD12	18	0.23
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD13	18	0.23
(1,764)	1:88:A:LEU:HA	1:92:A:TYR:H	9	0.23
(1,764)	1:88:A:LEU:HA	1:92:A:TYR:H	19	0.23
(1,751)	1:89:A:ILE:HG21	1:91:A:GLY:H	5	0.23
(1,751)	1:89:A:ILE:HG22	1:91:A:GLY:H	5	0.23
(1,751)	1:89:A:ILE:HG23	1:91:A:GLY:H	5	0.23
(1,748)	1:87:A:GLU:HA	1:91:A:GLY:H	13	0.23
(1,743)	1:89:A:ILE:HG13	1:90:A:ASN:H	1	0.23
(1,743)	1:89:A:ILE:HG13	1:90:A:ASN:H	4	0.23
(1,743)	1:89:A:ILE:HG13	1:90:A:ASN:H	16	0.23
(1,743)	1:89:A:ILE:HG13	1:90:A:ASN:H	20	0.23
(1,735)	1:89:A:ILE:HB	1:158:A:ILE:HD11	10	0.23
(1,735)	1:89:A:ILE:HB	1:158:A:ILE:HD12	10	0.23
(1,735)	1:89:A:ILE:HB	1:158:A:ILE:HD13	10	0.23
(1,692)	1:86:A:LEU:HG	1:90:A:ASN:HD22	2	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,669)	1:84:A:GLU:H	1:87:A:GLU:H	4	0.23
(1,663)	1:82:A:LYS:HB3	1:83:A:GLU:H	1	0.23
(1,663)	1:82:A:LYS:HB3	1:83:A:GLU:H	8	0.23
(1,663)	1:82:A:LYS:HB3	1:83:A:GLU:H	19	0.23
(1,654)	1:82:A:LYS:HG2	1:84:A:GLU:H	4	0.23
(1,654)	1:82:A:LYS:HG3	1:84:A:GLU:H	4	0.23
(1,618)	1:78:A:ILE:HA	1:80:A:ARG:H	19	0.23
(1,611)	1:75:A:GLN:HE21	1:78:A:ILE:HD11	13	0.23
(1,611)	1:75:A:GLN:HE21	1:78:A:ILE:HD12	13	0.23
(1,611)	1:75:A:GLN:HE21	1:78:A:ILE:HD13	13	0.23
(1,569)	1:73:A:TRP:HE1	1:74:A:ARG:HB2	3	0.23
(1,551)	1:70:A:PRO:HB3	1:71:A:SER:H	11	0.23
(1,521)	1:64:A:HIS:H	1:66:A:GLN:H	1	0.23
(1,521)	1:64:A:HIS:H	1:66:A:GLN:H	14	0.23
(1,513)	1:62:A:VAL:H	1:158:A:ILE:H	6	0.23
(1,496)	1:62:A:VAL:HG11	1:88:A:LEU:H	20	0.23
(1,496)	1:62:A:VAL:HG12	1:88:A:LEU:H	20	0.23
(1,496)	1:62:A:VAL:HG13	1:88:A:LEU:H	20	0.23
(1,480)	1:61:A:LEU:HD21	1:156:A:ILE:H	18	0.23
(1,480)	1:61:A:LEU:HD22	1:156:A:ILE:H	18	0.23
(1,480)	1:61:A:LEU:HD23	1:156:A:ILE:H	18	0.23
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB1	15	0.23
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB2	15	0.23
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB3	15	0.23
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB1	19	0.23
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB2	19	0.23
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB3	19	0.23
(1,435)	1:58:A:SER:HA	1:122:A:LEU:HG	2	0.23
(1,387)	1:35:A:GLU:HB2	1:36:A:ARG:H	3	0.23
(1,377)	1:33:A:GLN:HG2	1:35:A:GLU:H	10	0.23
(1,364)	1:24:A:TYR:HD1	1:33:A:GLN:H	6	0.23
(1,364)	1:24:A:TYR:HD2	1:33:A:GLN:H	6	0.23
(1,364)	1:24:A:TYR:HD1	1:33:A:GLN:H	7	0.23
(1,364)	1:24:A:TYR:HD2	1:33:A:GLN:H	7	0.23
(1,363)	1:11:A:TRP:HE3	1:33:A:GLN:H	13	0.23
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB1	6	0.23
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB2	6	0.23
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB3	6	0.23
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB1	5	0.23
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB2	5	0.23
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB3	5	0.23
(1,335)	1:29:A:THR:H	1:31:A:ALA:H	20	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,242)	1:10:A:GLY:H	1:26:A:ASN:HD21	2	0.23
(1,213)	1:11:A:TRP:HA	1:25:A:PHE:H	18	0.23
(1,194)	1:13:A:LYS:HG2	1:24:A:TYR:HA	18	0.23
(1,189)	1:13:A:LYS:H	1:24:A:TYR:HA	9	0.23
(1,189)	1:13:A:LYS:H	1:24:A:TYR:HA	20	0.23
(1,130)	1:16:A:SER:H	1:21:A:ARG:HA	10	0.23
(1,108)	1:15:A:MET:H	1:22:A:VAL:HA	19	0.23
(1,100)	1:14:A:ARG:HE	1:15:A:MET:H	16	0.23
(1,98)	1:14:A:ARG:H	1:24:A:TYR:H	5	0.23
(1,79)	1:13:A:LYS:H	1:24:A:TYR:HD1	11	0.23
(1,79)	1:13:A:LYS:H	1:24:A:TYR:HD2	11	0.23
(1,75)	1:13:A:LYS:HA	1:23:A:TYR:H	1	0.23
(1,66)	1:12:A:GLU:H	1:25:A:PHE:HE1	11	0.23
(1,66)	1:12:A:GLU:H	1:25:A:PHE:HE2	11	0.23
(1,64)	1:12:A:GLU:H	1:24:A:TYR:HD1	15	0.23
(1,64)	1:12:A:GLU:H	1:24:A:TYR:HD2	15	0.23
(1,11)	1:4:A:GLU:H	1:6:A:LYS:H	8	0.23
(1,7)	1:3:A:ASP:HA	1:4:A:GLU:H	17	0.23
(3,65)	1:91:A:GLY:O	1:95:A:LYS:N	20	0.22
(3,49)	1:82:A:LYS:O	1:86:A:LEU:N	4	0.22
(3,49)	1:82:A:LYS:O	1:86:A:LEU:N	19	0.22
(3,45)	1:70:A:PRO:O	1:78:A:ILE:N	16	0.22
(2,97)	1:94:A:GLN:HE21	2:640:B:LEU:HG	15	0.22
(2,82)	2:660:B:SEP:HA	2:661:B:PHE:HD1	9	0.22
(2,82)	2:660:B:SEP:HA	2:661:B:PHE:HD2	9	0.22
(2,20)	1:68:A:ARG:H	1:153:A:ASP:HB2	13	0.22
(2,20)	1:68:A:ARG:H	1:153:A:ASP:HB3	13	0.22
(1,2582)	1:34:A:TRP:HE1	2:642:B:PRO:HB2	16	0.22
(1,2582)	1:34:A:TRP:HE1	2:642:B:PRO:HB3	16	0.22
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG21	9	0.22
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG22	9	0.22
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG23	9	0.22
(1,2538)	2:649:B:ARG:H	2:650:B:ASN:HD21	15	0.22
(1,2526)	2:646:B:GLU:HB2	2:648:B:ILE:H	17	0.22
(1,2510)	2:645:B:GLN:H	2:647:B:VAL:H	14	0.22
(1,2357)	1:160:A:LEU:H	1:160:A:LEU:HD11	8	0.22
(1,2357)	1:160:A:LEU:H	1:160:A:LEU:HD12	8	0.22
(1,2357)	1:160:A:LEU:H	1:160:A:LEU:HD13	8	0.22
(1,2158)	1:119:A:ARG:H	1:119:A:ARG:HD2	18	0.22
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG21	5	0.22
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG22	5	0.22
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG23	5	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2036)	1:96:A:ILE:H	1:96:A:ILE:HD11	4	0.22
(1,2036)	1:96:A:ILE:H	1:96:A:ILE:HD12	4	0.22
(1,2036)	1:96:A:ILE:H	1:96:A:ILE:HD13	4	0.22
(1,2036)	1:96:A:ILE:H	1:96:A:ILE:HD11	5	0.22
(1,2036)	1:96:A:ILE:H	1:96:A:ILE:HD12	5	0.22
(1,2036)	1:96:A:ILE:H	1:96:A:ILE:HD13	5	0.22
(1,2033)	1:95:A:LYS:H	1:95:A:LYS:HD2	17	0.22
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD11	14	0.22
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD12	14	0.22
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD13	14	0.22
(1,1913)	1:82:A:LYS:H	1:82:A:LYS:HD2	5	0.22
(1,1913)	1:82:A:LYS:H	1:82:A:LYS:HD2	17	0.22
(1,1913)	1:82:A:LYS:H	1:82:A:LYS:HD2	19	0.22
(1,1751)	1:56:A:ARG:H	1:56:A:ARG:HG3	8	0.22
(1,1750)	1:56:A:ARG:HA	1:56:A:ARG:HE	4	0.22
(1,1750)	1:56:A:ARG:HA	1:56:A:ARG:HE	11	0.22
(1,1750)	1:56:A:ARG:HA	1:56:A:ARG:HE	17	0.22
(1,1694)	1:35:A:GLU:H	1:35:A:GLU:HG3	2	0.22
(1,1694)	1:35:A:GLU:H	1:35:A:GLU:HG3	8	0.22
(1,1694)	1:35:A:GLU:H	1:35:A:GLU:HG3	16	0.22
(1,1568)	1:21:A:ARG:HB2	1:21:A:ARG:HE	13	0.22
(1,1457)	1:6:A:LYS:H	1:6:A:LYS:HG2	11	0.22
(1,1457)	1:6:A:LYS:H	1:6:A:LYS:HG2	20	0.22
(1,1455)	1:6:A:LYS:H	1:6:A:LYS:HB3	18	0.22
(1,1424)	1:55:A:VAL:HG21	1:163:A:GLU:H	9	0.22
(1,1424)	1:55:A:VAL:HG22	1:163:A:GLU:H	9	0.22
(1,1424)	1:55:A:VAL:HG23	1:163:A:GLU:H	9	0.22
(1,1424)	1:55:A:VAL:HG11	1:163:A:GLU:H	9	0.22
(1,1424)	1:55:A:VAL:HG12	1:163:A:GLU:H	9	0.22
(1,1424)	1:55:A:VAL:HG13	1:163:A:GLU:H	9	0.22
(1,1363)	1:96:A:ILE:HG21	1:160:A:LEU:HD11	13	0.22
(1,1363)	1:96:A:ILE:HG21	1:160:A:LEU:HD12	13	0.22
(1,1363)	1:96:A:ILE:HG21	1:160:A:LEU:HD13	13	0.22
(1,1363)	1:96:A:ILE:HG22	1:160:A:LEU:HD11	13	0.22
(1,1363)	1:96:A:ILE:HG22	1:160:A:LEU:HD12	13	0.22
(1,1363)	1:96:A:ILE:HG22	1:160:A:LEU:HD13	13	0.22
(1,1363)	1:96:A:ILE:HG23	1:160:A:LEU:HD11	13	0.22
(1,1363)	1:96:A:ILE:HG23	1:160:A:LEU:HD12	13	0.22
(1,1363)	1:96:A:ILE:HG23	1:160:A:LEU:HD13	13	0.22
(1,1353)	1:57:A:CYS:HB3	1:160:A:LEU:H	6	0.22
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG21	14	0.22
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG22	14	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG23	14	0.22
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG21	19	0.22
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG22	19	0.22
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG23	19	0.22
(1,1206)	1:145:A:GLU:HB3	1:146:A:MET:HB2	14	0.22
(1,1200)	1:143:A:THR:H	1:144:A:GLY:H	8	0.22
(1,1200)	1:143:A:THR:H	1:144:A:GLY:H	19	0.22
(1,1199)	1:142:A:ARG:HG2	1:143:A:THR:H	19	0.22
(1,1193)	1:141:A:LEU:HD11	1:148:A:GLY:H	13	0.22
(1,1193)	1:141:A:LEU:HD12	1:148:A:GLY:H	13	0.22
(1,1193)	1:141:A:LEU:HD13	1:148:A:GLY:H	13	0.22
(1,1178)	1:137:A:ALA:HA	1:141:A:LEU:H	15	0.22
(1,1152)	1:135:A:GLU:HG2	1:136:A:ASP:H	20	0.22
(1,1141)	1:130:A:MET:HB2	1:134:A:PHE:H	7	0.22
(1,1141)	1:130:A:MET:HB2	1:134:A:PHE:H	10	0.22
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE1	11	0.22
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE2	11	0.22
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE3	11	0.22
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE1	11	0.22
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE2	11	0.22
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE3	11	0.22
(1,1038)	1:119:A:ARG:HA	1:121:A:ASP:H	5	0.22
(1,1038)	1:119:A:ARG:HA	1:121:A:ASP:H	18	0.22
(1,1020)	1:116:A:ALA:HA	1:118:A:ALA:H	14	0.22
(1,1000)	1:113:A:CYS:H	1:116:A:ALA:H	5	0.22
(1,970)	1:108:A:SER:H	1:110:A:PHE:H	2	0.22
(1,970)	1:108:A:SER:H	1:110:A:PHE:H	17	0.22
(1,961)	1:108:A:SER:H	1:119:A:ARG:HG2	20	0.22
(1,934)	1:104:A:GLU:HA	1:107:A:ALA:H	19	0.22
(1,914)	1:104:A:GLU:H	1:106:A:LEU:HB3	13	0.22
(1,888)	1:103:A:PHE:HE1	1:120:A:GLY:H	20	0.22
(1,888)	1:103:A:PHE:HE2	1:120:A:GLY:H	20	0.22
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD11	9	0.22
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD12	9	0.22
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD13	9	0.22
(1,772)	1:92:A:TYR:H	1:93:A:ILE:HB	5	0.22
(1,743)	1:89:A:ILE:HG13	1:90:A:ASN:H	19	0.22
(1,742)	1:89:A:ILE:HD11	1:90:A:ASN:H	8	0.22
(1,742)	1:89:A:ILE:HD12	1:90:A:ASN:H	8	0.22
(1,742)	1:89:A:ILE:HD13	1:90:A:ASN:H	8	0.22
(1,735)	1:89:A:ILE:HB	1:158:A:ILE:HD11	18	0.22
(1,735)	1:89:A:ILE:HB	1:158:A:ILE:HD12	18	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,735)	1:89:A:ILE:HB	1:158:A:ILE:HD13	18	0.22
(1,695)	1:86:A:LEU:HD21	1:149:A:PRO:HD3	7	0.22
(1,695)	1:86:A:LEU:HD22	1:149:A:PRO:HD3	7	0.22
(1,695)	1:86:A:LEU:HD23	1:149:A:PRO:HD3	7	0.22
(1,619)	1:78:A:ILE:HB	1:80:A:ARG:H	18	0.22
(1,569)	1:73:A:TRP:HE1	1:74:A:ARG:HB2	6	0.22
(1,569)	1:73:A:TRP:HE1	1:74:A:ARG:HB2	11	0.22
(1,564)	1:72:A:SER:H	1:78:A:ILE:HG12	12	0.22
(1,529)	1:64:A:HIS:HE1	1:67:A:SER:H	19	0.22
(1,521)	1:64:A:HIS:H	1:66:A:GLN:H	15	0.22
(1,514)	1:63:A:LYS:HB2	1:70:A:PRO:HA	11	0.22
(1,436)	1:58:A:SER:H	1:160:A:LEU:HG	17	0.22
(1,388)	1:35:A:GLU:HG2	1:36:A:ARG:H	12	0.22
(1,369)	1:33:A:GLN:HG2	1:34:A:TRP:H	12	0.22
(1,362)	1:11:A:TRP:HH2	1:33:A:GLN:HE21	12	0.22
(1,355)	1:25:A:PHE:HE1	1:32:A:SER:HB2	11	0.22
(1,355)	1:25:A:PHE:HE2	1:32:A:SER:HB2	11	0.22
(1,347)	1:31:A:ALA:HB1	1:33:A:GLN:H	14	0.22
(1,347)	1:31:A:ALA:HB2	1:33:A:GLN:H	14	0.22
(1,347)	1:31:A:ALA:HB3	1:33:A:GLN:H	14	0.22
(1,347)	1:31:A:ALA:HB1	1:33:A:GLN:H	17	0.22
(1,347)	1:31:A:ALA:HB2	1:33:A:GLN:H	17	0.22
(1,347)	1:31:A:ALA:HB3	1:33:A:GLN:H	17	0.22
(1,347)	1:31:A:ALA:HB1	1:33:A:GLN:H	20	0.22
(1,347)	1:31:A:ALA:HB2	1:33:A:GLN:H	20	0.22
(1,347)	1:31:A:ALA:HB3	1:33:A:GLN:H	20	0.22
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB1	5	0.22
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB2	5	0.22
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB3	5	0.22
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB1	15	0.22
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB2	15	0.22
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB3	15	0.22
(1,336)	1:29:A:THR:HG21	1:31:A:ALA:H	20	0.22
(1,336)	1:29:A:THR:HG22	1:31:A:ALA:H	20	0.22
(1,336)	1:29:A:THR:HG23	1:31:A:ALA:H	20	0.22
(1,287)	1:26:A:ASN:H	1:32:A:SER:HB2	2	0.22
(1,277)	1:26:A:ASN:H	1:30:A:ASN:H	17	0.22
(1,262)	1:25:A:PHE:HE1	1:26:A:ASN:HA	6	0.22
(1,262)	1:25:A:PHE:HE2	1:26:A:ASN:HA	6	0.22
(1,208)	1:24:A:TYR:H	1:34:A:TRP:HB3	19	0.22
(1,205)	1:24:A:TYR:H	1:33:A:GLN:HG2	1	0.22
(1,205)	1:24:A:TYR:H	1:33:A:GLN:HG2	8	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,196)	1:23:A:TYR:HB3	1:24:A:TYR:H	11	0.22
(1,178)	1:23:A:TYR:HE1	1:33:A:GLN:H	10	0.22
(1,178)	1:23:A:TYR:HE2	1:33:A:GLN:H	10	0.22
(1,157)	1:16:A:SER:H	1:22:A:VAL:HG11	15	0.22
(1,157)	1:16:A:SER:H	1:22:A:VAL:HG12	15	0.22
(1,157)	1:16:A:SER:H	1:22:A:VAL:HG13	15	0.22
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG11	2	0.22
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG12	2	0.22
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG13	2	0.22
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG11	2	0.22
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG12	2	0.22
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG13	2	0.22
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG11	2	0.22
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG12	2	0.22
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG13	2	0.22
(1,117)	1:16:A:SER:H	1:23:A:TYR:HE1	11	0.22
(1,117)	1:16:A:SER:H	1:23:A:TYR:HE2	11	0.22
(1,116)	1:16:A:SER:H	1:20:A:GLY:HA2	5	0.22
(1,69)	1:7:A:LEU:HD21	1:13:A:LYS:HE2	12	0.22
(1,69)	1:7:A:LEU:HD22	1:13:A:LYS:HE2	12	0.22
(1,69)	1:7:A:LEU:HD23	1:13:A:LYS:HE2	12	0.22
(1,69)	1:7:A:LEU:HD11	1:13:A:LYS:HE2	12	0.22
(1,69)	1:7:A:LEU:HD12	1:13:A:LYS:HE2	12	0.22
(1,69)	1:7:A:LEU:HD13	1:13:A:LYS:HE2	12	0.22
(1,64)	1:12:A:GLU:H	1:24:A:TYR:HD1	11	0.22
(1,64)	1:12:A:GLU:H	1:24:A:TYR:HD2	11	0.22
(1,16)	1:6:A:LYS:HE2	1:7:A:LEU:H	19	0.22
(3,63)	1:90:A:ASN:O	1:94:A:GLN:N	18	0.21
(3,51)	1:83:A:GLU:O	1:87:A:GLU:N	11	0.21
(3,47)	1:81:A:THR:O	1:85:A:ALA:N	19	0.21
(3,10)	1:16:A:SER:O	1:19:A:SER:H	10	0.21
(2,55)	1:150:A:VAL:HG21	1:158:A:ILE:HA	17	0.21
(2,55)	1:150:A:VAL:HG22	1:158:A:ILE:HA	17	0.21
(2,55)	1:150:A:VAL:HG23	1:158:A:ILE:HA	17	0.21
(2,25)	1:88:A:LEU:HG	1:92:A:TYR:H	16	0.21
(2,21)	1:73:A:TRP:HE1	1:74:A:ARG:HG3	4	0.21
(1,2572)	1:16:A:SER:HB2	2:641:B:TPO:HG21	1	0.21
(1,2572)	1:16:A:SER:HB2	2:641:B:TPO:HG22	1	0.21
(1,2572)	1:16:A:SER:HB2	2:641:B:TPO:HG23	1	0.21
(1,2527)	2:646:B:GLU:H	2:648:B:ILE:H	16	0.21
(1,2526)	2:646:B:GLU:HB2	2:648:B:ILE:H	5	0.21
(1,2523)	2:647:B:VAL:HA	2:649:B:ARG:H	14	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2496)	2:659:B:PHE:H	2:659:B:PHE:HE1	4	0.21
(1,2496)	2:659:B:PHE:H	2:659:B:PHE:HE2	4	0.21
(1,2481)	2:656:B:PHE:H	2:656:B:PHE:HE1	17	0.21
(1,2481)	2:656:B:PHE:H	2:656:B:PHE:HE2	17	0.21
(1,2074)	1:104:A:GLU:H	1:104:A:GLU:HG2	10	0.21
(1,2046)	1:97:A:LYS:H	1:97:A:LYS:HB2	17	0.21
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG21	1	0.21
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG22	1	0.21
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG23	1	0.21
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG21	3	0.21
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG22	3	0.21
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG23	3	0.21
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG21	4	0.21
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG22	4	0.21
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG23	4	0.21
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG21	9	0.21
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG22	9	0.21
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG23	9	0.21
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG21	12	0.21
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG22	12	0.21
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG23	12	0.21
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD11	3	0.21
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD12	3	0.21
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD13	3	0.21
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD11	3	0.21
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD12	3	0.21
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD13	3	0.21
(1,1751)	1:56:A:ARG:H	1:56:A:ARG:HG3	7	0.21
(1,1747)	1:56:A:ARG:H	1:56:A:ARG:HD2	20	0.21
(1,1694)	1:35:A:GLU:H	1:35:A:GLU:HG3	3	0.21
(1,1535)	1:14:A:ARG:HB2	1:14:A:ARG:HE	1	0.21
(1,1489)	1:11:A:TRP:H	1:11:A:TRP:HE1	8	0.21
(1,1355)	1:57:A:CYS:HB2	1:160:A:LEU:H	2	0.21
(1,1347)	1:148:A:GLY:H	1:159:A:ILE:HD11	17	0.21
(1,1347)	1:148:A:GLY:H	1:159:A:ILE:HD12	17	0.21
(1,1347)	1:148:A:GLY:H	1:159:A:ILE:HD13	17	0.21
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG21	10	0.21
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG22	10	0.21
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG23	10	0.21
(1,1280)	1:64:A:HIS:HD2	1:156:A:ILE:HG12	4	0.21
(1,1259)	1:151:A:PHE:HB2	1:152:A:THR:H	5	0.21
(1,1244)	1:150:A:VAL:HG21	1:157:A:HIS:HB2	17	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1244)	1:150:A:VAL:HG21	1:157:A:HIS:HB3	17	0.21
(1,1244)	1:150:A:VAL:HG22	1:157:A:HIS:HB2	17	0.21
(1,1244)	1:150:A:VAL:HG22	1:157:A:HIS:HB3	17	0.21
(1,1244)	1:150:A:VAL:HG23	1:157:A:HIS:HB2	17	0.21
(1,1244)	1:150:A:VAL:HG23	1:157:A:HIS:HB3	17	0.21
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG21	4	0.21
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG22	4	0.21
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG23	4	0.21
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG21	4	0.21
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG22	4	0.21
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG23	4	0.21
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG21	4	0.21
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG22	4	0.21
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG23	4	0.21
(1,1212)	1:146:A:MET:HG2	1:160:A:LEU:HG	3	0.21
(1,1200)	1:143:A:THR:H	1:144:A:GLY:H	9	0.21
(1,1038)	1:119:A:ARG:HA	1:121:A:ASP:H	6	0.21
(1,1036)	1:118:A:ALA:HB1	1:119:A:ARG:H	2	0.21
(1,1036)	1:118:A:ALA:HB2	1:119:A:ARG:H	2	0.21
(1,1036)	1:118:A:ALA:HB3	1:119:A:ARG:H	2	0.21
(1,1015)	1:116:A:ALA:HB1	1:120:A:GLY:H	2	0.21
(1,1015)	1:116:A:ALA:HB2	1:120:A:GLY:H	2	0.21
(1,1015)	1:116:A:ALA:HB3	1:120:A:GLY:H	2	0.21
(1,1012)	1:116:A:ALA:H	1:119:A:ARG:H	16	0.21
(1,1001)	1:113:A:CYS:H	1:116:A:ALA:HB1	19	0.21
(1,1001)	1:113:A:CYS:H	1:116:A:ALA:HB2	19	0.21
(1,1001)	1:113:A:CYS:H	1:116:A:ALA:HB3	19	0.21
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB1	9	0.21
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB2	9	0.21
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB3	9	0.21
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB1	10	0.21
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB2	10	0.21
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB3	10	0.21
(1,995)	1:108:A:SER:HA	1:116:A:ALA:H	5	0.21
(1,985)	1:61:A:LEU:HD21	1:113:A:CYS:HA	7	0.21
(1,985)	1:61:A:LEU:HD22	1:113:A:CYS:HA	7	0.21
(1,985)	1:61:A:LEU:HD23	1:113:A:CYS:HA	7	0.21
(1,959)	1:108:A:SER:HA	1:111:A:SER:H	1	0.21
(1,959)	1:108:A:SER:HA	1:111:A:SER:H	4	0.21
(1,941)	1:106:A:LEU:HD11	1:107:A:ALA:H	19	0.21
(1,941)	1:106:A:LEU:HD12	1:107:A:ALA:H	19	0.21
(1,941)	1:106:A:LEU:HD13	1:107:A:ALA:H	19	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,940)	1:106:A:LEU:HG	1:107:A:ALA:H	7	0.21
(1,920)	1:106:A:LEU:HB3	1:108:A:SER:H	11	0.21
(1,857)	1:101:A:GLU:HG2	1:106:A:LEU:HD11	8	0.21
(1,857)	1:101:A:GLU:HG2	1:106:A:LEU:HD12	8	0.21
(1,857)	1:101:A:GLU:HG2	1:106:A:LEU:HD13	8	0.21
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD11	6	0.21
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD12	6	0.21
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD13	6	0.21
(1,756)	1:90:A:ASN:HD21	1:91:A:GLY:H	17	0.21
(1,747)	1:90:A:ASN:HA	1:158:A:ILE:HD11	16	0.21
(1,747)	1:90:A:ASN:HA	1:158:A:ILE:HD12	16	0.21
(1,747)	1:90:A:ASN:HA	1:158:A:ILE:HD13	16	0.21
(1,743)	1:89:A:ILE:HG13	1:90:A:ASN:H	17	0.21
(1,740)	1:89:A:ILE:HG12	1:90:A:ASN:H	12	0.21
(1,735)	1:89:A:ILE:HB	1:158:A:ILE:HD11	13	0.21
(1,735)	1:89:A:ILE:HB	1:158:A:ILE:HD12	13	0.21
(1,735)	1:89:A:ILE:HB	1:158:A:ILE:HD13	13	0.21
(1,695)	1:86:A:LEU:HD21	1:149:A:PRO:HD3	8	0.21
(1,695)	1:86:A:LEU:HD22	1:149:A:PRO:HD3	8	0.21
(1,695)	1:86:A:LEU:HD23	1:149:A:PRO:HD3	8	0.21
(1,669)	1:84:A:GLU:H	1:87:A:GLU:H	19	0.21
(1,654)	1:82:A:LYS:HG2	1:84:A:GLU:H	16	0.21
(1,654)	1:82:A:LYS:HG3	1:84:A:GLU:H	16	0.21
(1,648)	1:66:A:GLN:HE22	1:82:A:LYS:HG3	11	0.21
(1,634)	1:80:A:ARG:HB2	1:81:A:THR:H	16	0.21
(1,538)	1:66:A:GLN:HG2	1:67:A:SER:H	4	0.21
(1,531)	1:64:A:HIS:HE1	1:67:A:SER:HB2	1	0.21
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB1	12	0.21
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB2	12	0.21
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB3	12	0.21
(1,435)	1:58:A:SER:HA	1:122:A:LEU:HG	10	0.21
(1,424)	1:56:A:ARG:HE	1:57:A:CYS:H	5	0.21
(1,424)	1:56:A:ARG:HE	1:57:A:CYS:H	6	0.21
(1,391)	1:35:A:GLU:HB3	1:36:A:ARG:H	1	0.21
(1,363)	1:11:A:TRP:HE3	1:33:A:GLN:H	9	0.21
(1,355)	1:25:A:PHE:HE1	1:32:A:SER:HB2	18	0.21
(1,355)	1:25:A:PHE:HE2	1:32:A:SER:HB2	18	0.21
(1,347)	1:31:A:ALA:HB1	1:33:A:GLN:H	1	0.21
(1,347)	1:31:A:ALA:HB2	1:33:A:GLN:H	1	0.21
(1,347)	1:31:A:ALA:HB3	1:33:A:GLN:H	1	0.21
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB1	2	0.21
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB2	2	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB3	2	0.21
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB1	8	0.21
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB2	8	0.21
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB3	8	0.21
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB1	19	0.21
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB2	19	0.21
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB3	19	0.21
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB1	4	0.21
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB2	4	0.21
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB3	4	0.21
(1,334)	1:27:A:HIS:HA	1:31:A:ALA:H	7	0.21
(1,333)	1:25:A:PHE:HA	1:31:A:ALA:H	1	0.21
(1,333)	1:25:A:PHE:HA	1:31:A:ALA:H	19	0.21
(1,287)	1:26:A:ASN:H	1:32:A:SER:HB2	16	0.21
(1,262)	1:25:A:PHE:HE1	1:26:A:ASN:HA	8	0.21
(1,262)	1:25:A:PHE:HE2	1:26:A:ASN:HA	8	0.21
(1,189)	1:13:A:LYS:H	1:24:A:TYR:HA	5	0.21
(1,189)	1:13:A:LYS:H	1:24:A:TYR:HA	13	0.21
(1,180)	1:23:A:TYR:HD1	1:33:A:GLN:HA	2	0.21
(1,180)	1:23:A:TYR:HD2	1:33:A:GLN:HA	2	0.21
(1,176)	1:23:A:TYR:HB3	1:24:A:TYR:HD1	5	0.21
(1,176)	1:23:A:TYR:HB3	1:24:A:TYR:HD2	5	0.21
(1,103)	1:14:A:ARG:HG2	1:15:A:MET:H	2	0.21
(1,87)	1:13:A:LYS:HG3	1:14:A:ARG:H	17	0.21
(1,75)	1:13:A:LYS:HA	1:23:A:TYR:H	20	0.21
(1,66)	1:12:A:GLU:H	1:25:A:PHE:HE1	9	0.21
(1,66)	1:12:A:GLU:H	1:25:A:PHE:HE2	9	0.21
(1,56)	1:11:A:TRP:HE1	1:31:A:ALA:HB1	5	0.21
(1,56)	1:11:A:TRP:HE1	1:31:A:ALA:HB2	5	0.21
(1,56)	1:11:A:TRP:HE1	1:31:A:ALA:HB3	5	0.21
(1,28)	1:7:A:LEU:HD21	1:13:A:LYS:HG3	10	0.21
(1,28)	1:7:A:LEU:HD22	1:13:A:LYS:HG3	10	0.21
(1,28)	1:7:A:LEU:HD23	1:13:A:LYS:HG3	10	0.21
(1,7)	1:3:A:ASP:HA	1:4:A:GLU:H	7	0.21
(1,7)	1:3:A:ASP:HA	1:4:A:GLU:H	19	0.21
(3,47)	1:81:A:THR:O	1:85:A:ALA:N	4	0.2
(3,27)	1:56:A:ARG:N	1:163:A:GLU:O	11	0.2
(2,107)	1:140:A:ALA:HB1	2:651:B:ILE:HA	19	0.2
