Full wwPDB NMR Structure Validation Report (i)

Mar 26, 2026 – 02:25 AM UTC

PDB ID	:	2KZU / pdb_00002kzu
BMRB ID	:	17019
Title	:	DAXX helical bundle (DHB) domain / Rassf1C complex
Authors	:	Escobar-Cabrera, E.; Lau, D.K.W.; Giovinazzi, S.; Ishov, A.M.; McIntosh, L.P.
Deposited on	:	2010-06-25

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

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

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

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

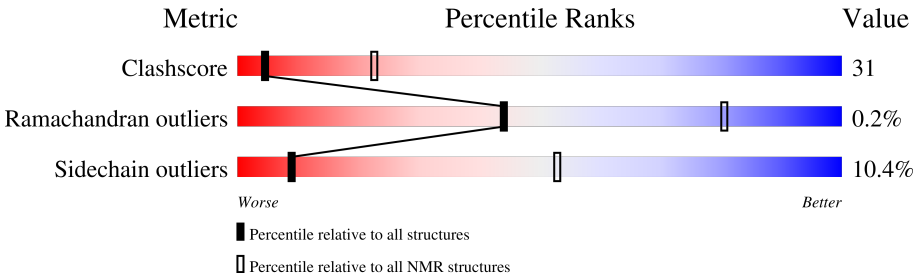
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment is 83%.

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	94	43% 37% 5% 15%
2	B	18	17% 50% 6% 28%

2 Ensemble composition and analysis

This entry contains 25 models. Model 15 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:59-A:138, B:27-B:39 (93)	0.35	15

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

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

The models can be grouped into 5 clusters and 3 single-model clusters were found.

Cluster number	Models
1	2, 9, 15, 18, 20, 24
2	1, 6, 8, 11, 14
3	4, 5, 7, 12, 22
4	13, 17, 23, 25
5	3, 10
Single-model clusters	16; 19; 21

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1836 atoms, of which 917 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Death-associated protein 6.

Mol	Chain	Residues	Atoms						Trace
1	A	94	Total	C	H	N	O	S	0
			1558	489	791	138	134	6	

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	51	GLY	-	expression tag	UNP Q4VX54
A	52	SER	-	expression tag	UNP Q4VX54
A	53	HIS	-	expression tag	UNP Q4VX54
A	54	MET	-	expression tag	UNP Q4VX54

- Molecule 2 is a protein called Ras association (RalGDS/AF-6) domain family 1.

Mol	Chain	Residues	Atoms					Trace
2	B	18	Total	C	H	N	O	0
			278	92	126	24	36	

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	22	GLY	-	expression tag	UNP Q5TZT2
B	39	TRP	-	expression tag	UNP Q5TZT2

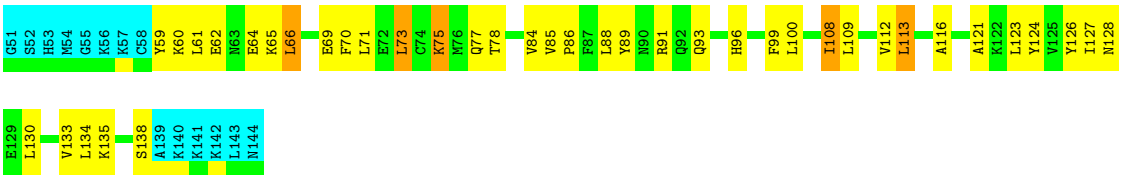
4 Residue-property plots

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: Death-associated protein 6

Chain A:



• Molecule 2: Ras association (RalGDS/AF-6) domain family 1

Chain B:

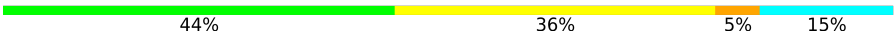
4.2 Scores per residue for each member of the ensemble

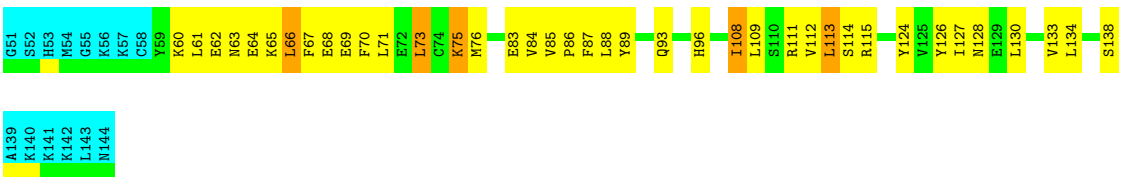
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Death-associated protein 6

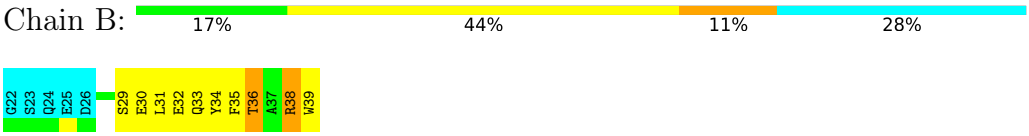
Chain A:





• Molecule 2: Ras association (RalGDS/AF-6) domain family 1

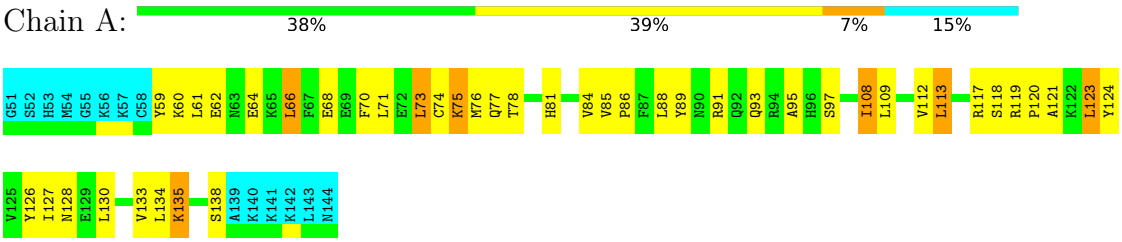
Chain B:



4.2.2 Score per residue for model 2

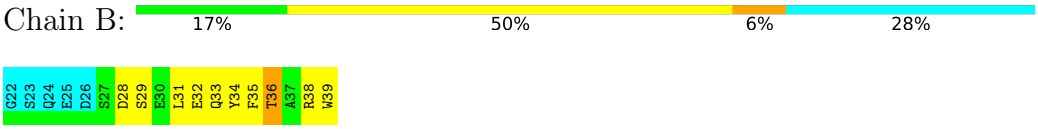
• Molecule 1: Death-associated protein 6

Chain A:



• Molecule 2: Ras association (RalGDS/AF-6) domain family 1

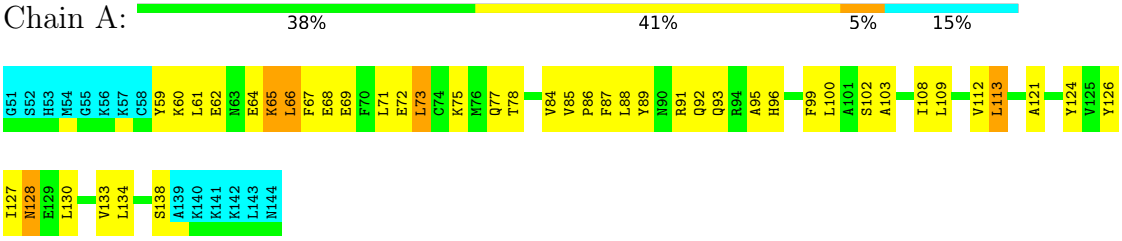
Chain B:



4.2.3 Score per residue for model 3

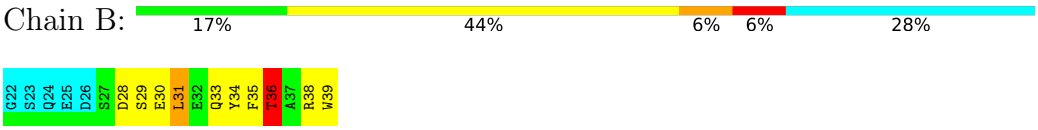
• Molecule 1: Death-associated protein 6

Chain A:



• Molecule 2: Ras association (RalGDS/AF-6) domain family 1

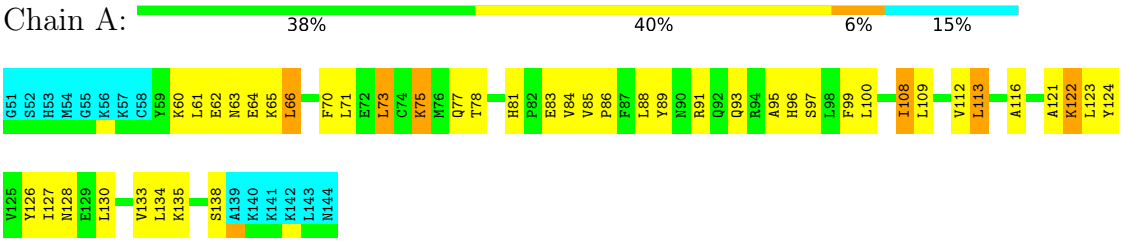
Chain B:



4.2.4 Score per residue for model 4

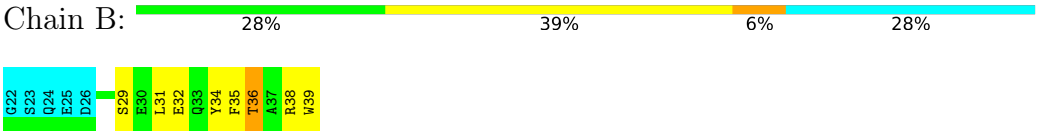
• Molecule 1: Death-associated protein 6

Chain A:



• Molecule 2: Ras association (RalGDS/AF-6) domain family 1

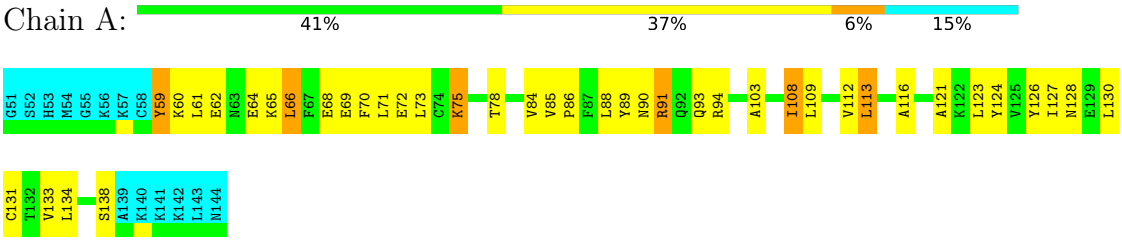
Chain B:



4.2.5 Score per residue for model 5

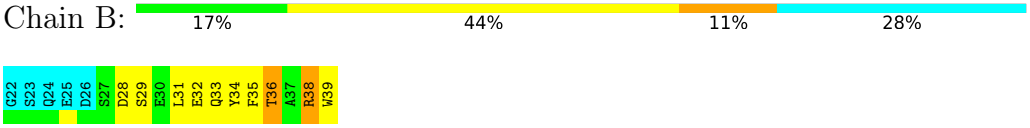
• Molecule 1: Death-associated protein 6

Chain A:



• Molecule 2: Ras association (RalGDS/AF-6) domain family 1

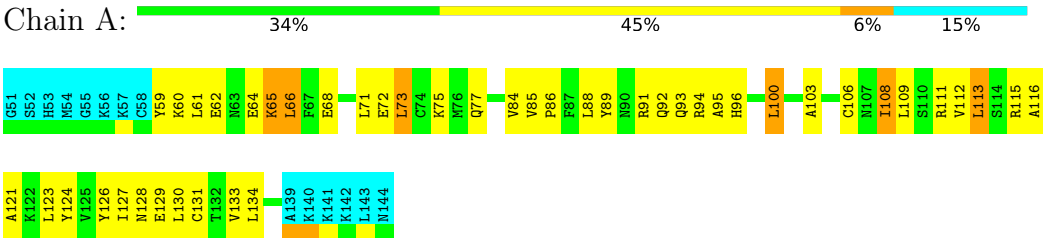
Chain B:



4.2.6 Score per residue for model 6

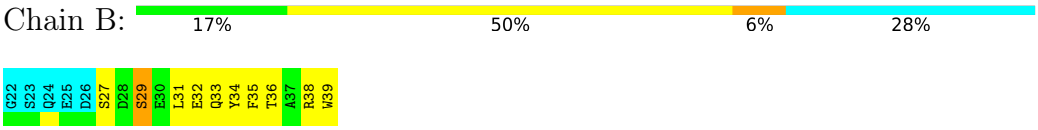
• Molecule 1: Death-associated protein 6

Chain A:



• Molecule 2: Ras association (RalGDS/AF-6) domain family 1

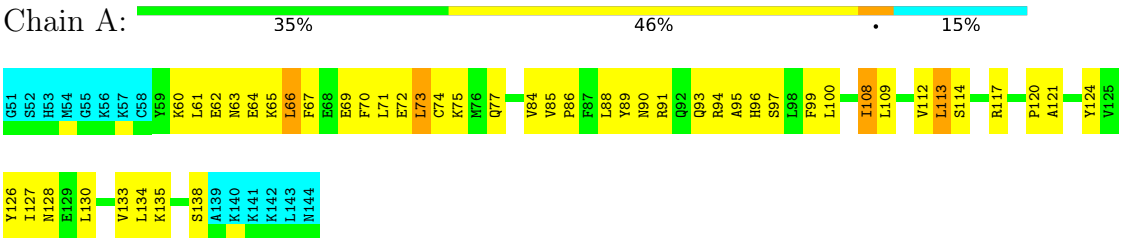
Chain B:



4.2.7 Score per residue for model 7

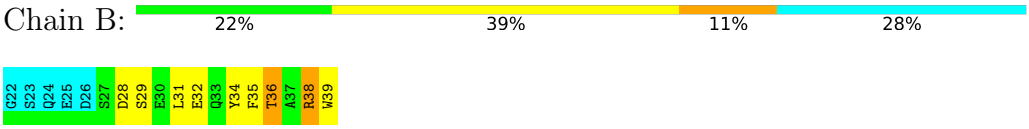
• Molecule 1: Death-associated protein 6

Chain A:



• Molecule 2: Ras association (RalGDS/AF-6) domain family 1

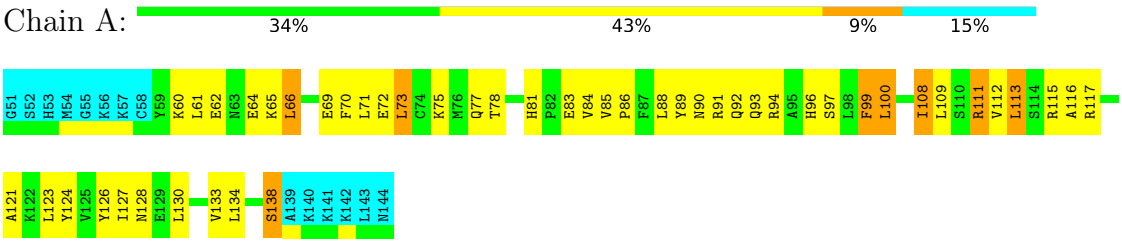
Chain B:



4.2.8 Score per residue for model 8

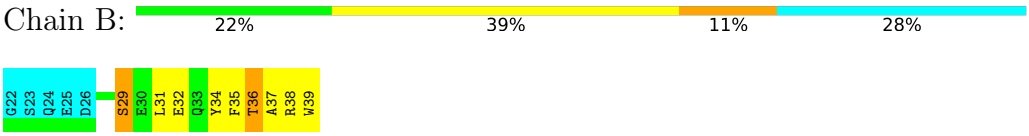
• Molecule 1: Death-associated protein 6

Chain A:



• Molecule 2: Ras association (RalGDS/AF-6) domain family 1

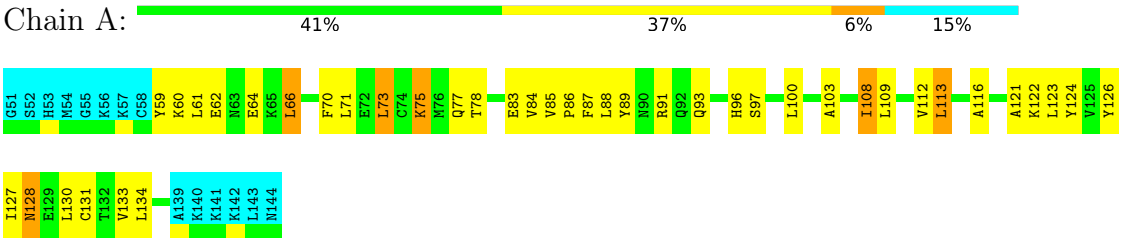
Chain B:



4.2.9 Score per residue for model 9

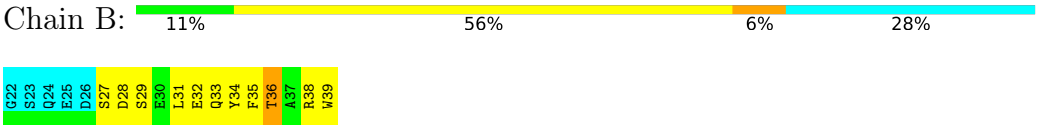
• Molecule 1: Death-associated protein 6

Chain A:



• Molecule 2: Ras association (RalGDS/AF-6) domain family 1

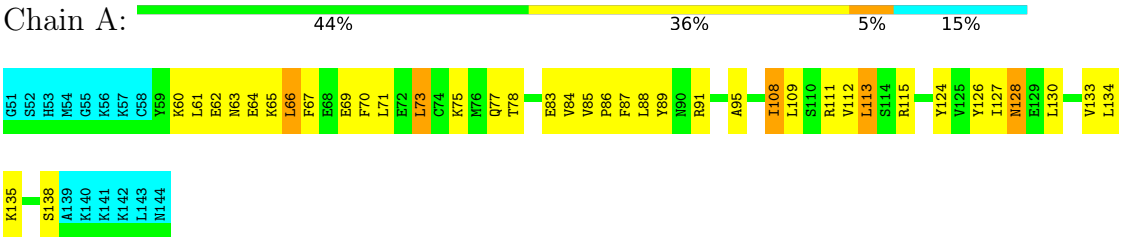
Chain B:



4.2.10 Score per residue for model 10

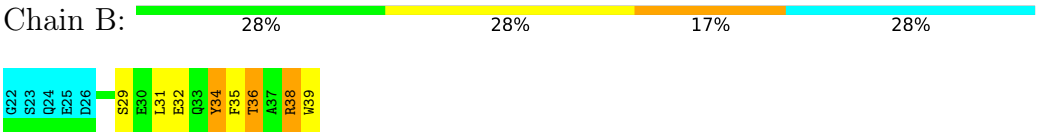
• Molecule 1: Death-associated protein 6

Chain A:



• Molecule 2: Ras association (RalGDS/AF-6) domain family 1

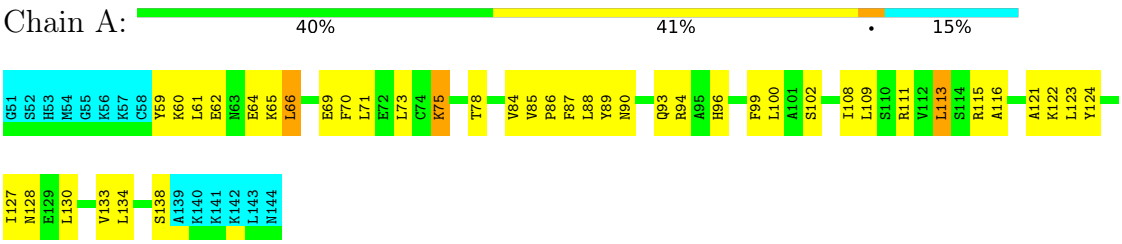
Chain B:



4.2.11 Score per residue for model 11

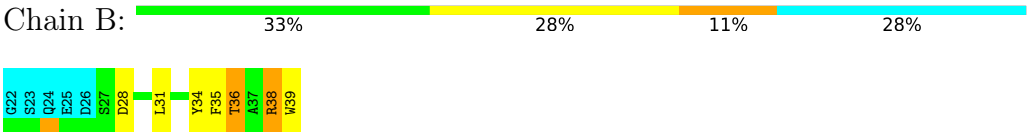
• Molecule 1: Death-associated protein 6

Chain A:



• Molecule 2: Ras association (RalGDS/AF-6) domain family 1

Chain B:



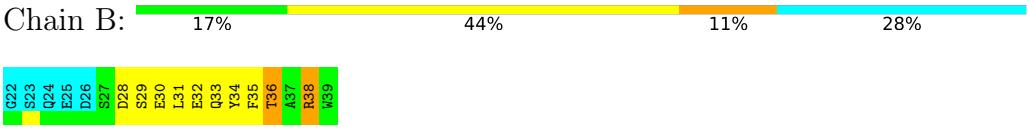
4.2.12 Score per residue for model 12

• Molecule 1: Death-associated protein 6

Chain A:

• Molecule 2: Ras association (RalGDS/AF-6) domain family 1

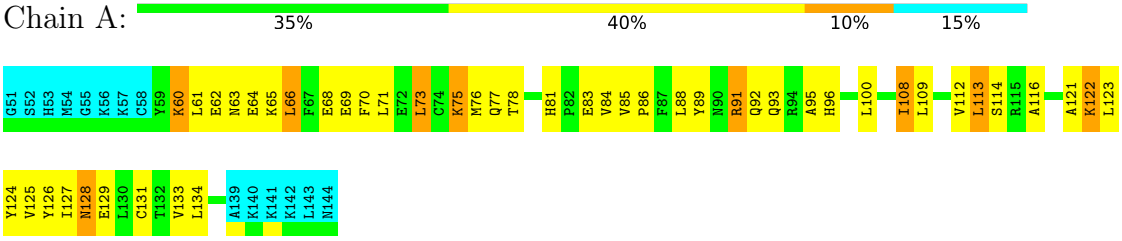
Chain B:



4.2.13 Score per residue for model 13

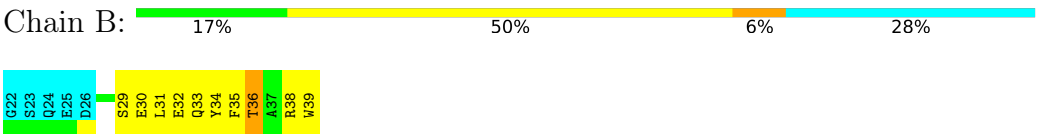
• Molecule 1: Death-associated protein 6

Chain A:



• Molecule 2: Ras association (RalGDS/AF-6) domain family 1

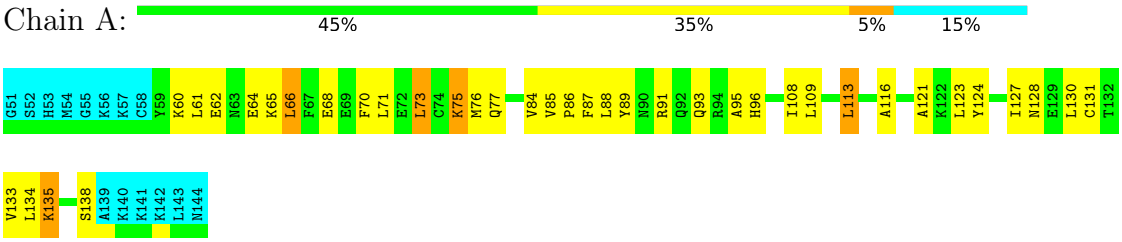
Chain B:



4.2.14 Score per residue for model 14

• Molecule 1: Death-associated protein 6

Chain A:



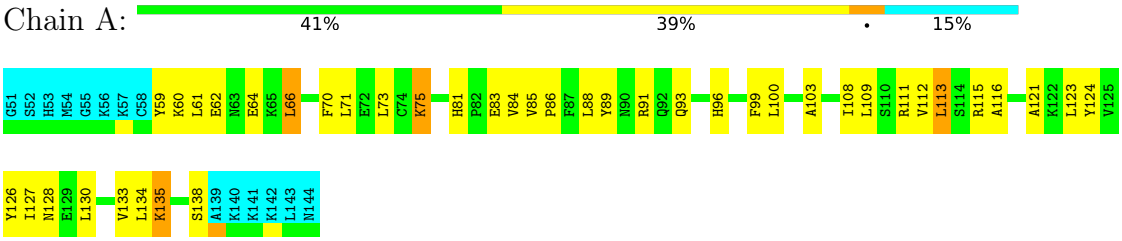
• Molecule 2: Ras association (RalGDS/AF-6) domain family 1

Chain B:

4.2.15 Score per residue for model 15 (medoid)

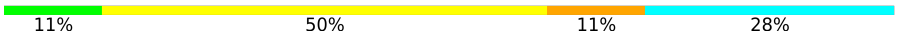
• Molecule 1: Death-associated protein 6

Chain A:



• Molecule 2: Ras association (RalGDS/AF-6) domain family 1

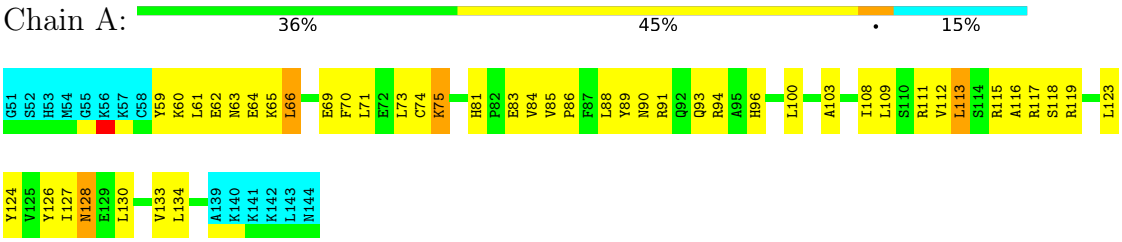
Chain B:



4.2.16 Score per residue for model 16

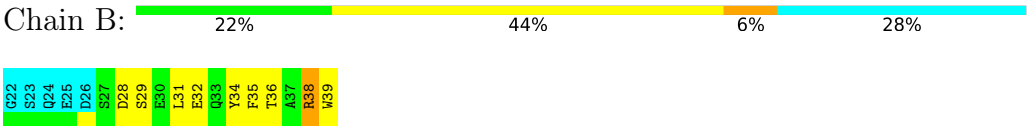
• Molecule 1: Death-associated protein 6

Chain A:



• Molecule 2: Ras association (RalGDS/AF-6) domain family 1

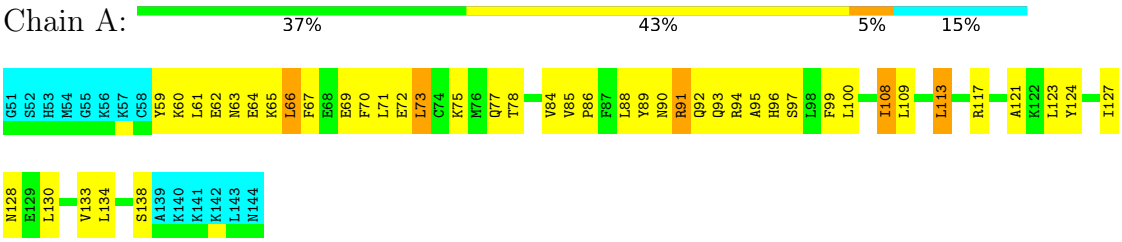
Chain B:



4.2.17 Score per residue for model 17

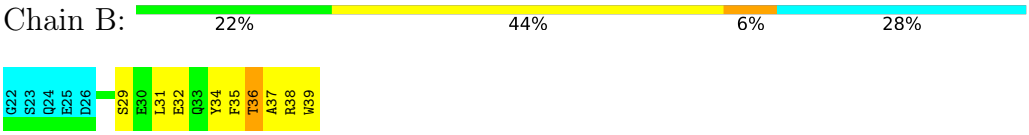
• Molecule 1: Death-associated protein 6

Chain A:



• Molecule 2: Ras association (RalGDS/AF-6) domain family 1

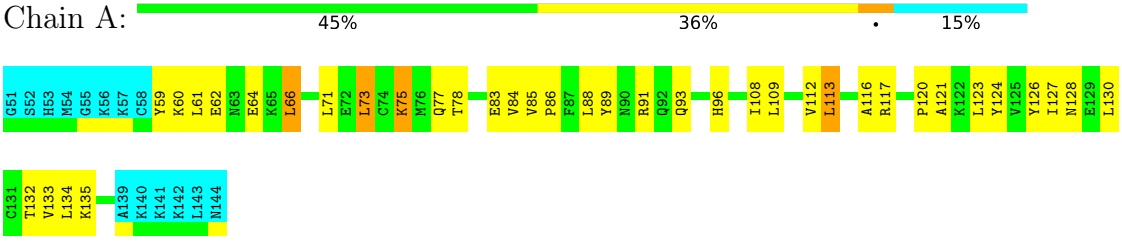
Chain B:



4.2.18 Score per residue for model 18

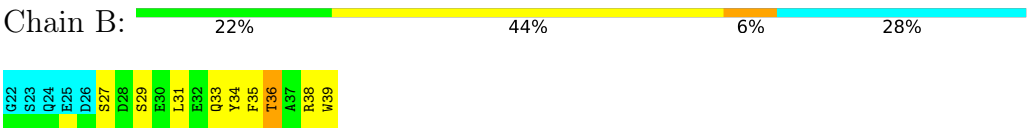
• Molecule 1: Death-associated protein 6

Chain A:



• Molecule 2: Ras association (RalGDS/AF-6) domain family 1

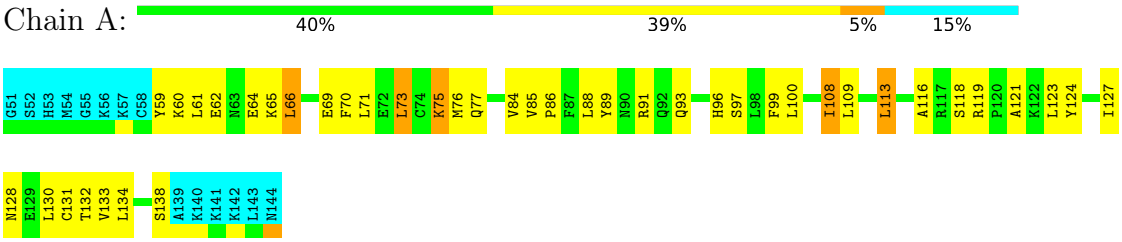
Chain B:



4.2.19 Score per residue for model 19

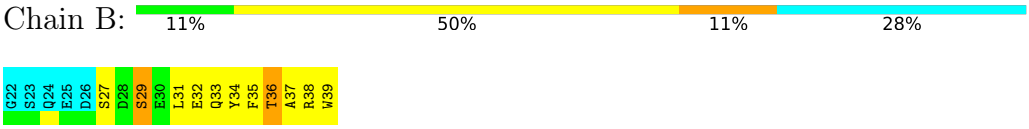
• Molecule 1: Death-associated protein 6

Chain A:



• Molecule 2: Ras association (RalGDS/AF-6) domain family 1

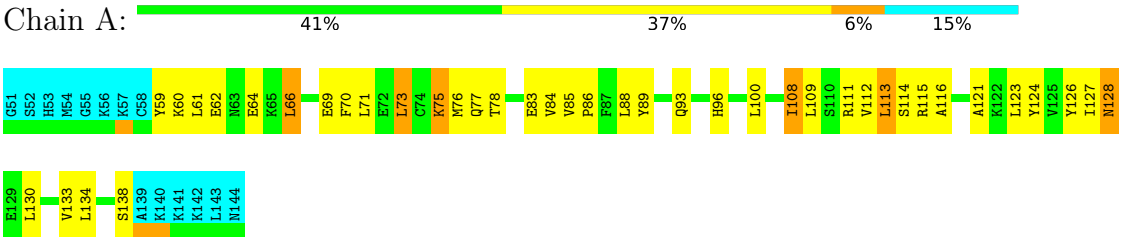
Chain B:



4.2.20 Score per residue for model 20

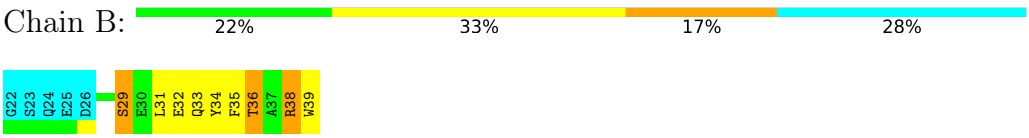
• Molecule 1: Death-associated protein 6

Chain A:



• Molecule 2: Ras association (RalGDS/AF-6) domain family 1

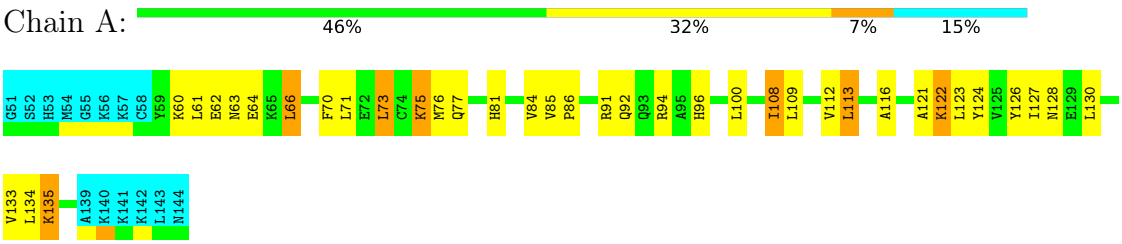
Chain B:



4.2.21 Score per residue for model 21

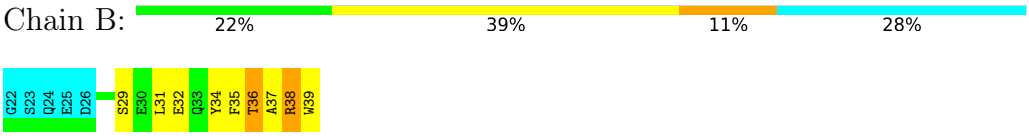
• Molecule 1: Death-associated protein 6

Chain A:



• Molecule 2: Ras association (RalGDS/AF-6) domain family 1

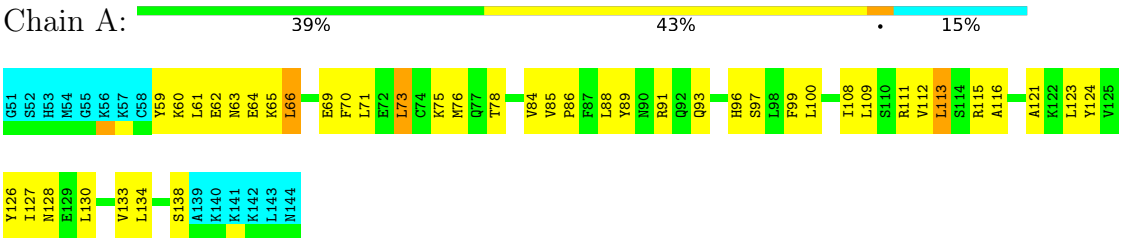
Chain B:



4.2.22 Score per residue for model 22

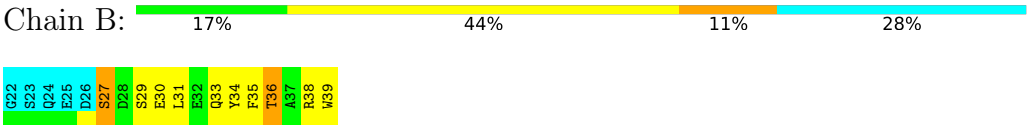
• Molecule 1: Death-associated protein 6

Chain A:



• Molecule 2: Ras association (RalGDS/AF-6) domain family 1

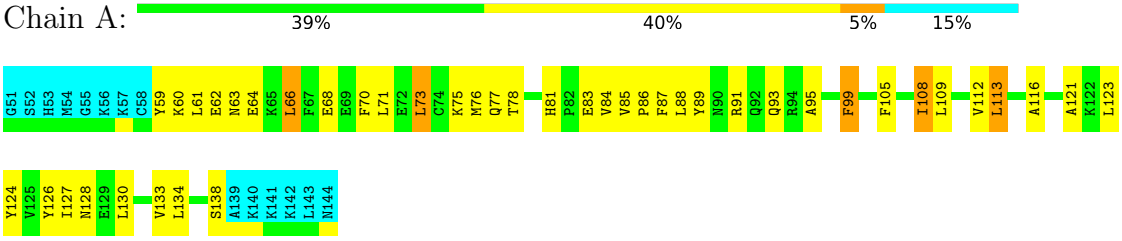
Chain B:



4.2.23 Score per residue for model 23

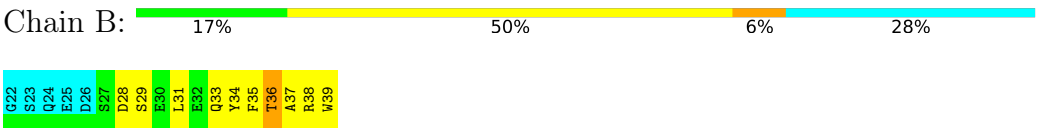
• Molecule 1: Death-associated protein 6

Chain A:



• Molecule 2: Ras association (RalGDS/AF-6) domain family 1

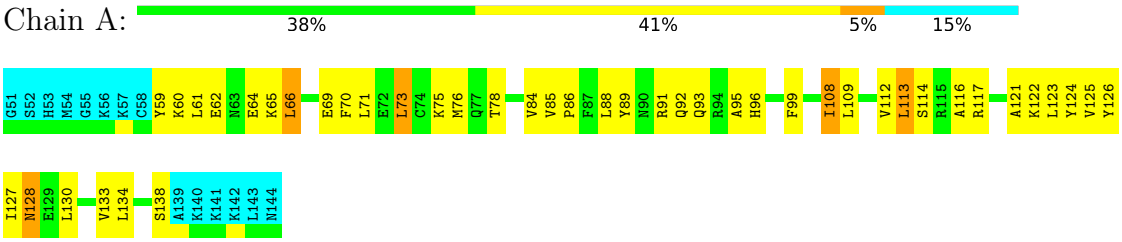
Chain B:



4.2.24 Score per residue for model 24

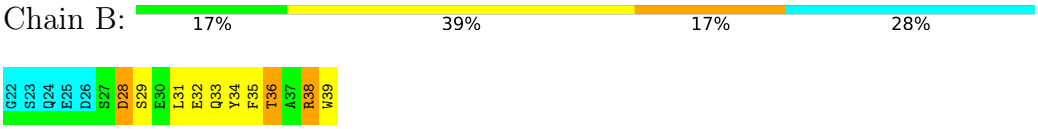
• Molecule 1: Death-associated protein 6

Chain A:



• Molecule 2: Ras association (RalGDS/AF-6) domain family 1

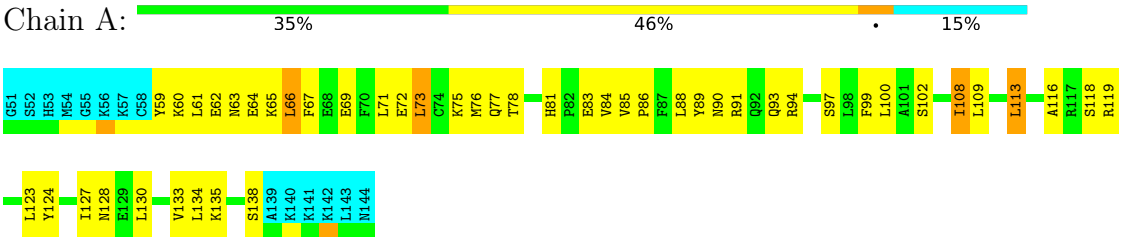
Chain B:



4.2.25 Score per residue for model 25

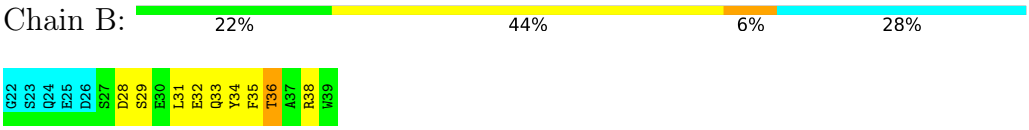
• Molecule 1: Death-associated protein 6

Chain A:



• Molecule 2: Ras association (RalGDS/AF-6) domain family 1

Chain B:



5 Refinement protocol and experimental data overview

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

Of the 120 calculated structures, 25 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
ARIA	structure solution	2.2
ARIA	refinement	2.2

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1292
Number of shifts mapped to atoms	1292
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	83%

6 Model quality

6.1 Standard geometry

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	0.54±0.03	0±0/677 (0.0± 0.1%)	0.86±0.01	0±0/914 (0.0± 0.0%)
2	B	0.51±0.03	0±0/119 (0.0± 0.0%)	0.83±0.03	0±0/159 (0.0± 0.0%)
All	All	0.53	2/19900 (0.0%)	0.85	0/26825 (0.0%)

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
1	A	59	TYR	CE1-CZ	-5.81	1.24	1.38	5	1
1	A	59	TYR	CE2-CZ	5.61	1.51	1.38	5	1

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	662	670	668	40±4
2	B	116	98	98	14±2
All	All	19450	19200	19150	1196

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 31.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:72:GLU:HA	1:A:75:LYS:HD3	0.96	1.37	7	4
1:A:99:PHE:HB3	1:A:138:SER:HB3	0.93	1.38	24	10
1:A:71:LEU:HA	1:A:74:CYS:SG	0.92	2.03	16	1
1:A:122:LYS:HD3	2:B:39:TRP:HA	0.89	1.44	13	3
1:A:74:CYS:SG	1:A:85:VAL:HG22	0.82	2.14	16	1
1:A:128:ASN:HB3	2:B:28:ASP:HA	0.78	1.56	24	3
1:A:108:ILE:HG21	1:A:133:VAL:HG11	0.76	1.58	19	25
1:A:66:LEU:HD22	1:A:109:LEU:HB3	0.76	1.56	7	25
1:A:84:VAL:HG11	1:A:127:ILE:HD13	0.75	1.57	3	25
1:A:118:SER:HB3	1:A:119:ARG:HD2	0.75	1.56	2	5
1:A:72:GLU:HA	1:A:75:LYS:HG2	0.75	1.58	17	1
1:A:128:ASN:ND2	2:B:31:LEU:HG	0.75	1.97	3	25
1:A:124:TYR:HA	1:A:127:ILE:HD12	0.74	1.57	13	25
1:A:112:VAL:HB	1:A:126:TYR:HB3	0.73	1.60	9	20
1:A:99:PHE:HD2	1:A:138:SER:HB3	0.73	1.41	23	2
2:B:38:ARG:HG2	2:B:39:TRP:N	0.73	1.97	15	20
1:A:96:HIS:HB3	1:A:138:SER:HB2	0.72	1.60	19	4
1:A:128:ASN:HD22	2:B:31:LEU:HG	0.71	1.44	24	3
1:A:121:ALA:HB1	2:B:38:ARG:HD3	0.70	1.63	14	16
1:A:71:LEU:HD22	1:A:85:VAL:HG13	0.68	1.63	16	22
1:A:85:VAL:HB	1:A:86:PRO:HD3	0.68	1.65	13	25
1:A:89:TYR:O	1:A:93:GLN:HG2	0.67	1.88	20	23
1:A:73:LEU:HD13	1:A:117:ARG:HD2	0.67	1.67	24	5
1:A:97:SER:HA	1:A:100:LEU:HD23	0.67	1.66	8	1
1:A:130:LEU:O	1:A:134:LEU:HG	0.67	1.90	9	24
1:A:60:LYS:O	1:A:64:GLU:HG3	0.66	1.90	10	24
1:A:65:LYS:O	1:A:68:GLU:HG3	0.66	1.90	13	1
1:A:121:ALA:HB1	2:B:38:ARG:HD2	0.64	1.67	12	1
1:A:99:PHE:HE2	1:A:134:LEU:HA	0.64	1.52	23	1
1:A:62:GLU:O	1:A:66:LEU:HB2	0.64	1.93	5	25
1:A:73:LEU:HA	1:A:76:MET:HE2	0.63	1.70	19	11
1:A:75:LYS:HD3	1:A:85:VAL:HG21	0.63	1.70	19	10
2:B:31:LEU:HD12	2:B:35:PHE:HE1	0.63	1.53	24	25
1:A:78:THR:OG1	1:A:81:HIS:HB2	0.63	1.94	2	1
1:A:99:PHE:CD2	1:A:138:SER:HB3	0.62	2.27	23	3
1:A:70:PHE:CD2	1:A:113:LEU:HA	0.62	2.29	20	21
2:B:31:LEU:HD12	2:B:35:PHE:CE1	0.61	2.29	24	25
1:A:78:THR:HG21	1:A:84:VAL:HG21	0.61	1.72	9	16
1:A:90:ASN:O	1:A:94:ARG:HG2	0.60	1.95	12	8
1:A:84:VAL:HG22	2:B:35:PHE:CZ	0.60	2.32	19	25
1:A:126:TYR:HA	1:A:129:GLU:CG	0.60	2.27	13	1
1:A:109:LEU:O	1:A:113:LEU:HB3	0.60	1.97	20	23

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:132:THR:HG23	2:B:27:SER:HB3	0.59	1.73	19	1
1:A:125:VAL:O	1:A:129:GLU:HG2	0.59	1.98	13	1
2:B:35:PHE:O	2:B:36:THR:HG23	0.59	1.97	21	25
1:A:125:VAL:HA	1:A:128:ASN:OD1	0.58	1.98	24	1
1:A:71:LEU:O	1:A:75:LYS:HG3	0.58	1.98	10	2
2:B:29:SER:HA	2:B:32:GLU:HG3	0.58	1.76	17	16
2:B:37:ALA:HB3	2:B:39:TRP:CD1	0.57	2.34	21	6
1:A:116:ALA:HB1	1:A:123:LEU:HD12	0.57	1.75	23	17
2:B:32:GLU:HA	2:B:36:THR:HG23	0.57	1.77	24	5
1:A:122:LYS:HE2	2:B:39:TRP:HA	0.57	1.75	11	1
1:A:97:SER:HA	1:A:100:LEU:HD12	0.57	1.77	19	6
1:A:71:LEU:HD13	1:A:89:TYR:CE2	0.57	2.35	23	20
1:A:91:ARG:HG3	1:A:134:LEU:HD12	0.57	1.76	4	17
1:A:65:LYS:O	1:A:69:GLU:HG3	0.56	2.00	16	13
1:A:113:LEU:O	1:A:117:ARG:HG2	0.56	1.99	18	3
1:A:84:VAL:HG22	2:B:35:PHE:CE1	0.56	2.36	22	22
1:A:61:LEU:HD23	1:A:61:LEU:H	0.56	1.60	14	22
2:B:29:SER:O	2:B:33:GLN:HG2	0.55	2.01	2	17
1:A:96:HIS:CB	1:A:138:SER:HB2	0.55	2.31	19	2
1:A:71:LEU:HD21	1:A:88:LEU:HB2	0.55	1.79	7	19
1:A:95:ALA:HB2	1:A:134:LEU:HB3	0.54	1.80	3	9
1:A:99:PHE:CE2	1:A:134:LEU:HA	0.54	2.35	23	1
1:A:91:ARG:HD2	1:A:135:LYS:HG2	0.54	1.78	21	8
1:A:96:HIS:O	1:A:100:LEU:HG	0.53	2.03	19	13
1:A:60:LYS:HG3	1:A:61:LEU:H	0.53	1.64	20	3
1:A:63:ASN:HA	1:A:66:LEU:HB2	0.53	1.80	4	10
1:A:61:LEU:O	1:A:65:LYS:HG2	0.52	2.03	10	1
1:A:91:ARG:HH11	1:A:135:LYS:HG3	0.52	1.64	14	1
1:A:121:ALA:HB1	2:B:38:ARG:CD	0.52	2.35	24	3
1:A:83:GLU:HB2	2:B:35:PHE:CE2	0.51	2.41	18	9
1:A:92:GLN:HA	1:A:134:LEU:HD13	0.51	1.83	3	7
1:A:65:LYS:O	1:A:69:GLU:HG2	0.51	2.05	17	1
1:A:92:GLN:CA	1:A:134:LEU:HD13	0.51	2.36	8	2
1:A:64:GLU:O	1:A:68:GLU:HG2	0.51	2.04	14	3
2:B:29:SER:HA	2:B:32:GLU:CG	0.51	2.35	12	10
1:A:128:ASN:HB3	2:B:28:ASP:CB	0.51	2.35	11	4
1:A:65:LYS:HA	1:A:68:GLU:HG2	0.51	1.83	1	2
1:A:111:ARG:O	1:A:115:ARG:HG2	0.50	2.06	1	8
1:A:75:LYS:HD2	1:A:85:VAL:HG21	0.50	1.82	2	1
1:A:116:ALA:HB1	1:A:123:LEU:CD1	0.50	2.36	24	16
1:A:113:LEU:HG	1:A:114:SER:N	0.50	2.21	1	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:121:ALA:HA	2:B:38:ARG:NH1	0.50	2.21	22	3
1:A:88:LEU:HD21	1:A:127:ILE:HG23	0.50	1.83	14	15
1:A:77:GLN:CB	1:A:123:LEU:HD22	0.50	2.36	2	7
1:A:84:VAL:HG11	1:A:127:ILE:CD1	0.49	2.36	21	19
1:A:84:VAL:HG13	1:A:127:ILE:HG21	0.49	1.85	20	10
1:A:108:ILE:O	1:A:112:VAL:HG22	0.49	2.08	20	7
2:B:38:ARG:HG3	2:B:39:TRP:N	0.49	2.22	14	1
1:A:75:LYS:HD2	1:A:85:VAL:HG11	0.49	1.84	20	4
1:A:85:VAL:HG12	1:A:89:TYR:CE2	0.49	2.43	10	3
1:A:111:ARG:O	1:A:115:ARG:HD3	0.49	2.08	15	1
1:A:84:VAL:CG1	1:A:127:ILE:HD13	0.49	2.37	17	8
1:A:83:GLU:HB2	2:B:35:PHE:HE2	0.48	1.66	8	8
1:A:77:GLN:HB2	1:A:123:LEU:HD22	0.48	1.85	2	2
1:A:115:ARG:HB3	1:A:126:TYR:CZ	0.48	2.43	15	2
1:A:65:LYS:HA	1:A:68:GLU:HG3	0.48	1.84	14	1
1:A:119:ARG:HD2	1:A:119:ARG:N	0.48	2.24	2	1
2:B:31:LEU:N	2:B:31:LEU:HD22	0.48	2.24	2	21
1:A:105:PHE:CZ	1:A:134:LEU:HD21	0.48	2.43	23	1
1:A:128:ASN:HB3	2:B:28:ASP:HB3	0.48	1.86	11	2
1:A:91:ARG:HG3	1:A:134:LEU:CD1	0.47	2.38	4	7
1:A:128:ASN:OD1	2:B:28:ASP:HB3	0.47	2.09	12	2
1:A:96:HIS:N	1:A:138:SER:HB2	0.47	2.25	24	1
1:A:73:LEU:O	1:A:77:GLN:HG2	0.47	2.09	25	17
1:A:59:TYR:CE1	1:A:103:ALA:HB2	0.47	2.44	15	4
1:A:65:LYS:NZ	1:A:65:LYS:HB3	0.47	2.23	13	2
1:A:124:TYR:HE2	2:B:35:PHE:CD1	0.47	2.27	14	1
1:A:74:CYS:O	1:A:78:THR:HG22	0.47	2.09	2	1
1:A:124:TYR:O	1:A:127:ILE:HB	0.47	2.09	24	6
2:B:36:THR:HG22	2:B:39:TRP:CZ2	0.47	2.45	5	4
1:A:77:GLN:NE2	1:A:120:PRO:HB3	0.47	2.24	7	3
1:A:66:LEU:HB3	1:A:109:LEU:HD13	0.46	1.87	5	25
1:A:75:LYS:CD	1:A:85:VAL:HG21	0.46	2.41	2	1
1:A:61:LEU:HG	1:A:62:GLU:N	0.46	2.26	15	11
1:A:128:ASN:OD1	2:B:39:TRP:HH2	0.46	1.94	2	5
1:A:71:LEU:CA	1:A:74:CYS:SG	0.46	2.93	16	1
1:A:72:GLU:HA	1:A:75:LYS:CG	0.46	2.35	17	1
1:A:113:LEU:HD11	1:A:117:ARG:HE	0.45	1.69	7	1
1:A:59:TYR:CD2	1:A:102:SER:HA	0.45	2.46	11	2
1:A:75:LYS:CD	1:A:85:VAL:HG11	0.45	2.40	20	5
2:B:38:ARG:CG	2:B:39:TRP:N	0.45	2.80	19	2
1:A:72:GLU:CA	1:A:75:LYS:HG2	0.45	2.36	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:59:TYR:HB3	1:A:106:CYS:SG	0.45	2.52	6	1
1:A:75:LYS:HE2	1:A:85:VAL:HG11	0.45	1.87	17	2
1:A:91:ARG:HG2	1:A:131:CYS:SG	0.45	2.51	19	6
1:A:65:LYS:HA	1:A:68:GLU:CG	0.45	2.42	14	1
1:A:60:LYS:HG3	1:A:61:LEU:N	0.45	2.26	23	3
1:A:129:GLU:O	1:A:133:VAL:HG23	0.44	2.12	13	2
1:A:83:GLU:O	1:A:87:PHE:HB2	0.44	2.11	10	1
1:A:111:ARG:N	1:A:111:ARG:HD2	0.44	2.27	8	1
2:B:38:ARG:HG3	2:B:39:TRP:H	0.44	1.72	14	1
1:A:61:LEU:H	1:A:61:LEU:HD23	0.44	1.72	23	2
1:A:60:LYS:HA	1:A:63:ASN:HD21	0.44	1.72	23	1
1:A:87:PHE:C	1:A:87:PHE:CD1	0.44	2.94	3	5
1:A:59:TYR:O	1:A:62:GLU:HB2	0.44	2.12	5	1
1:A:91:ARG:CG	1:A:134:LEU:HD12	0.44	2.43	23	4
2:B:38:ARG:HG2	2:B:38:ARG:HH11	0.44	1.72	21	1
1:A:78:THR:HG22	1:A:124:TYR:CZ	0.43	2.48	17	1
1:A:74:CYS:HB3	1:A:85:VAL:HG22	0.43	1.90	7	1
1:A:87:PHE:CZ	2:B:30:GLU:HG2	0.43	2.49	3	2
2:B:29:SER:HA	2:B:32:GLU:OE1	0.43	2.14	2	1
1:A:68:GLU:O	1:A:72:GLU:HG2	0.43	2.13	5	1
1:A:128:ASN:OD1	2:B:28:ASP:HB2	0.43	2.13	15	4
1:A:59:TYR:CZ	1:A:103:ALA:HB2	0.43	2.49	16	1
1:A:118:SER:HB3	1:A:119:ARG:CD	0.43	2.35	2	1
1:A:67:PHE:CE2	1:A:88:LEU:HB3	0.43	2.48	3	1
1:A:99:PHE:HD2	1:A:138:SER:OG	0.43	1.97	8	1
1:A:124:TYR:CE2	2:B:35:PHE:CD1	0.43	3.06	14	2
1:A:121:ALA:HB1	2:B:38:ARG:NE	0.43	2.28	21	1
1:A:63:ASN:O	1:A:67:PHE:HB2	0.43	2.13	1	2
1:A:81:HIS:C	1:A:83:GLU:H	0.43	2.22	15	7
2:B:37:ALA:HB3	2:B:39:TRP:HD1	0.42	1.74	21	1
2:B:34:TYR:CE1	2:B:35:PHE:CE2	0.42	3.08	10	1
1:A:73:LEU:HD13	1:A:117:ARG:HD3	0.42	1.91	2	1
1:A:61:LEU:HD23	1:A:61:LEU:N	0.42	2.28	9	1
2:B:31:LEU:N	2:B:31:LEU:CD2	0.42	2.83	3	7
1:A:128:ASN:ND2	2:B:31:LEU:CG	0.42	2.83	2	1
1:A:61:LEU:O	1:A:65:LYS:HG3	0.42	2.14	25	3
1:A:72:GLU:CA	1:A:75:LYS:HD3	0.42	2.35	25	1
1:A:65:LYS:HG3	1:A:66:LEU:N	0.42	2.30	10	1
2:B:38:ARG:CG	2:B:39:TRP:H	0.42	2.28	14	2
1:A:66:LEU:O	1:A:69:GLU:HB2	0.42	2.15	20	1
1:A:99:PHE:CD2	1:A:138:SER:OG	0.42	2.72	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:73:LEU:HD11	1:A:77:GLN:HE21	0.42	1.74	18	1
1:A:81:HIS:O	1:A:84:VAL:HG23	0.42	2.15	21	1
1:A:67:PHE:CD2	1:A:109:LEU:HD21	0.42	2.50	7	4
1:A:124:TYR:HB2	2:B:39:TRP:CZ2	0.41	2.50	2	1
1:A:95:ALA:HB1	1:A:138:SER:OG	0.41	2.15	24	2
1:A:99:PHE:O	1:A:102:SER:HB3	0.41	2.15	3	1
1:A:124:TYR:CB	2:B:39:TRP:HZ2	0.41	2.28	2	1
2:B:39:TRP:CD1	2:B:39:TRP:N	0.41	2.89	19	1
1:A:121:ALA:HB1	2:B:38:ARG:CG	0.41	2.46	5	1
2:B:31:LEU:HD22	2:B:31:LEU:N	0.41	2.31	20	3
1:A:65:LYS:HA	1:A:68:GLU:OE2	0.41	2.16	6	1
1:A:66:LEU:HD23	1:A:113:LEU:HD23	0.41	1.93	16	1
2:B:27:SER:O	2:B:30:GLU:HG3	0.41	2.15	22	1
1:A:96:HIS:O	1:A:100:LEU:HD22	0.41	2.16	6	1
1:A:132:THR:OG1	2:B:27:SER:HB3	0.40	2.16	18	1
1:A:61:LEU:HA	1:A:64:GLU:OE2	0.40	2.16	13	1
1:A:71:LEU:HD22	1:A:85:VAL:CG1	0.40	2.43	16	1
1:A:71:LEU:HD21	1:A:88:LEU:CB	0.40	2.46	16	1
1:A:68:GLU:O	1:A:72:GLU:HG3	0.40	2.15	3	1
1:A:128:ASN:HD22	1:A:128:ASN:N	0.40	2.14	10	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	80/94 (85%)	76±1 (95±1%)	4±1 (5±1%)	0±0 (0±0%)	100 100
2	B	12/18 (67%)	9±0 (77±4%)	3±1 (21±5%)	0±0 (2±3%)	9 53
All	All	2300/2800 (82%)	2138 (93%)	157 (7%)	5 (0%)	44 80

All 2 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	27	SER	4

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Mol	Chain	Res	Type	Models (Total)
2	B	36	THR	1

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	73/84 (87%)	67±2 (92±2%)	6±2 (8±2%)	12 59
2	B	12/16 (75%)	9±1 (78±5%)	3±1 (22±5%)	2 30
All	All	2125/2500 (85%)	1904 (90%)	221 (10%)	9 53

All 25 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	66	LEU	25
1	A	73	LEU	25
1	A	113	LEU	25
2	B	34	TYR	25
2	B	36	THR	23
1	A	75	LYS	18
1	A	108	ILE	17
2	B	38	ARG	12
1	A	138	SER	7
1	A	128	ASN	7
1	A	135	LYS	5
1	A	122	LYS	5
1	A	91	ARG	5
2	B	29	SER	4
1	A	123	LEU	3
1	A	97	SER	2
1	A	65	LYS	2
1	A	100	LEU	2
1	A	117	ARG	2
1	A	99	PHE	2
2	B	31	LEU	1
1	A	94	ARG	1
1	A	111	ARG	1

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Mol	Chain	Res	Type	Models (Total)
1	A	60	LYS	1
2	B	28	ASP	1

6.3.3 RNA

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates

There are no oligosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 83% for the well-defined parts and 82% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	1292
Number of shifts mapped to atoms	1292
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	110	-0.68 ± 0.15	Should be checked
$^{13}C_{\beta}$	108	0.15 ± 0.11	None needed (< 0.5 ppm)
$^{13}C'$	0	—	None (insufficient data)
^{15}N	104	-0.40 ± 0.23	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 83%, i.e. 1112 atoms were assigned a chemical shift out of a possible 1346. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	366/459 (80%)	183/183 (100%)	93/186 (50%)	90/90 (100%)
Sidechain	644/747 (86%)	437/484 (90%)	199/229 (87%)	8/34 (24%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	102/140 (73%)	62/68 (91%)	39/66 (59%)	1/6 (17%)
Overall	1112/1346 (83%)	682/735 (93%)	331/481 (69%)	99/130 (76%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 82%, i.e. 1292 atoms were assigned a chemical shift out of a possible 1583. 0 out of 19 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	430/557 (77%)	216/224 (96%)	110/224 (49%)	104/109 (95%)
Sidechain	756/879 (86%)	510/567 (90%)	236/271 (87%)	10/41 (24%)
Aromatic	106/147 (72%)	64/72 (89%)	41/68 (60%)	1/7 (14%)
Overall	1292/1583 (82%)	790/863 (92%)	387/563 (69%)	115/157 (73%)

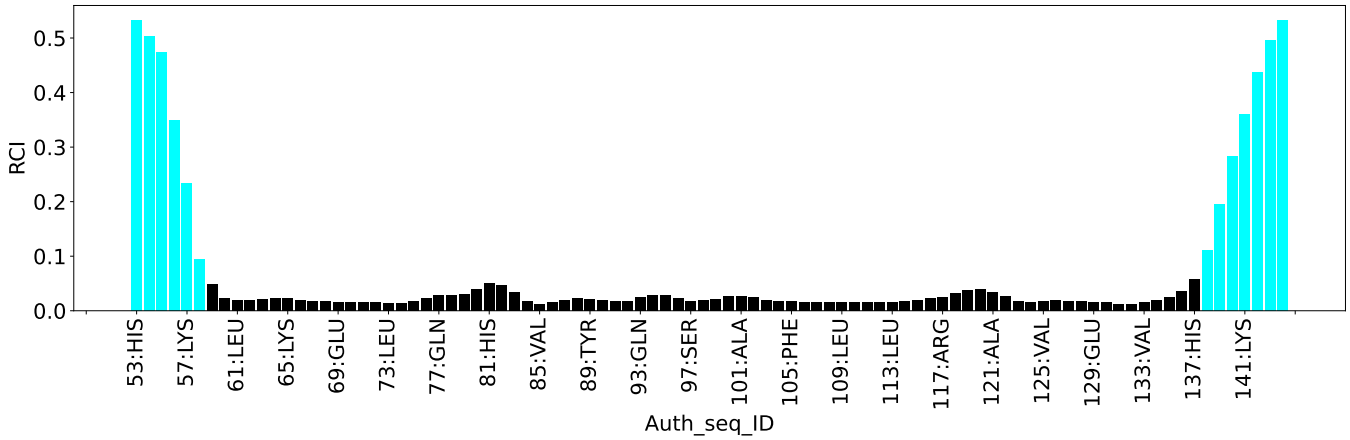
7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

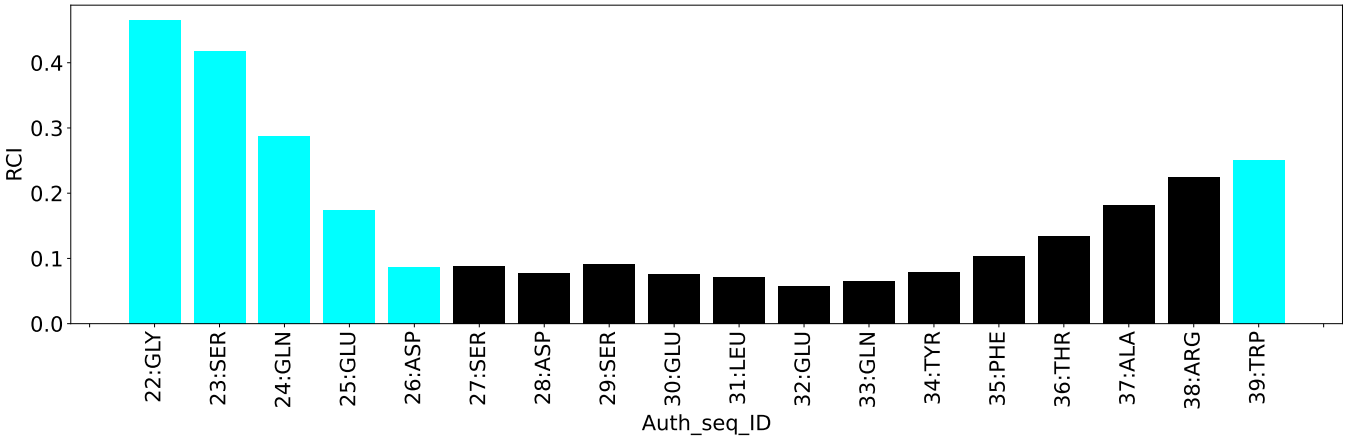
7.1.5 Random Coil Index (RCI) plots (i)

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

Random coil index (RCI) for chain A:



Random coil index (RCI) for chain B:


RCI
0.0
0.1
0.2
0.3
0.4
22:GLY
23:SER
24:GLN
25:GLU
26:ASP
27:SER
28:ASP
29:SER
30:GLU
31:LEU
32:GLU
33:GLN
34:TYR
35:PHE
36:THR
37:ALA
38:ARG
39:TRP
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	2287
Intra-residue (|i-j|=0)	949
Sequential (|i-j|=1)	480
Medium range (|i-j|>1 and |i-j|<5)	409
Long range (|i-j|≥5)	340
Inter-chain	109
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	162
Number of unmapped restraints	0
Number of restraints per residue	21.9
Number of long range restraints per residue[1]	3.0

[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)	108.6	0.2
0.2-0.5 (Medium)	242.8	0.5
>0.5 (Large)	218.0	4.35

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)	12.9	7.01
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis (i)

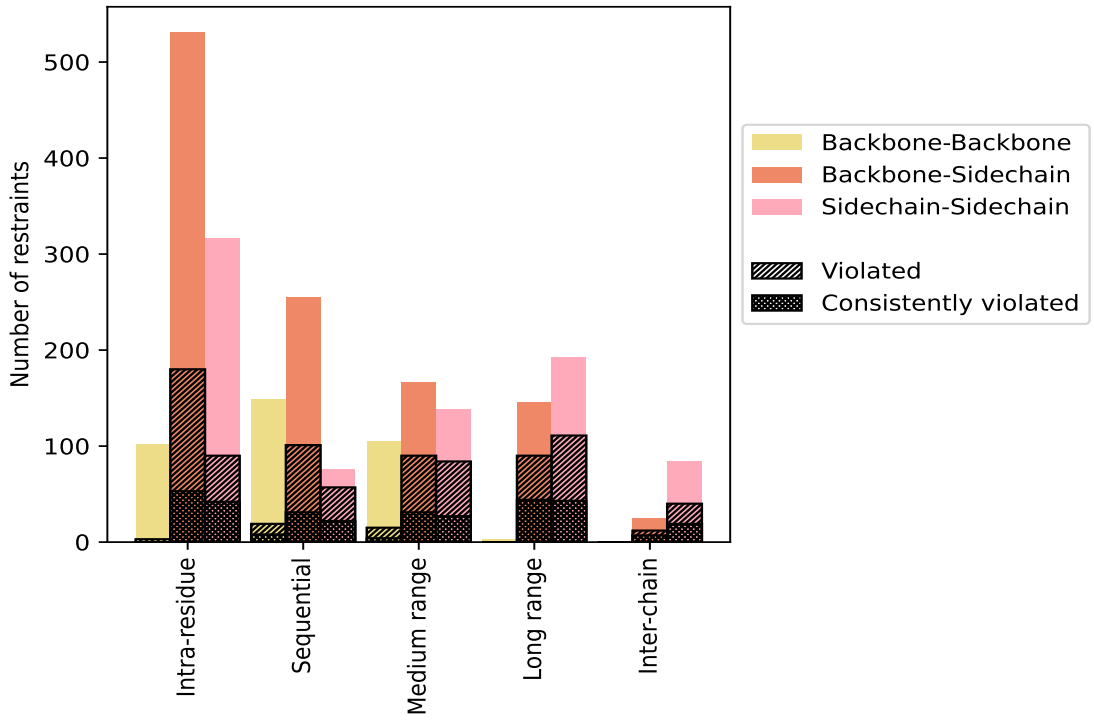
9.1 Summary of distance violations (i)

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)	949	41.5	273	28.8	11.9	95	10.0	4.2
Backbone-Backbone	102	4.5	3	2.9	0.1	0	0.0	0.0
Backbone-Sidechain	531	23.2	180	33.9	7.9	53	10.0	2.3
Sidechain-Sidechain	316	13.8	90	28.5	3.9	42	13.3	1.8
Sequential (|i-j|=1)	480	21.0	177	36.9	7.7	61	12.7	2.7
Backbone-Backbone	149	6.5	19	12.8	0.8	8	5.4	0.3
Backbone-Sidechain	255	11.1	101	39.6	4.4	31	12.2	1.4
Sidechain-Sidechain	76	3.3	57	75.0	2.5	22	28.9	1.0
Medium range (|i-j|>1 & |i-j|<5)	409	17.9	189	46.2	8.3	62	15.2	2.7
Backbone-Backbone	105	4.6	15	14.3	0.7	4	3.8	0.2
Backbone-Sidechain	166	7.3	90	54.2	3.9	31	18.7	1.4
Sidechain-Sidechain	138	6.0	84	60.9	3.7	27	19.6	1.2
Long range (|i-j|≥5)	340	14.9	201	59.1	8.8	87	25.6	3.8
Backbone-Backbone	3	0.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	145	6.3	90	62.1	3.9	44	30.3	1.9
Sidechain-Sidechain	192	8.4	111	57.8	4.9	43	22.4	1.9
Inter-chain	109	4.8	52	47.7	2.3	26	23.9	1.1
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	25	1.1	12	48.0	0.5	7	28.0	0.3
Sidechain-Sidechain	84	3.7	40	47.6	1.7	19	22.6	0.8
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	2287	100.0	892	39.0	39.0	331	14.5	14.5
Backbone-Backbone	359	15.7	37	10.3	1.6	12	3.3	0.5
Backbone-Sidechain	1122	49.1	473	42.2	20.7	166	14.8	7.3
Sidechain-Sidechain	806	35.2	382	47.4	16.7	153	19.0	6.7