(2,107)	1:140:A:ALA:HB2	2:651:B:ILE:HA	19	0.2
(2,107)	1:140:A:ALA:HB3	2:651:B:ILE:HA	19	0.2
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD11	7	0.2
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD12	7	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD13	7	0.2
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG11	5	0.2
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG12	5	0.2
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG13	5	0.2
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG21	5	0.2
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG22	5	0.2
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG23	5	0.2
(2,52)	1:141:A:LEU:HD21	1:148:A:GLY:H	15	0.2
(2,52)	1:141:A:LEU:HD22	1:148:A:GLY:H	15	0.2
(2,52)	1:141:A:LEU:HD23	1:148:A:GLY:H	15	0.2
(2,52)	1:141:A:LEU:HD21	1:148:A:GLY:H	16	0.2
(2,52)	1:141:A:LEU:HD22	1:148:A:GLY:H	16	0.2
(2,52)	1:141:A:LEU:HD23	1:148:A:GLY:H	16	0.2
(2,26)	1:94:A:GLN:HE21	1:97:A:LYS:HB3	8	0.2
(2,4)	1:21:A:ARG:HE	1:22:A:VAL:H	20	0.2
(1,2551)	2:652:B:ASP:H	2:654:B:SER:H	19	0.2
(1,2530)	2:648:B:ILE:HD11	2:649:B:ARG:H	4	0.2
(1,2530)	2:648:B:ILE:HD12	2:649:B:ARG:H	4	0.2
(1,2530)	2:648:B:ILE:HD13	2:649:B:ARG:H	4	0.2
(1,2530)	2:648:B:ILE:HD11	2:649:B:ARG:H	7	0.2
(1,2530)	2:648:B:ILE:HD12	2:649:B:ARG:H	7	0.2
(1,2530)	2:648:B:ILE:HD13	2:649:B:ARG:H	7	0.2
(1,2510)	2:645:B:GLN:H	2:647:B:VAL:H	3	0.2
(1,2496)	2:659:B:PHE:H	2:659:B:PHE:HE1	3	0.2
(1,2496)	2:659:B:PHE:H	2:659:B:PHE:HE2	3	0.2
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG21	8	0.2
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG22	8	0.2
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG23	8	0.2
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG21	14	0.2
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG22	14	0.2
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG23	14	0.2
(1,2033)	1:95:A:LYS:H	1:95:A:LYS:HD2	13	0.2
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD11	1	0.2
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD12	1	0.2
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD13	1	0.2
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD11	15	0.2
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD12	15	0.2
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD13	15	0.2
(1,1910)	1:82:A:LYS:H	1:82:A:LYS:HE2	1	0.2
(1,1751)	1:56:A:ARG:H	1:56:A:ARG:HG3	3	0.2
(1,1751)	1:56:A:ARG:H	1:56:A:ARG:HG3	12	0.2
(1,1751)	1:56:A:ARG:H	1:56:A:ARG:HG3	14	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1751)	1:56:A:ARG:H	1:56:A:ARG:HG3	15	0.2
(1,1703)	1:36:A:ARG:H	1:36:A:ARG:HD2	5	0.2
(1,1694)	1:35:A:GLU:H	1:35:A:GLU:HG3	1	0.2
(1,1694)	1:35:A:GLU:H	1:35:A:GLU:HG3	6	0.2
(1,1525)	1:14:A:ARG:H	1:14:A:ARG:HE	10	0.2
(1,1508)	1:13:A:LYS:H	1:13:A:LYS:HB3	15	0.2
(1,1457)	1:6:A:LYS:H	1:6:A:LYS:HG2	4	0.2
(1,1450)	1:4:A:GLU:HA	1:4:A:GLU:HG2	18	0.2
(1,1424)	1:55:A:VAL:HG21	1:163:A:GLU:H	19	0.2
(1,1424)	1:55:A:VAL:HG22	1:163:A:GLU:H	19	0.2
(1,1424)	1:55:A:VAL:HG23	1:163:A:GLU:H	19	0.2
(1,1424)	1:55:A:VAL:HG11	1:163:A:GLU:H	19	0.2
(1,1424)	1:55:A:VAL:HG12	1:163:A:GLU:H	19	0.2
(1,1424)	1:55:A:VAL:HG13	1:163:A:GLU:H	19	0.2
(1,1423)	1:55:A:VAL:HB	1:163:A:GLU:H	1	0.2
(1,1411)	1:56:A:ARG:H	1:162:A:THR:H	19	0.2
(1,1403)	1:144:A:GLY:H	1:161:A:ARG:HG2	20	0.2
(1,1399)	1:143:A:THR:H	1:161:A:ARG:HD2	15	0.2
(1,1382)	1:159:A:ILE:HG12	1:160:A:LEU:H	4	0.2
(1,1331)	1:146:A:MET:HG2	1:158:A:ILE:HG21	9	0.2
(1,1331)	1:146:A:MET:HG2	1:158:A:ILE:HG22	9	0.2
(1,1331)	1:146:A:MET:HG2	1:158:A:ILE:HG23	9	0.2
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG21	3	0.2
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG22	3	0.2
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG23	3	0.2
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG21	10	0.2
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG22	10	0.2
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG23	10	0.2
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG21	13	0.2
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG22	13	0.2
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG23	13	0.2
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG21	15	0.2
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG22	15	0.2
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG23	15	0.2
(1,1320)	1:60:A:LEU:HD11	1:158:A:ILE:HB	2	0.2
(1,1320)	1:60:A:LEU:HD12	1:158:A:ILE:HB	2	0.2
(1,1320)	1:60:A:LEU:HD13	1:158:A:ILE:HB	2	0.2
(1,1320)	1:60:A:LEU:HD21	1:158:A:ILE:HB	2	0.2
(1,1320)	1:60:A:LEU:HD22	1:158:A:ILE:HB	2	0.2
(1,1320)	1:60:A:LEU:HD23	1:158:A:ILE:HB	2	0.2
(1,1276)	1:63:A:LYS:HA	1:155:A:GLY:HA2	1	0.2
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG21	8	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG22	8	0.2
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG23	8	0.2
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG21	8	0.2
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG22	8	0.2
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG23	8	0.2
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG21	8	0.2
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG22	8	0.2
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG23	8	0.2
(1,1212)	1:146:A:MET:HG2	1:160:A:LEU:HG	1	0.2
(1,1212)	1:146:A:MET:HG2	1:160:A:LEU:HG	16	0.2
(1,1200)	1:143:A:THR:H	1:144:A:GLY:H	2	0.2
(1,1200)	1:143:A:THR:H	1:144:A:GLY:H	12	0.2
(1,1190)	1:141:A:LEU:HD21	1:142:A:ARG:HB2	6	0.2
(1,1190)	1:141:A:LEU:HD22	1:142:A:ARG:HB2	6	0.2
(1,1190)	1:141:A:LEU:HD23	1:142:A:ARG:HB2	6	0.2
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE1	15	0.2
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE2	15	0.2
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE3	15	0.2
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE1	15	0.2
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE2	15	0.2
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE3	15	0.2
(1,1078)	1:122:A:LEU:HG	1:123:A:GLY:H	16	0.2
(1,1051)	1:57:A:CYS:H	1:122:A:LEU:HD21	4	0.2
(1,1051)	1:57:A:CYS:H	1:122:A:LEU:HD22	4	0.2
(1,1051)	1:57:A:CYS:H	1:122:A:LEU:HD23	4	0.2
(1,1038)	1:119:A:ARG:HA	1:121:A:ASP:H	19	0.2
(1,1032)	1:107:A:ALA:HB1	1:119:A:ARG:H	15	0.2
(1,1032)	1:107:A:ALA:HB2	1:119:A:ARG:H	15	0.2
(1,1032)	1:107:A:ALA:HB3	1:119:A:ARG:H	15	0.2
(1,1031)	1:118:A:ALA:HB1	1:121:A:ASP:HB2	5	0.2
(1,1031)	1:118:A:ALA:HB2	1:121:A:ASP:HB2	5	0.2
(1,1031)	1:118:A:ALA:HB3	1:121:A:ASP:HB2	5	0.2
(1,1012)	1:116:A:ALA:H	1:119:A:ARG:H	6	0.2
(1,1011)	1:116:A:ALA:HB1	1:119:A:ARG:H	5	0.2
(1,1011)	1:116:A:ALA:HB2	1:119:A:ARG:H	5	0.2
(1,1011)	1:116:A:ALA:HB3	1:119:A:ARG:H	5	0.2
(1,970)	1:108:A:SER:H	1:110:A:PHE:H	15	0.2
(1,941)	1:106:A:LEU:HD11	1:107:A:ALA:H	3	0.2
(1,941)	1:106:A:LEU:HD12	1:107:A:ALA:H	3	0.2
(1,941)	1:106:A:LEU:HD13	1:107:A:ALA:H	3	0.2
(1,941)	1:106:A:LEU:HD11	1:107:A:ALA:H	4	0.2
(1,941)	1:106:A:LEU:HD12	1:107:A:ALA:H	4	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,941)	1:106:A:LEU:HD13	1:107:A:ALA:H	4	0.2
(1,923)	1:106:A:LEU:HA	1:110:A:PHE:H	18	0.2
(1,921)	1:106:A:LEU:H	1:109:A:GLN:H	2	0.2
(1,920)	1:106:A:LEU:HB3	1:108:A:SER:H	3	0.2
(1,889)	1:103:A:PHE:HE1	1:146:A:MET:HE1	9	0.2
(1,889)	1:103:A:PHE:HE1	1:146:A:MET:HE2	9	0.2
(1,889)	1:103:A:PHE:HE1	1:146:A:MET:HE3	9	0.2
(1,889)	1:103:A:PHE:HE2	1:146:A:MET:HE1	9	0.2
(1,889)	1:103:A:PHE:HE2	1:146:A:MET:HE2	9	0.2
(1,889)	1:103:A:PHE:HE2	1:146:A:MET:HE3	9	0.2
(1,862)	1:101:A:GLU:HG2	1:102:A:ASP:H	3	0.2
(1,854)	1:98:A:SER:H	1:101:A:GLU:H	5	0.2
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD11	15	0.2
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD12	15	0.2
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD13	15	0.2
(1,764)	1:88:A:LEU:HA	1:92:A:TYR:H	10	0.2
(1,748)	1:87:A:GLU:HA	1:91:A:GLY:H	11	0.2
(1,740)	1:89:A:ILE:HG12	1:90:A:ASN:H	13	0.2
(1,735)	1:89:A:ILE:HB	1:158:A:ILE:HD11	12	0.2
(1,735)	1:89:A:ILE:HB	1:158:A:ILE:HD12	12	0.2
(1,735)	1:89:A:ILE:HB	1:158:A:ILE:HD13	12	0.2
(1,674)	1:81:A:THR:H	1:85:A:ALA:H	5	0.2
(1,674)	1:81:A:THR:H	1:85:A:ALA:H	17	0.2
(1,671)	1:64:A:HIS:HB2	1:85:A:ALA:H	4	0.2
(1,663)	1:82:A:LYS:HB3	1:83:A:GLU:H	11	0.2
(1,663)	1:82:A:LYS:HB3	1:83:A:GLU:H	18	0.2
(1,647)	1:65:A:SER:H	1:82:A:LYS:H	11	0.2
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG21	1	0.2
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG22	1	0.2
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG23	1	0.2
(1,592)	1:75:A:GLN:HB2	1:77:A:LYS:H	4	0.2
(1,589)	1:74:A:ARG:H	1:112:A:ASP:HA	6	0.2
(1,576)	1:73:A:TRP:HE1	1:115:A:SER:H	3	0.2
(1,551)	1:70:A:PRO:HB3	1:71:A:SER:H	6	0.2
(1,541)	1:67:A:SER:HB3	1:70:A:PRO:HA	17	0.2
(1,476)	1:61:A:LEU:H	1:113:A:CYS:HB2	6	0.2
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG21	9	0.2
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG22	9	0.2
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG23	9	0.2
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG21	9	0.2
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG22	9	0.2
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG23	9	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG21	9	0.2
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG22	9	0.2
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG23	9	0.2
(1,435)	1:58:A:SER:HA	1:122:A:LEU:HG	18	0.2
(1,424)	1:56:A:ARG:HE	1:57:A:CYS:H	1	0.2
(1,401)	1:54:A:ARG:HD2	1:55:A:VAL:HA	7	0.2
(1,377)	1:33:A:GLN:HG2	1:35:A:GLU:H	4	0.2
(1,364)	1:24:A:TYR:HD1	1:33:A:GLN:H	18	0.2
(1,364)	1:24:A:TYR:HD2	1:33:A:GLN:H	18	0.2
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB1	3	0.2
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB2	3	0.2
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB3	3	0.2
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB1	11	0.2
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB2	11	0.2
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB3	11	0.2
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB1	11	0.2
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB2	11	0.2
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB3	11	0.2
(1,334)	1:27:A:HIS:HA	1:31:A:ALA:H	19	0.2
(1,321)	1:25:A:PHE:HZ	1:30:A:ASN:H	4	0.2
(1,302)	1:27:A:HIS:HD2	1:28:A:ILE:H	7	0.2
(1,278)	1:26:A:ASN:HB2	1:30:A:ASN:H	11	0.2
(1,262)	1:25:A:PHE:HE1	1:26:A:ASN:HA	3	0.2
(1,262)	1:25:A:PHE:HE2	1:26:A:ASN:HA	3	0.2
(1,262)	1:25:A:PHE:HE1	1:26:A:ASN:HA	9	0.2
(1,262)	1:25:A:PHE:HE2	1:26:A:ASN:HA	9	0.2
(1,256)	1:23:A:TYR:HE1	1:26:A:ASN:H	12	0.2
(1,256)	1:23:A:TYR:HE2	1:26:A:ASN:H	12	0.2
(1,244)	1:11:A:TRP:H	1:26:A:ASN:HB2	10	0.2
(1,189)	1:13:A:LYS:H	1:24:A:TYR:HA	8	0.2
(1,178)	1:23:A:TYR:HE1	1:33:A:GLN:H	15	0.2
(1,178)	1:23:A:TYR:HE2	1:33:A:GLN:H	15	0.2
(1,178)	1:23:A:TYR:HE1	1:33:A:GLN:H	16	0.2
(1,178)	1:23:A:TYR:HE2	1:33:A:GLN:H	16	0.2
(1,170)	1:16:A:SER:H	1:23:A:TYR:H	15	0.2
(1,130)	1:16:A:SER:H	1:21:A:ARG:HA	5	0.2
(1,123)	1:15:A:MET:HE1	1:20:A:GLY:H	15	0.2
(1,123)	1:15:A:MET:HE2	1:20:A:GLY:H	15	0.2
(1,123)	1:15:A:MET:HE3	1:20:A:GLY:H	15	0.2
(1,108)	1:15:A:MET:H	1:22:A:VAL:HA	3	0.2
(1,108)	1:15:A:MET:H	1:22:A:VAL:HA	10	0.2
(1,96)	1:14:A:ARG:H	1:23:A:TYR:HD1	14	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,96)	1:14:A:ARG:H	1:23:A:TYR:HD2	14	0.2
(1,93)	1:14:A:ARG:H	1:22:A:VAL:HA	17	0.2
(1,89)	1:14:A:ARG:H	1:15:A:MET:HA	11	0.2
(1,44)	1:8:A:PRO:HB2	1:11:A:TRP:HE1	16	0.2
(1,28)	1:7:A:LEU:HD21	1:13:A:LYS:HG3	20	0.2
(1,28)	1:7:A:LEU:HD22	1:13:A:LYS:HG3	20	0.2
(1,28)	1:7:A:LEU:HD23	1:13:A:LYS:HG3	20	0.2
(1,17)	1:6:A:LYS:HB3	1:7:A:LEU:H	15	0.2
(1,7)	1:3:A:ASP:HA	1:4:A:GLU:H	10	0.2
(1,7)	1:3:A:ASP:HA	1:4:A:GLU:H	12	0.2
(3,79)	1:105:A:SER:O	1:109:A:GLN:N	8	0.19
(3,71)	1:94:A:GLN:O	1:98:A:SER:N	5	0.19
(3,43)	1:72:A:SER:O	1:75:A:GLN:N	7	0.19
(3,34)	1:60:A:LEU:H	1:158:A:ILE:O	19	0.19
(2,105)	1:138:A:SER:H	2:656:B:PHE:HD1	9	0.19
(2,105)	1:138:A:SER:H	2:656:B:PHE:HD2	9	0.19
(2,102)	1:135:A:GLU:H	2:656:B:PHE:HB2	19	0.19
(2,94)	1:93:A:ILE:HG21	2:643:B:PRO:HB3	17	0.19
(2,94)	1:93:A:ILE:HG22	2:643:B:PRO:HB3	17	0.19
(2,94)	1:93:A:ILE:HG23	2:643:B:PRO:HB3	17	0.19
(2,92)	1:58:A:SER:H	2:651:B:ILE:HG12	20	0.19
(2,92)	1:58:A:SER:H	2:651:B:ILE:HG13	20	0.19
(2,62)	1:160:A:LEU:HD11	1:162:A:THR:H	11	0.19
(2,62)	1:160:A:LEU:HD12	1:162:A:THR:H	11	0.19
(2,62)	1:160:A:LEU:HD13	1:162:A:THR:H	11	0.19
(2,41)	1:126:A:SER:H	1:129:A:GLN:H	17	0.19
(2,1)	1:10:A:GLY:H	1:11:A:TRP:HB3	4	0.19
(2,1)	1:10:A:GLY:H	1:11:A:TRP:HB3	16	0.19
(1,2597)	1:138:A:SER:H	2:656:B:PHE:HB2	17	0.19
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG21	20	0.19
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG22	20	0.19
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG23	20	0.19
(1,2561)	2:655:B:GLU:H	2:656:B:PHE:HD1	2	0.19
(1,2561)	2:655:B:GLU:H	2:656:B:PHE:HD2	2	0.19
(1,2532)	2:648:B:ILE:HG21	2:650:B:ASN:H	13	0.19
(1,2532)	2:648:B:ILE:HG22	2:650:B:ASN:H	13	0.19
(1,2532)	2:648:B:ILE:HG23	2:650:B:ASN:H	13	0.19
(1,2526)	2:646:B:GLU:HB2	2:648:B:ILE:H	16	0.19
(1,2524)	2:647:B:VAL:HG11	2:650:B:ASN:HD22	20	0.19
(1,2524)	2:647:B:VAL:HG12	2:650:B:ASN:HD22	20	0.19
(1,2524)	2:647:B:VAL:HG13	2:650:B:ASN:HD22	20	0.19
(1,2481)	2:656:B:PHE:H	2:656:B:PHE:HE1	15	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2481)	2:656:B:PHE:H	2:656:B:PHE:HE2	15	0.19
(1,2158)	1:119:A:ARG:H	1:119:A:ARG:HD2	20	0.19
(1,2056)	1:101:A:GLU:H	1:101:A:GLU:HG2	8	0.19
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG21	6	0.19
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG22	6	0.19
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG23	6	0.19
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD11	8	0.19
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD12	8	0.19
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD13	8	0.19
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD11	20	0.19
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD12	20	0.19
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD13	20	0.19
(1,1751)	1:56:A:ARG:H	1:56:A:ARG:HG3	6	0.19
(1,1747)	1:56:A:ARG:H	1:56:A:ARG:HD2	16	0.19
(1,1694)	1:35:A:GLU:H	1:35:A:GLU:HG3	9	0.19
(1,1500)	1:12:A:GLU:H	1:12:A:GLU:HB2	20	0.19
(1,1456)	1:6:A:LYS:H	1:6:A:LYS:HE2	13	0.19
(1,1450)	1:4:A:GLU:HA	1:4:A:GLU:HG2	1	0.19
(1,1428)	1:143:A:THR:HG21	1:163:A:GLU:H	2	0.19
(1,1428)	1:143:A:THR:HG22	1:163:A:GLU:H	2	0.19
(1,1428)	1:143:A:THR:HG23	1:163:A:GLU:H	2	0.19
(1,1410)	1:161:A:ARG:HE	1:163:A:GLU:HG2	16	0.19
(1,1378)	1:147:A:SER:H	1:160:A:LEU:H	5	0.19
(1,1369)	1:104:A:GLU:H	1:160:A:LEU:HD11	3	0.19
(1,1369)	1:104:A:GLU:H	1:160:A:LEU:HD12	3	0.19
(1,1369)	1:104:A:GLU:H	1:160:A:LEU:HD13	3	0.19
(1,1346)	1:148:A:GLY:H	1:159:A:ILE:H	4	0.19
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG21	14	0.19
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG22	14	0.19
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG23	14	0.19
(1,1276)	1:63:A:LYS:HA	1:155:A:GLY:HA2	13	0.19
(1,1262)	1:151:A:PHE:H	1:156:A:ILE:HA	11	0.19
(1,1262)	1:151:A:PHE:H	1:156:A:ILE:HA	20	0.19
(1,1242)	1:150:A:VAL:HG11	1:157:A:HIS:H	10	0.19
(1,1242)	1:150:A:VAL:HG12	1:157:A:HIS:H	10	0.19
(1,1242)	1:150:A:VAL:HG13	1:157:A:HIS:H	10	0.19
(1,1184)	1:140:A:ALA:H	1:141:A:LEU:HG	1	0.19
(1,1177)	1:137:A:ALA:HB1	1:141:A:LEU:H	20	0.19
(1,1177)	1:137:A:ALA:HB2	1:141:A:LEU:H	20	0.19
(1,1177)	1:137:A:ALA:HB3	1:141:A:LEU:H	20	0.19
(1,1156)	1:136:A:ASP:HB2	1:137:A:ALA:H	1	0.19
(1,1143)	1:130:A:MET:HB2	1:135:A:GLU:H	10	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE1	13	0.19
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE2	13	0.19
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE3	13	0.19
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE1	13	0.19
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE2	13	0.19
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE3	13	0.19
(1,1066)	1:122:A:LEU:HD21	1:125:A:PHE:HD1	4	0.19
(1,1066)	1:122:A:LEU:HD21	1:125:A:PHE:HD2	4	0.19
(1,1066)	1:122:A:LEU:HD22	1:125:A:PHE:HD1	4	0.19
(1,1066)	1:122:A:LEU:HD22	1:125:A:PHE:HD2	4	0.19
(1,1066)	1:122:A:LEU:HD23	1:125:A:PHE:HD1	4	0.19
(1,1066)	1:122:A:LEU:HD23	1:125:A:PHE:HD2	4	0.19
(1,1047)	1:119:A:ARG:HD2	1:121:A:ASP:H	2	0.19
(1,1038)	1:119:A:ARG:HA	1:121:A:ASP:H	8	0.19
(1,1038)	1:119:A:ARG:HA	1:121:A:ASP:H	11	0.19
(1,1038)	1:119:A:ARG:HA	1:121:A:ASP:H	13	0.19
(1,1012)	1:116:A:ALA:H	1:119:A:ARG:H	11	0.19
(1,1012)	1:116:A:ALA:H	1:119:A:ARG:H	19	0.19
(1,1011)	1:116:A:ALA:HB1	1:119:A:ARG:H	2	0.19
(1,1011)	1:116:A:ALA:HB2	1:119:A:ARG:H	2	0.19
(1,1011)	1:116:A:ALA:HB3	1:119:A:ARG:H	2	0.19
(1,995)	1:108:A:SER:HA	1:116:A:ALA:H	6	0.19
(1,970)	1:108:A:SER:H	1:110:A:PHE:H	13	0.19
(1,888)	1:103:A:PHE:HE1	1:120:A:GLY:H	1	0.19
(1,888)	1:103:A:PHE:HE2	1:120:A:GLY:H	1	0.19
(1,871)	1:96:A:ILE:HB	1:103:A:PHE:H	19	0.19
(1,854)	1:98:A:SER:H	1:101:A:GLU:H	19	0.19
(1,799)	1:93:A:ILE:HB	1:146:A:MET:HE1	6	0.19
(1,799)	1:93:A:ILE:HB	1:146:A:MET:HE2	6	0.19
(1,799)	1:93:A:ILE:HB	1:146:A:MET:HE3	6	0.19
(1,764)	1:88:A:LEU:HA	1:92:A:TYR:H	15	0.19
(1,764)	1:88:A:LEU:HA	1:92:A:TYR:H	17	0.19
(1,750)	1:88:A:LEU:H	1:91:A:GLY:H	18	0.19
(1,748)	1:87:A:GLU:HA	1:91:A:GLY:H	10	0.19
(1,742)	1:89:A:ILE:HD11	1:90:A:ASN:H	12	0.19
(1,742)	1:89:A:ILE:HD12	1:90:A:ASN:H	12	0.19
(1,742)	1:89:A:ILE:HD13	1:90:A:ASN:H	12	0.19
(1,742)	1:89:A:ILE:HD11	1:90:A:ASN:H	13	0.19
(1,742)	1:89:A:ILE:HD12	1:90:A:ASN:H	13	0.19
(1,742)	1:89:A:ILE:HD13	1:90:A:ASN:H	13	0.19
(1,737)	1:86:A:LEU:HB3	1:90:A:ASN:H	4	0.19
(1,735)	1:89:A:ILE:HB	1:158:A:ILE:HD11	5	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,735)	1:89:A:ILE:HB	1:158:A:ILE:HD12	5	0.19
(1,735)	1:89:A:ILE:HB	1:158:A:ILE:HD13	5	0.19
(1,663)	1:82:A:LYS:HB3	1:83:A:GLU:H	5	0.19
(1,654)	1:82:A:LYS:HG2	1:84:A:GLU:H	12	0.19
(1,654)	1:82:A:LYS:HG3	1:84:A:GLU:H	12	0.19
(1,649)	1:66:A:GLN:HE21	1:82:A:LYS:HB2	4	0.19
(1,644)	1:81:A:THR:HA	1:84:A:GLU:H	5	0.19
(1,644)	1:81:A:THR:HA	1:84:A:GLU:H	8	0.19
(1,551)	1:70:A:PRO:HB3	1:71:A:SER:H	13	0.19
(1,549)	1:70:A:PRO:HG2	1:71:A:SER:H	12	0.19
(1,549)	1:70:A:PRO:HG2	1:71:A:SER:H	15	0.19
(1,520)	1:64:A:HIS:HE1	1:66:A:GLN:HG2	11	0.19
(1,515)	1:63:A:LYS:H	1:156:A:ILE:H	1	0.19
(1,496)	1:62:A:VAL:HG11	1:88:A:LEU:H	11	0.19
(1,496)	1:62:A:VAL:HG12	1:88:A:LEU:H	11	0.19
(1,496)	1:62:A:VAL:HG13	1:88:A:LEU:H	11	0.19
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG21	20	0.19
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG22	20	0.19
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG23	20	0.19
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG21	20	0.19
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG22	20	0.19
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG23	20	0.19
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG21	20	0.19
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG22	20	0.19
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG23	20	0.19
(1,402)	1:55:A:VAL:HA	1:125:A:PHE:H	4	0.19
(1,397)	1:54:A:ARG:HG2	1:126:A:SER:H	16	0.19
(1,393)	1:53:A:ALA:HB1	1:54:A:ARG:H	20	0.19
(1,393)	1:53:A:ALA:HB2	1:54:A:ARG:H	20	0.19
(1,393)	1:53:A:ALA:HB3	1:54:A:ARG:H	20	0.19
(1,388)	1:35:A:GLU:HG2	1:36:A:ARG:H	4	0.19
(1,377)	1:33:A:GLN:HG2	1:35:A:GLU:H	2	0.19
(1,363)	1:11:A:TRP:HE3	1:33:A:GLN:H	3	0.19
(1,344)	1:31:A:ALA:HB1	1:32:A:SER:H	13	0.19
(1,344)	1:31:A:ALA:HB2	1:32:A:SER:H	13	0.19
(1,344)	1:31:A:ALA:HB3	1:32:A:SER:H	13	0.19
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB1	7	0.19
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB2	7	0.19
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB3	7	0.19
(1,311)	1:27:A:HIS:HB2	1:29:A:THR:H	11	0.19
(1,218)	1:12:A:GLU:HB2	1:25:A:PHE:H	4	0.19
(1,217)	1:12:A:GLU:H	1:25:A:PHE:HB3	20	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,208)	1:24:A:TYR:H	1:34:A:TRP:HB3	17	0.19
(1,143)	1:15:A:MET:HA	1:22:A:VAL:H	10	0.19
(1,111)	1:15:A:MET:H	1:23:A:TYR:HD1	15	0.19
(1,111)	1:15:A:MET:H	1:23:A:TYR:HD2	15	0.19
(1,108)	1:15:A:MET:H	1:22:A:VAL:HA	4	0.19
(1,64)	1:12:A:GLU:H	1:24:A:TYR:HD1	19	0.19
(1,64)	1:12:A:GLU:H	1:24:A:TYR:HD2	19	0.19
(1,28)	1:7:A:LEU:HD21	1:13:A:LYS:HG3	3	0.19
(1,28)	1:7:A:LEU:HD22	1:13:A:LYS:HG3	3	0.19
(1,28)	1:7:A:LEU:HD23	1:13:A:LYS:HG3	3	0.19
(1,11)	1:4:A:GLU:H	1:6:A:LYS:H	15	0.19
(3,71)	1:94:A:GLN:O	1:98:A:SER:N	8	0.18
(3,65)	1:91:A:GLY:O	1:95:A:LYS:N	12	0.18
(3,53)	1:84:A:GLU:O	1:88:A:LEU:N	10	0.18
(3,44)	1:72:A:SER:O	1:75:A:GLN:H	4	0.18
(3,39)	1:64:A:HIS:O	1:67:A:SER:N	10	0.18
(3,34)	1:60:A:LEU:H	1:158:A:ILE:O	18	0.18
(2,112)	1:161:A:ARG:HE	2:651:B:ILE:HG12	18	0.18
(2,112)	1:161:A:ARG:HE	2:651:B:ILE:HG13	18	0.18
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG11	7	0.18
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG12	7	0.18
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG13	7	0.18
(2,93)	1:93:A:ILE:HD11	2:643:B:PRO:HA	14	0.18
(2,93)	1:93:A:ILE:HD12	2:643:B:PRO:HA	14	0.18
(2,93)	1:93:A:ILE:HD13	2:643:B:PRO:HA	14	0.18
(2,52)	1:141:A:LEU:HD21	1:148:A:GLY:H	19	0.18
(2,52)	1:141:A:LEU:HD22	1:148:A:GLY:H	19	0.18
(2,52)	1:141:A:LEU:HD23	1:148:A:GLY:H	19	0.18
(2,39)	1:55:A:VAL:HG11	1:127:A:ARG:H	20	0.18
(2,39)	1:55:A:VAL:HG12	1:127:A:ARG:H	20	0.18
(2,39)	1:55:A:VAL:HG13	1:127:A:ARG:H	20	0.18
(1,2623)	1:51:A:GLU:H	1:51:A:GLU:HG2	18	0.18
(1,2597)	1:138:A:SER:H	2:656:B:PHE:HB2	18	0.18
(1,2591)	1:123:A:GLY:H	2:656:B:PHE:HE1	4	0.18
(1,2591)	1:123:A:GLY:H	2:656:B:PHE:HE2	4	0.18
(1,2572)	1:16:A:SER:HB2	2:641:B:TPO:HG21	9	0.18
(1,2572)	1:16:A:SER:HB2	2:641:B:TPO:HG22	9	0.18
(1,2572)	1:16:A:SER:HB2	2:641:B:TPO:HG23	9	0.18
(1,2557)	2:654:B:SER:H	2:655:B:GLU:H	6	0.18
(1,2551)	2:652:B:ASP:H	2:654:B:SER:H	12	0.18
(1,2496)	2:659:B:PHE:H	2:659:B:PHE:HE1	14	0.18
(1,2496)	2:659:B:PHE:H	2:659:B:PHE:HE2	14	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2481)	2:656:B:PHE:H	2:656:B:PHE:HE1	2	0.18
(1,2481)	2:656:B:PHE:H	2:656:B:PHE:HE2	2	0.18
(1,2383)	1:163:A:GLU:H	1:163:A:GLU:HB2	16	0.18
(1,2302)	1:151:A:PHE:H	1:151:A:PHE:HE1	11	0.18
(1,2302)	1:151:A:PHE:H	1:151:A:PHE:HE2	11	0.18
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG21	2	0.18
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG22	2	0.18
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG23	2	0.18
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG21	7	0.18
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG22	7	0.18
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG23	7	0.18
(1,2036)	1:96:A:ILE:H	1:96:A:ILE:HD11	1	0.18
(1,2036)	1:96:A:ILE:H	1:96:A:ILE:HD12	1	0.18
(1,2036)	1:96:A:ILE:H	1:96:A:ILE:HD13	1	0.18
(1,2036)	1:96:A:ILE:H	1:96:A:ILE:HD11	3	0.18
(1,2036)	1:96:A:ILE:H	1:96:A:ILE:HD12	3	0.18
(1,2036)	1:96:A:ILE:H	1:96:A:ILE:HD13	3	0.18
(1,2036)	1:96:A:ILE:H	1:96:A:ILE:HD11	9	0.18
(1,2036)	1:96:A:ILE:H	1:96:A:ILE:HD12	9	0.18
(1,2036)	1:96:A:ILE:H	1:96:A:ILE:HD13	9	0.18
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD11	5	0.18
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD12	5	0.18
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD13	5	0.18
(1,1729)	1:54:A:ARG:H	1:54:A:ARG:HD2	7	0.18
(1,1703)	1:36:A:ARG:H	1:36:A:ARG:HD2	18	0.18
(1,1700)	1:36:A:ARG:H	1:36:A:ARG:HG2	15	0.18
(1,1694)	1:35:A:GLU:H	1:35:A:GLU:HG3	13	0.18
(1,1694)	1:35:A:GLU:H	1:35:A:GLU:HG3	20	0.18
(1,1568)	1:21:A:ARG:HB2	1:21:A:ARG:HE	3	0.18
(1,1568)	1:21:A:ARG:HB2	1:21:A:ARG:HE	14	0.18
(1,1456)	1:6:A:LYS:H	1:6:A:LYS:HE2	11	0.18
(1,1455)	1:6:A:LYS:H	1:6:A:LYS:HB3	6	0.18
(1,1455)	1:6:A:LYS:H	1:6:A:LYS:HB3	13	0.18
(1,1406)	1:147:A:SER:H	1:161:A:ARG:H	4	0.18
(1,1384)	1:159:A:ILE:HD11	1:160:A:LEU:H	19	0.18
(1,1384)	1:159:A:ILE:HD12	1:160:A:LEU:H	19	0.18
(1,1384)	1:159:A:ILE:HD13	1:160:A:LEU:H	19	0.18
(1,1382)	1:159:A:ILE:HG12	1:160:A:LEU:H	1	0.18
(1,1353)	1:57:A:CYS:HB3	1:160:A:LEU:H	12	0.18
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG21	4	0.18
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG22	4	0.18
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG23	4	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG21	11	0.18
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG22	11	0.18
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG23	11	0.18
(1,1311)	1:152:A:THR:HG21	1:157:A:HIS:H	5	0.18
(1,1311)	1:152:A:THR:HG22	1:157:A:HIS:H	5	0.18
(1,1311)	1:152:A:THR:HG23	1:157:A:HIS:H	5	0.18
(1,1311)	1:152:A:THR:HG21	1:157:A:HIS:H	14	0.18
(1,1311)	1:152:A:THR:HG22	1:157:A:HIS:H	14	0.18
(1,1311)	1:152:A:THR:HG23	1:157:A:HIS:H	14	0.18
(1,1230)	1:149:A:PRO:HD3	1:150:A:VAL:H	11	0.18
(1,1200)	1:143:A:THR:H	1:144:A:GLY:H	3	0.18
(1,1200)	1:143:A:THR:H	1:144:A:GLY:H	7	0.18
(1,1187)	1:140:A:ALA:HB1	1:141:A:LEU:HD21	15	0.18
(1,1187)	1:140:A:ALA:HB1	1:141:A:LEU:HD22	15	0.18
(1,1187)	1:140:A:ALA:HB1	1:141:A:LEU:HD23	15	0.18
(1,1187)	1:140:A:ALA:HB2	1:141:A:LEU:HD21	15	0.18
(1,1187)	1:140:A:ALA:HB2	1:141:A:LEU:HD22	15	0.18
(1,1187)	1:140:A:ALA:HB2	1:141:A:LEU:HD23	15	0.18
(1,1187)	1:140:A:ALA:HB3	1:141:A:LEU:HD21	15	0.18
(1,1187)	1:140:A:ALA:HB3	1:141:A:LEU:HD22	15	0.18
(1,1187)	1:140:A:ALA:HB3	1:141:A:LEU:HD23	15	0.18
(1,1178)	1:137:A:ALA:HA	1:141:A:LEU:H	11	0.18
(1,1132)	1:131:A:GLN:HG2	1:132:A:LYS:H	3	0.18
(1,1038)	1:119:A:ARG:HA	1:121:A:ASP:H	17	0.18
(1,1021)	1:117:A:LYS:HG3	1:118:A:ALA:H	15	0.18
(1,1021)	1:117:A:LYS:HG2	1:118:A:ALA:H	15	0.18
(1,1020)	1:116:A:ALA:HA	1:118:A:ALA:H	1	0.18
(1,1011)	1:116:A:ALA:HB1	1:119:A:ARG:H	7	0.18
(1,1011)	1:116:A:ALA:HB2	1:119:A:ARG:H	7	0.18
(1,1011)	1:116:A:ALA:HB3	1:119:A:ARG:H	7	0.18
(1,959)	1:108:A:SER:HA	1:111:A:SER:H	18	0.18
(1,941)	1:106:A:LEU:HD11	1:107:A:ALA:H	8	0.18
(1,941)	1:106:A:LEU:HD12	1:107:A:ALA:H	8	0.18
(1,941)	1:106:A:LEU:HD13	1:107:A:ALA:H	8	0.18
(1,940)	1:106:A:LEU:HG	1:107:A:ALA:H	6	0.18
(1,940)	1:106:A:LEU:HG	1:107:A:ALA:H	19	0.18
(1,920)	1:106:A:LEU:HB3	1:108:A:SER:H	1	0.18
(1,914)	1:104:A:GLU:H	1:106:A:LEU:HB3	1	0.18
(1,914)	1:104:A:GLU:H	1:106:A:LEU:HB3	11	0.18
(1,913)	1:103:A:PHE:H	1:106:A:LEU:HB3	10	0.18
(1,846)	1:98:A:SER:HB2	1:100:A:GLU:HB2	15	0.18
(1,825)	1:96:A:ILE:HD11	1:106:A:LEU:HG	20	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,825)	1:96:A:ILE:HD12	1:106:A:LEU:HG	20	0.18
(1,825)	1:96:A:ILE:HD13	1:106:A:LEU:HG	20	0.18
(1,766)	1:89:A:ILE:HD11	1:92:A:TYR:HD1	13	0.18
(1,766)	1:89:A:ILE:HD11	1:92:A:TYR:HD2	13	0.18
(1,766)	1:89:A:ILE:HD12	1:92:A:TYR:HD1	13	0.18
(1,766)	1:89:A:ILE:HD12	1:92:A:TYR:HD2	13	0.18
(1,766)	1:89:A:ILE:HD13	1:92:A:TYR:HD1	13	0.18
(1,766)	1:89:A:ILE:HD13	1:92:A:TYR:HD2	13	0.18
(1,735)	1:89:A:ILE:HB	1:158:A:ILE:HD11	3	0.18
(1,735)	1:89:A:ILE:HB	1:158:A:ILE:HD12	3	0.18
(1,735)	1:89:A:ILE:HB	1:158:A:ILE:HD13	3	0.18
(1,695)	1:86:A:LEU:HD21	1:149:A:PRO:HD3	12	0.18
(1,695)	1:86:A:LEU:HD22	1:149:A:PRO:HD3	12	0.18
(1,695)	1:86:A:LEU:HD23	1:149:A:PRO:HD3	12	0.18
(1,674)	1:81:A:THR:H	1:85:A:ALA:H	4	0.18
(1,669)	1:84:A:GLU:H	1:87:A:GLU:H	2	0.18
(1,663)	1:82:A:LYS:HB3	1:83:A:GLU:H	15	0.18
(1,649)	1:66:A:GLN:HE21	1:82:A:LYS:HB2	17	0.18
(1,591)	1:74:A:ARG:HE	1:75:A:GLN:H	1	0.18
(1,554)	1:70:A:PRO:HG3	1:71:A:SER:H	1	0.18
(1,538)	1:66:A:GLN:HG2	1:67:A:SER:H	5	0.18
(1,510)	1:62:A:VAL:HG11	1:156:A:ILE:H	8	0.18
(1,510)	1:62:A:VAL:HG12	1:156:A:ILE:H	8	0.18
(1,510)	1:62:A:VAL:HG13	1:156:A:ILE:H	8	0.18
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD11	7	0.18
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD12	7	0.18
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD13	7	0.18
(1,475)	1:61:A:LEU:HD11	1:113:A:CYS:H	5	0.18
(1,475)	1:61:A:LEU:HD12	1:113:A:CYS:H	5	0.18
(1,475)	1:61:A:LEU:HD13	1:113:A:CYS:H	5	0.18
(1,475)	1:61:A:LEU:HD21	1:113:A:CYS:H	5	0.18
(1,475)	1:61:A:LEU:HD22	1:113:A:CYS:H	5	0.18
(1,475)	1:61:A:LEU:HD23	1:113:A:CYS:H	5	0.18
(1,457)	1:60:A:LEU:HD11	1:108:A:SER:H	4	0.18
(1,457)	1:60:A:LEU:HD12	1:108:A:SER:H	4	0.18
(1,457)	1:60:A:LEU:HD13	1:108:A:SER:H	4	0.18
(1,457)	1:60:A:LEU:HD11	1:108:A:SER:H	5	0.18
(1,457)	1:60:A:LEU:HD12	1:108:A:SER:H	5	0.18
(1,457)	1:60:A:LEU:HD13	1:108:A:SER:H	5	0.18
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG21	1	0.18
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG22	1	0.18
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG23	1	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG21	1	0.18
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG22	1	0.18
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG23	1	0.18
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG21	1	0.18
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG22	1	0.18
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG23	1	0.18
(1,424)	1:56:A:ARG:HE	1:57:A:CYS:H	2	0.18
(1,424)	1:56:A:ARG:HE	1:57:A:CYS:H	18	0.18
(1,383)	1:34:A:TRP:H	1:35:A:GLU:HB3	9	0.18
(1,378)	1:33:A:GLN:H	1:35:A:GLU:H	14	0.18
(1,367)	1:24:A:TYR:HD1	1:34:A:TRP:H	18	0.18
(1,367)	1:24:A:TYR:HD2	1:34:A:TRP:H	18	0.18
(1,364)	1:24:A:TYR:HD1	1:33:A:GLN:H	14	0.18
(1,364)	1:24:A:TYR:HD2	1:33:A:GLN:H	14	0.18
(1,364)	1:24:A:TYR:HD1	1:33:A:GLN:H	16	0.18
(1,364)	1:24:A:TYR:HD2	1:33:A:GLN:H	16	0.18
(1,363)	1:11:A:TRP:HE3	1:33:A:GLN:H	7	0.18
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB1	9	0.18
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB2	9	0.18
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB3	9	0.18
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB1	12	0.18
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB2	12	0.18
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB3	12	0.18
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB1	14	0.18
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB2	14	0.18
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB3	14	0.18
(1,318)	1:29:A:THR:H	1:30:A:ASN:HB3	6	0.18
(1,318)	1:29:A:THR:H	1:30:A:ASN:HB3	9	0.18
(1,318)	1:29:A:THR:H	1:30:A:ASN:HB3	19	0.18
(1,278)	1:26:A:ASN:HB2	1:30:A:ASN:H	13	0.18
(1,277)	1:26:A:ASN:H	1:30:A:ASN:H	16	0.18
(1,242)	1:10:A:GLY:H	1:26:A:ASN:HD21	3	0.18
(1,242)	1:10:A:GLY:H	1:26:A:ASN:HD21	11	0.18
(1,194)	1:13:A:LYS:HG2	1:24:A:TYR:HA	17	0.18
(1,188)	1:13:A:LYS:HG2	1:24:A:TYR:HE1	13	0.18
(1,188)	1:13:A:LYS:HG2	1:24:A:TYR:HE2	13	0.18
(1,143)	1:15:A:MET:HA	1:22:A:VAL:H	18	0.18
(1,130)	1:16:A:SER:H	1:21:A:ARG:HA	20	0.18
(1,116)	1:16:A:SER:H	1:20:A:GLY:HA2	7	0.18
(1,110)	1:15:A:MET:H	1:23:A:TYR:HE1	16	0.18
(1,110)	1:15:A:MET:H	1:23:A:TYR:HE2	16	0.18
(1,108)	1:15:A:MET:H	1:22:A:VAL:HA	13	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,98)	1:14:A:ARG:H	1:24:A:TYR:H	12	0.18
(1,96)	1:14:A:ARG:H	1:23:A:TYR:HD1	9	0.18
(1,96)	1:14:A:ARG:H	1:23:A:TYR:HD2	9	0.18
(1,89)	1:14:A:ARG:H	1:15:A:MET:HA	19	0.18
(1,75)	1:13:A:LYS:HA	1:23:A:TYR:H	18	0.18
(1,27)	1:7:A:LEU:HD21	1:13:A:LYS:H	18	0.18
(1,27)	1:7:A:LEU:HD22	1:13:A:LYS:H	18	0.18
(1,27)	1:7:A:LEU:HD23	1:13:A:LYS:H	18	0.18
(1,17)	1:6:A:LYS:HB3	1:7:A:LEU:H	8	0.18
(1,12)	1:5:A:GLU:HB2	1:6:A:LYS:H	17	0.18
(1,7)	1:3:A:ASP:HA	1:4:A:GLU:H	15	0.18
(3,81)	1:106:A:LEU:O	1:110:A:PHE:N	2	0.17
(3,71)	1:94:A:GLN:O	1:98:A:SER:N	7	0.17
(3,63)	1:90:A:ASN:O	1:94:A:GLN:N	13	0.17
(3,45)	1:70:A:PRO:O	1:78:A:ILE:N	6	0.17
(3,44)	1:72:A:SER:O	1:75:A:GLN:H	12	0.17
(3,43)	1:72:A:SER:O	1:75:A:GLN:N	2	0.17
(2,111)	1:160:A:LEU:H	2:651:B:ILE:HG12	7	0.17
(2,111)	1:160:A:LEU:H	2:651:B:ILE:HG13	7	0.17
(2,93)	1:93:A:ILE:HD11	2:643:B:PRO:HA	4	0.17
(2,93)	1:93:A:ILE:HD12	2:643:B:PRO:HA	4	0.17
(2,93)	1:93:A:ILE:HD13	2:643:B:PRO:HA	4	0.17
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD11	6	0.17
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD12	6	0.17
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD13	6	0.17
(2,70)	2:651:B:ILE:HG21	2:656:B:PHE:HE1	8	0.17
(2,70)	2:651:B:ILE:HG21	2:656:B:PHE:HE2	8	0.17
(2,70)	2:651:B:ILE:HG22	2:656:B:PHE:HE1	8	0.17
(2,70)	2:651:B:ILE:HG22	2:656:B:PHE:HE2	8	0.17
(2,70)	2:651:B:ILE:HG23	2:656:B:PHE:HE1	8	0.17
(2,70)	2:651:B:ILE:HG23	2:656:B:PHE:HE2	8	0.17
(2,9)	1:53:A:ALA:H	1:54:A:ARG:HD2	17	0.17
(2,1)	1:10:A:GLY:H	1:11:A:TRP:HB3	5	0.17
(1,2584)	1:114:A:SER:H	2:659:B:PHE:HD1	15	0.17
(1,2584)	1:114:A:SER:H	2:659:B:PHE:HD2	15	0.17
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG21	6	0.17
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG22	6	0.17
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG23	6	0.17
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG21	8	0.17
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG22	8	0.17
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG23	8	0.17
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG21	9	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG22	9	0.17
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG23	9	0.17
(1,2520)	2:646:B:GLU:HG3	2:647:B:VAL:H	14	0.17
(1,2517)	2:646:B:GLU:HG2	2:647:B:VAL:H	7	0.17
(1,2513)	2:646:B:GLU:HA	2:649:B:ARG:HD2	19	0.17
(1,2496)	2:659:B:PHE:H	2:659:B:PHE:HE1	6	0.17
(1,2496)	2:659:B:PHE:H	2:659:B:PHE:HE2	6	0.17
(1,2466)	2:651:B:ILE:H	2:651:B:ILE:HD11	19	0.17
(1,2466)	2:651:B:ILE:H	2:651:B:ILE:HD12	19	0.17
(1,2466)	2:651:B:ILE:H	2:651:B:ILE:HD13	19	0.17
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG21	10	0.17
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG22	10	0.17
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG23	10	0.17
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG21	11	0.17
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG22	11	0.17
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG23	11	0.17
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG21	13	0.17
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG22	13	0.17
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG23	13	0.17
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG21	16	0.17
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG22	16	0.17
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG23	16	0.17
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG21	17	0.17
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG22	17	0.17
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG23	17	0.17
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG21	18	0.17
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG22	18	0.17
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG23	18	0.17
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG21	20	0.17
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG22	20	0.17
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG23	20	0.17
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD11	6	0.17
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD12	6	0.17
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD13	6	0.17
(1,1910)	1:82:A:LYS:H	1:82:A:LYS:HE2	2	0.17
(1,1906)	1:81:A:THR:H	1:81:A:THR:HG21	1	0.17
(1,1906)	1:81:A:THR:H	1:81:A:THR:HG22	1	0.17
(1,1906)	1:81:A:THR:H	1:81:A:THR:HG23	1	0.17
(1,1906)	1:81:A:THR:H	1:81:A:THR:HG21	2	0.17
(1,1906)	1:81:A:THR:H	1:81:A:THR:HG22	2	0.17
(1,1906)	1:81:A:THR:H	1:81:A:THR:HG23	2	0.17
(1,1906)	1:81:A:THR:H	1:81:A:THR:HG21	17	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1906)	1:81:A:THR:H	1:81:A:THR:HG22	17	0.17
(1,1906)	1:81:A:THR:H	1:81:A:THR:HG23	17	0.17
(1,1751)	1:56:A:ARG:H	1:56:A:ARG:HG3	4	0.17
(1,1700)	1:36:A:ARG:H	1:36:A:ARG:HG2	2	0.17
(1,1694)	1:35:A:GLU:H	1:35:A:GLU:HG3	14	0.17
(1,1660)	1:32:A:SER:H	1:32:A:SER:HB3	18	0.17
(1,1568)	1:21:A:ARG:HB2	1:21:A:ARG:HE	5	0.17
(1,1568)	1:21:A:ARG:HB2	1:21:A:ARG:HE	15	0.17
(1,1425)	1:56:A:ARG:H	1:163:A:GLU:H	11	0.17
(1,1410)	1:161:A:ARG:HE	1:163:A:GLU:HG2	20	0.17
(1,1384)	1:159:A:ILE:HD11	1:160:A:LEU:H	5	0.17
(1,1384)	1:159:A:ILE:HD12	1:160:A:LEU:H	5	0.17
(1,1384)	1:159:A:ILE:HD13	1:160:A:LEU:H	5	0.17
(1,1384)	1:159:A:ILE:HD11	1:160:A:LEU:H	18	0.17
(1,1384)	1:159:A:ILE:HD12	1:160:A:LEU:H	18	0.17
(1,1384)	1:159:A:ILE:HD13	1:160:A:LEU:H	18	0.17
(1,1382)	1:159:A:ILE:HG12	1:160:A:LEU:H	3	0.17
(1,1382)	1:159:A:ILE:HG12	1:160:A:LEU:H	6	0.17
(1,1382)	1:159:A:ILE:HG12	1:160:A:LEU:H	8	0.17
(1,1382)	1:159:A:ILE:HG12	1:160:A:LEU:H	12	0.17
(1,1382)	1:159:A:ILE:HG12	1:160:A:LEU:H	14	0.17
(1,1369)	1:104:A:GLU:H	1:160:A:LEU:HD11	15	0.17
(1,1369)	1:104:A:GLU:H	1:160:A:LEU:HD12	15	0.17
(1,1369)	1:104:A:GLU:H	1:160:A:LEU:HD13	15	0.17
(1,1369)	1:104:A:GLU:H	1:160:A:LEU:HD11	19	0.17
(1,1369)	1:104:A:GLU:H	1:160:A:LEU:HD12	19	0.17
(1,1369)	1:104:A:GLU:H	1:160:A:LEU:HD13	19	0.17
(1,1368)	1:103:A:PHE:HB3	1:160:A:LEU:HD21	17	0.17
(1,1368)	1:103:A:PHE:HB3	1:160:A:LEU:HD22	17	0.17
(1,1368)	1:103:A:PHE:HB3	1:160:A:LEU:HD23	17	0.17
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD11	15	0.17
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD12	15	0.17
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD13	15	0.17
(1,1363)	1:96:A:ILE:HG21	1:160:A:LEU:HD11	19	0.17
(1,1363)	1:96:A:ILE:HG21	1:160:A:LEU:HD12	19	0.17
(1,1363)	1:96:A:ILE:HG21	1:160:A:LEU:HD13	19	0.17
(1,1363)	1:96:A:ILE:HG22	1:160:A:LEU:HD11	19	0.17
(1,1363)	1:96:A:ILE:HG22	1:160:A:LEU:HD12	19	0.17
(1,1363)	1:96:A:ILE:HG22	1:160:A:LEU:HD13	19	0.17
(1,1363)	1:96:A:ILE:HG23	1:160:A:LEU:HD11	19	0.17
(1,1363)	1:96:A:ILE:HG23	1:160:A:LEU:HD12	19	0.17
(1,1363)	1:96:A:ILE:HG23	1:160:A:LEU:HD13	19	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1346)	1:148:A:GLY:H	1:159:A:ILE:H	14	0.17
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG21	17	0.17
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG22	17	0.17
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG23	17	0.17
(1,1282)	1:82:A:LYS:HE2	1:156:A:ILE:HD11	1	0.17
(1,1282)	1:82:A:LYS:HE2	1:156:A:ILE:HD12	1	0.17
(1,1282)	1:82:A:LYS:HE2	1:156:A:ILE:HD13	1	0.17
(1,1262)	1:151:A:PHE:H	1:156:A:ILE:HA	15	0.17
(1,1259)	1:151:A:PHE:HB2	1:152:A:THR:H	1	0.17
(1,1259)	1:151:A:PHE:HB2	1:152:A:THR:H	12	0.17
(1,1242)	1:150:A:VAL:HG11	1:157:A:HIS:H	1	0.17
(1,1242)	1:150:A:VAL:HG12	1:157:A:HIS:H	1	0.17
(1,1242)	1:150:A:VAL:HG13	1:157:A:HIS:H	1	0.17
(1,1200)	1:143:A:THR:H	1:144:A:GLY:H	4	0.17
(1,1200)	1:143:A:THR:H	1:144:A:GLY:H	5	0.17
(1,1200)	1:143:A:THR:H	1:144:A:GLY:H	6	0.17
(1,1178)	1:137:A:ALA:HA	1:141:A:LEU:H	17	0.17
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE1	5	0.17
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE2	5	0.17
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE3	5	0.17
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE1	5	0.17
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE2	5	0.17
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE3	5	0.17
(1,1078)	1:122:A:LEU:HG	1:123:A:GLY:H	2	0.17
(1,1078)	1:122:A:LEU:HG	1:123:A:GLY:H	20	0.17
(1,1031)	1:118:A:ALA:HB1	1:121:A:ASP:HB2	15	0.17
(1,1031)	1:118:A:ALA:HB2	1:121:A:ASP:HB2	15	0.17
(1,1031)	1:118:A:ALA:HB3	1:121:A:ASP:HB2	15	0.17
(1,1020)	1:116:A:ALA:HA	1:118:A:ALA:H	7	0.17
(1,1015)	1:116:A:ALA:HB1	1:120:A:GLY:H	11	0.17
(1,1015)	1:116:A:ALA:HB2	1:120:A:GLY:H	11	0.17
(1,1015)	1:116:A:ALA:HB3	1:120:A:GLY:H	11	0.17
(1,1011)	1:116:A:ALA:HB1	1:119:A:ARG:H	19	0.17
(1,1011)	1:116:A:ALA:HB2	1:119:A:ARG:H	19	0.17
(1,1011)	1:116:A:ALA:HB3	1:119:A:ARG:H	19	0.17
(1,978)	1:107:A:ALA:HB1	1:111:A:SER:HA	13	0.17
(1,978)	1:107:A:ALA:HB2	1:111:A:SER:HA	13	0.17
(1,978)	1:107:A:ALA:HB3	1:111:A:SER:HA	13	0.17
(1,970)	1:108:A:SER:H	1:110:A:PHE:H	8	0.17
(1,960)	1:108:A:SER:H	1:111:A:SER:H	20	0.17
(1,959)	1:108:A:SER:HA	1:111:A:SER:H	6	0.17
(1,959)	1:108:A:SER:HA	1:111:A:SER:H	12	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,941)	1:106:A:LEU:HD11	1:107:A:ALA:H	10	0.17
(1,941)	1:106:A:LEU:HD12	1:107:A:ALA:H	10	0.17
(1,941)	1:106:A:LEU:HD13	1:107:A:ALA:H	10	0.17
(1,940)	1:106:A:LEU:HG	1:107:A:ALA:H	12	0.17
(1,920)	1:106:A:LEU:HB3	1:108:A:SER:H	10	0.17
(1,920)	1:106:A:LEU:HB3	1:108:A:SER:H	20	0.17
(1,843)	1:97:A:LYS:HB2	1:98:A:SER:H	17	0.17
(1,824)	1:96:A:ILE:HG21	1:98:A:SER:H	19	0.17
(1,824)	1:96:A:ILE:HG22	1:98:A:SER:H	19	0.17
(1,824)	1:96:A:ILE:HG23	1:98:A:SER:H	19	0.17
(1,805)	1:93:A:ILE:HG21	1:94:A:GLN:H	19	0.17
(1,805)	1:93:A:ILE:HG22	1:94:A:GLN:H	19	0.17
(1,805)	1:93:A:ILE:HG23	1:94:A:GLN:H	19	0.17
(1,751)	1:89:A:ILE:HG21	1:91:A:GLY:H	8	0.17
(1,751)	1:89:A:ILE:HG22	1:91:A:GLY:H	8	0.17
(1,751)	1:89:A:ILE:HG23	1:91:A:GLY:H	8	0.17
(1,750)	1:88:A:LEU:H	1:91:A:GLY:H	6	0.17
(1,750)	1:88:A:LEU:H	1:91:A:GLY:H	15	0.17
(1,695)	1:86:A:LEU:HD21	1:149:A:PRO:HD3	9	0.17
(1,695)	1:86:A:LEU:HD22	1:149:A:PRO:HD3	9	0.17
(1,695)	1:86:A:LEU:HD23	1:149:A:PRO:HD3	9	0.17
(1,681)	1:85:A:ALA:H	1:88:A:LEU:HD11	20	0.17
(1,681)	1:85:A:ALA:H	1:88:A:LEU:HD12	20	0.17
(1,681)	1:85:A:ALA:H	1:88:A:LEU:HD13	20	0.17
(1,674)	1:81:A:THR:H	1:85:A:ALA:H	3	0.17
(1,674)	1:81:A:THR:H	1:85:A:ALA:H	12	0.17
(1,669)	1:84:A:GLU:H	1:87:A:GLU:H	6	0.17
(1,659)	1:81:A:THR:HA	1:83:A:GLU:H	11	0.17
(1,641)	1:65:A:SER:HB2	1:81:A:THR:HG21	12	0.17
(1,641)	1:65:A:SER:HB2	1:81:A:THR:HG22	12	0.17
(1,641)	1:65:A:SER:HB2	1:81:A:THR:HG23	12	0.17
(1,637)	1:80:A:ARG:HE	1:85:A:ALA:H	15	0.17
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG21	16	0.17
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG22	16	0.17
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG23	16	0.17
(1,619)	1:78:A:ILE:HB	1:80:A:ARG:H	6	0.17
(1,571)	1:73:A:TRP:HE1	1:74:A:ARG:HB3	20	0.17
(1,569)	1:73:A:TRP:HE1	1:74:A:ARG:HB2	5	0.17
(1,564)	1:72:A:SER:H	1:78:A:ILE:HG12	3	0.17
(1,564)	1:72:A:SER:H	1:78:A:ILE:HG12	9	0.17
(1,554)	1:70:A:PRO:HG3	1:71:A:SER:H	12	0.17
(1,457)	1:60:A:LEU:HD11	1:108:A:SER:H	14	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,457)	1:60:A:LEU:HD12	1:108:A:SER:H	14	0.17
(1,457)	1:60:A:LEU:HD13	1:108:A:SER:H	14	0.17
(1,440)	1:59:A:HIS:H	1:115:A:SER:HB3	11	0.17
(1,436)	1:58:A:SER:H	1:160:A:LEU:HG	3	0.17
(1,435)	1:58:A:SER:HA	1:122:A:LEU:HG	20	0.17
(1,393)	1:53:A:ALA:HB1	1:54:A:ARG:H	11	0.17
(1,393)	1:53:A:ALA:HB2	1:54:A:ARG:H	11	0.17
(1,393)	1:53:A:ALA:HB3	1:54:A:ARG:H	11	0.17
(1,391)	1:35:A:GLU:HB3	1:36:A:ARG:H	13	0.17
(1,388)	1:35:A:GLU:HG2	1:36:A:ARG:H	14	0.17
(1,388)	1:35:A:GLU:HG2	1:36:A:ARG:H	19	0.17
(1,362)	1:11:A:TRP:HH2	1:33:A:GLN:HE21	7	0.17
(1,355)	1:25:A:PHE:HE1	1:32:A:SER:HB2	8	0.17
(1,355)	1:25:A:PHE:HE2	1:32:A:SER:HB2	8	0.17
(1,347)	1:31:A:ALA:HB1	1:33:A:GLN:H	12	0.17
(1,347)	1:31:A:ALA:HB2	1:33:A:GLN:H	12	0.17
(1,347)	1:31:A:ALA:HB3	1:33:A:GLN:H	12	0.17
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB1	17	0.17
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB2	17	0.17
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB3	17	0.17
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB1	18	0.17
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB2	18	0.17
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB3	18	0.17
(1,321)	1:25:A:PHE:HZ	1:30:A:ASN:H	7	0.17
(1,321)	1:25:A:PHE:HZ	1:30:A:ASN:H	18	0.17
(1,321)	1:25:A:PHE:HZ	1:30:A:ASN:H	19	0.17
(1,318)	1:29:A:THR:H	1:30:A:ASN:HB3	14	0.17
(1,311)	1:27:A:HIS:HB2	1:29:A:THR:H	5	0.17
(1,311)	1:27:A:HIS:HB2	1:29:A:THR:H	12	0.17
(1,302)	1:27:A:HIS:HD2	1:28:A:ILE:H	6	0.17
(1,211)	1:24:A:TYR:HE1	1:36:A:ARG:HD2	8	0.17
(1,211)	1:24:A:TYR:HE2	1:36:A:ARG:HD2	8	0.17
(1,208)	1:24:A:TYR:H	1:34:A:TRP:HB3	7	0.17
(1,189)	1:13:A:LYS:H	1:24:A:TYR:HA	16	0.17
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG11	18	0.17
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG12	18	0.17
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG13	18	0.17
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG11	18	0.17
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG12	18	0.17
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG13	18	0.17
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG11	18	0.17
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG12	18	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG13	18	0.17
(1,96)	1:14:A:ARG:H	1:23:A:TYR:HD1	1	0.17
(1,96)	1:14:A:ARG:H	1:23:A:TYR:HD2	1	0.17
(1,28)	1:7:A:LEU:HD21	1:13:A:LYS:HG3	18	0.17
(1,28)	1:7:A:LEU:HD22	1:13:A:LYS:HG3	18	0.17
(1,28)	1:7:A:LEU:HD23	1:13:A:LYS:HG3	18	0.17
(1,20)	1:7:A:LEU:HD11	1:11:A:TRP:H	2	0.17
(1,20)	1:7:A:LEU:HD12	1:11:A:TRP:H	2	0.17
(1,20)	1:7:A:LEU:HD13	1:11:A:TRP:H	2	0.17
(1,7)	1:3:A:ASP:HA	1:4:A:GLU:H	9	0.17
(1,7)	1:3:A:ASP:HA	1:4:A:GLU:H	13	0.17
(1,7)	1:3:A:ASP:HA	1:4:A:GLU:H	14	0.17
(1,7)	1:3:A:ASP:HA	1:4:A:GLU:H	20	0.17
(4,2774)	1:26:A:ASN:H	1:31:A:ALA:O	16	0.16
(3,46)	1:70:A:PRO:O	1:78:A:ILE:H	11	0.16
(3,43)	1:72:A:SER:O	1:75:A:GLN:N	8	0.16
(2,101)	1:129:A:GLN:HE21	2:657:B:GLU:HB2	15	0.16
(2,101)	1:129:A:GLN:HE21	2:657:B:GLU:HB3	15	0.16
(2,97)	1:94:A:GLN:HE21	2:640:B:LEU:HG	8	0.16
(2,93)	1:93:A:ILE:HD11	2:643:B:PRO:HA	1	0.16
(2,93)	1:93:A:ILE:HD12	2:643:B:PRO:HA	1	0.16
(2,93)	1:93:A:ILE:HD13	2:643:B:PRO:HA	1	0.16
(2,74)	2:656:B:PHE:HB2	2:659:B:PHE:HD1	5	0.16
(2,74)	2:656:B:PHE:HB2	2:659:B:PHE:HD2	5	0.16
(2,74)	2:656:B:PHE:HB3	2:659:B:PHE:HD1	5	0.16