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

9.1.1 Bar chart : Distribution of distance restraints and violations



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	159	116	134	132	33	574	0.6	3.59	0.58	0.4
2	165	121	132	122	37	577	0.58	3.73	0.58	0.4
3	163	118	132	126	35	574	0.56	3.64	0.54	0.39
4	156	119	132	126	35	568	0.57	3.69	0.56	0.39
5	168	118	134	129	37	586	0.57	3.66	0.56	0.4
6	163	122	125	124	33	567	0.62	4.35	0.61	0.42
7	163	117	132	132	32	576	0.57	3.57	0.56	0.4
8	156	117	127	129	32	561	0.6	3.69	0.58	0.4
9	154	122	139	126	35	576	0.59	3.76	0.6	0.39
10	158	129	131	133	32	583	0.59	3.57	0.57	0.42

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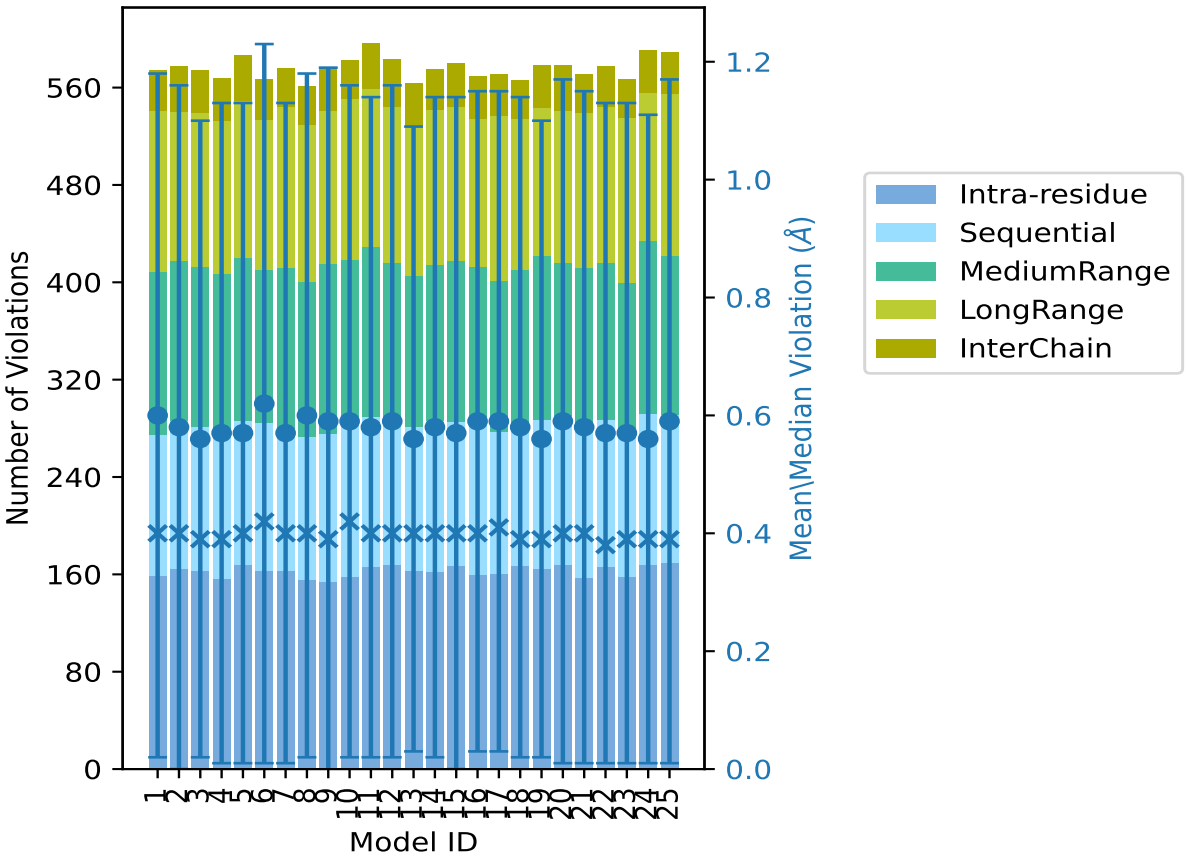
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
11	166	124	139	130	37	596	0.58	3.62	0.56	0.4
12	168	115	133	128	39	583	0.59	3.74	0.57	0.4
13	163	118	124	123	36	564	0.56	3.9	0.53	0.4
14	162	124	128	128	33	575	0.58	3.66	0.56	0.4
15	167	118	133	126	36	580	0.57	3.64	0.57	0.4
16	160	123	130	121	35	569	0.59	3.58	0.56	0.4
17	161	116	124	136	34	571	0.59	3.61	0.56	0.41
18	167	116	127	124	32	566	0.58	3.66	0.56	0.39
19	165	122	135	121	35	578	0.56	3.55	0.54	0.39
20	168	122	126	125	37	578	0.59	3.75	0.58	0.4
21	157	126	129	127	32	571	0.58	3.69	0.57	0.4
22	166	121	129	128	33	577	0.57	3.69	0.56	0.38
23	158	121	121	135	32	567	0.57	3.69	0.56	0.39
24	168	124	142	122	35	591	0.56	3.54	0.55	0.39
25	170	121	131	133	34	589	0.59	3.61	0.58	0.39

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

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



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

9.3 Distance violation statistics for the ensemble (i)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1395(IR:676, SQ:303, MR:220, LR:139, IC:57) 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]	%
27	8	15	12	6	68	1	4.0
14	7	7	6	3	37	2	8.0
14	10	11	9	1	45	3	12.0
11	11	4	5	1	32	4	16.0
10	10	2	4	1	27	5	20.0
9	10	4	3	0	26	6	24.0

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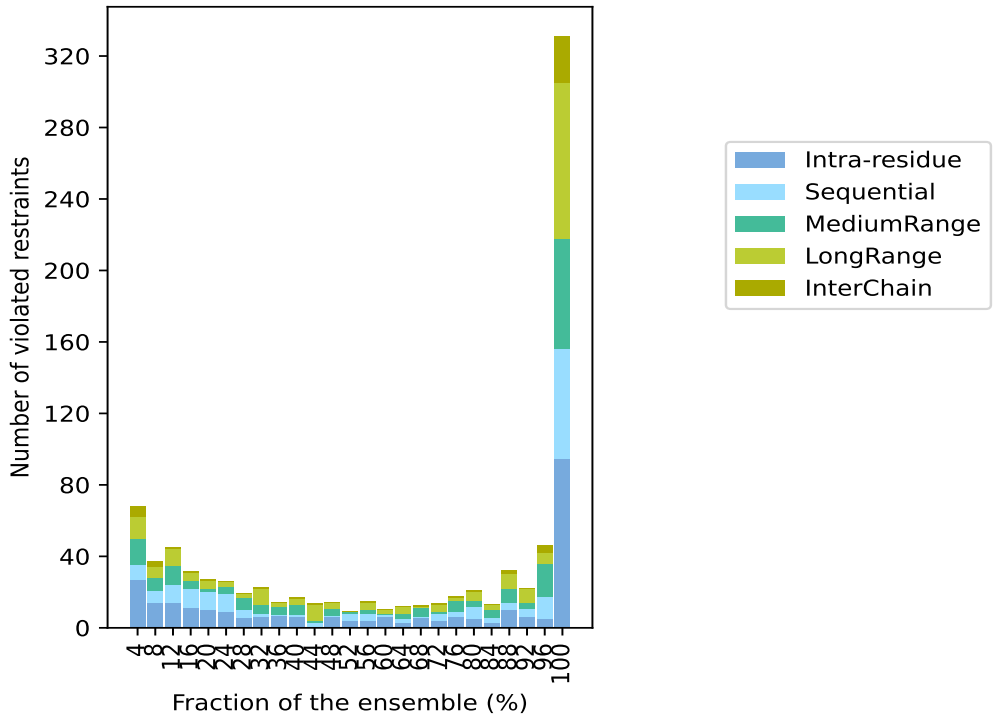
Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
6	4	7	2	0	19	7	28.0
6	2	5	9	1	23	8	32.0
7	0	5	2	0	14	9	36.0
6	1	6	3	1	17	10	40.0
0	3	1	9	1	14	11	44.0
6	1	4	3	0	14	12	48.0
4	4	1	0	0	9	13	52.0
4	4	2	4	1	15	14	56.0
6	1	1	2	0	10	15	60.0
3	2	3	4	0	12	16	64.0
6	0	5	1	1	13	17	68.0
4	4	1	4	1	14	18	72.0
6	3	6	2	1	18	19	76.0
5	7	3	5	1	21	20	80.0
3	3	4	3	0	13	21	84.0
10	4	8	8	2	32	22	88.0
6	5	3	8	0	22	23	92.0
5	12	19	6	4	46	24	96.0
95	61	62	87	26	331	25	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

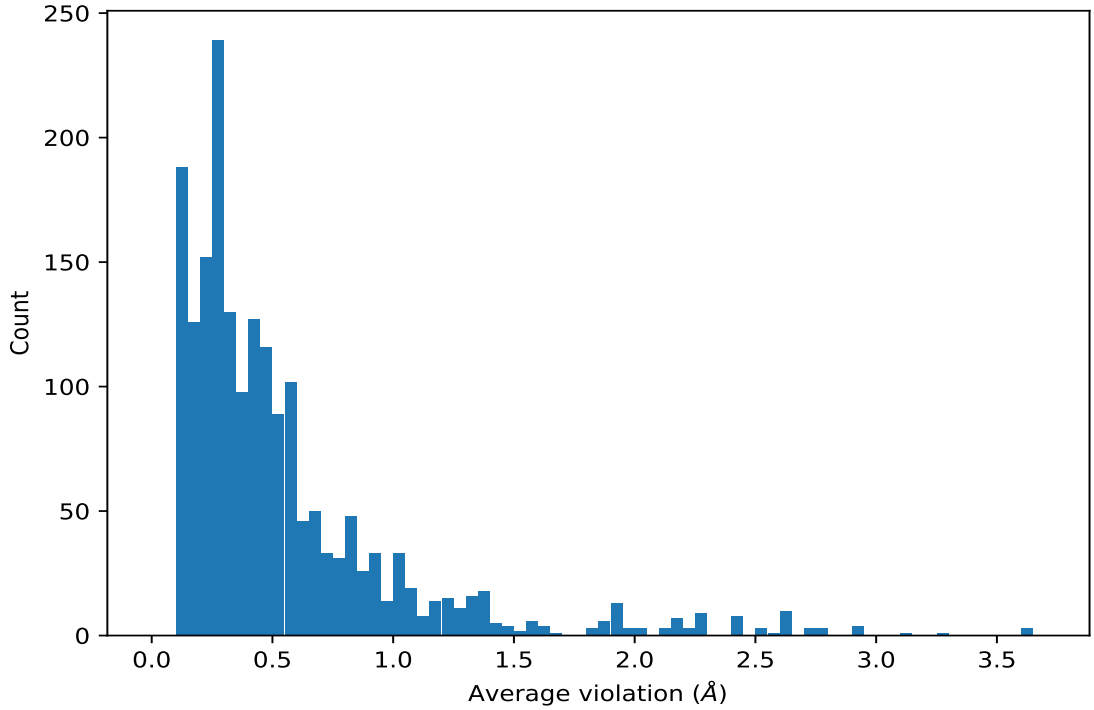
9.3.1 Bar graph : Distance violation statistics for the ensemble



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 (i)

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)
(1,761)	1:126:A:TYR:HD1	1:123:A:LEU:HD13	25	3.65	0.09	3.64
(1,761)	1:126:A:TYR:HD1	1:123:A:LEU:HD12	25	3.65	0.09	3.64
(1,761)	1:126:A:TYR:HD1	1:123:A:LEU:HD11	25	3.65	0.09	3.64
(1,764)	1:126:A:TYR:HE1	1:116:A:ALA:HA	25	3.27	0.1	3.27
(1,763)	1:126:A:TYR:HE1	1:122:A:LYS:H	25	3.13	0.18	3.13
(1,759)	1:126:A:TYR:HD1	1:116:A:ALA:HA	25	2.94	0.11	2.94
(1,1198)	1:89:A:TYR:HE1	1:85:A:VAL:HG11	25	2.92	0.23	2.87
(1,1198)	1:89:A:TYR:HE1	1:85:A:VAL:HG13	25	2.92	0.23	2.87
(1,1198)	1:89:A:TYR:HE1	1:85:A:VAL:HG12	25	2.92	0.23	2.87
(1,1195)	1:89:A:TYR:HD1	1:85:A:VAL:HG11	25	2.77	0.15	2.77
(1,1195)	1:89:A:TYR:HD1	1:85:A:VAL:HG13	25	2.77	0.15	2.77
(1,1195)	1:89:A:TYR:HD1	1:85:A:VAL:HG12	25	2.77	0.15	2.77
(1,1200)	1:89:A:TYR:HE1	1:71:A:LEU:HD22	25	2.7	0.17	2.69
(1,1200)	1:89:A:TYR:HE1	1:71:A:LEU:HD21	25	2.7	0.17	2.69
(1,1200)	1:89:A:TYR:HE1	1:71:A:LEU:HD23	25	2.7	0.17	2.69
(1,756)	1:126:A:TYR:HD1	1:123:A:LEU:HA	25	2.64	0.11	2.64

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1026)	1:109:A:LEU:HD13	1:67:A:PHE:HE1	25	2.63	0.89	2.95
(1,1026)	1:109:A:LEU:HD11	1:67:A:PHE:HE1	25	2.63	0.89	2.95
(1,1026)	1:109:A:LEU:HD12	1:67:A:PHE:HE1	25	2.63	0.89	2.95
(1,1105)	1:134:A:LEU:HD22	1:99:A:PHE:HE1	25	2.61	0.66	2.73
(1,1105)	1:134:A:LEU:HD21	1:99:A:PHE:HE1	25	2.61	0.66	2.73
(1,1105)	1:134:A:LEU:HD23	1:99:A:PHE:HE1	25	2.61	0.66	2.73
(1,765)	1:126:A:TYR:HE1	1:119:A:ARG:HB2	25	2.58	0.2	2.6
(1,1090)	1:100:A:LEU:HD21	1:99:A:PHE:HE1	25	2.5	0.62	2.42
(1,1090)	1:100:A:LEU:HD23	1:99:A:PHE:HE1	25	2.5	0.62	2.42
(1,1090)	1:100:A:LEU:HD22	1:99:A:PHE:HE1	25	2.5	0.62	2.42
(1,412)	1:131:A:CYS:H	1:87:A:PHE:HE1	25	2.44	0.2	2.48
(1,412)	1:131:A:CYS:H	1:87:A:PHE:HE2	25	2.44	0.2	2.48
(1,412)	1:131:A:CYS:H	1:87:A:PHE:HD2	25	2.44	0.2	2.48
(1,303)	2:36:B:THR:HG22	2:33:B:GLN:HB2	25	2.42	0.07	2.41
(1,303)	2:36:B:THR:HG21	2:33:B:GLN:HB2	25	2.42	0.07	2.41
(1,303)	2:36:B:THR:HG23	2:33:B:GLN:HB2	25	2.42	0.07	2.41
(1,303)	2:36:B:THR:HG21	1:125:A:VAL:HB	25	2.42	0.07	2.41
(1,303)	2:36:B:THR:HG22	1:125:A:VAL:HB	25	2.42	0.07	2.41
(1,298)	2:35:B:PHE:HB3	1:87:A:PHE:HD2	25	2.27	0.19	2.34
(1,298)	2:38:B:ARG:HD2	2:39:B:TRP:HZ2	25	2.27	0.19	2.34
(1,54)	1:124:A:TYR:HD1	1:84:A:VAL:HG21	25	2.27	1.12	2.81
(1,54)	1:124:A:TYR:HD1	1:84:A:VAL:HG22	25	2.27	1.12	2.81
(1,54)	1:127:A:ILE:HG23	1:124:A:TYR:HD1	25	2.27	1.12	2.81
(1,54)	1:127:A:ILE:HG22	1:124:A:TYR:HD1	25	2.27	1.12	2.81
(1,54)	1:124:A:TYR:HD1	1:84:A:VAL:HG23	25	2.27	1.12	2.81
(1,54)	1:127:A:ILE:HG21	1:124:A:TYR:HD1	25	2.27	1.12	2.81
(1,142)	1:89:A:TYR:HD1	1:88:A:LEU:HB2	25	2.25	0.07	2.25
(1,1027)	1:67:A:PHE:HE1	1:109:A:LEU:HD22	25	2.21	0.75	2.49
(1,1027)	1:67:A:PHE:HE1	1:109:A:LEU:HD21	25	2.21	0.75	2.49
(1,1027)	1:67:A:PHE:HE1	1:109:A:LEU:HD23	25	2.21	0.75	2.49
(1,382)	1:64:A:GLU:HG3	1:100:A:LEU:HD12	25	2.16	0.28	2.19
(1,382)	1:64:A:GLU:HG3	1:100:A:LEU:HD11	25	2.16	0.28	2.19
(1,382)	1:72:A:GLU:HG2	1:85:A:VAL:HG21	25	2.16	0.28	2.19
(1,382)	1:64:A:GLU:HG3	1:100:A:LEU:HD13	25	2.16	0.28	2.19
(1,382)	1:72:A:GLU:HG2	1:85:A:VAL:HG23	25	2.16	0.28	2.19
(1,382)	1:72:A:GLU:HG2	1:85:A:VAL:HG22	25	2.16	0.28	2.19
(1,382)	1:104:A:GLU:HG2	1:100:A:LEU:HD13	25	2.16	0.28	2.19
(1,1710)	2:32:B:GLU:HG2	1:125:A:VAL:HG21	25	2.12	0.16	2.16
(1,1710)	2:32:B:GLU:HG2	1:125:A:VAL:HG22	25	2.12	0.16	2.16
(1,1710)	2:32:B:GLU:HG2	1:125:A:VAL:HG23	25	2.12	0.16	2.16
(1,832)	1:121:A:ALA:HB3	1:120:A:PRO:HG3	25	2.01	0.02	2.01
(1,832)	1:121:A:ALA:HB1	1:120:A:PRO:HG3	25	2.01	0.02	2.01

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,832)	1:121:A:ALA:HB2	1:120:A:PRO:HG3	25	2.01	0.02	2.01
(1,760)	1:126:A:TYR:HD1	1:116:A:ALA:HB2	25	1.94	0.13	1.92
(1,760)	1:126:A:TYR:HD1	1:116:A:ALA:HB3	25	1.94	0.13	1.92
(1,760)	1:126:A:TYR:HD1	1:116:A:ALA:HB1	25	1.94	0.13	1.92
(1,1660)	2:36:B:THR:HG23	1:122:A:LYS:HD2	25	1.93	0.38	1.91
(1,1660)	2:36:B:THR:HG22	1:122:A:LYS:HD3	25	1.93	0.38	1.91
(1,1660)	2:36:B:THR:HG21	1:122:A:LYS:HD3	25	1.93	0.38	1.91
(1,1660)	2:36:B:THR:HG23	1:122:A:LYS:HD3	25	1.93	0.38	1.91
(1,1660)	2:36:B:THR:HG22	1:122:A:LYS:HD2	25	1.93	0.38	1.91
(1,1660)	2:36:B:THR:HG21	1:122:A:LYS:HD2	25	1.93	0.38	1.91
(1,1680)	2:35:B:PHE:HE1	1:124:A:TYR:HB2	25	1.91	0.04	1.9
(1,263)	1:132:A:THR:HG21	2:28:B:ASP:HB3	25	1.85	0.8	1.64
(1,263)	1:132:A:THR:HG22	2:28:B:ASP:HB3	25	1.85	0.8	1.64
(1,263)	1:132:A:THR:HG23	2:28:B:ASP:HB3	25	1.85	0.8	1.64
(1,263)	1:132:A:THR:HG22	2:28:B:ASP:HB2	25	1.85	0.8	1.64
(1,263)	1:132:A:THR:HG23	2:28:B:ASP:HB2	25	1.85	0.8	1.64
(1,263)	1:132:A:THR:HG21	2:28:B:ASP:HB2	25	1.85	0.8	1.64
(1,1586)	2:36:B:THR:HG23	1:125:A:VAL:H	25	1.84	0.14	1.82
(1,1586)	2:36:B:THR:HG22	1:125:A:VAL:H	25	1.84	0.14	1.82
(1,1586)	2:36:B:THR:HG21	1:125:A:VAL:H	25	1.84	0.14	1.82
(1,1330)	1:77:A:GLN:HG2	1:76:A:MET:HB3	25	1.67	0.05	1.67
(1,661)	1:133:A:VAL:HG13	1:99:A:PHE:HE1	25	1.62	0.36	1.69
(1,661)	1:133:A:VAL:HG12	1:99:A:PHE:HE1	25	1.62	0.36	1.69
(1,661)	1:133:A:VAL:HG11	1:99:A:PHE:HE1	25	1.62	0.36	1.69
(1,914)	1:61:A:LEU:HD12	1:61:A:LEU:H	25	1.56	0.07	1.57
(1,914)	1:61:A:LEU:HD13	1:61:A:LEU:H	25	1.56	0.07	1.57
(1,914)	1:61:A:LEU:HD11	1:61:A:LEU:H	25	1.56	0.07	1.57
(1,46)	1:126:A:TYR:HE1	1:122:A:LYS:HB3	25	1.49	0.4	1.46
(1,904)	1:115:A:ARG:HD3	1:126:A:TYR:HE2	25	1.46	0.42	1.61
(1,904)	1:115:A:ARG:HD3	1:126:A:TYR:HE1	25	1.46	0.42	1.61
(1,365)	2:29:B:SER:HB2	2:31:B:LEU:HB2	25	1.41	0.11	1.42
(1,365)	1:118:A:SER:HB3	1:116:A:ALA:HB2	25	1.41	0.11	1.42
(1,1255)	1:86:A:PRO:HD2	1:85:A:VAL:HG11	25	1.41	0.03	1.4
(1,1255)	1:86:A:PRO:HD2	1:85:A:VAL:HG13	25	1.41	0.03	1.4
(1,1255)	1:86:A:PRO:HD2	1:85:A:VAL:HG12	25	1.41	0.03	1.4
(1,1062)	1:103:A:ALA:HB3	1:59:A:TYR:HB3	25	1.36	0.43	1.49
(1,1062)	1:103:A:ALA:HB1	1:59:A:TYR:HB3	25	1.36	0.43	1.49
(1,1062)	1:103:A:ALA:HB2	1:59:A:TYR:HB3	25	1.36	0.43	1.49
(1,2113)	1:76:A:MET:H	1:77:A:GLN:HB3	25	1.35	0.05	1.34
(1,1449)	1:69:A:GLU:HG2	1:113:A:LEU:HD21	25	1.33	0.1	1.32
(1,1449)	1:69:A:GLU:HG2	1:113:A:LEU:HD23	25	1.33	0.1	1.32
(1,1449)	1:69:A:GLU:HG2	1:113:A:LEU:HD22	25	1.33	0.1	1.32

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1582)	2:37:B:ALA:HB3	1:125:A:VAL:HG23	25	1.31	0.17	1.3
(1,1582)	2:37:B:ALA:HB2	1:125:A:VAL:HG21	25	1.31	0.17	1.3
(1,1582)	2:37:B:ALA:HB1	1:125:A:VAL:HG23	25	1.31	0.17	1.3
(1,1582)	2:37:B:ALA:HB3	1:125:A:VAL:HG21	25	1.31	0.17	1.3
(1,1582)	2:37:B:ALA:HB2	1:125:A:VAL:HG23	25	1.31	0.17	1.3
(1,1582)	2:37:B:ALA:HB1	1:125:A:VAL:HG22	25	1.31	0.17	1.3
(1,1582)	2:37:B:ALA:HB2	1:125:A:VAL:HG22	25	1.31	0.17	1.3
(1,1582)	2:37:B:ALA:HB1	1:125:A:VAL:HG21	25	1.31	0.17	1.3
(1,381)	2:30:B:GLU:HG2	2:31:B:LEU:HB2	25	1.31	0.42	1.56
(1,63)	1:67:A:PHE:HA	1:109:A:LEU:HG	25	1.26	0.1	1.28
(1,63)	1:123:A:LEU:HD22	1:124:A:TYR:HA	25	1.26	0.1	1.28
(1,63)	1:123:A:LEU:HD21	1:124:A:TYR:HA	25	1.26	0.1	1.28
(1,63)	1:123:A:LEU:HD23	1:124:A:TYR:HA	25	1.26	0.1	1.28
(1,63)	1:123:A:LEU:HA	1:123:A:LEU:HD22	25	1.26	0.1	1.28
(1,671)	1:133:A:VAL:HG21	1:99:A:PHE:HZ	25	1.25	0.15	1.23
(1,671)	1:133:A:VAL:HG23	1:99:A:PHE:HZ	25	1.25	0.15	1.23
(1,671)	1:133:A:VAL:HG22	1:99:A:PHE:HZ	25	1.25	0.15	1.23
(1,2274)	2:39:B:TRP:HE1	2:38:B:ARG:HD2	25	1.24	0.51	1.32
(1,2274)	2:39:B:TRP:HE1	2:38:B:ARG:HD3	25	1.24	0.51	1.32
(1,795)	1:127:A:ILE:HD13	1:124:A:TYR:HE1	25	1.23	0.5	1.46
(1,795)	1:127:A:ILE:HD11	1:124:A:TYR:HE1	25	1.23	0.5	1.46
(1,795)	1:127:A:ILE:HD12	1:124:A:TYR:HE1	25	1.23	0.5	1.46
(1,1192)	1:89:A:TYR:HD1	1:89:A:TYR:H	25	1.23	0.05	1.23
(1,1470)	1:66:A:LEU:HD11	1:62:A:GLU:HG3	25	1.23	0.5	1.49
(1,1470)	1:66:A:LEU:HD12	1:62:A:GLU:HG3	25	1.23	0.5	1.49
(1,1470)	1:66:A:LEU:HD13	1:62:A:GLU:HG3	25	1.23	0.5	1.49
(1,534)	1:109:A:LEU:H	1:113:A:LEU:HB3	25	1.22	0.33	1.3
(1,534)	1:121:A:ALA:H	1:119:A:ARG:HG3	25	1.22	0.33	1.3
(1,534)	1:121:A:ALA:H	1:119:A:ARG:HG2	25	1.22	0.33	1.3
(1,534)	1:109:A:LEU:H	1:111:A:ARG:HG2	25	1.22	0.33	1.3
(1,710)	1:130:A:LEU:HD22	1:109:A:LEU:HD13	25	1.18	0.11	1.16
(1,710)	1:130:A:LEU:HD21	1:109:A:LEU:HD11	25	1.18	0.11	1.16
(1,710)	1:130:A:LEU:HD22	1:109:A:LEU:HD11	25	1.18	0.11	1.16
(1,710)	1:130:A:LEU:HD23	1:109:A:LEU:HD13	25	1.18	0.11	1.16
(1,710)	1:130:A:LEU:HD21	1:109:A:LEU:HD13	25	1.18	0.11	1.16
(1,710)	1:130:A:LEU:HD22	1:109:A:LEU:HD12	25	1.18	0.11	1.16
(1,710)	1:130:A:LEU:HD23	1:109:A:LEU:HD11	25	1.18	0.11	1.16
(1,710)	1:130:A:LEU:HD21	1:109:A:LEU:HD12	25	1.18	0.11	1.16
(1,710)	1:130:A:LEU:HD23	1:109:A:LEU:HD12	25	1.18	0.11	1.16
(1,1656)	2:37:B:ALA:HB3	2:39:B:TRP:HZ2	25	1.17	0.15	1.18
(1,1656)	2:37:B:ALA:HB2	2:39:B:TRP:HZ2	25	1.17	0.15	1.18
(1,1656)	2:37:B:ALA:HB1	2:39:B:TRP:HZ2	25	1.17	0.15	1.18

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1071)	1:101:A:ALA:HB2	1:63:A:ASN:HD21	25	1.12	0.37	1.26
(1,1071)	1:101:A:ALA:HB3	1:63:A:ASN:HD21	25	1.12	0.37	1.26
(1,1071)	1:101:A:ALA:HB1	1:63:A:ASN:HD21	25	1.12	0.37	1.26
(1,143)	1:89:A:TYR:HD2	1:86:A:PRO:HB2	25	1.09	0.2	1.05
(1,143)	1:92:A:GLN:HB2	1:89:A:TYR:HD1	25	1.09	0.2	1.05
(1,341)	2:31:B:LEU:HD13	1:84:A:VAL:H	25	1.09	0.05	1.08
(1,341)	2:31:B:LEU:HD12	1:84:A:VAL:H	25	1.09	0.05	1.08
(1,341)	2:31:B:LEU:HD11	1:84:A:VAL:H	25	1.09	0.05	1.08
(1,40)	1:127:A:ILE:HD11	1:74:A:CYS:HA	25	1.08	0.1	1.11
(1,40)	1:127:A:ILE:HD12	1:74:A:CYS:HA	25	1.08	0.1	1.11
(1,40)	1:127:A:ILE:HD12	1:127:A:ILE:HA	25	1.08	0.1	1.11
(1,40)	1:127:A:ILE:HD13	1:74:A:CYS:HA	25	1.08	0.1	1.11
(1,86)	1:98:A:LEU:HD11	1:99:A:PHE:H	25	1.08	0.07	1.08
(1,86)	1:113:A:LEU:HD12	1:73:A:LEU:H	25	1.08	0.07	1.08
(1,86)	1:113:A:LEU:HD13	1:73:A:LEU:H	25	1.08	0.07	1.08
(1,86)	1:98:A:LEU:HD13	1:99:A:PHE:H	25	1.08	0.07	1.08
(1,86)	1:98:A:LEU:HD12	1:99:A:PHE:H	25	1.08	0.07	1.08
(1,86)	1:113:A:LEU:HD11	1:73:A:LEU:H	25	1.08	0.07	1.08
(1,577)	1:75:A:LYS:HE2	1:71:A:LEU:HB3	25	1.07	0.73	0.79
(1,91)	1:109:A:LEU:HD11	1:64:A:GLU:H	25	1.04	0.04	1.05
(1,91)	1:109:A:LEU:HD12	1:64:A:GLU:H	25	1.04	0.04	1.05
(1,91)	1:109:A:LEU:HD13	1:64:A:GLU:H	25	1.04	0.04	1.05
(1,59)	1:123:A:LEU:HA	1:123:A:LEU:HD23	25	1.03	0.03	1.04
(1,59)	1:123:A:LEU:HA	1:123:A:LEU:HD22	25	1.03	0.03	1.04
(1,59)	1:123:A:LEU:HA	1:73:A:LEU:HD21	25	1.03	0.03	1.04
(1,59)	1:123:A:LEU:HA	1:123:A:LEU:HD21	25	1.03	0.03	1.04
(1,149)	1:88:A:LEU:HD23	1:89:A:TYR:H	25	1.02	0.06	1.04
(1,149)	1:88:A:LEU:HD22	1:89:A:TYR:H	25	1.02	0.06	1.04
(1,149)	1:88:A:LEU:HD12	1:89:A:TYR:H	25	1.02	0.06	1.04
(1,149)	1:88:A:LEU:HD21	1:89:A:TYR:H	25	1.02	0.06	1.04
(1,282)	2:31:B:LEU:HD13	1:124:A:TYR:HA	25	1.02	0.04	1.02
(1,282)	2:31:B:LEU:HD12	1:124:A:TYR:HA	25	1.02	0.04	1.02
(1,282)	2:31:B:LEU:HD23	1:131:A:CYS:HA	25	1.02	0.04	1.02
(1,282)	2:31:B:LEU:HD11	1:124:A:TYR:HA	25	1.02	0.04	1.02
(1,23)	1:130:A:LEU:HD21	1:113:A:LEU:H	25	1.02	0.07	1.04
(1,23)	1:130:A:LEU:HD23	1:130:A:LEU:H	25	1.02	0.07	1.04
(1,23)	1:130:A:LEU:HD21	1:130:A:LEU:H	25	1.02	0.07	1.04
(1,23)	1:130:A:LEU:HD22	1:130:A:LEU:H	25	1.02	0.07	1.04
(1,23)	1:130:A:LEU:HD23	1:113:A:LEU:H	25	1.02	0.07	1.04
(1,23)	1:130:A:LEU:HD22	1:113:A:LEU:H	25	1.02	0.07	1.04
(1,300)	2:37:B:ALA:HB1	1:123:A:LEU:HB2	25	1.02	0.18	1.0
(1,300)	2:37:B:ALA:HB3	1:123:A:LEU:HB2	25	1.02	0.18	1.0

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,300)	2:37:B:ALA:HB2	1:123:A:LEU:HB2	25	1.02	0.18	1.0
(1,120)	1:95:A:ALA:HB2	1:93:A:GLN:H	25	1.01	0.08	1.0
(1,120)	1:95:A:ALA:HB1	1:100:A:LEU:H	25	1.01	0.08	1.0
(1,120)	1:95:A:ALA:HB1	1:93:A:GLN:H	25	1.01	0.08	1.0
(1,120)	1:95:A:ALA:HB3	1:100:A:LEU:H	25	1.01	0.08	1.0
(1,120)	1:95:A:ALA:HB3	1:93:A:GLN:H	25	1.01	0.08	1.0
(1,120)	1:95:A:ALA:HB2	1:100:A:LEU:H	25	1.01	0.08	1.0
(1,400)	1:136:A:ALA:HB1	1:135:A:LYS:H	25	1.0	0.03	1.01
(1,400)	1:136:A:ALA:HB3	1:135:A:LYS:H	25	1.0	0.03	1.01
(1,400)	1:136:A:ALA:HB2	1:135:A:LYS:H	25	1.0	0.03	1.01
(1,1196)	1:89:A:TYR:HD1	1:71:A:LEU:HD12	25	0.98	0.13	1.02
(1,1196)	1:89:A:TYR:HD1	1:71:A:LEU:HD13	25	0.98	0.13	1.02
(1,1196)	1:89:A:TYR:HD1	1:71:A:LEU:HD11	25	0.98	0.13	1.02
(1,306)	2:36:B:THR:HG22	1:124:A:TYR:HE2	25	0.98	0.09	1.0
(1,306)	2:36:B:THR:HG21	1:124:A:TYR:HE2	25	0.98	0.09	1.0
(1,306)	2:36:B:THR:HG23	1:124:A:TYR:HE2	25	0.98	0.09	1.0
(1,306)	2:36:B:THR:HG22	1:124:A:TYR:HE1	25	0.98	0.09	1.0
(1,306)	2:36:B:THR:HG23	1:124:A:TYR:HE1	25	0.98	0.09	1.0
(1,306)	2:36:B:THR:HG21	1:124:A:TYR:HE1	25	0.98	0.09	1.0
(1,1311)	1:82:A:PRO:HD2	1:82:A:PRO:HB3	25	0.96	0.01	0.97
(1,443)	1:117:A:ARG:H	1:126:A:TYR:HE2	25	0.95	0.09	0.95
(1,443)	2:36:B:THR:H	2:34:B:TYR:HD1	25	0.95	0.09	0.95
(1,1194)	1:89:A:TYR:HB2	1:89:A:TYR:HD1	25	0.94	0.01	0.94
(1,174)	1:84:A:VAL:HG11	1:124:A:TYR:HA	25	0.93	0.07	0.93
(1,174)	1:84:A:VAL:HG13	1:124:A:TYR:HA	25	0.93	0.07	0.93
(1,174)	1:84:A:VAL:HG12	1:124:A:TYR:HA	25	0.93	0.07	0.93
(1,2119)	1:122:A:LYS:HB3	1:122:A:LYS:H	25	0.93	0.05	0.94
(1,9)	1:134:A:LEU:HD21	1:131:A:CYS:HA	25	0.92	0.07	0.91
(1,9)	1:134:A:LEU:HD23	1:131:A:CYS:HA	25	0.92	0.07	0.91
(1,9)	1:134:A:LEU:HD22	1:131:A:CYS:HA	25	0.92	0.07	0.91
(1,1722)	2:31:B:LEU:HD22	1:128:A:ASN:HB2	25	0.9	0.11	0.91
(1,1722)	2:31:B:LEU:HD23	1:128:A:ASN:HB2	25	0.9	0.11	0.91
(1,1722)	2:31:B:LEU:HD21	1:128:A:ASN:HB2	25	0.9	0.11	0.91
(1,1518)	1:61:A:LEU:HB2	1:61:A:LEU:HD23	25	0.9	0.04	0.91
(1,1518)	1:61:A:LEU:HB2	1:61:A:LEU:HD22	25	0.9	0.04	0.91
(1,1518)	1:61:A:LEU:HB2	1:61:A:LEU:HD21	25	0.9	0.04	0.91
(1,2061)	1:87:A:PHE:H	1:85:A:VAL:HG21	25	0.9	0.04	0.89
(1,2061)	1:87:A:PHE:H	1:85:A:VAL:HG22	25	0.9	0.04	0.89
(1,2061)	1:87:A:PHE:H	1:85:A:VAL:HG23	25	0.9	0.04	0.89
(1,150)	1:88:A:LEU:HD22	1:128:A:ASN:H	25	0.89	0.08	0.88
(1,150)	1:88:A:LEU:HD21	1:128:A:ASN:H	25	0.89	0.08	0.88
(1,150)	1:88:A:LEU:HD23	1:128:A:ASN:H	25	0.89	0.08	0.88

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1649)	2:37:B:ALA:HB2	2:38:B:ARG:HB2	25	0.89	0.16	0.92
(1,1649)	2:37:B:ALA:HB1	2:38:B:ARG:HB2	25	0.89	0.16	0.92
(1,1649)	2:37:B:ALA:HB3	2:38:B:ARG:HB2	25	0.89	0.16	0.92
(1,164)	1:87:A:PHE:HB3	1:87:A:PHE:HE2	25	0.89	0.06	0.9
(1,401)	1:113:A:LEU:HD23	1:113:A:LEU:H	25	0.87	0.07	0.87
(1,401)	1:113:A:LEU:HD21	1:113:A:LEU:H	25	0.87	0.07	0.87
(1,401)	1:113:A:LEU:HD22	1:113:A:LEU:H	25	0.87	0.07	0.87
(1,128)	1:93:A:GLN:HG2	1:94:A:ARG:H	25	0.87	0.12	0.9
(1,128)	1:93:A:GLN:HG2	1:89:A:TYR:HD1	25	0.87	0.12	0.9
(1,208)	1:71:A:LEU:HD23	1:88:A:LEU:H	25	0.87	0.07	0.86
(1,208)	1:71:A:LEU:HD22	1:88:A:LEU:H	25	0.87	0.07	0.86
(1,208)	1:71:A:LEU:HD21	1:88:A:LEU:H	25	0.87	0.07	0.86
(1,1375)	1:74:A:CYS:HA	1:77:A:GLN:HB3	25	0.86	0.14	0.85
(1,16)	1:132:A:THR:HG23	1:133:A:VAL:H	25	0.86	0.09	0.84
(1,16)	1:132:A:THR:HG21	1:133:A:VAL:H	25	0.86	0.09	0.84
(1,16)	1:132:A:THR:HG22	1:133:A:VAL:H	25	0.86	0.09	0.84
(1,184)	1:79:A:ALA:HB3	1:75:A:LYS:HA	25	0.85	0.17	0.83
(1,184)	1:79:A:ALA:HB1	1:75:A:LYS:HA	25	0.85	0.17	0.83
(1,184)	1:79:A:ALA:HB2	1:75:A:LYS:HA	25	0.85	0.17	0.83
(1,694)	1:113:A:LEU:HB2	1:114:A:SER:H	25	0.85	0.04	0.86
(1,1261)	1:86:A:PRO:HD2	1:85:A:VAL:HG21	25	0.84	0.03	0.85
(1,1261)	1:86:A:PRO:HD2	1:85:A:VAL:HG22	25	0.84	0.03	0.85
(1,1261)	1:86:A:PRO:HD2	1:85:A:VAL:HG23	25	0.84	0.03	0.85
(1,205)	1:71:A:LEU:HD13	1:75:A:LYS:HE2	25	0.84	0.19	0.76
(1,205)	1:71:A:LEU:HD11	1:75:A:LYS:HE2	25	0.84	0.19	0.76
(1,205)	1:71:A:LEU:HD12	1:70:A:PHE:HB3	25	0.84	0.19	0.76
(1,205)	1:71:A:LEU:HD13	1:70:A:PHE:HB3	25	0.84	0.19	0.76
(1,205)	1:71:A:LEU:HD12	1:75:A:LYS:HE2	25	0.84	0.19	0.76
(1,1611)	2:39:B:TRP:HZ3	2:39:B:TRP:HB2	25	0.83	0.06	0.83
(1,15)	1:132:A:THR:HG22	2:27:B:SER:H	25	0.83	0.15	0.88
(1,15)	1:132:A:THR:HG21	1:135:A:LYS:H	25	0.83	0.15	0.88
(1,15)	1:132:A:THR:HG21	2:27:B:SER:H	25	0.83	0.15	0.88
(1,15)	1:132:A:THR:HG22	1:135:A:LYS:H	25	0.83	0.15	0.88
(1,15)	1:132:A:THR:HG23	1:135:A:LYS:H	25	0.83	0.15	0.88
(1,15)	1:132:A:THR:HG23	2:27:B:SER:H	25	0.83	0.15	0.88
(1,218)	1:116:A:ALA:HB1	1:70:A:PHE:HD2	25	0.83	0.06	0.83
(1,218)	1:116:A:ALA:HB2	1:70:A:PHE:HD2	25	0.83	0.06	0.83
(1,218)	1:116:A:ALA:HB3	1:70:A:PHE:HD2	25	0.83	0.06	0.83
(1,530)	1:66:A:LEU:HD22	1:67:A:PHE:H	25	0.82	0.04	0.82
(1,530)	1:66:A:LEU:HD21	1:67:A:PHE:H	25	0.82	0.04	0.82
(1,530)	1:66:A:LEU:HD23	1:67:A:PHE:H	25	0.82	0.04	0.82
(1,304)	2:36:B:THR:HG22	2:35:B:PHE:HB2	25	0.81	0.07	0.81

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,304)	2:36:B:THR:HG21	2:35:B:PHE:HB2	25	0.81	0.07	0.81
(1,304)	2:36:B:THR:HG23	2:35:B:PHE:HB2	25	0.81	0.07	0.81
(1,280)	2:31:B:LEU:HG	1:87:A:PHE:HE2	25	0.81	0.2	0.77
(1,280)	2:31:B:LEU:HG	1:87:A:PHE:HD2	25	0.81	0.2	0.77
(1,221)	1:130:A:LEU:HD23	1:70:A:PHE:HZ	25	0.8	0.07	0.83
(1,221)	1:130:A:LEU:HD22	1:70:A:PHE:HZ	25	0.8	0.07	0.83
(1,221)	1:112:A:VAL:HG22	1:70:A:PHE:HZ	25	0.8	0.07	0.83
(1,221)	1:130:A:LEU:HD21	1:70:A:PHE:HZ	25	0.8	0.07	0.83
(1,221)	1:112:A:VAL:HG21	1:70:A:PHE:HZ	25	0.8	0.07	0.83
(1,221)	1:112:A:VAL:HG23	1:70:A:PHE:HZ	25	0.8	0.07	0.83
(1,136)	1:91:A:ARG:HG3	1:91:A:ARG:H	25	0.79	0.03	0.8
(1,200)	1:72:A:GLU:HG2	1:71:A:LEU:HD11	25	0.77	0.03	0.76
(1,200)	1:72:A:GLU:HG2	1:71:A:LEU:HD12	25	0.77	0.03	0.76
(1,200)	1:72:A:GLU:HG3	1:71:A:LEU:HD11	25	0.77	0.03	0.76
(1,200)	1:72:A:GLU:HG3	1:71:A:LEU:HD13	25	0.77	0.03	0.76
(1,200)	1:72:A:GLU:HG2	1:71:A:LEU:HD13	25	0.77	0.03	0.76
(1,200)	1:72:A:GLU:HG3	1:71:A:LEU:HD12	25	0.77	0.03	0.76
(1,153)	1:88:A:LEU:HD22	1:128:A:ASN:HA	25	0.77	0.06	0.78
(1,153)	1:88:A:LEU:HD21	1:128:A:ASN:HA	25	0.77	0.06	0.78
(1,153)	1:88:A:LEU:HD23	1:128:A:ASN:HA	25	0.77	0.06	0.78
(1,35)	1:127:A:ILE:HG22	1:88:A:LEU:H	25	0.75	0.07	0.74
(1,35)	1:127:A:ILE:HG21	1:88:A:LEU:H	25	0.75	0.07	0.74
(1,35)	1:127:A:ILE:HG23	1:88:A:LEU:H	25	0.75	0.07	0.74
(1,332)	1:127:A:ILE:HG12	1:124:A:TYR:HD2	25	0.75	0.06	0.74
(1,332)	1:127:A:ILE:HG12	1:124:A:TYR:HD1	25	0.75	0.06	0.74
(1,533)	1:109:A:LEU:H	1:112:A:VAL:HG22	25	0.75	0.04	0.75
(1,533)	1:109:A:LEU:H	1:112:A:VAL:HG23	25	0.75	0.04	0.75
(1,533)	1:109:A:LEU:H	1:112:A:VAL:HG21	25	0.75	0.04	0.75
(1,178)	1:84:A:VAL:HG21	1:78:A:THR:H	25	0.75	0.07	0.74
(1,178)	1:84:A:VAL:HG22	1:78:A:THR:H	25	0.75	0.07	0.74
(1,178)	1:84:A:VAL:HG23	1:78:A:THR:H	25	0.75	0.07	0.74
(1,39)	1:127:A:ILE:HD12	1:124:A:TYR:HE2	25	0.74	0.03	0.74
(1,39)	1:127:A:ILE:HD13	1:124:A:TYR:HE2	25	0.74	0.03	0.74
(1,39)	1:127:A:ILE:HD13	1:124:A:TYR:HE1	25	0.74	0.03	0.74
(1,39)	1:127:A:ILE:HD12	1:124:A:TYR:HE1	25	0.74	0.03	0.74
(1,39)	1:127:A:ILE:HD11	1:124:A:TYR:HE1	25	0.74	0.03	0.74
(1,39)	1:127:A:ILE:HD11	1:124:A:TYR:HE2	25	0.74	0.03	0.74
(1,413)	1:131:A:CYS:H	1:134:A:LEU:HD12	25	0.74	0.07	0.76
(1,413)	1:131:A:CYS:H	1:130:A:LEU:HD13	25	0.74	0.07	0.76
(1,413)	1:131:A:CYS:H	1:134:A:LEU:HD13	25	0.74	0.07	0.76
(1,413)	1:131:A:CYS:H	1:130:A:LEU:HD11	25	0.74	0.07	0.76
(1,413)	1:131:A:CYS:H	1:134:A:LEU:HD11	25	0.74	0.07	0.76

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,413)	1:131:A:CYS:H	1:130:A:LEU:HD23	25	0.74	0.07	0.76
(1,413)	1:131:A:CYS:H	1:130:A:LEU:HD12	25	0.74	0.07	0.76
(1,207)	1:109:A:LEU:HD23	1:113:A:LEU:H	25	0.74	0.09	0.74
(1,207)	1:109:A:LEU:HD22	1:113:A:LEU:H	25	0.74	0.09	0.74
(1,207)	1:109:A:LEU:HD21	1:113:A:LEU:H	25	0.74	0.09	0.74
(1,961)	1:109:A:LEU:HD11	1:109:A:LEU:HA	25	0.73	0.01	0.73
(1,961)	1:109:A:LEU:HD12	1:109:A:LEU:HA	25	0.73	0.01	0.73
(1,961)	1:109:A:LEU:HD13	1:109:A:LEU:HA	25	0.73	0.01	0.73
(1,395)	1:138:A:SER:H	1:95:A:ALA:HB1	25	0.72	0.15	0.75
(1,395)	1:138:A:SER:H	1:139:A:ALA:HB1	25	0.72	0.15	0.75
(1,395)	1:138:A:SER:H	1:95:A:ALA:HB3	25	0.72	0.15	0.75
(1,395)	1:138:A:SER:H	1:139:A:ALA:HB3	25	0.72	0.15	0.75
(1,395)	1:138:A:SER:H	1:95:A:ALA:HB2	25	0.72	0.15	0.75
(1,212)	1:71:A:LEU:HD21	1:71:A:LEU:HB2	25	0.71	0.1	0.73
(1,212)	1:71:A:LEU:HD23	1:74:A:CYS:HG	25	0.71	0.1	0.73
(1,212)	1:71:A:LEU:HD22	1:74:A:CYS:HG	25	0.71	0.1	0.73
(1,212)	1:71:A:LEU:HD23	1:71:A:LEU:HB2	25	0.71	0.1	0.73
(1,212)	1:71:A:LEU:HD22	1:71:A:LEU:HB2	25	0.71	0.1	0.73
(1,793)	1:124:A:TYR:HE1	1:124:A:TYR:H	25	0.69	0.1	0.7
(1,793)	1:124:A:TYR:HE2	1:124:A:TYR:H	25	0.69	0.1	0.7
(1,1341)	1:76:A:MET:HB3	1:73:A:LEU:HA	25	0.68	0.13	0.68
(1,484)	1:134:A:LEU:HD11	1:94:A:ARG:H	25	0.68	0.12	0.68
(1,484)	1:134:A:LEU:HD13	1:94:A:ARG:H	25	0.68	0.12	0.68
(1,484)	1:134:A:LEU:HD12	1:94:A:ARG:H	25	0.68	0.12	0.68
(1,923)	1:112:A:VAL:HA	1:112:A:VAL:HG21	25	0.67	0.01	0.67
(1,923)	1:112:A:VAL:HA	1:112:A:VAL:HG22	25	0.67	0.01	0.67
(1,923)	1:112:A:VAL:HA	1:112:A:VAL:HG23	25	0.67	0.01	0.67
(1,216)	1:113:A:LEU:HD11	1:70:A:PHE:HD2	25	0.67	0.11	0.65
(1,216)	1:113:A:LEU:HD12	1:70:A:PHE:HD2	25	0.67	0.11	0.65
(1,216)	1:113:A:LEU:HD13	1:70:A:PHE:HD2	25	0.67	0.11	0.65
(1,1004)	1:108:A:ILE:HD12	1:109:A:LEU:H	25	0.67	0.04	0.68
(1,1004)	1:108:A:ILE:HD13	1:109:A:LEU:H	25	0.67	0.04	0.68
(1,1004)	1:108:A:ILE:HD11	1:109:A:LEU:H	25	0.67	0.04	0.68
(1,502)	1:81:A:HIS:H	1:82:A:PRO:HB3	25	0.66	0.18	0.73
(1,427)	1:126:A:TYR:H	1:127:A:ILE:HD13	25	0.66	0.06	0.65
(1,427)	1:126:A:TYR:H	1:127:A:ILE:HD11	25	0.66	0.06	0.65
(1,427)	1:126:A:TYR:H	1:127:A:ILE:HD12	25	0.66	0.06	0.65
(1,323)	1:84:A:VAL:HG23	2:34:B:TYR:HD1	25	0.66	0.07	0.67
(1,323)	1:84:A:VAL:HG21	2:34:B:TYR:HD1	25	0.66	0.07	0.67
(1,323)	1:84:A:VAL:HG22	2:34:B:TYR:HD1	25	0.66	0.07	0.67
(1,310)	2:35:B:PHE:HD1	1:127:A:ILE:HB	25	0.66	0.09	0.65
(1,498)	1:87:A:PHE:H	1:84:A:VAL:HG13	25	0.66	0.07	0.64

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,498)	1:87:A:PHE:H	1:84:A:VAL:HG12	25	0.66	0.07	0.64
(1,498)	1:87:A:PHE:H	1:84:A:VAL:HG11	25	0.66	0.07	0.64
(1,1503)	1:64:A:GLU:HB2	1:64:A:GLU:HG2	25	0.65	0.01	0.65
(1,333)	1:127:A:ILE:HG12	1:130:A:LEU:HD23	25	0.64	0.1	0.68
(1,333)	1:127:A:ILE:HG12	1:130:A:LEU:HD22	25	0.64	0.1	0.68
(1,333)	1:127:A:ILE:HG12	1:130:A:LEU:HD21	25	0.64	0.1	0.68
(1,519)	1:74:A:CYS:H	1:85:A:VAL:HG22	25	0.64	0.05	0.63
(1,519)	1:74:A:CYS:H	1:85:A:VAL:HG23	25	0.64	0.05	0.63
(1,519)	1:74:A:CYS:H	1:85:A:VAL:HG21	25	0.64	0.05	0.63
(1,293)	2:39:B:TRP:HD1	2:38:B:ARG:HB3	25	0.63	0.16	0.7
(1,293)	2:39:B:TRP:HD1	1:121:A:ALA:HB2	25	0.63	0.16	0.7
(1,293)	2:39:B:TRP:HD1	1:121:A:ALA:HB1	25	0.63	0.16	0.7
(1,170)	1:85:A:VAL:HG12	1:75:A:LYS:H	25	0.63	0.08	0.63
(1,170)	1:85:A:VAL:HG13	1:89:A:TYR:H	25	0.63	0.08	0.63
(1,170)	1:85:A:VAL:HG11	1:89:A:TYR:H	25	0.63	0.08	0.63
(1,170)	1:85:A:VAL:HG13	1:75:A:LYS:H	25	0.63	0.08	0.63
(1,170)	1:85:A:VAL:HG11	1:75:A:LYS:H	25	0.63	0.08	0.63
(1,170)	1:85:A:VAL:HG12	1:89:A:TYR:H	25	0.63	0.08	0.63
(1,499)	1:85:A:VAL:H	1:74:A:CYS:HB3	25	0.63	0.13	0.6
(1,499)	1:85:A:VAL:H	1:86:A:PRO:HG3	25	0.63	0.13	0.6
(1,144)	1:89:A:TYR:HB2	1:89:A:TYR:HE2	25	0.62	0.01	0.63
(1,144)	1:59:A:TYR:HE2	1:59:A:TYR:HB2	25	0.62	0.01	0.63
(1,407)	1:133:A:VAL:H	1:130:A:LEU:HD12	25	0.62	0.04	0.62
(1,407)	1:133:A:VAL:H	1:130:A:LEU:HD13	25	0.62	0.04	0.62
(1,407)	1:133:A:VAL:H	1:130:A:LEU:HD11	25	0.62	0.04	0.62
(1,290)	2:39:B:TRP:HH2	2:36:B:THR:HB	25	0.62	0.14	0.65
(1,290)	2:39:B:TRP:HH2	2:36:B:THR:HA	25	0.62	0.14	0.65
(1,152)	1:67:A:PHE:HE1	1:88:A:LEU:HD12	25	0.61	0.06	0.61
(1,152)	1:67:A:PHE:HE1	1:88:A:LEU:HD11	25	0.61	0.06	0.61
(1,152)	1:67:A:PHE:HE2	1:88:A:LEU:HD11	25	0.61	0.06	0.61
(1,152)	1:67:A:PHE:HE1	1:88:A:LEU:HD13	25	0.61	0.06	0.61
(1,529)	1:67:A:PHE:H	1:68:A:GLU:HB3	25	0.61	0.13	0.65
(1,529)	1:67:A:PHE:H	1:68:A:GLU:HB2	25	0.61	0.13	0.65
(1,529)	1:67:A:PHE:H	1:69:A:GLU:HB2	25	0.61	0.13	0.65
(1,1861)	1:123:A:LEU:HD22	1:123:A:LEU:H	25	0.6	0.04	0.61
(1,1861)	1:123:A:LEU:HD21	1:123:A:LEU:H	25	0.6	0.04	0.61
(1,1861)	1:123:A:LEU:HD23	1:123:A:LEU:H	25	0.6	0.04	0.61
(1,2082)	1:81:A:HIS:H	1:79:A:ALA:HB2	25	0.6	0.05	0.61
(1,2082)	1:81:A:HIS:H	1:79:A:ALA:HB3	25	0.6	0.05	0.61
(1,2082)	1:81:A:HIS:H	1:79:A:ALA:HB1	25	0.6	0.05	0.61
(1,1738)	2:31:B:LEU:HB3	2:31:B:LEU:HD22	25	0.6	0.01	0.6
(1,1738)	2:31:B:LEU:HB3	2:31:B:LEU:HD23	25	0.6	0.01	0.6

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1738)	2:31:B:LEU:HB3	2:31:B:LEU:HD21	25	0.6	0.01	0.6
(1,203)	1:71:A:LEU:HD11	1:68:A:GLU:H	25	0.59	0.15	0.58
(1,203)	1:71:A:LEU:HD12	1:68:A:GLU:H	25	0.59	0.15	0.58
(1,203)	1:71:A:LEU:HD13	1:68:A:GLU:H	25	0.59	0.15	0.58
(1,203)	1:71:A:LEU:HD13	1:72:A:GLU:H	25	0.59	0.15	0.58
(1,141)	1:93:A:GLN:HG2	1:89:A:TYR:HD1	25	0.59	0.21	0.58
(1,141)	1:89:A:TYR:HD2	1:86:A:PRO:HB2	25	0.59	0.21	0.58
(1,265)	1:127:A:ILE:HD12	2:35:B:PHE:HE1	25	0.58	0.07	0.59
(1,265)	1:127:A:ILE:HD13	2:35:B:PHE:HE1	25	0.58	0.07	0.59
(1,265)	1:127:A:ILE:HD11	2:35:B:PHE:HE1	25	0.58	0.07	0.59
(1,319)	2:34:B:TYR:HE1	1:84:A:VAL:HG23	25	0.58	0.05	0.59
(1,319)	2:34:B:TYR:HE1	1:84:A:VAL:HG21	25	0.58	0.05	0.59
(1,319)	2:34:B:TYR:HE1	1:84:A:VAL:HG22	25	0.58	0.05	0.59
(1,932)	1:112:A:VAL:HG23	1:126:A:TYR:HA	25	0.58	0.04	0.58
(1,932)	1:112:A:VAL:HG21	1:126:A:TYR:HA	25	0.58	0.04	0.58
(1,932)	1:112:A:VAL:HG22	1:126:A:TYR:HA	25	0.58	0.04	0.58
(1,825)	1:122:A:LYS:HG2	1:125:A:VAL:HG23	25	0.57	0.05	0.58
(1,825)	1:122:A:LYS:HG2	1:125:A:VAL:HG21	25	0.57	0.05	0.58
(1,825)	1:122:A:LYS:HG2	1:125:A:VAL:HG22	25	0.57	0.05	0.58
(1,1338)	1:76:A:MET:HB3	1:76:A:MET:H	25	0.57	0.02	0.58
(1,2017)	1:93:A:GLN:HE22	1:89:A:TYR:HB3	25	0.57	0.15	0.53
(1,434)	1:74:A:CYS:H	1:123:A:LEU:HD11	25	0.56	0.11	0.61
(1,434)	1:74:A:CYS:H	1:123:A:LEU:HD13	25	0.56	0.11	0.61
(1,434)	1:74:A:CYS:H	1:123:A:LEU:HD12	25	0.56	0.11	0.61
(1,1457)	1:68:A:GLU:HB2	1:68:A:GLU:HG2	25	0.56	0.2	0.69
(1,232)	1:66:A:LEU:HD11	1:62:A:GLU:HA	25	0.56	0.09	0.57
(1,232)	1:66:A:LEU:HD12	1:62:A:GLU:HA	25	0.56	0.09	0.57
(1,232)	1:66:A:LEU:HD11	1:110:A:SER:HA	25	0.56	0.09	0.57
(1,232)	1:66:A:LEU:HD13	1:110:A:SER:HA	25	0.56	0.09	0.57
(1,232)	1:66:A:LEU:HD13	1:62:A:GLU:HA	25	0.56	0.09	0.57
(1,232)	1:66:A:LEU:HD12	1:110:A:SER:HA	25	0.56	0.09	0.57
(1,1629)	2:38:B:ARG:HG2	2:38:B:ARG:HA	25	0.56	0.04	0.55
(1,1629)	2:38:B:ARG:HG3	2:38:B:ARG:HA	25	0.56	0.04	0.55
(1,338)	2:31:B:LEU:HD22	2:32:B:GLU:HG3	25	0.55	0.04	0.55
(1,338)	2:31:B:LEU:HD23	2:32:B:GLU:HG3	25	0.55	0.04	0.55
(1,338)	2:31:B:LEU:HD21	2:32:B:GLU:HG3	25	0.55	0.04	0.55
(1,1910)	1:109:A:LEU:HD23	1:110:A:SER:H	25	0.55	0.02	0.55
(1,1910)	1:109:A:LEU:HD22	1:110:A:SER:H	25	0.55	0.02	0.55
(1,1910)	1:109:A:LEU:HD21	1:110:A:SER:H	25	0.55	0.02	0.55
(1,230)	1:66:A:LEU:HA	1:113:A:LEU:HD21	25	0.55	0.1	0.56
(1,230)	1:66:A:LEU:HA	1:113:A:LEU:HD22	25	0.55	0.1	0.56
(1,230)	1:66:A:LEU:HA	1:113:A:LEU:HD23	25	0.55	0.1	0.56

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1501)	1:64:A:GLU:HG2	1:65:A:LYS:H	25	0.55	0.05	0.56
(1,848)	1:120:A:PRO:HG3	1:119:A:ARG:HA	25	0.55	0.04	0.55
(1,44)	1:126:A:TYR:HE1	1:112:A:VAL:HA	25	0.55	0.1	0.58
(1,44)	1:126:A:TYR:HE2	1:126:A:TYR:HB2	25	0.55	0.1	0.58
(1,398)	1:135:A:LYS:HG2	1:136:A:ALA:H	25	0.54	0.11	0.51
(1,1421)	1:71:A:LEU:HD21	1:71:A:LEU:H	25	0.54	0.04	0.54
(1,1421)	1:71:A:LEU:HD23	1:71:A:LEU:H	25	0.54	0.04	0.54
(1,1421)	1:71:A:LEU:HD22	1:71:A:LEU:H	25	0.54	0.04	0.54
(1,454)	1:114:A:SER:H	1:112:A:VAL:HG21	25	0.53	0.06	0.53
(1,454)	1:114:A:SER:H	1:112:A:VAL:HG22	25	0.53	0.06	0.53
(1,454)	1:114:A:SER:H	1:112:A:VAL:HG23	25	0.53	0.06	0.53
(1,340)	2:31:B:LEU:HD11	1:88:A:LEU:H	25	0.53	0.12	0.54
(1,340)	2:31:B:LEU:HD13	1:88:A:LEU:H	25	0.53	0.12	0.54
(1,340)	2:31:B:LEU:HD12	1:88:A:LEU:H	25	0.53	0.12	0.54
(1,555)	2:36:B:THR:H	2:35:B:PHE:H	25	0.53	0.03	0.54
(1,555)	2:36:B:THR:H	2:37:B:ALA:H	25	0.53	0.03	0.54
(1,1329)	1:77:A:GLN:HG2	1:77:A:GLN:HB3	25	0.52	0.13	0.57
(1,1496)	1:64:A:GLU:HG3	1:64:A:GLU:HA	25	0.52	0.06	0.53
(1,607)	1:136:A:ALA:HB3	1:137:A:HIS:HA	25	0.52	0.05	0.53
(1,607)	1:136:A:ALA:HB1	1:137:A:HIS:HA	25	0.52	0.05	0.53
(1,607)	1:136:A:ALA:HB2	1:137:A:HIS:HA	25	0.52	0.05	0.53
(1,2124)	1:73:A:LEU:HD23	1:73:A:LEU:H	25	0.52	0.03	0.53
(1,2124)	1:73:A:LEU:HD21	1:73:A:LEU:H	25	0.52	0.03	0.53
(1,2124)	1:73:A:LEU:HD22	1:73:A:LEU:H	25	0.52	0.03	0.53
(1,199)	1:72:A:GLU:HG2	1:71:A:LEU:HB3	25	0.52	0.08	0.51
(1,199)	1:72:A:GLU:HG3	1:71:A:LEU:HB3	25	0.52	0.08	0.51
(1,552)	2:35:B:PHE:H	2:33:B:GLN:HA	25	0.52	0.06	0.53
(1,552)	2:36:B:THR:HA	2:35:B:PHE:H	25	0.52	0.06	0.53
(1,1576)	1:73:A:LEU:HD11	1:117:A:ARG:H	25	0.51	0.05	0.5
(1,1576)	1:73:A:LEU:HD13	1:117:A:ARG:H	25	0.51	0.05	0.5
(1,1576)	1:73:A:LEU:HD12	1:117:A:ARG:H	25	0.51	0.05	0.5
(1,281)	2:31:B:LEU:HD21	1:128:A:ASN:H	25	0.51	0.1	0.53
(1,281)	2:31:B:LEU:HD22	1:128:A:ASN:H	25	0.51	0.1	0.53
(1,281)	2:31:B:LEU:HD23	1:128:A:ASN:H	25	0.51	0.1	0.53
(1,151)	1:88:A:LEU:HD13	1:70:A:PHE:HD1	25	0.5	0.05	0.49
(1,151)	1:88:A:LEU:HD12	1:70:A:PHE:HD1	25	0.5	0.05	0.49
(1,151)	1:88:A:LEU:HD11	1:70:A:PHE:HD1	25	0.5	0.05	0.49
(1,455)	1:112:A:VAL:H	1:113:A:LEU:HB3	25	0.5	0.05	0.5
(1,2012)	1:94:A:ARG:HB3	1:94:A:ARG:H	25	0.5	0.06	0.52
(1,2013)	1:94:A:ARG:H	1:95:A:ALA:HB2	25	0.5	0.07	0.51
(1,2013)	1:94:A:ARG:H	1:95:A:ALA:HB1	25	0.5	0.07	0.51
(1,2013)	1:94:A:ARG:H	1:95:A:ALA:HB3	25	0.5	0.07	0.51

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,457)	1:111:A:ARG:H	1:109:A:LEU:HB3	25	0.49	0.05	0.49
(1,325)	2:33:B:GLN:HG2	2:31:B:LEU:HB2	25	0.49	0.03	0.48
(1,1736)	2:31:B:LEU:HB2	2:31:B:LEU:HD12	25	0.48	0.01	0.49
(1,1736)	2:31:B:LEU:HB2	2:31:B:LEU:HD11	25	0.48	0.01	0.49
(1,1736)	2:31:B:LEU:HB2	2:31:B:LEU:HD13	25	0.48	0.01	0.49
(1,195)	1:73:A:LEU:HD23	1:70:A:PHE:HA	25	0.48	0.07	0.5
(1,195)	1:73:A:LEU:HD21	1:70:A:PHE:HA	25	0.48	0.07	0.5
(1,195)	1:73:A:LEU:HD22	1:70:A:PHE:HA	25	0.48	0.07	0.5
(1,195)	1:73:A:LEU:HD22	1:117:A:ARG:HA	25	0.48	0.07	0.5
(1,195)	1:73:A:LEU:HD23	1:117:A:ARG:HA	25	0.48	0.07	0.5
(1,1076)	1:101:A:ALA:HB1	1:98:A:LEU:HD21	25	0.48	0.17	0.46
(1,1076)	1:101:A:ALA:HB2	1:98:A:LEU:HD21	25	0.48	0.17	0.46
(1,1076)	1:101:A:ALA:HB3	1:98:A:LEU:HD21	25	0.48	0.17	0.46
(1,1076)	1:101:A:ALA:HB2	1:98:A:LEU:HD23	25	0.48	0.17	0.46
(1,1076)	1:101:A:ALA:HB3	1:98:A:LEU:HD22	25	0.48	0.17	0.46
(1,1076)	1:101:A:ALA:HB1	1:98:A:LEU:HD22	25	0.48	0.17	0.46
(1,1076)	1:101:A:ALA:HB2	1:98:A:LEU:HD22	25	0.48	0.17	0.46
(1,1076)	1:101:A:ALA:HB1	1:98:A:LEU:HD23	25	0.48	0.17	0.46
(1,1076)	1:101:A:ALA:HB3	1:98:A:LEU:HD23	25	0.48	0.17	0.46
(1,1477)	1:66:A:LEU:HD22	1:113:A:LEU:HB3	25	0.48	0.14	0.43
(1,1477)	1:66:A:LEU:HD21	1:113:A:LEU:HB3	25	0.48	0.14	0.43
(1,1477)	1:66:A:LEU:HD23	1:113:A:LEU:HB3	25	0.48	0.14	0.43
(1,1199)	1:89:A:TYR:HE1	1:71:A:LEU:HD11	25	0.47	0.17	0.46
(1,1199)	1:89:A:TYR:HE1	1:71:A:LEU:HD12	25	0.47	0.17	0.46
(1,1199)	1:89:A:TYR:HE1	1:71:A:LEU:HD13	25	0.47	0.17	0.46
(1,1447)	1:69:A:GLU:HA	1:69:A:GLU:HG3	25	0.47	0.22	0.37
(1,289)	2:39:B:TRP:HZ3	2:36:B:THR:HB	25	0.47	0.07	0.47
(1,835)	1:120:A:PRO:HB3	1:120:A:PRO:HD2	25	0.47	0.01	0.47
(1,444)	1:73:A:LEU:HD11	1:117:A:ARG:H	25	0.47	0.05	0.46
(1,444)	1:73:A:LEU:HD13	1:117:A:ARG:H	25	0.47	0.05	0.46
(1,444)	1:73:A:LEU:HD12	1:117:A:ARG:H	25	0.47	0.05	0.46
(1,705)	1:130:A:LEU:HD13	1:109:A:LEU:HD13	25	0.46	0.04	0.47
(1,705)	1:130:A:LEU:HD11	1:109:A:LEU:HD11	25	0.46	0.04	0.47
(1,705)	1:130:A:LEU:HD13	1:109:A:LEU:HD11	25	0.46	0.04	0.47
(1,705)	1:130:A:LEU:HD12	1:109:A:LEU:HD13	25	0.46	0.04	0.47
(1,705)	1:130:A:LEU:HD13	1:109:A:LEU:HD12	25	0.46	0.04	0.47
(1,705)	1:130:A:LEU:HD11	1:109:A:LEU:HD12	25	0.46	0.04	0.47
(1,705)	1:130:A:LEU:HD11	1:109:A:LEU:HD13	25	0.46	0.04	0.47
(1,705)	1:130:A:LEU:HD12	1:109:A:LEU:HD12	25	0.46	0.04	0.47
(1,705)	1:130:A:LEU:HD12	1:109:A:LEU:HD11	25	0.46	0.04	0.47
(1,219)	1:70:A:PHE:HD1	1:73:A:LEU:HB3	25	0.46	0.03	0.46
(1,6)	1:130:A:LEU:HD21	1:70:A:PHE:HE2	25	0.46	0.05	0.46