(2,74)	2:656:B:PHE:HB3	2:659:B:PHE:HD2	5	0.16
(2,72)	2:653:B:GLN:HA	2:656:B:PHE:HE1	6	0.16
(2,72)	2:653:B:GLN:HA	2:656:B:PHE:HE2	6	0.16
(2,58)	1:152:A:THR:HG21	1:157:A:HIS:HB3	19	0.16
(2,58)	1:152:A:THR:HG22	1:157:A:HIS:HB3	19	0.16
(2,58)	1:152:A:THR:HG23	1:157:A:HIS:HB3	19	0.16
(2,42)	1:130:A:MET:HB2	1:134:A:PHE:HD1	14	0.16
(2,42)	1:130:A:MET:HB2	1:134:A:PHE:HD2	14	0.16
(2,38)	1:126:A:SER:H	1:129:A:GLN:HB2	15	0.16
(2,1)	1:10:A:GLY:H	1:11:A:TRP:HB3	18	0.16
(1,2598)	1:146:A:MET:HE1	2:642:B:PRO:HB2	11	0.16
(1,2598)	1:146:A:MET:HE1	2:642:B:PRO:HB3	11	0.16
(1,2598)	1:146:A:MET:HE2	2:642:B:PRO:HB2	11	0.16
(1,2598)	1:146:A:MET:HE2	2:642:B:PRO:HB3	11	0.16
(1,2598)	1:146:A:MET:HE3	2:642:B:PRO:HB2	11	0.16
(1,2598)	1:146:A:MET:HE3	2:642:B:PRO:HB3	11	0.16
(1,2582)	1:34:A:TRP:HE1	2:642:B:PRO:HB2	6	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2582)	1:34:A:TRP:HE1	2:642:B:PRO:HB3	6	0.16
(1,2561)	2:655:B:GLU:H	2:656:B:PHE:HD1	16	0.16
(1,2561)	2:655:B:GLU:H	2:656:B:PHE:HD2	16	0.16
(1,2517)	2:646:B:GLU:HG2	2:647:B:VAL:H	8	0.16
(1,2488)	2:656:B:PHE:HA	2:656:B:PHE:HE1	13	0.16
(1,2488)	2:656:B:PHE:HA	2:656:B:PHE:HE2	13	0.16
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE1	16	0.16
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE2	16	0.16
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE3	16	0.16
(1,2056)	1:101:A:GLU:H	1:101:A:GLU:HG2	1	0.16
(1,2056)	1:101:A:GLU:H	1:101:A:GLU:HG2	5	0.16
(1,2056)	1:101:A:GLU:H	1:101:A:GLU:HG2	9	0.16
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG21	15	0.16
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG22	15	0.16
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG23	15	0.16
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG21	19	0.16
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG22	19	0.16
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG23	19	0.16
(1,2033)	1:95:A:LYS:H	1:95:A:LYS:HD2	12	0.16
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD11	2	0.16
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD12	2	0.16
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD13	2	0.16
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD11	8	0.16
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD12	8	0.16
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD13	8	0.16
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD11	12	0.16
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD12	12	0.16
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD13	12	0.16
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD11	18	0.16
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD12	18	0.16
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD13	18	0.16
(1,1913)	1:82:A:LYS:H	1:82:A:LYS:HD2	4	0.16
(1,1913)	1:82:A:LYS:H	1:82:A:LYS:HD2	11	0.16
(1,1913)	1:82:A:LYS:H	1:82:A:LYS:HD2	20	0.16
(1,1751)	1:56:A:ARG:H	1:56:A:ARG:HG3	2	0.16
(1,1703)	1:36:A:ARG:H	1:36:A:ARG:HD2	19	0.16
(1,1694)	1:35:A:GLU:H	1:35:A:GLU:HG3	4	0.16
(1,1660)	1:32:A:SER:H	1:32:A:SER:HB3	14	0.16
(1,1660)	1:32:A:SER:H	1:32:A:SER:HB3	15	0.16
(1,1568)	1:21:A:ARG:HB2	1:21:A:ARG:HE	11	0.16
(1,1568)	1:21:A:ARG:HB2	1:21:A:ARG:HE	17	0.16
(1,1455)	1:6:A:LYS:H	1:6:A:LYS:HB3	14	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1382)	1:159:A:ILE:HG12	1:160:A:LEU:H	9	0.16
(1,1324)	1:89:A:ILE:HA	1:158:A:ILE:HG21	7	0.16
(1,1324)	1:89:A:ILE:HA	1:158:A:ILE:HG22	7	0.16
(1,1324)	1:89:A:ILE:HA	1:158:A:ILE:HG23	7	0.16
(1,1306)	1:89:A:ILE:HD11	1:157:A:HIS:HD2	15	0.16
(1,1306)	1:89:A:ILE:HD12	1:157:A:HIS:HD2	15	0.16
(1,1306)	1:89:A:ILE:HD13	1:157:A:HIS:HD2	15	0.16
(1,1262)	1:151:A:PHE:H	1:156:A:ILE:HA	6	0.16
(1,1262)	1:151:A:PHE:H	1:156:A:ILE:HA	17	0.16
(1,1259)	1:151:A:PHE:HB2	1:152:A:THR:H	8	0.16
(1,1259)	1:151:A:PHE:HB2	1:152:A:THR:H	14	0.16
(1,1259)	1:151:A:PHE:HB2	1:152:A:THR:H	19	0.16
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG21	3	0.16
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG22	3	0.16
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG23	3	0.16
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG21	3	0.16
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG22	3	0.16
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG23	3	0.16
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG21	3	0.16
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG22	3	0.16
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG23	3	0.16
(1,1200)	1:143:A:THR:H	1:144:A:GLY:H	13	0.16
(1,1199)	1:142:A:ARG:HG2	1:143:A:THR:H	20	0.16
(1,1085)	1:56:A:ARG:HE	1:124:A:ALA:H	18	0.16
(1,1047)	1:119:A:ARG:HD2	1:121:A:ASP:H	7	0.16
(1,1038)	1:119:A:ARG:HA	1:121:A:ASP:H	16	0.16
(1,1031)	1:118:A:ALA:HB1	1:121:A:ASP:HB2	16	0.16
(1,1031)	1:118:A:ALA:HB2	1:121:A:ASP:HB2	16	0.16
(1,1031)	1:118:A:ALA:HB3	1:121:A:ASP:HB2	16	0.16
(1,1029)	1:118:A:ALA:H	1:121:A:ASP:H	9	0.16
(1,1015)	1:116:A:ALA:HB1	1:120:A:GLY:H	4	0.16
(1,1015)	1:116:A:ALA:HB2	1:120:A:GLY:H	4	0.16
(1,1015)	1:116:A:ALA:HB3	1:120:A:GLY:H	4	0.16
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB1	1	0.16
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB2	1	0.16
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB3	1	0.16
(1,978)	1:107:A:ALA:HB1	1:111:A:SER:HA	10	0.16
(1,978)	1:107:A:ALA:HB2	1:111:A:SER:HA	10	0.16
(1,978)	1:107:A:ALA:HB3	1:111:A:SER:HA	10	0.16
(1,970)	1:108:A:SER:H	1:110:A:PHE:H	12	0.16
(1,941)	1:106:A:LEU:HD11	1:107:A:ALA:H	5	0.16
(1,941)	1:106:A:LEU:HD12	1:107:A:ALA:H	5	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,941)	1:106:A:LEU:HD13	1:107:A:ALA:H	5	0.16
(1,926)	1:60:A:LEU:HD11	1:107:A:ALA:H	6	0.16
(1,926)	1:60:A:LEU:HD12	1:107:A:ALA:H	6	0.16
(1,926)	1:60:A:LEU:HD13	1:107:A:ALA:H	6	0.16
(1,921)	1:106:A:LEU:H	1:109:A:GLN:H	12	0.16
(1,920)	1:106:A:LEU:HB3	1:108:A:SER:H	9	0.16
(1,862)	1:101:A:GLU:HG2	1:102:A:ASP:H	8	0.16
(1,828)	1:96:A:ILE:H	1:146:A:MET:HE1	12	0.16
(1,828)	1:96:A:ILE:H	1:146:A:MET:HE2	12	0.16
(1,828)	1:96:A:ILE:H	1:146:A:MET:HE3	12	0.16
(1,811)	1:94:A:GLN:H	1:96:A:ILE:H	14	0.16
(1,811)	1:94:A:GLN:H	1:96:A:ILE:H	19	0.16
(1,799)	1:93:A:ILE:HB	1:146:A:MET:HE1	3	0.16
(1,799)	1:93:A:ILE:HB	1:146:A:MET:HE2	3	0.16
(1,799)	1:93:A:ILE:HB	1:146:A:MET:HE3	3	0.16
(1,799)	1:93:A:ILE:HB	1:146:A:MET:HE1	18	0.16
(1,799)	1:93:A:ILE:HB	1:146:A:MET:HE2	18	0.16
(1,799)	1:93:A:ILE:HB	1:146:A:MET:HE3	18	0.16
(1,772)	1:92:A:TYR:H	1:93:A:ILE:HB	12	0.16
(1,751)	1:89:A:ILE:HG21	1:91:A:GLY:H	12	0.16
(1,751)	1:89:A:ILE:HG22	1:91:A:GLY:H	12	0.16
(1,751)	1:89:A:ILE:HG23	1:91:A:GLY:H	12	0.16
(1,698)	1:86:A:LEU:HD11	1:87:A:GLU:H	11	0.16
(1,698)	1:86:A:LEU:HD12	1:87:A:GLU:H	11	0.16
(1,698)	1:86:A:LEU:HD13	1:87:A:GLU:H	11	0.16
(1,692)	1:86:A:LEU:HG	1:90:A:ASN:HD22	13	0.16
(1,668)	1:83:A:GLU:HB2	1:84:A:GLU:H	10	0.16
(1,659)	1:81:A:THR:HA	1:83:A:GLU:H	8	0.16
(1,659)	1:81:A:THR:HA	1:83:A:GLU:H	15	0.16
(1,647)	1:65:A:SER:H	1:82:A:LYS:H	4	0.16
(1,639)	1:65:A:SER:HB3	1:81:A:THR:HG21	13	0.16
(1,639)	1:65:A:SER:HB3	1:81:A:THR:HG22	13	0.16
(1,639)	1:65:A:SER:HB3	1:81:A:THR:HG23	13	0.16
(1,634)	1:80:A:ARG:HB2	1:81:A:THR:H	11	0.16
(1,540)	1:67:A:SER:HA	1:69:A:ARG:H	11	0.16
(1,527)	1:66:A:GLN:HG2	1:81:A:THR:HG21	12	0.16
(1,527)	1:66:A:GLN:HG2	1:81:A:THR:HG22	12	0.16
(1,527)	1:66:A:GLN:HG2	1:81:A:THR:HG23	12	0.16
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD11	12	0.16
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD12	12	0.16
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD13	12	0.16
(1,469)	1:60:A:LEU:HB2	1:61:A:LEU:H	5	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,402)	1:55:A:VAL:HA	1:125:A:PHE:H	11	0.16
(1,391)	1:35:A:GLU:HB3	1:36:A:ARG:H	9	0.16
(1,388)	1:35:A:GLU:HG2	1:36:A:ARG:H	20	0.16
(1,387)	1:35:A:GLU:HB2	1:36:A:ARG:H	1	0.16
(1,383)	1:34:A:TRP:H	1:35:A:GLU:HB3	3	0.16
(1,373)	1:34:A:TRP:HD1	1:35:A:GLU:H	10	0.16
(1,369)	1:33:A:GLN:HG2	1:34:A:TRP:H	13	0.16
(1,367)	1:24:A:TYR:HD1	1:34:A:TRP:H	10	0.16
(1,367)	1:24:A:TYR:HD2	1:34:A:TRP:H	10	0.16
(1,364)	1:24:A:TYR:HD1	1:33:A:GLN:H	19	0.16
(1,364)	1:24:A:TYR:HD2	1:33:A:GLN:H	19	0.16
(1,347)	1:31:A:ALA:HB1	1:33:A:GLN:H	11	0.16
(1,347)	1:31:A:ALA:HB2	1:33:A:GLN:H	11	0.16
(1,347)	1:31:A:ALA:HB3	1:33:A:GLN:H	11	0.16
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB1	15	0.16
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB2	15	0.16
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB3	15	0.16
(1,333)	1:25:A:PHE:HA	1:31:A:ALA:H	2	0.16
(1,296)	1:27:A:HIS:HA	1:30:A:ASN:HD21	13	0.16
(1,262)	1:25:A:PHE:HE1	1:26:A:ASN:HA	17	0.16
(1,262)	1:25:A:PHE:HE2	1:26:A:ASN:HA	17	0.16
(1,208)	1:24:A:TYR:H	1:34:A:TRP:HB3	5	0.16
(1,189)	1:13:A:LYS:H	1:24:A:TYR:HA	7	0.16
(1,112)	1:15:A:MET:H	1:23:A:TYR:H	13	0.16
(1,111)	1:15:A:MET:H	1:23:A:TYR:HD1	12	0.16
(1,111)	1:15:A:MET:H	1:23:A:TYR:HD2	12	0.16
(1,108)	1:15:A:MET:H	1:22:A:VAL:HA	20	0.16
(1,35)	1:9:A:PRO:HG2	1:10:A:GLY:H	18	0.16
(1,2)	1:2:A:ALA:HA	1:3:A:ASP:H	19	0.16
(3,46)	1:70:A:PRO:O	1:78:A:ILE:H	16	0.15
(3,45)	1:70:A:PRO:O	1:78:A:ILE:N	17	0.15
(3,43)	1:72:A:SER:O	1:75:A:GLN:N	3	0.15
(2,108)	1:140:A:ALA:HB1	2:649:B:ARG:HA	2	0.15
(2,108)	1:140:A:ALA:HB2	2:649:B:ARG:HA	2	0.15
(2,108)	1:140:A:ALA:HB3	2:649:B:ARG:HA	2	0.15
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG11	9	0.15
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG12	9	0.15
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG13	9	0.15
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG11	11	0.15
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG12	11	0.15
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG13	11	0.15
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG21	11	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG22	11	0.15
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG23	11	0.15
(2,74)	2:656:B:PHE:HB2	2:659:B:PHE:HD1	15	0.15
(2,74)	2:656:B:PHE:HB2	2:659:B:PHE:HD2	15	0.15
(2,74)	2:656:B:PHE:HB3	2:659:B:PHE:HD1	15	0.15
(2,74)	2:656:B:PHE:HB3	2:659:B:PHE:HD2	15	0.15
(2,39)	1:55:A:VAL:HG11	1:127:A:ARG:H	17	0.15
(2,39)	1:55:A:VAL:HG12	1:127:A:ARG:H	17	0.15
(2,39)	1:55:A:VAL:HG13	1:127:A:ARG:H	17	0.15
(1,2572)	1:16:A:SER:HB2	2:641:B:TPO:HG21	3	0.15
(1,2572)	1:16:A:SER:HB2	2:641:B:TPO:HG22	3	0.15
(1,2572)	1:16:A:SER:HB2	2:641:B:TPO:HG23	3	0.15
(1,2572)	1:16:A:SER:HB2	2:641:B:TPO:HG21	6	0.15
(1,2572)	1:16:A:SER:HB2	2:641:B:TPO:HG22	6	0.15
(1,2572)	1:16:A:SER:HB2	2:641:B:TPO:HG23	6	0.15
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG21	2	0.15
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG22	2	0.15
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG23	2	0.15
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG21	3	0.15
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG22	3	0.15
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG23	3	0.15
(1,2561)	2:655:B:GLU:H	2:656:B:PHE:HD1	20	0.15
(1,2561)	2:655:B:GLU:H	2:656:B:PHE:HD2	20	0.15
(1,2523)	2:647:B:VAL:HA	2:649:B:ARG:H	3	0.15
(1,2517)	2:646:B:GLU:HG2	2:647:B:VAL:H	3	0.15
(1,2481)	2:656:B:PHE:H	2:656:B:PHE:HE1	20	0.15
(1,2481)	2:656:B:PHE:H	2:656:B:PHE:HE2	20	0.15
(1,2386)	1:163:A:GLU:H	1:163:A:GLU:HG2	11	0.15
(1,2383)	1:163:A:GLU:H	1:163:A:GLU:HB2	2	0.15
(1,2161)	1:119:A:ARG:H	1:119:A:ARG:HD3	13	0.15
(1,2036)	1:96:A:ILE:H	1:96:A:ILE:HD11	12	0.15
(1,2036)	1:96:A:ILE:H	1:96:A:ILE:HD12	12	0.15
(1,2036)	1:96:A:ILE:H	1:96:A:ILE:HD13	12	0.15
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD11	13	0.15
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD12	13	0.15
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD13	13	0.15
(1,1913)	1:82:A:LYS:H	1:82:A:LYS:HD2	6	0.15
(1,1913)	1:82:A:LYS:H	1:82:A:LYS:HD2	12	0.15
(1,1913)	1:82:A:LYS:H	1:82:A:LYS:HD2	14	0.15
(1,1751)	1:56:A:ARG:H	1:56:A:ARG:HG3	16	0.15
(1,1747)	1:56:A:ARG:H	1:56:A:ARG:HD2	13	0.15
(1,1694)	1:35:A:GLU:H	1:35:A:GLU:HG3	5	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1660)	1:32:A:SER:H	1:32:A:SER:HB3	4	0.15
(1,1660)	1:32:A:SER:H	1:32:A:SER:HB3	9	0.15
(1,1660)	1:32:A:SER:H	1:32:A:SER:HB3	10	0.15
(1,1660)	1:32:A:SER:H	1:32:A:SER:HB3	19	0.15
(1,1611)	1:25:A:PHE:H	1:25:A:PHE:HD1	16	0.15
(1,1611)	1:25:A:PHE:H	1:25:A:PHE:HD2	16	0.15
(1,1568)	1:21:A:ARG:HB2	1:21:A:ARG:HE	12	0.15
(1,1568)	1:21:A:ARG:HB2	1:21:A:ARG:HE	20	0.15
(1,1450)	1:4:A:GLU:HA	1:4:A:GLU:HG2	9	0.15
(1,1450)	1:4:A:GLU:HA	1:4:A:GLU:HG2	10	0.15
(1,1450)	1:4:A:GLU:HA	1:4:A:GLU:HG2	15	0.15
(1,1406)	1:147:A:SER:H	1:161:A:ARG:H	5	0.15
(1,1402)	1:143:A:THR:HG21	1:161:A:ARG:HD2	10	0.15
(1,1402)	1:143:A:THR:HG22	1:161:A:ARG:HD2	10	0.15
(1,1402)	1:143:A:THR:HG23	1:161:A:ARG:HD2	10	0.15
(1,1402)	1:143:A:THR:HG21	1:161:A:ARG:HD2	14	0.15
(1,1402)	1:143:A:THR:HG22	1:161:A:ARG:HD2	14	0.15
(1,1402)	1:143:A:THR:HG23	1:161:A:ARG:HD2	14	0.15
(1,1348)	1:157:A:HIS:HB2	1:159:A:ILE:HD11	18	0.15
(1,1348)	1:157:A:HIS:HB2	1:159:A:ILE:HD12	18	0.15
(1,1348)	1:157:A:HIS:HB2	1:159:A:ILE:HD13	18	0.15
(1,1348)	1:157:A:HIS:HB3	1:159:A:ILE:HD11	18	0.15
(1,1348)	1:157:A:HIS:HB3	1:159:A:ILE:HD12	18	0.15
(1,1348)	1:157:A:HIS:HB3	1:159:A:ILE:HD13	18	0.15
(1,1330)	1:92:A:TYR:HD1	1:158:A:ILE:HG21	4	0.15
(1,1330)	1:92:A:TYR:HD1	1:158:A:ILE:HG22	4	0.15
(1,1330)	1:92:A:TYR:HD1	1:158:A:ILE:HG23	4	0.15
(1,1330)	1:92:A:TYR:HD2	1:158:A:ILE:HG21	4	0.15
(1,1330)	1:92:A:TYR:HD2	1:158:A:ILE:HG22	4	0.15
(1,1330)	1:92:A:TYR:HD2	1:158:A:ILE:HG23	4	0.15
(1,1309)	1:150:A:VAL:HB	1:157:A:HIS:H	17	0.15
(1,1306)	1:89:A:ILE:HD11	1:157:A:HIS:HD2	19	0.15
(1,1306)	1:89:A:ILE:HD12	1:157:A:HIS:HD2	19	0.15
(1,1306)	1:89:A:ILE:HD13	1:157:A:HIS:HD2	19	0.15
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD11	4	0.15
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD12	4	0.15
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD13	4	0.15
(1,1259)	1:151:A:PHE:HB2	1:152:A:THR:H	3	0.15
(1,1259)	1:151:A:PHE:HB2	1:152:A:THR:H	7	0.15
(1,1206)	1:145:A:GLU:HB3	1:146:A:MET:HB2	10	0.15
(1,1190)	1:141:A:LEU:HD21	1:142:A:ARG:HB2	8	0.15
(1,1190)	1:141:A:LEU:HD22	1:142:A:ARG:HB2	8	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1190)	1:141:A:LEU:HD23	1:142:A:ARG:HB2	8	0.15
(1,1161)	1:136:A:ASP:HB2	1:138:A:SER:H	2	0.15
(1,1114)	1:126:A:SER:HB2	1:127:A:ARG:H	13	0.15
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE1	7	0.15
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE2	7	0.15
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE3	7	0.15
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE1	7	0.15
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE2	7	0.15
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE3	7	0.15
(1,1038)	1:119:A:ARG:HA	1:121:A:ASP:H	3	0.15
(1,1038)	1:119:A:ARG:HA	1:121:A:ASP:H	14	0.15
(1,1020)	1:116:A:ALA:HA	1:118:A:ALA:H	11	0.15
(1,1020)	1:116:A:ALA:HA	1:118:A:ALA:H	19	0.15
(1,1012)	1:116:A:ALA:H	1:119:A:ARG:H	7	0.15
(1,1001)	1:113:A:CYS:H	1:116:A:ALA:HB1	12	0.15
(1,1001)	1:113:A:CYS:H	1:116:A:ALA:HB2	12	0.15
(1,1001)	1:113:A:CYS:H	1:116:A:ALA:HB3	12	0.15
(1,970)	1:108:A:SER:H	1:110:A:PHE:H	6	0.15
(1,970)	1:108:A:SER:H	1:110:A:PHE:H	19	0.15
(1,970)	1:108:A:SER:H	1:110:A:PHE:H	20	0.15
(1,934)	1:104:A:GLU:HA	1:107:A:ALA:H	10	0.15
(1,920)	1:106:A:LEU:HB3	1:108:A:SER:H	13	0.15
(1,914)	1:104:A:GLU:H	1:106:A:LEU:HB3	3	0.15
(1,914)	1:104:A:GLU:H	1:106:A:LEU:HB3	6	0.15
(1,871)	1:96:A:ILE:HB	1:103:A:PHE:H	11	0.15
(1,871)	1:96:A:ILE:HB	1:103:A:PHE:H	16	0.15
(1,862)	1:101:A:GLU:HG2	1:102:A:ASP:H	4	0.15
(1,845)	1:97:A:LYS:HD2	1:98:A:SER:H	19	0.15
(1,844)	1:97:A:LYS:HG2	1:98:A:SER:H	19	0.15
(1,843)	1:97:A:LYS:HB2	1:98:A:SER:H	14	0.15
(1,822)	1:96:A:ILE:HD11	1:97:A:LYS:H	12	0.15
(1,822)	1:96:A:ILE:HD12	1:97:A:LYS:H	12	0.15
(1,822)	1:96:A:ILE:HD13	1:97:A:LYS:H	12	0.15
(1,811)	1:94:A:GLN:H	1:96:A:ILE:H	16	0.15
(1,805)	1:93:A:ILE:HG21	1:94:A:GLN:H	12	0.15
(1,805)	1:93:A:ILE:HG22	1:94:A:GLN:H	12	0.15
(1,805)	1:93:A:ILE:HG23	1:94:A:GLN:H	12	0.15
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE1	11	0.15
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE2	11	0.15
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE3	11	0.15
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD11	13	0.15
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD12	13	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD13	13	0.15
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD11	13	0.15
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD12	13	0.15
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD13	13	0.15
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD11	12	0.15
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD12	12	0.15
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD13	12	0.15
(1,750)	1:88:A:LEU:H	1:91:A:GLY:H	13	0.15
(1,723)	1:86:A:LEU:HD21	1:89:A:ILE:HB	7	0.15
(1,723)	1:86:A:LEU:HD22	1:89:A:ILE:HB	7	0.15
(1,723)	1:86:A:LEU:HD23	1:89:A:ILE:HB	7	0.15
(1,723)	1:86:A:LEU:HD21	1:89:A:ILE:HB	18	0.15
(1,723)	1:86:A:LEU:HD22	1:89:A:ILE:HB	18	0.15
(1,723)	1:86:A:LEU:HD23	1:89:A:ILE:HB	18	0.15
(1,692)	1:86:A:LEU:HG	1:90:A:ASN:HD22	1	0.15
(1,669)	1:84:A:GLU:H	1:87:A:GLU:H	3	0.15
(1,669)	1:84:A:GLU:H	1:87:A:GLU:H	5	0.15
(1,669)	1:84:A:GLU:H	1:87:A:GLU:H	7	0.15
(1,647)	1:65:A:SER:H	1:82:A:LYS:H	3	0.15
(1,619)	1:78:A:ILE:HB	1:80:A:ARG:H	13	0.15
(1,554)	1:70:A:PRO:HG3	1:71:A:SER:H	4	0.15
(1,554)	1:70:A:PRO:HG3	1:71:A:SER:H	5	0.15
(1,527)	1:66:A:GLN:HG2	1:81:A:THR:HG21	6	0.15
(1,527)	1:66:A:GLN:HG2	1:81:A:THR:HG22	6	0.15
(1,527)	1:66:A:GLN:HG2	1:81:A:THR:HG23	6	0.15
(1,514)	1:63:A:LYS:HB2	1:70:A:PRO:HA	15	0.15
(1,510)	1:62:A:VAL:HG11	1:156:A:ILE:H	4	0.15
(1,510)	1:62:A:VAL:HG12	1:156:A:ILE:H	4	0.15
(1,510)	1:62:A:VAL:HG13	1:156:A:ILE:H	4	0.15
(1,469)	1:60:A:LEU:HB2	1:61:A:LEU:H	12	0.15
(1,457)	1:60:A:LEU:HD11	1:108:A:SER:H	3	0.15
(1,457)	1:60:A:LEU:HD12	1:108:A:SER:H	3	0.15
(1,457)	1:60:A:LEU:HD13	1:108:A:SER:H	3	0.15
(1,424)	1:56:A:ARG:HE	1:57:A:CYS:H	3	0.15
(1,391)	1:35:A:GLU:HB3	1:36:A:ARG:H	3	0.15
(1,391)	1:35:A:GLU:HB3	1:36:A:ARG:H	5	0.15
(1,388)	1:35:A:GLU:HG2	1:36:A:ARG:H	17	0.15
(1,388)	1:35:A:GLU:HG2	1:36:A:ARG:H	18	0.15
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB1	4	0.15
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB2	4	0.15
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB3	4	0.15
(1,318)	1:29:A:THR:H	1:30:A:ASN:HB3	2	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,318)	1:29:A:THR:H	1:30:A:ASN:HB3	8	0.15
(1,318)	1:29:A:THR:H	1:30:A:ASN:HB3	17	0.15
(1,205)	1:24:A:TYR:H	1:33:A:GLN:HG2	11	0.15
(1,170)	1:16:A:SER:H	1:23:A:TYR:H	13	0.15
(1,129)	1:16:A:SER:HB2	1:21:A:ARG:H	10	0.15
(1,129)	1:16:A:SER:HB2	1:21:A:ARG:H	11	0.15
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG21	13	0.15
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG22	13	0.15
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG23	13	0.15
(1,75)	1:13:A:LYS:HA	1:23:A:TYR:H	17	0.15
(1,52)	1:11:A:TRP:HE1	1:26:A:ASN:HB2	11	0.15
(1,52)	1:11:A:TRP:HE1	1:26:A:ASN:HB3	11	0.15
(1,35)	1:9:A:PRO:HG2	1:10:A:GLY:H	12	0.15
(1,23)	1:7:A:LEU:HA	1:11:A:TRP:HB3	2	0.15
(3,80)	1:105:A:SER:O	1:109:A:GLN:H	1	0.14
(3,80)	1:105:A:SER:O	1:109:A:GLN:H	20	0.14
(3,47)	1:81:A:THR:O	1:85:A:ALA:N	17	0.14
(3,43)	1:72:A:SER:O	1:75:A:GLN:N	17	0.14
(2,111)	1:160:A:LEU:H	2:651:B:ILE:HG12	5	0.14
(2,111)	1:160:A:LEU:H	2:651:B:ILE:HG13	5	0.14
(2,93)	1:93:A:ILE:HD11	2:643:B:PRO:HA	12	0.14
(2,93)	1:93:A:ILE:HD12	2:643:B:PRO:HA	12	0.14
(2,93)	1:93:A:ILE:HD13	2:643:B:PRO:HA	12	0.14
(2,1)	1:10:A:GLY:H	1:11:A:TRP:HB3	10	0.14
(2,1)	1:10:A:GLY:H	1:11:A:TRP:HB3	13	0.14
(1,2591)	1:123:A:GLY:H	2:656:B:PHE:HE1	10	0.14
(1,2591)	1:123:A:GLY:H	2:656:B:PHE:HE2	10	0.14
(1,2582)	1:34:A:TRP:HE1	2:642:B:PRO:HB2	12	0.14
(1,2582)	1:34:A:TRP:HE1	2:642:B:PRO:HB3	12	0.14
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG21	1	0.14
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG22	1	0.14
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG23	1	0.14
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG21	17	0.14
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG22	17	0.14
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG23	17	0.14
(1,2532)	2:648:B:ILE:HG21	2:650:B:ASN:H	19	0.14
(1,2532)	2:648:B:ILE:HG22	2:650:B:ASN:H	19	0.14
(1,2532)	2:648:B:ILE:HG23	2:650:B:ASN:H	19	0.14
(1,2488)	2:656:B:PHE:HA	2:656:B:PHE:HE1	8	0.14
(1,2488)	2:656:B:PHE:HA	2:656:B:PHE:HE2	8	0.14
(1,2383)	1:163:A:GLU:H	1:163:A:GLU:HB2	13	0.14
(1,2056)	1:101:A:GLU:H	1:101:A:GLU:HG2	4	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2056)	1:101:A:GLU:H	1:101:A:GLU:HG2	12	0.14
(1,1869)	1:75:A:GLN:H	1:75:A:GLN:HE22	12	0.14
(1,1751)	1:56:A:ARG:H	1:56:A:ARG:HG3	13	0.14
(1,1751)	1:56:A:ARG:H	1:56:A:ARG:HG3	19	0.14
(1,1751)	1:56:A:ARG:H	1:56:A:ARG:HG3	20	0.14
(1,1747)	1:56:A:ARG:H	1:56:A:ARG:HD2	18	0.14
(1,1703)	1:36:A:ARG:H	1:36:A:ARG:HD2	11	0.14
(1,1660)	1:32:A:SER:H	1:32:A:SER:HB3	2	0.14
(1,1660)	1:32:A:SER:H	1:32:A:SER:HB3	3	0.14
(1,1660)	1:32:A:SER:H	1:32:A:SER:HB3	7	0.14
(1,1660)	1:32:A:SER:H	1:32:A:SER:HB3	8	0.14
(1,1660)	1:32:A:SER:H	1:32:A:SER:HB3	17	0.14
(1,1611)	1:25:A:PHE:H	1:25:A:PHE:HD1	5	0.14
(1,1611)	1:25:A:PHE:H	1:25:A:PHE:HD2	5	0.14
(1,1611)	1:25:A:PHE:H	1:25:A:PHE:HD1	10	0.14
(1,1611)	1:25:A:PHE:H	1:25:A:PHE:HD2	10	0.14
(1,1547)	1:15:A:MET:H	1:15:A:MET:HB2	3	0.14
(1,1456)	1:6:A:LYS:H	1:6:A:LYS:HE2	4	0.14
(1,1450)	1:4:A:GLU:HA	1:4:A:GLU:HG2	17	0.14
(1,1441)	1:162:A:THR:HG21	1:163:A:GLU:HG3	9	0.14
(1,1441)	1:162:A:THR:HG22	1:163:A:GLU:HG3	9	0.14
(1,1441)	1:162:A:THR:HG23	1:163:A:GLU:HG3	9	0.14
(1,1423)	1:55:A:VAL:HB	1:163:A:GLU:H	15	0.14
(1,1402)	1:143:A:THR:HG21	1:161:A:ARG:HD2	3	0.14
(1,1402)	1:143:A:THR:HG22	1:161:A:ARG:HD2	3	0.14
(1,1402)	1:143:A:THR:HG23	1:161:A:ARG:HD2	3	0.14
(1,1382)	1:159:A:ILE:HG12	1:160:A:LEU:H	7	0.14
(1,1368)	1:103:A:PHE:HB3	1:160:A:LEU:HD21	1	0.14
(1,1368)	1:103:A:PHE:HB3	1:160:A:LEU:HD22	1	0.14
(1,1368)	1:103:A:PHE:HB3	1:160:A:LEU:HD23	1	0.14
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD11	4	0.14
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD12	4	0.14
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD13	4	0.14
(1,1348)	1:157:A:HIS:HB2	1:159:A:ILE:HD11	1	0.14
(1,1348)	1:157:A:HIS:HB2	1:159:A:ILE:HD12	1	0.14
(1,1348)	1:157:A:HIS:HB2	1:159:A:ILE:HD13	1	0.14
(1,1348)	1:157:A:HIS:HB3	1:159:A:ILE:HD11	1	0.14
(1,1348)	1:157:A:HIS:HB3	1:159:A:ILE:HD12	1	0.14
(1,1348)	1:157:A:HIS:HB3	1:159:A:ILE:HD13	1	0.14
(1,1331)	1:146:A:MET:HG2	1:158:A:ILE:HG21	19	0.14
(1,1331)	1:146:A:MET:HG2	1:158:A:ILE:HG22	19	0.14
(1,1331)	1:146:A:MET:HG2	1:158:A:ILE:HG23	19	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG21	1	0.14
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG22	1	0.14
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG23	1	0.14
(1,1311)	1:152:A:THR:HG21	1:157:A:HIS:H	15	0.14
(1,1311)	1:152:A:THR:HG22	1:157:A:HIS:H	15	0.14
(1,1311)	1:152:A:THR:HG23	1:157:A:HIS:H	15	0.14
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG21	7	0.14
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG22	7	0.14
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG23	7	0.14
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG21	7	0.14
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG22	7	0.14
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG23	7	0.14
(1,1262)	1:151:A:PHE:H	1:156:A:ILE:HA	3	0.14
(1,1259)	1:151:A:PHE:HB2	1:152:A:THR:H	4	0.14
(1,1259)	1:151:A:PHE:HB2	1:152:A:THR:H	6	0.14
(1,1259)	1:151:A:PHE:HB2	1:152:A:THR:H	9	0.14
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG21	2	0.14
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG22	2	0.14
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG23	2	0.14
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG21	2	0.14
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG22	2	0.14
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG23	2	0.14
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG21	2	0.14
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG22	2	0.14
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG23	2	0.14
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG21	9	0.14
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG22	9	0.14
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG23	9	0.14
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG21	9	0.14
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG22	9	0.14
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG23	9	0.14
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG21	9	0.14
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG22	9	0.14
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG23	9	0.14
(1,1232)	1:149:A:PRO:HB3	1:150:A:VAL:H	13	0.14
(1,1200)	1:143:A:THR:H	1:144:A:GLY:H	16	0.14
(1,1199)	1:142:A:ARG:HG2	1:143:A:THR:H	15	0.14
(1,1038)	1:119:A:ARG:HA	1:121:A:ASP:H	15	0.14
(1,1036)	1:118:A:ALA:HB1	1:119:A:ARG:H	11	0.14
(1,1036)	1:118:A:ALA:HB2	1:119:A:ARG:H	11	0.14
(1,1036)	1:118:A:ALA:HB3	1:119:A:ARG:H	11	0.14
(1,1020)	1:116:A:ALA:HA	1:118:A:ALA:H	2	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1020)	1:116:A:ALA:HA	1:118:A:ALA:H	8	0.14
(1,998)	1:111:A:SER:H	1:116:A:ALA:HB1	10	0.14
(1,998)	1:111:A:SER:H	1:116:A:ALA:HB2	10	0.14
(1,998)	1:111:A:SER:H	1:116:A:ALA:HB3	10	0.14
(1,970)	1:108:A:SER:H	1:110:A:PHE:H	7	0.14
(1,920)	1:106:A:LEU:HB3	1:108:A:SER:H	15	0.14
(1,889)	1:103:A:PHE:HE1	1:146:A:MET:HE1	8	0.14
(1,889)	1:103:A:PHE:HE1	1:146:A:MET:HE2	8	0.14
(1,889)	1:103:A:PHE:HE1	1:146:A:MET:HE3	8	0.14
(1,889)	1:103:A:PHE:HE2	1:146:A:MET:HE1	8	0.14
(1,889)	1:103:A:PHE:HE2	1:146:A:MET:HE2	8	0.14
(1,889)	1:103:A:PHE:HE2	1:146:A:MET:HE3	8	0.14
(1,889)	1:103:A:PHE:HE1	1:146:A:MET:HE1	16	0.14
(1,889)	1:103:A:PHE:HE1	1:146:A:MET:HE2	16	0.14
(1,889)	1:103:A:PHE:HE1	1:146:A:MET:HE3	16	0.14
(1,889)	1:103:A:PHE:HE2	1:146:A:MET:HE1	16	0.14
(1,889)	1:103:A:PHE:HE2	1:146:A:MET:HE2	16	0.14
(1,889)	1:103:A:PHE:HE2	1:146:A:MET:HE3	16	0.14
(1,854)	1:98:A:SER:H	1:101:A:GLU:H	6	0.14
(1,854)	1:98:A:SER:H	1:101:A:GLU:H	18	0.14
(1,843)	1:97:A:LYS:HB2	1:98:A:SER:H	13	0.14
(1,831)	1:93:A:ILE:HG21	1:97:A:LYS:HB3	2	0.14
(1,831)	1:93:A:ILE:HG22	1:97:A:LYS:HB3	2	0.14
(1,831)	1:93:A:ILE:HG23	1:97:A:LYS:HB3	2	0.14
(1,807)	1:93:A:ILE:HD11	1:94:A:GLN:H	4	0.14
(1,807)	1:93:A:ILE:HD12	1:94:A:GLN:H	4	0.14
(1,807)	1:93:A:ILE:HD13	1:94:A:GLN:H	4	0.14
(1,800)	1:93:A:ILE:HB	1:158:A:ILE:HD11	8	0.14
(1,800)	1:93:A:ILE:HB	1:158:A:ILE:HD12	8	0.14
(1,800)	1:93:A:ILE:HB	1:158:A:ILE:HD13	8	0.14
(1,737)	1:86:A:LEU:HB3	1:90:A:ASN:H	3	0.14
(1,654)	1:82:A:LYS:HG2	1:84:A:GLU:H	8	0.14
(1,654)	1:82:A:LYS:HG3	1:84:A:GLU:H	8	0.14
(1,644)	1:81:A:THR:HA	1:84:A:GLU:H	1	0.14
(1,644)	1:81:A:THR:HA	1:84:A:GLU:H	14	0.14
(1,619)	1:78:A:ILE:HB	1:80:A:ARG:H	2	0.14
(1,605)	1:72:A:SER:HA	1:78:A:ILE:HD11	17	0.14
(1,605)	1:72:A:SER:HA	1:78:A:ILE:HD12	17	0.14
(1,605)	1:72:A:SER:HA	1:78:A:ILE:HD13	17	0.14
(1,589)	1:74:A:ARG:H	1:112:A:ASP:HA	8	0.14
(1,520)	1:64:A:HIS:HE1	1:66:A:GLN:HG2	5	0.14
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD11	20	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD12	20	0.14
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD13	20	0.14
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB1	2	0.14
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB2	2	0.14
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB3	2	0.14
(1,422)	1:56:A:ARG:HG2	1:162:A:THR:HB	1	0.14
(1,422)	1:56:A:ARG:HG2	1:162:A:THR:HB	18	0.14
(1,393)	1:53:A:ALA:HB1	1:54:A:ARG:H	17	0.14
(1,393)	1:53:A:ALA:HB2	1:54:A:ARG:H	17	0.14
(1,393)	1:53:A:ALA:HB3	1:54:A:ARG:H	17	0.14
(1,391)	1:35:A:GLU:HB3	1:36:A:ARG:H	7	0.14
(1,388)	1:35:A:GLU:HG2	1:36:A:ARG:H	6	0.14
(1,387)	1:35:A:GLU:HB2	1:36:A:ARG:H	13	0.14
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB1	10	0.14
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB2	10	0.14
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB3	10	0.14
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB1	20	0.14
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB2	20	0.14
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB3	20	0.14
(1,334)	1:27:A:HIS:HA	1:31:A:ALA:H	2	0.14
(1,333)	1:25:A:PHE:HA	1:31:A:ALA:H	10	0.14
(1,318)	1:29:A:THR:H	1:30:A:ASN:HB3	18	0.14
(1,265)	1:26:A:ASN:H	1:27:A:HIS:H	14	0.14
(1,265)	1:26:A:ASN:H	1:27:A:HIS:H	20	0.14
(1,262)	1:25:A:PHE:HE1	1:26:A:ASN:HA	13	0.14
(1,262)	1:25:A:PHE:HE2	1:26:A:ASN:HA	13	0.14
(1,189)	1:13:A:LYS:H	1:24:A:TYR:HA	10	0.14
(1,178)	1:23:A:TYR:HE1	1:33:A:GLN:H	6	0.14
(1,178)	1:23:A:TYR:HE2	1:33:A:GLN:H	6	0.14
(1,165)	1:22:A:VAL:H	1:23:A:TYR:H	17	0.14
(1,157)	1:16:A:SER:H	1:22:A:VAL:HG11	13	0.14
(1,157)	1:16:A:SER:H	1:22:A:VAL:HG12	13	0.14
(1,157)	1:16:A:SER:H	1:22:A:VAL:HG13	13	0.14
(1,130)	1:16:A:SER:H	1:21:A:ARG:HA	7	0.14
(1,116)	1:16:A:SER:H	1:20:A:GLY:HA2	17	0.14
(1,108)	1:15:A:MET:H	1:22:A:VAL:HA	12	0.14
(1,102)	1:14:A:ARG:HD2	1:15:A:MET:H	13	0.14
(1,102)	1:14:A:ARG:HD3	1:15:A:MET:H	13	0.14
(1,89)	1:14:A:ARG:H	1:15:A:MET:HA	5	0.14
(1,89)	1:14:A:ARG:H	1:15:A:MET:HA	6	0.14
(1,89)	1:14:A:ARG:H	1:15:A:MET:HA	12	0.14
(1,89)	1:14:A:ARG:H	1:15:A:MET:HA	14	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,79)	1:13:A:LYS:H	1:24:A:TYR:HD1	20	0.14
(1,79)	1:13:A:LYS:H	1:24:A:TYR:HD2	20	0.14
(1,35)	1:9:A:PRO:HG2	1:10:A:GLY:H	6	0.14
(1,35)	1:9:A:PRO:HG2	1:10:A:GLY:H	10	0.14
(1,28)	1:7:A:LEU:HD21	1:13:A:LYS:HG3	14	0.14
(1,28)	1:7:A:LEU:HD22	1:13:A:LYS:HG3	14	0.14
(1,28)	1:7:A:LEU:HD23	1:13:A:LYS:HG3	14	0.14
(1,20)	1:7:A:LEU:HD11	1:11:A:TRP:H	13	0.14
(1,20)	1:7:A:LEU:HD12	1:11:A:TRP:H	13	0.14
(1,20)	1:7:A:LEU:HD13	1:11:A:TRP:H	13	0.14
(4,2593)	2:640:B:LEU:H	2:641:B:TPO:H	10	0.13
(4,2532)	2:649:B:ARG:H	2:649:B:ARG:HD2	10	0.13
(3,71)	1:94:A:GLN:O	1:98:A:SER:N	17	0.13
(3,63)	1:90:A:ASN:O	1:94:A:GLN:N	4	0.13
(2,111)	1:160:A:LEU:H	2:651:B:ILE:HG12	4	0.13
(2,111)	1:160:A:LEU:H	2:651:B:ILE:HG13	4	0.13
(2,102)	1:135:A:GLU:H	2:656:B:PHE:HB2	6	0.13
(2,70)	2:651:B:ILE:HG21	2:656:B:PHE:HE1	5	0.13
(2,70)	2:651:B:ILE:HG21	2:656:B:PHE:HE2	5	0.13
(2,70)	2:651:B:ILE:HG22	2:656:B:PHE:HE1	5	0.13
(2,70)	2:651:B:ILE:HG22	2:656:B:PHE:HE2	5	0.13
(2,70)	2:651:B:ILE:HG23	2:656:B:PHE:HE1	5	0.13
(2,70)	2:651:B:ILE:HG23	2:656:B:PHE:HE2	5	0.13
(2,34)	1:59:A:HIS:H	1:122:A:LEU:HB2	15	0.13
(1,2591)	1:123:A:GLY:H	2:656:B:PHE:HE1	5	0.13
(1,2591)	1:123:A:GLY:H	2:656:B:PHE:HE2	5	0.13
(1,2589)	1:122:A:LEU:HD21	2:656:B:PHE:HE1	20	0.13
(1,2589)	1:122:A:LEU:HD21	2:656:B:PHE:HE2	20	0.13
(1,2589)	1:122:A:LEU:HD22	2:656:B:PHE:HE1	20	0.13
(1,2589)	1:122:A:LEU:HD22	2:656:B:PHE:HE2	20	0.13
(1,2589)	1:122:A:LEU:HD23	2:656:B:PHE:HE1	20	0.13
(1,2589)	1:122:A:LEU:HD23	2:656:B:PHE:HE2	20	0.13
(1,2588)	1:122:A:LEU:H	2:656:B:PHE:HE1	10	0.13
(1,2588)	1:122:A:LEU:H	2:656:B:PHE:HE2	10	0.13
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG21	13	0.13
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG22	13	0.13
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG23	13	0.13
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG21	12	0.13
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG22	12	0.13
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG23	12	0.13
(1,2530)	2:648:B:ILE:HD11	2:649:B:ARG:H	12	0.13
(1,2530)	2:648:B:ILE:HD12	2:649:B:ARG:H	12	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2530)	2:648:B:ILE:HD13	2:649:B:ARG:H	12	0.13
(1,2524)	2:647:B:VAL:HG11	2:650:B:ASN:HD22	9	0.13
(1,2524)	2:647:B:VAL:HG12	2:650:B:ASN:HD22	9	0.13
(1,2524)	2:647:B:VAL:HG13	2:650:B:ASN:HD22	9	0.13
(1,2488)	2:656:B:PHE:HA	2:656:B:PHE:HE1	9	0.13
(1,2488)	2:656:B:PHE:HA	2:656:B:PHE:HE2	9	0.13
(1,2383)	1:163:A:GLU:H	1:163:A:GLU:HB2	17	0.13
(1,1751)	1:56:A:ARG:H	1:56:A:ARG:HG3	17	0.13
(1,1694)	1:35:A:GLU:H	1:35:A:GLU:HG3	7	0.13
(1,1660)	1:32:A:SER:H	1:32:A:SER:HB3	1	0.13
(1,1660)	1:32:A:SER:H	1:32:A:SER:HB3	6	0.13
(1,1611)	1:25:A:PHE:H	1:25:A:PHE:HD1	1	0.13
(1,1611)	1:25:A:PHE:H	1:25:A:PHE:HD2	1	0.13
(1,1611)	1:25:A:PHE:H	1:25:A:PHE:HD1	13	0.13
(1,1611)	1:25:A:PHE:H	1:25:A:PHE:HD2	13	0.13
(1,1568)	1:21:A:ARG:HB2	1:21:A:ARG:HE	8	0.13
(1,1456)	1:6:A:LYS:H	1:6:A:LYS:HE2	20	0.13
(1,1453)	1:5:A:GLU:H	1:5:A:GLU:HA	14	0.13
(1,1453)	1:5:A:GLU:H	1:5:A:GLU:HA	16	0.13
(1,1450)	1:4:A:GLU:HA	1:4:A:GLU:HG2	7	0.13
(1,1450)	1:4:A:GLU:HA	1:4:A:GLU:HG2	14	0.13
(1,1428)	1:143:A:THR:HG21	1:163:A:GLU:H	19	0.13
(1,1428)	1:143:A:THR:HG22	1:163:A:GLU:H	19	0.13
(1,1428)	1:143:A:THR:HG23	1:163:A:GLU:H	19	0.13
(1,1335)	1:57:A:CYS:HA	1:159:A:ILE:HG21	8	0.13
(1,1335)	1:57:A:CYS:HA	1:159:A:ILE:HG22	8	0.13
(1,1335)	1:57:A:CYS:HA	1:159:A:ILE:HG23	8	0.13
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG21	6	0.13
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG22	6	0.13
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG23	6	0.13
(1,1324)	1:89:A:ILE:HA	1:158:A:ILE:HG21	6	0.13
(1,1324)	1:89:A:ILE:HA	1:158:A:ILE:HG22	6	0.13
(1,1324)	1:89:A:ILE:HA	1:158:A:ILE:HG23	6	0.13
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG21	16	0.13
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG22	16	0.13
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG23	16	0.13
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG21	3	0.13
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG22	3	0.13
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG23	3	0.13
(1,1259)	1:151:A:PHE:HB2	1:152:A:THR:H	2	0.13
(1,1235)	1:150:A:VAL:H	1:152:A:THR:HG21	13	0.13
(1,1235)	1:150:A:VAL:H	1:152:A:THR:HG22	13	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1235)	1:150:A:VAL:H	1:152:A:THR:HG23	13	0.13
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG11	11	0.13
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG12	11	0.13
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG13	11	0.13
(1,1208)	1:103:A:PHE:HD1	1:146:A:MET:HB2	8	0.13
(1,1208)	1:103:A:PHE:HD2	1:146:A:MET:HB2	8	0.13
(1,1193)	1:141:A:LEU:HD11	1:148:A:GLY:H	16	0.13
(1,1193)	1:141:A:LEU:HD12	1:148:A:GLY:H	16	0.13
(1,1193)	1:141:A:LEU:HD13	1:148:A:GLY:H	16	0.13
(1,1192)	1:141:A:LEU:HD21	1:146:A:MET:H	7	0.13
(1,1192)	1:141:A:LEU:HD22	1:146:A:MET:H	7	0.13
(1,1192)	1:141:A:LEU:HD23	1:146:A:MET:H	7	0.13
(1,1192)	1:141:A:LEU:HD21	1:146:A:MET:H	18	0.13
(1,1192)	1:141:A:LEU:HD22	1:146:A:MET:H	18	0.13
(1,1192)	1:141:A:LEU:HD23	1:146:A:MET:H	18	0.13
(1,1184)	1:140:A:ALA:H	1:141:A:LEU:HG	20	0.13
(1,1177)	1:137:A:ALA:HB1	1:141:A:LEU:H	4	0.13
(1,1177)	1:137:A:ALA:HB2	1:141:A:LEU:H	4	0.13
(1,1177)	1:137:A:ALA:HB3	1:141:A:LEU:H	4	0.13
(1,1072)	1:121:A:ASP:HB2	1:123:A:GLY:H	14	0.13
(1,1047)	1:119:A:ARG:HD2	1:121:A:ASP:H	6	0.13
(1,1038)	1:119:A:ARG:HA	1:121:A:ASP:H	20	0.13
(1,1036)	1:118:A:ALA:HB1	1:119:A:ARG:H	5	0.13
(1,1036)	1:118:A:ALA:HB2	1:119:A:ARG:H	5	0.13
(1,1036)	1:118:A:ALA:HB3	1:119:A:ARG:H	5	0.13
(1,1036)	1:118:A:ALA:HB1	1:119:A:ARG:H	8	0.13
(1,1036)	1:118:A:ALA:HB2	1:119:A:ARG:H	8	0.13
(1,1036)	1:118:A:ALA:HB3	1:119:A:ARG:H	8	0.13
(1,1036)	1:118:A:ALA:HB1	1:119:A:ARG:H	10	0.13
(1,1036)	1:118:A:ALA:HB2	1:119:A:ARG:H	10	0.13
(1,1036)	1:118:A:ALA:HB3	1:119:A:ARG:H	10	0.13
(1,1036)	1:118:A:ALA:HB1	1:119:A:ARG:H	13	0.13
(1,1036)	1:118:A:ALA:HB2	1:119:A:ARG:H	13	0.13
(1,1036)	1:118:A:ALA:HB3	1:119:A:ARG:H	13	0.13
(1,978)	1:107:A:ALA:HB1	1:111:A:SER:HA	20	0.13
(1,978)	1:107:A:ALA:HB2	1:111:A:SER:HA	20	0.13
(1,978)	1:107:A:ALA:HB3	1:111:A:SER:HA	20	0.13
(1,961)	1:108:A:SER:H	1:119:A:ARG:HG2	6	0.13
(1,961)	1:108:A:SER:H	1:119:A:ARG:HG2	12	0.13
(1,952)	1:107:A:ALA:HB1	1:111:A:SER:H	3	0.13
(1,952)	1:107:A:ALA:HB2	1:111:A:SER:H	3	0.13
(1,952)	1:107:A:ALA:HB3	1:111:A:SER:H	3	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,923)	1:106:A:LEU:HA	1:110:A:PHE:H	17	0.13
(1,914)	1:104:A:GLU:H	1:106:A:LEU:HB3	9	0.13
(1,888)	1:103:A:PHE:HE1	1:120:A:GLY:H	7	0.13
(1,888)	1:103:A:PHE:HE2	1:120:A:GLY:H	7	0.13
(1,878)	1:102:A:ASP:H	1:103:A:PHE:H	1	0.13
(1,878)	1:102:A:ASP:H	1:103:A:PHE:H	9	0.13
(1,854)	1:98:A:SER:H	1:101:A:GLU:H	15	0.13
(1,832)	1:93:A:ILE:HG21	1:97:A:LYS:HG2	13	0.13
(1,832)	1:93:A:ILE:HG22	1:97:A:LYS:HG2	13	0.13
(1,832)	1:93:A:ILE:HG23	1:97:A:LYS:HG2	13	0.13
(1,799)	1:93:A:ILE:HB	1:146:A:MET:HE1	14	0.13
(1,799)	1:93:A:ILE:HB	1:146:A:MET:HE2	14	0.13
(1,799)	1:93:A:ILE:HB	1:146:A:MET:HE3	14	0.13
(1,737)	1:86:A:LEU:HB3	1:90:A:ASN:H	9	0.13
(1,698)	1:86:A:LEU:HD11	1:87:A:GLU:H	16	0.13
(1,698)	1:86:A:LEU:HD12	1:87:A:GLU:H	16	0.13
(1,698)	1:86:A:LEU:HD13	1:87:A:GLU:H	16	0.13
(1,674)	1:81:A:THR:H	1:85:A:ALA:H	16	0.13
(1,654)	1:82:A:LYS:HG2	1:84:A:GLU:H	3	0.13
(1,654)	1:82:A:LYS:HG3	1:84:A:GLU:H	3	0.13
(1,649)	1:66:A:GLN:HE21	1:82:A:LYS:HB2	5	0.13
(1,649)	1:66:A:GLN:HE21	1:82:A:LYS:HB2	6	0.13
(1,647)	1:65:A:SER:H	1:82:A:LYS:H	18	0.13
(1,644)	1:81:A:THR:HA	1:84:A:GLU:H	2	0.13
(1,644)	1:81:A:THR:HA	1:84:A:GLU:H	7	0.13
(1,644)	1:81:A:THR:HA	1:84:A:GLU:H	11	0.13
(1,591)	1:74:A:ARG:HE	1:75:A:GLN:H	6	0.13
(1,586)	1:73:A:TRP:HB3	1:74:A:ARG:H	17	0.13
(1,551)	1:70:A:PRO:HB3	1:71:A:SER:H	10	0.13
(1,523)	1:64:A:HIS:HE1	1:66:A:GLN:H	5	0.13
(1,510)	1:62:A:VAL:HG11	1:156:A:ILE:H	1	0.13
(1,510)	1:62:A:VAL:HG12	1:156:A:ILE:H	1	0.13
(1,510)	1:62:A:VAL:HG13	1:156:A:ILE:H	1	0.13
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD11	8	0.13
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD12	8	0.13
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD13	8	0.13
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD11	13	0.13
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD12	13	0.13
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD13	13	0.13
(1,424)	1:56:A:ARG:HE	1:57:A:CYS:H	4	0.13
(1,424)	1:56:A:ARG:HE	1:57:A:CYS:H	13	0.13
(1,388)	1:35:A:GLU:HG2	1:36:A:ARG:H	11	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,383)	1:34:A:TRP:H	1:35:A:GLU:HB3	11	0.13
(1,378)	1:33:A:GLN:H	1:35:A:GLU:H	3	0.13
(1,378)	1:33:A:GLN:H	1:35:A:GLU:H	18	0.13
(1,363)	1:11:A:TRP:HE3	1:33:A:GLN:H	17	0.13
(1,317)	1:28:A:ILE:HG12	1:29:A:THR:H	8	0.13
(1,302)	1:27:A:HIS:HD2	1:28:A:ILE:H	5	0.13
(1,302)	1:27:A:HIS:HD2	1:28:A:ILE:H	14	0.13
(1,284)	1:26:A:ASN:HA	1:31:A:ALA:HB1	11	0.13
(1,284)	1:26:A:ASN:HA	1:31:A:ALA:HB2	11	0.13
(1,284)	1:26:A:ASN:HA	1:31:A:ALA:HB3	11	0.13
(1,277)	1:26:A:ASN:H	1:30:A:ASN:H	4	0.13
(1,277)	1:26:A:ASN:H	1:30:A:ASN:H	5	0.13
(1,262)	1:25:A:PHE:HE1	1:26:A:ASN:HA	15	0.13
(1,262)	1:25:A:PHE:HE2	1:26:A:ASN:HA	15	0.13
(1,208)	1:24:A:TYR:H	1:34:A:TRP:HB3	10	0.13
(1,205)	1:24:A:TYR:H	1:33:A:GLN:HG2	13	0.13
(1,199)	1:23:A:TYR:H	1:24:A:TYR:H	12	0.13
(1,189)	1:13:A:LYS:H	1:24:A:TYR:HA	3	0.13
(1,176)	1:23:A:TYR:HB3	1:24:A:TYR:HD1	17	0.13
(1,176)	1:23:A:TYR:HB3	1:24:A:TYR:HD2	17	0.13
(1,176)	1:23:A:TYR:HB3	1:24:A:TYR:HD1	19	0.13
(1,176)	1:23:A:TYR:HB3	1:24:A:TYR:HD2	19	0.13
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG11	7	0.13
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG12	7	0.13
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG13	7	0.13
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG11	7	0.13
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG12	7	0.13
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG13	7	0.13
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG11	7	0.13
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG12	7	0.13
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG13	7	0.13
(1,134)	1:20:A:GLY:H	1:21:A:ARG:HA	13	0.13
(1,108)	1:15:A:MET:H	1:22:A:VAL:HA	6	0.13
(1,96)	1:14:A:ARG:H	1:23:A:TYR:HD1	7	0.13
(1,96)	1:14:A:ARG:H	1:23:A:TYR:HD2	7	0.13
(1,89)	1:14:A:ARG:H	1:15:A:MET:HA	2	0.13
(1,89)	1:14:A:ARG:H	1:15:A:MET:HA	20	0.13
(1,87)	1:13:A:LYS:HG3	1:14:A:ARG:H	11	0.13
(1,81)	1:12:A:GLU:H	1:14:A:ARG:H	4	0.13
(1,35)	1:9:A:PRO:HG2	1:10:A:GLY:H	4	0.13
(1,12)	1:5:A:GLU:HB2	1:6:A:LYS:H	13	0.13
(1,7)	1:3:A:ASP:HA	1:4:A:GLU:H	2	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,7)	1:3:A:ASP:HA	1:4:A:GLU:H	3	0.13
(4,2784)	1:56:A:ARG:H	1:163:A:GLU:O	2	0.12
(4,2760)	1:12:A:GLU:H	1:25:A:PHE:O	7	0.12
(4,2672)	2:657:B:GLU:HG2	2:658:B:GLY:H	7	0.12
(4,1761)	1:33:A:GLN:HB3	1:33:A:GLN:HE21	11	0.12
(4,1761)	1:33:A:GLN:HB2	1:33:A:GLN:HE21	11	0.12
(4,1761)	1:33:A:GLN:HB3	1:33:A:GLN:HE22	11	0.12
(3,59)	1:88:A:LEU:O	1:92:A:TYR:N	6	0.12
(3,43)	1:72:A:SER:O	1:75:A:GLN:N	9	0.12
(3,10)	1:16:A:SER:O	1:19:A:SER:H	13	0.12
(2,34)	1:59:A:HIS:H	1:122:A:LEU:HB2	6	0.12
(2,1)	1:10:A:GLY:H	1:11:A:TRP:HB3	2	0.12
(2,1)	1:10:A:GLY:H	1:11:A:TRP:HB3	12	0.12
(1,2551)	2:652:B:ASP:H	2:654:B:SER:H	1	0.12
(1,2530)	2:648:B:ILE:HD11	2:649:B:ARG:H	2	0.12
(1,2530)	2:648:B:ILE:HD12	2:649:B:ARG:H	2	0.12
(1,2530)	2:648:B:ILE:HD13	2:649:B:ARG:H	2	0.12
(1,2488)	2:656:B:PHE:HA	2:656:B:PHE:HE1	5	0.12
(1,2488)	2:656:B:PHE:HA	2:656:B:PHE:HE2	5	0.12
(1,2477)	2:653:B:GLN:HA	2:653:B:GLN:HE22	2	0.12
(1,2466)	2:651:B:ILE:H	2:651:B:ILE:HD11	6	0.12
(1,2466)	2:651:B:ILE:H	2:651:B:ILE:HD12	6	0.12
(1,2466)	2:651:B:ILE:H	2:651:B:ILE:HD13	6	0.12
(1,2036)	1:96:A:ILE:H	1:96:A:ILE:HD11	6	0.12
(1,2036)	1:96:A:ILE:H	1:96:A:ILE:HD12	6	0.12
(1,2036)	1:96:A:ILE:H	1:96:A:ILE:HD13	6	0.12
(1,1751)	1:56:A:ARG:H	1:56:A:ARG:HG3	11	0.12
(1,1751)	1:56:A:ARG:H	1:56:A:ARG:HG3	18	0.12
(1,1747)	1:56:A:ARG:H	1:56:A:ARG:HD2	11	0.12
(1,1747)	1:56:A:ARG:H	1:56:A:ARG:HD2	19	0.12
(1,1703)	1:36:A:ARG:H	1:36:A:ARG:HD2	7	0.12
(1,1660)	1:32:A:SER:H	1:32:A:SER:HB3	20	0.12
(1,1611)	1:25:A:PHE:H	1:25:A:PHE:HD1	4	0.12
(1,1611)	1:25:A:PHE:H	1:25:A:PHE:HD2	4	0.12
(1,1611)	1:25:A:PHE:H	1:25:A:PHE:HD1	15	0.12
(1,1611)	1:25:A:PHE:H	1:25:A:PHE:HD2	15	0.12
(1,1568)	1:21:A:ARG:HB2	1:21:A:ARG:HE	9	0.12
(1,1547)	1:15:A:MET:H	1:15:A:MET:HB2	4	0.12
(1,1485)	1:11:A:TRP:HD1	1:11:A:TRP:HE3	12	0.12
(1,1453)	1:5:A:GLU:H	1:5:A:GLU:HA	2	0.12
(1,1453)	1:5:A:GLU:H	1:5:A:GLU:HA	4	0.12
(1,1453)	1:5:A:GLU:H	1:5:A:GLU:HA	19	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1450)	1:4:A:GLU:HA	1:4:A:GLU:HG2	4	0.12
(1,1450)	1:4:A:GLU:HA	1:4:A:GLU:HG2	12	0.12
(1,1441)	1:162:A:THR:HG21	1:163:A:GLU:HG3	5	0.12
(1,1441)	1:162:A:THR:HG22	1:163:A:GLU:HG3	5	0.12
(1,1441)	1:162:A:THR:HG23	1:163:A:GLU:HG3	5	0.12
(1,1431)	1:161:A:ARG:HA	1:163:A:GLU:H	10	0.12
(1,1361)	1:59:A:HIS:HB2	1:160:A:LEU:H	16	0.12
(1,1361)	1:59:A:HIS:HB3	1:160:A:LEU:H	16	0.12
(1,1353)	1:57:A:CYS:HB3	1:160:A:LEU:H	4	0.12
(1,1346)	1:148:A:GLY:H	1:159:A:ILE:H	17	0.12
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG21	20	0.12
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG22	20	0.12
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG23	20	0.12
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG21	6	0.12
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG22	6	0.12
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG23	6	0.12
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG21	6	0.12
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG22	6	0.12
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG23	6	0.12
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG21	6	0.12
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG22	6	0.12
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG23	6	0.12
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG21	14	0.12
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG22	14	0.12
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG23	14	0.12
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG21	14	0.12
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG22	14	0.12
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG23	14	0.12
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG21	14	0.12
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG22	14	0.12
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG23	14	0.12
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG21	15	0.12
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG22	15	0.12
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG23	15	0.12
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG21	15	0.12
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG22	15	0.12
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG23	15	0.12
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG21	15	0.12
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG22	15	0.12
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG23	15	0.12
(1,1233)	1:149:A:PRO:HD2	1:150:A:VAL:H	2	0.12
(1,1231)	1:149:A:PRO:HG2	1:150:A:VAL:H	11	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1199)	1:142:A:ARG:HG2	1:143:A:THR:H	16	0.12
(1,1178)	1:137:A:ALA:HA	1:141:A:LEU:H	12	0.12
(1,1161)	1:136:A:ASP:HB2	1:138:A:SER:H	18	0.12
(1,1096)	1:56:A:ARG:HA	1:125:A:PHE:HD1	2	0.12
(1,1096)	1:56:A:ARG:HA	1:125:A:PHE:HD2	2	0.12
(1,1072)	1:121:A:ASP:HB2	1:123:A:GLY:H	13	0.12