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,6)	1:130:A:LEU:HD23	1:70:A:PHE:HE2	25	0.46	0.05	0.46
(1,6)	1:130:A:LEU:HD22	1:70:A:PHE:HE2	25	0.46	0.05	0.46
(1,1337)	1:76:A:MET:HA	1:76:A:MET:HG3	25	0.46	0.03	0.46
(1,1228)	1:87:A:PHE:HD1	1:88:A:LEU:HD23	25	0.46	0.48	0.26
(1,1228)	1:87:A:PHE:HD1	1:88:A:LEU:HD22	25	0.46	0.48	0.26
(1,1228)	1:87:A:PHE:HD1	1:88:A:LEU:HD21	25	0.46	0.48	0.26
(1,1059)	1:103:A:ALA:HB2	1:104:A:GLU:HA	25	0.45	0.04	0.45
(1,1059)	1:103:A:ALA:HB3	1:104:A:GLU:HA	25	0.45	0.04	0.45
(1,1059)	1:103:A:ALA:HB1	1:104:A:GLU:HA	25	0.45	0.04	0.45
(1,201)	2:25:B:GLU:HG3	2:25:B:GLU:HB2	25	0.45	0.05	0.46
(1,201)	1:72:A:GLU:HG3	1:72:A:GLU:HB2	25	0.45	0.05	0.46
(1,201)	2:25:B:GLU:HG2	2:25:B:GLU:HB2	25	0.45	0.05	0.46
(1,201)	2:30:B:GLU:HG3	2:30:B:GLU:HB2	25	0.45	0.05	0.46
(1,2063)	1:85:A:VAL:H	1:71:A:LEU:HD22	25	0.45	0.03	0.44
(1,2063)	1:85:A:VAL:H	1:71:A:LEU:HD21	25	0.45	0.03	0.44
(1,2063)	1:85:A:VAL:H	1:71:A:LEU:HD23	25	0.45	0.03	0.44
(1,1431)	1:70:A:PHE:HB2	1:70:A:PHE:HD1	25	0.45	0.0	0.45
(1,194)	1:73:A:LEU:HD23	1:70:A:PHE:HD1	25	0.44	0.05	0.44
(1,194)	1:73:A:LEU:HD21	1:70:A:PHE:HD1	25	0.44	0.05	0.44
(1,194)	1:73:A:LEU:HD22	1:70:A:PHE:HD1	25	0.44	0.05	0.44
(1,1475)	1:66:A:LEU:HD23	1:109:A:LEU:HD21	25	0.44	0.04	0.44
(1,1475)	1:66:A:LEU:HD22	1:109:A:LEU:HD23	25	0.44	0.04	0.44
(1,1475)	1:66:A:LEU:HD21	1:109:A:LEU:HD23	25	0.44	0.04	0.44
(1,1475)	1:66:A:LEU:HD23	1:109:A:LEU:HD22	25	0.44	0.04	0.44
(1,1475)	1:66:A:LEU:HD22	1:109:A:LEU:HD22	25	0.44	0.04	0.44
(1,1475)	1:66:A:LEU:HD23	1:109:A:LEU:HD23	25	0.44	0.04	0.44
(1,1475)	1:66:A:LEU:HD21	1:109:A:LEU:HD22	25	0.44	0.04	0.44
(1,1475)	1:66:A:LEU:HD21	1:109:A:LEU:HD21	25	0.44	0.04	0.44
(1,1475)	1:66:A:LEU:HD22	1:109:A:LEU:HD21	25	0.44	0.04	0.44
(1,2060)	1:86:A:PRO:HB3	1:87:A:PHE:H	25	0.44	0.04	0.44
(1,399)	1:135:A:LYS:H	1:133:A:VAL:HA	25	0.44	0.03	0.44
(1,670)	1:133:A:VAL:HG22	1:105:A:PHE:HE1	25	0.44	0.03	0.44
(1,670)	1:133:A:VAL:HG21	1:105:A:PHE:HE1	25	0.44	0.03	0.44
(1,670)	1:133:A:VAL:HG23	1:105:A:PHE:HE1	25	0.44	0.03	0.44
(1,97)	1:105:A:PHE:HD1	1:134:A:LEU:HA	25	0.44	0.13	0.41
(1,97)	1:105:A:PHE:HD1	1:100:A:LEU:HA	25	0.44	0.13	0.41
(1,180)	1:82:A:PRO:HA	1:82:A:PRO:HG2	25	0.44	0.01	0.44
(1,1422)	1:71:A:LEU:HD21	1:74:A:CYS:H	25	0.43	0.02	0.43
(1,1422)	1:71:A:LEU:HD23	1:74:A:CYS:H	25	0.43	0.02	0.43
(1,1422)	1:71:A:LEU:HD22	1:74:A:CYS:H	25	0.43	0.02	0.43
(1,48)	1:126:A:TYR:HE1	1:125:A:VAL:HG12	25	0.43	0.07	0.42
(1,48)	1:126:A:TYR:HE1	1:125:A:VAL:HG11	25	0.43	0.07	0.42

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,48)	1:126:A:TYR:HE1	1:125:A:VAL:HG13	25	0.43	0.07	0.42
(1,1303)	1:137:A:HIS:HE1	1:136:A:ALA:HB2	25	0.43	0.05	0.43
(1,1303)	1:137:A:HIS:HE1	1:136:A:ALA:HB3	25	0.43	0.05	0.43
(1,1303)	1:137:A:HIS:HE1	1:136:A:ALA:HB1	25	0.43	0.05	0.43
(1,888)	1:116:A:ALA:HB3	1:123:A:LEU:H	25	0.42	0.03	0.43
(1,888)	1:116:A:ALA:HB1	1:123:A:LEU:H	25	0.42	0.03	0.43
(1,888)	1:116:A:ALA:HB2	1:123:A:LEU:H	25	0.42	0.03	0.43
(1,1924)	1:108:A:ILE:HG23	1:108:A:ILE:H	25	0.42	0.02	0.42
(1,1924)	1:108:A:ILE:HG21	1:108:A:ILE:H	25	0.42	0.02	0.42
(1,1924)	1:108:A:ILE:HG22	1:108:A:ILE:H	25	0.42	0.02	0.42
(1,989)	1:108:A:ILE:HG21	1:105:A:PHE:HA	25	0.42	0.06	0.43
(1,989)	1:108:A:ILE:HG22	1:105:A:PHE:HA	25	0.42	0.06	0.43
(1,989)	1:108:A:ILE:HG23	1:105:A:PHE:HA	25	0.42	0.06	0.43
(1,171)	1:84:A:VAL:HG13	1:85:A:VAL:H	25	0.42	0.02	0.42
(1,171)	1:84:A:VAL:HG12	1:85:A:VAL:H	25	0.42	0.02	0.42
(1,171)	1:84:A:VAL:HG11	1:85:A:VAL:H	25	0.42	0.02	0.42
(1,1481)	1:66:A:LEU:HD22	1:69:A:GLU:H	25	0.42	0.04	0.41
(1,1481)	1:66:A:LEU:HD21	1:69:A:GLU:H	25	0.42	0.04	0.41
(1,1481)	1:66:A:LEU:HD23	1:69:A:GLU:H	25	0.42	0.04	0.41
(1,1788)	1:139:A:ALA:H	1:135:A:LYS:HD3	25	0.42	0.1	0.42
(1,1788)	1:139:A:ALA:H	1:135:A:LYS:HD2	25	0.42	0.1	0.42
(1,1830)	1:128:A:ASN:H	1:128:A:ASN:HB3	25	0.42	0.02	0.42
(1,13)	1:133:A:VAL:HG12	1:108:A:ILE:HB	25	0.42	0.1	0.41
(1,13)	1:133:A:VAL:HG11	1:108:A:ILE:HB	25	0.42	0.1	0.41
(1,13)	1:133:A:VAL:HG13	1:108:A:ILE:HB	25	0.42	0.1	0.41
(1,2106)	1:76:A:MET:HB3	1:77:A:GLN:H	25	0.42	0.1	0.44
(1,494)	1:90:A:ASN:H	1:88:A:LEU:HB2	25	0.42	0.03	0.42
(1,67)	1:116:A:ALA:HB3	1:120:A:PRO:HA	25	0.41	0.1	0.42
(1,67)	1:116:A:ALA:HB1	1:120:A:PRO:HA	25	0.41	0.1	0.42
(1,67)	1:116:A:ALA:HB2	1:120:A:PRO:HA	25	0.41	0.1	0.42
(1,1385)	1:73:A:LEU:HB2	1:74:A:CYS:H	25	0.4	0.03	0.41
(1,132)	1:92:A:GLN:HB3	1:89:A:TYR:HD1	25	0.4	0.14	0.41
(1,132)	1:67:A:PHE:HE2	1:92:A:GLN:HB3	25	0.4	0.14	0.41
(1,132)	1:67:A:PHE:HE1	1:92:A:GLN:HB3	25	0.4	0.14	0.41
(1,1248)	1:85:A:VAL:HA	1:71:A:LEU:HD13	25	0.4	0.02	0.4
(1,1248)	1:85:A:VAL:HA	1:71:A:LEU:HD11	25	0.4	0.02	0.4
(1,1248)	1:85:A:VAL:HA	1:71:A:LEU:HD12	25	0.4	0.02	0.4
(1,1851)	1:124:A:TYR:HB3	1:124:A:TYR:H	25	0.4	0.01	0.4
(1,419)	1:129:A:GLU:H	1:126:A:TYR:H	25	0.4	0.04	0.39
(1,155)	1:88:A:LEU:HD22	1:131:A:CYS:HB3	25	0.4	0.07	0.39
(1,155)	1:88:A:LEU:HD21	1:131:A:CYS:HB3	25	0.4	0.07	0.39
(1,155)	1:88:A:LEU:HD12	1:74:A:CYS:HB2	25	0.4	0.07	0.39

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,155)	1:88:A:LEU:HD13	1:74:A:CYS:HB2	25	0.4	0.07	0.39
(1,155)	1:88:A:LEU:HD23	1:131:A:CYS:HB3	25	0.4	0.07	0.39
(1,155)	1:88:A:LEU:HD11	1:74:A:CYS:HB2	25	0.4	0.07	0.39
(1,1480)	1:66:A:LEU:HD23	1:63:A:ASN:HA	25	0.4	0.05	0.4
(1,1480)	1:66:A:LEU:HD22	1:63:A:ASN:HA	25	0.4	0.05	0.4
(1,1480)	1:66:A:LEU:HD21	1:63:A:ASN:HA	25	0.4	0.05	0.4
(1,1336)	1:76:A:MET:HA	1:76:A:MET:HB2	25	0.4	0.01	0.39
(1,1094)	1:100:A:LEU:HD23	1:138:A:SER:HB2	25	0.39	0.12	0.42
(1,1094)	1:100:A:LEU:HD22	1:138:A:SER:HB2	25	0.39	0.12	0.42
(1,1094)	1:100:A:LEU:HD21	1:138:A:SER:HB2	25	0.39	0.12	0.42
(1,917)	1:113:A:LEU:HB2	1:113:A:LEU:HD21	25	0.39	0.03	0.38
(1,917)	1:113:A:LEU:HB2	1:113:A:LEU:HD22	25	0.39	0.03	0.38
(1,917)	1:113:A:LEU:HB2	1:113:A:LEU:HD23	25	0.39	0.03	0.38
(1,1416)	1:71:A:LEU:HD11	1:71:A:LEU:H	25	0.39	0.05	0.39
(1,1416)	1:71:A:LEU:HD12	1:71:A:LEU:H	25	0.39	0.05	0.39
(1,1416)	1:71:A:LEU:HD13	1:71:A:LEU:H	25	0.39	0.05	0.39
(1,743)	1:127:A:ILE:HG21	1:124:A:TYR:HA	25	0.38	0.03	0.38
(1,743)	1:127:A:ILE:HG23	1:124:A:TYR:HA	25	0.38	0.03	0.38
(1,743)	1:127:A:ILE:HG22	1:124:A:TYR:HA	25	0.38	0.03	0.38
(1,312)	2:35:B:PHE:HE1	1:124:A:TYR:HA	25	0.38	0.06	0.4
(1,312)	2:35:B:PHE:HE1	2:36:B:THR:HA	25	0.38	0.06	0.4
(1,37)	1:127:A:ILE:HG23	1:128:A:ASN:HD22	25	0.38	0.06	0.38
(1,37)	1:127:A:ILE:HG22	1:128:A:ASN:HD22	25	0.38	0.06	0.38
(1,37)	1:127:A:ILE:HG21	1:128:A:ASN:HD22	25	0.38	0.06	0.38
(1,1568)	1:57:A:LYS:HD2	1:57:A:LYS:HE2	25	0.38	0.01	0.38
(1,693)	1:130:A:LEU:HA	1:130:A:LEU:HB3	25	0.38	0.01	0.38
(1,476)	1:96:A:HIS:H	1:95:A:ALA:H	25	0.37	0.04	0.37
(1,476)	1:96:A:HIS:H	1:138:A:SER:H	25	0.37	0.04	0.37
(1,98)	1:105:A:PHE:HD1	1:100:A:LEU:HD21	25	0.37	0.33	0.28
(1,98)	1:105:A:PHE:HD1	1:100:A:LEU:HD23	25	0.37	0.33	0.28
(1,98)	1:105:A:PHE:HD1	1:109:A:LEU:HD23	25	0.37	0.33	0.28
(1,98)	1:105:A:PHE:HD1	1:100:A:LEU:HD22	25	0.37	0.33	0.28
(1,1466)	1:109:A:LEU:HD11	1:66:A:LEU:HG	25	0.37	0.03	0.37
(1,1466)	1:109:A:LEU:HD12	1:66:A:LEU:HG	25	0.37	0.03	0.37
(1,1466)	1:109:A:LEU:HD13	1:66:A:LEU:HG	25	0.37	0.03	0.37
(1,809)	1:123:A:LEU:HD12	1:123:A:LEU:HD23	25	0.37	0.02	0.37
(1,809)	1:123:A:LEU:HD13	1:123:A:LEU:HD23	25	0.37	0.02	0.37
(1,809)	1:123:A:LEU:HD11	1:123:A:LEU:HD22	25	0.37	0.02	0.37
(1,809)	1:123:A:LEU:HD13	1:123:A:LEU:HD22	25	0.37	0.02	0.37
(1,809)	1:123:A:LEU:HD12	1:123:A:LEU:HD21	25	0.37	0.02	0.37
(1,809)	1:123:A:LEU:HD13	1:123:A:LEU:HD21	25	0.37	0.02	0.37
(1,809)	1:123:A:LEU:HD11	1:123:A:LEU:HD23	25	0.37	0.02	0.37

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,809)	1:123:A:LEU:HD12	1:123:A:LEU:HD22	25	0.37	0.02	0.37
(1,809)	1:123:A:LEU:HD11	1:123:A:LEU:HD21	25	0.37	0.02	0.37
(1,445)	1:116:A:ALA:H	1:112:A:VAL:HA	25	0.37	0.09	0.37
(1,668)	1:133:A:VAL:HG12	1:130:A:LEU:HD12	25	0.37	0.03	0.37
(1,668)	1:133:A:VAL:HG11	1:130:A:LEU:HD13	25	0.37	0.03	0.37
(1,668)	1:133:A:VAL:HG12	1:130:A:LEU:HD13	25	0.37	0.03	0.37
(1,668)	1:133:A:VAL:HG13	1:130:A:LEU:HD13	25	0.37	0.03	0.37
(1,668)	1:133:A:VAL:HG11	1:130:A:LEU:HD12	25	0.37	0.03	0.37
(1,668)	1:133:A:VAL:HG13	1:130:A:LEU:HD11	25	0.37	0.03	0.37
(1,668)	1:133:A:VAL:HG12	1:130:A:LEU:HD11	25	0.37	0.03	0.37
(1,668)	1:133:A:VAL:HG11	1:130:A:LEU:HD11	25	0.37	0.03	0.37
(1,668)	1:133:A:VAL:HG13	1:130:A:LEU:HD12	25	0.37	0.03	0.37
(1,996)	1:108:A:ILE:HG22	1:112:A:VAL:HG11	25	0.37	0.11	0.34
(1,996)	1:108:A:ILE:HG23	1:112:A:VAL:HG12	25	0.37	0.11	0.34
(1,996)	1:108:A:ILE:HG23	1:112:A:VAL:HG13	25	0.37	0.11	0.34
(1,996)	1:108:A:ILE:HG23	1:112:A:VAL:HG11	25	0.37	0.11	0.34
(1,996)	1:108:A:ILE:HG21	1:112:A:VAL:HG11	25	0.37	0.11	0.34
(1,996)	1:108:A:ILE:HG21	1:112:A:VAL:HG12	25	0.37	0.11	0.34
(1,996)	1:108:A:ILE:HG22	1:112:A:VAL:HG12	25	0.37	0.11	0.34
(1,996)	1:108:A:ILE:HG21	1:112:A:VAL:HG13	25	0.37	0.11	0.34
(1,996)	1:108:A:ILE:HG22	1:112:A:VAL:HG13	25	0.37	0.11	0.34
(1,81)	1:116:A:ALA:HB2	1:70:A:PHE:HZ	25	0.36	0.09	0.35
(1,81)	1:116:A:ALA:HB3	1:70:A:PHE:HZ	25	0.36	0.09	0.35
(1,81)	1:116:A:ALA:HB1	1:70:A:PHE:HZ	25	0.36	0.09	0.35
(1,541)	1:61:A:LEU:HB3	1:62:A:GLU:H	25	0.35	0.05	0.34
(1,1768)	2:24:B:GLN:HB2	2:24:B:GLN:HG2	25	0.35	0.05	0.34
(1,1768)	2:24:B:GLN:HG3	2:24:B:GLN:HB2	25	0.35	0.05	0.34
(1,1282)	1:84:A:VAL:HG22	1:85:A:VAL:H	25	0.35	0.03	0.35
(1,1282)	1:84:A:VAL:HG23	1:85:A:VAL:H	25	0.35	0.03	0.35
(1,1282)	1:84:A:VAL:HG21	1:85:A:VAL:H	25	0.35	0.03	0.35
(1,220)	1:70:A:PHE:HE2	1:113:A:LEU:HB2	25	0.35	0.08	0.33
(1,1618)	2:39:B:TRP:HD1	2:39:B:TRP:HB3	25	0.35	0.01	0.35
(1,87)	1:112:A:VAL:HG13	1:130:A:LEU:H	25	0.34	0.05	0.35
(1,87)	1:112:A:VAL:HG11	1:130:A:LEU:H	25	0.34	0.05	0.35
(1,87)	1:112:A:VAL:HG12	1:130:A:LEU:H	25	0.34	0.05	0.35
(1,94)	1:107:A:ASN:HA	1:108:A:ILE:H	25	0.34	0.01	0.34
(1,94)	1:90:A:ASN:HA	1:91:A:ARG:H	25	0.34	0.01	0.34
(1,936)	1:112:A:VAL:HG13	1:112:A:VAL:HG23	25	0.34	0.02	0.34
(1,936)	1:112:A:VAL:HG11	1:112:A:VAL:HG23	25	0.34	0.02	0.34
(1,936)	1:112:A:VAL:HG12	1:112:A:VAL:HG23	25	0.34	0.02	0.34
(1,936)	1:112:A:VAL:HG13	1:112:A:VAL:HG21	25	0.34	0.02	0.34
(1,936)	1:112:A:VAL:HG13	1:112:A:VAL:HG22	25	0.34	0.02	0.34

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,936)	1:112:A:VAL:HG11	1:112:A:VAL:HG22	25	0.34	0.02	0.34
(1,936)	1:112:A:VAL:HG12	1:112:A:VAL:HG21	25	0.34	0.02	0.34
(1,936)	1:112:A:VAL:HG11	1:112:A:VAL:HG21	25	0.34	0.02	0.34
(1,936)	1:112:A:VAL:HG12	1:112:A:VAL:HG22	25	0.34	0.02	0.34
(1,51)	1:126:A:TYR:HD1	1:125:A:VAL:HG12	25	0.34	0.07	0.33
(1,51)	1:126:A:TYR:HD1	1:125:A:VAL:HG11	25	0.34	0.07	0.33
(1,51)	1:126:A:TYR:HD1	1:125:A:VAL:HG13	25	0.34	0.07	0.33
(1,2173)	1:63:A:ASN:H	1:109:A:LEU:HD11	25	0.34	0.08	0.36
(1,2173)	1:63:A:ASN:H	1:109:A:LEU:HD13	25	0.34	0.08	0.36
(1,2173)	1:63:A:ASN:H	1:109:A:LEU:HD12	25	0.34	0.08	0.36
(1,886)	1:116:A:ALA:HA	1:123:A:LEU:HD13	25	0.34	0.05	0.33
(1,886)	1:116:A:ALA:HA	1:123:A:LEU:HD12	25	0.34	0.05	0.33
(1,886)	1:116:A:ALA:HA	1:123:A:LEU:HD11	25	0.34	0.05	0.33
(1,500)	1:85:A:VAL:H	1:83:A:GLU:H	25	0.33	0.08	0.35
(1,2142)	1:109:A:LEU:HD21	1:68:A:GLU:H	25	0.33	0.04	0.34
(1,2142)	1:109:A:LEU:HD23	1:68:A:GLU:H	25	0.33	0.04	0.34
(1,2142)	1:109:A:LEU:HD22	1:68:A:GLU:H	25	0.33	0.04	0.34
(1,1577)	1:77:A:GLN:HG3	1:73:A:LEU:HD13	25	0.33	0.12	0.3
(1,1577)	1:77:A:GLN:HG3	1:73:A:LEU:HD12	25	0.33	0.12	0.3
(1,1577)	1:77:A:GLN:HG3	1:73:A:LEU:HD11	25	0.33	0.12	0.3
(1,1577)	1:77:A:GLN:HG2	1:73:A:LEU:HD12	25	0.33	0.12	0.3
(1,1577)	1:77:A:GLN:HG2	1:73:A:LEU:HD13	25	0.33	0.12	0.3
(1,244)	1:111:A:ARG:HA	1:115:A:ARG:HG2	25	0.33	0.08	0.35
(1,244)	1:61:A:LEU:HG	1:61:A:LEU:HA	25	0.33	0.08	0.35
(1,643)	1:134:A:LEU:HD21	1:134:A:LEU:HD13	25	0.33	0.02	0.32
(1,643)	1:134:A:LEU:HD23	1:134:A:LEU:HD13	25	0.33	0.02	0.32
(1,643)	1:134:A:LEU:HD22	1:134:A:LEU:HD12	25	0.33	0.02	0.32
(1,643)	1:134:A:LEU:HD22	1:134:A:LEU:HD13	25	0.33	0.02	0.32
(1,643)	1:134:A:LEU:HD23	1:134:A:LEU:HD11	25	0.33	0.02	0.32
(1,643)	1:134:A:LEU:HD22	1:134:A:LEU:HD11	25	0.33	0.02	0.32
(1,643)	1:134:A:LEU:HD21	1:134:A:LEU:HD12	25	0.33	0.02	0.32
(1,1720)	2:34:B:TYR:HE1	2:31:B:LEU:HD23	25	0.32	0.03	0.33
(1,1720)	2:34:B:TYR:HE1	2:31:B:LEU:HD21	25	0.32	0.03	0.33
(1,1720)	2:34:B:TYR:HE1	2:31:B:LEU:HD22	25	0.32	0.03	0.33
(1,1318)	1:79:A:ALA:HA	1:79:A:ALA:HB1	25	0.32	0.01	0.33
(1,1318)	1:79:A:ALA:HA	1:79:A:ALA:HB2	25	0.32	0.01	0.33
(1,1318)	1:79:A:ALA:HA	1:79:A:ALA:HB3	25	0.32	0.01	0.33
(1,1854)	1:124:A:TYR:H	1:125:A:VAL:HG23	25	0.32	0.03	0.32
(1,1854)	1:124:A:TYR:H	1:125:A:VAL:HG21	25	0.32	0.03	0.32
(1,1854)	1:124:A:TYR:H	1:125:A:VAL:HG22	25	0.32	0.03	0.32
(1,172)	1:85:A:VAL:HG13	1:74:A:CYS:HB3	25	0.32	0.07	0.31
(1,172)	1:85:A:VAL:HG12	1:74:A:CYS:HB3	25	0.32	0.07	0.31

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,172)	1:85:A:VAL:HG11	1:74:A:CYS:HB3	25	0.32	0.07	0.31
(1,172)	1:85:A:VAL:HG13	1:88:A:LEU:HB2	25	0.32	0.07	0.31
(1,558)	2:32:B:GLU:HA	2:31:B:LEU:H	25	0.32	0.04	0.32
(1,1727)	2:31:B:LEU:HD12	2:31:B:LEU:H	25	0.31	0.05	0.32
(1,1727)	2:31:B:LEU:HD11	2:31:B:LEU:H	25	0.31	0.05	0.32
(1,1727)	2:31:B:LEU:HD13	2:31:B:LEU:H	25	0.31	0.05	0.32
(1,52)	1:125:A:VAL:HG11	1:128:A:ASN:HB2	25	0.31	0.12	0.37
(1,52)	1:125:A:VAL:HG13	1:128:A:ASN:HB2	25	0.31	0.12	0.37
(1,52)	1:125:A:VAL:HG12	1:128:A:ASN:HB2	25	0.31	0.12	0.37
(1,36)	1:127:A:ILE:HG21	1:124:A:TYR:HD2	25	0.31	0.07	0.3
(1,36)	1:127:A:ILE:HG23	1:124:A:TYR:HD2	25	0.31	0.07	0.3
(1,36)	1:127:A:ILE:HG23	1:124:A:TYR:HD1	25	0.31	0.07	0.3
(1,36)	1:127:A:ILE:HG22	1:124:A:TYR:HD1	25	0.31	0.07	0.3
(1,36)	1:127:A:ILE:HG22	1:124:A:TYR:HD2	25	0.31	0.07	0.3
(1,36)	1:127:A:ILE:HG21	1:124:A:TYR:HD1	25	0.31	0.07	0.3
(1,1622)	2:39:B:TRP:HE3	2:39:B:TRP:HB2	25	0.31	0.07	0.3
(1,1345)	1:76:A:MET:HG2	1:77:A:GLN:H	25	0.3	0.06	0.31
(1,2097)	1:77:A:GLN:HE21	1:77:A:GLN:HA	25	0.3	0.09	0.27
(1,24)	1:85:A:VAL:HG22	1:71:A:LEU:HA	25	0.3	0.05	0.3
(1,24)	1:85:A:VAL:HG23	1:71:A:LEU:HA	25	0.3	0.05	0.3
(1,24)	1:85:A:VAL:HG21	1:71:A:LEU:HA	25	0.3	0.05	0.3
(1,24)	1:85:A:VAL:HG22	1:86:A:PRO:HD3	25	0.3	0.05	0.3
(1,24)	1:85:A:VAL:HG23	1:86:A:PRO:HD3	25	0.3	0.05	0.3
(1,2006)	1:134:A:LEU:HD23	1:95:A:ALA:H	25	0.3	0.04	0.3
(1,2006)	1:134:A:LEU:HD22	1:95:A:ALA:H	25	0.3	0.04	0.3
(1,2006)	1:134:A:LEU:HD21	1:95:A:ALA:H	25	0.3	0.04	0.3
(1,1139)	1:134:A:LEU:HD23	1:95:A:ALA:HB2	25	0.3	0.09	0.3
(1,1139)	1:134:A:LEU:HD22	1:95:A:ALA:HB2	25	0.3	0.09	0.3
(1,1139)	1:134:A:LEU:HD22	1:95:A:ALA:HB1	25	0.3	0.09	0.3
(1,1139)	1:134:A:LEU:HD21	1:95:A:ALA:HB1	25	0.3	0.09	0.3
(1,1139)	1:134:A:LEU:HD21	1:95:A:ALA:HB3	25	0.3	0.09	0.3
(1,1139)	1:134:A:LEU:HD23	1:95:A:ALA:HB3	25	0.3	0.09	0.3
(1,1139)	1:134:A:LEU:HD23	1:95:A:ALA:HB1	25	0.3	0.09	0.3
(1,1139)	1:134:A:LEU:HD21	1:95:A:ALA:HB2	25	0.3	0.09	0.3
(1,794)	1:124:A:TYR:HE2	1:124:A:TYR:HD2	25	0.3	0.0	0.3
(1,794)	1:124:A:TYR:HD1	1:124:A:TYR:HE1	25	0.3	0.0	0.3
(1,210)	1:105:A:PHE:HZ	1:109:A:LEU:HD22	25	0.3	0.05	0.29
(1,210)	1:105:A:PHE:HZ	1:109:A:LEU:HD21	25	0.3	0.05	0.29
(1,210)	1:105:A:PHE:HZ	1:109:A:LEU:HD23	25	0.3	0.05	0.29
(1,492)	1:91:A:ARG:H	1:88:A:LEU:HD23	25	0.3	0.09	0.3
(1,492)	1:91:A:ARG:H	1:88:A:LEU:HD22	25	0.3	0.09	0.3
(1,492)	1:91:A:ARG:H	1:88:A:LEU:HD21	25	0.3	0.09	0.3

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1209)	1:88:A:LEU:HD11	1:70:A:PHE:HE1	25	0.29	0.03	0.3
(1,1209)	1:88:A:LEU:HD13	1:70:A:PHE:HE1	25	0.29	0.03	0.3
(1,1209)	1:88:A:LEU:HD12	1:70:A:PHE:HE1	25	0.29	0.03	0.3
(1,229)	1:105:A:PHE:HE2	1:67:A:PHE:HB2	25	0.29	0.05	0.3
(1,1269)	1:84:A:VAL:HG13	1:85:A:VAL:H	25	0.29	0.02	0.29
(1,1269)	1:84:A:VAL:HG12	1:85:A:VAL:H	25	0.29	0.02	0.29
(1,1269)	1:84:A:VAL:HG11	1:85:A:VAL:H	25	0.29	0.02	0.29
(1,608)	1:136:A:ALA:HA	1:136:A:ALA:HB2	25	0.29	0.01	0.29
(1,608)	1:136:A:ALA:HA	1:136:A:ALA:HB1	25	0.29	0.01	0.29
(1,608)	1:136:A:ALA:HA	1:136:A:ALA:HB3	25	0.29	0.01	0.29
(1,1042)	1:62:A:GLU:HB2	1:62:A:GLU:HA	25	0.29	0.02	0.29
(1,521)	1:71:A:LEU:H	1:113:A:LEU:HD11	25	0.29	0.08	0.28
(1,521)	1:71:A:LEU:H	1:113:A:LEU:HD12	25	0.29	0.08	0.28
(1,521)	1:71:A:LEU:H	1:113:A:LEU:HD13	25	0.29	0.08	0.28
(1,909)	1:114:A:SER:HB2	1:113:A:LEU:HG	25	0.28	0.2	0.19
(1,92)	1:109:A:LEU:HD21	1:67:A:PHE:H	25	0.28	0.04	0.27
(1,92)	1:109:A:LEU:HD23	1:67:A:PHE:H	25	0.28	0.04	0.27
(1,92)	1:109:A:LEU:HD22	1:67:A:PHE:H	25	0.28	0.04	0.27
(1,662)	1:133:A:VAL:HA	1:133:A:VAL:HG13	25	0.28	0.02	0.27
(1,662)	1:133:A:VAL:HA	1:133:A:VAL:HG12	25	0.28	0.02	0.27
(1,662)	1:133:A:VAL:HA	1:133:A:VAL:HG11	25	0.28	0.02	0.27
(1,2018)	1:93:A:GLN:HE22	1:93:A:GLN:HG2	25	0.27	0.06	0.26
(1,2018)	1:93:A:GLN:HE22	1:93:A:GLN:HG3	25	0.27	0.06	0.26
(1,1627)	2:39:B:TRP:HB2	2:39:B:TRP:HA	25	0.27	0.01	0.27
(1,246)	1:61:A:LEU:HG	1:61:A:LEU:HD22	25	0.27	0.02	0.27
(1,246)	1:61:A:LEU:HG	1:61:A:LEU:HD21	25	0.27	0.02	0.27
(1,246)	1:61:A:LEU:HG	1:61:A:LEU:HD23	25	0.27	0.02	0.27
(1,831)	1:121:A:ALA:HA	1:121:A:ALA:HB1	25	0.27	0.01	0.27
(1,831)	1:121:A:ALA:HA	1:121:A:ALA:HB2	25	0.27	0.01	0.27
(1,831)	1:121:A:ALA:HA	1:121:A:ALA:HB3	25	0.27	0.01	0.27
(1,520)	1:130:A:LEU:H	1:112:A:VAL:HG23	25	0.26	0.1	0.25
(1,520)	1:130:A:LEU:H	1:112:A:VAL:HG21	25	0.26	0.1	0.25
(1,520)	1:130:A:LEU:H	1:112:A:VAL:HG22	25	0.26	0.1	0.25
(1,1713)	2:31:B:LEU:HG	2:31:B:LEU:H	25	0.26	0.02	0.27
(1,2244)	2:36:B:THR:HG22	2:36:B:THR:H	25	0.26	0.08	0.29
(1,2244)	2:36:B:THR:HG21	2:36:B:THR:H	25	0.26	0.08	0.29
(1,2244)	2:36:B:THR:HG23	2:36:B:THR:H	25	0.26	0.08	0.29
(1,1450)	1:85:A:VAL:HB	1:86:A:PRO:HD3	25	0.26	0.02	0.26
(1,586)	1:139:A:ALA:HA	1:139:A:ALA:HB1	25	0.26	0.01	0.26
(1,586)	1:139:A:ALA:HA	1:139:A:ALA:HB3	25	0.26	0.01	0.26
(1,586)	1:139:A:ALA:HA	1:139:A:ALA:HB2	25	0.26	0.01	0.26
(1,1591)	1:84:A:VAL:HA	2:31:B:LEU:HD13	25	0.26	0.04	0.26

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1591)	1:84:A:VAL:HA	2:31:B:LEU:HD12	25	0.26	0.04	0.26
(1,1591)	1:84:A:VAL:HA	2:31:B:LEU:HD11	25	0.26	0.04	0.26
(1,490)	1:91:A:ARG:H	1:94:A:ARG:H	25	0.26	0.09	0.24
(1,14)	1:133:A:VAL:HG23	1:132:A:THR:H	25	0.26	0.04	0.26
(1,14)	1:133:A:VAL:HG22	1:132:A:THR:H	25	0.26	0.04	0.26
(1,14)	1:133:A:VAL:HG21	1:132:A:THR:H	25	0.26	0.04	0.26
(1,505)	1:79:A:ALA:H	1:76:A:MET:HA	25	0.26	0.07	0.27
(1,95)	1:107:A:ASN:HB2	1:108:A:ILE:HB	25	0.26	0.06	0.26
(1,1191)	1:89:A:TYR:HB2	1:89:A:TYR:HE2	25	0.26	0.0	0.26
(1,2228)	2:35:B:PHE:H	2:34:B:TYR:HB3	25	0.25	0.04	0.24
(1,258)	1:113:A:LEU:HG	1:113:A:LEU:HD22	25	0.25	0.03	0.26
(1,258)	1:113:A:LEU:HD13	1:113:A:LEU:HG	25	0.25	0.03	0.26
(1,258)	1:113:A:LEU:HD11	1:113:A:LEU:HG	25	0.25	0.03	0.26
(1,258)	1:113:A:LEU:HD12	1:113:A:LEU:HG	25	0.25	0.03	0.26
(1,258)	1:113:A:LEU:HG	1:113:A:LEU:HD21	25	0.25	0.03	0.26
(1,258)	1:113:A:LEU:HG	1:113:A:LEU:HD23	25	0.25	0.03	0.26
(1,664)	1:133:A:VAL:HG12	1:130:A:LEU:HA	25	0.25	0.02	0.25
(1,664)	1:133:A:VAL:HG11	1:130:A:LEU:HA	25	0.25	0.02	0.25
(1,664)	1:133:A:VAL:HG13	1:130:A:LEU:HA	25	0.25	0.02	0.25
(1,1542)	1:59:A:TYR:HE2	1:59:A:TYR:HD2	25	0.25	0.0	0.25
(1,1542)	1:59:A:TYR:HD1	1:59:A:TYR:HE1	25	0.25	0.0	0.25
(1,1562)	1:57:A:LYS:HD2	1:57:A:LYS:HG2	25	0.25	0.03	0.26
(1,1664)	2:36:B:THR:HG23	2:36:B:THR:HB	25	0.25	0.01	0.25
(1,1664)	2:36:B:THR:HG22	2:36:B:THR:HB	25	0.25	0.01	0.25
(1,1664)	2:36:B:THR:HG21	2:36:B:THR:HB	25	0.25	0.01	0.25
(1,1667)	2:36:B:THR:HB	2:36:B:THR:H	25	0.24	0.03	0.25
(1,2287)	2:33:B:GLN:HE22	2:33:B:GLN:HB3	25	0.24	0.02	0.24
(1,1741)	2:29:B:SER:HA	2:30:B:GLU:H	25	0.23	0.02	0.23
(1,1036)	1:62:A:GLU:HB3	1:62:A:GLU:H	25	0.23	0.02	0.23
(1,522)	1:70:A:PHE:H	1:73:A:LEU:H	25	0.23	0.05	0.22
(1,634)	1:134:A:LEU:HD12	1:134:A:LEU:H	25	0.23	0.04	0.22
(1,634)	1:134:A:LEU:HD11	1:134:A:LEU:H	25	0.23	0.04	0.22
(1,634)	1:134:A:LEU:HD13	1:134:A:LEU:H	25	0.23	0.04	0.22
(1,1703)	2:33:B:GLN:HG2	2:31:B:LEU:HD23	25	0.23	0.07	0.23
(1,1703)	2:33:B:GLN:HG2	2:31:B:LEU:HD21	25	0.23	0.07	0.23
(1,1703)	2:33:B:GLN:HG2	2:31:B:LEU:HD22	25	0.23	0.07	0.23
(1,551)	2:34:B:TYR:H	2:35:B:PHE:HA	25	0.22	0.04	0.22
(1,1636)	2:35:B:PHE:HB3	2:34:B:TYR:HE1	25	0.22	0.04	0.21
(1,1117)	1:98:A:LEU:HG	1:98:A:LEU:HD23	25	0.21	0.01	0.21
(1,1117)	1:98:A:LEU:HG	1:98:A:LEU:HD22	25	0.21	0.01	0.21
(1,1117)	1:98:A:LEU:HG	1:98:A:LEU:HD21	25	0.21	0.01	0.21
(1,775)	1:126:A:TYR:HE1	1:125:A:VAL:HG12	25	0.21	0.06	0.2

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,775)	1:126:A:TYR:HE1	1:125:A:VAL:HG11	25	0.21	0.06	0.2
(1,775)	1:126:A:TYR:HE1	1:125:A:VAL:HG13	25	0.21	0.06	0.2
(1,1595)	2:31:B:LEU:HD13	1:127:A:ILE:HB	25	0.21	0.05	0.2
(1,1595)	2:31:B:LEU:HD12	1:127:A:ILE:HB	25	0.21	0.05	0.2
(1,1595)	2:31:B:LEU:HD11	1:127:A:ILE:HB	25	0.21	0.05	0.2
(1,757)	1:126:A:TYR:HD1	1:126:A:TYR:HB2	25	0.21	0.01	0.21
(1,1919)	1:109:A:LEU:HB3	1:109:A:LEU:H	25	0.2	0.01	0.2
(1,1316)	1:79:A:ALA:HB2	1:79:A:ALA:H	25	0.2	0.02	0.21
(1,1316)	1:79:A:ALA:HB1	1:79:A:ALA:H	25	0.2	0.02	0.21
(1,1316)	1:79:A:ALA:HB3	1:79:A:ALA:H	25	0.2	0.02	0.21
(1,844)	1:120:A:PRO:HB2	1:120:A:PRO:HD2	25	0.2	0.01	0.2
(1,702)	1:85:A:VAL:HG22	1:85:A:VAL:HA	25	0.2	0.01	0.19
(1,702)	1:85:A:VAL:HG23	1:85:A:VAL:HA	25	0.2	0.01	0.19
(1,702)	1:85:A:VAL:HG21	1:85:A:VAL:HA	25	0.2	0.01	0.19
(1,438)	1:66:A:LEU:HD11	1:66:A:LEU:H	25	0.19	0.04	0.19
(1,438)	1:66:A:LEU:HD12	1:66:A:LEU:H	25	0.19	0.04	0.19
(1,438)	1:66:A:LEU:HD13	1:66:A:LEU:H	25	0.19	0.04	0.19
(1,160)	1:67:A:PHE:HD1	1:68:A:GLU:H	25	0.19	0.04	0.19
(1,160)	1:67:A:PHE:HD2	1:68:A:GLU:H	25	0.19	0.04	0.19
(1,264)	1:127:A:ILE:HG21	2:35:B:PHE:HE1	25	0.19	0.03	0.19
(1,264)	1:127:A:ILE:HG23	2:35:B:PHE:HE1	25	0.19	0.03	0.19
(1,264)	1:127:A:ILE:HG22	2:35:B:PHE:HE1	25	0.19	0.03	0.19
(1,1118)	1:98:A:LEU:HB3	1:98:A:LEU:HD22	25	0.19	0.21	0.15
(1,1118)	1:98:A:LEU:HB3	1:98:A:LEU:HD21	25	0.19	0.21	0.15
(1,1118)	1:98:A:LEU:HB3	1:98:A:LEU:HD23	25	0.19	0.21	0.15
(1,1097)	1:100:A:LEU:HD23	1:100:A:LEU:HD11	25	0.19	0.03	0.19
(1,1097)	1:100:A:LEU:HD21	1:100:A:LEU:HD11	25	0.19	0.03	0.19
(1,1097)	1:100:A:LEU:HD22	1:100:A:LEU:HD13	25	0.19	0.03	0.19
(1,1097)	1:100:A:LEU:HD22	1:100:A:LEU:HD12	25	0.19	0.03	0.19
(1,1097)	1:100:A:LEU:HD23	1:100:A:LEU:HD12	25	0.19	0.03	0.19
(1,1097)	1:100:A:LEU:HD21	1:100:A:LEU:HD12	25	0.19	0.03	0.19
(1,1097)	1:100:A:LEU:HD22	1:100:A:LEU:HD11	25	0.19	0.03	0.19
(1,1097)	1:100:A:LEU:HD21	1:100:A:LEU:HD13	25	0.19	0.03	0.19
(1,1097)	1:100:A:LEU:HD23	1:100:A:LEU:HD13	25	0.19	0.03	0.19
(1,1606)	2:32:B:GLU:HA	2:32:B:GLU:HB2	25	0.18	0.01	0.18
(1,991)	1:108:A:ILE:HA	1:108:A:ILE:HG22	25	0.18	0.02	0.19
(1,991)	1:108:A:ILE:HA	1:108:A:ILE:HG23	25	0.18	0.02	0.19
(1,991)	1:108:A:ILE:HA	1:108:A:ILE:HG21	25	0.18	0.02	0.19
(1,1432)	1:70:A:PHE:HA	1:70:A:PHE:HD1	25	0.18	0.02	0.18
(1,76)	1:118:A:SER:HA	1:118:A:SER:HB3	25	0.17	0.03	0.16
(1,76)	1:118:A:SER:HA	1:118:A:SER:HB2	25	0.17	0.03	0.16
(1,157)	1:130:A:LEU:HD23	1:88:A:LEU:HD12	25	0.17	0.04	0.17

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,157)	1:130:A:LEU:HD22	1:88:A:LEU:HD11	25	0.17	0.04	0.17
(1,157)	1:130:A:LEU:HD22	1:88:A:LEU:HD12	25	0.17	0.04	0.17
(1,157)	1:130:A:LEU:HD21	1:88:A:LEU:HD12	25	0.17	0.04	0.17
(1,157)	1:130:A:LEU:HD23	1:88:A:LEU:HD11	25	0.17	0.04	0.17
(1,157)	1:130:A:LEU:HD21	1:88:A:LEU:HD13	25	0.17	0.04	0.17
(1,157)	1:130:A:LEU:HD22	1:88:A:LEU:HD13	25	0.17	0.04	0.17
(1,157)	1:130:A:LEU:HD21	1:88:A:LEU:HD11	25	0.17	0.04	0.17
(1,157)	1:130:A:LEU:HD23	1:88:A:LEU:HD13	25	0.17	0.04	0.17
(1,1350)	1:76:A:MET:HB3	1:76:A:MET:HG3	25	0.17	0.0	0.17
(1,1705)	2:33:B:GLN:HA	2:34:B:TYR:H	25	0.16	0.01	0.16
(1,789)	1:124:A:TYR:HD1	1:124:A:TYR:HE1	25	0.16	0.02	0.17
(1,2107)	1:77:A:GLN:H	1:77:A:GLN:HB3	25	0.16	0.02	0.16
(1,604)	1:136:A:ALA:HB1	1:136:A:ALA:H	25	0.15	0.02	0.16
(1,604)	1:136:A:ALA:HB3	1:136:A:ALA:H	25	0.15	0.02	0.16
(1,604)	1:136:A:ALA:HB2	1:136:A:ALA:H	25	0.15	0.02	0.16
(1,1718)	2:31:B:LEU:HD22	2:32:B:GLU:H	25	0.15	0.03	0.14
(1,1718)	2:31:B:LEU:HD23	2:32:B:GLU:H	25	0.15	0.03	0.14
(1,1718)	2:31:B:LEU:HD21	2:32:B:GLU:H	25	0.15	0.03	0.14
(1,2095)	1:77:A:GLN:HG2	1:77:A:GLN:HE22	25	0.14	0.01	0.14
(1,599)	1:137:A:HIS:HA	1:137:A:HIS:HB2	25	0.14	0.01	0.14
(1,937)	1:112:A:VAL:HG21	1:113:A:LEU:HA	25	0.13	0.01	0.13
(1,937)	1:112:A:VAL:HG22	1:113:A:LEU:HA	25	0.13	0.01	0.13
(1,937)	1:112:A:VAL:HG23	1:113:A:LEU:HA	25	0.13	0.01	0.13
(1,870)	1:118:A:SER:HA	1:119:A:ARG:H	25	0.13	0.01	0.13
(1,2165)	1:63:A:ASN:HD22	1:63:A:ASN:HD21	25	0.13	0.01	0.13
(1,1707)	2:33:B:GLN:HB2	2:33:B:GLN:HA	25	0.11	0.0	0.11
(1,196)	1:73:A:LEU:HD23	1:76:A:MET:HE3	24	1.36	0.12	1.34
(1,196)	1:73:A:LEU:HD22	1:76:A:MET:HE2	24	1.36	0.12	1.34
(1,196)	1:73:A:LEU:HD23	1:76:A:MET:HE2	24	1.36	0.12	1.34
(1,196)	1:73:A:LEU:HD21	1:74:A:CYS:HB3	24	1.36	0.12	1.34
(1,196)	1:73:A:LEU:HD23	1:74:A:CYS:HB3	24	1.36	0.12	1.34
(1,196)	1:73:A:LEU:HD22	1:74:A:CYS:HB3	24	1.36	0.12	1.34
(1,196)	1:73:A:LEU:HD22	1:76:A:MET:HE3	24	1.36	0.12	1.34
(1,196)	1:73:A:LEU:HD21	1:76:A:MET:HE3	24	1.36	0.12	1.34
(1,196)	1:73:A:LEU:HD21	1:76:A:MET:HE1	24	1.36	0.12	1.34
(1,196)	1:73:A:LEU:HD22	1:76:A:MET:HE1	24	1.36	0.12	1.34
(1,450)	1:114:A:SER:H	1:126:A:TYR:HB3	24	1.28	0.15	1.29
(1,450)	1:114:A:SER:H	1:117:A:ARG:HD3	24	1.28	0.15	1.29
(1,450)	1:114:A:SER:H	1:115:A:ARG:HD2	24	1.28	0.15	1.29
(1,368)	2:26:B:ASP:HB3	1:87:A:PHE:HZ	24	1.21	0.45	1.27
(1,503)	1:81:A:HIS:H	1:84:A:VAL:HG22	24	0.85	0.1	0.86
(1,503)	1:78:A:THR:HG21	1:81:A:HIS:H	24	0.85	0.1	0.86

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,503)	1:81:A:HIS:H	1:84:A:VAL:HG21	24	0.85	0.1	0.86
(1,503)	1:81:A:HIS:H	1:84:A:VAL:HG23	24	0.85	0.1	0.86
(1,503)	1:78:A:THR:HG23	1:81:A:HIS:H	24	0.85	0.1	0.86
(1,503)	1:78:A:THR:HG22	1:81:A:HIS:H	24	0.85	0.1	0.86
(1,563)	1:134:A:LEU:H	1:135:A:LYS:HB2	24	0.79	0.07	0.81
(1,563)	2:26:B:ASP:H	2:30:B:GLU:HB3	24	0.79	0.07	0.81
(1,563)	1:113:A:LEU:H	1:111:A:ARG:HB2	24	0.79	0.07	0.81
(1,1137)	1:95:A:ALA:HB3	1:91:A:ARG:HD3	24	0.77	0.64	0.4
(1,1137)	1:95:A:ALA:HB2	1:91:A:ARG:HD3	24	0.77	0.64	0.4
(1,1137)	1:95:A:ALA:HB1	1:91:A:ARG:HD3	24	0.77	0.64	0.4
(1,307)	2:39:B:TRP:HE3	2:36:B:THR:HG21	24	0.7	0.23	0.69
(1,307)	2:39:B:TRP:HE3	2:36:B:THR:HG23	24	0.7	0.23	0.69
(1,307)	2:36:B:THR:HG21	1:128:A:ASN:HD21	24	0.7	0.23	0.69
(1,307)	2:39:B:TRP:HE3	2:36:B:THR:HG22	24	0.7	0.23	0.69
(1,307)	2:36:B:THR:HG22	1:128:A:ASN:HD21	24	0.7	0.23	0.69
(1,307)	2:36:B:THR:HG23	1:128:A:ASN:HD21	24	0.7	0.23	0.69
(1,122)	1:95:A:ALA:HB3	1:91:A:ARG:HD3	24	0.62	0.46	0.36
(1,122)	1:95:A:ALA:HB2	1:91:A:ARG:HD3	24	0.62	0.46	0.36
(1,122)	1:95:A:ALA:HB3	1:96:A:HIS:HB3	24	0.62	0.46	0.36
(1,122)	1:95:A:ALA:HB1	1:91:A:ARG:HD3	24	0.62	0.46	0.36
(1,122)	1:95:A:ALA:HB2	1:96:A:HIS:HB3	24	0.62	0.46	0.36
(1,122)	1:95:A:ALA:HB1	1:96:A:HIS:HB3	24	0.62	0.46	0.36
(1,379)	2:31:B:LEU:HB2	2:28:B:ASP:HB2	24	0.6	0.43	0.4
(1,189)	1:85:A:VAL:HG12	1:75:A:LYS:HA	24	0.55	0.1	0.57
(1,189)	1:85:A:VAL:HG13	1:75:A:LYS:HA	24	0.55	0.1	0.57
(1,189)	1:85:A:VAL:HG11	1:75:A:LYS:HA	24	0.55	0.1	0.57
(1,1088)	1:100:A:LEU:HD21	1:105:A:PHE:HD2	24	0.55	0.61	0.39
(1,1088)	1:100:A:LEU:HD23	1:105:A:PHE:HD2	24	0.55	0.61	0.39
(1,1088)	1:100:A:LEU:HD22	1:105:A:PHE:HD2	24	0.55	0.61	0.39
(1,2089)	1:79:A:ALA:H	1:78:A:THR:HG23	24	0.52	0.02	0.52
(1,2089)	1:79:A:ALA:H	1:78:A:THR:HG22	24	0.52	0.02	0.52
(1,2089)	1:79:A:ALA:H	1:78:A:THR:HG21	24	0.52	0.02	0.52
(1,228)	1:62:A:GLU:HG2	1:61:A:LEU:HD21	24	0.51	0.13	0.55
(1,228)	1:62:A:GLU:HG2	1:61:A:LEU:HD23	24	0.51	0.13	0.55
(1,228)	1:62:A:GLU:HG2	1:66:A:LEU:HD12	24	0.51	0.13	0.55
(1,228)	1:62:A:GLU:HG2	1:66:A:LEU:HD13	24	0.51	0.13	0.55
(1,228)	1:62:A:GLU:HG2	1:66:A:LEU:HD11	24	0.51	0.13	0.55
(1,1331)	1:77:A:GLN:HG2	1:73:A:LEU:HD13	24	0.5	0.29	0.42
(1,1331)	1:77:A:GLN:HG2	1:73:A:LEU:HD11	24	0.5	0.29	0.42
(1,1331)	1:77:A:GLN:HG2	1:73:A:LEU:HD12	24	0.5	0.29	0.42
(1,1070)	1:101:A:ALA:HB1	1:102:A:SER:H	24	0.49	0.15	0.55
(1,1070)	1:101:A:ALA:HB2	1:102:A:SER:H	24	0.49	0.15	0.55

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1070)	1:101:A:ALA:HB3	1:102:A:SER:H	24	0.49	0.15	0.55
(1,465)	1:106:A:CYS:H	1:103:A:ALA:HB1	24	0.49	0.18	0.44
(1,465)	1:106:A:CYS:H	1:103:A:ALA:HB2	24	0.49	0.18	0.44
(1,465)	1:106:A:CYS:H	1:103:A:ALA:HB3	24	0.49	0.18	0.44
(1,465)	1:108:A:ILE:HD12	1:106:A:CYS:H	24	0.49	0.18	0.44
(1,465)	1:108:A:ILE:HD13	1:106:A:CYS:H	24	0.49	0.18	0.44
(1,465)	1:108:A:ILE:HD11	1:106:A:CYS:H	24	0.49	0.18	0.44
(1,1115)	1:98:A:LEU:HD23	1:96:A:HIS:HE1	24	0.48	0.08	0.5
(1,1115)	1:98:A:LEU:HD22	1:96:A:HIS:HE1	24	0.48	0.08	0.5
(1,1115)	1:98:A:LEU:HD21	1:96:A:HIS:HE1	24	0.48	0.08	0.5
(1,1986)	1:99:A:PHE:H	1:98:A:LEU:HD21	24	0.48	0.03	0.49
(1,1986)	1:99:A:PHE:H	1:98:A:LEU:HD23	24	0.48	0.03	0.49
(1,1986)	1:99:A:PHE:H	1:98:A:LEU:HD22	24	0.48	0.03	0.49
(1,766)	1:126:A:TYR:HE1	1:115:A:ARG:HB2	24	0.42	0.16	0.43
(1,1716)	2:31:B:LEU:HG	2:32:B:GLU:HG3	24	0.41	0.09	0.4
(1,1716)	2:32:B:GLU:HG2	2:31:B:LEU:HG	24	0.41	0.09	0.4
(1,1798)	1:136:A:ALA:H	1:135:A:LYS:HD3	24	0.41	0.12	0.46
(1,1798)	1:136:A:ALA:H	1:135:A:LYS:HD2	24	0.41	0.12	0.46
(1,483)	1:93:A:GLN:HG2	1:94:A:ARG:H	24	0.4	0.03	0.4
(1,2019)	1:93:A:GLN:HE22	1:93:A:GLN:HB3	24	0.4	0.03	0.39
(1,191)	1:84:A:VAL:HG13	1:74:A:CYS:HB2	24	0.37	0.07	0.37
(1,191)	1:78:A:THR:HG21	1:74:A:CYS:HB2	24	0.37	0.07	0.37
(1,191)	1:84:A:VAL:HG11	1:74:A:CYS:HB2	24	0.37	0.07	0.37
(1,191)	1:84:A:VAL:HG12	1:74:A:CYS:HB2	24	0.37	0.07	0.37
(1,191)	1:85:A:VAL:HG12	1:74:A:CYS:HB2	24	0.37	0.07	0.37
(1,191)	1:85:A:VAL:HG13	1:74:A:CYS:HB2	24	0.37	0.07	0.37
(1,428)	1:128:A:ASN:HD22	1:128:A:ASN:HB3	24	0.37	0.07	0.38
(1,30)	1:129:A:GLU:HG3	1:130:A:LEU:H	24	0.36	0.07	0.35
(1,421)	1:128:A:ASN:H	1:70:A:PHE:HZ	24	0.36	0.08	0.36
(1,421)	1:72:A:GLU:H	1:70:A:PHE:HD1	24	0.36	0.08	0.36
(1,240)	1:104:A:GLU:HB3	1:105:A:PHE:HA	24	0.35	0.07	0.36
(1,240)	1:104:A:GLU:HB3	1:99:A:PHE:HA	24	0.35	0.07	0.36
(1,240)	2:33:B:GLN:HB2	2:34:B:TYR:HA	24	0.35	0.07	0.36
(1,116)	1:100:A:LEU:HD22	1:105:A:PHE:HE2	24	0.34	0.28	0.28
(1,116)	1:100:A:LEU:HD21	1:105:A:PHE:HE2	24	0.34	0.28	0.28
(1,116)	1:100:A:LEU:HD23	1:95:A:ALA:H	24	0.34	0.28	0.28
(1,116)	1:100:A:LEU:HD23	1:105:A:PHE:HE2	24	0.34	0.28	0.28
(1,275)	1:84:A:VAL:HG12	2:35:B:PHE:HE1	24	0.31	0.05	0.32
(1,275)	1:84:A:VAL:HG11	2:35:B:PHE:HE1	24	0.31	0.05	0.32
(1,275)	1:84:A:VAL:HG13	2:35:B:PHE:HE1	24	0.31	0.05	0.32
(1,275)	1:84:A:VAL:HG11	2:35:B:PHE:HZ	24	0.31	0.05	0.32
(1,275)	1:84:A:VAL:HG13	2:35:B:PHE:HZ	24	0.31	0.05	0.32

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,426)	1:125:A:VAL:HG12	1:126:A:TYR:H	24	0.3	0.05	0.31
(1,426)	1:125:A:VAL:HG11	1:126:A:TYR:H	24	0.3	0.05	0.31
(1,426)	1:125:A:VAL:HG13	1:126:A:TYR:H	24	0.3	0.05	0.31
(1,515)	1:73:A:LEU:HG	1:76:A:MET:H	24	0.3	0.06	0.3
(1,900)	1:115:A:ARG:HB3	1:115:A:ARG:HG2	24	0.3	0.01	0.3
(1,361)	2:29:B:SER:HB2	2:32:B:GLU:HG3	24	0.3	0.15	0.24
(1,361)	2:29:B:SER:HB2	2:30:B:GLU:HG2	24	0.3	0.15	0.24
(1,1419)	1:71:A:LEU:HD12	1:89:A:TYR:H	24	0.3	0.1	0.3
(1,1419)	1:71:A:LEU:HD13	1:89:A:TYR:H	24	0.3	0.1	0.3
(1,1419)	1:71:A:LEU:HD11	1:89:A:TYR:H	24	0.3	0.1	0.3
(1,257)	1:113:A:LEU:HD11	1:113:A:LEU:HB2	24	0.29	0.07	0.27
(1,257)	1:113:A:LEU:HD13	1:117:A:ARG:HG2	24	0.29	0.07	0.27
(1,257)	1:113:A:LEU:HD12	1:113:A:LEU:HB2	24	0.29	0.07	0.27
(1,257)	1:113:A:LEU:HD13	1:113:A:LEU:HB2	24	0.29	0.07	0.27
(1,257)	1:113:A:LEU:HD12	1:117:A:ARG:HG2	24	0.29	0.07	0.27
(1,257)	1:113:A:LEU:HD11	1:117:A:ARG:HG3	24	0.29	0.07	0.27
(1,257)	1:113:A:LEU:HD13	1:117:A:ARG:HG3	24	0.29	0.07	0.27
(1,342)	2:31:B:LEU:HD13	1:124:A:TYR:HB3	24	0.28	0.07	0.29
(1,342)	2:31:B:LEU:HD11	1:124:A:TYR:HB3	24	0.28	0.07	0.29
(1,342)	2:31:B:LEU:HD12	1:124:A:TYR:HB3	24	0.28	0.07	0.29
(1,236)	1:64:A:GLU:HA	1:67:A:PHE:H	24	0.28	0.08	0.3
(1,145)	1:88:A:LEU:HB3	1:85:A:VAL:HA	24	0.25	0.04	0.24
(1,1440)	1:127:A:ILE:HD13	1:70:A:PHE:HZ	24	0.25	0.06	0.24
(1,1440)	1:127:A:ILE:HD12	1:70:A:PHE:HZ	24	0.25	0.06	0.24
(1,1440)	1:127:A:ILE:HD11	1:70:A:PHE:HZ	24	0.25	0.06	0.24
(1,1295)	1:82:A:PRO:HG2	1:81:A:HIS:HA	24	0.24	0.1	0.2
(1,1486)	1:65:A:LYS:HA	1:65:A:LYS:HB2	24	0.18	0.01	0.18
(1,1721)	2:31:B:LEU:HD23	2:31:B:LEU:HA	24	0.16	0.02	0.16
(1,1721)	2:31:B:LEU:HD21	2:31:B:LEU:HA	24	0.16	0.02	0.16
(1,1721)	2:31:B:LEU:HD22	2:31:B:LEU:HA	24	0.16	0.02	0.16
(1,1346)	1:76:A:MET:HG2	1:73:A:LEU:HA	24	0.15	0.02	0.16
(1,1608)	2:32:B:GLU:HA	2:33:B:GLN:H	24	0.12	0.01	0.12
(1,383)	2:30:B:GLU:HB2	2:31:B:LEU:HB2	23	1.5	0.08	1.5
(1,4)	1:130:A:LEU:HD23	1:127:A:ILE:HA	23	0.99	0.11	1.01
(1,4)	1:130:A:LEU:HD22	1:127:A:ILE:HA	23	0.99	0.11	1.01
(1,4)	1:130:A:LEU:HD21	1:127:A:ILE:HA	23	0.99	0.11	1.01
(1,1651)	2:38:B:ARG:HG2	2:37:B:ALA:HB2	23	0.92	0.18	0.96
(1,1651)	2:38:B:ARG:HG2	2:37:B:ALA:HB1	23	0.92	0.18	0.96
(1,1651)	2:38:B:ARG:HG2	2:37:B:ALA:HB3	23	0.92	0.18	0.96
(1,1046)	2:30:B:GLU:HG3	2:30:B:GLU:H	23	0.9	0.05	0.91
(1,902)	1:115:A:ARG:HD2	1:115:A:ARG:H	23	0.59	0.05	0.58
(1,5)	1:100:A:LEU:HD13	1:100:A:LEU:H	23	0.58	0.06	0.57

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,5)	1:100:A:LEU:HD12	1:100:A:LEU:H	23	0.58	0.06	0.57
(1,5)	1:100:A:LEU:HD11	1:100:A:LEU:H	23	0.58	0.06	0.57
(1,723)	1:129:A:GLU:HG2	1:125:A:VAL:HG12	23	0.55	0.06	0.55
(1,723)	1:129:A:GLU:HG2	1:125:A:VAL:HG11	23	0.55	0.06	0.55
(1,723)	1:129:A:GLU:HG2	1:125:A:VAL:HG13	23	0.55	0.06	0.55
(1,243)	1:66:A:LEU:HD11	1:62:A:GLU:HG3	23	0.53	0.21	0.51
(1,243)	1:62:A:GLU:HG3	1:61:A:LEU:HD21	23	0.53	0.21	0.51
(1,243)	1:62:A:GLU:HG3	1:61:A:LEU:HD22	23	0.53	0.21	0.51
(1,243)	1:62:A:GLU:HG3	1:61:A:LEU:HD23	23	0.53	0.21	0.51
(1,243)	1:66:A:LEU:HD13	1:62:A:GLU:HG3	23	0.53	0.21	0.51
(1,1122)	1:96:A:HIS:HA	1:139:A:ALA:HB3	23	0.52	0.32	0.4
(1,1122)	1:96:A:HIS:HA	1:139:A:ALA:HB2	23	0.52	0.32	0.4
(1,1122)	1:96:A:HIS:HA	1:139:A:ALA:HB1	23	0.52	0.32	0.4
(1,1089)	1:105:A:PHE:HZ	1:100:A:LEU:HD22	23	0.5	0.85	0.24
(1,1089)	1:105:A:PHE:HZ	1:100:A:LEU:HD21	23	0.5	0.85	0.24
(1,1089)	1:105:A:PHE:HZ	1:100:A:LEU:HD23	23	0.5	0.85	0.24
(1,1971)	1:100:A:LEU:HD21	1:101:A:ALA:H	23	0.37	0.07	0.4
(1,1971)	1:100:A:LEU:HD23	1:101:A:ALA:H	23	0.37	0.07	0.4
(1,1971)	1:100:A:LEU:HD22	1:101:A:ALA:H	23	0.37	0.07	0.4
(1,225)	1:129:A:GLU:HG2	1:125:A:VAL:HG12	23	0.31	0.06	0.32
(1,225)	1:129:A:GLU:HG2	1:125:A:VAL:HG11	23	0.31	0.06	0.32
(1,225)	1:129:A:GLU:HG2	1:125:A:VAL:HG13	23	0.31	0.06	0.32
(1,2007)	1:100:A:LEU:HD23	1:95:A:ALA:H	23	0.29	0.08	0.3
(1,2007)	1:100:A:LEU:HD22	1:95:A:ALA:H	23	0.29	0.08	0.3
(1,2007)	1:100:A:LEU:HD21	1:95:A:ALA:H	23	0.29	0.08	0.3
(1,934)	1:112:A:VAL:HG12	1:126:A:TYR:HB3	23	0.29	0.09	0.32
(1,934)	1:112:A:VAL:HG13	1:126:A:TYR:HB3	23	0.29	0.09	0.32
(1,934)	1:112:A:VAL:HG11	1:126:A:TYR:HB3	23	0.29	0.09	0.32
(1,56)	1:124:A:TYR:HE2	2:35:B:PHE:HB3	23	0.27	0.12	0.25
(1,56)	1:124:A:TYR:HE1	2:35:B:PHE:HB3	23	0.27	0.12	0.25
(1,27)	1:130:A:LEU:HD22	1:67:A:PHE:HA	23	0.25	0.08	0.25
(1,27)	1:130:A:LEU:HD21	1:67:A:PHE:HA	23	0.25	0.08	0.25
(1,27)	1:130:A:LEU:HD23	1:67:A:PHE:HA	23	0.25	0.08	0.25
(1,147)	1:137:A:HIS:HB3	1:138:A:SER:H	23	0.24	0.09	0.22
(1,2108)	1:77:A:GLN:H	1:78:A:THR:HG23	23	0.22	0.04	0.22
(1,2108)	1:77:A:GLN:H	1:78:A:THR:HG21	23	0.22	0.04	0.22
(1,2108)	1:77:A:GLN:H	1:78:A:THR:HG22	23	0.22	0.04	0.22
(1,998)	1:108:A:ILE:HD11	1:105:A:PHE:HD1	23	0.21	0.02	0.22
(1,998)	1:108:A:ILE:HD12	1:105:A:PHE:HD1	23	0.21	0.02	0.22
(1,998)	1:108:A:ILE:HD13	1:105:A:PHE:HD1	23	0.21	0.02	0.22
(1,913)	1:113:A:LEU:HG	1:113:A:LEU:H	23	0.2	0.03	0.21
(1,25)	1:85:A:VAL:HG22	1:74:A:CYS:HB2	23	0.19	0.05	0.17

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,25)	1:85:A:VAL:HG23	1:74:A:CYS:HB2	23	0.19	0.05	0.17
(1,25)	1:85:A:VAL:HG21	1:74:A:CYS:HB2	23	0.19	0.05	0.17
(1,1491)	1:65:A:LYS:HB2	1:65:A:LYS:HG2	23	0.15	0.01	0.15
(1,1234)	1:67:A:PHE:HD1	1:109:A:LEU:HD13	22	1.99	0.11	2.04
(1,1234)	1:67:A:PHE:HD1	1:109:A:LEU:HD11	22	1.99	0.11	2.04
(1,1234)	1:67:A:PHE:HD1	1:109:A:LEU:HD12	22	1.99	0.11	2.04
(1,1233)	1:109:A:LEU:HD22	1:67:A:PHE:HD1	22	1.91	0.06	1.91
(1,1233)	1:109:A:LEU:HD21	1:67:A:PHE:HD1	22	1.91	0.06	1.91
(1,1233)	1:109:A:LEU:HD23	1:67:A:PHE:HD1	22	1.91	0.06	1.91
(1,1144)	1:111:A:ARG:HG2	1:107:A:ASN:HA	22	1.62	0.47	1.77
(1,162)	1:67:A:PHE:HD1	1:130:A:LEU:HD22	22	1.59	0.13	1.58
(1,162)	1:67:A:PHE:HD1	1:130:A:LEU:HD21	22	1.59	0.13	1.58
(1,162)	1:67:A:PHE:HD1	1:130:A:LEU:HD23	22	1.59	0.13	1.58
(1,1229)	1:67:A:PHE:HD1	1:67:A:PHE:H	22	1.13	0.01	1.13
(1,868)	1:119:A:ARG:HD2	1:119:A:ARG:HB2	22	0.71	0.21	0.75
(1,510)	1:73:A:LEU:HD23	1:77:A:GLN:HE22	22	0.65	0.08	0.64
(1,510)	1:73:A:LEU:HD21	1:77:A:GLN:HE22	22	0.65	0.08	0.64
(1,510)	1:73:A:LEU:HD22	1:77:A:GLN:HE22	22	0.65	0.08	0.64
(1,1232)	1:67:A:PHE:HD1	1:67:A:PHE:HB2	22	0.63	0.01	0.63
(1,2114)	1:75:A:LYS:HG2	1:75:A:LYS:H	22	0.61	0.05	0.62
(1,1489)	1:65:A:LYS:HG2	1:66:A:LEU:H	22	0.57	0.07	0.57
(1,1650)	2:37:B:ALA:HB2	1:121:A:ALA:HB1	22	0.56	0.21	0.55
(1,1650)	2:37:B:ALA:HB1	1:121:A:ALA:HB1	22	0.56	0.21	0.55
(1,1650)	2:37:B:ALA:HB3	1:121:A:ALA:HB2	22	0.56	0.21	0.55
(1,1650)	2:37:B:ALA:HB2	1:121:A:ALA:HB3	22	0.56	0.21	0.55
(1,1650)	2:37:B:ALA:HB1	1:121:A:ALA:HB3	22	0.56	0.21	0.55
(1,1650)	2:37:B:ALA:HB3	1:121:A:ALA:HB1	22	0.56	0.21	0.55
(1,1650)	2:37:B:ALA:HB1	1:121:A:ALA:HB2	22	0.56	0.21	0.55
(1,1650)	2:37:B:ALA:HB3	1:121:A:ALA:HB3	22	0.56	0.21	0.55
(1,1650)	2:37:B:ALA:HB2	1:121:A:ALA:HB2	22	0.56	0.21	0.55
(1,366)	1:100:A:LEU:HD11	1:138:A:SER:HB3	22	0.5	0.15	0.56
(1,366)	1:100:A:LEU:HD13	1:138:A:SER:HB3	22	0.5	0.15	0.56
(1,366)	1:100:A:LEU:HD12	1:138:A:SER:HB3	22	0.5	0.15	0.56
(1,17)	1:133:A:VAL:HG13	1:137:A:HIS:HB2	22	0.48	0.22	0.48
(1,17)	1:133:A:VAL:HG12	1:137:A:HIS:HB2	22	0.48	0.22	0.48
(1,17)	1:133:A:VAL:HG11	1:137:A:HIS:HB2	22	0.48	0.22	0.48
(1,1231)	1:67:A:PHE:HA	1:67:A:PHE:HD1	22	0.47	0.04	0.46
(1,1633)	2:38:B:ARG:HD2	2:38:B:ARG:HB2	22	0.47	0.09	0.48
(1,318)	2:34:B:TYR:HE1	1:83:A:GLU:HB3	22	0.47	0.15	0.42
(1,318)	2:34:B:TYR:HE1	2:30:B:GLU:HB2	22	0.47	0.15	0.42
(1,321)	2:34:B:TYR:HD1	1:83:A:GLU:HB3	22	0.46	0.19	0.47
(1,321)	2:34:B:TYR:HD1	2:33:B:GLN:HG2	22	0.46	0.19	0.47

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1183)	1:90:A:ASN:HB2	1:87:A:PHE:HD1	22	0.41	0.15	0.44
(1,1326)	1:77:A:GLN:HG2	1:77:A:GLN:HA	22	0.41	0.04	0.42
(1,1395)	1:116:A:ALA:HB3	1:73:A:LEU:HD22	22	0.41	0.14	0.39
(1,1395)	1:116:A:ALA:HB3	1:73:A:LEU:HD23	22	0.41	0.14	0.39
(1,1395)	1:116:A:ALA:HB1	1:73:A:LEU:HD22	22	0.41	0.14	0.39
(1,1395)	1:116:A:ALA:HB1	1:73:A:LEU:HD23	22	0.41	0.14	0.39
(1,1395)	1:116:A:ALA:HB2	1:73:A:LEU:HD21	22	0.41	0.14	0.39
(1,1395)	1:116:A:ALA:HB3	1:73:A:LEU:HD21	22	0.41	0.14	0.39
(1,1395)	1:116:A:ALA:HB2	1:73:A:LEU:HD23	22	0.41	0.14	0.39
(1,1395)	1:116:A:ALA:HB1	1:73:A:LEU:HD21	22	0.41	0.14	0.39
(1,2005)	1:95:A:ALA:H	1:94:A:ARG:HG3	22	0.39	0.22	0.31
(1,2005)	1:95:A:ALA:H	1:94:A:ARG:HG2	22	0.39	0.22	0.31
(1,1996)	1:97:A:SER:H	1:139:A:ALA:HB3	22	0.38	0.11	0.38
(1,1996)	1:97:A:SER:H	1:139:A:ALA:HB2	22	0.38	0.11	0.38
(1,1996)	1:97:A:SER:H	1:139:A:ALA:HB1	22	0.38	0.11	0.38
(1,538)	1:63:A:ASN:H	1:61:A:LEU:HA	22	0.31	0.1	0.32
(1,1670)	2:37:B:ALA:HB1	2:36:B:THR:HA	22	0.3	0.09	0.28
(1,1670)	2:37:B:ALA:HB3	2:36:B:THR:HA	22	0.3	0.09	0.28
(1,1670)	2:37:B:ALA:HB2	2:36:B:THR:HA	22	0.3	0.09	0.28
(1,960)	1:67:A:PHE:HA	1:109:A:LEU:HD13	22	0.28	0.1	0.28
(1,960)	1:67:A:PHE:HA	1:109:A:LEU:HD11	22	0.28	0.1	0.28
(1,960)	1:67:A:PHE:HA	1:109:A:LEU:HD12	22	0.28	0.1	0.28
(1,666)	1:134:A:LEU:HD22	1:133:A:VAL:HG11	22	0.27	0.03	0.28
(1,666)	1:134:A:LEU:HD21	1:133:A:VAL:HG13	22	0.27	0.03	0.28
(1,666)	1:134:A:LEU:HD23	1:133:A:VAL:HG13	22	0.27	0.03	0.28
(1,666)	1:134:A:LEU:HD23	1:133:A:VAL:HG12	22	0.27	0.03	0.28
(1,666)	1:134:A:LEU:HD22	1:133:A:VAL:HG12	22	0.27	0.03	0.28
(1,666)	1:134:A:LEU:HD23	1:133:A:VAL:HG11	22	0.27	0.03	0.28
(1,666)	1:134:A:LEU:HD22	1:133:A:VAL:HG13	22	0.27	0.03	0.28
(1,337)	2:31:B:LEU:HD22	2:28:B:ASP:HB2	22	0.26	0.07	0.24
(1,337)	2:31:B:LEU:HD23	2:28:B:ASP:HB2	22	0.26	0.07	0.24
(1,337)	2:31:B:LEU:HD21	2:28:B:ASP:HB2	22	0.26	0.07	0.24
(1,337)	2:31:B:LEU:HD23	2:28:B:ASP:HB3	22	0.26	0.07	0.24
(1,337)	2:31:B:LEU:HD21	2:28:B:ASP:HB3	22	0.26	0.07	0.24
(1,337)	2:31:B:LEU:HD22	2:28:B:ASP:HB3	22	0.26	0.07	0.24
(1,1197)	1:89:A:TYR:HD2	1:71:A:LEU:HD22	22	0.22	0.05	0.22
(1,1197)	1:89:A:TYR:HD2	1:71:A:LEU:HD23	22	0.22	0.05	0.22
(1,1197)	1:89:A:TYR:HD2	1:71:A:LEU:HD21	22	0.22	0.05	0.22
(1,1803)	1:135:A:LYS:HB3	1:135:A:LYS:H	22	0.2	0.03	0.2
(1,1356)	1:75:A:LYS:HA	1:75:A:LYS:HG2	22	0.2	0.02	0.2
(1,1975)	1:100:A:LEU:HD13	1:100:A:LEU:H	22	0.18	0.06	0.16
(1,1975)	1:100:A:LEU:HD12	1:100:A:LEU:H	22	0.18	0.06	0.16

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1975)	1:100:A:LEU:HD11	1:100:A:LEU:H	22	0.18	0.06	0.16
(1,1370)	1:75:A:LYS:HE3	1:72:A:GLU:HB3	21	0.56	0.64	0.26
(1,134)	1:92:A:GLN:HG2	1:95:A:ALA:H	21	0.46	0.13	0.48
(1,134)	1:105:A:PHE:HE2	1:92:A:GLN:HG2	21	0.46	0.13	0.48
(1,2051)	1:89:A:TYR:H	1:90:A:ASN:HB3	21	0.43	0.13	0.44
(1,42)	1:126:A:TYR:HD1	1:125:A:VAL:HB	21	0.32	0.16	0.29
(1,140)	2:35:B:PHE:HB3	2:35:B:PHE:HE2	21	0.31	0.1	0.38
(1,140)	1:99:A:PHE:HB3	1:138:A:SER:H	21	0.31	0.1	0.38
(1,414)	1:72:A:GLU:H	1:68:A:GLU:HA	21	0.28	0.08	0.27
(1,414)	1:72:A:GLU:H	1:69:A:GLU:HA	21	0.28	0.08	0.27
(1,1074)	1:101:A:ALA:HB2	1:60:A:LYS:HA	21	0.27	0.05	0.28
(1,1074)	1:101:A:ALA:HB3	1:60:A:LYS:HA	21	0.27	0.05	0.28
(1,1074)	1:101:A:ALA:HB1	1:60:A:LYS:HA	21	0.27	0.05	0.28
(1,1391)	1:74:A:CYS:HA	1:73:A:LEU:HD23	21	0.24	0.08	0.25
(1,1391)	1:74:A:CYS:HA	1:73:A:LEU:HD21	21	0.24	0.08	0.25
(1,1391)	1:74:A:CYS:HA	1:73:A:LEU:HD22	21	0.24	0.08	0.25
(1,139)	1:128:A:ASN:HB2	1:128:A:ASN:HD22	21	0.2	0.06	0.19
(1,139)	1:90:A:ASN:HB2	1:90:A:ASN:HD22	21	0.2	0.06	0.19
(1,84)	1:113:A:LEU:HA	1:113:A:LEU:HG	21	0.17	0.04	0.16
(1,84)	1:114:A:SER:HB2	1:113:A:LEU:HG	21	0.17	0.04	0.16
(1,773)	1:125:A:VAL:HA	1:125:A:VAL:HG11	21	0.14	0.03	0.14
(1,773)	1:125:A:VAL:HA	1:125:A:VAL:HG13	21	0.14	0.03	0.14
(1,773)	1:125:A:VAL:HA	1:125:A:VAL:HG12	21	0.14	0.03	0.14
(1,1423)	1:71:A:LEU:HD21	1:70:A:PHE:HD1	21	0.12	0.01	0.11
(1,1423)	1:71:A:LEU:HD23	1:70:A:PHE:HD1	21	0.12	0.01	0.11
(1,1423)	1:71:A:LEU:HD22	1:70:A:PHE:HD1	21	0.12	0.01	0.11
(1,1109)	1:98:A:LEU:HB3	1:98:A:LEU:H	21	0.12	0.01	0.12
(1,355)	2:29:B:SER:HB3	2:31:B:LEU:H	20	0.94	0.22	1.03
(1,355)	2:29:B:SER:HB3	2:33:B:GLN:H	20	0.94	0.22	1.03
(1,907)	1:114:A:SER:HB2	1:115:A:ARG:H	20	0.86	0.05	0.86
(1,117)	1:100:A:LEU:HD22	1:92:A:GLN:HG2	20	0.68	0.16	0.76
(1,117)	1:100:A:LEU:HB2	1:100:A:LEU:HD23	20	0.68	0.16	0.76
(1,117)	1:100:A:LEU:HD21	1:92:A:GLN:HG2	20	0.68	0.16	0.76
(1,117)	1:100:A:LEU:HB2	1:100:A:LEU:HD21	20	0.68	0.16	0.76
(1,117)	1:100:A:LEU:HD23	1:92:A:GLN:HG2	20	0.68	0.16	0.76
(1,117)	1:100:A:LEU:HB2	1:100:A:LEU:HD22	20	0.68	0.16	0.76
(1,619)	1:135:A:LYS:HG2	1:91:A:ARG:HD3	20	0.64	0.46	0.65
(1,585)	1:139:A:ALA:HB2	1:140:A:LYS:H	20	0.62	0.21	0.63
(1,585)	1:139:A:ALA:HB3	1:140:A:LYS:H	20	0.62	0.21	0.63
(1,585)	1:139:A:ALA:HB1	1:140:A:LYS:H	20	0.62	0.21	0.63
(1,197)	1:73:A:LEU:HD22	1:123:A:LEU:HB2	20	0.42	0.15	0.48
(1,197)	1:73:A:LEU:HD23	1:123:A:LEU:HB2	20	0.42	0.15	0.48

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,197)	1:73:A:LEU:HD21	1:123:A:LEU:HB2	20	0.42	0.15	0.48
(1,197)	1:73:A:LEU:HD23	1:117:A:ARG:HB2	20	0.42	0.15	0.48
(1,197)	1:73:A:LEU:HD22	1:117:A:ARG:HB2	20	0.42	0.15	0.48
(1,1040)	1:62:A:GLU:HB3	1:59:A:TYR:HA	20	0.38	0.13	0.38
(1,2265)	2:26:B:ASP:HB3	2:26:B:ASP:H	20	0.36	0.08	0.37
(1,1098)	1:100:A:LEU:HD22	1:92:A:GLN:HA	20	0.35	0.19	0.3
(1,1098)	1:100:A:LEU:HD23	1:92:A:GLN:HA	20	0.35	0.19	0.3
(1,1098)	1:100:A:LEU:HD21	1:92:A:GLN:HA	20	0.35	0.19	0.3
(1,1185)	1:90:A:ASN:HB2	1:90:A:ASN:HD22	20	0.35	0.01	0.35
(1,1538)	1:59:A:TYR:HB3	1:59:A:TYR:HD1	20	0.33	0.01	0.33
(1,1619)	2:39:B:TRP:HD1	2:38:B:ARG:HB2	20	0.3	0.06	0.3
(1,1723)	2:31:B:LEU:HD23	2:30:B:GLU:HB2	20	0.28	0.12	0.26
(1,1723)	2:31:B:LEU:HD22	2:30:B:GLU:HB2	20	0.28	0.12	0.26
(1,1723)	2:31:B:LEU:HD21	2:30:B:GLU:HB2	20	0.28	0.12	0.26
(1,209)	1:67:A:PHE:HE1	1:71:A:LEU:HD23	20	0.26	0.1	0.29
(1,209)	1:71:A:LEU:HD21	1:67:A:PHE:HE2	20	0.26	0.1	0.29
(1,209)	1:67:A:PHE:HE1	1:71:A:LEU:HD22	20	0.26	0.1	0.29
(1,209)	1:67:A:PHE:HE1	1:71:A:LEU:HD21	20	0.26	0.1	0.29
(1,209)	1:71:A:LEU:HD22	1:67:A:PHE:HE2	20	0.26	0.1	0.29
(1,209)	1:71:A:LEU:HD23	1:67:A:PHE:HE2	20	0.26	0.1	0.29
(1,453)	1:114:A:SER:H	1:113:A:LEU:HD23	20	0.24	0.06	0.24
(1,453)	1:114:A:SER:H	1:113:A:LEU:HD21	20	0.24	0.06	0.24
(1,453)	1:114:A:SER:H	1:113:A:LEU:HD22	20	0.24	0.06	0.24
(1,1592)	1:84:A:VAL:HG21	2:35:B:PHE:HB2	20	0.23	0.06	0.23
(1,1592)	1:84:A:VAL:HG23	2:35:B:PHE:HB2	20	0.23	0.06	0.23
(1,1592)	1:84:A:VAL:HG22	2:35:B:PHE:HB2	20	0.23	0.06	0.23
(1,1961)	1:102:A:SER:H	1:59:A:TYR:HD1	20	0.23	0.06	0.22
(1,1648)	2:38:B:ARG:HA	2:37:B:ALA:HB2	20	0.22	0.06	0.2
(1,1648)	2:38:B:ARG:HA	2:37:B:ALA:HB1	20	0.22	0.06	0.2
(1,1648)	2:38:B:ARG:HA	2:37:B:ALA:HB3	20	0.22	0.06	0.2
(1,873)	1:118:A:SER:HB2	1:119:A:ARG:H	20	0.17	0.02	0.18
(1,410)	1:134:A:LEU:H	1:132:A:THR:H	20	0.15	0.03	0.15
(1,66)	1:121:A:ALA:HA	1:121:A:ALA:H	20	0.13	0.02	0.12
(1,66)	1:80:A:ASP:HA	1:80:A:ASP:H	20	0.13	0.02	0.12
(1,767)	1:124:A:TYR:HE1	1:84:A:VAL:HG21	19	2.62	0.22	2.63
(1,767)	1:124:A:TYR:HE1	1:84:A:VAL:HG22	19	2.62	0.22	2.63
(1,767)	1:124:A:TYR:HE1	1:84:A:VAL:HG23	19	2.62	0.22	2.63
(1,1251)	1:68:A:GLU:HB2	1:68:A:GLU:H	19	0.88	0.02	0.88
(1,869)	1:119:A:ARG:HD3	1:119:A:ARG:HB2	19	0.81	0.05	0.81
(1,792)	1:127:A:ILE:HD13	1:124:A:TYR:HD1	19	0.69	0.1	0.71
(1,792)	1:127:A:ILE:HD11	1:124:A:TYR:HD1	19	0.69	0.1	0.71
(1,792)	1:127:A:ILE:HD12	1:124:A:TYR:HD1	19	0.69	0.1	0.71

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,380)	2:27:B:SER:HA	2:30:B:GLU:HB3	19	0.49	0.24	0.46
(1,380)	2:27:B:SER:HA	2:25:B:GLU:HB3	19	0.49	0.24	0.46
(1,790)	1:124:A:TYR:HD1	1:124:A:TYR:HA	19	0.49	0.05	0.48
(1,1781)	1:140:A:LYS:H	1:141:A:LYS:HB3	19	0.44	0.51	0.17
(1,227)	1:62:A:GLU:HG2	1:61:A:LEU:HG	19	0.43	0.16	0.41
(1,356)	2:29:B:SER:HB2	2:31:B:LEU:H	19	0.34	0.21	0.27
(1,356)	2:29:B:SER:HB2	2:33:B:GLN:H	19	0.34	0.21	0.27
(1,1280)	1:84:A:VAL:HG22	1:81:A:HIS:HB2	19	0.32	0.09	0.33
(1,1280)	1:84:A:VAL:HG21	1:81:A:HIS:HB2	19	0.32	0.09	0.33
(1,1280)	1:84:A:VAL:HG23	1:81:A:HIS:HB2	19	0.32	0.09	0.33
(1,858)	1:119:A:ARG:HG3	1:119:A:ARG:HA	19	0.29	0.05	0.3
(1,1044)	1:62:A:GLU:HB3	1:62:A:GLU:HG3	19	0.25	0.01	0.25
(1,2202)	1:125:A:VAL:H	1:122:A:LYS:HD2	19	0.21	0.09	0.18
(1,2202)	1:125:A:VAL:H	1:122:A:LYS:HD3	19	0.21	0.09	0.18
(1,811)	1:123:A:LEU:HD21	1:70:A:PHE:HE1	19	0.18	0.06	0.18
(1,811)	1:123:A:LEU:HD23	1:70:A:PHE:HE1	19	0.18	0.06	0.18
(1,811)	1:123:A:LEU:HD22	1:70:A:PHE:HE1	19	0.18	0.06	0.18
(1,673)	1:133:A:VAL:HG21	1:130:A:LEU:HA	19	0.17	0.05	0.15
(1,673)	1:133:A:VAL:HG22	1:130:A:LEU:HA	19	0.17	0.05	0.15
(1,673)	1:133:A:VAL:HG23	1:130:A:LEU:HA	19	0.17	0.05	0.15
(1,288)	2:32:B:GLU:HA	2:35:B:PHE:HD1	19	0.15	0.03	0.15
(1,1319)	1:77:A:GLN:HB3	1:78:A:THR:H	19	0.14	0.03	0.13
(1,1603)	2:33:B:GLN:HG2	2:33:B:GLN:HB2	19	0.11	0.01	0.11
(1,618)	1:56:A:LYS:HG2	1:57:A:LYS:H	18	0.73	0.52	0.6
(1,80)	1:94:A:ARG:HD2	1:93:A:GLN:HB2	18	0.52	0.15	0.57
(1,80)	1:94:A:ARG:HD3	1:94:A:ARG:HB2	18	0.52	0.15	0.57
(1,80)	1:94:A:ARG:HD3	1:93:A:GLN:HB2	18	0.52	0.15	0.57
(1,80)	1:94:A:ARG:HD2	1:94:A:ARG:HB2	18	0.52	0.15	0.57
(1,369)	2:26:B:ASP:HB2	1:87:A:PHE:HZ	18	0.5	0.33	0.36
(1,369)	2:26:B:ASP:HB2	2:33:B:GLN:HE21	18	0.5	0.33	0.36
(1,1549)	1:58:A:CYS:HB2	1:57:A:LYS:HA	18	0.44	0.48	0.2
(1,1361)	1:75:A:LYS:HE2	1:75:A:LYS:HG3	18	0.33	0.02	0.33
(1,62)	1:123:A:LEU:HD23	1:70:A:PHE:HE1	18	0.29	0.06	0.29
(1,62)	1:123:A:LEU:HD22	1:70:A:PHE:HE1	18	0.29	0.06	0.29
(1,62)	1:123:A:LEU:HD21	1:70:A:PHE:HE1	18	0.29	0.06	0.29
(1,392)	1:139:A:ALA:H	1:96:A:HIS:HD2	18	0.28	0.1	0.29
(1,392)	1:139:A:ALA:H	1:138:A:SER:H	18	0.28	0.1	0.29
(1,1745)	2:29:B:SER:HB3	2:30:B:GLU:H	18	0.26	0.1	0.25
(1,1142)	1:94:A:ARG:HD2	1:94:A:ARG:HB2	18	0.23	0.04	0.24
(1,1142)	1:94:A:ARG:HD3	1:94:A:ARG:HB2	18	0.23	0.04	0.24
(1,1283)	1:84:A:VAL:HG21	1:127:A:ILE:HD12	18	0.21	0.11	0.17
(1,1283)	1:84:A:VAL:HG22	1:127:A:ILE:HD12	18	0.21	0.11	0.17

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1283)	1:84:A:VAL:HG21	1:127:A:ILE:HD13	18	0.21	0.11	0.17
(1,1283)	1:84:A:VAL:HG23	1:127:A:ILE:HD12	18	0.21	0.11	0.17
(1,1283)	1:84:A:VAL:HG22	1:127:A:ILE:HD13	18	0.21	0.11	0.17
(1,1283)	1:84:A:VAL:HG23	1:127:A:ILE:HD13	18	0.21	0.11	0.17
(1,1283)	1:84:A:VAL:HG23	1:127:A:ILE:HD11	18	0.21	0.11	0.17
(1,540)	1:63:A:ASN:H	1:61:A:LEU:HG	18	0.2	0.05	0.18
(1,1171)	1:91:A:ARG:HG2	1:91:A:ARG:HA	18	0.16	0.04	0.16
(1,930)	1:126:A:TYR:HD1	1:112:A:VAL:HG13	18	0.14	0.02	0.14
(1,930)	1:126:A:TYR:HD1	1:112:A:VAL:HG11	18	0.14	0.02	0.14
(1,930)	1:126:A:TYR:HD1	1:112:A:VAL:HG12	18	0.14	0.02	0.14
(1,1003)	1:108:A:ILE:HB	1:108:A:ILE:HD11	18	0.12	0.02	0.11
(1,1003)	1:108:A:ILE:HB	1:108:A:ILE:HD12	18	0.12	0.02	0.11
(1,1003)	1:108:A:ILE:HB	1:108:A:ILE:HD13	18	0.12	0.02	0.11
(1,1456)	1:69:A:GLU:HG2	1:66:A:LEU:HA	17	0.57	0.36	0.4
(1,478)	1:95:A:ALA:H	1:91:A:ARG:HD2	17	0.49	0.17	0.49
(1,387)	1:141:A:LYS:H	1:141:A:LYS:HG2	17	0.45	0.09	0.45
(1,387)	1:141:A:LYS:H	1:141:A:LYS:HG3	17	0.45	0.09	0.45
(1,387)	1:141:A:LYS:H	1:139:A:ALA:HB3	17	0.45	0.09	0.45
(1,1367)	1:75:A:LYS:HD2	1:75:A:LYS:HA	17	0.28	0.34	0.16
(1,1091)	1:100:A:LEU:HD21	1:92:A:GLN:HE21	17	0.25	0.19	0.2
(1,1091)	1:100:A:LEU:HD23	1:92:A:GLN:HE21	17	0.25	0.19	0.2
(1,1091)	1:100:A:LEU:HD22	1:92:A:GLN:HE21	17	0.25	0.19	0.2
(1,1133)	1:95:A:ALA:HB1	1:99:A:PHE:HD2	17	0.23	0.07	0.21
(1,1133)	1:95:A:ALA:HB3	1:99:A:PHE:HD2	17	0.23	0.07	0.21
(1,1133)	1:95:A:ALA:HB2	1:99:A:PHE:HD2	17	0.23	0.07	0.21
(1,1588)	1:87:A:PHE:HB2	2:31:B:LEU:HD12	17	0.23	0.07	0.24
(1,1588)	1:87:A:PHE:HB2	2:31:B:LEU:HD11	17	0.23	0.07	0.24
(1,1588)	1:87:A:PHE:HB2	2:31:B:LEU:HD13	17	0.23	0.07	0.24
(1,542)	1:61:A:LEU:HG	1:61:A:LEU:H	17	0.16	0.01	0.16
(1,746)	1:127:A:ILE:HD13	1:127:A:ILE:H	17	0.15	0.05	0.14
(1,746)	1:127:A:ILE:HD11	1:127:A:ILE:H	17	0.15	0.05	0.14
(1,746)	1:127:A:ILE:HD12	1:127:A:ILE:H	17	0.15	0.05	0.14
(1,911)	1:113:A:LEU:HB2	1:113:A:LEU:H	17	0.15	0.04	0.13
(1,1317)	1:79:A:ALA:HB3	1:76:A:MET:HA	17	0.15	0.03	0.14
(1,1317)	1:79:A:ALA:HB1	1:76:A:MET:HA	17	0.15	0.03	0.14
(1,1317)	1:79:A:ALA:HB2	1:76:A:MET:HA	17	0.15	0.03	0.14
(1,1186)	1:90:A:ASN:HB3	1:90:A:ASN:HA	17	0.11	0.01	0.11
(1,1724)	2:31:B:LEU:HG	2:31:B:LEU:HD22	17	0.11	0.0	0.11
(1,1724)	2:31:B:LEU:HG	2:31:B:LEU:HD21	17	0.11	0.0	0.11
(1,1724)	2:31:B:LEU:HG	2:31:B:LEU:HD23	17	0.11	0.0	0.11
(1,1771)	1:142:A:LYS:H	1:142:A:LYS:HD2	16	0.66	0.44	0.7
(1,451)	1:114:A:SER:H	1:117:A:ARG:HB2	16	0.54	0.16	0.52

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1252)	1:69:A:GLU:HB2	1:69:A:GLU:HG2	16	0.34	0.01	0.35
(1,2004)	1:95:A:ALA:H	1:94:A:ARG:HB3	16	0.29	0.08	0.3
(1,1000)	1:108:A:ILE:HD11	1:99:A:PHE:HE1	16	0.27	0.06	0.27
(1,1000)	1:108:A:ILE:HD12	1:99:A:PHE:HE1	16	0.27	0.06	0.27
(1,1000)	1:108:A:ILE:HD13	1:99:A:PHE:HE1	16	0.27	0.06	0.27
(1,526)	1:69:A:GLU:H	1:113:A:LEU:HD21	16	0.26	0.08	0.26
(1,526)	1:69:A:GLU:H	1:113:A:LEU:HD22	16	0.26	0.08	0.26
(1,526)	1:69:A:GLU:H	1:113:A:LEU:HD23	16	0.26	0.08	0.26
(1,1057)	1:103:A:ALA:HB3	1:59:A:TYR:HD1	16	0.24	0.08	0.25
(1,1057)	1:103:A:ALA:HB2	1:59:A:TYR:HD1	16	0.24	0.08	0.25
(1,1057)	1:103:A:ALA:HB1	1:59:A:TYR:HD1	16	0.24	0.08	0.25
(1,1751)	2:27:B:SER:HA	2:28:B:ASP:H	16	0.19	0.03	0.19
(1,807)	1:123:A:LEU:HD11	1:74:A:CYS:HB2	16	0.15	0.09	0.13
(1,807)	1:123:A:LEU:HD13	1:74:A:CYS:HB2	16	0.15	0.09	0.13
(1,807)	1:123:A:LEU:HD12	1:74:A:CYS:HB2	16	0.15	0.09	0.13
(1,456)	1:112:A:VAL:H	1:108:A:ILE:HG23	16	0.15	0.03	0.15
(1,456)	1:112:A:VAL:H	1:108:A:ILE:HG21	16	0.15	0.03	0.15
(1,456)	1:112:A:VAL:H	1:108:A:ILE:HG22	16	0.15	0.03	0.15
(1,509)	1:77:A:GLN:HE22	1:73:A:LEU:HG	16	0.14	0.02	0.13
(1,1776)	1:144:A:ASN:HA	1:144:A:ASN:H	16	0.12	0.01	0.12
(1,367)	2:26:B:ASP:HB3	2:31:B:LEU:H	15	0.31	0.21	0.22
(1,1761)	2:25:B:GLU:HA	2:25:B:GLU:HB2	15	0.26	0.02	0.26
(1,1987)	1:99:A:PHE:H	1:99:A:PHE:HD2	15	0.2	0.05	0.2
(1,1837)	1:127:A:ILE:H	1:123:A:LEU:HD13	15	0.19	0.08	0.16
(1,1837)	1:127:A:ILE:H	1:123:A:LEU:HD12	15	0.19	0.08	0.16
(1,1837)	1:127:A:ILE:H	1:123:A:LEU:HD11	15	0.19	0.08	0.16
(1,83)	1:113:A:LEU:HA	1:116:A:ALA:HB1	15	0.18	0.06	0.17
(1,83)	1:113:A:LEU:HA	1:116:A:ALA:HB3	15	0.18	0.06	0.17
(1,83)	1:113:A:LEU:HA	1:116:A:ALA:HB2	15	0.18	0.06	0.17
(1,1315)	1:79:A:ALA:HB2	1:80:A:ASP:H	15	0.15	0.02	0.14
(1,1315)	1:79:A:ALA:HB3	1:80:A:ASP:H	15	0.15	0.02	0.14
(1,1315)	1:79:A:ALA:HB1	1:80:A:ASP:H	15	0.15	0.02	0.14
(1,107)	1:69:A:GLU:HA	1:69:A:GLU:HB3	15	0.14	0.03	0.13
(1,995)	1:108:A:ILE:HG21	1:130:A:LEU:HD12	15	0.14	0.03	0.13
(1,995)	1:108:A:ILE:HG22	1:130:A:LEU:HD11	15	0.14	0.03	0.13
(1,995)	1:108:A:ILE:HG22	1:130:A:LEU:HD13	15	0.14	0.03	0.13
(1,995)	1:108:A:ILE:HG21	1:130:A:LEU:HD13	15	0.14	0.03	0.13
(1,995)	1:108:A:ILE:HG21	1:130:A:LEU:HD11	15	0.14	0.03	0.13
(1,995)	1:108:A:ILE:HG23	1:130:A:LEU:HD12	15	0.14	0.03	0.13
(1,995)	1:108:A:ILE:HG23	1:130:A:LEU:HD11	15	0.14	0.03	0.13
(1,779)	1:125:A:VAL:HB	1:125:A:VAL:HG12	15	0.13	0.02	0.13
(1,779)	1:125:A:VAL:HB	1:125:A:VAL:HG11	15	0.13	0.02	0.13

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,779)	1:125:A:VAL:HB	1:125:A:VAL:HG13	15	0.13	0.02	0.13
(1,601)	1:137:A:HIS:HB3	1:137:A:HIS:H	15	0.12	0.02	0.12
(1,1940)	1:106:A:CYS:H	1:63:A:ASN:HD22	14	1.34	0.1	1.33
(1,946)	1:110:A:SER:HB2	1:66:A:LEU:HD12	14	0.86	0.31	0.86
(1,946)	1:110:A:SER:HB2	1:66:A:LEU:HD11	14	0.86	0.31	0.86
(1,946)	1:110:A:SER:HB2	1:66:A:LEU:HD13	14	0.86	0.31	0.86
(1,1553)	1:59:A:TYR:HD1	1:57:A:LYS:HB2	14	0.79	0.5	0.86
(1,1635)	2:39:B:TRP:HA	2:38:B:ARG:HD2	14	0.59	0.38	0.42
(1,572)	1:143:A:LEU:HB2	1:143:A:LEU:HD11	14	0.54	0.57	0.14
(1,572)	1:143:A:LEU:HB2	1:143:A:LEU:HD13	14	0.54	0.57	0.14
(1,572)	1:143:A:LEU:HB2	1:143:A:LEU:HD12	14	0.54	0.57	0.14
(1,488)	1:92:A:GLN:HE22	1:64:A:GLU:HG3	14	0.43	0.19	0.44
(1,561)	2:27:B:SER:H	2:30:B:GLU:HB3	14	0.38	0.23	0.3
(1,561)	2:27:B:SER:H	2:25:B:GLU:HB3	14	0.38	0.23	0.3
(1,2197)	1:55:A:GLY:HA2	1:56:A:LYS:H	14	0.37	0.14	0.43
(1,1754)	2:30:B:GLU:HG2	2:31:B:LEU:H	14	0.34	0.1	0.36
(1,1126)	1:96:A:HIS:HD2	1:139:A:ALA:HB3	14	0.26	0.06	0.26
(1,1126)	1:96:A:HIS:HD2	1:139:A:ALA:HB2	14	0.26	0.06	0.26
(1,1126)	1:96:A:HIS:HD2	1:139:A:ALA:HB1	14	0.26	0.06	0.26
(1,1789)	1:139:A:ALA:H	1:139:A:ALA:HB3	14	0.23	0.05	0.24
(1,1789)	1:139:A:ALA:H	1:139:A:ALA:HB2	14	0.23	0.05	0.24
(1,1789)	1:139:A:ALA:H	1:139:A:ALA:HB1	14	0.23	0.05	0.24
(1,1725)	2:31:B:LEU:HD23	1:127:A:ILE:HG22	14	0.19	0.06	0.18
(1,1725)	2:31:B:LEU:HD22	1:127:A:ILE:HG22	14	0.19	0.06	0.18
(1,1725)	2:31:B:LEU:HD22	1:127:A:ILE:HG21	14	0.19	0.06	0.18
(1,1725)	2:31:B:LEU:HD21	1:127:A:ILE:HG22	14	0.19	0.06	0.18
(1,1725)	2:31:B:LEU:HD22	1:127:A:ILE:HG23	14	0.19	0.06	0.18
(1,1725)	2:31:B:LEU:HD21	1:127:A:ILE:HG21	14	0.19	0.06	0.18
(1,1725)	2:31:B:LEU:HD21	1:127:A:ILE:HG23	14	0.19	0.06	0.18
(1,596)	1:137:A:HIS:HA	1:138:A:SER:H	14	0.17	0.05	0.16
(1,1552)	1:57:A:LYS:HB2	1:57:A:LYS:HA	14	0.16	0.03	0.16
(1,2161)	1:64:A:GLU:HB3	1:64:A:GLU:H	14	0.11	0.01	0.11
(1,575)	1:143:A:LEU:HA	1:143:A:LEU:HD21	13	1.36	0.58	1.64
(1,575)	1:143:A:LEU:HA	1:143:A:LEU:HD22	13	1.36	0.58	1.64
(1,575)	1:143:A:LEU:HA	1:143:A:LEU:HD23	13	1.36	0.58	1.64
(1,591)	1:138:A:SER:HB3	1:138:A:SER:H	13	0.57	0.34	0.79
(1,1874)	1:118:A:SER:H	1:117:A:ARG:HG3	13	0.38	0.1	0.38
(1,1874)	1:118:A:SER:H	1:117:A:ARG:HG2	13	0.38	0.1	0.38
(1,2151)	1:65:A:LYS:HG3	1:66:A:LEU:H	13	0.29	0.36	0.13
(1,2136)	1:69:A:GLU:H	1:70:A:PHE:HB2	13	0.25	0.12	0.18
(1,2136)	1:69:A:GLU:H	1:70:A:PHE:HB3	13	0.25	0.12	0.18
(1,512)	1:77:A:GLN:H	1:123:A:LEU:HD22	13	0.22	0.07	0.25

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,512)	1:77:A:GLN:H	1:123:A:LEU:HD21	13	0.22	0.07	0.25
(1,512)	1:77:A:GLN:H	1:123:A:LEU:HD23	13	0.22	0.07	0.25
(1,394)	1:137:A:HIS:HB3	1:138:A:SER:H	13	0.2	0.05	0.22
(1,944)	1:110:A:SER:HB2	1:110:A:SER:H	13	0.18	0.01	0.18
(1,940)	1:111:A:ARG:HB3	1:111:A:ARG:H	13	0.11	0.01	0.11
(1,827)	1:122:A:LYS:HD2	1:122:A:LYS:HA	12	0.48	0.21	0.54
(1,233)	1:66:A:LEU:HD13	1:63:A:ASN:HB3	12	0.45	0.28	0.27
(1,233)	1:62:A:GLU:HG2	1:66:A:LEU:HD12	12	0.45	0.28	0.27
(1,233)	1:62:A:GLU:HG2	1:66:A:LEU:HD11	12	0.45	0.28	0.27
(1,233)	1:66:A:LEU:HD11	1:63:A:ASN:HB3	12	0.45	0.28	0.27
(1,233)	1:62:A:GLU:HG2	1:66:A:LEU:HD13	12	0.45	0.28	0.27
(1,233)	1:66:A:LEU:HD12	1:63:A:ASN:HB3	12	0.45	0.28	0.27
(1,1801)	1:135:A:LYS:H	1:91:A:ARG:HD3	12	0.43	0.23	0.38
(1,111)	1:62:A:GLU:HB3	1:59:A:TYR:HD2	12	0.4	0.27	0.26
(1,111)	1:62:A:GLU:HB3	1:59:A:TYR:HD1	12	0.4	0.27	0.26
(1,111)	1:104:A:GLU:HB3	1:106:A:CYS:H	12	0.4	0.27	0.26
(1,1755)	2:30:B:GLU:HG2	2:30:B:GLU:HA	12	0.36	0.02	0.36
(1,1753)	2:27:B:SER:HB2	2:27:B:SER:HA	12	0.35	0.22	0.18
(1,1147)	1:94:A:ARG:HG2	1:94:A:ARG:HA	12	0.24	0.14	0.16
(1,1570)	1:57:A:LYS:HE2	1:59:A:TYR:HE1	12	0.23	0.06	0.24
(1,123)	1:95:A:ALA:HB2	1:134:A:LEU:HB2	12	0.22	0.15	0.17
(1,123)	1:95:A:ALA:HB1	1:134:A:LEU:HB2	12	0.22	0.15	0.17
(1,123)	1:95:A:ALA:HB3	1:134:A:LEU:HB2	12	0.22	0.15	0.17
(1,2100)	1:77:A:GLN:HE21	1:76:A:MET:HE1	12	0.22	0.09	0.18
(1,2100)	1:77:A:GLN:HE21	1:76:A:MET:HE3	12	0.22	0.09	0.18
(1,2100)	1:77:A:GLN:HE21	1:76:A:MET:HE2	12	0.22	0.09	0.18
(1,1759)	2:30:B:GLU:HA	2:30:B:GLU:HG3	12	0.21	0.05	0.22
(1,1072)	1:101:A:ALA:HB1	1:58:A:CYS:HA	12	0.2	0.06	0.19
(1,1072)	1:101:A:ALA:HB2	1:58:A:CYS:HA	12	0.2	0.06	0.19
(1,1072)	1:101:A:ALA:HB3	1:58:A:CYS:HA	12	0.2	0.06	0.19
(1,2032)	1:90:A:ASN:HD22	1:93:A:GLN:HB2	12	0.19	0.03	0.2
(1,1653)	2:37:B:ALA:HB1	2:37:B:ALA:HA	12	0.12	0.01	0.12
(1,1653)	2:37:B:ALA:HB2	2:37:B:ALA:HA	12	0.12	0.01	0.12
(1,1653)	2:37:B:ALA:HB3	2:37:B:ALA:HA	12	0.12	0.01	0.12
(1,206)	1:73:A:LEU:HD21	1:117:A:ARG:HD3	11	0.57	0.2	0.62
(1,206)	1:71:A:LEU:HD11	1:89:A:TYR:HB2	11	0.57	0.2	0.62
(1,206)	1:73:A:LEU:HD22	1:117:A:ARG:HD3	11	0.57	0.2	0.62
(1,206)	1:73:A:LEU:HD23	1:117:A:ARG:HD3	11	0.57	0.2	0.62
(1,206)	1:71:A:LEU:HD12	1:89:A:TYR:HB2	11	0.57	0.2	0.62
(1,206)	1:73:A:LEU:HD22	1:117:A:ARG:HD2	11	0.57	0.2	0.62
(1,206)	1:71:A:LEU:HD13	1:89:A:TYR:HB2	11	0.57	0.2	0.62
(1,1554)	1:59:A:TYR:HE1	1:57:A:LYS:HB2	11	0.49	0.2	0.53

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1968)	1:101:A:ALA:H	1:63:A:ASN:HD22	11	0.36	0.1	0.37
(1,1168)	1:100:A:LEU:HD21	1:92:A:GLN:HG2	11	0.32	0.15	0.27
(1,1168)	1:100:A:LEU:HD23	1:92:A:GLN:HG2	11	0.32	0.15	0.27
(1,1168)	1:100:A:LEU:HD22	1:92:A:GLN:HG2	11	0.32	0.15	0.27
(1,473)	1:101:A:ALA:H	1:100:A:LEU:HG	11	0.31	0.04	0.32
(1,473)	1:101:A:ALA:H	1:100:A:LEU:HB3	11	0.31	0.04	0.32
(1,121)	1:95:A:ALA:HB1	1:138:A:SER:HB3	11	0.28	0.11	0.3
(1,121)	1:95:A:ALA:HB3	1:134:A:LEU:HA	11	0.28	0.11	0.3
(1,121)	1:95:A:ALA:HB2	1:134:A:LEU:HA	11	0.28	0.11	0.3
(1,121)	1:95:A:ALA:HB1	1:134:A:LEU:HA	11	0.28	0.11	0.3
(1,8)	1:134:A:LEU:HD21	1:105:A:PHE:HD1	11	0.27	0.09	0.3
(1,8)	1:134:A:LEU:HD22	1:67:A:PHE:HZ	11	0.27	0.09	0.3
(1,8)	1:134:A:LEU:HD21	1:67:A:PHE:HZ	11	0.27	0.09	0.3
(1,8)	1:134:A:LEU:HD23	1:105:A:PHE:HD1	11	0.27	0.09	0.3
(1,8)	1:134:A:LEU:HD23	1:67:A:PHE:HZ	11	0.27	0.09	0.3
(1,163)	1:67:A:PHE:HD2	1:92:A:GLN:HG3	11	0.23	0.09	0.22
(1,163)	1:87:A:PHE:HD1	1:88:A:LEU:HD22	11	0.23	0.09	0.22
(1,163)	1:67:A:PHE:HD1	1:92:A:GLN:HG3	11	0.23	0.09	0.22
(1,163)	1:87:A:PHE:HD1	1:88:A:LEU:HD21	11	0.23	0.09	0.22
(1,1175)	1:91:A:ARG:HG2	1:134:A:LEU:HB2	11	0.2	0.08	0.16
(1,915)	1:113:A:LEU:HD22	1:69:A:GLU:HB3	11	0.2	0.08	0.15
(1,915)	1:113:A:LEU:HD21	1:69:A:GLU:HB3	11	0.2	0.08	0.15
(1,915)	1:113:A:LEU:HD23	1:69:A:GLU:HB3	11	0.2	0.08	0.15
(1,2248)	2:30:B:GLU:HB2	2:31:B:LEU:H	11	0.15	0.04	0.14
(1,2094)	1:79:A:ALA:HB3	1:78:A:THR:H	11	0.15	0.05	0.12
(1,2094)	1:79:A:ALA:HB1	1:78:A:THR:H	11	0.15	0.05	0.12
(1,2094)	1:79:A:ALA:HB2	1:78:A:THR:H	11	0.15	0.05	0.12
(1,285)	2:31:B:LEU:HD13	1:127:A:ILE:HB	11	0.13	0.03	0.12
(1,285)	2:31:B:LEU:HD12	1:127:A:ILE:HB	11	0.13	0.03	0.12
(1,285)	2:31:B:LEU:HD11	1:127:A:ILE:HB	11	0.13	0.03	0.12
(1,1257)	1:85:A:VAL:HG12	1:71:A:LEU:HA	11	0.12	0.02	0.11
(1,1257)	1:85:A:VAL:HG13	1:71:A:LEU:HA	11	0.12	0.02	0.11
(1,1257)	1:85:A:VAL:HG11	1:71:A:LEU:HA	11	0.12	0.02	0.11
(1,1989)	1:98:A:LEU:H	1:138:A:SER:HB2	10	1.35	0.62	1.65
(1,879)	1:94:A:ARG:HD3	1:90:A:ASN:HD22	10	0.87	0.33	0.98
(1,879)	1:94:A:ARG:HD2	1:90:A:ASN:HD22	10	0.87	0.33	0.98
(1,2026)	1:67:A:PHE:HD1	1:92:A:GLN:HE22	10	0.5	0.16	0.54
(1,2026)	1:67:A:PHE:HD2	1:92:A:GLN:HE21	10	0.5	0.16	0.54
(1,2026)	1:67:A:PHE:HD2	1:92:A:GLN:HE22	10	0.5	0.16	0.54
(1,881)	1:117:A:ARG:HD2	1:117:A:ARG:HB2	10	0.43	0.35	0.27
(1,881)	1:117:A:ARG:HD2	1:117:A:ARG:HB3	10	0.43	0.35	0.27
(1,364)	2:29:B:SER:HB3	2:32:B:GLU:HB2	10	0.35	0.18	0.32

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1775)	1:143:A:LEU:H	1:141:A:LYS:HG3	10	0.33	0.13	0.32
(1,1775)	1:143:A:LEU:H	1:141:A:LYS:HG2	10	0.33	0.13	0.32
(1,2188)	1:59:A:TYR:H	1:58:A:CYS:HB3	10	0.28	0.06	0.28
(1,2188)	1:59:A:TYR:H	1:58:A:CYS:HB2	10	0.28	0.06	0.28
(1,942)	1:111:A:ARG:HB2	1:111:A:ARG:HD2	10	0.27	0.06	0.28
(1,1666)	2:36:B:THR:HG22	1:124:A:TYR:H	10	0.25	0.06	0.29
(1,1666)	2:36:B:THR:HG23	1:124:A:TYR:H	10	0.25	0.06	0.29
(1,1666)	2:36:B:THR:HG21	1:124:A:TYR:H	10	0.25	0.06	0.29
(1,1536)	1:59:A:TYR:HD1	1:59:A:TYR:HA	10	0.14	0.04	0.12
(1,1708)	2:32:B:GLU:HG2	2:39:B:TRP:HZ2	10	0.13	0.05	0.12
(1,1247)	1:88:A:LEU:HD13	1:85:A:VAL:HA	10	0.13	0.02	0.13
(1,1247)	1:88:A:LEU:HD12	1:85:A:VAL:HA	10	0.13	0.02	0.13
(1,1247)	1:88:A:LEU:HD11	1:85:A:VAL:HA	10	0.13	0.02	0.13
(1,464)	1:107:A:ASN:H	1:108:A:ILE:HB	10	0.12	0.02	0.13
(1,1764)	2:24:B:GLN:HB3	2:24:B:GLN:HG3	10	0.12	0.01	0.11
(1,1764)	2:24:B:GLN:HB3	2:24:B:GLN:HG2	10	0.12	0.01	0.11
(1,578)	1:57:A:LYS:HA	1:57:A:LYS:H	10	0.11	0.01	0.11
(1,1690)	2:34:B:TYR:HE1	2:34:B:TYR:HD1	10	0.1	0.0	0.1
(1,254)	1:57:A:LYS:HE3	1:54:A:MET:HG3	9	0.95	0.67	0.84
(1,254)	1:57:A:LYS:HE2	1:54:A:MET:HG3	9	0.95	0.67	0.84
(1,2195)	1:56:A:LYS:H	1:56:A:LYS:HG2	9	0.66	0.29	0.67
(1,1392)	1:73:A:LEU:HD22	1:117:A:ARG:HD3	9	0.58	0.14	0.66
(1,1392)	1:73:A:LEU:HD21	1:117:A:ARG:HD2	9	0.58	0.14	0.66
(1,1392)	1:73:A:LEU:HD23	1:117:A:ARG:HD3	9	0.58	0.14	0.66
(1,1392)	1:73:A:LEU:HD23	1:117:A:ARG:HD2	9	0.58	0.14	0.66
(1,1392)	1:73:A:LEU:HD22	1:117:A:ARG:HD2	9	0.58	0.14	0.66
(1,1371)	1:75:A:LYS:HE3	1:72:A:GLU:HG2	9	0.56	0.6	0.16
(1,826)	1:117:A:ARG:HG2	1:117:A:ARG:H	9	0.54	0.04	0.53
(1,253)	1:57:A:LYS:HE3	1:54:A:MET:HG2	9	0.43	0.38	0.28
(1,253)	1:57:A:LYS:HE2	1:54:A:MET:HG3	9	0.43	0.38	0.28
(1,253)	1:57:A:LYS:HE3	1:54:A:MET:HG3	9	0.43	0.38	0.28
(1,2011)	1:94:A:ARG:HD2	1:94:A:ARG:H	9	0.43	0.07	0.38
(1,576)	1:142:A:LYS:HB2	1:142:A:LYS:H	9	0.35	0.13	0.31
(1,2138)	1:69:A:GLU:HG3	1:69:A:GLU:H	9	0.27	0.03	0.28
(1,2273)	2:25:B:GLU:HB3	2:25:B:GLU:H	9	0.23	0.06	0.22
(1,633)	1:100:A:LEU:HD12	1:92:A:GLN:HE21	9	0.22	0.11	0.2
(1,633)	1:100:A:LEU:HD11	1:92:A:GLN:HE21	9	0.22	0.11	0.2
(1,633)	1:100:A:LEU:HD13	1:92:A:GLN:HE21	9	0.22	0.11	0.2
(1,778)	1:125:A:VAL:HG23	1:122:A:LYS:HA	9	0.21	0.08	0.18
(1,778)	1:125:A:VAL:HG21	1:122:A:LYS:HA	9	0.21	0.08	0.18
(1,778)	1:125:A:VAL:HG22	1:122:A:LYS:HA	9	0.21	0.08	0.18
(1,672)	1:133:A:VAL:HG23	1:137:A:HIS:HD2	9	0.18	0.03	0.18

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,672)	1:133:A:VAL:HG21	1:137:A:HIS:HD2	9	0.18	0.03	0.18
(1,672)	1:133:A:VAL:HG22	1:137:A:HIS:HD2	9	0.18	0.03	0.18
(1,79)	1:117:A:ARG:HD3	1:117:A:ARG:HG2	9	0.12	0.01	0.12
(1,79)	1:111:A:ARG:HD3	1:111:A:ARG:HG2	9	0.12	0.01	0.12
(1,570)	1:143:A:LEU:HB2	1:144:A:ASN:HD21	8	1.23	0.49	1.36
(1,1049)	1:108:A:ILE:HD12	1:104:A:GLU:HG2	8	1.14	0.42	1.3
(1,1049)	1:108:A:ILE:HD11	1:104:A:GLU:HG2	8	1.14	0.42	1.3
(1,1049)	1:108:A:ILE:HD13	1:104:A:GLU:HG2	8	1.14	0.42	1.3
(1,1976)	1:100:A:LEU:H	1:138:A:SER:HB2	8	1.06	0.23	1.04
(1,1983)	1:99:A:PHE:H	1:138:A:SER:HB2	8	0.5	0.19	0.45
(1,1123)	1:83:A:GLU:HA	1:83:A:GLU:HG3	8	0.46	0.16	0.54
(1,324)	2:33:B:GLN:HG2	2:26:B:ASP:HB2	8	0.28	0.11	0.28
(1,324)	2:33:B:GLN:HG2	2:26:B:ASP:HB3	8	0.28	0.11	0.28
(1,343)	2:31:B:LEU:HB2	1:87:A:PHE:HE2	8	0.26	0.12	0.22
(1,593)	1:138:A:SER:HA	1:138:A:SER:HB2	8	0.24	0.02	0.24
(1,878)	1:117:A:ARG:HG2	1:114:A:SER:HA	8	0.2	0.05	0.19
(1,1558)	1:57:A:LYS:HB2	1:57:A:LYS:HG3	8	0.2	0.01	0.21
(1,2207)	2:38:B:ARG:HB2	2:39:B:TRP:H	8	0.19	0.05	0.19
(1,1279)	1:84:A:VAL:HG23	1:81:A:HIS:HB3	8	0.19	0.05	0.21
(1,1279)	1:84:A:VAL:HG21	1:81:A:HIS:HB3	8	0.19	0.05	0.21
(1,1279)	1:84:A:VAL:HG22	1:81:A:HIS:HB3	8	0.19	0.05	0.21
(1,466)	1:106:A:CYS:H	1:63:A:ASN:HD21	8	0.18	0.07	0.15
(1,1)	1:141:A:LYS:HG3	1:141:A:LYS:HA	8	0.17	0.06	0.14
(1,1746)	1:100:A:LEU:HD11	1:138:A:SER:HB2	8	0.16	0.05	0.14
(1,1746)	1:100:A:LEU:HD13	1:138:A:SER:HB2	8	0.16	0.05	0.14
(1,1746)	1:100:A:LEU:HD12	1:138:A:SER:HB2	8	0.16	0.05	0.14
(1,812)	1:123:A:LEU:HD23	1:77:A:GLN:HE21	8	0.16	0.02	0.16
(1,812)	1:123:A:LEU:HD22	1:77:A:GLN:HE21	8	0.16	0.02	0.16
(1,812)	1:123:A:LEU:HD21	1:77:A:GLN:HE21	8	0.16	0.02	0.16
(1,704)	1:130:A:LEU:HD13	1:109:A:LEU:HD22	8	0.15	0.04	0.15
(1,704)	1:130:A:LEU:HD11	1:109:A:LEU:HD21	8	0.15	0.04	0.15
(1,704)	1:130:A:LEU:HD12	1:109:A:LEU:HD23	8	0.15	0.04	0.15
(1,999)	1:108:A:ILE:HD12	1:99:A:PHE:HZ	8	0.15	0.03	0.14
(1,999)	1:108:A:ILE:HD11	1:99:A:PHE:HZ	8	0.15	0.03	0.14
(1,999)	1:108:A:ILE:HD13	1:99:A:PHE:HZ	8	0.15	0.03	0.14
(1,19)	1:133:A:VAL:HG21	1:130:A:LEU:HA	8	0.13	0.02	0.12
(1,19)	1:133:A:VAL:HG23	1:130:A:LEU:HA	8	0.13	0.02	0.12
(1,19)	1:133:A:VAL:HG22	1:130:A:LEU:HA	8	0.13	0.02	0.12
(1,1512)	1:62:A:GLU:HG2	1:62:A:GLU:H	8	0.13	0.03	0.12
(1,2153)	1:109:A:LEU:HD11	1:66:A:LEU:H	8	0.13	0.02	0.12
(1,2153)	1:109:A:LEU:HD12	1:66:A:LEU:H	8	0.13	0.02	0.12
(1,2153)	1:109:A:LEU:HD13	1:66:A:LEU:H	8	0.13	0.02	0.12

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1411)	1:71:A:LEU:HD23	1:71:A:LEU:HB2	8	0.12	0.01	0.12
(1,1411)	1:71:A:LEU:HD22	1:71:A:LEU:HB2	8	0.12	0.01	0.12
(1,1369)	1:75:A:LYS:HE3	1:72:A:GLU:HA	8	0.11	0.01	0.11
(1,1415)	1:71:A:LEU:HB2	1:75:A:LYS:HE2	7	0.95	0.46	1.15
(1,1143)	1:94:A:ARG:HG2	1:94:A:ARG:H	7	0.93	0.11	0.9
(1,1075)	1:101:A:ALA:HB2	1:60:A:LYS:HB2	7	0.81	0.35	0.98
(1,1075)	1:101:A:ALA:HB3	1:60:A:LYS:HB2	7	0.81	0.35	0.98
(1,1075)	1:101:A:ALA:HB1	1:60:A:LYS:HB2	7	0.81	0.35	0.98
(1,1047)	1:104:A:GLU:HG2	1:105:A:PHE:H	7	0.45	0.1	0.44
(1,2037)	1:90:A:ASN:HD21	1:94:A:ARG:HD3	7	0.43	0.1	0.45
(1,2037)	1:90:A:ASN:HD21	1:94:A:ARG:HD2	7	0.43	0.1	0.45
(1,45)	1:59:A:TYR:HE1	1:57:A:LYS:HD2	7	0.31	0.16	0.24
(1,45)	1:59:A:TYR:HE1	1:57:A:LYS:HD3	7	0.31	0.16	0.24
(1,45)	1:59:A:TYR:HE2	1:57:A:LYS:HD3	7	0.31	0.16	0.24
(1,1454)	1:68:A:GLU:HG2	1:69:A:GLU:H	7	0.28	0.15	0.22
(1,469)	1:102:A:SER:H	1:100:A:LEU:HB2	7	0.26	0.09	0.25
(1,469)	1:102:A:SER:H	1:104:A:GLU:HB3	7	0.26	0.09	0.25
(1,389)	1:143:A:LEU:H	1:142:A:LYS:HD2	7	0.24	0.1	0.24
(1,389)	1:143:A:LEU:H	1:142:A:LYS:HB2	7	0.24	0.1	0.24
(1,1702)	2:33:B:GLN:HG3	2:34:B:TYR:HE2	7	0.23	0.13	0.17
(1,1495)	1:64:A:GLU:HA	1:67:A:PHE:HB2	7	0.21	0.06	0.23
(1,1615)	2:39:B:TRP:HE3	2:36:B:THR:HG22	7	0.21	0.06	0.21
(1,1615)	2:39:B:TRP:HE3	2:36:B:THR:HG21	7	0.21	0.06	0.21
(1,1615)	2:39:B:TRP:HE3	2:36:B:THR:HG23	7	0.21	0.06	0.21
(1,1446)	1:69:A:GLU:HG2	1:69:A:GLU:H	7	0.16	0.03	0.15
(1,2054)	1:85:A:VAL:HG12	1:89:A:TYR:H	7	0.15	0.03	0.15
(1,2054)	1:85:A:VAL:HG13	1:89:A:TYR:H	7	0.15	0.03	0.15
(1,2054)	1:85:A:VAL:HG11	1:89:A:TYR:H	7	0.15	0.03	0.15
(1,475)	1:98:A:LEU:HD23	1:98:A:LEU:H	7	0.15	0.02	0.15
(1,475)	1:98:A:LEU:HD22	1:98:A:LEU:H	7	0.15	0.02	0.15
(1,2080)	1:81:A:HIS:H	1:81:A:HIS:HB3	7	0.13	0.02	0.13
(1,537)	1:63:A:ASN:H	1:61:A:LEU:H	7	0.13	0.02	0.12
(1,1715)	2:31:B:LEU:HG	2:31:B:LEU:HA	7	0.11	0.0	0.11
(1,2286)	2:33:B:GLN:HG2	2:33:B:GLN:HE22	7	0.1	0.0	0.1
(1,2189)	1:59:A:TYR:H	1:60:A:LYS:HB2	6	1.18	0.19	1.19
(1,706)	1:85:A:VAL:HG23	1:75:A:LYS:HD2	6	0.9	0.93	0.38
(1,706)	1:85:A:VAL:HG22	1:75:A:LYS:HD2	6	0.9	0.93	0.38
(1,706)	1:85:A:VAL:HG21	1:75:A:LYS:HD2	6	0.9	0.93	0.38
(1,791)	1:124:A:TYR:HB2	1:124:A:TYR:HD1	6	0.76	0.01	0.76
(1,1066)	1:101:A:ALA:HA	1:60:A:LYS:HB2	6	0.65	0.35	0.57
(1,1634)	2:38:B:ARG:HD2	2:37:B:ALA:HB2	6	0.59	0.54	0.28
(1,1634)	2:38:B:ARG:HD2	2:37:B:ALA:HB1	6	0.59	0.54	0.28

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1634)	2:38:B:ARG:HD2	2:37:B:ALA:HB3	6	0.59	0.54	0.28
(1,1652)	2:38:B:ARG:HD2	2:37:B:ALA:HB2	6	0.51	0.16	0.56
(1,1652)	2:37:B:ALA:HB2	2:38:B:ARG:HD3	6	0.51	0.16	0.56
(1,1652)	2:38:B:ARG:HD2	2:37:B:ALA:HB3	6	0.51	0.16	0.56
(1,1652)	2:37:B:ALA:HB1	2:38:B:ARG:HD3	6	0.51	0.16	0.56
(1,857)	1:119:A:ARG:HB2	1:119:A:ARG:HG3	6	0.41	0.02	0.4
(1,1513)	1:62:A:GLU:HA	1:62:A:GLU:HG3	6	0.39	0.03	0.41
(1,1772)	1:142:A:LYS:H	1:141:A:LYS:HG2	6	0.34	0.15	0.34
(1,1772)	1:142:A:LYS:H	1:141:A:LYS:HG3	6	0.34	0.15	0.34
(1,2179)	1:60:A:LYS:HB3	1:61:A:LEU:H	6	0.29	0.02	0.29
(1,222)	1:68:A:GLU:HA	1:71:A:LEU:HG	6	0.29	0.07	0.32
(1,867)	1:119:A:ARG:HD3	1:119:A:ARG:HA	6	0.26	0.06	0.26
(1,391)	1:144:A:ASN:H	1:142:A:LYS:HB2	6	0.26	0.13	0.2
(1,614)	1:135:A:LYS:HA	1:135:A:LYS:HD2	6	0.25	0.14	0.2
(1,2071)	1:83:A:GLU:HG3	1:83:A:GLU:H	6	0.24	0.07	0.27
(1,1453)	1:68:A:GLU:HG3	1:69:A:GLU:H	6	0.22	0.03	0.2
(1,1068)	1:101:A:ALA:HB2	1:59:A:TYR:H	6	0.19	0.04	0.18
(1,1068)	1:101:A:ALA:HB3	1:59:A:TYR:H	6	0.19	0.04	0.18
(1,2194)	1:56:A:LYS:HB3	1:56:A:LYS:H	6	0.19	0.15	0.12
(1,814)	1:123:A:LEU:HD23	1:120:A:PRO:HA	6	0.19	0.05	0.2
(1,814)	1:123:A:LEU:HD22	1:120:A:PRO:HA	6	0.19	0.05	0.2
(1,814)	1:123:A:LEU:HD21	1:120:A:PRO:HA	6	0.19	0.05	0.2
(1,20)	1:61:A:LEU:HA	1:64:A:GLU:HB2	6	0.16	0.05	0.14
(1,20)	1:66:A:LEU:HA	1:69:A:GLU:HB2	6	0.16	0.05	0.14
(1,262)	1:80:A:ASP:HB2	1:81:A:HIS:HD2	6	0.16	0.02	0.17
(1,262)	1:80:A:ASP:HB3	1:81:A:HIS:HD2	6	0.16	0.02	0.17
(1,1132)	1:95:A:ALA:HB1	1:96:A:HIS:H	6	0.15	0.03	0.16
(1,1132)	1:95:A:ALA:HB3	1:96:A:HIS:H	6	0.15	0.03	0.16
(1,1132)	1:95:A:ALA:HB2	1:96:A:HIS:H	6	0.15	0.03	0.16
(1,1556)	1:57:A:LYS:HG2	1:57:A:LYS:HA	6	0.15	0.03	0.15
(1,1343)	1:76:A:MET:HG2	1:76:A:MET:H	6	0.14	0.02	0.16
(1,1617)	2:39:B:TRP:HD1	2:38:B:ARG:HA	6	0.13	0.02	0.13
(1,1740)	2:31:B:LEU:HA	2:32:B:GLU:H	6	0.1	0.0	0.1
(1,1397)	1:72:A:GLU:HG2	1:71:A:LEU:H	5	1.53	0.06	1.52
(1,1398)	1:72:A:GLU:HG2	1:71:A:LEU:HB2	5	1.3	0.08	1.27
(1,1637)	2:38:B:ARG:HD2	2:39:B:TRP:HD1	5	0.96	0.44	0.9
(1,1396)	1:72:A:GLU:HG2	1:72:A:GLU:H	5	0.83	0.05	0.8
(1,1561)	1:57:A:LYS:HD2	1:57:A:LYS:HA	5	0.58	0.26	0.58
(1,2193)	1:58:A:CYS:H	1:57:A:LYS:HG2	5	0.5	0.2	0.48
(1,1765)	2:24:B:GLN:HB2	2:24:B:GLN:HG2	5	0.47	0.17	0.55
(1,376)	2:29:B:SER:HB2	2:26:B:ASP:HB3	5	0.4	0.29	0.35
(1,376)	2:27:B:SER:HB3	2:26:B:ASP:HB3	5	0.4	0.29	0.35

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,376)	2:27:B:SER:HB3	2:28:B:ASP:HB3	5	0.4	0.29	0.35
(1,1534)	1:59:A:TYR:HD1	1:59:A:TYR:H	5	0.3	0.03	0.3
(1,574)	1:143:A:LEU:HG	1:143:A:LEU:H	5	0.29	0.06	0.3
(1,1544)	1:103:A:ALA:HA	1:59:A:TYR:HE1	5	0.27	0.1	0.25
(1,344)	2:31:B:LEU:HB3	1:87:A:PHE:HD2	5	0.26	0.1	0.27
(1,344)	2:31:B:LEU:HB3	1:87:A:PHE:HE2	5	0.26	0.1	0.27
(1,1958)	1:103:A:ALA:H	1:102:A:SER:HB3	5	0.25	0.12	0.26
(1,922)	1:112:A:VAL:HA	1:115:A:ARG:HG3	5	0.21	0.09	0.17
(1,922)	1:112:A:VAL:HA	1:115:A:ARG:HG2	5	0.21	0.09	0.17
(1,161)	1:87:A:PHE:HE2	2:34:B:TYR:HE1	5	0.21	0.06	0.21
(1,1550)	1:141:A:LYS:HG3	1:141:A:LYS:HA	5	0.18	0.06	0.16
(1,1550)	1:141:A:LYS:HG2	1:141:A:LYS:HA	5	0.18	0.06	0.16
(1,1539)	1:62:A:GLU:HB3	1:59:A:TYR:HD1	5	0.18	0.04	0.18
(1,2075)	1:81:A:HIS:H	1:81:A:HIS:HD2	5	0.17	0.02	0.17
(1,582)	1:139:A:ALA:HA	1:96:A:HIS:HB2	5	0.16	0.02	0.16
(1,821)	1:122:A:LYS:HG3	1:122:A:LYS:H	5	0.15	0.04	0.13
(1,388)	1:57:A:LYS:HA	1:57:A:LYS:H	5	0.14	0.0	0.14
(1,963)	1:109:A:LEU:HD12	1:63:A:ASN:HB2	5	0.14	0.02	0.13
(1,963)	1:109:A:LEU:HD13	1:63:A:ASN:HB2	5	0.14	0.02	0.13
(1,963)	1:109:A:LEU:HD11	1:63:A:ASN:HB2	5	0.14	0.02	0.13
(1,1529)	1:59:A:TYR:HB2	1:59:A:TYR:HD1	5	0.14	0.01	0.15
(1,860)	1:119:A:ARG:HG2	1:119:A:ARG:H	5	0.14	0.01	0.15
(1,78)	1:118:A:SER:HB3	1:119:A:ARG:HG3	5	0.12	0.01	0.12
(1,553)	2:29:B:SER:HB2	2:30:B:GLU:H	5	0.11	0.01	0.11
(1,837)	1:120:A:PRO:HD2	1:119:A:ARG:H	5	0.11	0.01	0.1
(1,1766)	2:24:B:GLN:HG2	2:23:B:SER:HA	4	1.1	0.41	1.16
(1,1096)	1:100:A:LEU:HD23	1:92:A:GLN:HG3	4	1.06	0.92	0.76
(1,1096)	1:100:A:LEU:HD22	1:92:A:GLN:HG3	4	1.06	0.92	0.76
(1,1929)	1:107:A:ASN:HD21	1:103:A:ALA:HB3	4	0.51	0.06	0.5
(1,1929)	1:107:A:ASN:HD21	1:103:A:ALA:HB1	4	0.51	0.06	0.5
(1,1929)	1:107:A:ASN:HD21	1:103:A:ALA:HB2	4	0.51	0.06	0.5
(1,1273)	1:85:A:VAL:HG13	1:75:A:LYS:HE2	4	0.48	0.07	0.48
(1,1273)	1:85:A:VAL:HG11	1:75:A:LYS:HE2	4	0.48	0.07	0.48
(1,1275)	1:78:A:THR:HG21	1:77:A:GLN:HB3	4	0.48	0.56	0.18
(1,1275)	1:78:A:THR:HG22	1:77:A:GLN:HB3	4	0.48	0.56	0.18
(1,375)	2:27:B:SER:HB2	2:28:B:ASP:HB3	4	0.47	0.21	0.5
(1,375)	2:27:B:SER:HB3	2:28:B:ASP:HB3	4	0.47	0.21	0.5
(1,375)	2:29:B:SER:HB2	2:26:B:ASP:HB2	4	0.47	0.21	0.5
(1,1770)	1:141:A:LYS:HB3	1:141:A:LYS:H	4	0.46	0.19	0.45
(1,2086)	1:80:A:ASP:HB2	1:80:A:ASP:H	4	0.45	0.02	0.45
(1,2271)	2:25:B:GLU:H	2:25:B:GLU:HG3	4	0.42	0.04	0.41
(1,2271)	2:25:B:GLU:H	2:25:B:GLU:HG2	4	0.42	0.04	0.41