(1,1051)	1:57:A:CYS:H	1:122:A:LEU:HD21	1	0.12
(1,1051)	1:57:A:CYS:H	1:122:A:LEU:HD22	1	0.12
(1,1051)	1:57:A:CYS:H	1:122:A:LEU:HD23	1	0.12
(1,1038)	1:119:A:ARG:HA	1:121:A:ASP:H	4	0.12
(1,1036)	1:118:A:ALA:HB1	1:119:A:ARG:H	17	0.12
(1,1036)	1:118:A:ALA:HB2	1:119:A:ARG:H	17	0.12
(1,1036)	1:118:A:ALA:HB3	1:119:A:ARG:H	17	0.12
(1,1026)	1:118:A:ALA:H	1:119:A:ARG:HA	1	0.12
(1,1001)	1:113:A:CYS:H	1:116:A:ALA:HB1	9	0.12
(1,1001)	1:113:A:CYS:H	1:116:A:ALA:HB2	9	0.12
(1,1001)	1:113:A:CYS:H	1:116:A:ALA:HB3	9	0.12
(1,961)	1:108:A:SER:H	1:119:A:ARG:HG2	19	0.12
(1,921)	1:106:A:LEU:H	1:109:A:GLN:H	20	0.12
(1,914)	1:104:A:GLU:H	1:106:A:LEU:HB3	16	0.12
(1,888)	1:103:A:PHE:HE1	1:120:A:GLY:H	12	0.12
(1,888)	1:103:A:PHE:HE2	1:120:A:GLY:H	12	0.12
(1,888)	1:103:A:PHE:HE1	1:120:A:GLY:H	16	0.12
(1,888)	1:103:A:PHE:HE2	1:120:A:GLY:H	16	0.12
(1,885)	1:103:A:PHE:HA	1:106:A:LEU:HD11	2	0.12
(1,885)	1:103:A:PHE:HA	1:106:A:LEU:HD12	2	0.12
(1,885)	1:103:A:PHE:HA	1:106:A:LEU:HD13	2	0.12
(1,878)	1:102:A:ASP:H	1:103:A:PHE:H	3	0.12
(1,878)	1:102:A:ASP:H	1:103:A:PHE:H	19	0.12
(1,868)	1:60:A:LEU:HD21	1:103:A:PHE:HE1	10	0.12
(1,868)	1:60:A:LEU:HD21	1:103:A:PHE:HE2	10	0.12
(1,868)	1:60:A:LEU:HD22	1:103:A:PHE:HE1	10	0.12
(1,868)	1:60:A:LEU:HD22	1:103:A:PHE:HE2	10	0.12
(1,868)	1:60:A:LEU:HD23	1:103:A:PHE:HE1	10	0.12
(1,868)	1:60:A:LEU:HD23	1:103:A:PHE:HE2	10	0.12
(1,857)	1:101:A:GLU:HG2	1:106:A:LEU:HD11	12	0.12
(1,857)	1:101:A:GLU:HG2	1:106:A:LEU:HD12	12	0.12
(1,857)	1:101:A:GLU:HG2	1:106:A:LEU:HD13	12	0.12
(1,807)	1:93:A:ILE:HD11	1:94:A:GLN:H	5	0.12
(1,807)	1:93:A:ILE:HD12	1:94:A:GLN:H	5	0.12
(1,807)	1:93:A:ILE:HD13	1:94:A:GLN:H	5	0.12
(1,728)	1:89:A:ILE:HD11	1:92:A:TYR:HE1	14	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,728)	1:89:A:ILE:HD11	1:92:A:TYR:HE2	14	0.12
(1,728)	1:89:A:ILE:HD12	1:92:A:TYR:HE1	14	0.12
(1,728)	1:89:A:ILE:HD12	1:92:A:TYR:HE2	14	0.12
(1,728)	1:89:A:ILE:HD13	1:92:A:TYR:HE1	14	0.12
(1,728)	1:89:A:ILE:HD13	1:92:A:TYR:HE2	14	0.12
(1,681)	1:85:A:ALA:H	1:88:A:LEU:HD11	7	0.12
(1,681)	1:85:A:ALA:H	1:88:A:LEU:HD12	7	0.12
(1,681)	1:85:A:ALA:H	1:88:A:LEU:HD13	7	0.12
(1,659)	1:81:A:THR:HA	1:83:A:GLU:H	6	0.12
(1,648)	1:66:A:GLN:HE22	1:82:A:LYS:HG3	6	0.12
(1,647)	1:65:A:SER:H	1:82:A:LYS:H	14	0.12
(1,644)	1:81:A:THR:HA	1:84:A:GLU:H	3	0.12
(1,599)	1:70:A:PRO:HB2	1:78:A:ILE:H	11	0.12
(1,538)	1:66:A:GLN:HG2	1:67:A:SER:H	18	0.12
(1,537)	1:66:A:GLN:HB3	1:67:A:SER:H	17	0.12
(1,532)	1:64:A:HIS:H	1:67:A:SER:H	1	0.12
(1,531)	1:64:A:HIS:HE1	1:67:A:SER:HB2	6	0.12
(1,523)	1:64:A:HIS:HE1	1:66:A:GLN:H	2	0.12
(1,515)	1:63:A:LYS:H	1:156:A:ILE:H	4	0.12
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD11	9	0.12
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD12	9	0.12
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD13	9	0.12
(1,469)	1:60:A:LEU:HB2	1:61:A:LEU:H	13	0.12
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB1	13	0.12
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB2	13	0.12
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB3	13	0.12
(1,450)	1:60:A:LEU:HD11	1:89:A:ILE:HD11	8	0.12
(1,450)	1:60:A:LEU:HD11	1:89:A:ILE:HD12	8	0.12
(1,450)	1:60:A:LEU:HD11	1:89:A:ILE:HD13	8	0.12
(1,450)	1:60:A:LEU:HD12	1:89:A:ILE:HD11	8	0.12
(1,450)	1:60:A:LEU:HD12	1:89:A:ILE:HD12	8	0.12
(1,450)	1:60:A:LEU:HD12	1:89:A:ILE:HD13	8	0.12
(1,450)	1:60:A:LEU:HD13	1:89:A:ILE:HD11	8	0.12
(1,450)	1:60:A:LEU:HD13	1:89:A:ILE:HD12	8	0.12
(1,450)	1:60:A:LEU:HD13	1:89:A:ILE:HD13	8	0.12
(1,436)	1:58:A:SER:H	1:160:A:LEU:HG	2	0.12
(1,436)	1:58:A:SER:H	1:160:A:LEU:HG	14	0.12
(1,391)	1:35:A:GLU:HB3	1:36:A:ARG:H	19	0.12
(1,387)	1:35:A:GLU:HB2	1:36:A:ARG:H	5	0.12
(1,387)	1:35:A:GLU:HB2	1:36:A:ARG:H	12	0.12
(1,387)	1:35:A:GLU:HB2	1:36:A:ARG:H	17	0.12
(1,377)	1:33:A:GLN:HG2	1:35:A:GLU:H	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,377)	1:33:A:GLN:HG2	1:35:A:GLU:H	15	0.12
(1,365)	1:32:A:SER:H	1:33:A:GLN:H	5	0.12
(1,364)	1:24:A:TYR:HD1	1:33:A:GLN:H	5	0.12
(1,364)	1:24:A:TYR:HD2	1:33:A:GLN:H	5	0.12
(1,363)	1:11:A:TRP:HE3	1:33:A:GLN:H	11	0.12
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB1	16	0.12
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB2	16	0.12
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB3	16	0.12
(1,321)	1:25:A:PHE:HZ	1:30:A:ASN:H	8	0.12
(1,318)	1:29:A:THR:H	1:30:A:ASN:HB3	11	0.12
(1,317)	1:28:A:ILE:HG12	1:29:A:THR:H	12	0.12
(1,277)	1:26:A:ASN:H	1:30:A:ASN:H	2	0.12
(1,277)	1:26:A:ASN:H	1:30:A:ASN:H	19	0.12
(1,223)	1:14:A:ARG:HB2	1:25:A:PHE:H	17	0.12
(1,208)	1:24:A:TYR:H	1:34:A:TRP:HB3	12	0.12
(1,205)	1:24:A:TYR:H	1:33:A:GLN:HG2	9	0.12
(1,199)	1:23:A:TYR:H	1:24:A:TYR:H	7	0.12
(1,189)	1:13:A:LYS:H	1:24:A:TYR:HA	1	0.12
(1,189)	1:13:A:LYS:H	1:24:A:TYR:HA	14	0.12
(1,143)	1:15:A:MET:HA	1:22:A:VAL:H	11	0.12
(1,125)	1:15:A:MET:HA	1:21:A:ARG:H	18	0.12
(1,121)	1:17:A:ARG:HB2	1:18:A:SER:H	5	0.12
(1,121)	1:17:A:ARG:HB2	1:18:A:SER:H	10	0.12
(1,121)	1:17:A:ARG:HB2	1:18:A:SER:H	20	0.12
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG21	10	0.12
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG22	10	0.12
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG23	10	0.12
(1,98)	1:14:A:ARG:H	1:24:A:TYR:H	7	0.12
(1,89)	1:14:A:ARG:H	1:15:A:MET:HA	8	0.12
(1,35)	1:9:A:PRO:HG2	1:10:A:GLY:H	17	0.12
(1,20)	1:7:A:LEU:HD11	1:11:A:TRP:H	19	0.12
(1,20)	1:7:A:LEU:HD12	1:11:A:TRP:H	19	0.12
(1,20)	1:7:A:LEU:HD13	1:11:A:TRP:H	19	0.12
(4,2798)	1:72:A:SER:H	1:75:A:GLN:O	7	0.11
(4,2798)	1:72:A:SER:H	1:75:A:GLN:O	8	0.11
(4,2774)	1:26:A:ASN:H	1:31:A:ALA:O	11	0.11
(4,1958)	1:75:A:GLN:HB2	1:75:A:GLN:HE21	2	0.11
(4,1958)	1:75:A:GLN:HB2	1:75:A:GLN:HE22	2	0.11
(4,1958)	1:75:A:GLN:HB2	1:75:A:GLN:HE21	15	0.11
(4,1958)	1:75:A:GLN:HB2	1:75:A:GLN:HE22	15	0.11
(4,1958)	1:75:A:GLN:HB2	1:75:A:GLN:HE21	18	0.11
(4,1958)	1:75:A:GLN:HB2	1:75:A:GLN:HE22	18	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,71)	1:94:A:GLN:O	1:98:A:SER:N	10	0.11
(3,63)	1:90:A:ASN:O	1:94:A:GLN:N	16	0.11
(3,10)	1:16:A:SER:O	1:19:A:SER:H	5	0.11
(3,9)	1:16:A:SER:O	1:19:A:SER:N	18	0.11
(2,113)	1:162:A:THR:H	2:651:B:ILE:HG12	20	0.11
(2,113)	1:162:A:THR:H	2:651:B:ILE:HG13	20	0.11
(2,107)	1:140:A:ALA:HB1	2:651:B:ILE:HA	15	0.11
(2,107)	1:140:A:ALA:HB2	2:651:B:ILE:HA	15	0.11
(2,107)	1:140:A:ALA:HB3	2:651:B:ILE:HA	15	0.11
(2,91)	1:57:A:CYS:H	2:651:B:ILE:HG12	13	0.11
(2,91)	1:57:A:CYS:H	2:651:B:ILE:HG13	13	0.11
(2,67)	2:646:B:GLU:HA	2:647:B:VAL:HG11	1	0.11
(2,67)	2:646:B:GLU:HA	2:647:B:VAL:HG12	1	0.11
(2,67)	2:646:B:GLU:HA	2:647:B:VAL:HG13	1	0.11
(2,67)	2:646:B:GLU:HA	2:647:B:VAL:HG11	9	0.11
(2,67)	2:646:B:GLU:HA	2:647:B:VAL:HG12	9	0.11
(2,67)	2:646:B:GLU:HA	2:647:B:VAL:HG13	9	0.11
(2,52)	1:141:A:LEU:HD21	1:148:A:GLY:H	3	0.11
(2,52)	1:141:A:LEU:HD22	1:148:A:GLY:H	3	0.11
(2,52)	1:141:A:LEU:HD23	1:148:A:GLY:H	3	0.11
(2,52)	1:141:A:LEU:HD21	1:148:A:GLY:H	18	0.11
(2,52)	1:141:A:LEU:HD22	1:148:A:GLY:H	18	0.11
(2,52)	1:141:A:LEU:HD23	1:148:A:GLY:H	18	0.11
(2,1)	1:10:A:GLY:H	1:11:A:TRP:HB3	1	0.11
(2,1)	1:10:A:GLY:H	1:11:A:TRP:HB3	9	0.11
(1,2597)	1:138:A:SER:H	2:656:B:PHE:HB2	5	0.11
(1,2593)	1:129:A:GLN:HE21	2:656:B:PHE:HE1	20	0.11
(1,2593)	1:129:A:GLN:HE21	2:656:B:PHE:HE2	20	0.11
(1,2551)	2:652:B:ASP:H	2:654:B:SER:H	5	0.11
(1,2551)	2:652:B:ASP:H	2:654:B:SER:H	17	0.11
(1,2527)	2:646:B:GLU:H	2:648:B:ILE:H	19	0.11
(1,2526)	2:646:B:GLU:HB2	2:648:B:ILE:H	2	0.11
(1,2506)	2:644:B:ASP:H	2:645:B:GLN:HA	16	0.11
(1,2488)	2:656:B:PHE:HA	2:656:B:PHE:HE1	3	0.11
(1,2488)	2:656:B:PHE:HA	2:656:B:PHE:HE2	3	0.11
(1,2488)	2:656:B:PHE:HA	2:656:B:PHE:HE1	4	0.11
(1,2488)	2:656:B:PHE:HA	2:656:B:PHE:HE2	4	0.11
(1,2386)	1:163:A:GLU:H	1:163:A:GLU:HG2	14	0.11
(1,2074)	1:104:A:GLU:H	1:104:A:GLU:HG2	19	0.11
(1,2056)	1:101:A:GLU:H	1:101:A:GLU:HG2	6	0.11
(1,2036)	1:96:A:ILE:H	1:96:A:ILE:HD11	8	0.11
(1,2036)	1:96:A:ILE:H	1:96:A:ILE:HD12	8	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2036)	1:96:A:ILE:H	1:96:A:ILE:HD13	8	0.11
(1,1913)	1:82:A:LYS:H	1:82:A:LYS:HD2	16	0.11
(1,1869)	1:75:A:GLN:H	1:75:A:GLN:HE22	14	0.11
(1,1747)	1:56:A:ARG:H	1:56:A:ARG:HD2	2	0.11
(1,1660)	1:32:A:SER:H	1:32:A:SER:HB3	12	0.11
(1,1611)	1:25:A:PHE:H	1:25:A:PHE:HD1	18	0.11
(1,1611)	1:25:A:PHE:H	1:25:A:PHE:HD2	18	0.11
(1,1571)	1:21:A:ARG:H	1:21:A:ARG:HD2	5	0.11
(1,1571)	1:21:A:ARG:H	1:21:A:ARG:HD2	8	0.11
(1,1571)	1:21:A:ARG:H	1:21:A:ARG:HD2	15	0.11
(1,1571)	1:21:A:ARG:H	1:21:A:ARG:HD2	16	0.11
(1,1521)	1:14:A:ARG:H	1:14:A:ARG:HG3	15	0.11
(1,1485)	1:11:A:TRP:HD1	1:11:A:TRP:HE3	1	0.11
(1,1485)	1:11:A:TRP:HD1	1:11:A:TRP:HE3	2	0.11
(1,1485)	1:11:A:TRP:HD1	1:11:A:TRP:HE3	3	0.11
(1,1485)	1:11:A:TRP:HD1	1:11:A:TRP:HE3	4	0.11
(1,1485)	1:11:A:TRP:HD1	1:11:A:TRP:HE3	5	0.11
(1,1485)	1:11:A:TRP:HD1	1:11:A:TRP:HE3	6	0.11
(1,1485)	1:11:A:TRP:HD1	1:11:A:TRP:HE3	7	0.11
(1,1485)	1:11:A:TRP:HD1	1:11:A:TRP:HE3	8	0.11
(1,1485)	1:11:A:TRP:HD1	1:11:A:TRP:HE3	9	0.11
(1,1485)	1:11:A:TRP:HD1	1:11:A:TRP:HE3	10	0.11
(1,1485)	1:11:A:TRP:HD1	1:11:A:TRP:HE3	11	0.11
(1,1485)	1:11:A:TRP:HD1	1:11:A:TRP:HE3	14	0.11
(1,1485)	1:11:A:TRP:HD1	1:11:A:TRP:HE3	15	0.11
(1,1485)	1:11:A:TRP:HD1	1:11:A:TRP:HE3	16	0.11
(1,1485)	1:11:A:TRP:HD1	1:11:A:TRP:HE3	17	0.11
(1,1485)	1:11:A:TRP:HD1	1:11:A:TRP:HE3	18	0.11
(1,1485)	1:11:A:TRP:HD1	1:11:A:TRP:HE3	19	0.11
(1,1485)	1:11:A:TRP:HD1	1:11:A:TRP:HE3	20	0.11
(1,1455)	1:6:A:LYS:H	1:6:A:LYS:HB3	15	0.11
(1,1453)	1:5:A:GLU:H	1:5:A:GLU:HA	1	0.11
(1,1453)	1:5:A:GLU:H	1:5:A:GLU:HA	10	0.11
(1,1453)	1:5:A:GLU:H	1:5:A:GLU:HA	15	0.11
(1,1452)	1:5:A:GLU:H	1:5:A:GLU:HB3	16	0.11
(1,1450)	1:4:A:GLU:HA	1:4:A:GLU:HG2	5	0.11
(1,1450)	1:4:A:GLU:HA	1:4:A:GLU:HG2	6	0.11
(1,1435)	1:161:A:ARG:HG3	1:163:A:GLU:H	19	0.11
(1,1369)	1:104:A:GLU:H	1:160:A:LEU:HD11	16	0.11
(1,1369)	1:104:A:GLU:H	1:160:A:LEU:HD12	16	0.11
(1,1369)	1:104:A:GLU:H	1:160:A:LEU:HD13	16	0.11
(1,1340)	1:147:A:SER:HB2	1:159:A:ILE:HD11	17	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1340)	1:147:A:SER:HB2	1:159:A:ILE:HD12	17	0.11
(1,1340)	1:147:A:SER:HB2	1:159:A:ILE:HD13	17	0.11
(1,1324)	1:89:A:ILE:HA	1:158:A:ILE:HG21	1	0.11
(1,1324)	1:89:A:ILE:HA	1:158:A:ILE:HG22	1	0.11
(1,1324)	1:89:A:ILE:HA	1:158:A:ILE:HG23	1	0.11
(1,1322)	1:61:A:LEU:HA	1:158:A:ILE:H	6	0.11
(1,1311)	1:152:A:THR:HG21	1:157:A:HIS:H	10	0.11
(1,1311)	1:152:A:THR:HG22	1:157:A:HIS:H	10	0.11
(1,1311)	1:152:A:THR:HG23	1:157:A:HIS:H	10	0.11
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG21	19	0.11
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG22	19	0.11
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG23	19	0.11
(1,1262)	1:151:A:PHE:H	1:156:A:ILE:HA	18	0.11
(1,1259)	1:151:A:PHE:HB2	1:152:A:THR:H	13	0.11
(1,1259)	1:151:A:PHE:HB2	1:152:A:THR:H	15	0.11
(1,1259)	1:151:A:PHE:HB2	1:152:A:THR:H	16	0.11
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG11	18	0.11
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG12	18	0.11
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG13	18	0.11
(1,1141)	1:130:A:MET:HB2	1:134:A:PHE:H	13	0.11
(1,1088)	1:56:A:ARG:HD2	1:124:A:ALA:HA	13	0.11
(1,1079)	1:123:A:GLY:H	1:125:A:PHE:HD1	15	0.11
(1,1079)	1:123:A:GLY:H	1:125:A:PHE:HD2	15	0.11
(1,1052)	1:58:A:SER:HB2	1:122:A:LEU:H	17	0.11
(1,1038)	1:119:A:ARG:HA	1:121:A:ASP:H	12	0.11
(1,1026)	1:118:A:ALA:H	1:119:A:ARG:HA	9	0.11
(1,998)	1:111:A:SER:H	1:116:A:ALA:HB1	2	0.11
(1,998)	1:111:A:SER:H	1:116:A:ALA:HB2	2	0.11
(1,998)	1:111:A:SER:H	1:116:A:ALA:HB3	2	0.11
(1,970)	1:108:A:SER:H	1:110:A:PHE:H	14	0.11
(1,941)	1:106:A:LEU:HD11	1:107:A:ALA:H	16	0.11
(1,941)	1:106:A:LEU:HD12	1:107:A:ALA:H	16	0.11
(1,941)	1:106:A:LEU:HD13	1:107:A:ALA:H	16	0.11
(1,926)	1:60:A:LEU:HD11	1:107:A:ALA:H	1	0.11
(1,926)	1:60:A:LEU:HD12	1:107:A:ALA:H	1	0.11
(1,926)	1:60:A:LEU:HD13	1:107:A:ALA:H	1	0.11
(1,926)	1:60:A:LEU:HD11	1:107:A:ALA:H	18	0.11
(1,926)	1:60:A:LEU:HD12	1:107:A:ALA:H	18	0.11
(1,926)	1:60:A:LEU:HD13	1:107:A:ALA:H	18	0.11
(1,925)	1:60:A:LEU:HG	1:107:A:ALA:H	17	0.11
(1,921)	1:106:A:LEU:H	1:109:A:GLN:H	7	0.11
(1,878)	1:102:A:ASP:H	1:103:A:PHE:H	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,868)	1:60:A:LEU:HD21	1:103:A:PHE:HE1	16	0.11
(1,868)	1:60:A:LEU:HD21	1:103:A:PHE:HE2	16	0.11
(1,868)	1:60:A:LEU:HD22	1:103:A:PHE:HE1	16	0.11
(1,868)	1:60:A:LEU:HD22	1:103:A:PHE:HE2	16	0.11
(1,868)	1:60:A:LEU:HD23	1:103:A:PHE:HE1	16	0.11
(1,868)	1:60:A:LEU:HD23	1:103:A:PHE:HE2	16	0.11
(1,843)	1:97:A:LYS:HB2	1:98:A:SER:H	7	0.11
(1,828)	1:96:A:ILE:H	1:146:A:MET:HE1	19	0.11
(1,828)	1:96:A:ILE:H	1:146:A:MET:HE2	19	0.11
(1,828)	1:96:A:ILE:H	1:146:A:MET:HE3	19	0.11
(1,816)	1:95:A:LYS:HD2	1:96:A:ILE:H	4	0.11
(1,772)	1:92:A:TYR:H	1:93:A:ILE:HB	17	0.11
(1,750)	1:88:A:LEU:H	1:91:A:GLY:H	2	0.11
(1,669)	1:84:A:GLU:H	1:87:A:GLU:H	20	0.11
(1,663)	1:82:A:LYS:HB3	1:83:A:GLU:H	20	0.11
(1,659)	1:81:A:THR:HA	1:83:A:GLU:H	1	0.11
(1,659)	1:81:A:THR:HA	1:83:A:GLU:H	7	0.11
(1,659)	1:81:A:THR:HA	1:83:A:GLU:H	16	0.11
(1,619)	1:78:A:ILE:HB	1:80:A:ARG:H	11	0.11
(1,619)	1:78:A:ILE:HB	1:80:A:ARG:H	17	0.11
(1,586)	1:73:A:TRP:HB3	1:74:A:ARG:H	2	0.11
(1,586)	1:73:A:TRP:HB3	1:74:A:ARG:H	18	0.11
(1,554)	1:70:A:PRO:HG3	1:71:A:SER:H	11	0.11
(1,538)	1:66:A:GLN:HG2	1:67:A:SER:H	3	0.11
(1,469)	1:60:A:LEU:HB2	1:61:A:LEU:H	8	0.11
(1,469)	1:60:A:LEU:HB2	1:61:A:LEU:H	10	0.11
(1,469)	1:60:A:LEU:HB2	1:61:A:LEU:H	14	0.11
(1,436)	1:58:A:SER:H	1:160:A:LEU:HG	6	0.11
(1,387)	1:35:A:GLU:HB2	1:36:A:ARG:H	7	0.11
(1,387)	1:35:A:GLU:HB2	1:36:A:ARG:H	9	0.11
(1,387)	1:35:A:GLU:HB2	1:36:A:ARG:H	11	0.11
(1,387)	1:35:A:GLU:HB2	1:36:A:ARG:H	18	0.11
(1,384)	1:7:A:LEU:HD21	1:36:A:ARG:HA	18	0.11
(1,384)	1:7:A:LEU:HD22	1:36:A:ARG:HA	18	0.11
(1,384)	1:7:A:LEU:HD23	1:36:A:ARG:HA	18	0.11
(1,378)	1:33:A:GLN:H	1:35:A:GLU:H	1	0.11
(1,378)	1:33:A:GLN:H	1:35:A:GLU:H	6	0.11
(1,377)	1:33:A:GLN:HG2	1:35:A:GLU:H	17	0.11
(1,373)	1:34:A:TRP:HD1	1:35:A:GLU:H	11	0.11
(1,373)	1:34:A:TRP:HD1	1:35:A:GLU:H	15	0.11
(1,367)	1:24:A:TYR:HD1	1:34:A:TRP:H	16	0.11
(1,367)	1:24:A:TYR:HD2	1:34:A:TRP:H	16	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,364)	1:24:A:TYR:HD1	1:33:A:GLN:H	17	0.11
(1,364)	1:24:A:TYR:HD2	1:33:A:GLN:H	17	0.11
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB1	16	0.11
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB2	16	0.11
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB3	16	0.11
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB1	12	0.11
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB2	12	0.11
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB3	12	0.11
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB1	19	0.11
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB2	19	0.11
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB3	19	0.11
(1,318)	1:29:A:THR:H	1:30:A:ASN:HB3	10	0.11
(1,318)	1:29:A:THR:H	1:30:A:ASN:HB3	13	0.11
(1,278)	1:26:A:ASN:HB2	1:30:A:ASN:H	5	0.11
(1,278)	1:26:A:ASN:HB2	1:30:A:ASN:H	17	0.11
(1,265)	1:26:A:ASN:H	1:27:A:HIS:H	5	0.11
(1,265)	1:26:A:ASN:H	1:27:A:HIS:H	7	0.11
(1,262)	1:25:A:PHE:HE1	1:26:A:ASN:HA	20	0.11
(1,262)	1:25:A:PHE:HE2	1:26:A:ASN:HA	20	0.11
(1,242)	1:10:A:GLY:H	1:26:A:ASN:HD21	7	0.11
(1,236)	1:25:A:PHE:HA	1:31:A:ALA:HB1	13	0.11
(1,236)	1:25:A:PHE:HA	1:31:A:ALA:HB2	13	0.11
(1,236)	1:25:A:PHE:HA	1:31:A:ALA:HB3	13	0.11
(1,199)	1:23:A:TYR:H	1:24:A:TYR:H	6	0.11
(1,199)	1:23:A:TYR:H	1:24:A:TYR:H	8	0.11
(1,199)	1:23:A:TYR:H	1:24:A:TYR:H	9	0.11
(1,199)	1:23:A:TYR:H	1:24:A:TYR:H	11	0.11
(1,199)	1:23:A:TYR:H	1:24:A:TYR:H	15	0.11
(1,199)	1:23:A:TYR:H	1:24:A:TYR:H	16	0.11
(1,181)	1:23:A:TYR:HB2	1:34:A:TRP:HE3	19	0.11
(1,180)	1:23:A:TYR:HD1	1:33:A:GLN:HA	12	0.11
(1,180)	1:23:A:TYR:HD2	1:33:A:GLN:HA	12	0.11
(1,165)	1:22:A:VAL:H	1:23:A:TYR:H	2	0.11
(1,165)	1:22:A:VAL:H	1:23:A:TYR:H	3	0.11
(1,130)	1:16:A:SER:H	1:21:A:ARG:HA	14	0.11
(1,110)	1:15:A:MET:H	1:23:A:TYR:HE1	10	0.11
(1,110)	1:15:A:MET:H	1:23:A:TYR:HE2	10	0.11
(1,110)	1:15:A:MET:H	1:23:A:TYR:HE1	19	0.11
(1,110)	1:15:A:MET:H	1:23:A:TYR:HE2	19	0.11
(1,108)	1:15:A:MET:H	1:22:A:VAL:HA	9	0.11
(1,104)	1:15:A:MET:H	1:16:A:SER:H	13	0.11
(1,98)	1:14:A:ARG:H	1:24:A:TYR:H	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,84)	1:13:A:LYS:HG2	1:14:A:ARG:H	9	0.11
(1,67)	1:12:A:GLU:HB3	1:27:A:HIS:HD2	13	0.11
(1,61)	1:11:A:TRP:HA	1:12:A:GLU:HB3	17	0.11
(1,52)	1:11:A:TRP:HE1	1:26:A:ASN:HB2	6	0.11
(1,52)	1:11:A:TRP:HE1	1:26:A:ASN:HB3	6	0.11
(1,42)	1:10:A:GLY:H	1:28:A:ILE:HD11	20	0.11
(1,42)	1:10:A:GLY:H	1:28:A:ILE:HD12	20	0.11
(1,42)	1:10:A:GLY:H	1:28:A:ILE:HD13	20	0.11
(1,41)	1:10:A:GLY:H	1:27:A:HIS:HD2	18	0.11
(1,20)	1:7:A:LEU:HD11	1:11:A:TRP:H	14	0.11
(1,20)	1:7:A:LEU:HD12	1:11:A:TRP:H	14	0.11
(1,20)	1:7:A:LEU:HD13	1:11:A:TRP:H	14	0.11
(1,2)	1:2:A:ALA:HA	1:3:A:ASP:H	10	0.11
(4,2764)	1:16:A:SER:H	1:21:A:ARG:O	3	0.1
(4,2764)	1:16:A:SER:H	1:21:A:ARG:O	12	0.1
(4,2656)	2:654:B:SER:H	2:655:B:GLU:H	19	0.1
(2,92)	1:58:A:SER:H	2:651:B:ILE:HG12	1	0.1
(2,92)	1:58:A:SER:H	2:651:B:ILE:HG13	1	0.1
(1,2530)	2:648:B:ILE:HD11	2:649:B:ARG:H	14	0.1
(1,2530)	2:648:B:ILE:HD12	2:649:B:ARG:H	14	0.1
(1,2530)	2:648:B:ILE:HD13	2:649:B:ARG:H	14	0.1
(1,2488)	2:656:B:PHE:HA	2:656:B:PHE:HE1	1	0.1
(1,2488)	2:656:B:PHE:HA	2:656:B:PHE:HE2	1	0.1
(1,2488)	2:656:B:PHE:HA	2:656:B:PHE:HE1	6	0.1
(1,2488)	2:656:B:PHE:HA	2:656:B:PHE:HE2	6	0.1
(1,2466)	2:651:B:ILE:H	2:651:B:ILE:HD11	14	0.1
(1,2466)	2:651:B:ILE:H	2:651:B:ILE:HD12	14	0.1
(1,2466)	2:651:B:ILE:H	2:651:B:ILE:HD13	14	0.1
(1,2083)	1:106:A:LEU:H	1:106:A:LEU:HG	7	0.1
(1,2083)	1:106:A:LEU:H	1:106:A:LEU:HG	19	0.1
(1,2074)	1:104:A:GLU:H	1:104:A:GLU:HG2	5	0.1
(1,1869)	1:75:A:GLN:H	1:75:A:GLN:HE22	5	0.1
(1,1694)	1:35:A:GLU:H	1:35:A:GLU:HG3	19	0.1
(1,1611)	1:25:A:PHE:H	1:25:A:PHE:HD1	6	0.1
(1,1611)	1:25:A:PHE:H	1:25:A:PHE:HD2	6	0.1
(1,1611)	1:25:A:PHE:H	1:25:A:PHE:HD1	8	0.1
(1,1611)	1:25:A:PHE:H	1:25:A:PHE:HD2	8	0.1
(1,1547)	1:15:A:MET:H	1:15:A:MET:HB2	1	0.1
(1,1485)	1:11:A:TRP:HD1	1:11:A:TRP:HE3	13	0.1
(1,1453)	1:5:A:GLU:H	1:5:A:GLU:HA	5	0.1
(1,1453)	1:5:A:GLU:H	1:5:A:GLU:HA	9	0.1
(1,1453)	1:5:A:GLU:H	1:5:A:GLU:HA	13	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1453)	1:5:A:GLU:H	1:5:A:GLU:HA	18	0.1
(1,1412)	1:56:A:ARG:HB2	1:162:A:THR:HG21	13	0.1
(1,1412)	1:56:A:ARG:HB2	1:162:A:THR:HG22	13	0.1
(1,1412)	1:56:A:ARG:HB2	1:162:A:THR:HG23	13	0.1
(1,1363)	1:96:A:ILE:HG21	1:160:A:LEU:HD11	7	0.1
(1,1363)	1:96:A:ILE:HG21	1:160:A:LEU:HD12	7	0.1
(1,1363)	1:96:A:ILE:HG21	1:160:A:LEU:HD13	7	0.1
(1,1363)	1:96:A:ILE:HG22	1:160:A:LEU:HD11	7	0.1
(1,1363)	1:96:A:ILE:HG22	1:160:A:LEU:HD12	7	0.1
(1,1363)	1:96:A:ILE:HG22	1:160:A:LEU:HD13	7	0.1
(1,1363)	1:96:A:ILE:HG23	1:160:A:LEU:HD11	7	0.1
(1,1363)	1:96:A:ILE:HG23	1:160:A:LEU:HD12	7	0.1
(1,1363)	1:96:A:ILE:HG23	1:160:A:LEU:HD13	7	0.1
(1,1331)	1:146:A:MET:HG2	1:158:A:ILE:HG21	14	0.1
(1,1331)	1:146:A:MET:HG2	1:158:A:ILE:HG22	14	0.1
(1,1331)	1:146:A:MET:HG2	1:158:A:ILE:HG23	14	0.1
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG21	12	0.1
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG22	12	0.1
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG23	12	0.1
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG21	12	0.1
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG22	12	0.1
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG23	12	0.1
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG21	12	0.1
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG22	12	0.1
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG23	12	0.1
(1,1235)	1:150:A:VAL:H	1:152:A:THR:HG21	17	0.1
(1,1235)	1:150:A:VAL:H	1:152:A:THR:HG22	17	0.1
(1,1235)	1:150:A:VAL:H	1:152:A:THR:HG23	17	0.1
(1,1206)	1:145:A:GLU:HB3	1:146:A:MET:HB2	15	0.1
(1,1200)	1:143:A:THR:H	1:144:A:GLY:H	20	0.1
(1,1130)	1:131:A:GLN:HE21	1:153:A:ASP:HB2	4	0.1
(1,1130)	1:131:A:GLN:HE21	1:153:A:ASP:HB3	4	0.1
(1,1130)	1:131:A:GLN:HE21	1:153:A:ASP:HB2	9	0.1
(1,1130)	1:131:A:GLN:HE21	1:153:A:ASP:HB3	9	0.1
(1,1089)	1:57:A:CYS:H	1:124:A:ALA:HA	9	0.1
(1,1085)	1:56:A:ARG:HE	1:124:A:ALA:H	15	0.1
(1,1085)	1:56:A:ARG:HE	1:124:A:ALA:H	16	0.1
(1,1047)	1:119:A:ARG:HD2	1:121:A:ASP:H	16	0.1
(1,1036)	1:118:A:ALA:HB1	1:119:A:ARG:H	3	0.1
(1,1036)	1:118:A:ALA:HB2	1:119:A:ARG:H	3	0.1
(1,1036)	1:118:A:ALA:HB3	1:119:A:ARG:H	3	0.1
(1,941)	1:106:A:LEU:HD11	1:107:A:ALA:H	2	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,941)	1:106:A:LEU:HD12	1:107:A:ALA:H	2	0.1
(1,941)	1:106:A:LEU:HD13	1:107:A:ALA:H	2	0.1
(1,843)	1:97:A:LYS:HB2	1:98:A:SER:H	8	0.1
(1,843)	1:97:A:LYS:HB2	1:98:A:SER:H	10	0.1
(1,841)	1:97:A:LYS:HB3	1:98:A:SER:H	11	0.1
(1,805)	1:93:A:ILE:HG21	1:94:A:GLN:H	8	0.1
(1,805)	1:93:A:ILE:HG22	1:94:A:GLN:H	8	0.1
(1,805)	1:93:A:ILE:HG23	1:94:A:GLN:H	8	0.1
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE1	5	0.1
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE2	5	0.1
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE3	5	0.1
(1,702)	1:87:A:GLU:HA	1:90:A:ASN:H	20	0.1
(1,681)	1:85:A:ALA:H	1:88:A:LEU:HD11	11	0.1
(1,681)	1:85:A:ALA:H	1:88:A:LEU:HD12	11	0.1
(1,681)	1:85:A:ALA:H	1:88:A:LEU:HD13	11	0.1
(1,644)	1:81:A:THR:HA	1:84:A:GLU:H	12	0.1
(1,554)	1:70:A:PRO:HG3	1:71:A:SER:H	18	0.1
(1,538)	1:66:A:GLN:HG2	1:67:A:SER:H	8	0.1
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB1	17	0.1
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB2	17	0.1
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB3	17	0.1
(1,436)	1:58:A:SER:H	1:160:A:LEU:HG	9	0.1
(1,391)	1:35:A:GLU:HB3	1:36:A:ARG:H	4	0.1
(1,354)	1:24:A:TYR:H	1:32:A:SER:HB3	8	0.1
(1,320)	1:25:A:PHE:HE1	1:30:A:ASN:H	1	0.1
(1,320)	1:25:A:PHE:HE2	1:30:A:ASN:H	1	0.1
(1,318)	1:29:A:THR:H	1:30:A:ASN:HB3	4	0.1
(1,318)	1:29:A:THR:H	1:30:A:ASN:HB3	5	0.1
(1,277)	1:26:A:ASN:H	1:30:A:ASN:H	11	0.1
(1,277)	1:26:A:ASN:H	1:30:A:ASN:H	15	0.1
(1,236)	1:25:A:PHE:HA	1:31:A:ALA:HB1	2	0.1
(1,236)	1:25:A:PHE:HA	1:31:A:ALA:HB2	2	0.1
(1,236)	1:25:A:PHE:HA	1:31:A:ALA:HB3	2	0.1
(1,199)	1:23:A:TYR:H	1:24:A:TYR:H	1	0.1
(1,199)	1:23:A:TYR:H	1:24:A:TYR:H	4	0.1
(1,199)	1:23:A:TYR:H	1:24:A:TYR:H	18	0.1
(1,165)	1:22:A:VAL:H	1:23:A:TYR:H	8	0.1
(1,110)	1:15:A:MET:H	1:23:A:TYR:HE1	14	0.1
(1,110)	1:15:A:MET:H	1:23:A:TYR:HE2	14	0.1
(1,108)	1:15:A:MET:H	1:22:A:VAL:HA	8	0.1
(1,96)	1:14:A:ARG:H	1:23:A:TYR:HD1	5	0.1
(1,96)	1:14:A:ARG:H	1:23:A:TYR:HD2	5	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,90)	1:14:A:ARG:H	1:15:A:MET:H	19	0.1
(1,35)	1:9:A:PRO:HG2	1:10:A:GLY:H	3	0.1