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,363)	2:29:B:SER:HB2	2:32:B:GLU:HB2	4	0.4	0.29	0.26
(1,363)	1:118:A:SER:HB3	1:119:A:ARG:HB2	4	0.4	0.29	0.26
(1,359)	2:27:B:SER:HB2	2:28:B:ASP:HB3	4	0.39	0.21	0.28
(1,359)	2:29:B:SER:HB2	2:26:B:ASP:HB3	4	0.39	0.21	0.28
(1,501)	1:80:A:ASP:HB3	1:81:A:HIS:H	4	0.37	0.05	0.4
(1,501)	1:80:A:ASP:HB2	1:81:A:HIS:H	4	0.37	0.05	0.4
(1,360)	2:29:B:SER:HB3	2:26:B:ASP:HB3	4	0.36	0.27	0.26
(1,360)	2:27:B:SER:HB3	2:26:B:ASP:HB3	4	0.36	0.27	0.26
(1,360)	2:27:B:SER:HB3	2:28:B:ASP:HB3	4	0.36	0.27	0.26
(1,89)	1:94:A:ARG:HD2	1:94:A:ARG:HA	4	0.35	0.23	0.36
(1,89)	1:94:A:ARG:HD3	1:94:A:ARG:HA	4	0.35	0.23	0.36
(1,255)	1:56:A:LYS:HA	1:56:A:LYS:HB3	4	0.33	0.05	0.34
(1,480)	1:134:A:LEU:HD11	1:95:A:ALA:H	4	0.29	0.13	0.27
(1,480)	1:100:A:LEU:HD12	1:95:A:ALA:H	4	0.29	0.13	0.27
(1,480)	1:134:A:LEU:HD12	1:95:A:ALA:H	4	0.29	0.13	0.27
(1,480)	1:100:A:LEU:HD11	1:95:A:ALA:H	4	0.29	0.13	0.27
(1,799)	1:111:A:ARG:HA	1:111:A:ARG:HG3	4	0.26	0.01	0.26
(1,898)	1:115:A:ARG:HA	1:115:A:ARG:HG2	4	0.26	0.26	0.11
(1,569)	1:143:A:LEU:HB2	1:144:A:ASN:H	4	0.24	0.06	0.26
(1,813)	1:123:A:LEU:HD21	1:124:A:TYR:HE2	4	0.22	0.04	0.22
(1,813)	1:123:A:LEU:HD23	1:124:A:TYR:HE2	4	0.22	0.04	0.22
(1,562)	2:26:B:ASP:H	2:25:B:GLU:HG3	4	0.22	0.09	0.22
(1,562)	2:26:B:ASP:H	2:25:B:GLU:HG2	4	0.22	0.09	0.22
(1,2196)	1:56:A:LYS:H	1:56:A:LYS:HB2	4	0.2	0.02	0.21
(1,270)	1:88:A:LEU:HD23	2:31:B:LEU:HD13	4	0.18	0.08	0.15
(1,270)	1:88:A:LEU:HD21	2:31:B:LEU:HD11	4	0.18	0.08	0.15
(1,270)	1:88:A:LEU:HD22	2:31:B:LEU:HD12	4	0.18	0.08	0.15
(1,270)	1:88:A:LEU:HD23	2:31:B:LEU:HD12	4	0.18	0.08	0.15
(1,2268)	2:26:B:ASP:H	2:25:B:GLU:HB3	4	0.17	0.06	0.15
(1,477)	1:93:A:GLN:HA	1:95:A:ALA:H	4	0.17	0.05	0.16
(1,532)	1:66:A:LEU:H	1:64:A:GLU:HB2	4	0.14	0.03	0.12
(1,594)	1:95:A:ALA:HB3	1:138:A:SER:HB3	4	0.13	0.01	0.13
(1,594)	1:95:A:ALA:HB1	1:138:A:SER:HB3	4	0.13	0.01	0.13
(1,594)	1:95:A:ALA:HB2	1:138:A:SER:HB3	4	0.13	0.01	0.13
(1,1014)	1:74:A:CYS:HA	1:78:A:THR:HG21	4	0.12	0.01	0.12
(1,1014)	1:74:A:CYS:HA	1:78:A:THR:HG22	4	0.12	0.01	0.12
(1,1014)	1:74:A:CYS:HA	1:78:A:THR:HG23	4	0.12	0.01	0.12
(1,1212)	1:88:A:LEU:HB2	1:88:A:LEU:HD12	4	0.12	0.02	0.12
(1,1212)	1:88:A:LEU:HB2	1:88:A:LEU:HD13	4	0.12	0.02	0.12
(1,1639)	2:38:B:ARG:HD2	2:38:B:ARG:H	4	0.12	0.02	0.12
(1,1777)	1:144:A:ASN:HB3	1:144:A:ASN:H	4	0.12	0.02	0.12
(1,459)	1:111:A:ARG:HB2	1:110:A:SER:H	4	0.12	0.01	0.12

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1327)	1:77:A:GLN:HG2	1:73:A:LEU:HA	3	1.48	0.03	1.46
(1,237)	1:64:A:GLU:HB2	1:65:A:LYS:HG3	3	1.32	0.06	1.31
(1,237)	1:85:A:VAL:HB	1:71:A:LEU:HB3	3	1.32	0.06	1.31
(1,1333)	1:77:A:GLN:HG2	1:73:A:LEU:HG	3	0.94	0.02	0.96
(1,1368)	1:75:A:LYS:HD3	1:75:A:LYS:HB2	3	0.77	0.27	0.58
(1,1328)	1:77:A:GLN:HG2	1:74:A:CYS:HA	3	0.76	0.09	0.76
(1,1760)	2:24:B:GLN:HG2	2:24:B:GLN:HA	3	0.72	0.12	0.65
(1,2)	1:141:A:LYS:HA	1:141:A:LYS:HB2	3	0.7	0.01	0.7
(1,187)	1:77:A:GLN:HG3	1:73:A:LEU:HD13	3	0.7	0.02	0.7
(1,508)	1:77:A:GLN:HE22	1:76:A:MET:HE2	3	0.61	0.17	0.65
(1,508)	1:77:A:GLN:HE22	1:120:A:PRO:HG2	3	0.61	0.17	0.65
(1,1642)	2:38:B:ARG:HB3	2:38:B:ARG:HD2	3	0.61	0.0	0.61
(1,249)	1:56:A:LYS:HA	1:57:A:LYS:H	3	0.53	0.25	0.53
(1,1324)	1:77:A:GLN:HG2	1:77:A:GLN:H	3	0.52	0.04	0.52
(1,1632)	2:38:B:ARG:HG2	2:38:B:ARG:HD2	3	0.52	0.02	0.53
(1,1393)	1:77:A:GLN:HG3	1:73:A:LEU:HD23	3	0.48	0.02	0.48
(1,1393)	1:77:A:GLN:HG3	1:73:A:LEU:HD22	3	0.48	0.02	0.48
(1,1393)	1:77:A:GLN:HG3	1:73:A:LEU:HD21	3	0.48	0.02	0.48
(1,1620)	2:39:B:TRP:HD1	2:38:B:ARG:HG2	3	0.47	0.06	0.5
(1,584)	1:139:A:ALA:HB3	1:96:A:HIS:H	3	0.44	0.09	0.45
(1,584)	1:139:A:ALA:HB1	1:96:A:HIS:H	3	0.44	0.09	0.45
(1,1559)	1:57:A:LYS:HB2	1:57:A:LYS:HG2	3	0.42	0.08	0.46
(1,186)	1:123:A:LEU:HD21	1:77:A:GLN:HG3	3	0.39	0.07	0.38
(1,186)	1:123:A:LEU:HD23	1:77:A:GLN:HG3	3	0.39	0.07	0.38
(1,2033)	1:90:A:ASN:HD22	1:94:A:ARG:HG2	3	0.39	0.13	0.35
(1,1747)	2:26:B:ASP:HB3	2:27:B:SER:HA	3	0.36	0.16	0.27
(1,1061)	1:103:A:ALA:HB1	1:106:A:CYS:HB3	3	0.35	0.25	0.18
(1,1484)	1:65:A:LYS:HA	1:65:A:LYS:HG2	3	0.29	0.25	0.14
(1,2260)	2:27:B:SER:HB2	2:27:B:SER:H	3	0.29	0.01	0.29
(1,1906)	1:111:A:ARG:H	1:111:A:ARG:HD2	3	0.28	0.02	0.28
(1,1886)	1:88:A:LEU:H	1:87:A:PHE:HD1	3	0.27	0.04	0.28
(1,1886)	1:88:A:LEU:H	1:87:A:PHE:HD2	3	0.27	0.04	0.28
(1,631)	1:73:A:LEU:HD13	1:117:A:ARG:HA	3	0.26	0.07	0.29
(1,631)	1:73:A:LEU:HD11	1:117:A:ARG:HA	3	0.26	0.07	0.29
(1,631)	1:73:A:LEU:HD12	1:117:A:ARG:HA	3	0.26	0.07	0.29
(1,2027)	1:92:A:GLN:HE22	1:64:A:GLU:HA	3	0.25	0.02	0.25
(1,2259)	2:27:B:SER:HB3	2:27:B:SER:H	3	0.25	0.11	0.24
(1,642)	1:134:A:LEU:HD21	1:92:A:GLN:HG3	3	0.23	0.06	0.26
(1,642)	1:134:A:LEU:HD22	1:92:A:GLN:HG3	3	0.23	0.06	0.26
(1,448)	1:116:A:ALA:H	1:126:A:TYR:HE2	3	0.23	0.12	0.17
(1,2031)	1:91:A:ARG:H	1:134:A:LEU:HD12	3	0.22	0.08	0.18
(1,2031)	1:91:A:ARG:H	1:134:A:LEU:HD13	3	0.22	0.08	0.18

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1569)	1:57:A:LYS:HE3	1:59:A:TYR:HE1	3	0.22	0.11	0.19
(1,589)	2:27:B:SER:HA	1:132:A:THR:HG21	3	0.21	0.03	0.22
(1,1545)	1:59:A:TYR:HE1	1:57:A:LYS:HB3	3	0.18	0.05	0.2
(1,1545)	1:59:A:TYR:HE1	1:57:A:LYS:HB2	3	0.18	0.05	0.2
(1,2267)	2:26:B:ASP:H	2:25:B:GLU:HB2	3	0.17	0.06	0.14
(1,55)	1:124:A:TYR:HE2	1:81:A:HIS:HB3	3	0.16	0.03	0.14
(1,55)	1:124:A:TYR:HE2	2:35:B:PHE:HB3	3	0.16	0.03	0.14
(1,109)	1:64:A:GLU:HB3	1:65:A:LYS:H	3	0.16	0.03	0.14
(1,100)	1:67:A:PHE:HE1	1:88:A:LEU:HD13	3	0.14	0.02	0.14
(1,100)	1:67:A:PHE:HE1	1:88:A:LEU:HD11	3	0.14	0.02	0.14
(1,100)	1:67:A:PHE:HE2	1:88:A:LEU:HD11	3	0.14	0.02	0.14
(1,238)	1:66:A:LEU:HD13	1:62:A:GLU:HA	3	0.14	0.01	0.14
(1,238)	1:66:A:LEU:HD11	1:62:A:GLU:HA	3	0.14	0.01	0.14
(1,61)	1:61:A:LEU:HD22	1:59:A:TYR:HA	3	0.13	0.01	0.13
(1,61)	1:123:A:LEU:HD12	1:120:A:PRO:HA	3	0.13	0.01	0.13
(1,61)	1:123:A:LEU:HD13	1:120:A:PRO:HA	3	0.13	0.01	0.13
(1,830)	1:121:A:ALA:HB1	1:122:A:LYS:H	3	0.12	0.01	0.11
(1,830)	1:121:A:ALA:HB3	1:122:A:LYS:H	3	0.12	0.01	0.11
(1,2185)	1:59:A:TYR:HE1	1:59:A:TYR:H	3	0.12	0.01	0.12
(1,636)	1:134:A:LEU:HD23	1:134:A:LEU:H	3	0.12	0.02	0.11
(1,931)	1:112:A:VAL:HG11	1:126:A:TYR:HA	3	0.12	0.01	0.12
(1,931)	1:112:A:VAL:HG13	1:126:A:TYR:HA	3	0.12	0.01	0.12
(1,353)	2:29:B:SER:HB2	2:29:B:SER:H	3	0.11	0.01	0.1
(1,353)	2:27:B:SER:HB2	2:27:B:SER:H	3	0.11	0.01	0.1
(1,1093)	1:100:A:LEU:HA	1:100:A:LEU:HD22	2	1.16	0.08	1.16
(1,1366)	1:75:A:LYS:HD3	1:75:A:LYS:H	2	0.84	0.01	0.84
(1,1259)	1:85:A:VAL:HG11	1:75:A:LYS:HD2	2	0.74	0.06	0.74
(1,1557)	1:57:A:LYS:HG3	1:57:A:LYS:HA	2	0.6	0.01	0.6
(1,980)	1:108:A:ILE:HA	1:108:A:ILE:HD13	2	0.58	0.26	0.58
(1,980)	1:108:A:ILE:HA	1:108:A:ILE:HD11	2	0.58	0.26	0.58
(1,211)	1:71:A:LEU:HD23	1:70:A:PHE:HB3	2	0.44	0.32	0.44
(1,211)	1:71:A:LEU:HD21	1:74:A:CYS:HB2	2	0.44	0.32	0.44
(1,1644)	2:31:B:LEU:HA	1:128:A:ASN:HD22	2	0.4	0.26	0.4
(1,1974)	1:100:A:LEU:HG	1:100:A:LEU:H	2	0.34	0.0	0.34
(1,722)	1:129:A:GLU:HG3	1:125:A:VAL:HG12	2	0.32	0.07	0.32
(1,2264)	2:25:B:GLU:HA	2:26:B:ASP:H	2	0.3	0.05	0.3
(1,945)	1:110:A:SER:HB2	1:111:A:ARG:H	2	0.24	0.04	0.24
(1,1567)	1:57:A:LYS:HG3	1:57:A:LYS:HE2	2	0.23	0.12	0.23
(1,559)	2:31:B:LEU:H	2:30:B:GLU:HB3	2	0.22	0.01	0.22
(1,58)	1:123:A:LEU:HA	1:123:A:LEU:HB3	2	0.22	0.0	0.22
(1,1002)	1:108:A:ILE:HD13	1:104:A:GLU:HG2	2	0.22	0.02	0.22
(1,1002)	1:108:A:ILE:HD12	1:104:A:GLU:HG2	2	0.22	0.02	0.22

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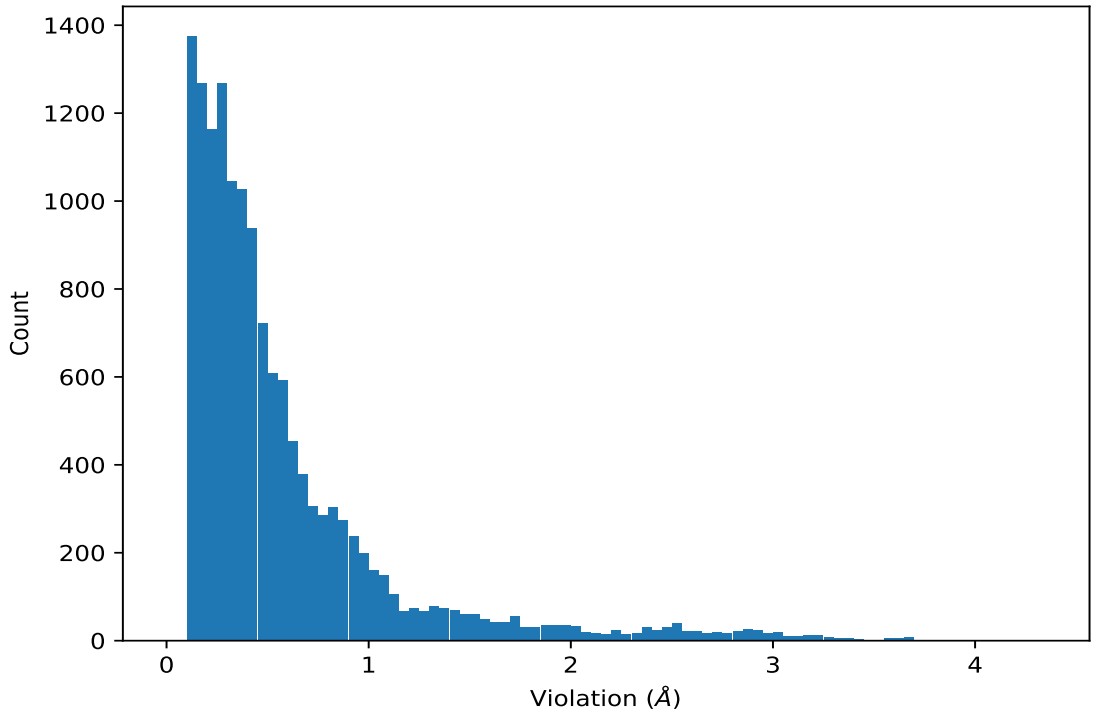
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1792)	1:138:A:SER:H	1:135:A:LYS:HD3	2	0.22	0.1	0.22
(1,771)	1:125:A:VAL:HA	1:128:A:ASN:HD21	2	0.2	0.01	0.2
(1,708)	1:130:A:LEU:HD21	1:70:A:PHE:HD2	2	0.19	0.04	0.19
(1,708)	1:130:A:LEU:HD23	1:70:A:PHE:HD2	2	0.19	0.04	0.19
(1,198)	2:30:B:GLU:HG3	1:87:A:PHE:HZ	2	0.16	0.01	0.16
(1,2272)	2:25:B:GLU:H	2:25:B:GLU:HB2	2	0.16	0.02	0.16
(1,549)	2:39:B:TRP:HE1	1:127:A:ILE:HG13	2	0.15	0.0	0.15
(1,549)	2:39:B:TRP:HE1	1:78:A:THR:HG21	2	0.15	0.0	0.15
(1,897)	1:115:A:ARG:HA	1:115:A:ARG:HD3	2	0.14	0.01	0.14
(1,1769)	2:26:B:ASP:HB3	2:30:B:GLU:HG2	2	0.14	0.02	0.14
(1,1769)	2:26:B:ASP:HB3	2:30:B:GLU:HG3	2	0.14	0.02	0.14
(1,1056)	1:103:A:ALA:HB1	1:104:A:GLU:H	2	0.13	0.02	0.13
(1,26)	1:134:A:LEU:HD13	1:67:A:PHE:HE2	2	0.12	0.02	0.12
(1,26)	1:134:A:LEU:HD13	1:67:A:PHE:HE1	2	0.12	0.02	0.12
(1,113)	1:93:A:GLN:HA	1:94:A:ARG:H	2	0.12	0.02	0.12
(1,156)	1:88:A:LEU:HB3	1:88:A:LEU:HD11	2	0.12	0.01	0.12
(1,1488)	1:65:A:LYS:HG3	1:65:A:LYS:H	2	0.12	0.02	0.12
(1,638)	1:134:A:LEU:HD23	1:99:A:PHE:HE2	2	0.12	0.01	0.12
(1,859)	1:119:A:ARG:HG2	1:119:A:ARG:HA	2	0.12	0.0	0.12
(1,1028)	1:67:A:PHE:HE1	1:88:A:LEU:HB3	2	0.12	0.02	0.12
(1,2255)	2:28:B:ASP:H	2:27:B:SER:HB2	2	0.12	0.02	0.12
(1,711)	1:130:A:LEU:HD21	1:109:A:LEU:HD21	2	0.12	0.0	0.12
(1,75)	1:119:A:ARG:HG2	1:119:A:ARG:HD3	2	0.11	0.0	0.11
(1,751)	1:127:A:ILE:HG23	1:127:A:ILE:HD13	2	0.11	0.0	0.11
(1,751)	1:127:A:ILE:HG21	1:127:A:ILE:HD12	2	0.11	0.0	0.11
(1,924)	1:112:A:VAL:HA	1:115:A:ARG:HB3	2	0.11	0.01	0.11
(1,1077)	1:101:A:ALA:HB1	1:98:A:LEU:HA	2	0.11	0.0	0.11