10 Dihedral-angle violation analysis

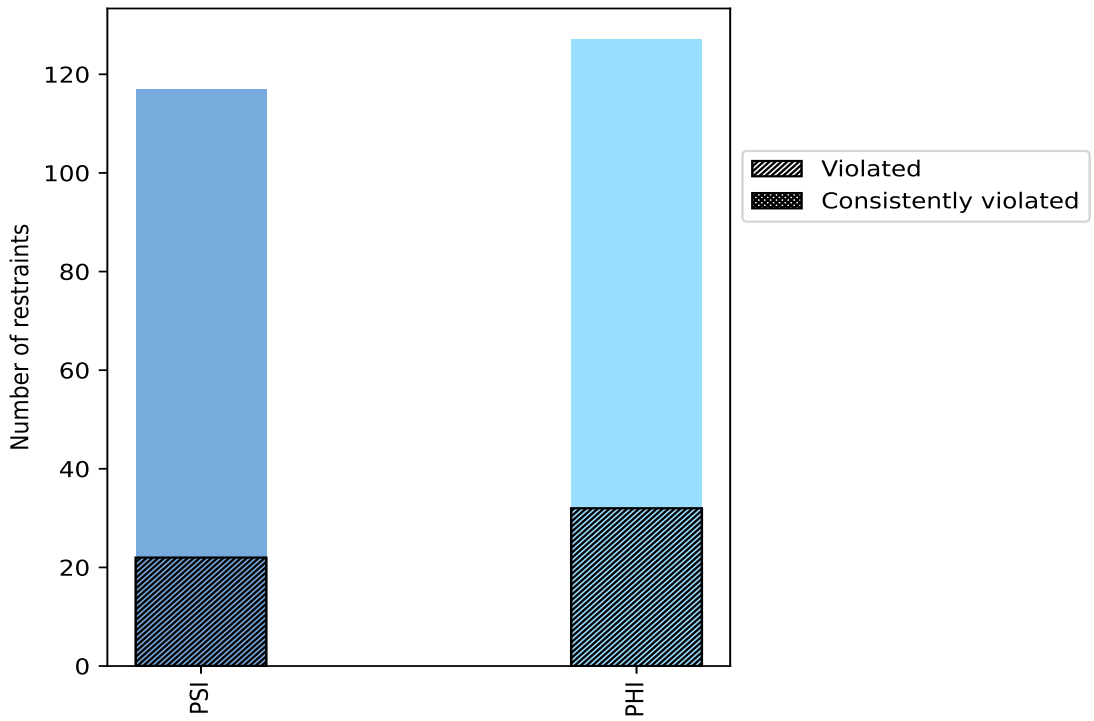
10.1 Summary of dihedral-angle violations

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

Angle type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
PSI	117	48.0	22	18.8	9.0	0	0.0	0.0
PHI	127	52.0	32	25.2	13.1	0	0.0	0.0
Total	244	100.0	54	22.1	22.1	0	0.0	0.0

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

10.1.1 Bar chart : Distribution of dihedral-angles and violations



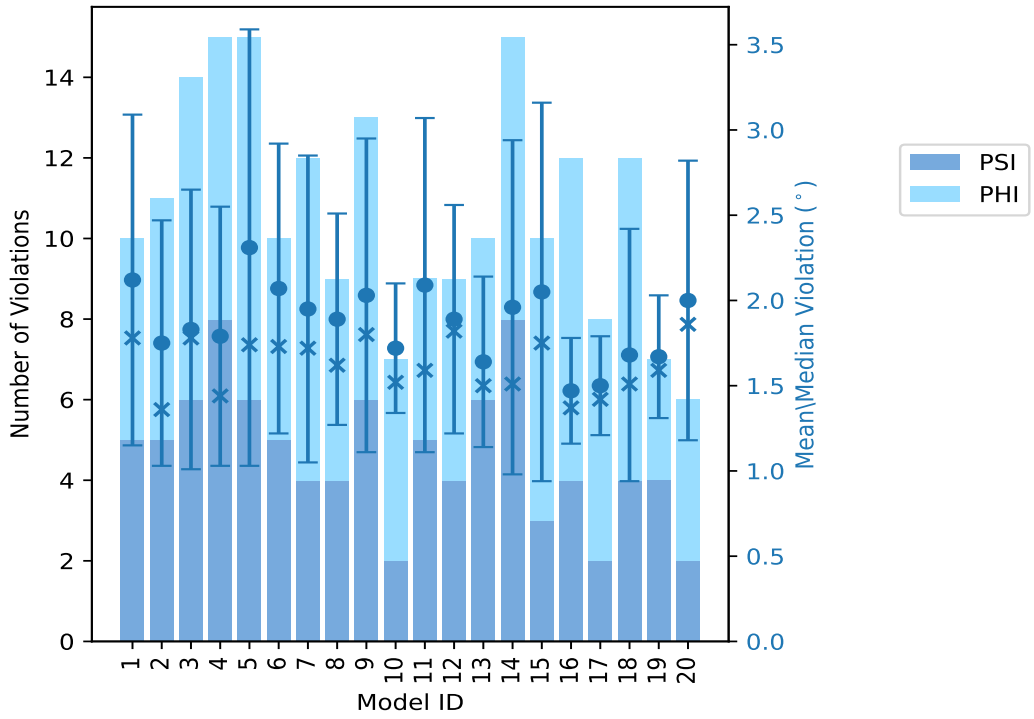
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	PHI	Total				
1	5	5	10	2.12	4.52	0.97	1.78
2	5	6	11	1.75	3.45	0.72	1.36
3	6	8	14	1.83	4.56	0.82	1.78
4	8	7	15	1.79	3.34	0.76	1.44
5	6	9	15	2.31	5.69	1.28	1.74
6	5	5	10	2.07	4.2	0.85	1.73
7	4	8	12	1.95	4.06	0.9	1.72
8	4	5	9	1.89	3.18	0.62	1.62
9	6	7	13	2.03	4.38	0.92	1.8
10	2	5	7	1.72	2.3	0.38	1.52
11	5	4	9	2.09	3.26	0.98	1.59
12	4	5	9	1.89	3.44	0.67	1.82
13	6	4	10	1.64	2.44	0.5	1.5
14	8	7	15	1.96	4.09	0.98	1.51
15	3	7	10	2.05	4.89	1.11	1.75
16	4	8	12	1.47	2.1	0.31	1.37
17	2	6	8	1.5	2.2	0.29	1.42
18	4	8	12	1.68	3.69	0.74	1.51
19	4	3	7	1.67	2.3	0.36	1.59
20	2	4	6	2.0	3.59	0.82	1.86

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	
PSI	PHI	Total	Count[1]	%
12	11	23	1	5.0
1	7	8	2	10.0
0	5	5	3	15.0
3	2	5	4	20.0
1	1	2	5	25.0
0	1	1	6	30.0
1	0	1	7	35.0
0	2	2	8	40.0
0	0	0	9	45.0
1	0	1	10	50.0
0	0	0	11	55.0

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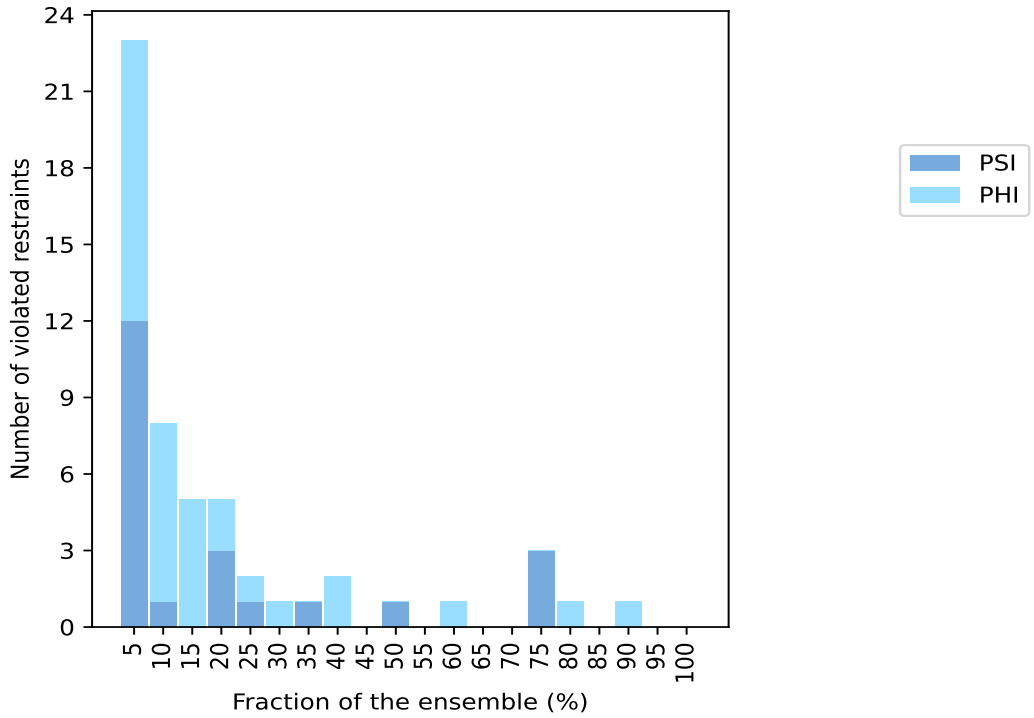
Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count[1]	%
0	1	1	12	60.0
0	0	0	13	65.0
0	0	0	14	70.0
3	0	3	15	75.0
0	1	1	16	80.0
0	0	0	17	85.0
0	1	1	18	90.0
0	0	0	19	95.0
0	0	0	20	100.0

[1] Number of models with violations

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

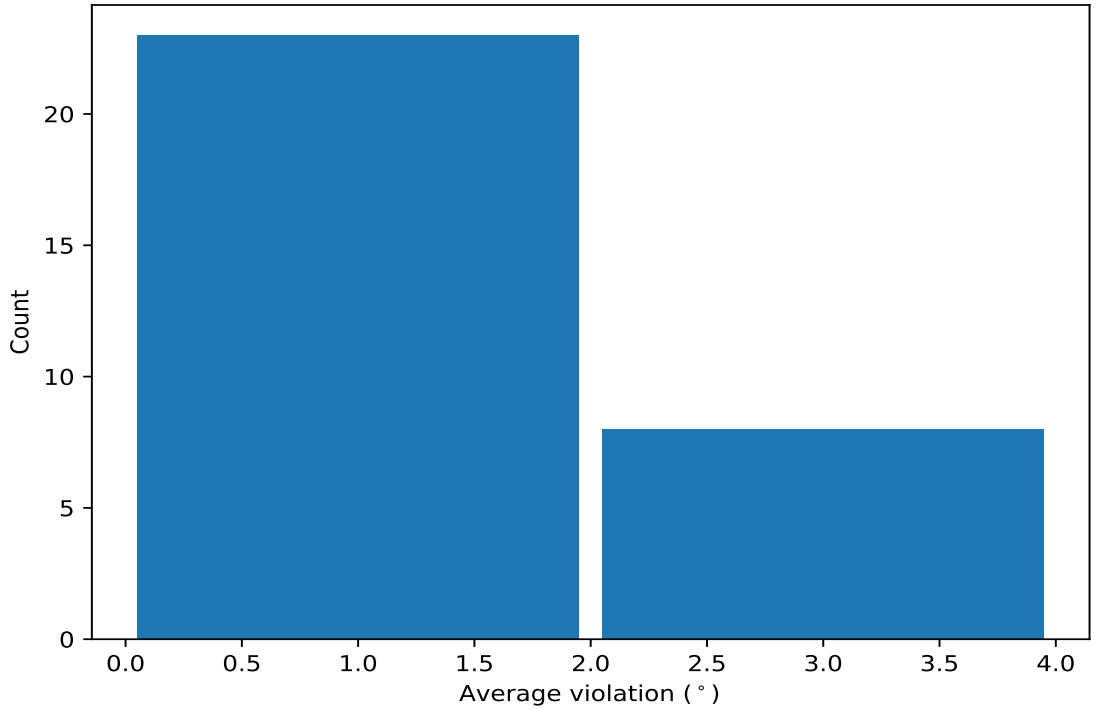


10.4 Most violated dihedral-angle restraints in the ensemble

10.4.1 Histogram : Distribution of mean dihedral-angle violations

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

in the ensemble



10.4.2 Table: Most violated dihedral-angle restraints

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,227)	1:151:A:PHE:C	1:152:A:THR:N	1:152:A:THR:CA	1:152:A:THR:C	18	2.09	0.6	1.92
(1,91)	1:62:A:VAL:C	1:63:A:LYS:N	1:63:A:LYS:CA	1:63:A:LYS:C	16	1.71	0.39	1.72
(1,107)	1:77:A:LYS:N	1:77:A:LYS:CA	1:77:A:LYS:C	1:78:A:ILE:N	15	2.55	1.32	1.99
(1,228)	1:152:A:THR:N	1:152:A:THR:CA	1:152:A:THR:C	1:153:A:ASP:N	15	2.49	1.04	2.13
(1,211)	1:139:A:PHE:N	1:139:A:PHE:CA	1:139:A:PHE:C	1:140:A:ALA:N	15	1.82	0.5	1.87
(1,99)	1:68:A:ARG:C	1:69:A:ARG:N	1:69:A:ARG:CA	1:69:A:ARG:C	12	3.36	1.11	3.39
(1,42)	1:30:A:ASN:N	1:30:A:ASN:CA	1:30:A:ASN:C	1:31:A:ALA:N	10	1.77	0.59	1.82
(1,220)	1:144:A:GLY:C	1:145:A:GLU:N	1:145:A:GLU:CA	1:145:A:GLU:C	8	1.68	0.44	1.86
(1,97)	1:66:A:GLN:C	1:67:A:SER:N	1:67:A:SER:CA	1:67:A:SER:C	8	1.64	0.43	1.54
(1,213)	1:140:A:ALA:N	1:140:A:ALA:CA	1:140:A:ALA:C	1:141:A:LEU:N	7	1.44	0.23	1.44
(1,235)	1:156:A:ILE:C	1:157:A:HIS:N	1:157:A:HIS:CA	1:157:A:HIS:C	6	1.85	0.4	1.8
(1,61)	1:42:A:SER:N	1:42:A:SER:CA	1:42:A:SER:C	1:43:A:SER:N	5	2.13	0.7	1.88
(1,110)	1:79:A:THR:C	1:80:A:ARG:N	1:80:A:ARG:CA	1:80:A:ARG:C	5	1.37	0.15	1.29
(1,201)	1:134:A:PHE:N	1:134:A:PHE:CA	1:134:A:PHE:C	1:135:A:GLU:N	4	2.42	1.03	2.46
(1,205)	1:136:A:ASP:N	1:136:A:ASP:CA	1:136:A:ASP:C	1:137:A:ALA:N	4	2.03	0.74	1.73
(1,62)	1:42:A:SER:C	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	4	1.66	0.62	1.46
(1,204)	1:135:A:GLU:C	1:136:A:ASP:N	1:136:A:ASP:CA	1:136:A:ASP:C	4	1.35	0.24	1.33
(1,96)	1:65:A:SER:N	1:65:A:SER:CA	1:65:A:SER:C	1:66:A:GLN:N	4	1.28	0.21	1.23
(1,51)	1:34:A:TRP:C	1:35:A:GLU:N	1:35:A:GLU:CA	1:35:A:GLU:C	3	1.53	0.53	1.35
(1,66)	1:46:A:LYS:C	1:47:A:ASN:N	1:47:A:ASN:CA	1:47:A:ASN:C	3	1.53	0.38	1.47

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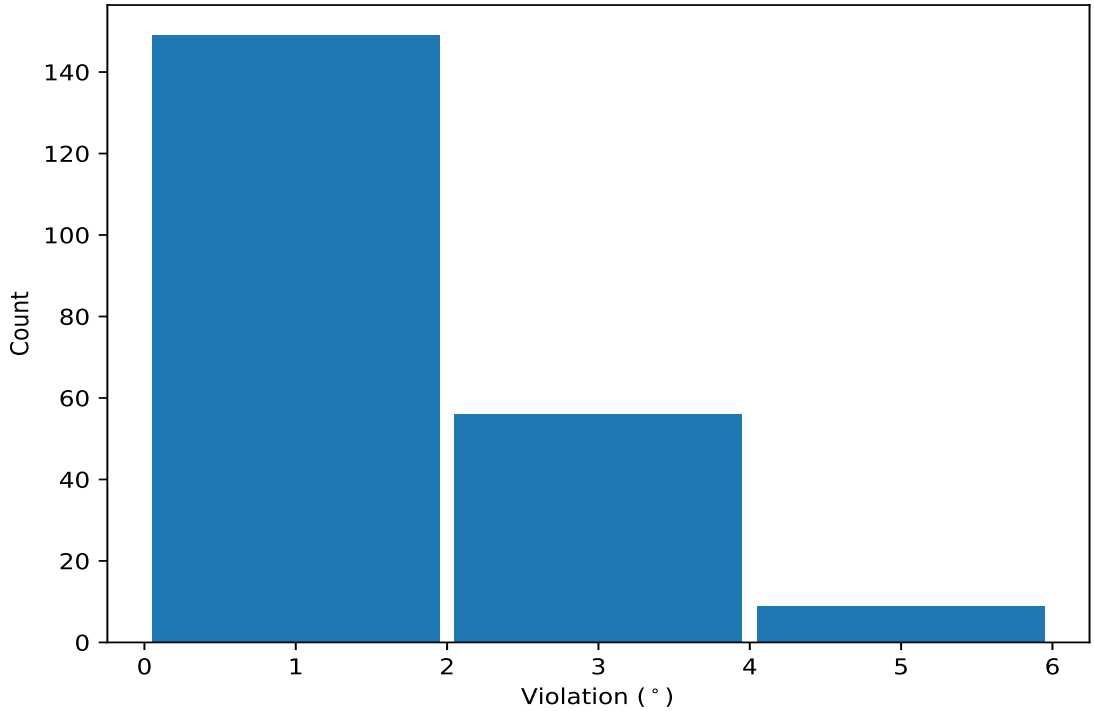
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,168)	1:112:A:ASP:C	1:113:A:CYS:N	1:113:A:CYS:CA	1:113:A:CYS:C	3	1.31	0.14	1.39
(1,210)	1:138:A:SER:C	1:139:A:PHE:N	1:139:A:PHE:CA	1:139:A:PHE:C	3	1.3	0.19	1.34
(1,10)	1:9:A:PRO:C	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	3	1.26	0.12	1.35
(1,108)	1:77:A:LYS:C	1:78:A:ILE:N	1:78:A:ILE:CA	1:78:A:ILE:C	2	2.04	0.78	2.04
(1,1)	1:2:A:ALA:C	1:3:A:ASP:N	1:3:A:ASP:CA	1:3:A:ASP:C	2	1.93	0.13	1.93
(1,69)	1:49:A:GLN:C	1:50:A:GLY:N	1:50:A:GLY:CA	1:50:A:GLY:C	2	1.56	0.3	1.56
(1,45)	1:31:A:ALA:C	1:32:A:SER:N	1:32:A:SER:CA	1:32:A:SER:C	2	1.54	0.17	1.54
(1,35)	1:26:A:ASN:C	1:27:A:HIS:N	1:27:A:HIS:CA	1:27:A:HIS:C	2	1.42	0.08	1.42
(1,5)	1:4:A:GLU:C	1:5:A:GLU:N	1:5:A:GLU:CA	1:5:A:GLU:C	2	1.42	0.12	1.42
(1,64)	1:44:A:GLY:C	1:45:A:GLY:N	1:45:A:GLY:CA	1:45:A:GLY:C	2	1.22	0.11	1.22
(1,167)	1:110:A:PHE:N	1:110:A:PHE:CA	1:110:A:PHE:C	1:111:A:SER:N	2	1.19	0.0	1.19