[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)
(1,1090)	1:100:A:LEU:HD22	1:99:A:PHE:HE1	6	4.35
(1,761)	1:126:A:TYR:HD1	1:123:A:LEU:HD12	13	3.9
(1,761)	1:126:A:TYR:HD1	1:123:A:LEU:HD12	9	3.76
(1,761)	1:126:A:TYR:HD1	1:123:A:LEU:HD13	20	3.75
(1,761)	1:126:A:TYR:HD1	1:123:A:LEU:HD11	12	3.74
(1,761)	1:126:A:TYR:HD1	1:123:A:LEU:HD13	2	3.73
(1,763)	1:126:A:TYR:HE1	1:122:A:LYS:H	21	3.69
(1,761)	1:126:A:TYR:HD1	1:123:A:LEU:HD12	4	3.69
(1,761)	1:126:A:TYR:HD1	1:123:A:LEU:HD11	8	3.69
(1,761)	1:126:A:TYR:HD1	1:123:A:LEU:HD12	23	3.69
(1,761)	1:126:A:TYR:HD1	1:123:A:LEU:HD12	22	3.68
(1,761)	1:126:A:TYR:HD1	1:123:A:LEU:HD11	5	3.66
(1,761)	1:126:A:TYR:HD1	1:123:A:LEU:HD11	14	3.66
(1,761)	1:126:A:TYR:HD1	1:123:A:LEU:HD13	18	3.66
(1,761)	1:126:A:TYR:HD1	1:123:A:LEU:HD12	3	3.64
(1,761)	1:126:A:TYR:HD1	1:123:A:LEU:HD12	15	3.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,761)	1:126:A:TYR:HD1	1:123:A:LEU:HD11	11	3.62
(1,761)	1:126:A:TYR:HD1	1:123:A:LEU:HD13	17	3.61
(1,761)	1:126:A:TYR:HD1	1:123:A:LEU:HD13	25	3.61
(1,761)	1:126:A:TYR:HD1	1:123:A:LEU:HD13	1	3.59
(1,761)	1:126:A:TYR:HD1	1:123:A:LEU:HD13	16	3.58
(1,761)	1:126:A:TYR:HD1	1:123:A:LEU:HD12	7	3.57
(1,761)	1:126:A:TYR:HD1	1:123:A:LEU:HD13	10	3.57
(1,761)	1:126:A:TYR:HD1	1:123:A:LEU:HD13	6	3.55
(1,761)	1:126:A:TYR:HD1	1:123:A:LEU:HD12	19	3.55
(1,764)	1:126:A:TYR:HE1	1:116:A:ALA:HA	2	3.54
(1,761)	1:126:A:TYR:HD1	1:123:A:LEU:HD11	24	3.54
(1,761)	1:126:A:TYR:HD1	1:123:A:LEU:HD11	21	3.47
(1,764)	1:126:A:TYR:HE1	1:116:A:ALA:HA	24	3.45
(1,263)	1:132:A:THR:HG21	2:28:B:ASP:HB2	10	3.44
(1,764)	1:126:A:TYR:HE1	1:116:A:ALA:HA	25	3.42
(1,763)	1:126:A:TYR:HE1	1:122:A:LYS:H	15	3.4
(1,764)	1:126:A:TYR:HE1	1:116:A:ALA:HA	20	3.37
(1,1198)	1:89:A:TYR:HE1	1:85:A:VAL:HG13	9	3.36
(1,764)	1:126:A:TYR:HE1	1:116:A:ALA:HA	9	3.36
(1,764)	1:126:A:TYR:HE1	1:116:A:ALA:HA	18	3.36
(1,763)	1:126:A:TYR:HE1	1:122:A:LYS:H	25	3.36
(1,764)	1:126:A:TYR:HE1	1:116:A:ALA:HA	10	3.33
(1,759)	1:126:A:TYR:HD1	1:116:A:ALA:HA	2	3.31
(1,1105)	1:134:A:LEU:HD23	1:99:A:PHE:HE1	10	3.3
(1,764)	1:126:A:TYR:HE1	1:116:A:ALA:HA	4	3.3
(1,764)	1:126:A:TYR:HE1	1:116:A:ALA:HA	17	3.3
(1,1198)	1:89:A:TYR:HE1	1:85:A:VAL:HG13	23	3.29
(1,1105)	1:134:A:LEU:HD23	1:99:A:PHE:HE1	5	3.29
(1,764)	1:126:A:TYR:HE1	1:116:A:ALA:HA	3	3.27
(1,764)	1:126:A:TYR:HE1	1:116:A:ALA:HA	7	3.27
(1,764)	1:126:A:TYR:HE1	1:116:A:ALA:HA	12	3.27
(1,764)	1:126:A:TYR:HE1	1:116:A:ALA:HA	22	3.27
(1,763)	1:126:A:TYR:HE1	1:122:A:LYS:H	11	3.27
(1,764)	1:126:A:TYR:HE1	1:116:A:ALA:HA	1	3.25
(1,764)	1:126:A:TYR:HE1	1:116:A:ALA:HA	8	3.25
(1,1198)	1:89:A:TYR:HE1	1:85:A:VAL:HG13	2	3.24
(1,1089)	1:105:A:PHE:HZ	1:100:A:LEU:HD23	6	3.24
(1,1089)	1:105:A:PHE:HZ	1:100:A:LEU:HD23	8	3.24
(1,764)	1:126:A:TYR:HE1	1:116:A:ALA:HA	21	3.24
(1,763)	1:126:A:TYR:HE1	1:122:A:LYS:H	1	3.24
(1,763)	1:126:A:TYR:HE1	1:122:A:LYS:H	16	3.24
(1,764)	1:126:A:TYR:HE1	1:116:A:ALA:HA	6	3.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,263)	1:132:A:THR:HG23	2:28:B:ASP:HB2	9	3.23
(1,1198)	1:89:A:TYR:HE1	1:85:A:VAL:HG11	15	3.22
(1,764)	1:126:A:TYR:HE1	1:116:A:ALA:HA	5	3.22
(1,764)	1:126:A:TYR:HE1	1:116:A:ALA:HA	15	3.22
(1,763)	1:126:A:TYR:HE1	1:122:A:LYS:H	23	3.21
(1,763)	1:126:A:TYR:HE1	1:122:A:LYS:H	14	3.2
(1,1198)	1:89:A:TYR:HE1	1:85:A:VAL:HG13	14	3.19
(1,764)	1:126:A:TYR:HE1	1:116:A:ALA:HA	19	3.19
(1,763)	1:126:A:TYR:HE1	1:122:A:LYS:H	4	3.19
(1,763)	1:126:A:TYR:HE1	1:122:A:LYS:H	10	3.19
(1,1105)	1:134:A:LEU:HD22	1:99:A:PHE:HE1	9	3.18
(1,54)	1:124:A:TYR:HD1	1:84:A:VAL:HG23	7	3.18
(1,764)	1:126:A:TYR:HE1	1:116:A:ALA:HA	11	3.17
(1,54)	1:124:A:TYR:HD1	1:84:A:VAL:HG22	2	3.17
(1,1198)	1:89:A:TYR:HE1	1:85:A:VAL:HG11	4	3.16
(1,1198)	1:89:A:TYR:HE1	1:85:A:VAL:HG11	5	3.16
(1,764)	1:126:A:TYR:HE1	1:116:A:ALA:HA	23	3.15
(1,763)	1:126:A:TYR:HE1	1:122:A:LYS:H	19	3.15
(1,763)	1:126:A:TYR:HE1	1:122:A:LYS:H	20	3.15
(1,1105)	1:134:A:LEU:HD22	1:99:A:PHE:HE1	14	3.14
(1,764)	1:126:A:TYR:HE1	1:116:A:ALA:HA	13	3.14
(1,763)	1:126:A:TYR:HE1	1:122:A:LYS:H	5	3.13
(1,767)	1:124:A:TYR:HE1	1:84:A:VAL:HG22	2	3.11
(1,764)	1:126:A:TYR:HE1	1:116:A:ALA:HA	16	3.11
(1,763)	1:126:A:TYR:HE1	1:122:A:LYS:H	3	3.11
(1,1195)	1:89:A:TYR:HD1	1:85:A:VAL:HG13	9	3.1
(1,1105)	1:134:A:LEU:HD21	1:99:A:PHE:HE1	2	3.1
(1,764)	1:126:A:TYR:HE1	1:116:A:ALA:HA	14	3.1
(1,54)	1:124:A:TYR:HD1	1:84:A:VAL:HG21	1	3.1
(1,1026)	1:109:A:LEU:HD11	1:67:A:PHE:HE1	2	3.08
(1,763)	1:126:A:TYR:HE1	1:122:A:LYS:H	6	3.08
(1,1026)	1:109:A:LEU:HD11	1:67:A:PHE:HE1	9	3.07
(1,763)	1:126:A:TYR:HE1	1:122:A:LYS:H	12	3.07
(1,54)	1:124:A:TYR:HD1	1:84:A:VAL:HG21	25	3.07
(1,1200)	1:89:A:TYR:HE1	1:71:A:LEU:HD21	2	3.06
(1,1026)	1:109:A:LEU:HD13	1:67:A:PHE:HE1	24	3.06
(1,759)	1:126:A:TYR:HD1	1:116:A:ALA:HA	9	3.05
(1,54)	1:124:A:TYR:HD1	1:84:A:VAL:HG22	8	3.05
(1,54)	1:124:A:TYR:HD1	1:84:A:VAL:HG21	15	3.05
(1,1105)	1:134:A:LEU:HD22	1:99:A:PHE:HE1	1	3.04
(1,1026)	1:109:A:LEU:HD13	1:67:A:PHE:HE1	1	3.04
(1,1026)	1:109:A:LEU:HD13	1:67:A:PHE:HE1	8	3.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1026)	1:109:A:LEU:HD11	1:67:A:PHE:HE1	15	3.04
(1,1026)	1:109:A:LEU:HD13	1:67:A:PHE:HE1	20	3.04
(1,759)	1:126:A:TYR:HD1	1:116:A:ALA:HA	25	3.04
(1,54)	1:124:A:TYR:HD1	1:84:A:VAL:HG23	19	3.04
(1,1198)	1:89:A:TYR:HE1	1:85:A:VAL:HG11	3	3.03
(1,1026)	1:109:A:LEU:HD11	1:67:A:PHE:HE1	6	3.03
(1,1026)	1:109:A:LEU:HD12	1:67:A:PHE:HE1	14	3.03
(1,759)	1:126:A:TYR:HD1	1:116:A:ALA:HA	7	3.03
(1,763)	1:126:A:TYR:HE1	1:122:A:LYS:H	7	3.02
(1,763)	1:126:A:TYR:HE1	1:122:A:LYS:H	18	3.02
(1,759)	1:126:A:TYR:HD1	1:116:A:ALA:HA	24	3.02
(1,1026)	1:109:A:LEU:HD11	1:67:A:PHE:HE1	18	3.01
(1,759)	1:126:A:TYR:HD1	1:116:A:ALA:HA	10	3.01
(1,1198)	1:89:A:TYR:HE1	1:85:A:VAL:HG11	1	3.0
(1,1026)	1:109:A:LEU:HD12	1:67:A:PHE:HE1	11	3.0
(1,759)	1:126:A:TYR:HD1	1:116:A:ALA:HA	20	3.0
(1,1195)	1:89:A:TYR:HD1	1:85:A:VAL:HG13	14	2.99
(1,1090)	1:100:A:LEU:HD21	1:99:A:PHE:HE1	12	2.99
(1,759)	1:126:A:TYR:HD1	1:116:A:ALA:HA	18	2.99
(1,1195)	1:89:A:TYR:HD1	1:85:A:VAL:HG13	23	2.98
(1,765)	1:126:A:TYR:HE1	1:119:A:ARG:HB2	20	2.98
(1,759)	1:126:A:TYR:HD1	1:116:A:ALA:HA	3	2.98
(1,759)	1:126:A:TYR:HD1	1:116:A:ALA:HA	13	2.98
(1,759)	1:126:A:TYR:HD1	1:116:A:ALA:HA	17	2.98
(1,1198)	1:89:A:TYR:HE1	1:85:A:VAL:HG12	6	2.96
(1,1105)	1:134:A:LEU:HD23	1:99:A:PHE:HE1	12	2.96
(1,1105)	1:134:A:LEU:HD22	1:99:A:PHE:HE1	16	2.96
(1,1090)	1:100:A:LEU:HD22	1:99:A:PHE:HE1	14	2.96
(1,1026)	1:109:A:LEU:HD12	1:67:A:PHE:HE1	23	2.96
(1,765)	1:126:A:TYR:HE1	1:119:A:ARG:HB2	25	2.96
(1,759)	1:126:A:TYR:HD1	1:116:A:ALA:HA	12	2.96
(1,1026)	1:109:A:LEU:HD11	1:67:A:PHE:HE1	4	2.95
(1,763)	1:126:A:TYR:HE1	1:122:A:LYS:H	24	2.95
(1,54)	1:124:A:TYR:HD1	1:84:A:VAL:HG23	12	2.95
(1,763)	1:126:A:TYR:HE1	1:122:A:LYS:H	2	2.94
(1,763)	1:126:A:TYR:HE1	1:122:A:LYS:H	9	2.94
(1,763)	1:126:A:TYR:HE1	1:122:A:LYS:H	22	2.94
(1,759)	1:126:A:TYR:HD1	1:116:A:ALA:HA	1	2.94
(1,759)	1:126:A:TYR:HD1	1:116:A:ALA:HA	6	2.94
(1,759)	1:126:A:TYR:HD1	1:116:A:ALA:HA	22	2.94
(1,1090)	1:100:A:LEU:HD23	1:99:A:PHE:HE1	5	2.93
(1,759)	1:126:A:TYR:HD1	1:116:A:ALA:HA	4	2.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,577)	1:75:A:LYS:HE2	1:71:A:LEU:HB3	7	2.93
(1,54)	1:124:A:TYR:HD1	1:84:A:VAL:HG23	23	2.93
(1,1200)	1:89:A:TYR:HE1	1:71:A:LEU:HD23	23	2.92
(1,1090)	1:100:A:LEU:HD21	1:99:A:PHE:HE1	1	2.92
(1,1090)	1:100:A:LEU:HD23	1:99:A:PHE:HE1	2	2.92
(1,759)	1:126:A:TYR:HD1	1:116:A:ALA:HA	8	2.92
(1,1200)	1:89:A:TYR:HE1	1:71:A:LEU:HD22	5	2.91
(1,1195)	1:89:A:TYR:HD1	1:85:A:VAL:HG11	3	2.91
(1,1026)	1:109:A:LEU:HD13	1:67:A:PHE:HE1	16	2.91
(1,763)	1:126:A:TYR:HE1	1:122:A:LYS:H	17	2.91
(1,263)	1:132:A:THR:HG23	2:28:B:ASP:HB2	12	2.91
(1,1195)	1:89:A:TYR:HD1	1:85:A:VAL:HG12	6	2.9
(1,1195)	1:89:A:TYR:HD1	1:85:A:VAL:HG11	15	2.9
(1,763)	1:126:A:TYR:HE1	1:122:A:LYS:H	8	2.9
(1,759)	1:126:A:TYR:HD1	1:116:A:ALA:HA	15	2.9
(1,54)	1:124:A:TYR:HD1	1:84:A:VAL:HG21	3	2.9
(1,1660)	2:36:B:THR:HG22	1:122:A:LYS:HD2	25	2.89
(1,1200)	1:89:A:TYR:HE1	1:71:A:LEU:HD21	14	2.89
(1,1198)	1:89:A:TYR:HE1	1:85:A:VAL:HG13	13	2.89
(1,1026)	1:109:A:LEU:HD11	1:67:A:PHE:HE1	21	2.89
(1,767)	1:124:A:TYR:HE1	1:84:A:VAL:HG21	25	2.89
(1,765)	1:126:A:TYR:HE1	1:119:A:ARG:HB2	4	2.89
(1,1026)	1:109:A:LEU:HD12	1:67:A:PHE:HE1	17	2.88
(1,1200)	1:89:A:TYR:HE1	1:71:A:LEU:HD23	3	2.87
(1,1198)	1:89:A:TYR:HE1	1:85:A:VAL:HG11	19	2.87
(1,1198)	1:89:A:TYR:HE1	1:85:A:VAL:HG12	20	2.87
(1,1026)	1:109:A:LEU:HD13	1:67:A:PHE:HE1	7	2.87
(1,1200)	1:89:A:TYR:HE1	1:71:A:LEU:HD21	4	2.86
(1,1195)	1:89:A:TYR:HD1	1:85:A:VAL:HG11	4	2.86
(1,1195)	1:89:A:TYR:HD1	1:85:A:VAL:HG11	19	2.86
(1,1105)	1:134:A:LEU:HD23	1:99:A:PHE:HE1	25	2.86
(1,1090)	1:100:A:LEU:HD21	1:99:A:PHE:HE1	10	2.86
(1,1026)	1:109:A:LEU:HD12	1:67:A:PHE:HE1	25	2.86
(1,763)	1:126:A:TYR:HE1	1:122:A:LYS:H	13	2.86
(1,1200)	1:89:A:TYR:HE1	1:71:A:LEU:HD21	9	2.85
(1,1200)	1:89:A:TYR:HE1	1:71:A:LEU:HD22	15	2.85
(1,1198)	1:89:A:TYR:HE1	1:85:A:VAL:HG11	11	2.85
(1,1195)	1:89:A:TYR:HD1	1:85:A:VAL:HG11	1	2.85
(1,1195)	1:89:A:TYR:HD1	1:85:A:VAL:HG13	13	2.85
(1,1026)	1:109:A:LEU:HD13	1:67:A:PHE:HE1	10	2.85
(1,759)	1:126:A:TYR:HD1	1:116:A:ALA:HA	21	2.85
(1,54)	1:124:A:TYR:HD1	1:84:A:VAL:HG23	11	2.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,54)	1:124:A:TYR:HD1	1:84:A:VAL:HG23	20	2.85
(1,767)	1:124:A:TYR:HE1	1:84:A:VAL:HG23	7	2.84
(1,759)	1:126:A:TYR:HD1	1:116:A:ALA:HA	5	2.84
(1,263)	1:132:A:THR:HG22	2:28:B:ASP:HB2	20	2.84
(1,46)	1:126:A:TYR:HE1	1:122:A:LYS:HB3	21	2.84
(1,1195)	1:89:A:TYR:HD1	1:85:A:VAL:HG13	2	2.83
(1,1105)	1:134:A:LEU:HD23	1:99:A:PHE:HE1	7	2.83
(1,1026)	1:109:A:LEU:HD11	1:67:A:PHE:HE1	12	2.83
(1,756)	1:126:A:TYR:HD1	1:123:A:LEU:HA	21	2.83
(1,1195)	1:89:A:TYR:HD1	1:85:A:VAL:HG11	5	2.82
(1,1105)	1:134:A:LEU:HD23	1:99:A:PHE:HE1	22	2.82
(1,756)	1:126:A:TYR:HD1	1:123:A:LEU:HA	11	2.82
(1,767)	1:124:A:TYR:HE1	1:84:A:VAL:HG21	15	2.81
(1,759)	1:126:A:TYR:HD1	1:116:A:ALA:HA	16	2.81
(1,54)	1:124:A:TYR:HD1	1:84:A:VAL:HG23	9	2.81
(1,1200)	1:89:A:TYR:HE1	1:71:A:LEU:HD22	1	2.8
(1,1198)	1:89:A:TYR:HE1	1:85:A:VAL:HG13	12	2.8
(1,1198)	1:89:A:TYR:HE1	1:85:A:VAL:HG13	17	2.8
(1,1198)	1:89:A:TYR:HE1	1:85:A:VAL:HG12	25	2.8
(1,1026)	1:109:A:LEU:HD12	1:67:A:PHE:HE1	22	2.8
(1,756)	1:126:A:TYR:HD1	1:123:A:LEU:HA	1	2.8
(1,756)	1:126:A:TYR:HD1	1:123:A:LEU:HA	13	2.8
(1,1198)	1:89:A:TYR:HE1	1:85:A:VAL:HG13	7	2.79
(1,1090)	1:100:A:LEU:HD22	1:99:A:PHE:HE1	9	2.79
(1,1090)	1:100:A:LEU:HD23	1:99:A:PHE:HE1	24	2.79
(1,1026)	1:109:A:LEU:HD11	1:67:A:PHE:HE1	5	2.79
(1,759)	1:126:A:TYR:HD1	1:116:A:ALA:HA	19	2.79
(1,759)	1:126:A:TYR:HD1	1:116:A:ALA:HA	23	2.79
(1,54)	1:124:A:TYR:HD1	1:84:A:VAL:HG21	22	2.79
(1,759)	1:126:A:TYR:HD1	1:116:A:ALA:HA	11	2.78
(1,1198)	1:89:A:TYR:HE1	1:85:A:VAL:HG11	16	2.77
(1,1195)	1:89:A:TYR:HD1	1:85:A:VAL:HG13	17	2.77
(1,767)	1:124:A:TYR:HE1	1:84:A:VAL:HG22	8	2.77
(1,767)	1:124:A:TYR:HE1	1:84:A:VAL:HG23	19	2.77
(1,765)	1:126:A:TYR:HE1	1:119:A:ARG:HB2	2	2.77
(1,263)	1:132:A:THR:HG22	2:28:B:ASP:HB2	4	2.77
(1,1200)	1:89:A:TYR:HE1	1:71:A:LEU:HD21	11	2.76
(1,765)	1:126:A:TYR:HE1	1:119:A:ARG:HB2	9	2.76
(1,759)	1:126:A:TYR:HD1	1:116:A:ALA:HA	14	2.76
(1,263)	1:132:A:THR:HG21	2:28:B:ASP:HB2	18	2.76
(1,1200)	1:89:A:TYR:HE1	1:71:A:LEU:HD21	16	2.74
(1,1198)	1:89:A:TYR:HE1	1:85:A:VAL:HG11	22	2.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1195)	1:89:A:TYR:HD1	1:85:A:VAL:HG12	25	2.74
(1,1105)	1:134:A:LEU:HD23	1:99:A:PHE:HE1	24	2.74
(1,1090)	1:100:A:LEU:HD22	1:99:A:PHE:HE1	8	2.74
(1,765)	1:126:A:TYR:HE1	1:119:A:ARG:HB2	24	2.74
(1,756)	1:126:A:TYR:HD1	1:123:A:LEU:HA	4	2.74
(1,756)	1:126:A:TYR:HD1	1:123:A:LEU:HA	23	2.74
(1,54)	1:124:A:TYR:HD1	1:84:A:VAL:HG22	17	2.74
(1,1200)	1:89:A:TYR:HE1	1:71:A:LEU:HD23	17	2.73
(1,1195)	1:89:A:TYR:HD1	1:85:A:VAL:HG11	11	2.73
(1,1105)	1:134:A:LEU:HD23	1:99:A:PHE:HE1	11	2.73
(1,1198)	1:89:A:TYR:HE1	1:85:A:VAL:HG11	18	2.72
(1,767)	1:124:A:TYR:HE1	1:84:A:VAL:HG21	1	2.72
(1,412)	1:131:A:CYS:H	1:87:A:PHE:HE1	2	2.72
(1,54)	1:124:A:TYR:HD1	1:84:A:VAL:HG21	6	2.72
(1,756)	1:126:A:TYR:HD1	1:123:A:LEU:HA	15	2.71
(1,756)	1:126:A:TYR:HD1	1:123:A:LEU:HA	19	2.71
(1,1195)	1:89:A:TYR:HD1	1:85:A:VAL:HG11	21	2.7
(1,756)	1:126:A:TYR:HD1	1:123:A:LEU:HA	20	2.7
(1,1200)	1:89:A:TYR:HE1	1:71:A:LEU:HD23	6	2.69
(1,1198)	1:89:A:TYR:HE1	1:85:A:VAL:HG11	21	2.69
(1,1195)	1:89:A:TYR:HD1	1:85:A:VAL:HG12	20	2.69
(1,1105)	1:134:A:LEU:HD23	1:99:A:PHE:HE1	20	2.69
(1,765)	1:126:A:TYR:HE1	1:119:A:ARG:HB2	16	2.69
(1,1195)	1:89:A:TYR:HD1	1:85:A:VAL:HG12	8	2.68
(1,1105)	1:134:A:LEU:HD21	1:99:A:PHE:HE1	3	2.68
(1,765)	1:126:A:TYR:HE1	1:119:A:ARG:HB2	17	2.68
(1,756)	1:126:A:TYR:HD1	1:123:A:LEU:HA	16	2.68
(1,54)	1:124:A:TYR:HD1	1:84:A:VAL:HG22	18	2.68
(1,765)	1:126:A:TYR:HE1	1:119:A:ARG:HB2	21	2.67
(1,1200)	1:89:A:TYR:HE1	1:71:A:LEU:HD23	20	2.66
(1,756)	1:126:A:TYR:HD1	1:123:A:LEU:HA	25	2.66
(1,1198)	1:89:A:TYR:HE1	1:85:A:VAL:HG13	24	2.65
(1,1195)	1:89:A:TYR:HD1	1:85:A:VAL:HG13	12	2.65
(1,577)	1:75:A:LYS:HE2	1:71:A:LEU:HB3	25	2.65
(1,412)	1:131:A:CYS:H	1:87:A:PHE:HE1	20	2.65
(1,767)	1:124:A:TYR:HE1	1:84:A:VAL:HG23	23	2.64
(1,765)	1:126:A:TYR:HE1	1:119:A:ARG:HB2	6	2.64
(1,756)	1:126:A:TYR:HD1	1:123:A:LEU:HA	5	2.64
(1,756)	1:126:A:TYR:HD1	1:123:A:LEU:HA	10	2.64
(1,756)	1:126:A:TYR:HD1	1:123:A:LEU:HA	14	2.64
(1,1200)	1:89:A:TYR:HE1	1:71:A:LEU:HD22	25	2.63
(1,1195)	1:89:A:TYR:HD1	1:85:A:VAL:HG13	7	2.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,767)	1:124:A:TYR:HE1	1:84:A:VAL:HG21	3	2.63
(1,767)	1:124:A:TYR:HE1	1:84:A:VAL:HG23	12	2.63
(1,765)	1:126:A:TYR:HE1	1:119:A:ARG:HB2	22	2.63
(1,756)	1:126:A:TYR:HD1	1:123:A:LEU:HA	22	2.63
(1,54)	1:124:A:TYR:HD1	1:84:A:VAL:HG23	14	2.63
(1,1198)	1:89:A:TYR:HE1	1:85:A:VAL:HG12	8	2.62
(1,1195)	1:89:A:TYR:HD1	1:85:A:VAL:HG11	18	2.62
(1,412)	1:131:A:CYS:H	1:87:A:PHE:HE1	12	2.62
(1,412)	1:131:A:CYS:H	1:87:A:PHE:HE2	16	2.62
(1,1195)	1:89:A:TYR:HD1	1:85:A:VAL:HG11	16	2.61
(1,765)	1:126:A:TYR:HE1	1:119:A:ARG:HB2	18	2.61
(1,577)	1:75:A:LYS:HE2	1:71:A:LEU:HB3	6	2.61
(1,1200)	1:89:A:TYR:HE1	1:71:A:LEU:HD23	18	2.6
(1,1200)	1:89:A:TYR:HE1	1:71:A:LEU:HD22	24	2.6
(1,765)	1:126:A:TYR:HE1	1:119:A:ARG:HB2	7	2.6
(1,1200)	1:89:A:TYR:HE1	1:71:A:LEU:HD23	22	2.59
(1,1195)	1:89:A:TYR:HD1	1:85:A:VAL:HG11	22	2.59
(1,767)	1:124:A:TYR:HE1	1:84:A:VAL:HG23	20	2.59
(1,756)	1:126:A:TYR:HD1	1:123:A:LEU:HA	3	2.59
(1,412)	1:131:A:CYS:H	1:87:A:PHE:HE1	5	2.59
(1,412)	1:131:A:CYS:H	1:87:A:PHE:HE2	19	2.59
(1,1200)	1:89:A:TYR:HE1	1:71:A:LEU:HD21	12	2.58
(1,1200)	1:89:A:TYR:HE1	1:71:A:LEU:HD22	19	2.58
(1,1105)	1:134:A:LEU:HD22	1:99:A:PHE:HE1	17	2.58
(1,1027)	1:67:A:PHE:HE1	1:109:A:LEU:HD21	14	2.58
(1,1200)	1:89:A:TYR:HE1	1:71:A:LEU:HD21	7	2.57
(1,756)	1:126:A:TYR:HD1	1:123:A:LEU:HA	6	2.57
(1,756)	1:126:A:TYR:HD1	1:123:A:LEU:HA	12	2.57
(1,1105)	1:134:A:LEU:HD21	1:99:A:PHE:HE1	21	2.56
(1,1088)	1:100:A:LEU:HD22	1:105:A:PHE:HD2	8	2.56
(1,1027)	1:67:A:PHE:HE1	1:109:A:LEU:HD21	2	2.56
(1,756)	1:126:A:TYR:HD1	1:123:A:LEU:HA	8	2.56
(1,298)	2:35:B:PHE:HB3	1:87:A:PHE:HD2	10	2.56
(1,1027)	1:67:A:PHE:HE1	1:109:A:LEU:HD23	4	2.55
(1,1027)	1:67:A:PHE:HE1	1:109:A:LEU:HD23	10	2.55
(1,1027)	1:67:A:PHE:HE1	1:109:A:LEU:HD23	18	2.55
(1,756)	1:126:A:TYR:HD1	1:123:A:LEU:HA	7	2.55
(1,1090)	1:100:A:LEU:HD22	1:99:A:PHE:HE1	11	2.54
(1,1027)	1:67:A:PHE:HE1	1:109:A:LEU:HD21	15	2.54
(1,767)	1:124:A:TYR:HE1	1:84:A:VAL:HG23	9	2.54
(1,756)	1:126:A:TYR:HD1	1:123:A:LEU:HA	9	2.54
(1,382)	1:64:A:GLU:HG3	1:100:A:LEU:HD13	22	2.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,303)	2:36:B:THR:HG21	2:33:B:GLN:HB2	2	2.54
(1,303)	2:36:B:THR:HG21	1:125:A:VAL:HB	17	2.54
(1,1195)	1:89:A:TYR:HD1	1:85:A:VAL:HG13	10	2.53
(1,1096)	1:100:A:LEU:HD23	1:92:A:GLN:HG3	8	2.53
(1,1088)	1:100:A:LEU:HD22	1:105:A:PHE:HD2	6	2.53
(1,1027)	1:67:A:PHE:HE1	1:109:A:LEU:HD22	20	2.53
(1,756)	1:126:A:TYR:HD1	1:123:A:LEU:HA	18	2.53
(1,412)	1:131:A:CYS:H	1:87:A:PHE:HE2	6	2.53
(1,412)	1:131:A:CYS:H	1:87:A:PHE:HE1	17	2.53
(1,412)	1:131:A:CYS:H	1:87:A:PHE:HE1	25	2.53
(1,298)	2:35:B:PHE:HB3	1:87:A:PHE:HD2	13	2.53
(1,1660)	2:36:B:THR:HG23	1:122:A:LYS:HD2	9	2.52
(1,1660)	2:36:B:THR:HG21	1:122:A:LYS:HD2	24	2.52
(1,1105)	1:134:A:LEU:HD22	1:99:A:PHE:HE1	18	2.52
(1,1027)	1:67:A:PHE:HE1	1:109:A:LEU:HD22	24	2.52
(1,767)	1:124:A:TYR:HE1	1:84:A:VAL:HG21	22	2.52
(1,1200)	1:89:A:TYR:HE1	1:71:A:LEU:HD21	13	2.51
(1,1195)	1:89:A:TYR:HD1	1:85:A:VAL:HG13	24	2.51
(1,1027)	1:67:A:PHE:HE1	1:109:A:LEU:HD22	1	2.51
(1,1027)	1:67:A:PHE:HE1	1:109:A:LEU:HD23	21	2.51
(1,767)	1:124:A:TYR:HE1	1:84:A:VAL:HG23	11	2.51
(1,767)	1:124:A:TYR:HE1	1:84:A:VAL:HG22	17	2.51
(1,765)	1:126:A:TYR:HE1	1:119:A:ARG:HB2	1	2.51
(1,765)	1:126:A:TYR:HE1	1:119:A:ARG:HB2	5	2.51
(1,765)	1:126:A:TYR:HE1	1:119:A:ARG:HB2	10	2.51
(1,756)	1:126:A:TYR:HD1	1:123:A:LEU:HA	2	2.51
(1,577)	1:75:A:LYS:HE2	1:71:A:LEU:HB3	8	2.51
(1,1198)	1:89:A:TYR:HE1	1:85:A:VAL:HG13	10	2.5
(1,1027)	1:67:A:PHE:HE1	1:109:A:LEU:HD21	9	2.5
(1,1027)	1:67:A:PHE:HE1	1:109:A:LEU:HD23	17	2.5
(1,756)	1:126:A:TYR:HD1	1:123:A:LEU:HA	24	2.5
(1,382)	1:72:A:GLU:HG2	1:85:A:VAL:HG23	15	2.5
(1,303)	2:36:B:THR:HG22	1:125:A:VAL:HB	12	2.5
(1,303)	2:36:B:THR:HG22	2:33:B:GLN:HB2	21	2.5
(1,1105)	1:134:A:LEU:HD21	1:99:A:PHE:HE1	6	2.49
(1,1027)	1:67:A:PHE:HE1	1:109:A:LEU:HD21	16	2.49
(1,765)	1:126:A:TYR:HE1	1:119:A:ARG:HB2	15	2.49
(1,412)	1:131:A:CYS:H	1:87:A:PHE:HE1	8	2.49
(1,412)	1:131:A:CYS:H	1:87:A:PHE:HE1	15	2.49
(1,412)	1:131:A:CYS:H	1:87:A:PHE:HE1	22	2.49
(1,303)	2:36:B:THR:HG21	2:33:B:GLN:HB2	23	2.49
(1,298)	2:35:B:PHE:HB3	1:87:A:PHE:HD2	5	2.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1027)	1:67:A:PHE:HE1	1:109:A:LEU:HD23	6	2.48
(1,1027)	1:67:A:PHE:HE1	1:109:A:LEU:HD23	8	2.48
(1,1027)	1:67:A:PHE:HE1	1:109:A:LEU:HD21	23	2.48
(1,765)	1:126:A:TYR:HE1	1:119:A:ARG:HB2	19	2.48
(1,765)	1:126:A:TYR:HE1	1:119:A:ARG:HB2	23	2.48
(1,412)	1:131:A:CYS:H	1:87:A:PHE:HE1	1	2.48
(1,263)	1:132:A:THR:HG22	2:28:B:ASP:HB2	6	2.48
(1,54)	1:124:A:TYR:HD1	1:84:A:VAL:HG23	21	2.48
(1,1105)	1:134:A:LEU:HD23	1:99:A:PHE:HE1	4	2.47
(1,1105)	1:134:A:LEU:HD23	1:99:A:PHE:HE1	15	2.47
(1,382)	1:64:A:GLU:HG3	1:100:A:LEU:HD11	21	2.47
(1,303)	2:36:B:THR:HG21	2:33:B:GLN:HB2	6	2.47
(1,412)	1:131:A:CYS:H	1:87:A:PHE:HE2	9	2.46
(1,382)	1:64:A:GLU:HG3	1:100:A:LEU:HD12	9	2.46
(1,303)	2:36:B:THR:HG23	2:33:B:GLN:HB2	7	2.46
(1,303)	2:36:B:THR:HG22	2:33:B:GLN:HB2	9	2.46
(1,303)	2:36:B:THR:HG23	2:33:B:GLN:HB2	18	2.46
(1,298)	2:35:B:PHE:HB3	1:87:A:PHE:HD2	24	2.46
(1,1200)	1:89:A:TYR:HE1	1:71:A:LEU:HD21	8	2.45
(1,1090)	1:100:A:LEU:HD22	1:99:A:PHE:HE1	18	2.45
(1,382)	1:72:A:GLU:HG2	1:85:A:VAL:HG21	17	2.45
(1,303)	2:36:B:THR:HG23	2:33:B:GLN:HB2	10	2.45
(1,1027)	1:67:A:PHE:HE1	1:109:A:LEU:HD22	22	2.44
(1,1027)	1:67:A:PHE:HE1	1:109:A:LEU:HD21	25	2.44
(1,1710)	2:32:B:GLU:HG2	1:125:A:VAL:HG21	10	2.43
(1,1660)	2:36:B:THR:HG21	1:122:A:LYS:HD3	18	2.43
(1,1200)	1:89:A:TYR:HE1	1:71:A:LEU:HD22	10	2.43
(1,1027)	1:67:A:PHE:HE1	1:109:A:LEU:HD21	11	2.43
(1,765)	1:126:A:TYR:HE1	1:119:A:ARG:HB2	8	2.43
(1,756)	1:126:A:TYR:HD1	1:123:A:LEU:HA	17	2.43
(1,412)	1:131:A:CYS:H	1:87:A:PHE:HE2	7	2.43
(1,1710)	2:32:B:GLU:HG2	1:125:A:VAL:HG23	21	2.42
(1,1200)	1:89:A:TYR:HE1	1:71:A:LEU:HD21	21	2.42
(1,1090)	1:100:A:LEU:HD23	1:99:A:PHE:HE1	25	2.42
(1,1027)	1:67:A:PHE:HE1	1:109:A:LEU:HD22	12	2.42
(1,303)	2:36:B:THR:HG23	2:33:B:GLN:HB2	3	2.42
(1,298)	2:35:B:PHE:HB3	1:87:A:PHE:HD2	2	2.42
(1,298)	2:35:B:PHE:HB3	1:87:A:PHE:HD2	7	2.42
(1,412)	1:131:A:CYS:H	1:87:A:PHE:HE2	21	2.41
(1,412)	1:131:A:CYS:H	1:87:A:PHE:HE1	23	2.41
(1,382)	1:64:A:GLU:HG3	1:100:A:LEU:HD13	20	2.41
(1,303)	2:36:B:THR:HG21	2:33:B:GLN:HB2	8	2.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,303)	2:36:B:THR:HG21	2:33:B:GLN:HB2	14	2.41
(1,298)	2:35:B:PHE:HB3	1:87:A:PHE:HD2	25	2.41
(1,303)	2:36:B:THR:HG23	2:33:B:GLN:HB2	11	2.4
(1,1105)	1:134:A:LEU:HD23	1:99:A:PHE:HE1	19	2.39
(1,1090)	1:100:A:LEU:HD21	1:99:A:PHE:HE1	16	2.39
(1,1090)	1:100:A:LEU:HD23	1:99:A:PHE:HE1	20	2.39
(1,767)	1:124:A:TYR:HE1	1:84:A:VAL:HG21	6	2.39
(1,765)	1:126:A:TYR:HE1	1:119:A:ARG:HB2	11	2.39
(1,412)	1:131:A:CYS:H	1:87:A:PHE:HE1	18	2.39
(1,382)	1:72:A:GLU:HG2	1:85:A:VAL:HG22	11	2.39
(1,303)	2:36:B:THR:HG22	2:33:B:GLN:HB2	1	2.39
(1,303)	2:36:B:THR:HG21	2:33:B:GLN:HB2	22	2.39
(1,298)	2:35:B:PHE:HB3	1:87:A:PHE:HD2	4	2.39
(1,142)	1:89:A:TYR:HD1	1:88:A:LEU:HB2	5	2.39
(1,1027)	1:67:A:PHE:HE1	1:109:A:LEU:HD21	7	2.38
(1,412)	1:131:A:CYS:H	1:87:A:PHE:HE2	13	2.38
(1,303)	2:36:B:THR:HG22	2:33:B:GLN:HB2	4	2.38
(1,303)	2:36:B:THR:HG22	2:33:B:GLN:HB2	13	2.38
(1,298)	2:35:B:PHE:HB3	1:87:A:PHE:HD2	12	2.38
(1,1027)	1:67:A:PHE:HE1	1:109:A:LEU:HD23	5	2.37
(1,303)	2:36:B:THR:HG21	1:125:A:VAL:HB	5	2.37
(1,298)	2:35:B:PHE:HB3	1:87:A:PHE:HD2	20	2.37
(1,1090)	1:100:A:LEU:HD21	1:99:A:PHE:HE1	21	2.36
(1,767)	1:124:A:TYR:HE1	1:84:A:VAL:HG22	18	2.36
(1,412)	1:131:A:CYS:H	1:87:A:PHE:HE1	4	2.36
(1,303)	2:36:B:THR:HG22	2:33:B:GLN:HB2	15	2.36
(1,263)	1:132:A:THR:HG23	2:28:B:ASP:HB3	24	2.36
(1,142)	1:89:A:TYR:HD1	1:88:A:LEU:HB2	2	2.36
(1,142)	1:89:A:TYR:HD1	1:88:A:LEU:HB2	11	2.36
(1,142)	1:89:A:TYR:HD1	1:88:A:LEU:HB2	17	2.36
(1,412)	1:131:A:CYS:H	1:87:A:PHE:HE1	14	2.35
(1,298)	2:35:B:PHE:HB3	1:87:A:PHE:HD2	19	2.35
(1,298)	2:35:B:PHE:HB3	1:87:A:PHE:HD2	22	2.35
(1,303)	2:36:B:THR:HG21	2:33:B:GLN:HB2	25	2.34
(1,298)	2:35:B:PHE:HB3	1:87:A:PHE:HD2	16	2.34
(1,412)	1:131:A:CYS:H	1:87:A:PHE:HE2	11	2.33
(1,382)	1:72:A:GLU:HG2	1:85:A:VAL:HG21	3	2.33
(1,303)	2:36:B:THR:HG23	2:33:B:GLN:HB2	19	2.33
(1,303)	2:36:B:THR:HG23	2:33:B:GLN:HB2	24	2.33
(1,1105)	1:134:A:LEU:HD23	1:99:A:PHE:HE1	13	2.32
(1,765)	1:126:A:TYR:HE1	1:119:A:ARG:HB2	12	2.32
(1,382)	1:72:A:GLU:HG2	1:85:A:VAL:HG23	6	2.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,303)	2:36:B:THR:HG22	2:33:B:GLN:HB2	20	2.32
(1,298)	2:35:B:PHE:HB3	1:87:A:PHE:HD2	9	2.32
(1,382)	1:72:A:GLU:HG2	1:85:A:VAL:HG23	19	2.31
(1,765)	1:126:A:TYR:HE1	1:119:A:ARG:HB2	14	2.3
(1,412)	1:131:A:CYS:H	1:87:A:PHE:HE2	24	2.3
(1,142)	1:89:A:TYR:HD1	1:88:A:LEU:HB2	3	2.3
(1,142)	1:89:A:TYR:HD1	1:88:A:LEU:HB2	14	2.3
(1,142)	1:89:A:TYR:HD1	1:88:A:LEU:HB2	18	2.3
(1,303)	2:36:B:THR:HG21	2:33:B:GLN:HB2	16	2.29
(1,142)	1:89:A:TYR:HD1	1:88:A:LEU:HB2	23	2.29
(1,1710)	2:32:B:GLU:HG2	1:125:A:VAL:HG22	13	2.28
(1,1710)	2:32:B:GLU:HG2	1:125:A:VAL:HG21	3	2.27
(1,1090)	1:100:A:LEU:HD22	1:99:A:PHE:HE1	22	2.27
(1,765)	1:126:A:TYR:HE1	1:119:A:ARG:HB2	3	2.27
(1,298)	2:35:B:PHE:HB3	1:87:A:PHE:HD2	11	2.27
(1,142)	1:89:A:TYR:HD1	1:88:A:LEU:HB2	4	2.27
(1,1710)	2:32:B:GLU:HG2	1:125:A:VAL:HG23	16	2.26
(1,142)	1:89:A:TYR:HD1	1:88:A:LEU:HB2	24	2.26
(1,142)	1:89:A:TYR:HD1	1:88:A:LEU:HB2	25	2.26
(1,767)	1:124:A:TYR:HE1	1:84:A:VAL:HG23	14	2.25
(1,263)	1:132:A:THR:HG22	2:28:B:ASP:HB3	2	2.25
(1,142)	1:89:A:TYR:HD1	1:88:A:LEU:HB2	9	2.25
(1,142)	1:89:A:TYR:HD1	1:88:A:LEU:HB2	15	2.25
(1,1710)	2:32:B:GLU:HG2	1:125:A:VAL:HG22	8	2.24
(1,765)	1:126:A:TYR:HE1	1:119:A:ARG:HB2	13	2.24
(1,382)	1:64:A:GLU:HG3	1:100:A:LEU:HD11	18	2.24
(1,142)	1:89:A:TYR:HD1	1:88:A:LEU:HB2	12	2.24
(1,142)	1:89:A:TYR:HD1	1:88:A:LEU:HB2	16	2.24
(1,142)	1:89:A:TYR:HD1	1:88:A:LEU:HB2	20	2.24
(1,142)	1:89:A:TYR:HD1	1:88:A:LEU:HB2	22	2.24
(1,1090)	1:100:A:LEU:HD23	1:99:A:PHE:HE1	3	2.23
(1,706)	1:85:A:VAL:HG21	1:75:A:LYS:HD2	24	2.23
(1,142)	1:89:A:TYR:HD1	1:88:A:LEU:HB2	1	2.23
(1,142)	1:89:A:TYR:HD1	1:88:A:LEU:HB2	6	2.23
(1,1710)	2:32:B:GLU:HG2	1:125:A:VAL:HG21	6	2.22
(1,1660)	2:36:B:THR:HG22	1:122:A:LYS:HD2	16	2.22
(1,1090)	1:100:A:LEU:HD23	1:99:A:PHE:HE1	17	2.22
(1,767)	1:124:A:TYR:HE1	1:84:A:VAL:HG23	21	2.22
(1,412)	1:131:A:CYS:H	1:87:A:PHE:HD2	10	2.22
(1,382)	1:72:A:GLU:HG2	1:85:A:VAL:HG23	23	2.22
(1,1710)	2:32:B:GLU:HG2	1:125:A:VAL:HG23	7	2.21
(1,298)	2:35:B:PHE:HB3	1:87:A:PHE:HD2	1	2.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,298)	2:35:B:PHE:HB3	1:87:A:PHE:HD2	18	2.21
(1,142)	1:89:A:TYR:HD1	1:88:A:LEU:HB2	8	2.21
(1,142)	1:89:A:TYR:HD1	1:88:A:LEU:HB2	10	2.21
(1,142)	1:89:A:TYR:HD1	1:88:A:LEU:HB2	19	2.21
(1,298)	2:38:B:ARG:HD2	2:39:B:TRP:HZ2	8	2.2
(1,1710)	2:32:B:GLU:HG2	1:125:A:VAL:HG21	1	2.19
(1,1090)	1:100:A:LEU:HD22	1:99:A:PHE:HE1	7	2.19
(1,382)	1:64:A:GLU:HG3	1:100:A:LEU:HD12	1	2.19
(1,1710)	2:32:B:GLU:HG2	1:125:A:VAL:HG22	9	2.18
(1,706)	1:85:A:VAL:HG21	1:75:A:LYS:HD2	10	2.18
(1,298)	2:35:B:PHE:HB3	1:87:A:PHE:HD2	15	2.18
(1,298)	2:35:B:PHE:HB3	1:87:A:PHE:HD2	23	2.18
(1,1710)	2:32:B:GLU:HG2	1:125:A:VAL:HG23	11	2.17
(1,1710)	2:32:B:GLU:HG2	1:125:A:VAL:HG22	23	2.17
(1,1090)	1:100:A:LEU:HD22	1:99:A:PHE:HE1	15	2.17
(1,1710)	2:32:B:GLU:HG2	1:125:A:VAL:HG23	17	2.16
(1,1586)	2:36:B:THR:HG21	1:125:A:VAL:H	19	2.16
(1,760)	1:126:A:TYR:HD1	1:116:A:ALA:HB3	2	2.16
(1,1710)	2:32:B:GLU:HG2	1:125:A:VAL:HG22	12	2.15
(1,1234)	1:67:A:PHE:HD1	1:109:A:LEU:HD11	2	2.15
(1,1234)	1:67:A:PHE:HD1	1:109:A:LEU:HD11	9	2.14
(1,760)	1:126:A:TYR:HD1	1:116:A:ALA:HB3	10	2.14
(1,382)	1:64:A:GLU:HG3	1:100:A:LEU:HD11	2	2.14
(1,382)	1:72:A:GLU:HG2	1:85:A:VAL:HG21	16	2.14
(1,382)	1:64:A:GLU:HG3	1:100:A:LEU:HD13	24	2.14
(1,142)	1:89:A:TYR:HD1	1:88:A:LEU:HB2	13	2.14
(1,1660)	2:36:B:THR:HG21	1:122:A:LYS:HD3	10	2.13
(1,1586)	2:36:B:THR:HG22	1:125:A:VAL:H	14	2.13
(1,661)	1:133:A:VAL:HG13	1:99:A:PHE:HE1	14	2.13
(1,382)	1:72:A:GLU:HG2	1:85:A:VAL:HG23	25	2.13
(1,1660)	2:36:B:THR:HG21	1:122:A:LYS:HD3	5	2.12
(1,1234)	1:67:A:PHE:HD1	1:109:A:LEU:HD13	8	2.12
(1,760)	1:126:A:TYR:HD1	1:116:A:ALA:HB1	3	2.11
(1,1234)	1:67:A:PHE:HD1	1:109:A:LEU:HD11	15	2.1
(1,1234)	1:67:A:PHE:HD1	1:109:A:LEU:HD13	24	2.1
(1,382)	1:64:A:GLU:HG3	1:100:A:LEU:HD13	13	2.1
(1,142)	1:89:A:TYR:HD1	1:88:A:LEU:HB2	21	2.1
(1,1710)	2:32:B:GLU:HG2	1:125:A:VAL:HG22	4	2.09
(1,1234)	1:67:A:PHE:HD1	1:109:A:LEU:HD13	1	2.09
(1,1234)	1:67:A:PHE:HD1	1:109:A:LEU:HD11	6	2.09
(1,760)	1:126:A:TYR:HD1	1:116:A:ALA:HB2	9	2.09
(1,760)	1:126:A:TYR:HD1	1:116:A:ALA:HB2	24	2.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1710)	2:32:B:GLU:HG2	1:125:A:VAL:HG21	15	2.08
(1,1660)	2:36:B:THR:HG23	1:122:A:LYS:HD3	4	2.08
(1,1660)	2:36:B:THR:HG22	1:122:A:LYS:HD2	6	2.08
(1,1234)	1:67:A:PHE:HD1	1:109:A:LEU:HD12	14	2.08
(1,1234)	1:67:A:PHE:HD1	1:109:A:LEU:HD13	20	2.08
(1,1228)	1:87:A:PHE:HD1	1:88:A:LEU:HD23	10	2.08
(1,1062)	1:103:A:ALA:HB3	1:59:A:TYR:HB3	12	2.08
(1,760)	1:126:A:TYR:HD1	1:116:A:ALA:HB1	7	2.08
(1,142)	1:89:A:TYR:HD1	1:88:A:LEU:HB2	7	2.08
(1,1234)	1:67:A:PHE:HD1	1:109:A:LEU:HD12	11	2.07
(1,832)	1:121:A:ALA:HB2	1:120:A:PRO:HG3	17	2.07
(1,1234)	1:67:A:PHE:HD1	1:109:A:LEU:HD11	18	2.06
(1,298)	2:35:B:PHE:HB3	1:87:A:PHE:HD2	6	2.06
(1,1710)	2:32:B:GLU:HG2	1:125:A:VAL:HG21	24	2.05
(1,832)	1:121:A:ALA:HB2	1:120:A:PRO:HG3	4	2.05
(1,1710)	2:32:B:GLU:HG2	1:125:A:VAL:HG23	20	2.04
(1,760)	1:126:A:TYR:HD1	1:116:A:ALA:HB1	12	2.04
(1,1710)	2:32:B:GLU:HG2	1:125:A:VAL:HG22	2	2.03
(1,1660)	2:36:B:THR:HG22	1:122:A:LYS:HD3	8	2.03
(1,1660)	2:36:B:THR:HG21	1:122:A:LYS:HD3	19	2.03
(1,832)	1:121:A:ALA:HB2	1:120:A:PRO:HG3	22	2.03
(1,760)	1:126:A:TYR:HD1	1:116:A:ALA:HB3	8	2.03
(1,760)	1:126:A:TYR:HD1	1:116:A:ALA:HB2	18	2.03
(1,382)	1:64:A:GLU:HG3	1:100:A:LEU:HD13	14	2.03
(1,298)	2:35:B:PHE:HB3	1:87:A:PHE:HD2	17	2.03
(1,1586)	2:36:B:THR:HG23	1:125:A:VAL:H	21	2.02
(1,832)	1:121:A:ALA:HB2	1:120:A:PRO:HG3	6	2.02
(1,832)	1:121:A:ALA:HB1	1:120:A:PRO:HG3	9	2.02
(1,832)	1:121:A:ALA:HB2	1:120:A:PRO:HG3	13	2.02
(1,832)	1:121:A:ALA:HB2	1:120:A:PRO:HG3	16	2.02
(1,832)	1:121:A:ALA:HB1	1:120:A:PRO:HG3	24	2.02
(1,661)	1:133:A:VAL:HG13	1:99:A:PHE:HE1	10	2.02
(1,1234)	1:67:A:PHE:HD1	1:109:A:LEU:HD12	23	2.01
(1,1090)	1:100:A:LEU:HD23	1:99:A:PHE:HE1	4	2.01
(1,1090)	1:100:A:LEU:HD22	1:99:A:PHE:HE1	13	2.01
(1,1090)	1:100:A:LEU:HD22	1:99:A:PHE:HE1	19	2.01
(1,832)	1:121:A:ALA:HB3	1:120:A:PRO:HG3	2	2.01
(1,832)	1:121:A:ALA:HB2	1:120:A:PRO:HG3	11	2.01
(1,832)	1:121:A:ALA:HB1	1:120:A:PRO:HG3	19	2.01
(1,832)	1:121:A:ALA:HB1	1:120:A:PRO:HG3	20	2.01
(1,832)	1:121:A:ALA:HB1	1:120:A:PRO:HG3	23	2.01
(1,1710)	2:32:B:GLU:HG2	1:125:A:VAL:HG22	5	2.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1233)	1:109:A:LEU:HD21	1:67:A:PHE:HD1	2	2.0
(1,832)	1:121:A:ALA:HB1	1:120:A:PRO:HG3	3	2.0
(1,832)	1:121:A:ALA:HB1	1:120:A:PRO:HG3	5	2.0
(1,832)	1:121:A:ALA:HB3	1:120:A:PRO:HG3	8	2.0
(1,832)	1:121:A:ALA:HB3	1:120:A:PRO:HG3	14	2.0
(1,832)	1:121:A:ALA:HB2	1:120:A:PRO:HG3	25	2.0
(1,1680)	2:35:B:PHE:HE1	1:124:A:TYR:HB2	14	1.99
(1,1233)	1:109:A:LEU:HD23	1:67:A:PHE:HD1	4	1.99
(1,1233)	1:109:A:LEU:HD21	1:67:A:PHE:HD1	14	1.99
(1,832)	1:121:A:ALA:HB3	1:120:A:PRO:HG3	1	1.99
(1,832)	1:121:A:ALA:HB3	1:120:A:PRO:HG3	7	1.99
(1,832)	1:121:A:ALA:HB1	1:120:A:PRO:HG3	10	1.99
(1,46)	1:126:A:TYR:HE1	1:122:A:LYS:HB3	14	1.99
(1,1234)	1:67:A:PHE:HD1	1:109:A:LEU:HD11	4	1.98
(1,1233)	1:109:A:LEU:HD23	1:67:A:PHE:HD1	10	1.98
(1,1233)	1:109:A:LEU:HD21	1:67:A:PHE:HD1	15	1.98
(1,832)	1:121:A:ALA:HB3	1:120:A:PRO:HG3	12	1.98
(1,832)	1:121:A:ALA:HB3	1:120:A:PRO:HG3	21	1.98
(1,760)	1:126:A:TYR:HD1	1:116:A:ALA:HB1	13	1.98
(1,2274)	2:39:B:TRP:HE1	2:38:B:ARG:HD3	5	1.97
(1,1680)	2:35:B:PHE:HE1	1:124:A:TYR:HB2	16	1.97
(1,1680)	2:35:B:PHE:HE1	1:124:A:TYR:HB2	19	1.97
(1,1586)	2:36:B:THR:HG22	1:125:A:VAL:H	25	1.97
(1,832)	1:121:A:ALA:HB2	1:120:A:PRO:HG3	15	1.97
(1,832)	1:121:A:ALA:HB3	1:120:A:PRO:HG3	18	1.97
(1,760)	1:126:A:TYR:HD1	1:116:A:ALA:HB2	17	1.97
(1,661)	1:133:A:VAL:HG13	1:99:A:PHE:HE1	1	1.97
(1,263)	1:132:A:THR:HG23	2:28:B:ASP:HB3	5	1.97
(1,2274)	2:39:B:TRP:HE1	2:38:B:ARG:HD2	12	1.96
(1,1680)	2:35:B:PHE:HE1	1:124:A:TYR:HB2	10	1.96
(1,1660)	2:36:B:THR:HG23	1:122:A:LYS:HD2	1	1.96
(1,1586)	2:36:B:THR:HG22	1:125:A:VAL:H	6	1.96
(1,1233)	1:109:A:LEU:HD23	1:67:A:PHE:HD1	18	1.96
(1,298)	2:35:B:PHE:HB3	1:87:A:PHE:HD2	21	1.96
(1,1680)	2:35:B:PHE:HE1	1:124:A:TYR:HB2	6	1.95
(1,1680)	2:35:B:PHE:HE1	1:124:A:TYR:HB2	7	1.95
(1,1680)	2:35:B:PHE:HE1	1:124:A:TYR:HB2	8	1.95
(1,1586)	2:36:B:THR:HG21	1:125:A:VAL:H	11	1.95
(1,1586)	2:36:B:THR:HG22	1:125:A:VAL:H	16	1.95
(1,1233)	1:109:A:LEU:HD21	1:67:A:PHE:HD1	9	1.95
(1,760)	1:126:A:TYR:HD1	1:116:A:ALA:HB3	6	1.95
(1,1680)	2:35:B:PHE:HE1	1:124:A:TYR:HB2	25	1.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1586)	2:36:B:THR:HG23	1:125:A:VAL:H	9	1.94
(1,1234)	1:67:A:PHE:HD1	1:109:A:LEU:HD13	16	1.94
(1,1233)	1:109:A:LEU:HD23	1:67:A:PHE:HD1	21	1.94
(1,1137)	1:95:A:ALA:HB2	1:91:A:ARG:HD3	9	1.94
(1,382)	1:104:A:GLU:HG2	1:100:A:LEU:HD13	8	1.94
(1,46)	1:126:A:TYR:HE1	1:122:A:LYS:HB3	15	1.94
(1,1710)	2:32:B:GLU:HG2	1:125:A:VAL:HG21	25	1.93
(1,1680)	2:35:B:PHE:HE1	1:124:A:TYR:HB2	21	1.93
(1,1680)	2:35:B:PHE:HE1	1:124:A:TYR:HB2	24	1.93
(1,1233)	1:109:A:LEU:HD22	1:67:A:PHE:HD1	20	1.93
(1,1233)	1:109:A:LEU:HD22	1:67:A:PHE:HD1	24	1.93
(1,368)	2:26:B:ASP:HB3	1:87:A:PHE:HZ	17	1.93
(1,1710)	2:32:B:GLU:HG2	1:125:A:VAL:HG21	18	1.92
(1,1370)	1:75:A:LYS:HE3	1:72:A:GLU:HB3	8	1.92
(1,760)	1:126:A:TYR:HD1	1:116:A:ALA:HB2	1	1.92
(1,1710)	2:32:B:GLU:HG2	1:125:A:VAL:HG21	19	1.91
(1,1710)	2:32:B:GLU:HG2	1:125:A:VAL:HG21	22	1.91
(1,1660)	2:36:B:THR:HG21	1:122:A:LYS:HD3	3	1.91
(1,1234)	1:67:A:PHE:HD1	1:109:A:LEU:HD11	21	1.91
(1,1233)	1:109:A:LEU:HD23	1:67:A:PHE:HD1	8	1.91
(1,1233)	1:109:A:LEU:HD23	1:67:A:PHE:HD1	17	1.91
(1,1233)	1:109:A:LEU:HD21	1:67:A:PHE:HD1	23	1.91
(1,1680)	2:35:B:PHE:HE1	1:124:A:TYR:HB2	1	1.9
(1,1680)	2:35:B:PHE:HE1	1:124:A:TYR:HB2	3	1.9
(1,1680)	2:35:B:PHE:HE1	1:124:A:TYR:HB2	5	1.9
(1,1680)	2:35:B:PHE:HE1	1:124:A:TYR:HB2	13	1.9
(1,1370)	1:75:A:LYS:HE3	1:72:A:GLU:HB3	6	1.9
(1,1370)	1:75:A:LYS:HE3	1:72:A:GLU:HB3	25	1.9
(1,1234)	1:67:A:PHE:HD1	1:109:A:LEU:HD13	7	1.9
(1,1137)	1:95:A:ALA:HB1	1:91:A:ARG:HD3	13	1.9
(1,760)	1:126:A:TYR:HD1	1:116:A:ALA:HB3	21	1.9
(1,661)	1:133:A:VAL:HG11	1:99:A:PHE:HE1	5	1.9
(1,575)	1:143:A:LEU:HA	1:143:A:LEU:HD21	17	1.9
(1,298)	2:35:B:PHE:HB3	1:87:A:PHE:HD2	3	1.9
(1,1680)	2:35:B:PHE:HE1	1:124:A:TYR:HB2	9	1.89
(1,1680)	2:35:B:PHE:HE1	1:124:A:TYR:HB2	11	1.89
(1,1680)	2:35:B:PHE:HE1	1:124:A:TYR:HB2	15	1.89
(1,1680)	2:35:B:PHE:HE1	1:124:A:TYR:HB2	22	1.89
(1,1586)	2:36:B:THR:HG23	1:125:A:VAL:H	15	1.89
(1,1586)	2:36:B:THR:HG21	1:125:A:VAL:H	18	1.89
(1,1233)	1:109:A:LEU:HD23	1:67:A:PHE:HD1	6	1.89
(1,1233)	1:109:A:LEU:HD21	1:67:A:PHE:HD1	16	1.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1680)	2:35:B:PHE:HE1	1:124:A:TYR:HB2	4	1.88
(1,1680)	2:35:B:PHE:HE1	1:124:A:TYR:HB2	12	1.88
(1,1680)	2:35:B:PHE:HE1	1:124:A:TYR:HB2	23	1.88
(1,1586)	2:36:B:THR:HG21	1:125:A:VAL:H	24	1.88
(1,1234)	1:67:A:PHE:HD1	1:109:A:LEU:HD12	17	1.88
(1,1234)	1:67:A:PHE:HD1	1:109:A:LEU:HD12	25	1.88
(1,1233)	1:109:A:LEU:HD22	1:67:A:PHE:HD1	1	1.88
(1,1233)	1:109:A:LEU:HD22	1:67:A:PHE:HD1	22	1.88
(1,760)	1:126:A:TYR:HD1	1:116:A:ALA:HB3	25	1.88
(1,661)	1:133:A:VAL:HG11	1:99:A:PHE:HE1	9	1.88
(1,382)	1:64:A:GLU:HG3	1:100:A:LEU:HD13	4	1.88
(1,298)	2:35:B:PHE:HB3	1:87:A:PHE:HD2	14	1.88
(1,1660)	2:36:B:THR:HG23	1:122:A:LYS:HD3	20	1.87
(1,1233)	1:109:A:LEU:HD22	1:67:A:PHE:HD1	12	1.87
(1,760)	1:126:A:TYR:HD1	1:116:A:ALA:HB1	14	1.87
(1,162)	1:67:A:PHE:HD1	1:130:A:LEU:HD22	10	1.87
(1,1680)	2:35:B:PHE:HE1	1:124:A:TYR:HB2	17	1.86
(1,1680)	2:35:B:PHE:HE1	1:124:A:TYR:HB2	18	1.86
(1,1144)	1:111:A:ARG:HG2	1:107:A:ASN:HA	15	1.86
(1,760)	1:126:A:TYR:HD1	1:116:A:ALA:HB2	5	1.86
(1,760)	1:126:A:TYR:HD1	1:116:A:ALA:HB3	16	1.86
(1,760)	1:126:A:TYR:HD1	1:116:A:ALA:HB3	22	1.86
(1,381)	2:30:B:GLU:HG2	2:31:B:LEU:HB2	25	1.86
(1,1680)	2:35:B:PHE:HE1	1:124:A:TYR:HB2	20	1.85
(1,1660)	2:36:B:THR:HG23	1:122:A:LYS:HD2	13	1.85
(1,1234)	1:67:A:PHE:HD1	1:109:A:LEU:HD11	12	1.85
(1,1144)	1:111:A:ARG:HG2	1:107:A:ASN:HA	16	1.85
(1,760)	1:126:A:TYR:HD1	1:116:A:ALA:HB1	4	1.85
(1,1586)	2:36:B:THR:HG22	1:125:A:VAL:H	23	1.84
(1,1234)	1:67:A:PHE:HD1	1:109:A:LEU:HD13	10	1.84
(1,760)	1:126:A:TYR:HD1	1:116:A:ALA:HB3	20	1.84
(1,661)	1:133:A:VAL:HG13	1:99:A:PHE:HE1	11	1.84
(1,575)	1:143:A:LEU:HA	1:143:A:LEU:HD23	14	1.84
(1,1233)	1:109:A:LEU:HD21	1:67:A:PHE:HD1	11	1.83
(1,1233)	1:109:A:LEU:HD21	1:67:A:PHE:HD1	25	1.83
(1,1137)	1:95:A:ALA:HB2	1:91:A:ARG:HD3	12	1.83
(1,661)	1:133:A:VAL:HG12	1:99:A:PHE:HE1	2	1.83
(1,263)	1:132:A:THR:HG23	2:28:B:ASP:HB2	14	1.83
(1,2274)	2:39:B:TRP:HE1	2:38:B:ARG:HD3	14	1.82
(1,1586)	2:36:B:THR:HG22	1:125:A:VAL:H	22	1.82
(1,1234)	1:67:A:PHE:HD1	1:109:A:LEU:HD11	5	1.82
(1,1144)	1:111:A:ARG:HG2	1:107:A:ASN:HA	13	1.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1144)	1:111:A:ARG:HG2	1:107:A:ASN:HA	19	1.82
(1,904)	1:115:A:ARG:HD3	1:126:A:TYR:HE2	20	1.82
(1,1680)	2:35:B:PHE:HE1	1:124:A:TYR:HB2	2	1.81
(1,1586)	2:36:B:THR:HG23	1:125:A:VAL:H	1	1.81
(1,1233)	1:109:A:LEU:HD23	1:67:A:PHE:HD1	5	1.81
(1,1233)	1:109:A:LEU:HD21	1:67:A:PHE:HD1	7	1.81
(1,1144)	1:111:A:ARG:HG2	1:107:A:ASN:HA	10	1.81
(1,1144)	1:111:A:ARG:HG2	1:107:A:ASN:HA	22	1.81
(1,575)	1:143:A:LEU:HA	1:143:A:LEU:HD23	9	1.81
(1,254)	1:57:A:LYS:HE2	1:54:A:MET:HG3	15	1.81
(1,1586)	2:36:B:THR:HG22	1:125:A:VAL:H	8	1.8
(1,1586)	2:36:B:THR:HG23	1:125:A:VAL:H	13	1.8
(1,1144)	1:111:A:ARG:HG2	1:107:A:ASN:HA	4	1.8
(1,760)	1:126:A:TYR:HD1	1:116:A:ALA:HB1	19	1.8
(1,575)	1:143:A:LEU:HA	1:143:A:LEU:HD23	13	1.8
(1,368)	2:26:B:ASP:HB3	1:87:A:PHE:HZ	3	1.8
(1,368)	2:26:B:ASP:HB3	1:87:A:PHE:HZ	9	1.8
(1,1553)	1:59:A:TYR:HD1	1:57:A:LYS:HB2	10	1.79
(1,1234)	1:67:A:PHE:HD1	1:109:A:LEU:HD12	22	1.79
(1,1062)	1:103:A:ALA:HB1	1:59:A:TYR:HB3	2	1.79
(1,575)	1:143:A:LEU:HA	1:143:A:LEU:HD21	11	1.79
(1,1586)	2:36:B:THR:HG21	1:125:A:VAL:H	10	1.78
(1,1582)	2:37:B:ALA:HB2	1:125:A:VAL:HG23	25	1.78
(1,1144)	1:111:A:ARG:HG2	1:107:A:ASN:HA	1	1.78
(1,1144)	1:111:A:ARG:HG2	1:107:A:ASN:HA	3	1.78
(1,1144)	1:111:A:ARG:HG2	1:107:A:ASN:HA	17	1.78
(1,661)	1:133:A:VAL:HG13	1:99:A:PHE:HE1	12	1.78
(1,46)	1:126:A:TYR:HE1	1:122:A:LYS:HB3	11	1.78
(1,1144)	1:111:A:ARG:HG2	1:107:A:ASN:HA	5	1.77
(1,1144)	1:111:A:ARG:HG2	1:107:A:ASN:HA	21	1.77
(1,1137)	1:95:A:ALA:HB2	1:91:A:ARG:HD3	5	1.77
(1,1062)	1:103:A:ALA:HB1	1:59:A:TYR:HB3	22	1.77
(1,904)	1:115:A:ARG:HD3	1:126:A:TYR:HE1	3	1.77
(1,661)	1:133:A:VAL:HG12	1:99:A:PHE:HE1	24	1.77
(1,263)	1:132:A:THR:HG22	2:28:B:ASP:HB3	13	1.77
(1,162)	1:67:A:PHE:HD1	1:130:A:LEU:HD21	4	1.77
(1,1989)	1:98:A:LEU:H	1:138:A:SER:HB2	12	1.76
(1,1710)	2:32:B:GLU:HG2	1:125:A:VAL:HG23	14	1.76
(1,1586)	2:36:B:THR:HG21	1:125:A:VAL:H	17	1.76
(1,1330)	1:77:A:GLN:HG2	1:76:A:MET:HB3	17	1.76
(1,1330)	1:77:A:GLN:HG2	1:76:A:MET:HB3	19	1.76
(1,904)	1:115:A:ARG:HD3	1:126:A:TYR:HE2	17	1.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,382)	1:72:A:GLU:HG2	1:85:A:VAL:HG22	7	1.76
(1,162)	1:67:A:PHE:HD1	1:130:A:LEU:HD21	21	1.76
(1,46)	1:126:A:TYR:HE1	1:122:A:LYS:HB3	23	1.76
(1,2274)	2:39:B:TRP:HE1	2:38:B:ARG:HD2	7	1.75
(1,1228)	1:87:A:PHE:HD1	1:88:A:LEU:HD21	13	1.75
(1,381)	2:30:B:GLU:HG2	2:31:B:LEU:HB2	18	1.75
(1,2274)	2:39:B:TRP:HE1	2:38:B:ARG:HD2	25	1.74
(1,1989)	1:98:A:LEU:H	1:138:A:SER:HB2	2	1.74
(1,1586)	2:36:B:THR:HG22	1:125:A:VAL:H	2	1.74
(1,1144)	1:111:A:ARG:HG2	1:107:A:ASN:HA	20	1.74
(1,1137)	1:95:A:ALA:HB2	1:91:A:ARG:HD3	17	1.74
(1,1062)	1:103:A:ALA:HB1	1:59:A:TYR:HB3	21	1.74
(1,1062)	1:103:A:ALA:HB3	1:59:A:TYR:HB3	23	1.74
(1,904)	1:115:A:ARG:HD3	1:126:A:TYR:HE2	1	1.74
(1,904)	1:115:A:ARG:HD3	1:126:A:TYR:HE1	13	1.74
(1,795)	1:127:A:ILE:HD13	1:124:A:TYR:HE1	25	1.74
(1,760)	1:126:A:TYR:HD1	1:116:A:ALA:HB2	11	1.74
(1,760)	1:126:A:TYR:HD1	1:116:A:ALA:HB3	23	1.74
(1,661)	1:133:A:VAL:HG13	1:99:A:PHE:HE1	17	1.74
(1,570)	1:143:A:LEU:HB2	1:144:A:ASN:HD21	11	1.74
(1,381)	2:30:B:GLU:HG2	2:31:B:LEU:HB2	4	1.74
(1,162)	1:67:A:PHE:HD1	1:130:A:LEU:HD21	23	1.74
(1,1660)	2:36:B:THR:HG21	1:122:A:LYS:HD2	7	1.73
(1,1330)	1:77:A:GLN:HG2	1:76:A:MET:HB3	10	1.73
(1,1144)	1:111:A:ARG:HG2	1:107:A:ASN:HA	6	1.73
(1,1144)	1:111:A:ARG:HG2	1:107:A:ASN:HA	9	1.73
(1,1071)	1:101:A:ALA:HB2	1:63:A:ASN:HD21	12	1.73
(1,1062)	1:103:A:ALA:HB3	1:59:A:TYR:HB3	4	1.73
(1,1062)	1:103:A:ALA:HB1	1:59:A:TYR:HB3	19	1.73
(1,661)	1:133:A:VAL:HG11	1:99:A:PHE:HE1	25	1.73
(1,162)	1:67:A:PHE:HD1	1:130:A:LEU:HD23	17	1.73
(1,46)	1:126:A:TYR:HE1	1:122:A:LYS:HB3	22	1.73
(1,2274)	2:39:B:TRP:HE1	2:38:B:ARG:HD2	16	1.72
(1,1989)	1:98:A:LEU:H	1:138:A:SER:HB2	9	1.72
(1,1470)	1:66:A:LEU:HD13	1:62:A:GLU:HG3	5	1.72
(1,1470)	1:66:A:LEU:HD12	1:62:A:GLU:HG3	10	1.72
(1,1330)	1:77:A:GLN:HG2	1:76:A:MET:HB3	25	1.72
(1,1144)	1:111:A:ARG:HG2	1:107:A:ASN:HA	24	1.72
(1,661)	1:133:A:VAL:HG11	1:99:A:PHE:HE1	7	1.72
(1,254)	1:57:A:LYS:HE3	1:54:A:MET:HG3	6	1.72
(1,162)	1:67:A:PHE:HD1	1:130:A:LEU:HD21	14	1.72
(1,2274)	2:39:B:TRP:HE1	2:38:B:ARG:HD3	15	1.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1660)	2:36:B:THR:HG22	1:122:A:LYS:HD2	22	1.71
(1,1586)	2:36:B:THR:HG21	1:125:A:VAL:H	7	1.71
(1,1370)	1:75:A:LYS:HE3	1:72:A:GLU:HB3	7	1.71
(1,1330)	1:77:A:GLN:HG2	1:76:A:MET:HB3	6	1.71
(1,1137)	1:95:A:ALA:HB3	1:91:A:ARG:HD3	16	1.71
(1,570)	1:143:A:LEU:HB2	1:144:A:ASN:HD21	14	1.71
(1,381)	2:30:B:GLU:HG2	2:31:B:LEU:HB2	8	1.71
(1,381)	2:30:B:GLU:HG2	2:31:B:LEU:HB2	20	1.71
(1,2274)	2:39:B:TRP:HE1	2:38:B:ARG:HD3	19	1.7
(1,1586)	2:36:B:THR:HG23	1:125:A:VAL:H	4	1.7
(1,1470)	1:66:A:LEU:HD12	1:62:A:GLU:HG3	25	1.7
(1,1330)	1:77:A:GLN:HG2	1:76:A:MET:HB3	8	1.7
(1,1330)	1:77:A:GLN:HG2	1:76:A:MET:HB3	16	1.7
(1,1330)	1:77:A:GLN:HG2	1:76:A:MET:HB3	21	1.7
(1,1144)	1:111:A:ARG:HG2	1:107:A:ASN:HA	11	1.7
(1,1144)	1:111:A:ARG:HG2	1:107:A:ASN:HA	25	1.7
(1,904)	1:115:A:ARG:HD3	1:126:A:TYR:HE2	8	1.7
(1,671)	1:133:A:VAL:HG23	1:99:A:PHE:HZ	23	1.7
(1,381)	2:30:B:GLU:HG2	2:31:B:LEU:HB2	19	1.7
(1,1660)	2:36:B:THR:HG23	1:122:A:LYS:HD2	21	1.69
(1,1330)	1:77:A:GLN:HG2	1:76:A:MET:HB3	4	1.69
(1,1330)	1:77:A:GLN:HG2	1:76:A:MET:HB3	5	1.69
(1,1144)	1:111:A:ARG:HG2	1:107:A:ASN:HA	12	1.69
(1,661)	1:133:A:VAL:HG13	1:99:A:PHE:HE1	3	1.69
(1,162)	1:67:A:PHE:HD1	1:130:A:LEU:HD22	25	1.69
(1,1989)	1:98:A:LEU:H	1:138:A:SER:HB2	14	1.68
(1,1586)	2:36:B:THR:HG22	1:125:A:VAL:H	12	1.68
(1,1586)	2:36:B:THR:HG23	1:125:A:VAL:H	20	1.68
(1,1330)	1:77:A:GLN:HG2	1:76:A:MET:HB3	22	1.68
(1,1062)	1:103:A:ALA:HB2	1:59:A:TYR:HB3	17	1.68
(1,914)	1:61:A:LEU:HD13	1:61:A:LEU:H	25	1.68
(1,575)	1:143:A:LEU:HA	1:143:A:LEU:HD23	25	1.68
(1,381)	2:30:B:GLU:HG2	2:31:B:LEU:HB2	23	1.68
(1,1989)	1:98:A:LEU:H	1:138:A:SER:HB2	1	1.67
(1,1586)	2:36:B:THR:HG21	1:125:A:VAL:H	3	1.67
(1,1330)	1:77:A:GLN:HG2	1:76:A:MET:HB3	7	1.67
(1,1330)	1:77:A:GLN:HG2	1:76:A:MET:HB3	9	1.67
(1,1330)	1:77:A:GLN:HG2	1:76:A:MET:HB3	15	1.67
(1,1330)	1:77:A:GLN:HG2	1:76:A:MET:HB3	18	1.67
(1,1330)	1:77:A:GLN:HG2	1:76:A:MET:HB3	20	1.67
(1,1330)	1:77:A:GLN:HG2	1:76:A:MET:HB3	24	1.67
(1,904)	1:115:A:ARG:HD3	1:126:A:TYR:HE2	9	1.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,661)	1:133:A:VAL:HG13	1:99:A:PHE:HE1	16	1.67
(1,382)	1:64:A:GLU:HG3	1:100:A:LEU:HD13	5	1.67
(1,382)	1:64:A:GLU:HG3	1:100:A:LEU:HD12	12	1.67
(1,2274)	2:39:B:TRP:HE1	2:38:B:ARG:HD3	11	1.66
(1,1330)	1:77:A:GLN:HG2	1:76:A:MET:HB3	13	1.66
(1,1330)	1:77:A:GLN:HG2	1:76:A:MET:HB3	14	1.66
(1,1144)	1:111:A:ARG:HG2	1:107:A:ASN:HA	7	1.66
(1,904)	1:115:A:ARG:HD3	1:126:A:TYR:HE2	2	1.66
(1,904)	1:115:A:ARG:HD3	1:126:A:TYR:HE1	11	1.66
(1,760)	1:126:A:TYR:HD1	1:116:A:ALA:HB3	15	1.66
(1,661)	1:133:A:VAL:HG13	1:99:A:PHE:HE1	22	1.66
(1,412)	1:131:A:CYS:H	1:87:A:PHE:HE1	3	1.66
(1,1330)	1:77:A:GLN:HG2	1:76:A:MET:HB3	3	1.65
(1,1330)	1:77:A:GLN:HG2	1:76:A:MET:HB3	23	1.65
(1,914)	1:61:A:LEU:HD13	1:61:A:LEU:H	5	1.65
(1,914)	1:61:A:LEU:HD12	1:61:A:LEU:H	10	1.65
(1,381)	2:30:B:GLU:HG2	2:31:B:LEU:HB2	22	1.65
(1,381)	2:30:B:GLU:HG2	2:31:B:LEU:HB2	24	1.65
(1,1989)	1:98:A:LEU:H	1:138:A:SER:HB2	5	1.64
(1,914)	1:61:A:LEU:HD11	1:61:A:LEU:H	20	1.64
(1,904)	1:115:A:ARG:HD3	1:126:A:TYR:HE2	5	1.64
(1,575)	1:143:A:LEU:HA	1:143:A:LEU:HD23	12	1.64
(1,570)	1:143:A:LEU:HB2	1:144:A:ASN:HD21	9	1.64
(1,381)	2:30:B:GLU:HG2	2:31:B:LEU:HB2	5	1.64
(1,263)	1:132:A:THR:HG21	2:28:B:ASP:HB3	7	1.64
(1,254)	1:57:A:LYS:HE3	1:54:A:MET:HG3	16	1.64
(1,1989)	1:98:A:LEU:H	1:138:A:SER:HB2	8	1.63
(1,1330)	1:77:A:GLN:HG2	1:76:A:MET:HB3	2	1.63
(1,1330)	1:77:A:GLN:HG2	1:76:A:MET:HB3	12	1.63
(1,904)	1:115:A:ARG:HD3	1:126:A:TYR:HE2	19	1.63
(1,904)	1:115:A:ARG:HD3	1:126:A:TYR:HE2	22	1.63
(1,795)	1:127:A:ILE:HD11	1:124:A:TYR:HE1	8	1.63
(1,575)	1:143:A:LEU:HA	1:143:A:LEU:HD22	16	1.63
(1,1415)	1:71:A:LEU:HB2	1:75:A:LYS:HE2	7	1.62
(1,1071)	1:101:A:ALA:HB3	1:63:A:ASN:HD21	3	1.62
(1,795)	1:127:A:ILE:HD13	1:124:A:TYR:HE1	7	1.62
(1,795)	1:127:A:ILE:HD11	1:124:A:TYR:HE1	12	1.62
(1,534)	1:109:A:LEU:H	1:113:A:LEU:HB3	14	1.62
(1,383)	2:30:B:GLU:HB2	2:31:B:LEU:HB2	11	1.62
(1,383)	2:30:B:GLU:HB2	2:31:B:LEU:HB2	17	1.62
(1,46)	1:126:A:TYR:HE1	1:122:A:LYS:HB3	13	1.62
(1,1766)	2:24:B:GLN:HG2	2:23:B:SER:HA	11	1.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1660)	2:36:B:THR:HG23	1:122:A:LYS:HD2	15	1.61
(1,1071)	1:101:A:ALA:HB3	1:63:A:ASN:HD21	13	1.61
(1,914)	1:61:A:LEU:HD12	1:61:A:LEU:H	7	1.61
(1,914)	1:61:A:LEU:HD12	1:61:A:LEU:H	16	1.61
(1,904)	1:115:A:ARG:HD3	1:126:A:TYR:HE2	12	1.61
(1,661)	1:133:A:VAL:HG11	1:99:A:PHE:HE1	20	1.61
(1,618)	1:56:A:LYS:HG2	1:57:A:LYS:H	25	1.61
(1,575)	1:143:A:LEU:HA	1:143:A:LEU:HD22	4	1.61
(1,534)	1:109:A:LEU:H	1:113:A:LEU:HB3	11	1.61
(1,383)	2:30:B:GLU:HB2	2:31:B:LEU:HB2	7	1.61
(1,383)	2:30:B:GLU:HB2	2:31:B:LEU:HB2	16	1.61
(1,1660)	2:36:B:THR:HG22	1:122:A:LYS:HD2	14	1.6
(1,1397)	1:72:A:GLU:HG2	1:71:A:LEU:H	10	1.6
(1,1397)	1:72:A:GLU:HG2	1:71:A:LEU:H	23	1.6
(1,914)	1:61:A:LEU:HD12	1:61:A:LEU:H	23	1.6
(1,904)	1:115:A:ARG:HD3	1:126:A:TYR:HE2	4	1.6
(1,381)	2:30:B:GLU:HG2	2:31:B:LEU:HB2	9	1.6
(1,368)	2:26:B:ASP:HB3	1:87:A:PHE:HZ	13	1.6
(1,162)	1:67:A:PHE:HD1	1:130:A:LEU:HD21	2	1.6
(1,1470)	1:66:A:LEU:HD13	1:62:A:GLU:HG3	23	1.59
(1,1062)	1:103:A:ALA:HB3	1:59:A:TYR:HB3	24	1.59
(1,914)	1:61:A:LEU:HD12	1:61:A:LEU:H	11	1.59
(1,368)	2:26:B:ASP:HB3	1:87:A:PHE:HZ	1	1.59
(1,368)	2:26:B:ASP:HB3	1:87:A:PHE:HZ	20	1.59
(1,46)	1:126:A:TYR:HE1	1:122:A:LYS:HB3	1	1.59
(1,914)	1:61:A:LEU:HD11	1:61:A:LEU:H	13	1.58
(1,914)	1:61:A:LEU:HD12	1:61:A:LEU:H	15	1.58
(1,914)	1:61:A:LEU:HD11	1:61:A:LEU:H	18	1.58
(1,795)	1:127:A:ILE:HD13	1:124:A:TYR:HE1	1	1.58
(1,661)	1:133:A:VAL:HG12	1:99:A:PHE:HE1	4	1.58
(1,383)	2:30:B:GLU:HB2	2:31:B:LEU:HB2	9	1.58
(1,381)	2:30:B:GLU:HG2	2:31:B:LEU:HB2	12	1.58
(1,162)	1:67:A:PHE:HD1	1:130:A:LEU:HD22	5	1.58
(1,162)	1:67:A:PHE:HD1	1:130:A:LEU:HD23	15	1.58
(1,162)	1:67:A:PHE:HD1	1:130:A:LEU:HD21	22	1.58
(1,1470)	1:66:A:LEU:HD13	1:62:A:GLU:HG3	11	1.57
(1,1062)	1:103:A:ALA:HB1	1:59:A:TYR:HB3	14	1.57
(1,914)	1:61:A:LEU:HD12	1:61:A:LEU:H	1	1.57
(1,914)	1:61:A:LEU:HD13	1:61:A:LEU:H	3	1.57
(1,914)	1:61:A:LEU:HD11	1:61:A:LEU:H	8	1.57