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

10.5 All violated dihedral-angle restraints

10.5.1 Histogram : Distribution of violations

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



10.5.2 Table: All violated dihedral-angle restraints

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

restraint.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,107)	1:77:A:LYS:N	1:77:A:LYS:CA	1:77:A:LYS:C	1:78:A:ILE:N	5	5.69
(1,107)	1:77:A:LYS:N	1:77:A:LYS:CA	1:77:A:LYS:C	1:78:A:ILE:N	15	4.89
(1,99)	1:68:A:ARG:C	1:69:A:ARG:N	1:69:A:ARG:CA	1:69:A:ARG:C	3	4.56
(1,228)	1:152:A:THR:N	1:152:A:THR:CA	1:152:A:THR:C	1:153:A:ASP:N	1	4.52
(1,99)	1:68:A:ARG:C	1:69:A:ARG:N	1:69:A:ARG:CA	1:69:A:ARG:C	5	4.5
(1,99)	1:68:A:ARG:C	1:69:A:ARG:N	1:69:A:ARG:CA	1:69:A:ARG:C	9	4.38
(1,99)	1:68:A:ARG:C	1:69:A:ARG:N	1:69:A:ARG:CA	1:69:A:ARG:C	6	4.2
(1,99)	1:68:A:ARG:C	1:69:A:ARG:N	1:69:A:ARG:CA	1:69:A:ARG:C	14	4.09
(1,228)	1:152:A:THR:N	1:152:A:THR:CA	1:152:A:THR:C	1:153:A:ASP:N	7	4.06
(1,228)	1:152:A:THR:N	1:152:A:THR:CA	1:152:A:THR:C	1:153:A:ASP:N	14	3.97
(1,107)	1:77:A:LYS:N	1:77:A:LYS:CA	1:77:A:LYS:C	1:78:A:ILE:N	18	3.69
(1,201)	1:134:A:PHE:N	1:134:A:PHE:CA	1:134:A:PHE:C	1:135:A:GLU:N	20	3.59
(1,107)	1:77:A:LYS:N	1:77:A:LYS:CA	1:77:A:LYS:C	1:78:A:ILE:N	2	3.45
(1,99)	1:68:A:ARG:C	1:69:A:ARG:N	1:69:A:ARG:CA	1:69:A:ARG:C	12	3.44
(1,99)	1:68:A:ARG:C	1:69:A:ARG:N	1:69:A:ARG:CA	1:69:A:ARG:C	4	3.34
(1,228)	1:152:A:THR:N	1:152:A:THR:CA	1:152:A:THR:C	1:153:A:ASP:N	4	3.26
(1,201)	1:134:A:PHE:N	1:134:A:PHE:CA	1:134:A:PHE:C	1:135:A:GLU:N	11	3.26
(1,205)	1:136:A:ASP:N	1:136:A:ASP:CA	1:136:A:ASP:C	1:137:A:ALA:N	11	3.24
(1,227)	1:151:A:PHE:C	1:152:A:THR:N	1:152:A:THR:CA	1:152:A:THR:C	5	3.23
(1,99)	1:68:A:ARG:C	1:69:A:ARG:N	1:69:A:ARG:CA	1:69:A:ARG:C	7	3.23
(1,99)	1:68:A:ARG:C	1:69:A:ARG:N	1:69:A:ARG:CA	1:69:A:ARG:C	8	3.18
(1,107)	1:77:A:LYS:N	1:77:A:LYS:CA	1:77:A:LYS:C	1:78:A:ILE:N	11	3.16
(1,61)	1:42:A:SER:N	1:42:A:SER:CA	1:42:A:SER:C	1:43:A:SER:N	9	3.14
(1,99)	1:68:A:ARG:C	1:69:A:ARG:N	1:69:A:ARG:CA	1:69:A:ARG:C	1	3.07
(1,227)	1:151:A:PHE:C	1:152:A:THR:N	1:152:A:THR:CA	1:152:A:THR:C	11	3.01
(1,228)	1:152:A:THR:N	1:152:A:THR:CA	1:152:A:THR:C	1:153:A:ASP:N	5	3.0
(1,108)	1:77:A:LYS:C	1:78:A:ILE:N	1:78:A:ILE:CA	1:78:A:ILE:C	15	2.82
(1,228)	1:152:A:THR:N	1:152:A:THR:CA	1:152:A:THR:C	1:153:A:ASP:N	8	2.8
(1,227)	1:151:A:PHE:C	1:152:A:THR:N	1:152:A:THR:CA	1:152:A:THR:C	2	2.79
(1,227)	1:151:A:PHE:C	1:152:A:THR:N	1:152:A:THR:CA	1:152:A:THR:C	9	2.75
(1,61)	1:42:A:SER:N	1:42:A:SER:CA	1:42:A:SER:C	1:43:A:SER:N	14	2.7
(1,62)	1:42:A:SER:C	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	14	2.69
(1,227)	1:151:A:PHE:C	1:152:A:THR:N	1:152:A:THR:CA	1:152:A:THR:C	4	2.68
(1,42)	1:30:A:ASN:N	1:30:A:ASN:CA	1:30:A:ASN:C	1:31:A:ALA:N	15	2.68
(1,97)	1:66:A:GLN:C	1:67:A:SER:N	1:67:A:SER:CA	1:67:A:SER:C	4	2.64
(1,87)	1:60:A:LEU:N	1:60:A:LEU:CA	1:60:A:LEU:C	1:61:A:LEU:N	6	2.57
(1,91)	1:62:A:VAL:C	1:63:A:LYS:N	1:63:A:LYS:CA	1:63:A:LYS:C	14	2.55
(1,211)	1:139:A:PHE:N	1:139:A:PHE:CA	1:139:A:PHE:C	1:140:A:ALA:N	1	2.54
(1,211)	1:139:A:PHE:N	1:139:A:PHE:CA	1:139:A:PHE:C	1:140:A:ALA:N	5	2.52
(1,228)	1:152:A:THR:N	1:152:A:THR:CA	1:152:A:THR:C	1:153:A:ASP:N	9	2.5
(1,227)	1:151:A:PHE:C	1:152:A:THR:N	1:152:A:THR:CA	1:152:A:THR:C	7	2.47
(1,235)	1:156:A:ILE:C	1:157:A:HIS:N	1:157:A:HIS:CA	1:157:A:HIS:C	6	2.44
(1,211)	1:139:A:PHE:N	1:139:A:PHE:CA	1:139:A:PHE:C	1:140:A:ALA:N	13	2.44
(1,107)	1:77:A:LYS:N	1:77:A:LYS:CA	1:77:A:LYS:C	1:78:A:ILE:N	7	2.42
(1,91)	1:62:A:VAL:C	1:63:A:LYS:N	1:63:A:LYS:CA	1:63:A:LYS:C	5	2.41
(1,42)	1:30:A:ASN:N	1:30:A:ASN:CA	1:30:A:ASN:C	1:31:A:ALA:N	6	2.41
(1,42)	1:30:A:ASN:N	1:30:A:ASN:CA	1:30:A:ASN:C	1:31:A:ALA:N	12	2.34
(1,227)	1:151:A:PHE:C	1:152:A:THR:N	1:152:A:THR:CA	1:152:A:THR:C	19	2.3
(1,107)	1:77:A:LYS:N	1:77:A:LYS:CA	1:77:A:LYS:C	1:78:A:ILE:N	10	2.3
(1,227)	1:151:A:PHE:C	1:152:A:THR:N	1:152:A:THR:CA	1:152:A:THR:C	20	2.25
(1,51)	1:34:A:TRP:C	1:35:A:GLU:N	1:35:A:GLU:CA	1:35:A:GLU:C	18	2.25

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,235)	1:156:A:ILE:C	1:157:A:HIS:N	1:157:A:HIS:CA	1:157:A:HIS:C	13	2.22
(1,211)	1:139:A:PHE:N	1:139:A:PHE:CA	1:139:A:PHE:C	1:140:A:ALA:N	17	2.2
(1,228)	1:152:A:THR:N	1:152:A:THR:CA	1:152:A:THR:C	1:153:A:ASP:N	13	2.13
(1,220)	1:144:A:GLY:C	1:145:A:GLU:N	1:145:A:GLU:CA	1:145:A:GLU:C	9	2.13
(1,220)	1:144:A:GLY:C	1:145:A:GLU:N	1:145:A:GLU:CA	1:145:A:GLU:C	3	2.12
(1,42)	1:30:A:ASN:N	1:30:A:ASN:CA	1:30:A:ASN:C	1:31:A:ALA:N	16	2.1
(1,211)	1:139:A:PHE:N	1:139:A:PHE:CA	1:139:A:PHE:C	1:140:A:ALA:N	2	2.09
(1,42)	1:30:A:ASN:N	1:30:A:ASN:CA	1:30:A:ASN:C	1:31:A:ALA:N	5	2.09
(1,220)	1:144:A:GLY:C	1:145:A:GLU:N	1:145:A:GLU:CA	1:145:A:GLU:C	13	2.06
(1,91)	1:62:A:VAL:C	1:63:A:LYS:N	1:63:A:LYS:CA	1:63:A:LYS:C	18	2.06
(1,1)	1:2:A:ALA:C	1:3:A:ASP:N	1:3:A:ASP:CA	1:3:A:ASP:C	10	2.06
(1,227)	1:151:A:PHE:C	1:152:A:THR:N	1:152:A:THR:CA	1:152:A:THR:C	10	2.03
(1,66)	1:46:A:LYS:C	1:47:A:ASN:N	1:47:A:ASN:CA	1:47:A:ASN:C	18	2.02
(1,205)	1:136:A:ASP:N	1:136:A:ASP:CA	1:136:A:ASP:C	1:137:A:ALA:N	20	2.01
(1,107)	1:77:A:LYS:N	1:77:A:LYS:CA	1:77:A:LYS:C	1:78:A:ILE:N	19	1.99
(1,228)	1:152:A:THR:N	1:152:A:THR:CA	1:152:A:THR:C	1:153:A:ASP:N	12	1.98
(1,220)	1:144:A:GLY:C	1:145:A:GLU:N	1:145:A:GLU:CA	1:145:A:GLU:C	16	1.96
(1,211)	1:139:A:PHE:N	1:139:A:PHE:CA	1:139:A:PHE:C	1:140:A:ALA:N	3	1.95
(1,107)	1:77:A:LYS:N	1:77:A:LYS:CA	1:77:A:LYS:C	1:78:A:ILE:N	3	1.95
(1,91)	1:62:A:VAL:C	1:63:A:LYS:N	1:63:A:LYS:CA	1:63:A:LYS:C	1	1.94
(1,211)	1:139:A:PHE:N	1:139:A:PHE:CA	1:139:A:PHE:C	1:140:A:ALA:N	7	1.91
(1,97)	1:66:A:GLN:C	1:67:A:SER:N	1:67:A:SER:CA	1:67:A:SER:C	8	1.88
(1,61)	1:42:A:SER:N	1:42:A:SER:CA	1:42:A:SER:C	1:43:A:SER:N	3	1.88
(1,211)	1:139:A:PHE:N	1:139:A:PHE:CA	1:139:A:PHE:C	1:140:A:ALA:N	4	1.87
(1,228)	1:152:A:THR:N	1:152:A:THR:CA	1:152:A:THR:C	1:153:A:ASP:N	3	1.86
(1,211)	1:139:A:PHE:N	1:139:A:PHE:CA	1:139:A:PHE:C	1:140:A:ALA:N	12	1.86
(1,69)	1:49:A:GLN:C	1:50:A:GLY:N	1:50:A:GLY:CA	1:50:A:GLY:C	9	1.85
(1,211)	1:139:A:PHE:N	1:139:A:PHE:CA	1:139:A:PHE:C	1:140:A:ALA:N	15	1.84
(1,91)	1:62:A:VAL:C	1:63:A:LYS:N	1:63:A:LYS:CA	1:63:A:LYS:C	6	1.84
(1,235)	1:156:A:ILE:C	1:157:A:HIS:N	1:157:A:HIS:CA	1:157:A:HIS:C	12	1.82
(1,91)	1:62:A:VAL:C	1:63:A:LYS:N	1:63:A:LYS:CA	1:63:A:LYS:C	7	1.82
(1,91)	1:62:A:VAL:C	1:63:A:LYS:N	1:63:A:LYS:CA	1:63:A:LYS:C	15	1.82
(1,227)	1:151:A:PHE:C	1:152:A:THR:N	1:152:A:THR:CA	1:152:A:THR:C	1	1.81
(1,216)	1:141:A:LEU:C	1:142:A:ARG:N	1:142:A:ARG:CA	1:142:A:ARG:C	18	1.8
(1,91)	1:62:A:VAL:C	1:63:A:LYS:N	1:63:A:LYS:CA	1:63:A:LYS:C	9	1.8
(1,1)	1:2:A:ALA:C	1:3:A:ASP:N	1:3:A:ASP:CA	1:3:A:ASP:C	19	1.8
(1,213)	1:140:A:ALA:N	1:140:A:ALA:CA	1:140:A:ALA:C	1:141:A:LEU:N	3	1.79
(1,235)	1:156:A:ILE:C	1:157:A:HIS:N	1:157:A:HIS:CA	1:157:A:HIS:C	8	1.78
(1,192)	1:128:A:GLY:C	1:129:A:GLN:N	1:129:A:GLN:CA	1:129:A:GLN:C	3	1.76
(1,220)	1:144:A:GLY:C	1:145:A:GLU:N	1:145:A:GLU:CA	1:145:A:GLU:C	1	1.75
(1,148)	1:100:A:GLU:C	1:101:A:GLU:N	1:101:A:GLU:CA	1:101:A:GLU:C	2	1.75
(1,61)	1:42:A:SER:N	1:42:A:SER:CA	1:42:A:SER:C	1:43:A:SER:N	5	1.74
(1,45)	1:31:A:ALA:C	1:32:A:SER:N	1:32:A:SER:CA	1:32:A:SER:C	2	1.71
(1,227)	1:151:A:PHE:C	1:152:A:THR:N	1:152:A:THR:CA	1:152:A:THR:C	12	1.7
(1,204)	1:135:A:GLU:C	1:136:A:ASP:N	1:136:A:ASP:CA	1:136:A:ASP:C	20	1.7
(1,200)	1:133:A:PRO:C	1:134:A:PHE:N	1:134:A:PHE:CA	1:134:A:PHE:C	12	1.7
(1,227)	1:151:A:PHE:C	1:152:A:THR:N	1:152:A:THR:CA	1:152:A:THR:C	15	1.68
(1,227)	1:151:A:PHE:C	1:152:A:THR:N	1:152:A:THR:CA	1:152:A:THR:C	17	1.67
(1,235)	1:156:A:ILE:C	1:157:A:HIS:N	1:157:A:HIS:CA	1:157:A:HIS:C	9	1.65
(1,201)	1:134:A:PHE:N	1:134:A:PHE:CA	1:134:A:PHE:C	1:135:A:GLU:N	16	1.65
(1,91)	1:62:A:VAL:C	1:63:A:LYS:N	1:63:A:LYS:CA	1:63:A:LYS:C	16	1.65

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,107)	1:77:A:LYS:N	1:77:A:LYS:CA	1:77:A:LYS:C	1:78:A:ILE:N	1	1.64
(1,107)	1:77:A:LYS:N	1:77:A:LYS:CA	1:77:A:LYS:C	1:78:A:ILE:N	14	1.64
(1,228)	1:152:A:THR:N	1:152:A:THR:CA	1:152:A:THR:C	1:153:A:ASP:N	6	1.62
(1,227)	1:151:A:PHE:C	1:152:A:THR:N	1:152:A:THR:CA	1:152:A:THR:C	14	1.62
(1,213)	1:140:A:ALA:N	1:140:A:ALA:CA	1:140:A:ALA:C	1:141:A:LEU:N	8	1.62
(1,97)	1:66:A:GLN:C	1:67:A:SER:N	1:67:A:SER:CA	1:67:A:SER:C	7	1.61
(1,96)	1:65:A:SER:N	1:65:A:SER:CA	1:65:A:SER:C	1:66:A:GLN:N	6	1.61
(1,213)	1:140:A:ALA:N	1:140:A:ALA:CA	1:140:A:ALA:C	1:141:A:LEU:N	1	1.6
(1,228)	1:152:A:THR:N	1:152:A:THR:CA	1:152:A:THR:C	1:153:A:ASP:N	11	1.59
(1,110)	1:79:A:THR:C	1:80:A:ARG:N	1:80:A:ARG:CA	1:80:A:ARG:C	13	1.59
(1,58)	1:40:A:ASN:N	1:40:A:ASN:CA	1:40:A:ASN:C	1:41:A:SER:N	19	1.59
(1,97)	1:66:A:GLN:C	1:67:A:SER:N	1:67:A:SER:CA	1:67:A:SER:C	18	1.56
(1,91)	1:62:A:VAL:C	1:63:A:LYS:N	1:63:A:LYS:CA	1:63:A:LYS:C	8	1.55
(1,227)	1:151:A:PHE:C	1:152:A:THR:N	1:152:A:THR:CA	1:152:A:THR:C	8	1.54
(1,42)	1:30:A:ASN:N	1:30:A:ASN:CA	1:30:A:ASN:C	1:31:A:ALA:N	4	1.54
(1,5)	1:4:A:GLU:C	1:5:A:GLU:N	1:5:A:GLU:CA	1:5:A:GLU:C	16	1.54
(1,211)	1:139:A:PHE:N	1:139:A:PHE:CA	1:139:A:PHE:C	1:140:A:ALA:N	10	1.52
(1,210)	1:138:A:SER:C	1:139:A:PHE:N	1:139:A:PHE:CA	1:139:A:PHE:C	10	1.51
(1,97)	1:66:A:GLN:C	1:67:A:SER:N	1:67:A:SER:CA	1:67:A:SER:C	14	1.51
(1,35)	1:26:A:ASN:C	1:27:A:HIS:N	1:27:A:HIS:CA	1:27:A:HIS:C	10	1.51
(1,110)	1:79:A:THR:C	1:80:A:ARG:N	1:80:A:ARG:CA	1:80:A:ARG:C	5	1.5
(1,62)	1:42:A:SER:C	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	9	1.5
(1,107)	1:77:A:LYS:N	1:77:A:LYS:CA	1:77:A:LYS:C	1:78:A:ILE:N	4	1.49
(1,66)	1:46:A:LYS:C	1:47:A:ASN:N	1:47:A:ASN:CA	1:47:A:ASN:C	17	1.47
(1,227)	1:151:A:PHE:C	1:152:A:THR:N	1:152:A:THR:CA	1:152:A:THR:C	18	1.46
(1,205)	1:136:A:ASP:N	1:136:A:ASP:CA	1:136:A:ASP:C	1:137:A:ALA:N	19	1.45
(1,213)	1:140:A:ALA:N	1:140:A:ALA:CA	1:140:A:ALA:C	1:141:A:LEU:N	4	1.44
(1,107)	1:77:A:LYS:N	1:77:A:LYS:CA	1:77:A:LYS:C	1:78:A:ILE:N	9	1.44
(1,91)	1:62:A:VAL:C	1:63:A:LYS:N	1:63:A:LYS:CA	1:63:A:LYS:C	17	1.44
(1,97)	1:66:A:GLN:C	1:67:A:SER:N	1:67:A:SER:CA	1:67:A:SER:C	5	1.43
(1,91)	1:62:A:VAL:C	1:63:A:LYS:N	1:63:A:LYS:CA	1:63:A:LYS:C	20	1.43
(1,168)	1:112:A:ASP:C	1:113:A:CYS:N	1:113:A:CYS:CA	1:113:A:CYS:C	3	1.42
(1,107)	1:77:A:LYS:N	1:77:A:LYS:CA	1:77:A:LYS:C	1:78:A:ILE:N	8	1.42
(1,205)	1:136:A:ASP:N	1:136:A:ASP:CA	1:136:A:ASP:C	1:137:A:ALA:N	13	1.41
(1,62)	1:42:A:SER:C	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	5	1.41
(1,204)	1:135:A:GLU:C	1:136:A:ASP:N	1:136:A:ASP:CA	1:136:A:ASP:C	17	1.39
(1,168)	1:112:A:ASP:C	1:113:A:CYS:N	1:113:A:CYS:CA	1:113:A:CYS:C	6	1.39
(1,208)	1:137:A:ALA:C	1:138:A:SER:N	1:138:A:SER:CA	1:138:A:SER:C	5	1.38
(1,45)	1:31:A:ALA:C	1:32:A:SER:N	1:32:A:SER:CA	1:32:A:SER:C	16	1.38
(1,228)	1:152:A:THR:N	1:152:A:THR:CA	1:152:A:THR:C	1:153:A:ASP:N	2	1.36
(1,228)	1:152:A:THR:N	1:152:A:THR:CA	1:152:A:THR:C	1:153:A:ASP:N	16	1.36
(1,227)	1:151:A:PHE:C	1:152:A:THR:N	1:152:A:THR:CA	1:152:A:THR:C	16	1.36
(1,91)	1:62:A:VAL:C	1:63:A:LYS:N	1:63:A:LYS:CA	1:63:A:LYS:C	3	1.36
(1,68)	1:49:A:GLN:N	1:49:A:GLN:CA	1:49:A:GLN:C	1:50:A:GLY:N	14	1.36
(1,97)	1:66:A:GLN:C	1:67:A:SER:N	1:67:A:SER:CA	1:67:A:SER:C	1	1.35
(1,51)	1:34:A:TRP:C	1:35:A:GLU:N	1:35:A:GLU:CA	1:35:A:GLU:C	15	1.35
(1,42)	1:30:A:ASN:N	1:30:A:ASN:CA	1:30:A:ASN:C	1:31:A:ALA:N	7	1.35
(1,10)	1:9:A:PRO:C	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	3	1.35
(1,10)	1:9:A:PRO:C	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	14	1.35
(1,210)	1:138:A:SER:C	1:139:A:PHE:N	1:139:A:PHE:CA	1:139:A:PHE:C	14	1.34
(1,35)	1:26:A:ASN:C	1:27:A:HIS:N	1:27:A:HIS:CA	1:27:A:HIS:C	15	1.34

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,176)	1:117:A:LYS:N	1:117:A:LYS:CA	1:117:A:LYS:C	1:118:A:ALA:N	4	1.33
(1,91)	1:62:A:VAL:C	1:63:A:LYS:N	1:63:A:LYS:CA	1:63:A:LYS:C	4	1.33
(1,86)	1:59:A:HIS:C	1:60:A:LEU:N	1:60:A:LEU:CA	1:60:A:LEU:C	11	1.33
(1,64)	1:44:A:GLY:C	1:45:A:GLY:N	1:45:A:GLY:CA	1:45:A:GLY:C	16	1.33
(1,213)	1:140:A:ALA:N	1:140:A:ALA:CA	1:140:A:ALA:C	1:141:A:LEU:N	5	1.32
(1,220)	1:144:A:GLY:C	1:145:A:GLU:N	1:145:A:GLU:CA	1:145:A:GLU:C	4	1.31
(1,170)	1:114:A:SER:N	1:114:A:SER:CA	1:114:A:SER:C	1:115:A:SER:N	4	1.31
(1,213)	1:140:A:ALA:N	1:140:A:ALA:CA	1:140:A:ALA:C	1:141:A:LEU:N	6	1.3
(1,5)	1:4:A:GLU:C	1:5:A:GLU:N	1:5:A:GLU:CA	1:5:A:GLU:C	2	1.3
(1,110)	1:79:A:THR:C	1:80:A:ARG:N	1:80:A:ARG:CA	1:80:A:ARG:C	6	1.29
(1,228)	1:152:A:THR:N	1:152:A:THR:CA	1:152:A:THR:C	1:153:A:ASP:N	17	1.28
(1,242)	1:160:A:LEU:N	1:160:A:LEU:CA	1:160:A:LEU:C	1:161:A:ARG:N	19	1.27
(1,204)	1:135:A:GLU:C	1:136:A:ASP:N	1:136:A:ASP:CA	1:136:A:ASP:C	2	1.27
(1,126)	1:87:A:GLU:C	1:88:A:LEU:N	1:88:A:LEU:CA	1:88:A:LEU:C	17	1.27
(1,99)	1:68:A:ARG:C	1:69:A:ARG:N	1:69:A:ARG:CA	1:69:A:ARG:C	19	1.27
(1,96)	1:65:A:SER:N	1:65:A:SER:CA	1:65:A:SER:C	1:66:A:GLN:N	8	1.27
(1,211)	1:139:A:PHE:N	1:139:A:PHE:CA	1:139:A:PHE:C	1:140:A:ALA:N	16	1.26
(1,108)	1:77:A:LYS:C	1:78:A:ILE:N	1:78:A:ILE:CA	1:78:A:ILE:C	5	1.26
(1,69)	1:49:A:GLN:C	1:50:A:GLY:N	1:50:A:GLY:CA	1:50:A:GLY:C	17	1.26
(1,110)	1:79:A:THR:C	1:80:A:ARG:N	1:80:A:ARG:CA	1:80:A:ARG:C	2	1.24
(1,227)	1:151:A:PHE:C	1:152:A:THR:N	1:152:A:THR:CA	1:152:A:THR:C	3	1.22
(1,110)	1:79:A:THR:C	1:80:A:ARG:N	1:80:A:ARG:CA	1:80:A:ARG:C	7	1.22
(1,235)	1:156:A:ILE:C	1:157:A:HIS:N	1:157:A:HIS:CA	1:157:A:HIS:C	3	1.21
(1,6)	1:5:A:GLU:N	1:5:A:GLU:CA	1:5:A:GLU:C	1:6:A:LYS:N	2	1.21
(1,96)	1:65:A:SER:N	1:65:A:SER:CA	1:65:A:SER:C	1:66:A:GLN:N	4	1.2
(1,91)	1:62:A:VAL:C	1:63:A:LYS:N	1:63:A:LYS:CA	1:63:A:LYS:C	13	1.2
(1,57)	1:39:A:GLY:C	1:40:A:ASN:N	1:40:A:ASN:CA	1:40:A:ASN:C	7	1.2
(1,167)	1:110:A:PHE:N	1:110:A:PHE:CA	1:110:A:PHE:C	1:111:A:SER:N	3	1.19
(1,167)	1:110:A:PHE:N	1:110:A:PHE:CA	1:110:A:PHE:C	1:111:A:SER:N	14	1.19
(1,211)	1:139:A:PHE:N	1:139:A:PHE:CA	1:139:A:PHE:C	1:140:A:ALA:N	9	1.18
(1,201)	1:134:A:PHE:N	1:134:A:PHE:CA	1:134:A:PHE:C	1:135:A:GLU:N	14	1.18
(1,106)	1:76:A:GLU:C	1:77:A:LYS:N	1:77:A:LYS:CA	1:77:A:LYS:C	5	1.17
(1,61)	1:42:A:SER:N	1:42:A:SER:CA	1:42:A:SER:C	1:43:A:SER:N	13	1.17
(1,220)	1:144:A:GLY:C	1:145:A:GLU:N	1:145:A:GLU:CA	1:145:A:GLU:C	18	1.14
(1,91)	1:62:A:VAL:C	1:63:A:LYS:N	1:63:A:LYS:CA	1:63:A:LYS:C	10	1.14
(1,105)	1:76:A:GLU:N	1:76:A:GLU:CA	1:76:A:GLU:C	1:77:A:LYS:N	13	1.13
(1,168)	1:112:A:ASP:C	1:113:A:CYS:N	1:113:A:CYS:CA	1:113:A:CYS:C	18	1.11
(1,64)	1:44:A:GLY:C	1:45:A:GLY:N	1:45:A:GLY:CA	1:45:A:GLY:C	4	1.11
(1,42)	1:30:A:ASN:N	1:30:A:ASN:CA	1:30:A:ASN:C	1:31:A:ALA:N	14	1.11
(1,97)	1:66:A:GLN:C	1:67:A:SER:N	1:67:A:SER:CA	1:67:A:SER:C	12	1.1
(1,66)	1:46:A:LYS:C	1:47:A:ASN:N	1:47:A:ASN:CA	1:47:A:ASN:C	15	1.1
(1,21)	1:18:A:SER:C	1:19:A:SER:N	1:19:A:SER:CA	1:19:A:SER:C	11	1.09
(1,10)	1:9:A:PRO:C	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	11	1.09
(1,42)	1:30:A:ASN:N	1:30:A:ASN:CA	1:30:A:ASN:C	1:31:A:ALA:N	9	1.08
(1,210)	1:138:A:SER:C	1:139:A:PHE:N	1:139:A:PHE:CA	1:139:A:PHE:C	16	1.06
(1,109)	1:78:A:ILE:N	1:78:A:ILE:CA	1:78:A:ILE:C	1:79:A:THR:N	18	1.05
(1,107)	1:77:A:LYS:N	1:77:A:LYS:CA	1:77:A:LYS:C	1:78:A:ILE:N	13	1.05
(1,62)	1:42:A:SER:C	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	7	1.05
(1,217)	1:142:A:ARG:N	1:142:A:ARG:CA	1:142:A:ARG:C	1:143:A:THR:N	2	1.04
(1,211)	1:139:A:PHE:N	1:139:A:PHE:CA	1:139:A:PHE:C	1:140:A:ALA:N	14	1.04
(1,99)	1:68:A:ARG:C	1:69:A:ARG:N	1:69:A:ARG:CA	1:69:A:ARG:C	16	1.04

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,96)	1:65:A:SER:N	1:65:A:SER:CA	1:65:A:SER:C	1:66:A:GLN:N	12	1.04
(1,213)	1:140:A:ALA:N	1:140:A:ALA:CA	1:140:A:ALA:C	1:141:A:LEU:N	9	1.03
(1,204)	1:135:A:GLU:C	1:136:A:ASP:N	1:136:A:ASP:CA	1:136:A:ASP:C	7	1.03
(1,42)	1:30:A:ASN:N	1:30:A:ASN:CA	1:30:A:ASN:C	1:31:A:ALA:N	18	1.03
(1,223)	1:149:A:PRO:C	1:150:A:VAL:N	1:150:A:VAL:CA	1:150:A:VAL:C	15	1.02
(1,211)	1:139:A:PHE:N	1:139:A:PHE:CA	1:139:A:PHE:C	1:140:A:ALA:N	11	1.02
(1,19)	1:16:A:SER:N	1:16:A:SER:CA	1:16:A:SER:C	1:17:A:ARG:N	18	1.01
(1,220)	1:144:A:GLY:C	1:145:A:GLU:N	1:145:A:GLU:CA	1:145:A:GLU:C	20	1.0
(1,51)	1:34:A:TRP:C	1:35:A:GLU:N	1:35:A:GLU:CA	1:35:A:GLU:C	4	1.0
(1,8)	1:6:A:LYS:N	1:6:A:LYS:CA	1:6:A:LYS:C	1:7:A:LEU:N	1	1.0