(1,618)	1:56:A:LYS:HG2	1:57:A:LYS:H	16	1.57
(1,196)	1:73:A:LEU:HD21	1:76:A:MET:HE3	12	1.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,162)	1:67:A:PHE:HD1	1:130:A:LEU:HD22	1	1.57
(1,162)	1:67:A:PHE:HD1	1:130:A:LEU:HD21	16	1.57
(1,46)	1:126:A:TYR:HE1	1:122:A:LYS:HB3	4	1.57
(1,1660)	2:36:B:THR:HG22	1:122:A:LYS:HD3	12	1.56
(1,1586)	2:36:B:THR:HG21	1:125:A:VAL:H	5	1.56
(1,1330)	1:77:A:GLN:HG2	1:76:A:MET:HB3	1	1.56
(1,1330)	1:77:A:GLN:HG2	1:76:A:MET:HB3	11	1.56
(1,914)	1:61:A:LEU:HD12	1:61:A:LEU:H	22	1.56
(1,795)	1:127:A:ILE:HD11	1:124:A:TYR:HE1	14	1.56
(1,661)	1:133:A:VAL:HG12	1:99:A:PHE:HE1	21	1.56
(1,534)	1:121:A:ALA:H	1:119:A:ARG:HG2	13	1.56
(1,383)	2:30:B:GLU:HB2	2:31:B:LEU:HB2	25	1.56
(1,381)	2:30:B:GLU:HG2	2:31:B:LEU:HB2	13	1.56
(1,162)	1:67:A:PHE:HD1	1:130:A:LEU:HD21	9	1.56
(1,1976)	1:100:A:LEU:H	1:138:A:SER:HB2	8	1.55
(1,1660)	2:36:B:THR:HG22	1:122:A:LYS:HD3	2	1.55
(1,1071)	1:101:A:ALA:HB3	1:63:A:ASN:HD21	5	1.55
(1,914)	1:61:A:LEU:HD13	1:61:A:LEU:H	4	1.55
(1,904)	1:115:A:ARG:HD3	1:126:A:TYR:HE1	7	1.55
(1,904)	1:115:A:ARG:HD3	1:126:A:TYR:HE1	16	1.55
(1,904)	1:115:A:ARG:HD3	1:126:A:TYR:HE2	18	1.55
(1,795)	1:127:A:ILE:HD13	1:124:A:TYR:HE1	2	1.55
(1,795)	1:127:A:ILE:HD12	1:124:A:TYR:HE1	23	1.55
(1,381)	2:30:B:GLU:HG2	2:31:B:LEU:HB2	2	1.55
(1,162)	1:67:A:PHE:HD1	1:130:A:LEU:HD23	18	1.55
(1,46)	1:126:A:TYR:HE1	1:122:A:LYS:HB3	6	1.55
(1,2274)	2:39:B:TRP:HE1	2:38:B:ARG:HD2	10	1.54
(1,1470)	1:66:A:LEU:HD13	1:62:A:GLU:HG3	4	1.54
(1,1470)	1:66:A:LEU:HD12	1:62:A:GLU:HG3	7	1.54
(1,1470)	1:66:A:LEU:HD13	1:62:A:GLU:HG3	16	1.54
(1,914)	1:61:A:LEU:HD12	1:61:A:LEU:H	2	1.54
(1,914)	1:61:A:LEU:HD13	1:61:A:LEU:H	24	1.54
(1,661)	1:133:A:VAL:HG12	1:99:A:PHE:HE1	18	1.54
(1,534)	1:109:A:LEU:H	1:113:A:LEU:HB3	1	1.54
(1,383)	2:30:B:GLU:HB2	2:31:B:LEU:HB2	8	1.54
(1,382)	1:64:A:GLU:HG3	1:100:A:LEU:HD13	10	1.54
(1,365)	2:29:B:SER:HB2	2:31:B:LEU:HB2	24	1.54
(1,196)	1:73:A:LEU:HD23	1:76:A:MET:HE2	3	1.54
(1,162)	1:67:A:PHE:HD1	1:130:A:LEU:HD23	12	1.54
(1,1582)	2:37:B:ALA:HB2	1:125:A:VAL:HG22	11	1.53
(1,1255)	1:86:A:PRO:HD2	1:85:A:VAL:HG11	16	1.53
(1,795)	1:127:A:ILE:HD11	1:124:A:TYR:HE1	15	1.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,795)	1:127:A:ILE:HD13	1:124:A:TYR:HE1	19	1.53
(1,661)	1:133:A:VAL:HG12	1:99:A:PHE:HE1	6	1.53
(1,534)	1:121:A:ALA:H	1:119:A:ARG:HG2	17	1.53
(1,365)	2:29:B:SER:HB2	2:31:B:LEU:HB2	4	1.53
(1,143)	1:89:A:TYR:HD2	1:86:A:PRO:HB2	2	1.53
(1,98)	1:105:A:PHE:HD1	1:109:A:LEU:HD23	6	1.53
(1,2274)	2:39:B:TRP:HE1	2:38:B:ARG:HD2	24	1.52
(1,1781)	1:140:A:LYS:H	1:141:A:LYS:HB3	24	1.52
(1,1660)	2:36:B:THR:HG22	1:122:A:LYS:HD3	23	1.52
(1,1470)	1:66:A:LEU:HD13	1:62:A:GLU:HG3	22	1.52
(1,1397)	1:72:A:GLU:HG2	1:71:A:LEU:H	16	1.52
(1,1327)	1:77:A:GLN:HG2	1:73:A:LEU:HA	19	1.52
(1,1062)	1:103:A:ALA:HB3	1:59:A:TYR:HB3	8	1.52
(1,1049)	1:108:A:ILE:HD11	1:104:A:GLU:HG2	11	1.52
(1,914)	1:61:A:LEU:HD12	1:61:A:LEU:H	6	1.52
(1,914)	1:61:A:LEU:HD13	1:61:A:LEU:H	12	1.52
(1,661)	1:133:A:VAL:HG11	1:99:A:PHE:HE1	19	1.52
(1,570)	1:143:A:LEU:HB2	1:144:A:ASN:HD21	13	1.52
(1,534)	1:121:A:ALA:H	1:119:A:ARG:HG2	15	1.52
(1,365)	2:29:B:SER:HB2	2:31:B:LEU:HB2	1	1.52
(1,1582)	2:37:B:ALA:HB2	1:125:A:VAL:HG21	2	1.51
(1,1470)	1:66:A:LEU:HD11	1:62:A:GLU:HG3	6	1.51
(1,1071)	1:101:A:ALA:HB3	1:63:A:ASN:HD21	10	1.51
(1,1062)	1:103:A:ALA:HB2	1:59:A:TYR:HB3	7	1.51
(1,450)	1:114:A:SER:H	1:126:A:TYR:HB3	25	1.51
(1,383)	2:30:B:GLU:HB2	2:31:B:LEU:HB2	3	1.51
(1,383)	2:30:B:GLU:HB2	2:31:B:LEU:HB2	15	1.51
(1,383)	2:30:B:GLU:HB2	2:31:B:LEU:HB2	20	1.51
(1,383)	2:30:B:GLU:HB2	2:31:B:LEU:HB2	23	1.51
(1,368)	2:26:B:ASP:HB3	1:87:A:PHE:HZ	8	1.51
(1,365)	1:118:A:SER:HB3	1:116:A:ALA:HB2	16	1.51
(1,254)	1:57:A:LYS:HE3	1:54:A:MET:HG3	1	1.51
(1,196)	1:73:A:LEU:HD22	1:76:A:MET:HE1	18	1.51
(1,46)	1:126:A:TYR:HE1	1:122:A:LYS:HB3	3	1.51
(1,1940)	1:106:A:CYS:H	1:63:A:ASN:HD22	25	1.5
(1,1582)	2:37:B:ALA:HB1	1:125:A:VAL:HG23	15	1.5
(1,914)	1:61:A:LEU:HD13	1:61:A:LEU:H	17	1.5
(1,914)	1:61:A:LEU:HD11	1:61:A:LEU:H	19	1.5
(1,914)	1:61:A:LEU:HD11	1:61:A:LEU:H	21	1.5
(1,383)	2:30:B:GLU:HB2	2:31:B:LEU:HB2	10	1.5
(1,383)	2:30:B:GLU:HB2	2:31:B:LEU:HB2	14	1.5
(1,365)	2:29:B:SER:HB2	2:31:B:LEU:HB2	5	1.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,365)	2:29:B:SER:HB2	2:31:B:LEU:HB2	8	1.5
(1,162)	1:67:A:PHE:HD1	1:130:A:LEU:HD23	20	1.5
(1,46)	1:126:A:TYR:HE1	1:122:A:LYS:HB3	17	1.5
(1,2113)	1:76:A:MET:H	1:77:A:GLN:HB3	1	1.49
(1,1940)	1:106:A:CYS:H	1:63:A:ASN:HD22	10	1.49
(1,1470)	1:66:A:LEU:HD13	1:62:A:GLU:HG3	13	1.49
(1,1470)	1:66:A:LEU:HD13	1:62:A:GLU:HG3	17	1.49
(1,1470)	1:66:A:LEU:HD11	1:62:A:GLU:HG3	20	1.49
(1,1449)	1:69:A:GLU:HG2	1:113:A:LEU:HD21	5	1.49
(1,1397)	1:72:A:GLU:HG2	1:71:A:LEU:H	3	1.49
(1,1062)	1:103:A:ALA:HB2	1:59:A:TYR:HB3	9	1.49
(1,904)	1:115:A:ARG:HD3	1:126:A:TYR:HE2	23	1.49
(1,534)	1:121:A:ALA:H	1:119:A:ARG:HG2	5	1.49
(1,534)	1:121:A:ALA:H	1:119:A:ARG:HG2	22	1.49
(1,383)	2:30:B:GLU:HB2	2:31:B:LEU:HB2	6	1.49
(1,368)	2:26:B:ASP:HB3	1:87:A:PHE:HZ	10	1.49
(1,263)	1:132:A:THR:HG23	2:28:B:ASP:HB3	3	1.49
(1,196)	1:73:A:LEU:HD22	1:76:A:MET:HE2	2	1.49
(1,196)	1:73:A:LEU:HD23	1:76:A:MET:HE3	14	1.49
(1,1660)	2:36:B:THR:HG21	1:122:A:LYS:HD3	17	1.48
(1,1470)	1:66:A:LEU:HD12	1:62:A:GLU:HG3	3	1.48
(1,795)	1:127:A:ILE:HD13	1:124:A:TYR:HE1	20	1.48
(1,795)	1:127:A:ILE:HD12	1:124:A:TYR:HE1	22	1.48
(1,534)	1:121:A:ALA:H	1:119:A:ARG:HG2	10	1.48
(1,383)	2:30:B:GLU:HB2	2:31:B:LEU:HB2	4	1.48
(1,383)	2:30:B:GLU:HB2	2:31:B:LEU:HB2	12	1.48
(1,365)	2:29:B:SER:HB2	2:31:B:LEU:HB2	15	1.48
(1,263)	1:132:A:THR:HG21	2:28:B:ASP:HB3	1	1.48
(1,196)	1:73:A:LEU:HD21	1:74:A:CYS:HB3	4	1.48
(1,196)	1:73:A:LEU:HD22	1:76:A:MET:HE3	9	1.48
(1,2113)	1:76:A:MET:H	1:77:A:GLN:HB3	19	1.47
(1,1582)	2:37:B:ALA:HB2	1:125:A:VAL:HG23	18	1.47
(1,1449)	1:69:A:GLU:HG2	1:113:A:LEU:HD21	12	1.47
(1,1449)	1:69:A:GLU:HG2	1:113:A:LEU:HD23	20	1.47
(1,263)	1:132:A:THR:HG23	2:28:B:ASP:HB3	21	1.47
(1,2113)	1:76:A:MET:H	1:77:A:GLN:HB3	11	1.46
(1,1781)	1:140:A:LYS:H	1:141:A:LYS:HB3	12	1.46
(1,1327)	1:77:A:GLN:HG2	1:73:A:LEU:HA	1	1.46
(1,1327)	1:77:A:GLN:HG2	1:73:A:LEU:HA	11	1.46
(1,1049)	1:108:A:ILE:HD11	1:104:A:GLU:HG2	15	1.46
(1,795)	1:127:A:ILE:HD11	1:124:A:TYR:HE1	21	1.46
(1,671)	1:133:A:VAL:HG23	1:99:A:PHE:HZ	14	1.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,450)	1:114:A:SER:H	1:126:A:TYR:HB3	5	1.46
(1,450)	1:114:A:SER:H	1:126:A:TYR:HB3	17	1.46
(1,383)	2:30:B:GLU:HB2	2:31:B:LEU:HB2	1	1.46
(1,365)	2:29:B:SER:HB2	2:31:B:LEU:HB2	3	1.46
(1,365)	2:29:B:SER:HB2	2:31:B:LEU:HB2	12	1.46
(1,196)	1:73:A:LEU:HD21	1:76:A:MET:HE1	21	1.46
(1,162)	1:67:A:PHE:HD1	1:130:A:LEU:HD21	8	1.46
(1,162)	1:67:A:PHE:HD1	1:130:A:LEU:HD22	11	1.46
(1,46)	1:126:A:TYR:HE1	1:122:A:LYS:HB3	10	1.46
(1,1989)	1:98:A:LEU:H	1:138:A:SER:HB2	10	1.45
(1,1940)	1:106:A:CYS:H	1:63:A:ASN:HD22	6	1.45
(1,1637)	2:38:B:ARG:HD2	2:39:B:TRP:HD1	11	1.45
(1,1449)	1:69:A:GLU:HG2	1:113:A:LEU:HD21	13	1.45
(1,1449)	1:69:A:GLU:HG2	1:113:A:LEU:HD23	25	1.45
(1,1371)	1:75:A:LYS:HE3	1:72:A:GLU:HG2	8	1.45
(1,1275)	1:78:A:THR:HG21	1:77:A:GLN:HB3	2	1.45
(1,1071)	1:101:A:ALA:HB2	1:63:A:ASN:HD21	22	1.45
(1,619)	1:135:A:LYS:HG2	1:91:A:ARG:HD3	17	1.45
(1,450)	1:114:A:SER:H	1:126:A:TYR:HB3	2	1.45
(1,383)	2:30:B:GLU:HB2	2:31:B:LEU:HB2	18	1.45
(1,263)	1:132:A:THR:HG23	2:28:B:ASP:HB3	16	1.45
(1,162)	1:67:A:PHE:HD1	1:130:A:LEU:HD21	6	1.45
(1,1637)	2:38:B:ARG:HD2	2:39:B:TRP:HD1	15	1.44
(1,1397)	1:72:A:GLU:HG2	1:71:A:LEU:H	7	1.44
(1,1255)	1:86:A:PRO:HD2	1:85:A:VAL:HG11	18	1.44
(1,1255)	1:86:A:PRO:HD2	1:85:A:VAL:HG11	21	1.44
(1,1255)	1:86:A:PRO:HD2	1:85:A:VAL:HG11	22	1.44
(1,1255)	1:86:A:PRO:HD2	1:85:A:VAL:HG13	23	1.44
(1,450)	1:114:A:SER:H	1:126:A:TYR:HB3	14	1.44
(1,365)	2:29:B:SER:HB2	2:31:B:LEU:HB2	10	1.44
(1,2274)	2:39:B:TRP:HE1	2:38:B:ARG:HD2	20	1.43
(1,1255)	1:86:A:PRO:HD2	1:85:A:VAL:HG13	9	1.43
(1,1129)	1:98:A:LEU:HD12	1:96:A:HIS:HE1	19	1.43
(1,1071)	1:101:A:ALA:HB1	1:63:A:ASN:HD21	21	1.43
(1,914)	1:61:A:LEU:HD12	1:61:A:LEU:H	14	1.43
(1,450)	1:114:A:SER:H	1:126:A:TYR:HB3	13	1.43
(1,450)	1:114:A:SER:H	1:126:A:TYR:HB3	23	1.43
(1,365)	2:29:B:SER:HB2	2:31:B:LEU:HB2	13	1.43
(1,365)	2:29:B:SER:HB2	2:31:B:LEU:HB2	20	1.43
(1,196)	1:73:A:LEU:HD21	1:74:A:CYS:HB3	20	1.43
(1,162)	1:67:A:PHE:HD1	1:130:A:LEU:HD23	7	1.43
(1,122)	1:95:A:ALA:HB2	1:96:A:HIS:HB3	13	1.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,46)	1:126:A:TYR:HE1	1:122:A:LYS:HB3	7	1.43
(1,2189)	1:59:A:TYR:H	1:60:A:LYS:HB2	25	1.42
(1,1656)	2:37:B:ALA:HB2	2:39:B:TRP:HZ2	18	1.42
(1,1582)	2:37:B:ALA:HB3	1:125:A:VAL:HG23	22	1.42
(1,1449)	1:69:A:GLU:HG2	1:113:A:LEU:HD22	24	1.42
(1,1371)	1:75:A:LYS:HE3	1:72:A:GLU:HG2	6	1.42
(1,1255)	1:86:A:PRO:HD2	1:85:A:VAL:HG11	4	1.42
(1,1255)	1:86:A:PRO:HD2	1:85:A:VAL:HG12	20	1.42
(1,1071)	1:101:A:ALA:HB2	1:63:A:ASN:HD21	4	1.42
(1,1062)	1:103:A:ALA:HB2	1:59:A:TYR:HB3	13	1.42
(1,1062)	1:103:A:ALA:HB3	1:59:A:TYR:HB3	18	1.42
(1,904)	1:115:A:ARG:HD3	1:126:A:TYR:HE1	14	1.42
(1,795)	1:127:A:ILE:HD11	1:124:A:TYR:HE1	3	1.42
(1,365)	2:29:B:SER:HB2	2:31:B:LEU:HB2	2	1.42
(1,365)	2:29:B:SER:HB2	2:31:B:LEU:HB2	21	1.42
(1,253)	1:57:A:LYS:HE3	1:54:A:MET:HG2	15	1.42
(1,196)	1:73:A:LEU:HD22	1:74:A:CYS:HB3	7	1.42
(1,143)	1:89:A:TYR:HD2	1:86:A:PRO:HB2	15	1.42
(1,1940)	1:106:A:CYS:H	1:63:A:ASN:HD22	5	1.41
(1,1781)	1:140:A:LYS:H	1:141:A:LYS:HB3	18	1.41
(1,1656)	2:37:B:ALA:HB3	2:39:B:TRP:HZ2	11	1.41
(1,1582)	2:37:B:ALA:HB1	1:125:A:VAL:HG21	12	1.41
(1,1549)	1:58:A:CYS:HB2	1:57:A:LYS:HA	20	1.41
(1,1449)	1:69:A:GLU:HG2	1:113:A:LEU:HD22	22	1.41
(1,1398)	1:72:A:GLU:HG2	1:71:A:LEU:HB2	23	1.41
(1,1255)	1:86:A:PRO:HD2	1:85:A:VAL:HG12	6	1.41
(1,1255)	1:86:A:PRO:HD2	1:85:A:VAL:HG11	19	1.41
(1,1255)	1:86:A:PRO:HD2	1:85:A:VAL:HG13	24	1.41
(1,1071)	1:101:A:ALA:HB2	1:63:A:ASN:HD21	6	1.41
(1,795)	1:127:A:ILE:HD13	1:124:A:TYR:HE1	9	1.41
(1,671)	1:133:A:VAL:HG21	1:99:A:PHE:HZ	8	1.41
(1,368)	2:26:B:ASP:HB3	1:87:A:PHE:HZ	7	1.41
(1,365)	2:29:B:SER:HB2	2:31:B:LEU:HB2	7	1.41
(1,365)	2:29:B:SER:HB2	2:31:B:LEU:HB2	23	1.41
(1,63)	1:123:A:LEU:HA	1:123:A:LEU:HD22	24	1.41
(1,46)	1:126:A:TYR:HE1	1:122:A:LYS:HB3	19	1.41
(1,1449)	1:69:A:GLU:HG2	1:113:A:LEU:HD21	6	1.4
(1,1255)	1:86:A:PRO:HD2	1:85:A:VAL:HG13	2	1.4
(1,1255)	1:86:A:PRO:HD2	1:85:A:VAL:HG13	13	1.4
(1,1255)	1:86:A:PRO:HD2	1:85:A:VAL:HG11	15	1.4
(1,1062)	1:103:A:ALA:HB1	1:59:A:TYR:HB3	15	1.4
(1,946)	1:110:A:SER:HB2	1:66:A:LEU:HD12	20	1.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,795)	1:127:A:ILE:HD13	1:124:A:TYR:HE1	6	1.4
(1,450)	1:114:A:SER:H	1:126:A:TYR:HB3	4	1.4
(1,383)	2:30:B:GLU:HB2	2:31:B:LEU:HB2	13	1.4
(1,383)	2:30:B:GLU:HB2	2:31:B:LEU:HB2	21	1.4
(1,365)	2:29:B:SER:HB2	2:31:B:LEU:HB2	17	1.4
(1,196)	1:73:A:LEU:HD21	1:74:A:CYS:HB3	13	1.4
(1,63)	1:123:A:LEU:HD23	1:124:A:TYR:HA	6	1.4
(1,2189)	1:59:A:TYR:H	1:60:A:LYS:HB2	20	1.39
(1,1940)	1:106:A:CYS:H	1:63:A:ASN:HD22	16	1.39
(1,1470)	1:66:A:LEU:HD13	1:62:A:GLU:HG3	12	1.39
(1,1255)	1:86:A:PRO:HD2	1:85:A:VAL:HG11	5	1.39
(1,1255)	1:86:A:PRO:HD2	1:85:A:VAL:HG13	12	1.39
(1,1255)	1:86:A:PRO:HD2	1:85:A:VAL:HG13	14	1.39
(1,1255)	1:86:A:PRO:HD2	1:85:A:VAL:HG13	17	1.39
(1,1255)	1:86:A:PRO:HD2	1:85:A:VAL:HG12	25	1.39
(1,383)	2:30:B:GLU:HB2	2:31:B:LEU:HB2	5	1.39
(1,368)	2:26:B:ASP:HB3	1:87:A:PHE:HZ	2	1.39
(1,237)	1:85:A:VAL:HB	1:71:A:LEU:HB3	5	1.39
(1,116)	1:100:A:LEU:HD23	1:95:A:ALA:H	6	1.39
(1,63)	1:123:A:LEU:HD21	1:124:A:TYR:HA	16	1.39
(1,1634)	2:38:B:ARG:HD2	2:37:B:ALA:HB1	15	1.38
(1,1582)	2:37:B:ALA:HB3	1:125:A:VAL:HG21	5	1.38
(1,1582)	2:37:B:ALA:HB2	1:125:A:VAL:HG22	17	1.38
(1,1255)	1:86:A:PRO:HD2	1:85:A:VAL:HG12	8	1.38
(1,1255)	1:86:A:PRO:HD2	1:85:A:VAL:HG13	10	1.38
(1,1255)	1:86:A:PRO:HD2	1:85:A:VAL:HG11	11	1.38
(1,1049)	1:108:A:ILE:HD11	1:104:A:GLU:HG2	25	1.38
(1,710)	1:130:A:LEU:HD21	1:109:A:LEU:HD12	19	1.38
(1,450)	1:114:A:SER:H	1:126:A:TYR:HB3	22	1.38
(1,379)	2:31:B:LEU:HB2	2:28:B:ASP:HB2	20	1.38
(1,365)	2:29:B:SER:HB2	2:31:B:LEU:HB2	9	1.38
(1,46)	1:126:A:TYR:HE1	1:122:A:LYS:HB3	16	1.38
(1,46)	1:126:A:TYR:HE1	1:122:A:LYS:HB3	20	1.38
(1,2113)	1:76:A:MET:H	1:77:A:GLN:HB3	8	1.37
(1,2113)	1:76:A:MET:H	1:77:A:GLN:HB3	17	1.37
(1,2113)	1:76:A:MET:H	1:77:A:GLN:HB3	22	1.37
(1,2113)	1:76:A:MET:H	1:77:A:GLN:HB3	23	1.37
(1,1656)	2:37:B:ALA:HB2	2:39:B:TRP:HZ2	15	1.37
(1,1470)	1:66:A:LEU:HD12	1:62:A:GLU:HG3	8	1.37
(1,1398)	1:72:A:GLU:HG2	1:71:A:LEU:HB2	10	1.37
(1,1255)	1:86:A:PRO:HD2	1:85:A:VAL:HG11	1	1.37
(1,1255)	1:86:A:PRO:HD2	1:85:A:VAL:HG11	3	1.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1255)	1:86:A:PRO:HD2	1:85:A:VAL:HG13	7	1.37
(1,795)	1:127:A:ILE:HD11	1:124:A:TYR:HE1	17	1.37
(1,795)	1:127:A:ILE:HD13	1:124:A:TYR:HE1	18	1.37
(1,671)	1:133:A:VAL:HG22	1:99:A:PHE:HZ	17	1.37
(1,661)	1:133:A:VAL:HG12	1:99:A:PHE:HE1	13	1.37
(1,534)	1:109:A:LEU:H	1:111:A:ARG:HG2	23	1.37
(1,383)	2:30:B:GLU:HB2	2:31:B:LEU:HB2	2	1.37
(1,365)	2:29:B:SER:HB2	2:31:B:LEU:HB2	11	1.37
(1,365)	2:29:B:SER:HB2	2:31:B:LEU:HB2	18	1.37
(1,365)	2:29:B:SER:HB2	2:31:B:LEU:HB2	19	1.37
(1,122)	1:95:A:ALA:HB1	1:96:A:HIS:HB3	16	1.37
(1,2113)	1:76:A:MET:H	1:77:A:GLN:HB3	5	1.36
(1,2113)	1:76:A:MET:H	1:77:A:GLN:HB3	12	1.36
(1,2113)	1:76:A:MET:H	1:77:A:GLN:HB3	13	1.36
(1,1470)	1:66:A:LEU:HD11	1:62:A:GLU:HG3	9	1.36
(1,914)	1:61:A:LEU:HD13	1:61:A:LEU:H	9	1.36
(1,904)	1:115:A:ARG:HD3	1:126:A:TYR:HE1	6	1.36
(1,795)	1:127:A:ILE:HD11	1:124:A:TYR:HE1	11	1.36
(1,710)	1:130:A:LEU:HD21	1:109:A:LEU:HD11	9	1.36
(1,671)	1:133:A:VAL:HG21	1:99:A:PHE:HZ	10	1.36
(1,671)	1:133:A:VAL:HG23	1:99:A:PHE:HZ	11	1.36
(1,534)	1:121:A:ALA:H	1:119:A:ARG:HG2	12	1.36
(1,450)	1:114:A:SER:H	1:126:A:TYR:HB3	19	1.36
(1,383)	2:30:B:GLU:HB2	2:31:B:LEU:HB2	24	1.36
(1,368)	2:26:B:ASP:HB3	1:87:A:PHE:HZ	24	1.36
(1,122)	1:95:A:ALA:HB3	1:96:A:HIS:HB3	5	1.36
(1,63)	1:67:A:PHE:HA	1:109:A:LEU:HG	11	1.36
(1,63)	1:123:A:LEU:HD21	1:124:A:TYR:HA	23	1.36
(1,1940)	1:106:A:CYS:H	1:63:A:ASN:HD22	21	1.35
(1,1582)	2:37:B:ALA:HB3	1:125:A:VAL:HG21	4	1.35
(1,1582)	2:37:B:ALA:HB3	1:125:A:VAL:HG21	13	1.35
(1,1449)	1:69:A:GLU:HG2	1:113:A:LEU:HD23	9	1.35
(1,534)	1:121:A:ALA:H	1:119:A:ARG:HG2	21	1.35
(1,263)	1:132:A:THR:HG23	2:28:B:ASP:HB3	23	1.35
(1,196)	1:73:A:LEU:HD22	1:74:A:CYS:HB3	24	1.35
(1,162)	1:67:A:PHE:HD1	1:130:A:LEU:HD21	24	1.35
(1,46)	1:126:A:TYR:HE1	1:122:A:LYS:HB3	2	1.35
(1,46)	1:126:A:TYR:HE1	1:122:A:LYS:HB3	12	1.35
(1,2113)	1:76:A:MET:H	1:77:A:GLN:HB3	4	1.34
(1,2113)	1:76:A:MET:H	1:77:A:GLN:HB3	15	1.34
(1,2113)	1:76:A:MET:H	1:77:A:GLN:HB3	18	1.34
(1,2113)	1:76:A:MET:H	1:77:A:GLN:HB3	20	1.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1449)	1:69:A:GLU:HG2	1:113:A:LEU:HD21	21	1.34
(1,1371)	1:75:A:LYS:HE3	1:72:A:GLU:HG2	25	1.34
(1,671)	1:133:A:VAL:HG21	1:99:A:PHE:HZ	4	1.34
(1,365)	2:29:B:SER:HB2	2:31:B:LEU:HB2	6	1.34
(1,263)	1:132:A:THR:HG21	2:28:B:ASP:HB3	11	1.34
(1,143)	1:89:A:TYR:HD2	1:86:A:PRO:HB2	4	1.34
(1,98)	1:105:A:PHE:HD1	1:109:A:LEU:HD23	8	1.34
(1,2113)	1:76:A:MET:H	1:77:A:GLN:HB3	6	1.33
(1,2113)	1:76:A:MET:H	1:77:A:GLN:HB3	9	1.33
(1,2113)	1:76:A:MET:H	1:77:A:GLN:HB3	10	1.33
(1,2113)	1:76:A:MET:H	1:77:A:GLN:HB3	21	1.33
(1,1940)	1:106:A:CYS:H	1:63:A:ASN:HD22	17	1.33
(1,1656)	2:37:B:ALA:HB1	2:39:B:TRP:HZ2	24	1.33
(1,1634)	2:38:B:ARG:HD2	2:37:B:ALA:HB1	11	1.33
(1,1549)	1:58:A:CYS:HB2	1:57:A:LYS:HA	1	1.33
(1,1449)	1:69:A:GLU:HG2	1:113:A:LEU:HD22	4	1.33
(1,1449)	1:69:A:GLU:HG2	1:113:A:LEU:HD21	11	1.33
(1,1192)	1:89:A:TYR:HD1	1:89:A:TYR:H	5	1.33
(1,1062)	1:103:A:ALA:HB3	1:59:A:TYR:HB3	1	1.33
(1,572)	1:143:A:LEU:HB2	1:143:A:LEU:HD11	1	1.33
(1,365)	2:29:B:SER:HB2	2:31:B:LEU:HB2	25	1.33
(1,196)	1:73:A:LEU:HD21	1:74:A:CYS:HB3	8	1.33
(1,143)	1:92:A:GLN:HB2	1:89:A:TYR:HD1	5	1.33
(1,122)	1:95:A:ALA:HB3	1:96:A:HIS:HB3	17	1.33
(1,63)	1:67:A:PHE:HA	1:109:A:LEU:HG	7	1.33
(1,2274)	2:39:B:TRP:HE1	2:38:B:ARG:HD2	1	1.32
(1,2113)	1:76:A:MET:H	1:77:A:GLN:HB3	7	1.32
(1,2113)	1:76:A:MET:H	1:77:A:GLN:HB3	16	1.32
(1,2113)	1:76:A:MET:H	1:77:A:GLN:HB3	24	1.32
(1,2113)	1:76:A:MET:H	1:77:A:GLN:HB3	25	1.32
(1,1940)	1:106:A:CYS:H	1:63:A:ASN:HD22	3	1.32
(1,1940)	1:106:A:CYS:H	1:63:A:ASN:HD22	7	1.32
(1,1940)	1:106:A:CYS:H	1:63:A:ASN:HD22	13	1.32
(1,1582)	2:37:B:ALA:HB3	1:125:A:VAL:HG21	23	1.32
(1,1553)	1:59:A:TYR:HD1	1:57:A:LYS:HB2	22	1.32
(1,1449)	1:69:A:GLU:HG2	1:113:A:LEU:HD21	2	1.32
(1,1449)	1:69:A:GLU:HG2	1:113:A:LEU:HD22	8	1.32
(1,1192)	1:89:A:TYR:HD1	1:89:A:TYR:H	2	1.32
(1,904)	1:115:A:ARG:HD3	1:126:A:TYR:HE2	25	1.32
(1,710)	1:130:A:LEU:HD23	1:109:A:LEU:HD13	20	1.32
(1,661)	1:133:A:VAL:HG12	1:99:A:PHE:HE1	15	1.32
(1,619)	1:135:A:LYS:HG2	1:91:A:ARG:HD3	3	1.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,63)	1:67:A:PHE:HA	1:109:A:LEU:HG	1	1.32
(1,63)	1:67:A:PHE:HA	1:109:A:LEU:HG	10	1.32
(1,1940)	1:106:A:CYS:H	1:63:A:ASN:HD22	12	1.31
(1,1766)	2:24:B:GLN:HG2	2:23:B:SER:HA	6	1.31
(1,904)	1:115:A:ARG:HD3	1:126:A:TYR:HE2	10	1.31
(1,879)	1:94:A:ARG:HD2	1:90:A:ASN:HD22	4	1.31
(1,710)	1:130:A:LEU:HD21	1:109:A:LEU:HD11	2	1.31
(1,450)	1:114:A:SER:H	1:126:A:TYR:HB3	8	1.31
(1,379)	2:31:B:LEU:HB2	2:28:B:ASP:HB2	14	1.31
(1,237)	1:64:A:GLU:HB2	1:65:A:LYS:HG3	10	1.31
(1,196)	1:73:A:LEU:HD21	1:74:A:CYS:HB3	6	1.31
(1,196)	1:73:A:LEU:HD21	1:74:A:CYS:HB3	23	1.31
(1,63)	1:67:A:PHE:HA	1:109:A:LEU:HG	21	1.31
(1,2113)	1:76:A:MET:H	1:77:A:GLN:HB3	3	1.3
(1,1582)	2:37:B:ALA:HB2	1:125:A:VAL:HG22	14	1.3
(1,1549)	1:58:A:CYS:HB2	1:57:A:LYS:HA	17	1.3
(1,1549)	1:58:A:CYS:HB2	1:57:A:LYS:HA	23	1.3
(1,1071)	1:101:A:ALA:HB3	1:63:A:ASN:HD21	7	1.3
(1,1071)	1:101:A:ALA:HB3	1:63:A:ASN:HD21	17	1.3
(1,1049)	1:108:A:ILE:HD12	1:104:A:GLU:HG2	22	1.3
(1,710)	1:130:A:LEU:HD21	1:109:A:LEU:HD13	24	1.3
(1,572)	1:143:A:LEU:HB2	1:143:A:LEU:HD12	6	1.3
(1,572)	1:143:A:LEU:HB2	1:143:A:LEU:HD11	23	1.3
(1,534)	1:121:A:ALA:H	1:119:A:ARG:HG2	8	1.3
(1,534)	1:121:A:ALA:H	1:119:A:ARG:HG2	24	1.3
(1,450)	1:114:A:SER:H	1:126:A:TYR:HB3	1	1.3
(1,379)	2:31:B:LEU:HB2	2:28:B:ASP:HB2	6	1.3
(1,368)	2:26:B:ASP:HB3	1:87:A:PHE:HZ	18	1.3
(1,196)	1:73:A:LEU:HD23	1:76:A:MET:HE3	1	1.3
(1,122)	1:95:A:ALA:HB3	1:96:A:HIS:HB3	9	1.3
(1,63)	1:123:A:LEU:HD21	1:124:A:TYR:HA	4	1.3
(1,63)	1:123:A:LEU:HD23	1:124:A:TYR:HA	22	1.3
(1,2113)	1:76:A:MET:H	1:77:A:GLN:HB3	14	1.29
(1,1635)	2:39:B:TRP:HA	2:38:B:ARG:HD2	14	1.29
(1,1415)	1:71:A:LEU:HB2	1:75:A:LYS:HE2	25	1.29
(1,1192)	1:89:A:TYR:HD1	1:89:A:TYR:H	24	1.29
(1,1075)	1:101:A:ALA:HB1	1:60:A:LYS:HB2	25	1.29
(1,1071)	1:101:A:ALA:HB1	1:63:A:ASN:HD21	23	1.29
(1,1049)	1:108:A:ILE:HD11	1:104:A:GLU:HG2	14	1.29
(1,881)	1:117:A:ARG:HD2	1:117:A:ARG:HB2	4	1.29
(1,710)	1:130:A:LEU:HD21	1:109:A:LEU:HD13	8	1.29
(1,710)	1:130:A:LEU:HD23	1:109:A:LEU:HD11	18	1.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,572)	1:143:A:LEU:HB2	1:143:A:LEU:HD13	3	1.29
(1,572)	1:143:A:LEU:HB2	1:143:A:LEU:HD11	19	1.29
(1,379)	2:31:B:LEU:HB2	2:28:B:ASP:HB2	4	1.29
(1,63)	1:67:A:PHE:HA	1:109:A:LEU:HG	25	1.29
(1,46)	1:126:A:TYR:HE1	1:122:A:LYS:HB3	8	1.29
(1,1781)	1:140:A:LYS:H	1:141:A:LYS:HB3	11	1.28
(1,1656)	2:37:B:ALA:HB3	2:39:B:TRP:HZ2	1	1.28
(1,1582)	2:37:B:ALA:HB2	1:125:A:VAL:HG23	6	1.28
(1,1470)	1:66:A:LEU:HD13	1:62:A:GLU:HG3	15	1.28
(1,1470)	1:66:A:LEU:HD13	1:62:A:GLU:HG3	24	1.28
(1,1449)	1:69:A:GLU:HG2	1:113:A:LEU:HD23	18	1.28
(1,1192)	1:89:A:TYR:HD1	1:89:A:TYR:H	16	1.28
(1,1076)	1:101:A:ALA:HB2	1:98:A:LEU:HD23	19	1.28
(1,671)	1:133:A:VAL:HG21	1:99:A:PHE:HZ	1	1.28
(1,671)	1:133:A:VAL:HG21	1:99:A:PHE:HZ	7	1.28
(1,450)	1:114:A:SER:H	1:126:A:TYR:HB3	11	1.28
(1,300)	2:37:B:ALA:HB1	1:123:A:LEU:HB2	8	1.28
(1,63)	1:123:A:LEU:HD23	1:124:A:TYR:HA	18	1.28
(1,63)	1:67:A:PHE:HA	1:109:A:LEU:HG	19	1.28
(1,2113)	1:76:A:MET:H	1:77:A:GLN:HB3	2	1.27
(1,1656)	2:37:B:ALA:HB2	2:39:B:TRP:HZ2	2	1.27
(1,1656)	2:37:B:ALA:HB3	2:39:B:TRP:HZ2	4	1.27
(1,1656)	2:37:B:ALA:HB2	2:39:B:TRP:HZ2	10	1.27
(1,1449)	1:69:A:GLU:HG2	1:113:A:LEU:HD23	10	1.27
(1,1449)	1:69:A:GLU:HG2	1:113:A:LEU:HD23	19	1.27
(1,1398)	1:72:A:GLU:HG2	1:71:A:LEU:HB2	16	1.27
(1,1192)	1:89:A:TYR:HD1	1:89:A:TYR:H	11	1.27
(1,1122)	1:96:A:HIS:HA	1:139:A:ALA:HB1	21	1.27
(1,619)	1:135:A:LYS:HG2	1:91:A:ARG:HD3	12	1.27
(1,577)	1:75:A:LYS:HE2	1:71:A:LEU:HB3	17	1.27
(1,450)	1:114:A:SER:H	1:126:A:TYR:HB3	7	1.27
(1,450)	1:114:A:SER:H	1:126:A:TYR:HB3	10	1.27
(1,300)	2:37:B:ALA:HB3	1:123:A:LEU:HB2	9	1.27
(1,205)	1:71:A:LEU:HD13	1:70:A:PHE:HB3	8	1.27
(1,143)	1:92:A:GLN:HB2	1:89:A:TYR:HD1	9	1.27
(1,63)	1:67:A:PHE:HA	1:109:A:LEU:HG	5	1.27
(1,1660)	2:36:B:THR:HG21	1:122:A:LYS:HD3	11	1.26
(1,1449)	1:69:A:GLU:HG2	1:113:A:LEU:HD22	17	1.26
(1,1331)	1:77:A:GLN:HG2	1:73:A:LEU:HD13	19	1.26
(1,1192)	1:89:A:TYR:HD1	1:89:A:TYR:H	17	1.26
(1,1071)	1:101:A:ALA:HB1	1:63:A:ASN:HD21	25	1.26
(1,618)	1:56:A:LYS:HG2	1:57:A:LYS:H	9	1.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,618)	1:56:A:LYS:HG2	1:57:A:LYS:H	19	1.26
(1,300)	2:37:B:ALA:HB3	1:123:A:LEU:HB2	10	1.26
(1,196)	1:73:A:LEU:HD22	1:74:A:CYS:HB3	25	1.26
(1,1656)	2:37:B:ALA:HB3	2:39:B:TRP:HZ2	13	1.25
(1,1449)	1:69:A:GLU:HG2	1:113:A:LEU:HD23	3	1.25
(1,1449)	1:69:A:GLU:HG2	1:113:A:LEU:HD23	7	1.25
(1,1398)	1:72:A:GLU:HG2	1:71:A:LEU:HB2	3	1.25
(1,1192)	1:89:A:TYR:HD1	1:89:A:TYR:H	4	1.25
(1,1192)	1:89:A:TYR:HD1	1:89:A:TYR:H	22	1.25
(1,671)	1:133:A:VAL:HG21	1:99:A:PHE:HZ	19	1.25
(1,671)	1:133:A:VAL:HG22	1:99:A:PHE:HZ	25	1.25
(1,379)	2:31:B:LEU:HB2	2:28:B:ASP:HB2	18	1.25
(1,368)	2:26:B:ASP:HB3	1:87:A:PHE:HZ	12	1.25
(1,300)	2:37:B:ALA:HB2	1:123:A:LEU:HB2	21	1.25
(1,237)	1:64:A:GLU:HB2	1:65:A:LYS:HG3	14	1.25
(1,184)	1:79:A:ALA:HB3	1:75:A:LYS:HA	25	1.25
(1,1656)	2:37:B:ALA:HB1	2:39:B:TRP:HZ2	16	1.24
(1,1656)	2:37:B:ALA:HB3	2:39:B:TRP:HZ2	25	1.24
(1,1449)	1:69:A:GLU:HG2	1:113:A:LEU:HD22	16	1.24
(1,1415)	1:71:A:LEU:HB2	1:75:A:LYS:HE2	6	1.24
(1,1192)	1:89:A:TYR:HD1	1:89:A:TYR:H	15	1.24
(1,1192)	1:89:A:TYR:HD1	1:89:A:TYR:H	18	1.24
(1,1192)	1:89:A:TYR:HD1	1:89:A:TYR:H	20	1.24
(1,1118)	1:98:A:LEU:HB3	1:98:A:LEU:HD23	19	1.24
(1,1093)	1:100:A:LEU:HA	1:100:A:LEU:HD22	6	1.24
(1,710)	1:130:A:LEU:HD22	1:109:A:LEU:HD13	1	1.24
(1,710)	1:130:A:LEU:HD21	1:109:A:LEU:HD11	6	1.24
(1,710)	1:130:A:LEU:HD23	1:109:A:LEU:HD11	15	1.24
(1,671)	1:133:A:VAL:HG22	1:99:A:PHE:HZ	6	1.24
(1,450)	1:114:A:SER:H	1:126:A:TYR:HB3	3	1.24
(1,196)	1:73:A:LEU:HD23	1:74:A:CYS:HB3	10	1.24
(1,196)	1:73:A:LEU:HD21	1:74:A:CYS:HB3	19	1.24
(1,40)	1:127:A:ILE:HD12	1:127:A:ILE:HA	5	1.24
(1,1582)	2:37:B:ALA:HB2	1:125:A:VAL:HG23	19	1.23
(1,1449)	1:69:A:GLU:HG2	1:113:A:LEU:HD21	1	1.23
(1,1331)	1:77:A:GLN:HG2	1:73:A:LEU:HD13	11	1.23
(1,1192)	1:89:A:TYR:HD1	1:89:A:TYR:H	3	1.23
(1,1192)	1:89:A:TYR:HD1	1:89:A:TYR:H	6	1.23
(1,1192)	1:89:A:TYR:HD1	1:89:A:TYR:H	8	1.23
(1,1192)	1:89:A:TYR:HD1	1:89:A:TYR:H	14	1.23
(1,1062)	1:103:A:ALA:HB2	1:59:A:TYR:HB3	3	1.23
(1,671)	1:133:A:VAL:HG23	1:99:A:PHE:HZ	3	1.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,671)	1:133:A:VAL:HG22	1:99:A:PHE:HZ	21	1.23
(1,499)	1:85:A:VAL:H	1:86:A:PRO:HG3	16	1.23
(1,196)	1:73:A:LEU:HD23	1:74:A:CYS:HB3	5	1.23
(1,196)	1:73:A:LEU:HD22	1:74:A:CYS:HB3	15	1.23
(1,143)	1:92:A:GLN:HB2	1:89:A:TYR:HD1	23	1.23
(1,63)	1:123:A:LEU:HD23	1:124:A:TYR:HA	20	1.23
(1,1582)	2:37:B:ALA:HB3	1:125:A:VAL:HG23	1	1.22
(1,1331)	1:77:A:GLN:HG2	1:73:A:LEU:HD13	1	1.22
(1,1192)	1:89:A:TYR:HD1	1:89:A:TYR:H	10	1.22
(1,1192)	1:89:A:TYR:HD1	1:89:A:TYR:H	12	1.22
(1,1192)	1:89:A:TYR:HD1	1:89:A:TYR:H	19	1.22
(1,1192)	1:89:A:TYR:HD1	1:89:A:TYR:H	23	1.22
(1,1122)	1:96:A:HIS:HA	1:139:A:ALA:HB1	12	1.22
(1,710)	1:130:A:LEU:HD22	1:109:A:LEU:HD12	11	1.22
(1,341)	2:31:B:LEU:HD12	1:84:A:VAL:H	7	1.22
(1,205)	1:71:A:LEU:HD12	1:70:A:PHE:HB3	25	1.22
(1,196)	1:73:A:LEU:HD22	1:74:A:CYS:HB3	11	1.22
(1,196)	1:73:A:LEU:HD21	1:76:A:MET:HE1	17	1.22
(1,143)	1:89:A:TYR:HD2	1:86:A:PRO:HB2	16	1.22
(1,40)	1:127:A:ILE:HD12	1:74:A:CYS:HA	17	1.22
(1,4)	1:130:A:LEU:HD22	1:127:A:ILE:HA	24	1.22
(1,2189)	1:59:A:TYR:H	1:60:A:LYS:HB2	17	1.21
(1,1449)	1:69:A:GLU:HG2	1:113:A:LEU:HD21	15	1.21
(1,1367)	1:75:A:LYS:HD2	1:75:A:LYS:HA	10	1.21
(1,1196)	1:89:A:TYR:HD1	1:71:A:LEU:HD13	2	1.21
(1,1192)	1:89:A:TYR:HD1	1:89:A:TYR:H	9	1.21
(1,1192)	1:89:A:TYR:HD1	1:89:A:TYR:H	25	1.21
(1,671)	1:133:A:VAL:HG22	1:99:A:PHE:HZ	5	1.21
(1,671)	1:133:A:VAL:HG23	1:99:A:PHE:HZ	13	1.21
(1,671)	1:133:A:VAL:HG22	1:99:A:PHE:HZ	22	1.21
(1,280)	2:31:B:LEU:HG	1:87:A:PHE:HE2	12	1.21
(1,205)	1:71:A:LEU:HD13	1:70:A:PHE:HB3	7	1.21
(1,143)	1:89:A:TYR:HD2	1:86:A:PRO:HB2	20	1.21
(1,63)	1:123:A:LEU:HD22	1:124:A:TYR:HA	8	1.21
(1,1940)	1:106:A:CYS:H	1:63:A:ASN:HD22	22	1.2
(1,1582)	2:37:B:ALA:HB1	1:125:A:VAL:HG23	3	1.2
(1,1449)	1:69:A:GLU:HG2	1:113:A:LEU:HD21	23	1.2
(1,1367)	1:75:A:LYS:HD2	1:75:A:LYS:HA	24	1.2
(1,1192)	1:89:A:TYR:HD1	1:89:A:TYR:H	1	1.2
(1,1192)	1:89:A:TYR:HD1	1:89:A:TYR:H	7	1.2
(1,946)	1:110:A:SER:HB2	1:66:A:LEU:HD11	19	1.2
(1,570)	1:143:A:LEU:HB2	1:144:A:ASN:HD21	1	1.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,450)	1:114:A:SER:H	1:115:A:ARG:HD2	21	1.2
(1,300)	2:37:B:ALA:HB2	1:123:A:LEU:HB2	3	1.2
(1,300)	2:37:B:ALA:HB3	1:123:A:LEU:HB2	14	1.2
(1,280)	2:31:B:LEU:HG	1:87:A:PHE:HE2	2	1.2
(1,86)	1:98:A:LEU:HD13	1:99:A:PHE:H	6	1.2
(1,40)	1:127:A:ILE:HD11	1:74:A:CYS:HA	7	1.2
(1,40)	1:127:A:ILE:HD11	1:74:A:CYS:HA	25	1.2
(1,1656)	2:37:B:ALA:HB1	2:39:B:TRP:HZ2	20	1.19
(1,1582)	2:37:B:ALA:HB2	1:125:A:VAL:HG21	9	1.19
(1,1582)	2:37:B:ALA:HB1	1:125:A:VAL:HG22	21	1.19
(1,1456)	1:69:A:GLU:HG2	1:66:A:LEU:HA	12	1.19
(1,1398)	1:72:A:GLU:HG2	1:71:A:LEU:HB2	7	1.19
(1,1228)	1:87:A:PHE:HD1	1:88:A:LEU:HD21	24	1.19
(1,450)	1:114:A:SER:H	1:126:A:TYR:HB3	9	1.19
(1,143)	1:89:A:TYR:HD2	1:86:A:PRO:HB2	14	1.19
(1,63)	1:123:A:LEU:HD21	1:124:A:TYR:HA	15	1.19
(1,1771)	1:142:A:LYS:H	1:142:A:LYS:HD2	13	1.18
(1,1771)	1:142:A:LYS:H	1:142:A:LYS:HD2	20	1.18
(1,1656)	2:37:B:ALA:HB1	2:39:B:TRP:HZ2	3	1.18
(1,1649)	2:37:B:ALA:HB1	2:38:B:ARG:HB2	18	1.18
(1,1582)	2:37:B:ALA:HB3	1:125:A:VAL:HG21	8	1.18
(1,1137)	1:95:A:ALA:HB2	1:91:A:ARG:HD3	24	1.18
(1,534)	1:121:A:ALA:H	1:119:A:ARG:HG2	20	1.18
(1,341)	2:31:B:LEU:HD12	1:84:A:VAL:H	16	1.18
(1,205)	1:71:A:LEU:HD12	1:70:A:PHE:HB3	6	1.18
(1,86)	1:98:A:LEU:HD12	1:99:A:PHE:H	18	1.18
(1,86)	1:113:A:LEU:HD11	1:73:A:LEU:H	19	1.18
(1,63)	1:123:A:LEU:HD21	1:124:A:TYR:HA	17	1.18
(1,40)	1:127:A:ILE:HD11	1:74:A:CYS:HA	18	1.18
(1,2189)	1:59:A:TYR:H	1:60:A:LYS:HB2	22	1.17
(1,1940)	1:106:A:CYS:H	1:63:A:ASN:HD22	4	1.17
(1,1940)	1:106:A:CYS:H	1:63:A:ASN:HD22	23	1.17
(1,1582)	2:37:B:ALA:HB1	1:125:A:VAL:HG22	20	1.17
(1,1096)	1:100:A:LEU:HD23	1:92:A:GLN:HG3	6	1.17
(1,1071)	1:101:A:ALA:HB3	1:63:A:ASN:HD21	16	1.17
(1,671)	1:133:A:VAL:HG22	1:99:A:PHE:HZ	12	1.17
(1,671)	1:133:A:VAL:HG22	1:99:A:PHE:HZ	24	1.17
(1,618)	1:56:A:LYS:HG2	1:57:A:LYS:H	18	1.17
(1,450)	1:114:A:SER:H	1:126:A:TYR:HB3	6	1.17
(1,368)	2:26:B:ASP:HB3	1:87:A:PHE:HZ	15	1.17
(1,341)	2:31:B:LEU:HD11	1:84:A:VAL:H	10	1.17
(1,300)	2:37:B:ALA:HB2	1:123:A:LEU:HB2	7	1.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,63)	1:123:A:LEU:HD21	1:124:A:TYR:HA	3	1.17
(1,40)	1:127:A:ILE:HD11	1:74:A:CYS:HA	9	1.17
(1,1976)	1:100:A:LEU:H	1:138:A:SER:HB2	9	1.16
(1,1229)	1:67:A:PHE:HD1	1:67:A:PHE:H	20	1.16
(1,1196)	1:89:A:TYR:HD1	1:71:A:LEU:HD11	5	1.16
(1,946)	1:110:A:SER:HB2	1:66:A:LEU:HD11	18	1.16
(1,710)	1:130:A:LEU:HD22	1:109:A:LEU:HD13	13	1.16
(1,710)	1:130:A:LEU:HD21	1:109:A:LEU:HD12	14	1.16
(1,671)	1:133:A:VAL:HG23	1:99:A:PHE:HZ	9	1.16
(1,534)	1:121:A:ALA:H	1:119:A:ARG:HG2	3	1.16
(1,534)	1:121:A:ALA:H	1:119:A:ARG:HG2	4	1.16
(1,355)	2:29:B:SER:HB3	2:31:B:LEU:H	21	1.16
(1,300)	2:37:B:ALA:HB2	1:123:A:LEU:HB2	16	1.16
(1,120)	1:95:A:ALA:HB3	1:93:A:GLN:H	18	1.16
(1,86)	1:113:A:LEU:HD11	1:73:A:LEU:H	10	1.16
(1,86)	1:98:A:LEU:HD11	1:99:A:PHE:H	20	1.16
(1,63)	1:123:A:LEU:HD21	1:124:A:TYR:HA	9	1.16
(1,46)	1:126:A:TYR:HE1	1:122:A:LYS:HB3	25	1.16
(1,40)	1:127:A:ILE:HD11	1:74:A:CYS:HA	20	1.16
(1,1771)	1:142:A:LYS:H	1:142:A:LYS:HD2	23	1.15
(1,1415)	1:71:A:LEU:HB2	1:75:A:LYS:HE2	8	1.15
(1,1375)	1:74:A:CYS:HA	1:77:A:GLN:HB3	19	1.15
(1,1368)	1:75:A:LYS:HD3	1:75:A:LYS:HB2	17	1.15
(1,1229)	1:67:A:PHE:HD1	1:67:A:PHE:H	4	1.15
(1,1229)	1:67:A:PHE:HD1	1:67:A:PHE:H	9	1.15
(1,879)	1:94:A:ARG:HD3	1:90:A:ASN:HD22	13	1.15
(1,710)	1:130:A:LEU:HD23	1:109:A:LEU:HD13	7	1.15
(1,368)	2:26:B:ASP:HB3	1:87:A:PHE:HZ	11	1.15
(1,341)	2:31:B:LEU:HD12	1:84:A:VAL:H	24	1.15
(1,122)	1:95:A:ALA:HB2	1:91:A:ARG:HD3	24	1.15
(1,40)	1:127:A:ILE:HD11	1:74:A:CYS:HA	6	1.15
(1,2274)	2:39:B:TRP:HE1	2:38:B:ARG:HD3	21	1.14
(1,2151)	1:65:A:LYS:HG3	1:66:A:LEU:H	14	1.14
(1,1771)	1:142:A:LYS:H	1:142:A:LYS:HD2	2	1.14
(1,1656)	2:37:B:ALA:HB2	2:39:B:TRP:HZ2	6	1.14
(1,1553)	1:59:A:TYR:HD1	1:57:A:LYS:HB2	25	1.14
(1,1449)	1:69:A:GLU:HG2	1:113:A:LEU:HD22	14	1.14
(1,1229)	1:67:A:PHE:HD1	1:67:A:PHE:H	18	1.14
(1,1229)	1:67:A:PHE:HD1	1:67:A:PHE:H	21	1.14
(1,1229)	1:67:A:PHE:HD1	1:67:A:PHE:H	22	1.14
(1,1196)	1:89:A:TYR:HD1	1:71:A:LEU:HD12	3	1.14
(1,1062)	1:103:A:ALA:HB3	1:59:A:TYR:HB3	6	1.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1062)	1:103:A:ALA:HB2	1:59:A:TYR:HB3	16	1.14
(1,946)	1:110:A:SER:HB2	1:66:A:LEU:HD12	1	1.14
(1,450)	1:114:A:SER:H	1:117:A:ARG:HD3	12	1.14
(1,365)	2:29:B:SER:HB2	2:31:B:LEU:HB2	14	1.14
(1,341)	2:31:B:LEU:HD13	1:84:A:VAL:H	1	1.14
(1,341)	2:31:B:LEU:HD12	1:84:A:VAL:H	12	1.14
(1,300)	2:37:B:ALA:HB1	1:123:A:LEU:HB2	5	1.14
(1,263)	1:132:A:THR:HG21	2:28:B:ASP:HB3	8	1.14
(1,196)	1:73:A:LEU:HD22	1:74:A:CYS:HB3	22	1.14
(1,174)	1:84:A:VAL:HG11	1:124:A:TYR:HA	16	1.14
(1,149)	1:88:A:LEU:HD23	1:89:A:TYR:H	10	1.14
(1,143)	1:89:A:TYR:HD2	1:86:A:PRO:HB2	6	1.14
(1,143)	1:89:A:TYR:HD2	1:86:A:PRO:HB2	22	1.14
(1,122)	1:95:A:ALA:HB3	1:96:A:HIS:HB3	12	1.14
(1,63)	1:123:A:LEU:HD23	1:124:A:TYR:HA	13	1.14
(1,1771)	1:142:A:LYS:H	1:142:A:LYS:HD2	6	1.13
(1,1656)	2:37:B:ALA:HB1	2:39:B:TRP:HZ2	12	1.13
(1,1582)	2:37:B:ALA:HB1	1:125:A:VAL:HG22	16	1.13
(1,1553)	1:59:A:TYR:HD1	1:57:A:LYS:HB2	11	1.13
(1,1229)	1:67:A:PHE:HD1	1:67:A:PHE:H	5	1.13
(1,1229)	1:67:A:PHE:HD1	1:67:A:PHE:H	11	1.13
(1,1229)	1:67:A:PHE:HD1	1:67:A:PHE:H	15	1.13
(1,1229)	1:67:A:PHE:HD1	1:67:A:PHE:H	17	1.13
(1,1229)	1:67:A:PHE:HD1	1:67:A:PHE:H	23	1.13
(1,1229)	1:67:A:PHE:HD1	1:67:A:PHE:H	24	1.13
(1,1192)	1:89:A:TYR:HD1	1:89:A:TYR:H	13	1.13
(1,1066)	1:101:A:ALA:HA	1:60:A:LYS:HB2	25	1.13
(1,710)	1:130:A:LEU:HD23	1:109:A:LEU:HD11	12	1.13
(1,40)	1:127:A:ILE:HD12	1:74:A:CYS:HA	4	1.13
(1,40)	1:127:A:ILE:HD12	1:74:A:CYS:HA	15	1.13
(1,1651)	2:38:B:ARG:HG2	2:37:B:ALA:HB3	24	1.12
(1,1553)	1:59:A:TYR:HD1	1:57:A:LYS:HB2	6	1.12
(1,1229)	1:67:A:PHE:HD1	1:67:A:PHE:H	1	1.12
(1,1229)	1:67:A:PHE:HD1	1:67:A:PHE:H	2	1.12
(1,1229)	1:67:A:PHE:HD1	1:67:A:PHE:H	6	1.12
(1,1229)	1:67:A:PHE:HD1	1:67:A:PHE:H	7	1.12
(1,1229)	1:67:A:PHE:HD1	1:67:A:PHE:H	8	1.12
(1,1229)	1:67:A:PHE:HD1	1:67:A:PHE:H	10	1.12
(1,1229)	1:67:A:PHE:HD1	1:67:A:PHE:H	12	1.12
(1,1229)	1:67:A:PHE:HD1	1:67:A:PHE:H	16	1.12
(1,710)	1:130:A:LEU:HD21	1:109:A:LEU:HD13	16	1.12
(1,710)	1:130:A:LEU:HD21	1:109:A:LEU:HD12	22	1.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,671)	1:133:A:VAL:HG22	1:99:A:PHE:HZ	18	1.12
(1,619)	1:135:A:LYS:HG2	1:91:A:ARG:HD3	13	1.12
(1,534)	1:121:A:ALA:H	1:119:A:ARG:HG3	16	1.12
(1,341)	2:31:B:LEU:HD12	1:84:A:VAL:H	13	1.12
(1,300)	2:37:B:ALA:HB2	1:123:A:LEU:HB2	24	1.12
(1,149)	1:88:A:LEU:HD12	1:89:A:TYR:H	3	1.12
(1,91)	1:109:A:LEU:HD11	1:64:A:GLU:H	20	1.12
(1,40)	1:127:A:ILE:HD13	1:74:A:CYS:HA	22	1.12
(1,40)	1:127:A:ILE:HD13	1:74:A:CYS:HA	23	1.12
(1,2151)	1:65:A:LYS:HG3	1:66:A:LEU:H	5	1.11
(1,1976)	1:100:A:LEU:H	1:138:A:SER:HB2	1	1.11
(1,1656)	2:37:B:ALA:HB1	2:39:B:TRP:HZ2	7	1.11
(1,1651)	2:38:B:ARG:HG2	2:37:B:ALA:HB1	2	1.11
(1,1582)	2:37:B:ALA:HB1	1:125:A:VAL:HG22	7	1.11
(1,1375)	1:74:A:CYS:HA	1:77:A:GLN:HB3	1	1.11
(1,1229)	1:67:A:PHE:HD1	1:67:A:PHE:H	25	1.11
(1,1196)	1:89:A:TYR:HD1	1:71:A:LEU:HD12	19	1.11
(1,1192)	1:89:A:TYR:HD1	1:89:A:TYR:H	21	1.11
(1,1143)	1:94:A:ARG:HG2	1:94:A:ARG:H	6	1.11
(1,671)	1:133:A:VAL:HG23	1:99:A:PHE:HZ	2	1.11
(1,671)	1:133:A:VAL:HG23	1:99:A:PHE:HZ	20	1.11
(1,306)	2:36:B:THR:HG21	1:124:A:TYR:HE1	16	1.11
(1,149)	1:88:A:LEU:HD21	1:89:A:TYR:H	13	1.11
(1,120)	1:95:A:ALA:HB2	1:93:A:GLN:H	1	1.11
(1,120)	1:95:A:ALA:HB1	1:100:A:LEU:H	23	1.11
(1,91)	1:109:A:LEU:HD12	1:64:A:GLU:H	9	1.11
(1,86)	1:98:A:LEU:HD12	1:99:A:PHE:H	8	1.11
(1,86)	1:113:A:LEU:HD13	1:73:A:LEU:H	14	1.11
(1,86)	1:113:A:LEU:HD13	1:73:A:LEU:H	16	1.11
(1,40)	1:127:A:ILE:HD12	1:74:A:CYS:HA	11	1.11
(1,40)	1:127:A:ILE:HD11	1:74:A:CYS:HA	13	1.11
(1,40)	1:127:A:ILE:HD12	1:74:A:CYS:HA	24	1.11
(1,1656)	2:37:B:ALA:HB2	2:39:B:TRP:HZ2	9	1.1
(1,1656)	2:37:B:ALA:HB2	2:39:B:TRP:HZ2	17	1.1
(1,1635)	2:39:B:TRP:HA	2:38:B:ARG:HD2	19	1.1
(1,1582)	2:37:B:ALA:HB1	1:125:A:VAL:HG23	24	1.1
(1,1456)	1:69:A:GLU:HG2	1:66:A:LEU:HA	16	1.1
(1,1229)	1:67:A:PHE:HD1	1:67:A:PHE:H	14	1.1
(1,1196)	1:89:A:TYR:HD1	1:71:A:LEU:HD11	9	1.1
(1,946)	1:110:A:SER:HB2	1:66:A:LEU:HD13	8	1.1
(1,710)	1:130:A:LEU:HD21	1:109:A:LEU:HD11	21	1.1
(1,355)	2:29:B:SER:HB3	2:31:B:LEU:H	4	1.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,341)	2:31:B:LEU:HD13	1:84:A:VAL:H	11	1.1
(1,341)	2:31:B:LEU:HD13	1:84:A:VAL:H	21	1.1
(1,306)	2:36:B:THR:HG23	1:124:A:TYR:HE2	19	1.1
(1,282)	2:31:B:LEU:HD13	1:124:A:TYR:HA	6	1.1
(1,141)	1:89:A:TYR:HD2	1:86:A:PRO:HB2	21	1.1
(1,120)	1:95:A:ALA:HB2	1:100:A:LEU:H	14	1.1
(1,120)	1:95:A:ALA:HB1	1:93:A:GLN:H	25	1.1
(1,86)	1:113:A:LEU:HD12	1:73:A:LEU:H	21	1.1
(1,9)	1:134:A:LEU:HD23	1:131:A:CYS:HA	3	1.1
(1,4)	1:130:A:LEU:HD21	1:127:A:ILE:HA	15	1.1
(1,4)	1:130:A:LEU:HD22	1:127:A:ILE:HA	19	1.1
(1,1722)	2:31:B:LEU:HD22	1:128:A:ASN:HB2	22	1.09
(1,1656)	2:37:B:ALA:HB3	2:39:B:TRP:HZ2	22	1.09
(1,1651)	2:38:B:ARG:HG2	2:37:B:ALA:HB2	1	1.09
(1,1196)	1:89:A:TYR:HD1	1:71:A:LEU:HD13	6	1.09
(1,1196)	1:89:A:TYR:HD1	1:71:A:LEU:HD12	14	1.09
(1,710)	1:130:A:LEU:HD21	1:109:A:LEU:HD11	4	1.09
(1,710)	1:130:A:LEU:HD21	1:109:A:LEU:HD12	23	1.09
(1,618)	1:56:A:LYS:HG2	1:57:A:LYS:H	20	1.09
(1,534)	1:121:A:ALA:H	1:119:A:ARG:HG2	18	1.09
(1,450)	1:114:A:SER:H	1:126:A:TYR:HB3	16	1.09
(1,341)	2:31:B:LEU:HD11	1:84:A:VAL:H	15	1.09
(1,306)	2:36:B:THR:HG21	1:124:A:TYR:HE2	25	1.09
(1,300)	2:37:B:ALA:HB1	1:123:A:LEU:HB2	13	1.09
(1,149)	1:88:A:LEU:HD22	1:89:A:TYR:H	18	1.09
(1,120)	1:95:A:ALA:HB1	1:100:A:LEU:H	16	1.09
(1,86)	1:98:A:LEU:HD13	1:99:A:PHE:H	22	1.09
(1,86)	1:98:A:LEU:HD13	1:99:A:PHE:H	25	1.09
(1,63)	1:123:A:LEU:HD22	1:124:A:TYR:HA	12	1.09
(1,63)	1:123:A:LEU:HD23	1:124:A:TYR:HA	14	1.09
(1,23)	1:130:A:LEU:HD23	1:130:A:LEU:H	6	1.09
(1,23)	1:130:A:LEU:HD23	1:130:A:LEU:H	22	1.09
(1,4)	1:130:A:LEU:HD23	1:127:A:ILE:HA	5	1.09
(1,2274)	2:39:B:TRP:HE1	2:38:B:ARG:HD2	2	1.08
(1,1722)	2:31:B:LEU:HD23	1:128:A:ASN:HB2	17	1.08
(1,1196)	1:89:A:TYR:HD1	1:71:A:LEU:HD11	11	1.08
(1,1143)	1:94:A:ARG:HG2	1:94:A:ARG:H	23	1.08
(1,1066)	1:101:A:ALA:HA	1:60:A:LYS:HB2	20	1.08
(1,879)	1:94:A:ARG:HD2	1:90:A:ASN:HD22	24	1.08
(1,618)	1:56:A:LYS:HG2	1:57:A:LYS:H	12	1.08
(1,577)	1:75:A:LYS:HE2	1:71:A:LEU:HB3	10	1.08
(1,443)	2:36:B:THR:H	2:34:B:TYR:HD1	20	1.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,355)	2:29:B:SER:HB3	2:31:B:LEU:H	5	1.08
(1,341)	2:31:B:LEU:HD11	1:84:A:VAL:H	3	1.08
(1,341)	2:31:B:LEU:HD12	1:84:A:VAL:H	14	1.08
(1,341)	2:31:B:LEU:HD13	1:84:A:VAL:H	23	1.08
(1,307)	2:39:B:TRP:HE3	2:36:B:THR:HG21	4	1.08
(1,307)	2:36:B:THR:HG22	1:128:A:ASN:HD21	8	1.08
(1,306)	2:36:B:THR:HG21	1:124:A:TYR:HE2	2	1.08
(1,306)	2:36:B:THR:HG23	1:124:A:TYR:HE1	10	1.08
(1,282)	2:31:B:LEU:HD11	1:124:A:TYR:HA	10	1.08
(1,282)	2:31:B:LEU:HD13	1:124:A:TYR:HA	21	1.08
(1,149)	1:88:A:LEU:HD21	1:89:A:TYR:H	4	1.08
(1,143)	1:89:A:TYR:HD2	1:86:A:PRO:HB2	12	1.08
(1,91)	1:109:A:LEU:HD12	1:64:A:GLU:H	2	1.08
(1,91)	1:109:A:LEU:HD12	1:64:A:GLU:H	5	1.08
(1,91)	1:109:A:LEU:HD11	1:64:A:GLU:H	7	1.08
(1,91)	1:109:A:LEU:HD12	1:64:A:GLU:H	12	1.08
(1,91)	1:109:A:LEU:HD13	1:64:A:GLU:H	19	1.08
(1,86)	1:113:A:LEU:HD12	1:73:A:LEU:H	2	1.08
(1,86)	1:113:A:LEU:HD13	1:73:A:LEU:H	23	1.08
(1,59)	1:123:A:LEU:HA	1:123:A:LEU:HD22	17	1.08
(1,23)	1:130:A:LEU:HD21	1:130:A:LEU:H	11	1.08
(1,23)	1:130:A:LEU:HD21	1:113:A:LEU:H	13	1.08
(1,23)	1:130:A:LEU:HD23	1:130:A:LEU:H	23	1.08
(1,4)	1:130:A:LEU:HD23	1:127:A:ILE:HA	1	1.08
(1,4)	1:130:A:LEU:HD22	1:127:A:ILE:HA	2	1.08
(1,4)	1:130:A:LEU:HD21	1:127:A:ILE:HA	20	1.08
(1,1553)	1:59:A:TYR:HD1	1:57:A:LYS:HB2	24	1.07
(1,1375)	1:74:A:CYS:HA	1:77:A:GLN:HB3	11	1.07
(1,1093)	1:100:A:LEU:HA	1:100:A:LEU:HD22	8	1.07
(1,1049)	1:108:A:ILE:HD11	1:104:A:GLU:HG2	16	1.07
(1,710)	1:130:A:LEU:HD23	1:109:A:LEU:HD12	17	1.07
(1,710)	1:130:A:LEU:HD22	1:109:A:LEU:HD12	25	1.07
(1,577)	1:75:A:LYS:HE2	1:71:A:LEU:HB3	24	1.07
(1,443)	1:117:A:ARG:H	1:126:A:TYR:HE2	4	1.07
(1,341)	2:31:B:LEU:HD12	1:84:A:VAL:H	20	1.07
(1,341)	2:31:B:LEU:HD12	1:84:A:VAL:H	22	1.07
(1,306)	2:36:B:THR:HG21	1:124:A:TYR:HE2	6	1.07
(1,306)	2:36:B:THR:HG22	1:124:A:TYR:HE1	13	1.07
(1,282)	2:31:B:LEU:HD12	1:124:A:TYR:HA	13	1.07
(1,282)	2:31:B:LEU:HD11	1:124:A:TYR:HA	15	1.07
(1,282)	2:31:B:LEU:HD12	1:124:A:TYR:HA	16	1.07
(1,184)	1:79:A:ALA:HB2	1:75:A:LYS:HA	8	1.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,91)	1:109:A:LEU:HD11	1:64:A:GLU:H	10	1.07
(1,91)	1:109:A:LEU:HD11	1:64:A:GLU:H	13	1.07
(1,91)	1:109:A:LEU:HD12	1:64:A:GLU:H	21	1.07
(1,91)	1:109:A:LEU:HD13	1:64:A:GLU:H	25	1.07
(1,59)	1:123:A:LEU:HA	1:123:A:LEU:HD21	9	1.07
(1,23)	1:130:A:LEU:HD23	1:130:A:LEU:H	8	1.07
(1,23)	1:130:A:LEU:HD23	1:130:A:LEU:H	14	1.07
(1,2274)	2:39:B:TRP:HE1	2:38:B:ARG:HD2	13	1.06
(1,1722)	2:31:B:LEU:HD23	1:128:A:ASN:HB2	14	1.06
(1,671)	1:133:A:VAL:HG23	1:99:A:PHE:HZ	16	1.06
(1,450)	1:114:A:SER:H	1:126:A:TYR:HB3	20	1.06
(1,443)	2:36:B:THR:H	2:34:B:TYR:HD1	16	1.06
(1,368)	2:26:B:ASP:HB3	1:87:A:PHE:HZ	19	1.06
(1,356)	2:29:B:SER:HB2	2:31:B:LEU:H	16	1.06
(1,341)	2:31:B:LEU:HD13	1:84:A:VAL:H	6	1.06
(1,282)	2:31:B:LEU:HD13	1:124:A:TYR:HA	1	1.06
(1,282)	2:31:B:LEU:HD12	1:124:A:TYR:HA	9	1.06
(1,282)	2:31:B:LEU:HD12	1:124:A:TYR:HA	20	1.06
(1,263)	1:132:A:THR:HG23	2:28:B:ASP:HB3	17	1.06
(1,149)	1:88:A:LEU:HD22	1:89:A:TYR:H	14	1.06
(1,149)	1:88:A:LEU:HD21	1:89:A:TYR:H	25	1.06
(1,116)	1:100:A:LEU:HD23	1:95:A:ALA:H	8	1.06
(1,91)	1:109:A:LEU:HD13	1:64:A:GLU:H	17	1.06
(1,86)	1:113:A:LEU:HD12	1:73:A:LEU:H	3	1.06
(1,86)	1:98:A:LEU:HD11	1:99:A:PHE:H	24	1.06
(1,59)	1:123:A:LEU:HA	1:123:A:LEU:HD23	8	1.06
(1,59)	1:123:A:LEU:HA	1:123:A:LEU:HD22	12	1.06
(1,59)	1:123:A:LEU:HA	1:123:A:LEU:HD22	15	1.06
(1,23)	1:130:A:LEU:HD23	1:130:A:LEU:H	2	1.06
(1,23)	1:130:A:LEU:HD22	1:130:A:LEU:H	7	1.06
(1,23)	1:130:A:LEU:HD23	1:113:A:LEU:H	16	1.06
(1,1976)	1:100:A:LEU:H	1:138:A:SER:HB2	2	1.05
(1,1722)	2:31:B:LEU:HD22	1:128:A:ASN:HB2	18	1.05
(1,1651)	2:38:B:ARG:HG2	2:37:B:ALA:HB1	17	1.05
(1,1649)	2:37:B:ALA:HB3	2:38:B:ARG:HB2	20	1.05
(1,1582)	2:37:B:ALA:HB2	1:125:A:VAL:HG23	10	1.05
(1,1196)	1:89:A:TYR:HD1	1:71:A:LEU:HD12	1	1.05
(1,1196)	1:89:A:TYR:HD1	1:71:A:LEU:HD13	15	1.05
(1,1196)	1:89:A:TYR:HD1	1:71:A:LEU:HD13	16	1.05
(1,1196)	1:89:A:TYR:HD1	1:71:A:LEU:HD13	23	1.05
(1,710)	1:130:A:LEU:HD21	1:109:A:LEU:HD11	3	1.05
(1,618)	1:56:A:LYS:HG2	1:57:A:LYS:H	6	1.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,577)	1:75:A:LYS:HE2	1:71:A:LEU:HB3	4	1.05
(1,443)	1:117:A:ARG:H	1:126:A:TYR:HE2	10	1.05
(1,400)	1:136:A:ALA:HB1	1:135:A:LYS:H	1	1.05
(1,400)	1:136:A:ALA:HB3	1:135:A:LYS:H	15	1.05
(1,400)	1:136:A:ALA:HB2	1:135:A:LYS:H	20	1.05
(1,369)	2:26:B:ASP:HB2	1:87:A:PHE:HZ	21	1.05
(1,368)	2:26:B:ASP:HB3	1:87:A:PHE:HZ	16	1.05
(1,365)	2:29:B:SER:HB2	2:31:B:LEU:HB2	22	1.05
(1,355)	2:29:B:SER:HB3	2:31:B:LEU:H	8	1.05
(1,355)	2:29:B:SER:HB3	2:31:B:LEU:H	13	1.05
(1,341)	2:31:B:LEU:HD12	1:84:A:VAL:H	17	1.05
(1,341)	2:31:B:LEU:HD13	1:84:A:VAL:H	19	1.05
(1,341)	2:31:B:LEU:HD12	1:84:A:VAL:H	25	1.05
(1,306)	2:36:B:THR:HG22	1:124:A:TYR:HE2	15	1.05
(1,306)	2:36:B:THR:HG23	1:124:A:TYR:HE1	24	1.05
(1,282)	2:31:B:LEU:HD12	1:124:A:TYR:HA	12	1.05
(1,280)	2:31:B:LEU:HG	1:87:A:PHE:HE2	4	1.05
(1,184)	1:79:A:ALA:HB3	1:75:A:LYS:HA	21	1.05
(1,150)	1:88:A:LEU:HD23	1:128:A:ASN:H	9	1.05
(1,150)	1:88:A:LEU:HD23	1:128:A:ASN:H	21	1.05
(1,149)	1:88:A:LEU:HD21	1:89:A:TYR:H	7	1.05
(1,149)	1:88:A:LEU:HD21	1:89:A:TYR:H	15	1.05
(1,143)	1:89:A:TYR:HD2	1:86:A:PRO:HB2	3	1.05
(1,143)	1:89:A:TYR:HD2	1:86:A:PRO:HB2	11	1.05
(1,143)	1:89:A:TYR:HD2	1:86:A:PRO:HB2	18	1.05
(1,120)	1:95:A:ALA:HB3	1:100:A:LEU:H	21	1.05
(1,91)	1:109:A:LEU:HD13	1:64:A:GLU:H	22	1.05
(1,86)	1:98:A:LEU:HD11	1:99:A:PHE:H	1	1.05
(1,86)	1:98:A:LEU:HD11	1:99:A:PHE:H	11	1.05
(1,59)	1:123:A:LEU:HA	1:123:A:LEU:HD21	6	1.05
(1,59)	1:123:A:LEU:HA	1:123:A:LEU:HD23	7	1.05
(1,59)	1:123:A:LEU:HA	1:123:A:LEU:HD21	13	1.05
(1,59)	1:123:A:LEU:HA	1:123:A:LEU:HD23	14	1.05
(1,59)	1:123:A:LEU:HA	1:123:A:LEU:HD21	20	1.05
(1,59)	1:123:A:LEU:HA	1:123:A:LEU:HD21	22	1.05
(1,1722)	2:31:B:LEU:HD22	1:128:A:ASN:HB2	25	1.04
(1,1375)	1:74:A:CYS:HA	1:77:A:GLN:HB3	2	1.04
(1,443)	1:117:A:ARG:H	1:126:A:TYR:HE2	6	1.04
(1,400)	1:136:A:ALA:HB3	1:135:A:LYS:H	21	1.04
(1,395)	1:138:A:SER:H	1:139:A:ALA:HB3	6	1.04
(1,379)	2:31:B:LEU:HB2	2:28:B:ASP:HB2	12	1.04
(1,369)	2:26:B:ASP:HB2	2:33:B:GLN:HE21	16	1.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,355)	2:29:B:SER:HB3	2:31:B:LEU:H	9	1.04
(1,355)	2:29:B:SER:HB3	2:31:B:LEU:H	23	1.04
(1,355)	2:29:B:SER:HB3	2:31:B:LEU:H	24	1.04
(1,341)	2:31:B:LEU:HD11	1:84:A:VAL:H	8	1.04
(1,341)	2:31:B:LEU:HD12	1:84:A:VAL:H	9	1.04
(1,307)	2:39:B:TRP:HE3	2:36:B:THR:HG22	5	1.04
(1,282)	2:31:B:LEU:HD12	1:124:A:TYR:HA	17	1.04
(1,280)	2:31:B:LEU:HG	1:87:A:PHE:HE2	5	1.04
(1,280)	2:31:B:LEU:HG	1:87:A:PHE:HE2	20	1.04
(1,184)	1:79:A:ALA:HB1	1:75:A:LYS:HA	19	1.04
(1,150)	1:88:A:LEU:HD23	1:128:A:ASN:H	16	1.04
(1,149)	1:88:A:LEU:HD22	1:89:A:TYR:H	8	1.04
(1,149)	1:88:A:LEU:HD23	1:89:A:TYR:H	12	1.04
(1,149)	1:88:A:LEU:HD23	1:89:A:TYR:H	17	1.04
(1,149)	1:88:A:LEU:HD21	1:89:A:TYR:H	24	1.04
(1,120)	1:95:A:ALA:HB1	1:100:A:LEU:H	2	1.04
(1,120)	1:95:A:ALA:HB1	1:93:A:GLN:H	11	1.04
(1,120)	1:95:A:ALA:HB2	1:100:A:LEU:H	13	1.04
(1,91)	1:109:A:LEU:HD11	1:64:A:GLU:H	24	1.04
(1,86)	1:113:A:LEU:HD13	1:73:A:LEU:H	5	1.04
(1,86)	1:98:A:LEU:HD11	1:99:A:PHE:H	15	1.04
(1,86)	1:113:A:LEU:HD12	1:73:A:LEU:H	17	1.04
(1,59)	1:123:A:LEU:HA	1:123:A:LEU:HD22	2	1.04
(1,59)	1:123:A:LEU:HA	1:123:A:LEU:HD21	21	1.04
(1,23)	1:130:A:LEU:HD23	1:130:A:LEU:H	9	1.04
(1,23)	1:130:A:LEU:HD22	1:130:A:LEU:H	12	1.04
(1,23)	1:130:A:LEU:HD23	1:130:A:LEU:H	21	1.04
(1,9)	1:134:A:LEU:HD22	1:131:A:CYS:HA	12	1.04
(1,4)	1:130:A:LEU:HD23	1:127:A:ILE:HA	25	1.04
(1,1976)	1:100:A:LEU:H	1:138:A:SER:HB2	14	1.03
(1,1771)	1:142:A:LYS:H	1:142:A:LYS:HD2	10	1.03
(1,1656)	2:37:B:ALA:HB3	2:39:B:TRP:HZ2	5	1.03
(1,1656)	2:37:B:ALA:HB2	2:39:B:TRP:HZ2	14	1.03
(1,879)	1:94:A:ARG:HD2	1:90:A:ASN:HD22	8	1.03
(1,450)	1:114:A:SER:H	1:117:A:ARG:HD3	18	1.03
(1,443)	2:36:B:THR:H	2:34:B:TYR:HD1	15	1.03
(1,400)	1:136:A:ALA:HB1	1:135:A:LYS:H	2	1.03
(1,400)	1:136:A:ALA:HB1	1:135:A:LYS:H	5	1.03
(1,400)	1:136:A:ALA:HB2	1:135:A:LYS:H	6	1.03
(1,355)	2:29:B:SER:HB3	2:31:B:LEU:H	3	1.03
(1,355)	2:29:B:SER:HB3	2:31:B:LEU:H	7	1.03
(1,355)	2:29:B:SER:HB3	2:31:B:LEU:H	18	1.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,341)	2:31:B:LEU:HD12	1:84:A:VAL:H	5	1.03
(1,341)	2:31:B:LEU:HD13	1:84:A:VAL:H	18	1.03
(1,307)	2:39:B:TRP:HE3	2:36:B:THR:HG22	7	1.03
(1,306)	2:36:B:THR:HG23	1:124:A:TYR:HE2	11	1.03
(1,306)	2:36:B:THR:HG22	1:124:A:TYR:HE2	20	1.03
(1,306)	2:36:B:THR:HG22	1:124:A:TYR:HE2	21	1.03
(1,282)	2:31:B:LEU:HD11	1:124:A:TYR:HA	8	1.03
(1,280)	2:31:B:LEU:HG	1:87:A:PHE:HE2	15	1.03
(1,184)	1:79:A:ALA:HB1	1:75:A:LYS:HA	5	1.03
(1,184)	1:79:A:ALA:HB3	1:75:A:LYS:HA	16	1.03
(1,149)	1:88:A:LEU:HD21	1:89:A:TYR:H	20	1.03
(1,149)	1:88:A:LEU:HD23	1:89:A:TYR:H	23	1.03
(1,143)	1:89:A:TYR:HD2	1:86:A:PRO:HB2	1	1.03
(1,143)	1:89:A:TYR:HD2	1:86:A:PRO:HB2	7	1.03
(1,120)	1:95:A:ALA:HB3	1:100:A:LEU:H	17	1.03
(1,91)	1:109:A:LEU:HD12	1:64:A:GLU:H	3	1.03
(1,91)	1:109:A:LEU:HD12	1:64:A:GLU:H	15	1.03
(1,91)	1:109:A:LEU:HD12	1:64:A:GLU:H	18	1.03
(1,86)	1:113:A:LEU:HD12	1:73:A:LEU:H	4	1.03
(1,59)	1:123:A:LEU:HA	1:123:A:LEU:HD21	18	1.03
(1,40)	1:127:A:ILE:HD12	1:74:A:CYS:HA	12	1.03
(1,23)	1:130:A:LEU:HD22	1:130:A:LEU:H	18	1.03
(1,4)	1:130:A:LEU:HD21	1:127:A:ILE:HA	7	1.03
(1,4)	1:130:A:LEU:HD23	1:127:A:ILE:HA	11	1.03
(1,2119)	1:122:A:LYS:HB3	1:122:A:LYS:H	21	1.02
(1,1649)	2:37:B:ALA:HB3	2:38:B:ARG:HB2	15	1.02
(1,1456)	1:69:A:GLU:HG2	1:66:A:LEU:HA	5	1.02
(1,1341)	1:76:A:MET:HB3	1:73:A:LEU:HA	17	1.02
(1,1196)	1:89:A:TYR:HD1	1:71:A:LEU:HD13	4	1.02
(1,1075)	1:101:A:ALA:HB2	1:60:A:LYS:HB2	17	1.02
(1,879)	1:94:A:ARG:HD2	1:90:A:ASN:HD22	5	1.02
(1,710)	1:130:A:LEU:HD22	1:109:A:LEU:HD11	5	1.02
(1,443)	2:36:B:THR:H	2:34:B:TYR:HD1	14	1.02
(1,400)	1:136:A:ALA:HB2	1:135:A:LYS:H	10	1.02
(1,400)	1:136:A:ALA:HB1	1:135:A:LYS:H	11	1.02
(1,400)	1:136:A:ALA:HB1	1:135:A:LYS:H	14	1.02
(1,400)	1:136:A:ALA:HB3	1:135:A:LYS:H	25	1.02
(1,379)	2:31:B:LEU:HB2	2:28:B:ASP:HB2	9	1.02
(1,368)	2:26:B:ASP:HB3	1:87:A:PHE:HZ	4	1.02
(1,355)	2:29:B:SER:HB3	2:31:B:LEU:H	11	1.02
(1,341)	2:31:B:LEU:HD12	1:84:A:VAL:H	2	1.02
(1,341)	2:31:B:LEU:HD11	1:84:A:VAL:H	4	1.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,300)	2:37:B:ALA:HB1	1:123:A:LEU:HB2	4	1.02
(1,282)	2:31:B:LEU:HD13	1:124:A:TYR:HA	11	1.02
(1,282)	2:31:B:LEU:HD12	1:124:A:TYR:HA	14	1.02
(1,143)	1:89:A:TYR:HD2	1:86:A:PRO:HB2	24	1.02
(1,143)	1:89:A:TYR:HD2	1:86:A:PRO:HB2	25	1.02
(1,91)	1:109:A:LEU:HD13	1:64:A:GLU:H	11	1.02
(1,63)	1:123:A:LEU:HD22	1:124:A:TYR:HA	2	1.02
(1,46)	1:126:A:TYR:HE1	1:122:A:LYS:HB3	18	1.02
(1,9)	1:134:A:LEU:HD23	1:131:A:CYS:HA	23	1.02
(1,1656)	2:37:B:ALA:HB3	2:39:B:TRP:HZ2	23	1.01
(1,1651)	2:38:B:ARG:HG2	2:37:B:ALA:HB1	6	1.01
(1,1651)	2:38:B:ARG:HG2	2:37:B:ALA:HB1	9	1.01
(1,1651)	2:38:B:ARG:HG2	2:37:B:ALA:HB1	10	1.01
(1,1649)	2:37:B:ALA:HB1	2:38:B:ARG:HB2	9	1.01
(1,1649)	2:37:B:ALA:HB1	2:38:B:ARG:HB2	10	1.01
(1,1635)	2:39:B:TRP:HA	2:38:B:ARG:HD2	11	1.01
(1,1498)	1:129:A:GLU:HB3	1:130:A:LEU:H	13	1.01
(1,443)	2:36:B:THR:H	2:34:B:TYR:HD1	17	1.01
(1,443)	2:36:B:THR:H	2:34:B:TYR:HD1	21	1.01
(1,400)	1:136:A:ALA:HB1	1:135:A:LYS:H	12	1.01
(1,400)	1:136:A:ALA:HB3	1:135:A:LYS:H	16	1.01
(1,355)	2:29:B:SER:HB3	2:31:B:LEU:H	10	1.01
(1,355)	2:29:B:SER:HB3	2:33:B:GLN:H	14	1.01
(1,184)	1:79:A:ALA:HB1	1:75:A:LYS:HA	10	1.01
(1,174)	1:84:A:VAL:HG13	1:124:A:TYR:HA	7	1.01
(1,174)	1:84:A:VAL:HG13	1:124:A:TYR:HA	9	1.01
(1,149)	1:88:A:LEU:HD22	1:89:A:TYR:H	22	1.01
(1,120)	1:95:A:ALA:HB1	1:93:A:GLN:H	24	1.01
(1,91)	1:109:A:LEU:HD12	1:64:A:GLU:H	4	1.01
(1,91)	1:109:A:LEU:HD11	1:64:A:GLU:H	16	1.01
(1,86)	1:98:A:LEU:HD13	1:99:A:PHE:H	7	1.01
(1,59)	1:123:A:LEU:HA	1:123:A:LEU:HD23	1	1.01
(1,59)	1:123:A:LEU:HA	1:73:A:LEU:HD21	3	1.01
(1,59)	1:123:A:LEU:HA	1:123:A:LEU:HD22	23	1.01
(1,23)	1:130:A:LEU:HD21	1:130:A:LEU:H	25	1.01
(1,16)	1:132:A:THR:HG21	1:133:A:VAL:H	2	1.01
(1,4)	1:130:A:LEU:HD22	1:127:A:ILE:HA	4	1.01
(1,4)	1:130:A:LEU:HD21	1:127:A:ILE:HA	18	1.01
(1,2119)	1:122:A:LYS:HB3	1:122:A:LYS:H	14	1.0
(1,1766)	2:24:B:GLN:HG2	2:23:B:SER:HA	24	1.0
(1,1649)	2:37:B:ALA:HB3	2:38:B:ARG:HB2	16	1.0
(1,1375)	1:74:A:CYS:HA	1:77:A:GLN:HB3	21	1.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1075)	1:101:A:ALA:HB3	1:60:A:LYS:HB2	20	1.0
(1,1049)	1:108:A:ILE:HD12	1:104:A:GLU:HG2	3	1.0
(1,401)	1:113:A:LEU:HD22	1:113:A:LEU:H	12	1.0
(1,400)	1:136:A:ALA:HB3	1:135:A:LYS:H	23	1.0
(1,368)	2:26:B:ASP:HB3	1:87:A:PHE:HZ	22	1.0
(1,306)	2:36:B:THR:HG23	1:124:A:TYR:HE2	17	1.0
(1,300)	2:37:B:ALA:HB3	1:123:A:LEU:HB2	17	1.0
(1,282)	2:31:B:LEU:HD23	1:131:A:CYS:HA	3	1.0
(1,282)	2:31:B:LEU:HD13	1:124:A:TYR:HA	18	1.0
(1,282)	2:31:B:LEU:HD13	1:124:A:TYR:HA	19	1.0
(1,282)	2:31:B:LEU:HD12	1:124:A:TYR:HA	24	1.0
(1,149)	1:88:A:LEU:HD23	1:89:A:TYR:H	5	1.0
(1,128)	1:93:A:GLN:HG2	1:94:A:ARG:H	25	1.0
(1,120)	1:95:A:ALA:HB1	1:93:A:GLN:H	4	1.0
(1,91)	1:109:A:LEU:HD11	1:64:A:GLU:H	8	1.0
(1,91)	1:109:A:LEU:HD13	1:64:A:GLU:H	23	1.0
(1,59)	1:123:A:LEU:HA	1:123:A:LEU:HD22	4	1.0
(1,59)	1:123:A:LEU:HA	1:123:A:LEU:HD21	10	1.0
(1,59)	1:123:A:LEU:HA	1:123:A:LEU:HD23	11	1.0
(1,59)	1:123:A:LEU:HA	1:123:A:LEU:HD22	16	1.0
(1,46)	1:126:A:TYR:HE1	1:122:A:LYS:HB3	9	1.0
(1,40)	1:127:A:ILE:HD11	1:74:A:CYS:HA	19	1.0
(1,23)	1:130:A:LEU:HD21	1:113:A:LEU:H	1	1.0
(1,23)	1:130:A:LEU:HD22	1:130:A:LEU:H	17	1.0
(1,16)	1:132:A:THR:HG21	1:133:A:VAL:H	20	1.0
(1,16)	1:132:A:THR:HG22	1:133:A:VAL:H	21	1.0
(1,15)	1:132:A:THR:HG23	1:135:A:LYS:H	18	1.0
(1,4)	1:130:A:LEU:HD22	1:127:A:ILE:HA	22	1.0
(1,1722)	2:31:B:LEU:HD23	1:128:A:ASN:HB2	4	0.99
(1,1651)	2:38:B:ARG:HG2	2:37:B:ALA:HB2	18	0.99
(1,1649)	2:37:B:ALA:HB1	2:38:B:ARG:HB2	2	0.99
(1,1649)	2:37:B:ALA:HB1	2:38:B:ARG:HB2	11	0.99
(1,619)	1:135:A:LYS:HG2	1:91:A:ARG:HD3	5	0.99
(1,619)	1:135:A:LYS:HG2	1:91:A:ARG:HD3	24	0.99
(1,400)	1:136:A:ALA:HB2	1:135:A:LYS:H	4	0.99
(1,400)	1:136:A:ALA:HB3	1:135:A:LYS:H	9	0.99
(1,400)	1:136:A:ALA:HB2	1:135:A:LYS:H	13	0.99
(1,369)	2:26:B:ASP:HB2	2:33:B:GLN:HE21	14	0.99
(1,282)	2:31:B:LEU:HD12	1:124:A:TYR:HA	7	0.99
(1,282)	2:31:B:LEU:HD13	1:124:A:TYR:HA	23	0.99
(1,282)	2:31:B:LEU:HD12	1:124:A:TYR:HA	25	0.99
(1,280)	2:31:B:LEU:HG	1:87:A:PHE:HE2	16	0.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,150)	1:88:A:LEU:HD23	1:128:A:ASN:H	6	0.99
(1,149)	1:88:A:LEU:HD23	1:89:A:TYR:H	1	0.99
(1,149)	1:88:A:LEU:HD22	1:89:A:TYR:H	2	0.99
(1,149)	1:88:A:LEU:HD21	1:89:A:TYR:H	6	0.99
(1,143)	1:89:A:TYR:HD2	1:86:A:PRO:HB2	19	0.99
(1,120)	1:95:A:ALA:HB3	1:93:A:GLN:H	7	0.99
(1,120)	1:95:A:ALA:HB2	1:100:A:LEU:H	20	0.99
(1,91)	1:109:A:LEU:HD11	1:64:A:GLU:H	1	0.99
(1,40)	1:127:A:ILE:HD11	1:74:A:CYS:HA	10	0.99
(1,40)	1:127:A:ILE:HD13	1:74:A:CYS:HA	16	0.99
(1,16)	1:132:A:THR:HG23	1:133:A:VAL:H	11	0.99
(1,4)	1:130:A:LEU:HD22	1:127:A:ILE:HA	14	0.99
(1,4)	1:130:A:LEU:HD22	1:127:A:ILE:HA	23	0.99
(1,2061)	1:87:A:PHE:H	1:85:A:VAL:HG22	20	0.98
(1,2061)	1:87:A:PHE:H	1:85:A:VAL:HG21	22	0.98
(1,1976)	1:100:A:LEU:H	1:138:A:SER:HB2	12	0.98
(1,1801)	1:135:A:LYS:H	1:91:A:ARG:HD3	17	0.98
(1,1771)	1:142:A:LYS:H	1:142:A:LYS:HD2	4	0.98
(1,1656)	2:37:B:ALA:HB2	2:39:B:TRP:HZ2	19	0.98
(1,1650)	2:37:B:ALA:HB2	1:121:A:ALA:HB3	22	0.98
(1,1649)	2:37:B:ALA:HB2	2:38:B:ARG:HB2	1	0.98
(1,1635)	2:39:B:TRP:HA	2:38:B:ARG:HD2	15	0.98
(1,1375)	1:74:A:CYS:HA	1:77:A:GLN:HB3	3	0.98
(1,1196)	1:89:A:TYR:HD1	1:71:A:LEU:HD11	17	0.98
(1,1075)	1:101:A:ALA:HB2	1:60:A:LYS:HB2	8	0.98
(1,907)	1:114:A:SER:HB2	1:115:A:ARG:H	2	0.98
(1,619)	1:135:A:LYS:HG2	1:91:A:ARG:HD3	9	0.98
(1,503)	1:81:A:HIS:H	1:84:A:VAL:HG21	12	0.98
(1,443)	2:36:B:THR:H	2:34:B:TYR:HD1	18	0.98
(1,400)	1:136:A:ALA:HB3	1:135:A:LYS:H	17	0.98
(1,400)	1:136:A:ALA:HB3	1:135:A:LYS:H	18	0.98
(1,400)	1:136:A:ALA:HB1	1:135:A:LYS:H	22	0.98
(1,300)	2:37:B:ALA:HB3	1:123:A:LEU:HB2	6	0.98
(1,216)	1:113:A:LEU:HD11	1:70:A:PHE:HD2	1	0.98
(1,207)	1:109:A:LEU:HD22	1:113:A:LEU:H	19	0.98
(1,174)	1:84:A:VAL:HG11	1:124:A:TYR:HA	4	0.98
(1,174)	1:84:A:VAL:HG12	1:124:A:TYR:HA	15	0.98
(1,174)	1:84:A:VAL:HG13	1:124:A:TYR:HA	23	0.98
(1,164)	1:87:A:PHE:HB3	1:87:A:PHE:HE2	3	0.98
(1,120)	1:95:A:ALA:HB1	1:93:A:GLN:H	3	0.98
(1,120)	1:95:A:ALA:HB3	1:100:A:LEU:H	5	0.98
(1,91)	1:109:A:LEU:HD13	1:64:A:GLU:H	14	0.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,59)	1:123:A:LEU:HA	1:123:A:LEU:HD22	5	0.98
(1,59)	1:123:A:LEU:HA	1:123:A:LEU:HD21	19	0.98
(1,59)	1:123:A:LEU:HA	1:123:A:LEU:HD22	24	0.98
(1,40)	1:127:A:ILE:HD11	1:74:A:CYS:HA	2	0.98
(1,23)	1:130:A:LEU:HD23	1:130:A:LEU:H	4	0.98
(1,23)	1:130:A:LEU:HD21	1:130:A:LEU:H	10	0.98
(1,23)	1:130:A:LEU:HD23	1:130:A:LEU:H	19	0.98
(1,23)	1:130:A:LEU:HD23	1:113:A:LEU:H	24	0.98
(1,16)	1:132:A:THR:HG22	1:133:A:VAL:H	3	0.98
(1,16)	1:132:A:THR:HG22	1:133:A:VAL:H	16	0.98
(1,9)	1:134:A:LEU:HD21	1:131:A:CYS:HA	1	0.98
(1,9)	1:134:A:LEU:HD21	1:131:A:CYS:HA	18	0.98
(1,9)	1:134:A:LEU:HD22	1:131:A:CYS:HA	22	0.98
(1,2195)	1:56:A:LYS:H	1:56:A:LYS:HG2	10	0.97
(1,2119)	1:122:A:LYS:HB3	1:122:A:LYS:H	7	0.97
(1,2119)	1:122:A:LYS:HB3	1:122:A:LYS:H	22	0.97
(1,2061)	1:87:A:PHE:H	1:85:A:VAL:HG21	8	0.97
(1,1722)	2:31:B:LEU:HD23	1:128:A:ASN:HB2	15	0.97
(1,1651)	2:38:B:ARG:HG2	2:37:B:ALA:HB1	16	0.97
(1,1651)	2:38:B:ARG:HG2	2:37:B:ALA:HB2	22	0.97
(1,1649)	2:37:B:ALA:HB3	2:38:B:ARG:HB2	7	0.97
(1,1635)	2:39:B:TRP:HA	2:38:B:ARG:HD2	21	0.97
(1,1311)	1:82:A:PRO:HD2	1:82:A:PRO:HB3	2	0.97
(1,1311)	1:82:A:PRO:HD2	1:82:A:PRO:HB3	4	0.97
(1,1311)	1:82:A:PRO:HD2	1:82:A:PRO:HB3	5	0.97
(1,1311)	1:82:A:PRO:HD2	1:82:A:PRO:HB3	6	0.97
(1,1311)	1:82:A:PRO:HD2	1:82:A:PRO:HB3	8	0.97
(1,1311)	1:82:A:PRO:HD2	1:82:A:PRO:HB3	10	0.97
(1,1311)	1:82:A:PRO:HD2	1:82:A:PRO:HB3	12	0.97
(1,1311)	1:82:A:PRO:HD2	1:82:A:PRO:HB3	13	0.97
(1,1311)	1:82:A:PRO:HD2	1:82:A:PRO:HB3	15	0.97
(1,1311)	1:82:A:PRO:HD2	1:82:A:PRO:HB3	16	0.97
(1,1311)	1:82:A:PRO:HD2	1:82:A:PRO:HB3	19	0.97
(1,1311)	1:82:A:PRO:HD2	1:82:A:PRO:HB3	23	0.97
(1,1311)	1:82:A:PRO:HD2	1:82:A:PRO:HB3	25	0.97
(1,1196)	1:89:A:TYR:HD1	1:71:A:LEU:HD13	20	0.97
(1,946)	1:110:A:SER:HB2	1:66:A:LEU:HD11	15	0.97
(1,503)	1:78:A:THR:HG22	1:81:A:HIS:H	13	0.97
(1,503)	1:78:A:THR:HG23	1:81:A:HIS:H	20	0.97
(1,443)	2:36:B:THR:H	2:34:B:TYR:HD1	3	0.97
(1,443)	1:117:A:ARG:H	1:126:A:TYR:HE2	7	0.97
(1,400)	1:136:A:ALA:HB3	1:135:A:LYS:H	3	0.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,400)	1:136:A:ALA:HB1	1:135:A:LYS:H	8	0.97
(1,306)	2:36:B:THR:HG22	1:124:A:TYR:HE2	1	0.97
(1,282)	2:31:B:LEU:HD12	1:124:A:TYR:HA	22	0.97
(1,243)	1:62:A:GLU:HG3	1:61:A:LEU:HD23	25	0.97
(1,205)	1:71:A:LEU:HD11	1:75:A:LYS:HE2	4	0.97
(1,184)	1:79:A:ALA:HB2	1:75:A:LYS:HA	17	0.97
(1,174)	1:84:A:VAL:HG13	1:124:A:TYR:HA	10	0.97
(1,174)	1:84:A:VAL:HG11	1:124:A:TYR:HA	25	0.97
(1,150)	1:88:A:LEU:HD22	1:128:A:ASN:H	19	0.97
(1,149)	1:88:A:LEU:HD21	1:89:A:TYR:H	21	0.97
(1,141)	1:89:A:TYR:HD2	1:86:A:PRO:HB2	10	0.97
(1,128)	1:93:A:GLN:HG2	1:94:A:ARG:H	8	0.97
(1,120)	1:95:A:ALA:HB3	1:93:A:GLN:H	22	0.97
(1,59)	1:123:A:LEU:HA	1:123:A:LEU:HD22	25	0.97
(1,9)	1:134:A:LEU:HD21	1:131:A:CYS:HA	8	0.97
(1,4)	1:130:A:LEU:HD22	1:127:A:ILE:HA	21	0.97
(1,2195)	1:56:A:LYS:H	1:56:A:LYS:HG2	13	0.96
(1,2189)	1:59:A:TYR:H	1:60:A:LYS:HB2	8	0.96
(1,2119)	1:122:A:LYS:HB3	1:122:A:LYS:H	2	0.96
(1,2119)	1:122:A:LYS:HB3	1:122:A:LYS:H	6	0.96
(1,1983)	1:99:A:PHE:H	1:138:A:SER:HB2	8	0.96
(1,1651)	2:38:B:ARG:HG2	2:37:B:ALA:HB3	3	0.96
(1,1651)	2:38:B:ARG:HG2	2:37:B:ALA:HB2	8	0.96
(1,1651)	2:38:B:ARG:HG2	2:37:B:ALA:HB2	13	0.96
(1,1651)	2:38:B:ARG:HG2	2:37:B:ALA:HB3	20	0.96
(1,1651)	2:38:B:ARG:HG2	2:37:B:ALA:HB2	23	0.96
(1,1553)	1:59:A:TYR:HD1	1:57:A:LYS:HB2	15	0.96
(1,1518)	1:61:A:LEU:HB2	1:61:A:LEU:HD22	9	0.96
(1,1375)	1:74:A:CYS:HA	1:77:A:GLN:HB3	14	0.96
(1,1333)	1:77:A:GLN:HG2	1:73:A:LEU:HG	1	0.96
(1,1333)	1:77:A:GLN:HG2	1:73:A:LEU:HG	19	0.96
(1,1311)	1:82:A:PRO:HD2	1:82:A:PRO:HB3	1	0.96
(1,1311)	1:82:A:PRO:HD2	1:82:A:PRO:HB3	3	0.96
(1,1311)	1:82:A:PRO:HD2	1:82:A:PRO:HB3	7	0.96
(1,1311)	1:82:A:PRO:HD2	1:82:A:PRO:HB3	9	0.96
(1,1311)	1:82:A:PRO:HD2	1:82:A:PRO:HB3	14	0.96
(1,1311)	1:82:A:PRO:HD2	1:82:A:PRO:HB3	17	0.96
(1,1311)	1:82:A:PRO:HD2	1:82:A:PRO:HB3	18	0.96
(1,1311)	1:82:A:PRO:HD2	1:82:A:PRO:HB3	20	0.96
(1,1311)	1:82:A:PRO:HD2	1:82:A:PRO:HB3	21	0.96
(1,1311)	1:82:A:PRO:HD2	1:82:A:PRO:HB3	22	0.96
(1,1311)	1:82:A:PRO:HD2	1:82:A:PRO:HB3	24	0.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1137)	1:95:A:ALA:HB2	1:91:A:ARG:HD3	3	0.96
(1,1098)	1:100:A:LEU:HD23	1:92:A:GLN:HA	6	0.96
(1,1046)	2:30:B:GLU:HG3	2:30:B:GLU:H	5	0.96
(1,946)	1:110:A:SER:HB2	1:66:A:LEU:HD11	11	0.96
(1,710)	1:130:A:LEU:HD22	1:109:A:LEU:HD13	10	0.96
(1,570)	1:143:A:LEU:HB2	1:144:A:ASN:HD21	17	0.96
(1,484)	1:134:A:LEU:HD11	1:94:A:ARG:H	15	0.96
(1,401)	1:113:A:LEU:HD23	1:113:A:LEU:H	16	0.96
(1,400)	1:136:A:ALA:HB3	1:135:A:LYS:H	19	0.96
(1,307)	2:36:B:THR:HG23	1:128:A:ASN:HD21	13	0.96
(1,300)	2:37:B:ALA:HB3	1:123:A:LEU:HB2	25	0.96
(1,218)	1:116:A:ALA:HB3	1:70:A:PHE:HD2	12	0.96
(1,208)	1:71:A:LEU:HD23	1:88:A:LEU:H	5	0.96
(1,208)	1:71:A:LEU:HD22	1:88:A:LEU:H	21	0.96
(1,208)	1:71:A:LEU:HD21	1:88:A:LEU:H	23	0.96
(1,164)	1:87:A:PHE:HB3	1:87:A:PHE:HE2	4	0.96
(1,120)	1:95:A:ALA:HB1	1:93:A:GLN:H	19	0.96
(1,86)	1:113:A:LEU:HD11	1:73:A:LEU:H	12	0.96
(1,40)	1:127:A:ILE:HD11	1:74:A:CYS:HA	1	0.96
(1,40)	1:127:A:ILE:HD12	1:74:A:CYS:HA	8	0.96
(1,23)	1:130:A:LEU:HD21	1:130:A:LEU:H	5	0.96
(1,23)	1:130:A:LEU:HD22	1:130:A:LEU:H	15	0.96
(1,16)	1:132:A:THR:HG22	1:133:A:VAL:H	17	0.96
(1,15)	1:132:A:THR:HG23	1:135:A:LYS:H	8	0.96
(1,15)	1:132:A:THR:HG22	1:135:A:LYS:H	24	0.96
(1,9)	1:134:A:LEU:HD22	1:131:A:CYS:HA	15	0.96
(1,2195)	1:56:A:LYS:H	1:56:A:LYS:HG2	16	0.95
(1,2119)	1:122:A:LYS:HB3	1:122:A:LYS:H	3	0.95
(1,2119)	1:122:A:LYS:HB3	1:122:A:LYS:H	10	0.95
(1,2119)	1:122:A:LYS:HB3	1:122:A:LYS:H	13	0.95
(1,1651)	2:38:B:ARG:HG2	2:37:B:ALA:HB2	4	0.95
(1,1651)	2:38:B:ARG:HG2	2:37:B:ALA:HB3	21	0.95
(1,1649)	2:37:B:ALA:HB3	2:38:B:ARG:HB2	24	0.95
(1,1611)	2:39:B:TRP:HZ3	2:39:B:TRP:HB2	11	0.95
(1,1311)	1:82:A:PRO:HD2	1:82:A:PRO:HB3	11	0.95
(1,1046)	2:30:B:GLU:HG3	2:30:B:GLU:H	4	0.95
(1,534)	1:121:A:ALA:H	1:119:A:ARG:HG3	19	0.95
(1,503)	1:81:A:HIS:H	1:84:A:VAL:HG21	24	0.95
(1,443)	1:117:A:ARG:H	1:126:A:TYR:HE2	11	0.95
(1,401)	1:113:A:LEU:HD23	1:113:A:LEU:H	22	0.95
(1,400)	1:136:A:ALA:HB2	1:135:A:LYS:H	7	0.95
(1,400)	1:136:A:ALA:HB1	1:135:A:LYS:H	24	0.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,355)	2:29:B:SER:HB3	2:31:B:LEU:H	25	0.95
(1,306)	2:36:B:THR:HG21	1:124:A:TYR:HE2	14	0.95
(1,306)	2:36:B:THR:HG21	1:124:A:TYR:HE2	22	0.95
(1,282)	2:31:B:LEU:HD12	1:124:A:TYR:HA	2	0.95
(1,282)	2:31:B:LEU:HD11	1:124:A:TYR:HA	4	0.95
(1,208)	1:71:A:LEU:HD23	1:88:A:LEU:H	19	0.95
(1,184)	1:79:A:ALA:HB2	1:75:A:LYS:HA	4	0.95
(1,174)	1:84:A:VAL:HG11	1:124:A:TYR:HA	5	0.95
(1,174)	1:84:A:VAL:HG13	1:124:A:TYR:HA	19	0.95
(1,164)	1:87:A:PHE:HB3	1:87:A:PHE:HE2	12	0.95
(1,150)	1:88:A:LEU:HD22	1:128:A:ASN:H	5	0.95
(1,150)	1:88:A:LEU:HD23	1:128:A:ASN:H	24	0.95
(1,120)	1:95:A:ALA:HB3	1:100:A:LEU:H	9	0.95
(1,86)	1:98:A:LEU:HD11	1:99:A:PHE:H	13	0.95
(1,9)	1:134:A:LEU:HD21	1:131:A:CYS:HA	14	0.95
(1,4)	1:130:A:LEU:HD21	1:127:A:ILE:HA	17	0.95
(1,2119)	1:122:A:LYS:HB3	1:122:A:LYS:H	1	0.94
(1,2119)	1:122:A:LYS:HB3	1:122:A:LYS:H	8	0.94
(1,2119)	1:122:A:LYS:HB3	1:122:A:LYS:H	12	0.94
(1,2119)	1:122:A:LYS:HB3	1:122:A:LYS:H	15	0.94
(1,2119)	1:122:A:LYS:HB3	1:122:A:LYS:H	23	0.94
(1,2061)	1:87:A:PHE:H	1:85:A:VAL:HG23	17	0.94
(1,2061)	1:87:A:PHE:H	1:85:A:VAL:HG21	25	0.94
(1,1651)	2:38:B:ARG:HG2	2:37:B:ALA:HB3	7	0.94
(1,1518)	1:61:A:LEU:HB2	1:61:A:LEU:HD23	21	0.94
(1,1194)	1:89:A:TYR:HB2	1:89:A:TYR:HD1	1	0.94
(1,1194)	1:89:A:TYR:HB2	1:89:A:TYR:HD1	2	0.94
(1,1194)	1:89:A:TYR:HB2	1:89:A:TYR:HD1	4	0.94
(1,1194)	1:89:A:TYR:HB2	1:89:A:TYR:HD1	5	0.94
(1,1194)	1:89:A:TYR:HB2	1:89:A:TYR:HD1	7	0.94
(1,1194)	1:89:A:TYR:HB2	1:89:A:TYR:HD1	9	0.94
(1,1194)	1:89:A:TYR:HB2	1:89:A:TYR:HD1	10	0.94
(1,1194)	1:89:A:TYR:HB2	1:89:A:TYR:HD1	12	0.94
(1,1194)	1:89:A:TYR:HB2	1:89:A:TYR:HD1	13	0.94
(1,1194)	1:89:A:TYR:HB2	1:89:A:TYR:HD1	15	0.94
(1,1194)	1:89:A:TYR:HB2	1:89:A:TYR:HD1	18	0.94
(1,1194)	1:89:A:TYR:HB2	1:89:A:TYR:HD1	22	0.94
(1,1194)	1:89:A:TYR:HB2	1:89:A:TYR:HD1	23	0.94
(1,1194)	1:89:A:TYR:HB2	1:89:A:TYR:HD1	24	0.94
(1,1046)	2:30:B:GLU:HG3	2:30:B:GLU:H	8	0.94
(1,1046)	2:30:B:GLU:HG3	2:30:B:GLU:H	18	0.94
(1,1046)	2:30:B:GLU:HG3	2:30:B:GLU:H	24	0.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,907)	1:114:A:SER:HB2	1:115:A:ARG:H	19	0.94
(1,671)	1:133:A:VAL:HG22	1:99:A:PHE:HZ	15	0.94
(1,450)	1:114:A:SER:H	1:117:A:ARG:HD3	24	0.94
(1,443)	1:117:A:ARG:H	1:126:A:TYR:HE2	8	0.94
(1,443)	1:117:A:ARG:H	1:126:A:TYR:HE2	12	0.94
(1,401)	1:113:A:LEU:HD21	1:113:A:LEU:H	4	0.94
(1,401)	1:113:A:LEU:HD21	1:113:A:LEU:H	10	0.94
(1,306)	2:36:B:THR:HG22	1:124:A:TYR:HE1	4	0.94
(1,306)	2:36:B:THR:HG23	1:124:A:TYR:HE2	7	0.94
(1,304)	2:36:B:THR:HG21	2:35:B:PHE:HB2	14	0.94
(1,300)	2:37:B:ALA:HB3	1:123:A:LEU:HB2	18	0.94
(1,300)	2:37:B:ALA:HB2	1:123:A:LEU:HB2	20	0.94
(1,282)	2:31:B:LEU:HD12	1:124:A:TYR:HA	5	0.94
(1,218)	1:116:A:ALA:HB2	1:70:A:PHE:HD2	6	0.94
(1,208)	1:71:A:LEU:HD22	1:88:A:LEU:H	13	0.94
(1,164)	1:87:A:PHE:HB3	1:87:A:PHE:HE2	5	0.94
(1,164)	1:87:A:PHE:HB3	1:87:A:PHE:HE2	17	0.94
(1,164)	1:87:A:PHE:HB3	1:87:A:PHE:HE2	18	0.94
(1,164)	1:87:A:PHE:HB3	1:87:A:PHE:HE2	20	0.94
(1,164)	1:87:A:PHE:HB3	1:87:A:PHE:HE2	22	0.94
(1,149)	1:88:A:LEU:HD21	1:89:A:TYR:H	9	0.94
(1,149)	1:88:A:LEU:HD22	1:89:A:TYR:H	11	0.94
(1,120)	1:95:A:ALA:HB3	1:100:A:LEU:H	10	0.94
(1,91)	1:109:A:LEU:HD12	1:64:A:GLU:H	6	0.94
(1,86)	1:113:A:LEU:HD13	1:73:A:LEU:H	9	0.94
(1,9)	1:134:A:LEU:HD21	1:131:A:CYS:HA	17	0.94
(1,9)	1:134:A:LEU:HD22	1:131:A:CYS:HA	24	0.94
(1,2189)	1:59:A:TYR:H	1:60:A:LYS:HB2	23	0.93
(1,2119)	1:122:A:LYS:HB3	1:122:A:LYS:H	4	0.93
(1,2119)	1:122:A:LYS:HB3	1:122:A:LYS:H	9	0.93
(1,2119)	1:122:A:LYS:HB3	1:122:A:LYS:H	19	0.93
(1,1722)	2:31:B:LEU:HD23	1:128:A:ASN:HB2	2	0.93
(1,1649)	2:37:B:ALA:HB2	2:38:B:ARG:HB2	13	0.93
(1,1518)	1:61:A:LEU:HB2	1:61:A:LEU:HD21	12	0.93
(1,1518)	1:61:A:LEU:HB2	1:61:A:LEU:HD22	14	0.93
(1,1518)	1:61:A:LEU:HB2	1:61:A:LEU:HD23	17	0.93
(1,1518)	1:61:A:LEU:HB2	1:61:A:LEU:HD22	19	0.93
(1,1456)	1:69:A:GLU:HG2	1:66:A:LEU:HA	25	0.93
(1,1196)	1:89:A:TYR:HD1	1:71:A:LEU:HD11	22	0.93
(1,1194)	1:89:A:TYR:HB2	1:89:A:TYR:HD1	3	0.93
(1,1194)	1:89:A:TYR:HB2	1:89:A:TYR:HD1	6	0.93
(1,1194)	1:89:A:TYR:HB2	1:89:A:TYR:HD1	8	0.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1194)	1:89:A:TYR:HB2	1:89:A:TYR:HD1	11	0.93
(1,1194)	1:89:A:TYR:HB2	1:89:A:TYR:HD1	14	0.93
(1,1194)	1:89:A:TYR:HB2	1:89:A:TYR:HD1	16	0.93
(1,1194)	1:89:A:TYR:HB2	1:89:A:TYR:HD1	17	0.93
(1,1194)	1:89:A:TYR:HB2	1:89:A:TYR:HD1	19	0.93
(1,1194)	1:89:A:TYR:HB2	1:89:A:TYR:HD1	21	0.93
(1,1194)	1:89:A:TYR:HB2	1:89:A:TYR:HD1	25	0.93
(1,1046)	2:30:B:GLU:HG3	2:30:B:GLU:H	13	0.93
(1,1046)	2:30:B:GLU:HG3	2:30:B:GLU:H	20	0.93
(1,1046)	2:30:B:GLU:HG3	2:30:B:GLU:H	23	0.93
(1,879)	1:94:A:ARG:HD2	1:90:A:ASN:HD22	10	0.93
(1,503)	1:81:A:HIS:H	1:84:A:VAL:HG22	1	0.93
(1,503)	1:78:A:THR:HG22	1:81:A:HIS:H	11	0.93
(1,484)	1:134:A:LEU:HD11	1:94:A:ARG:H	1	0.93
(1,401)	1:113:A:LEU:HD22	1:113:A:LEU:H	5	0.93
(1,401)	1:113:A:LEU:HD21	1:113:A:LEU:H	14	0.93
(1,307)	2:39:B:TRP:HE3	2:36:B:THR:HG23	12	0.93
(1,300)	2:37:B:ALA:HB1	1:123:A:LEU:HB2	22	0.93
(1,208)	1:71:A:LEU:HD22	1:88:A:LEU:H	14	0.93
(1,208)	1:71:A:LEU:HD22	1:88:A:LEU:H	16	0.93
(1,205)	1:71:A:LEU:HD12	1:75:A:LYS:HE2	13	0.93
(1,184)	1:79:A:ALA:HB2	1:75:A:LYS:HA	13	0.93
(1,174)	1:84:A:VAL:HG11	1:124:A:TYR:HA	1	0.93
(1,174)	1:84:A:VAL:HG12	1:124:A:TYR:HA	8	0.93
(1,174)	1:84:A:VAL:HG12	1:124:A:TYR:HA	18	0.93
(1,174)	1:84:A:VAL:HG12	1:124:A:TYR:HA	22	0.93
(1,164)	1:87:A:PHE:HB3	1:87:A:PHE:HE2	2	0.93
(1,164)	1:87:A:PHE:HB3	1:87:A:PHE:HE2	15	0.93
(1,150)	1:88:A:LEU:HD21	1:128:A:ASN:H	2	0.93
(1,128)	1:93:A:GLN:HG2	1:94:A:ARG:H	1	0.93
(1,128)	1:93:A:GLN:HG2	1:94:A:ARG:H	14	0.93
(1,122)	1:95:A:ALA:HB2	1:91:A:ARG:HD3	3	0.93
(1,46)	1:126:A:TYR:HE1	1:122:A:LYS:HB3	5	0.93
(1,40)	1:127:A:ILE:HD12	1:74:A:CYS:HA	21	0.93
(1,15)	1:132:A:THR:HG21	2:27:B:SER:H	3	0.93
(1,15)	1:132:A:THR:HG23	1:135:A:LYS:H	7	0.93
(1,4)	1:130:A:LEU:HD21	1:127:A:ILE:HA	12	0.93
(1,2061)	1:87:A:PHE:H	1:85:A:VAL:HG21	2	0.92
(1,2061)	1:87:A:PHE:H	1:85:A:VAL:HG23	11	0.92
(1,2061)	1:87:A:PHE:H	1:85:A:VAL:HG22	12	0.92
(1,1722)	2:31:B:LEU:HD21	1:128:A:ASN:HB2	5	0.92
(1,1722)	2:31:B:LEU:HD23	1:128:A:ASN:HB2	7	0.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1722)	2:31:B:LEU:HD22	1:128:A:ASN:HB2	23	0.92
(1,1649)	2:37:B:ALA:HB3	2:38:B:ARG:HB2	3	0.92
(1,1611)	2:39:B:TRP:HZ3	2:39:B:TRP:HB2	6	0.92
(1,1611)	2:39:B:TRP:HZ3	2:39:B:TRP:HB2	15	0.92
(1,1518)	1:61:A:LEU:HB2	1:61:A:LEU:HD23	1	0.92
(1,1518)	1:61:A:LEU:HB2	1:61:A:LEU:HD22	4	0.92
(1,1518)	1:61:A:LEU:HB2	1:61:A:LEU:HD23	6	0.92
(1,1375)	1:74:A:CYS:HA	1:77:A:GLN:HB3	12	0.92
(1,1196)	1:89:A:TYR:HD1	1:71:A:LEU:HD13	25	0.92
(1,1194)	1:89:A:TYR:HB2	1:89:A:TYR:HD1	20	0.92
(1,1046)	2:30:B:GLU:HG3	2:30:B:GLU:H	2	0.92
(1,1046)	2:30:B:GLU:HG3	2:30:B:GLU:H	25	0.92
(1,907)	1:114:A:SER:HB2	1:115:A:ARG:H	22	0.92
(1,907)	1:114:A:SER:HB2	1:115:A:ARG:H	25	0.92
(1,879)	1:94:A:ARG:HD2	1:90:A:ASN:HD22	16	0.92
(1,869)	1:119:A:ARG:HD3	1:119:A:ARG:HB2	12	0.92
(1,503)	1:81:A:HIS:H	1:84:A:VAL:HG21	23	0.92
(1,502)	1:81:A:HIS:H	1:82:A:PRO:HB3	23	0.92
(1,451)	1:114:A:SER:H	1:117:A:ARG:HB2	18	0.92
(1,401)	1:113:A:LEU:HD21	1:113:A:LEU:H	3	0.92
(1,306)	2:36:B:THR:HG23	1:124:A:TYR:HE2	3	0.92
(1,304)	2:36:B:THR:HG23	2:35:B:PHE:HB2	19	0.92
(1,218)	1:116:A:ALA:HB3	1:70:A:PHE:HD2	3	0.92
(1,174)	1:84:A:VAL:HG13	1:124:A:TYR:HA	11	0.92
(1,164)	1:87:A:PHE:HB3	1:87:A:PHE:HE2	25	0.92
(1,128)	1:93:A:GLN:HG2	1:89:A:TYR:HD1	9	0.92
(1,128)	1:93:A:GLN:HG2	1:94:A:ARG:H	12	0.92
(1,128)	1:93:A:GLN:HG2	1:94:A:ARG:H	16	0.92
(1,128)	1:93:A:GLN:HG2	1:94:A:ARG:H	17	0.92
(1,9)	1:134:A:LEU:HD23	1:131:A:CYS:HA	21	0.92
(1,2119)	1:122:A:LYS:HB3	1:122:A:LYS:H	17	0.91
(1,2119)	1:122:A:LYS:HB3	1:122:A:LYS:H	20	0.91
(1,2061)	1:87:A:PHE:H	1:85:A:VAL:HG23	5	0.91
(1,2061)	1:87:A:PHE:H	1:85:A:VAL:HG21	19	0.91
(1,2017)	1:93:A:GLN:HE22	1:89:A:TYR:HB3	18	0.91
(1,1722)	2:31:B:LEU:HD22	1:128:A:ASN:HB2	8	0.91
(1,1722)	2:31:B:LEU:HD23	1:128:A:ASN:HB2	12	0.91
(1,1722)	2:31:B:LEU:HD23	1:128:A:ASN:HB2	19	0.91
(1,1649)	2:37:B:ALA:HB1	2:38:B:ARG:HB2	6	0.91
(1,1649)	2:37:B:ALA:HB2	2:38:B:ARG:HB2	22	0.91
(1,1611)	2:39:B:TRP:HZ3	2:39:B:TRP:HB2	25	0.91
(1,1518)	1:61:A:LEU:HB2	1:61:A:LEU:HD22	2	0.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1518)	1:61:A:LEU:HB2	1:61:A:LEU:HD23	3	0.91
(1,1518)	1:61:A:LEU:HB2	1:61:A:LEU:HD23	8	0.91
(1,1518)	1:61:A:LEU:HB2	1:61:A:LEU:HD22	18	0.91
(1,1518)	1:61:A:LEU:HB2	1:61:A:LEU:HD21	22	0.91
(1,1518)	1:61:A:LEU:HB2	1:61:A:LEU:HD23	23	0.91
(1,1518)	1:61:A:LEU:HB2	1:61:A:LEU:HD22	24	0.91
(1,1333)	1:77:A:GLN:HG2	1:73:A:LEU:HG	11	0.91
(1,1091)	1:100:A:LEU:HD21	1:92:A:GLN:HE21	8	0.91
(1,1046)	2:30:B:GLU:HG3	2:30:B:GLU:H	9	0.91
(1,1046)	2:30:B:GLU:HG3	2:30:B:GLU:H	12	0.91
(1,1046)	2:30:B:GLU:HG3	2:30:B:GLU:H	16	0.91
(1,868)	1:119:A:ARG:HD2	1:119:A:ARG:HB2	17	0.91
(1,502)	1:81:A:HIS:H	1:82:A:PRO:HB3	8	0.91
(1,443)	1:117:A:ARG:H	1:126:A:TYR:HE2	9	0.91
(1,401)	1:113:A:LEU:HD23	1:113:A:LEU:H	15	0.91
(1,381)	2:30:B:GLU:HG2	2:31:B:LEU:HB2	3	0.91
(1,381)	2:30:B:GLU:HG2	2:31:B:LEU:HB2	14	0.91
(1,355)	2:29:B:SER:HB3	2:31:B:LEU:H	22	0.91
(1,304)	2:36:B:THR:HG23	2:35:B:PHE:HB2	11	0.91
(1,304)	2:36:B:THR:HG22	2:35:B:PHE:HB2	20	0.91
(1,221)	1:130:A:LEU:HD21	1:70:A:PHE:HZ	11	0.91
(1,218)	1:116:A:ALA:HB2	1:70:A:PHE:HD2	8	0.91
(1,208)	1:71:A:LEU:HD22	1:88:A:LEU:H	2	0.91
(1,174)	1:84:A:VAL:HG12	1:124:A:TYR:HA	3	0.91
(1,174)	1:84:A:VAL:HG13	1:124:A:TYR:HA	6	0.91
(1,174)	1:84:A:VAL:HG13	1:124:A:TYR:HA	12	0.91
(1,164)	1:87:A:PHE:HB3	1:87:A:PHE:HE2	16	0.91
(1,150)	1:88:A:LEU:HD22	1:128:A:ASN:H	3	0.91
(1,150)	1:88:A:LEU:HD22	1:128:A:ASN:H	12	0.91
(1,150)	1:88:A:LEU:HD21	1:128:A:ASN:H	18	0.91
(1,149)	1:88:A:LEU:HD23	1:89:A:TYR:H	19	0.91
(1,128)	1:93:A:GLN:HG2	1:94:A:ARG:H	6	0.91
(1,128)	1:93:A:GLN:HG2	1:94:A:ARG:H	7	0.91
(1,128)	1:93:A:GLN:HG2	1:94:A:ARG:H	13	0.91
(1,120)	1:95:A:ALA:HB2	1:100:A:LEU:H	8	0.91
(1,40)	1:127:A:ILE:HD12	1:74:A:CYS:HA	3	0.91
(1,16)	1:132:A:THR:HG21	1:133:A:VAL:H	4	0.91
(1,15)	1:132:A:THR:HG22	1:135:A:LYS:H	22	0.91
(1,9)	1:134:A:LEU:HD22	1:131:A:CYS:HA	19	0.91
(1,2119)	1:122:A:LYS:HB3	1:122:A:LYS:H	24	0.9
(1,2061)	1:87:A:PHE:H	1:85:A:VAL:HG23	18	0.9
(1,1722)	2:31:B:LEU:HD22	1:128:A:ASN:HB2	11	0.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1651)	2:38:B:ARG:HG2	2:37:B:ALA:HB1	15	0.9
(1,1649)	2:37:B:ALA:HB1	2:38:B:ARG:HB2	14	0.9
(1,1649)	2:37:B:ALA:HB1	2:38:B:ARG:HB2	19	0.9
(1,1637)	2:38:B:ARG:HD2	2:39:B:TRP:HD1	14	0.9
(1,1611)	2:39:B:TRP:HZ3	2:39:B:TRP:HB2	1	0.9
(1,1518)	1:61:A:LEU:HB2	1:61:A:LEU:HD22	15	0.9
(1,1396)	1:72:A:GLU:HG2	1:72:A:GLU:H	23	0.9
(1,1251)	1:68:A:GLU:HB2	1:68:A:GLU:H	21	0.9
(1,1251)	1:68:A:GLU:HB2	1:68:A:GLU:H	25	0.9
(1,1196)	1:89:A:TYR:HD1	1:71:A:LEU:HD11	8	0.9
(1,1196)	1:89:A:TYR:HD1	1:71:A:LEU:HD12	18	0.9
(1,1143)	1:94:A:ARG:HG2	1:94:A:ARG:H	2	0.9
(1,1143)	1:94:A:ARG:HG2	1:94:A:ARG:H	22	0.9
(1,1122)	1:96:A:HIS:HA	1:139:A:ALA:HB2	13	0.9
(1,1122)	1:96:A:HIS:HA	1:139:A:ALA:HB2	23	0.9
(1,1046)	2:30:B:GLU:HG3	2:30:B:GLU:H	11	0.9
(1,868)	1:119:A:ARG:HD2	1:119:A:ARG:HB2	11	0.9
(1,793)	1:124:A:TYR:HE1	1:124:A:TYR:H	14	0.9
(1,694)	1:113:A:LEU:HB2	1:114:A:SER:H	18	0.9
(1,561)	2:27:B:SER:H	2:30:B:GLU:HB3	9	0.9
(1,561)	2:27:B:SER:H	2:30:B:GLU:HB3	19	0.9
(1,503)	1:81:A:HIS:H	1:84:A:VAL:HG22	3	0.9
(1,503)	1:81:A:HIS:H	1:84:A:VAL:HG23	17	0.9
(1,503)	1:81:A:HIS:H	1:84:A:VAL:HG22	25	0.9
(1,443)	1:117:A:ARG:H	1:126:A:TYR:HE2	2	0.9
(1,443)	1:117:A:ARG:H	1:126:A:TYR:HE2	22	0.9
(1,401)	1:113:A:LEU:HD21	1:113:A:LEU:H	17	0.9
(1,376)	2:29:B:SER:HB2	2:26:B:ASP:HB3	14	0.9
(1,208)	1:71:A:LEU:HD21	1:88:A:LEU:H	3	0.9
(1,205)	1:71:A:LEU:HD12	1:75:A:LYS:HE2	12	0.9
(1,178)	1:84:A:VAL:HG23	1:78:A:THR:H	21	0.9
(1,164)	1:87:A:PHE:HB3	1:87:A:PHE:HE2	1	0.9
(1,164)	1:87:A:PHE:HB3	1:87:A:PHE:HE2	14	0.9
(1,153)	1:88:A:LEU:HD22	1:128:A:ASN:HA	3	0.9
(1,149)	1:88:A:LEU:HD21	1:89:A:TYR:H	16	0.9
(1,143)	1:89:A:TYR:HD2	1:86:A:PRO:HB2	13	0.9
(1,128)	1:93:A:GLN:HG2	1:94:A:ARG:H	10	0.9
(1,128)	1:93:A:GLN:HG2	1:89:A:TYR:HD1	23	0.9
(1,128)	1:93:A:GLN:HG2	1:94:A:ARG:H	24	0.9
(1,35)	1:127:A:ILE:HG23	1:88:A:LEU:H	9	0.9
(1,35)	1:127:A:ILE:HG22	1:88:A:LEU:H	16	0.9
(1,15)	1:132:A:THR:HG21	1:135:A:LYS:H	4	0.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,15)	1:132:A:THR:HG21	1:135:A:LYS:H	6	0.9
(1,9)	1:134:A:LEU:HD22	1:131:A:CYS:HA	10	0.9
(1,2195)	1:56:A:LYS:H	1:56:A:LYS:HG2	19	0.89
(1,2119)	1:122:A:LYS:HB3	1:122:A:LYS:H	11	0.89
(1,2061)	1:87:A:PHE:H	1:85:A:VAL:HG22	3	0.89
(1,2061)	1:87:A:PHE:H	1:85:A:VAL:HG22	6	0.89
(1,2061)	1:87:A:PHE:H	1:85:A:VAL:HG23	7	0.89
(1,2061)	1:87:A:PHE:H	1:85:A:VAL:HG23	9	0.89
(1,1760)	2:24:B:GLN:HG2	2:24:B:GLN:HA	11	0.89
(1,1518)	1:61:A:LEU:HB2	1:61:A:LEU:HD23	7	0.89
(1,1375)	1:74:A:CYS:HA	1:77:A:GLN:HB3	4	0.89
(1,1375)	1:74:A:CYS:HA	1:77:A:GLN:HB3	24	0.89
(1,1261)	1:86:A:PRO:HD2	1:85:A:VAL:HG23	7	0.89
(1,1251)	1:68:A:GLU:HB2	1:68:A:GLU:H	1	0.89
(1,1251)	1:68:A:GLU:HB2	1:68:A:GLU:H	5	0.89
(1,1251)	1:68:A:GLU:HB2	1:68:A:GLU:H	11	0.89
(1,1251)	1:68:A:GLU:HB2	1:68:A:GLU:H	20	0.89
(1,1251)	1:68:A:GLU:HB2	1:68:A:GLU:H	24	0.89
(1,1143)	1:94:A:ARG:HG2	1:94:A:ARG:H	1	0.89
(1,868)	1:119:A:ARG:HD2	1:119:A:ARG:HB2	10	0.89
(1,792)	1:127:A:ILE:HD13	1:124:A:TYR:HD1	25	0.89
(1,694)	1:113:A:LEU:HB2	1:114:A:SER:H	8	0.89
(1,694)	1:113:A:LEU:HB2	1:114:A:SER:H	10	0.89
(1,694)	1:113:A:LEU:HB2	1:114:A:SER:H	11	0.89
(1,694)	1:113:A:LEU:HB2	1:114:A:SER:H	19	0.89
(1,619)	1:135:A:LYS:HG2	1:91:A:ARG:HD3	16	0.89
(1,534)	1:121:A:ALA:H	1:119:A:ARG:HG2	9	0.89
(1,530)	1:66:A:LEU:HD22	1:67:A:PHE:H	25	0.89
(1,503)	1:78:A:THR:HG22	1:81:A:HIS:H	18	0.89
(1,488)	1:92:A:GLN:HE22	1:64:A:GLU:HG3	2	0.89
(1,443)	1:117:A:ARG:H	1:126:A:TYR:HE2	13	0.89
(1,395)	1:138:A:SER:H	1:95:A:ALA:HB3	4	0.89
(1,395)	1:138:A:SER:H	1:139:A:ALA:HB1	11	0.89
(1,380)	2:27:B:SER:HA	2:30:B:GLU:HB3	19	0.89
(1,363)	2:29:B:SER:HB2	2:32:B:GLU:HB2	1	0.89
(1,306)	2:36:B:THR:HG23	1:124:A:TYR:HE1	5	0.89
(1,304)	2:36:B:THR:HG22	2:35:B:PHE:HB2	15	0.89
(1,263)	1:132:A:THR:HG23	2:28:B:ASP:HB3	25	0.89
(1,221)	1:130:A:LEU:HD21	1:70:A:PHE:HZ	12	0.89
(1,221)	1:130:A:LEU:HD22	1:70:A:PHE:HZ	18	0.89
(1,208)	1:71:A:LEU:HD22	1:88:A:LEU:H	8	0.89
(1,174)	1:84:A:VAL:HG12	1:124:A:TYR:HA	20	0.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,174)	1:84:A:VAL:HG13	1:124:A:TYR:HA	24	0.89
(1,164)	1:87:A:PHE:HB3	1:87:A:PHE:HE2	8	0.89
(1,150)	1:88:A:LEU:HD21	1:128:A:ASN:H	8	0.89
(1,128)	1:93:A:GLN:HG2	1:94:A:ARG:H	3	0.89
(1,128)	1:93:A:GLN:HG2	1:89:A:TYR:HD1	5	0.89
(1,128)	1:93:A:GLN:HG2	1:89:A:TYR:HD1	18	0.89
(1,128)	1:93:A:GLN:HG2	1:94:A:ARG:H	19	0.89
(1,128)	1:93:A:GLN:HG2	1:94:A:ARG:H	22	0.89
(1,120)	1:95:A:ALA:HB2	1:93:A:GLN:H	15	0.89
(1,23)	1:130:A:LEU:HD22	1:113:A:LEU:H	20	0.89
(1,15)	1:132:A:THR:HG22	1:135:A:LYS:H	21	0.89
(1,9)	1:134:A:LEU:HD22	1:131:A:CYS:HA	4	0.89
(1,9)	1:134:A:LEU:HD22	1:131:A:CYS:HA	5	0.89
(1,9)	1:134:A:LEU:HD22	1:131:A:CYS:HA	13	0.89
(1,4)	1:130:A:LEU:HD22	1:127:A:ILE:HA	9	0.89
(1,2061)	1:87:A:PHE:H	1:85:A:VAL:HG23	4	0.88
(1,2061)	1:87:A:PHE:H	1:85:A:VAL:HG22	24	0.88
(1,1656)	2:37:B:ALA:HB3	2:39:B:TRP:HZ2	8	0.88
(1,1651)	2:38:B:ARG:HG2	2:37:B:ALA:HB2	11	0.88
(1,1650)	2:37:B:ALA:HB2	1:121:A:ALA:HB3	13	0.88
(1,1611)	2:39:B:TRP:HZ3	2:39:B:TRP:HB2	10	0.88
(1,1611)	2:39:B:TRP:HZ3	2:39:B:TRP:HB2	19	0.88
(1,1561)	1:57:A:LYS:HD2	1:57:A:LYS:HA	12	0.88
(1,1456)	1:69:A:GLU:HG2	1:66:A:LEU:HA	22	0.88
(1,1396)	1:72:A:GLU:HG2	1:72:A:GLU:H	10	0.88
(1,1375)	1:74:A:CYS:HA	1:77:A:GLN:HB3	9	0.88
(1,1261)	1:86:A:PRO:HD2	1:85:A:VAL:HG21	1	0.88
(1,1261)	1:86:A:PRO:HD2	1:85:A:VAL:HG23	21	0.88
(1,1251)	1:68:A:GLU:HB2	1:68:A:GLU:H	6	0.88
(1,1251)	1:68:A:GLU:HB2	1:68:A:GLU:H	7	0.88
(1,1251)	1:68:A:GLU:HB2	1:68:A:GLU:H	8	0.88
(1,1251)	1:68:A:GLU:HB2	1:68:A:GLU:H	13	0.88
(1,1251)	1:68:A:GLU:HB2	1:68:A:GLU:H	17	0.88
(1,1251)	1:68:A:GLU:HB2	1:68:A:GLU:H	18	0.88
(1,1046)	2:30:B:GLU:HG3	2:30:B:GLU:H	7	0.88
(1,1046)	2:30:B:GLU:HG3	2:30:B:GLU:H	10	0.88
(1,907)	1:114:A:SER:HB2	1:115:A:ARG:H	3	0.88
(1,869)	1:119:A:ARG:HD3	1:119:A:ARG:HB2	9	0.88
(1,694)	1:113:A:LEU:HB2	1:114:A:SER:H	9	0.88
(1,591)	1:138:A:SER:HB3	1:138:A:SER:H	1	0.88
(1,585)	1:139:A:ALA:HB1	1:140:A:LYS:H	25	0.88
(1,563)	1:113:A:LEU:H	1:111:A:ARG:HB2	12	0.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,530)	1:66:A:LEU:HD21	1:67:A:PHE:H	11	0.88
(1,478)	1:95:A:ALA:H	1:91:A:ARG:HD2	22	0.88
(1,401)	1:113:A:LEU:HD23	1:113:A:LEU:H	21	0.88
(1,401)	1:113:A:LEU:HD23	1:113:A:LEU:H	23	0.88
(1,395)	1:138:A:SER:H	1:95:A:ALA:HB1	1	0.88
(1,379)	2:31:B:LEU:HB2	2:28:B:ASP:HB2	10	0.88
(1,306)	2:36:B:THR:HG22	1:124:A:TYR:HE2	9	0.88
(1,300)	2:37:B:ALA:HB1	1:123:A:LEU:HB2	1	0.88
(1,221)	1:130:A:LEU:HD23	1:70:A:PHE:HZ	1	0.88
(1,216)	1:113:A:LEU:HD13	1:70:A:PHE:HD2	20	0.88
(1,208)	1:71:A:LEU:HD21	1:88:A:LEU:H	22	0.88
(1,164)	1:87:A:PHE:HB3	1:87:A:PHE:HE2	23	0.88
(1,150)	1:88:A:LEU:HD23	1:128:A:ASN:H	20	0.88
(1,143)	1:89:A:TYR:HD2	1:86:A:PRO:HB2	17	0.88
(1,120)	1:95:A:ALA:HB1	1:100:A:LEU:H	6	0.88
(1,40)	1:127:A:ILE:HD12	1:74:A:CYS:HA	14	0.88
(1,16)	1:132:A:THR:HG21	1:133:A:VAL:H	13	0.88
(1,15)	1:132:A:THR:HG22	2:27:B:SER:H	1	0.88
(1,15)	1:132:A:THR:HG23	1:135:A:LYS:H	11	0.88
(1,15)	1:132:A:THR:HG21	1:135:A:LYS:H	13	0.88
(1,15)	1:132:A:THR:HG23	2:27:B:SER:H	15	0.88
(1,15)	1:132:A:THR:HG22	1:135:A:LYS:H	19	0.88
(1,15)	1:132:A:THR:HG22	1:135:A:LYS:H	25	0.88
(1,9)	1:134:A:LEU:HD21	1:131:A:CYS:HA	9	0.88
(1,9)	1:134:A:LEU:HD22	1:131:A:CYS:HA	25	0.88
(1,4)	1:130:A:LEU:HD22	1:127:A:ILE:HA	16	0.88
(1,2119)	1:122:A:LYS:HB3	1:122:A:LYS:H	16	0.87
(1,2061)	1:87:A:PHE:H	1:85:A:VAL:HG22	14	0.87
(1,2061)	1:87:A:PHE:H	1:85:A:VAL:HG22	16	0.87
(1,1771)	1:142:A:LYS:H	1:142:A:LYS:HD2	15	0.87
(1,1650)	2:37:B:ALA:HB3	1:121:A:ALA:HB1	21	0.87
(1,1649)	2:37:B:ALA:HB2	2:38:B:ARG:HB2	4	0.87
(1,1611)	2:39:B:TRP:HZ3	2:39:B:TRP:HB2	16	0.87
(1,1611)	2:39:B:TRP:HZ3	2:39:B:TRP:HB2	18	0.87
(1,1554)	1:59:A:TYR:HE1	1:57:A:LYS:HB2	10	0.87
(1,1518)	1:61:A:LEU:HB2	1:61:A:LEU:HD23	16	0.87
(1,1375)	1:74:A:CYS:HA	1:77:A:GLN:HB3	18	0.87
(1,1261)	1:86:A:PRO:HD2	1:85:A:VAL:HG21	13	0.87
(1,1251)	1:68:A:GLU:HB2	1:68:A:GLU:H	19	0.87
(1,1251)	1:68:A:GLU:HB2	1:68:A:GLU:H	22	0.87
(1,1196)	1:89:A:TYR:HD1	1:71:A:LEU:HD11	21	0.87
(1,1046)	2:30:B:GLU:HG3	2:30:B:GLU:H	17	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,907)	1:114:A:SER:HB2	1:115:A:ARG:H	4	0.87
(1,907)	1:114:A:SER:HB2	1:115:A:ARG:H	11	0.87
(1,907)	1:114:A:SER:HB2	1:115:A:ARG:H	12	0.87
(1,907)	1:114:A:SER:HB2	1:115:A:ARG:H	15	0.87
(1,904)	1:115:A:ARG:HD3	1:126:A:TYR:HE2	24	0.87
(1,869)	1:119:A:ARG:HD3	1:119:A:ARG:HB2	8	0.87
(1,868)	1:119:A:ARG:HD2	1:119:A:ARG:HB2	22	0.87
(1,694)	1:113:A:LEU:HB2	1:114:A:SER:H	2	0.87
(1,694)	1:113:A:LEU:HB2	1:114:A:SER:H	3	0.87
(1,694)	1:113:A:LEU:HB2	1:114:A:SER:H	4	0.87
(1,694)	1:113:A:LEU:HB2	1:114:A:SER:H	5	0.87
(1,694)	1:113:A:LEU:HB2	1:114:A:SER:H	6	0.87
(1,676)	1:133:A:VAL:HG22	1:129:A:GLU:HB3	13	0.87
(1,591)	1:138:A:SER:HB3	1:138:A:SER:H	2	0.87
(1,591)	1:138:A:SER:HB3	1:138:A:SER:H	5	0.87
(1,585)	1:139:A:ALA:HB3	1:140:A:LYS:H	2	0.87
(1,530)	1:66:A:LEU:HD22	1:67:A:PHE:H	19	0.87
(1,510)	1:73:A:LEU:HD22	1:77:A:GLN:HE22	10	0.87
(1,503)	1:78:A:THR:HG21	1:81:A:HIS:H	22	0.87
(1,451)	1:114:A:SER:H	1:117:A:ARG:HB2	24	0.87
(1,443)	1:117:A:ARG:H	1:126:A:TYR:HE2	23	0.87
(1,401)	1:113:A:LEU:HD23	1:113:A:LEU:H	2	0.87
(1,401)	1:113:A:LEU:HD21	1:113:A:LEU:H	9	0.87
(1,401)	1:113:A:LEU:HD22	1:113:A:LEU:H	25	0.87
(1,381)	2:30:B:GLU:HG2	2:31:B:LEU:HB2	7	0.87
(1,355)	2:29:B:SER:HB3	2:33:B:GLN:H	20	0.87
(1,300)	2:37:B:ALA:HB3	1:123:A:LEU:HB2	2	0.87
(1,280)	2:31:B:LEU:HG	1:87:A:PHE:HE2	3	0.87
(1,263)	1:132:A:THR:HG22	2:28:B:ASP:HB3	15	0.87
(1,218)	1:116:A:ALA:HB3	1:70:A:PHE:HD2	7	0.87
(1,218)	1:116:A:ALA:HB2	1:70:A:PHE:HD2	10	0.87
(1,208)	1:71:A:LEU:HD23	1:88:A:LEU:H	15	0.87
(1,205)	1:71:A:LEU:HD12	1:75:A:LYS:HE2	9	0.87
(1,200)	1:72:A:GLU:HG3	1:71:A:LEU:HD13	7	0.87
(1,164)	1:87:A:PHE:HB3	1:87:A:PHE:HE2	21	0.87
(1,150)	1:88:A:LEU:HD22	1:128:A:ASN:H	10	0.87
(1,150)	1:88:A:LEU:HD22	1:128:A:ASN:H	17	0.87
(1,150)	1:88:A:LEU:HD22	1:128:A:ASN:H	23	0.87
(1,128)	1:93:A:GLN:HG2	1:94:A:ARG:H	2	0.87
(1,128)	1:93:A:GLN:HG2	1:94:A:ARG:H	21	0.87
(1,2274)	2:39:B:TRP:HE1	2:38:B:ARG:HD2	6	0.86
(1,2157)	1:65:A:LYS:HB2	1:65:A:LYS:H	10	0.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2061)	1:87:A:PHE:H	1:85:A:VAL:HG21	1	0.86
(1,2061)	1:87:A:PHE:H	1:85:A:VAL:HG21	23	0.86
(1,1649)	2:37:B:ALA:HB1	2:38:B:ARG:HB2	17	0.86
(1,1456)	1:69:A:GLU:HG2	1:66:A:LEU:HA	11	0.86
(1,1328)	1:77:A:GLN:HG2	1:74:A:CYS:HA	19	0.86
(1,1261)	1:86:A:PRO:HD2	1:85:A:VAL:HG22	3	0.86
(1,1261)	1:86:A:PRO:HD2	1:85:A:VAL:HG22	12	0.86
(1,1261)	1:86:A:PRO:HD2	1:85:A:VAL:HG22	15	0.86
(1,1261)	1:86:A:PRO:HD2	1:85:A:VAL:HG21	23	0.86
(1,1251)	1:68:A:GLU:HB2	1:68:A:GLU:H	10	0.86
(1,1251)	1:68:A:GLU:HB2	1:68:A:GLU:H	16	0.86
(1,907)	1:114:A:SER:HB2	1:115:A:ARG:H	5	0.86
(1,907)	1:114:A:SER:HB2	1:115:A:ARG:H	6	0.86
(1,907)	1:114:A:SER:HB2	1:115:A:ARG:H	23	0.86
(1,869)	1:119:A:ARG:HD3	1:119:A:ARG:HB2	3	0.86
(1,869)	1:119:A:ARG:HD3	1:119:A:ARG:HB2	5	0.86
(1,868)	1:119:A:ARG:HD2	1:119:A:ARG:HB2	15	0.86
(1,694)	1:113:A:LEU:HB2	1:114:A:SER:H	22	0.86
(1,694)	1:113:A:LEU:HB2	1:114:A:SER:H	23	0.86
(1,694)	1:113:A:LEU:HB2	1:114:A:SER:H	25	0.86
(1,585)	1:139:A:ALA:HB3	1:140:A:LYS:H	11	0.86
(1,570)	1:143:A:LEU:HB2	1:144:A:ASN:HD21	21	0.86
(1,563)	1:134:A:LEU:H	1:135:A:LYS:HB2	2	0.86
(1,530)	1:66:A:LEU:HD22	1:67:A:PHE:H	8	0.86
(1,530)	1:66:A:LEU:HD21	1:67:A:PHE:H	23	0.86
(1,502)	1:81:A:HIS:H	1:82:A:PRO:HB3	15	0.86
(1,484)	1:134:A:LEU:HD13	1:94:A:ARG:H	18	0.86
(1,401)	1:113:A:LEU:HD23	1:113:A:LEU:H	6	0.86
(1,381)	2:30:B:GLU:HG2	2:31:B:LEU:HB2	21	0.86
(1,367)	2:26:B:ASP:HB3	2:31:B:LEU:H	3	0.86
(1,332)	1:127:A:ILE:HG12	1:124:A:TYR:HD2	18	0.86
(1,307)	2:39:B:TRP:HE3	2:36:B:THR:HG21	21	0.86
(1,306)	2:36:B:THR:HG23	1:124:A:TYR:HE2	18	0.86
(1,306)	2:36:B:THR:HG21	1:124:A:TYR:HE2	23	0.86
(1,280)	2:31:B:LEU:HG	1:87:A:PHE:HE2	8	0.86
(1,221)	1:130:A:LEU:HD22	1:70:A:PHE:HZ	17	0.86
(1,221)	1:130:A:LEU:HD23	1:70:A:PHE:HZ	19	0.86
(1,221)	1:130:A:LEU:HD21	1:70:A:PHE:HZ	20	0.86
(1,221)	1:130:A:LEU:HD22	1:70:A:PHE:HZ	24	0.86
(1,218)	1:116:A:ALA:HB1	1:70:A:PHE:HD2	17	0.86
(1,218)	1:116:A:ALA:HB2	1:70:A:PHE:HD2	25	0.86
(1,208)	1:71:A:LEU:HD22	1:88:A:LEU:H	9	0.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,184)	1:79:A:ALA:HB2	1:75:A:LYS:HA	15	0.86
(1,184)	1:79:A:ALA:HB2	1:75:A:LYS:HA	23	0.86
(1,164)	1:87:A:PHE:HB3	1:87:A:PHE:HE2	6	0.86
(1,150)	1:88:A:LEU:HD21	1:128:A:ASN:H	11	0.86
(1,141)	1:93:A:GLN:HG2	1:89:A:TYR:HD1	13	0.86
(1,16)	1:132:A:THR:HG22	1:133:A:VAL:H	19	0.86
(1,9)	1:134:A:LEU:HD22	1:131:A:CYS:HA	7	0.86
(1,4)	1:130:A:LEU:HD22	1:127:A:ILE:HA	3	0.86
(1,2274)	2:39:B:TRP:HE1	2:38:B:ARG:HD2	4	0.85
(1,2193)	1:58:A:CYS:H	1:57:A:LYS:HG2	9	0.85
(1,2061)	1:87:A:PHE:H	1:85:A:VAL:HG22	15	0.85
(1,1976)	1:100:A:LEU:H	1:138:A:SER:HB2	5	0.85
(1,1722)	2:31:B:LEU:HD21	1:128:A:ASN:HB2	3	0.85
(1,1722)	2:31:B:LEU:HD23	1:128:A:ASN:HB2	9	0.85
(1,1722)	2:31:B:LEU:HD22	1:128:A:ASN:HB2	20	0.85
(1,1611)	2:39:B:TRP:HZ3	2:39:B:TRP:HB2	17	0.85
(1,1518)	1:61:A:LEU:HB2	1:61:A:LEU:HD22	20	0.85
(1,1375)	1:74:A:CYS:HA	1:77:A:GLN:HB3	23	0.85
(1,1366)	1:75:A:LYS:HD3	1:75:A:LYS:H	10	0.85
(1,1261)	1:86:A:PRO:HD2	1:85:A:VAL:HG23	4	0.85
(1,1261)	1:86:A:PRO:HD2	1:85:A:VAL:HG22	6	0.85
(1,1261)	1:86:A:PRO:HD2	1:85:A:VAL:HG22	10	0.85
(1,1261)	1:86:A:PRO:HD2	1:85:A:VAL:HG21	19	0.85
(1,1261)	1:86:A:PRO:HD2	1:85:A:VAL:HG22	20	0.85
(1,1261)	1:86:A:PRO:HD2	1:85:A:VAL:HG21	25	0.85
(1,1251)	1:68:A:GLU:HB2	1:68:A:GLU:H	3	0.85
(1,1196)	1:89:A:TYR:HD1	1:71:A:LEU:HD11	13	0.85
(1,1196)	1:89:A:TYR:HD1	1:71:A:LEU:HD12	24	0.85
(1,980)	1:108:A:ILE:HA	1:108:A:ILE:HD11	23	0.85
(1,907)	1:114:A:SER:HB2	1:115:A:ARG:H	21	0.85
(1,869)	1:119:A:ARG:HD3	1:119:A:ARG:HB2	18	0.85
(1,766)	1:126:A:TYR:HE1	1:115:A:ARG:HB2	24	0.85
(1,694)	1:113:A:LEU:HB2	1:114:A:SER:H	15	0.85
(1,694)	1:113:A:LEU:HB2	1:114:A:SER:H	17	0.85
(1,591)	1:138:A:SER:HB3	1:138:A:SER:H	9	0.85
(1,591)	1:138:A:SER:HB3	1:138:A:SER:H	12	0.85
(1,591)	1:138:A:SER:HB3	1:138:A:SER:H	14	0.85
(1,563)	1:134:A:LEU:H	1:135:A:LYS:HB2	14	0.85
(1,503)	1:78:A:THR:HG21	1:81:A:HIS:H	4	0.85
(1,401)	1:113:A:LEU:HD22	1:113:A:LEU:H	19	0.85
(1,401)	1:113:A:LEU:HD21	1:113:A:LEU:H	24	0.85
(1,395)	1:138:A:SER:H	1:95:A:ALA:HB3	17	0.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,381)	2:30:B:GLU:HG2	2:31:B:LEU:HB2	11	0.85
(1,332)	1:127:A:ILE:HG12	1:124:A:TYR:HD2	11	0.85
(1,318)	2:34:B:TYR:HE1	2:30:B:GLU:HB2	19	0.85
(1,306)	2:36:B:THR:HG21	1:124:A:TYR:HE2	8	0.85
(1,304)	2:36:B:THR:HG22	2:35:B:PHE:HB2	1	0.85
(1,304)	2:36:B:THR:HG23	2:35:B:PHE:HB2	10	0.85
(1,243)	1:62:A:GLU:HG3	1:61:A:LEU:HD23	13	0.85
(1,218)	1:116:A:ALA:HB2	1:70:A:PHE:HD2	16	0.85
(1,208)	1:71:A:LEU:HD21	1:88:A:LEU:H	6	0.85
(1,208)	1:71:A:LEU:HD21	1:88:A:LEU:H	18	0.85
(1,208)	1:71:A:LEU:HD21	1:88:A:LEU:H	20	0.85
(1,205)	1:71:A:LEU:HD11	1:75:A:LYS:HE2	2	0.85
(1,174)	1:84:A:VAL:HG13	1:124:A:TYR:HA	2	0.85
(1,174)	1:84:A:VAL:HG11	1:124:A:TYR:HA	14	0.85
(1,150)	1:88:A:LEU:HD22	1:128:A:ASN:H	1	0.85
(1,150)	1:88:A:LEU:HD23	1:128:A:ASN:H	4	0.85
(1,141)	1:93:A:GLN:HG2	1:89:A:TYR:HD1	17	0.85
(1,136)	1:91:A:ARG:HG3	1:91:A:ARG:H	4	0.85
(1,16)	1:132:A:THR:HG22	1:133:A:VAL:H	5	0.85
(1,16)	1:132:A:THR:HG22	1:133:A:VAL:H	24	0.85
(1,15)	1:132:A:THR:HG22	1:135:A:LYS:H	17	0.85
(1,9)	1:134:A:LEU:HD21	1:131:A:CYS:HA	16	0.85
(1,9)	1:134:A:LEU:HD22	1:131:A:CYS:HA	20	0.85
(1,4)	1:130:A:LEU:HD23	1:127:A:ILE:HA	10	0.85
(1,2119)	1:122:A:LYS:HB3	1:122:A:LYS:H	18	0.84
(1,1722)	2:31:B:LEU:HD23	1:128:A:ASN:HB2	16	0.84
(1,1611)	2:39:B:TRP:HZ3	2:39:B:TRP:HB2	20	0.84
(1,1341)	1:76:A:MET:HB3	1:73:A:LEU:HA	16	0.84
(1,1261)	1:86:A:PRO:HD2	1:85:A:VAL:HG21	8	0.84
(1,1261)	1:86:A:PRO:HD2	1:85:A:VAL:HG23	11	0.84
(1,1261)	1:86:A:PRO:HD2	1:85:A:VAL:HG22	14	0.84
(1,1261)	1:86:A:PRO:HD2	1:85:A:VAL:HG23	17	0.84
(1,1261)	1:86:A:PRO:HD2	1:85:A:VAL:HG23	18	0.84
(1,1199)	1:89:A:TYR:HE1	1:71:A:LEU:HD12	2	0.84
(1,1122)	1:96:A:HIS:HA	1:139:A:ALA:HB3	18	0.84
(1,1046)	2:30:B:GLU:HG3	2:30:B:GLU:H	6	0.84
(1,907)	1:114:A:SER:HB2	1:115:A:ARG:H	10	0.84
(1,869)	1:119:A:ARG:HD3	1:119:A:ARG:HB2	21	0.84
(1,868)	1:119:A:ARG:HD2	1:119:A:ARG:HB2	20	0.84
(1,694)	1:113:A:LEU:HB2	1:114:A:SER:H	12	0.84
(1,694)	1:113:A:LEU:HB2	1:114:A:SER:H	14	0.84
(1,694)	1:113:A:LEU:HB2	1:114:A:SER:H	16	0.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,694)	1:113:A:LEU:HB2	1:114:A:SER:H	21	0.84
(1,585)	1:139:A:ALA:HB3	1:140:A:LYS:H	17	0.84
(1,563)	1:113:A:LEU:H	1:111:A:ARG:HB2	13	0.84
(1,530)	1:66:A:LEU:HD21	1:67:A:PHE:H	3	0.84
(1,530)	1:66:A:LEU:HD21	1:67:A:PHE:H	16	0.84
(1,530)	1:66:A:LEU:HD22	1:67:A:PHE:H	21	0.84
(1,530)	1:66:A:LEU:HD21	1:67:A:PHE:H	22	0.84
(1,503)	1:81:A:HIS:H	1:84:A:VAL:HG22	15	0.84
(1,503)	1:78:A:THR:HG22	1:81:A:HIS:H	21	0.84
(1,502)	1:81:A:HIS:H	1:82:A:PRO:HB3	4	0.84
(1,443)	1:117:A:ARG:H	1:126:A:TYR:HE2	25	0.84
(1,413)	1:131:A:CYS:H	1:130:A:LEU:HD13	2	0.84
(1,381)	2:30:B:GLU:HG2	2:31:B:LEU:HB2	1	0.84
(1,368)	2:26:B:ASP:HB3	1:87:A:PHE:HZ	25	0.84
(1,364)	2:29:B:SER:HB3	2:32:B:GLU:HB2	16	0.84
(1,310)	2:35:B:PHE:HD1	1:127:A:ILE:HB	17	0.84
(1,307)	2:39:B:TRP:HE3	2:36:B:THR:HG22	24	0.84
(1,304)	2:36:B:THR:HG21	2:35:B:PHE:HB2	25	0.84
(1,254)	1:57:A:LYS:HE3	1:54:A:MET:HG3	17	0.84
(1,249)	1:56:A:LYS:HA	1:57:A:LYS:H	5	0.84
(1,233)	1:66:A:LEU:HD13	1:63:A:ASN:HB3	1	0.84
(1,233)	1:66:A:LEU:HD12	1:63:A:ASN:HB3	18	0.84
(1,221)	1:130:A:LEU:HD21	1:70:A:PHE:HZ	5	0.84
(1,221)	1:130:A:LEU:HD21	1:70:A:PHE:HZ	7	0.84
(1,221)	1:112:A:VAL:HG23	1:70:A:PHE:HZ	14	0.84
(1,208)	1:71:A:LEU:HD22	1:88:A:LEU:H	4	0.84
(1,200)	1:72:A:GLU:HG3	1:71:A:LEU:HD11	3	0.84
(1,178)	1:84:A:VAL:HG23	1:78:A:THR:H	14	0.84
(1,178)	1:84:A:VAL:HG22	1:78:A:THR:H	18	0.84
(1,170)	1:85:A:VAL:HG11	1:75:A:LYS:H	17	0.84
(1,164)	1:87:A:PHE:HB3	1:87:A:PHE:HE2	7	0.84
(1,164)	1:87:A:PHE:HB3	1:87:A:PHE:HE2	9	0.84
(1,153)	1:88:A:LEU:HD21	1:128:A:ASN:HA	18	0.84
(1,150)	1:88:A:LEU:HD21	1:128:A:ASN:H	22	0.84
(1,136)	1:91:A:ARG:HG3	1:91:A:ARG:H	5	0.84
(1,35)	1:127:A:ILE:HG22	1:88:A:LEU:H	19	0.84
(1,16)	1:132:A:THR:HG23	1:133:A:VAL:H	7	0.84
(1,16)	1:132:A:THR:HG22	1:133:A:VAL:H	14	0.84
(1,2119)	1:122:A:LYS:HB3	1:122:A:LYS:H	25	0.83
(1,2061)	1:87:A:PHE:H	1:85:A:VAL:HG23	21	0.83
(1,1722)	2:31:B:LEU:HD23	1:128:A:ASN:HB2	21	0.83
(1,1611)	2:39:B:TRP:HZ3	2:39:B:TRP:HB2	2	0.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1611)	2:39:B:TRP:HZ3	2:39:B:TRP:HB2	21	0.83
(1,1518)	1:61:A:LEU:HB2	1:61:A:LEU:HD22	10	0.83
(1,1518)	1:61:A:LEU:HB2	1:61:A:LEU:HD22	11	0.83
(1,1518)	1:61:A:LEU:HB2	1:61:A:LEU:HD22	13	0.83
(1,1366)	1:75:A:LYS:HD3	1:75:A:LYS:H	24	0.83
(1,1341)	1:76:A:MET:HB3	1:73:A:LEU:HA	10	0.83
(1,1261)	1:86:A:PRO:HD2	1:85:A:VAL:HG21	2	0.83
(1,1261)	1:86:A:PRO:HD2	1:85:A:VAL:HG23	5	0.83
(1,1261)	1:86:A:PRO:HD2	1:85:A:VAL:HG23	9	0.83
(1,1261)	1:86:A:PRO:HD2	1:85:A:VAL:HG22	24	0.83
(1,1251)	1:68:A:GLU:HB2	1:68:A:GLU:H	12	0.83
(1,1143)	1:94:A:ARG:HG2	1:94:A:ARG:H	15	0.83
(1,1046)	2:30:B:GLU:HG3	2:30:B:GLU:H	3	0.83
(1,1046)	2:30:B:GLU:HG3	2:30:B:GLU:H	14	0.83
(1,1046)	2:30:B:GLU:HG3	2:30:B:GLU:H	15	0.83
(1,1046)	2:30:B:GLU:HG3	2:30:B:GLU:H	21	0.83
(1,907)	1:114:A:SER:HB2	1:115:A:ARG:H	14	0.83
(1,869)	1:119:A:ARG:HD3	1:119:A:ARG:HB2	23	0.83
(1,868)	1:119:A:ARG:HD2	1:119:A:ARG:HB2	24	0.83
(1,694)	1:113:A:LEU:HB2	1:114:A:SER:H	20	0.83
(1,585)	1:139:A:ALA:HB1	1:140:A:LYS:H	3	0.83
(1,585)	1:139:A:ALA:HB3	1:140:A:LYS:H	10	0.83
(1,577)	1:75:A:LYS:HE2	1:71:A:LEU:HB3	2	0.83
(1,563)	1:134:A:LEU:H	1:135:A:LYS:HB2	4	0.83
(1,563)	1:134:A:LEU:H	1:135:A:LYS:HB2	5	0.83
(1,563)	1:134:A:LEU:H	1:135:A:LYS:HB2	17	0.83
(1,533)	1:109:A:LEU:H	1:112:A:VAL:HG23	19	0.83
(1,530)	1:66:A:LEU:HD22	1:67:A:PHE:H	5	0.83
(1,503)	1:81:A:HIS:H	1:84:A:VAL:HG23	8	0.83
(1,443)	1:117:A:ARG:H	1:126:A:TYR:HE2	1	0.83
(1,443)	1:117:A:ARG:H	1:126:A:TYR:HE2	24	0.83
(1,413)	1:131:A:CYS:H	1:130:A:LEU:HD13	3	0.83
(1,413)	1:131:A:CYS:H	1:130:A:LEU:HD11	21	0.83
(1,401)	1:113:A:LEU:HD22	1:113:A:LEU:H	18	0.83
(1,395)	1:138:A:SER:H	1:95:A:ALA:HB2	22	0.83
(1,381)	2:30:B:GLU:HG2	2:31:B:LEU:HB2	17	0.83
(1,380)	2:27:B:SER:HA	2:30:B:GLU:HB3	5	0.83
(1,380)	2:27:B:SER:HA	2:30:B:GLU:HB3	21	0.83
(1,332)	1:127:A:ILE:HG12	1:124:A:TYR:HD2	9	0.83
(1,332)	1:127:A:ILE:HG12	1:124:A:TYR:HD2	17	0.83
(1,318)	2:34:B:TYR:HE1	1:83:A:GLU:HB3	21	0.83
(1,304)	2:36:B:THR:HG21	2:35:B:PHE:HB2	6	0.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,304)	2:36:B:THR:HG23	2:35:B:PHE:HB2	18	0.83
(1,304)	2:36:B:THR:HG21	2:35:B:PHE:HB2	23	0.83
(1,290)	2:39:B:TRP:HH2	2:36:B:THR:HB	11	0.83
(1,221)	1:130:A:LEU:HD22	1:70:A:PHE:HZ	8	0.83
(1,221)	1:112:A:VAL:HG21	1:70:A:PHE:HZ	15	0.83
(1,218)	1:116:A:ALA:HB1	1:70:A:PHE:HD2	1	0.83
(1,218)	1:116:A:ALA:HB3	1:70:A:PHE:HD2	14	0.83
(1,218)	1:116:A:ALA:HB1	1:70:A:PHE:HD2	18	0.83
(1,218)	1:116:A:ALA:HB2	1:70:A:PHE:HD2	22	0.83
(1,216)	1:113:A:LEU:HD11	1:70:A:PHE:HD2	7	0.83
(1,207)	1:109:A:LEU:HD22	1:113:A:LEU:H	25	0.83
(1,203)	1:71:A:LEU:HD11	1:68:A:GLU:H	18	0.83
(1,203)	1:71:A:LEU:HD13	1:72:A:GLU:H	22	0.83
(1,184)	1:79:A:ALA:HB1	1:75:A:LYS:HA	22	0.83
(1,178)	1:84:A:VAL:HG21	1:78:A:THR:H	6	0.83
(1,178)	1:84:A:VAL:HG22	1:78:A:THR:H	17	0.83
(1,174)	1:84:A:VAL:HG13	1:124:A:TYR:HA	17	0.83
(1,174)	1:84:A:VAL:HG13	1:124:A:TYR:HA	21	0.83
(1,164)	1:87:A:PHE:HB3	1:87:A:PHE:HE2	11	0.83
(1,164)	1:87:A:PHE:HB3	1:87:A:PHE:HE2	19	0.83
(1,153)	1:88:A:LEU:HD23	1:128:A:ASN:HA	21	0.83
(1,150)	1:88:A:LEU:HD23	1:128:A:ASN:H	15	0.83
(1,143)	1:89:A:TYR:HD2	1:86:A:PRO:HB2	8	0.83
(1,35)	1:127:A:ILE:HG21	1:88:A:LEU:H	10	0.83
(1,35)	1:127:A:ILE:HG21	1:88:A:LEU:H	21	0.83
(1,16)	1:132:A:THR:HG23	1:133:A:VAL:H	8	0.83
(1,15)	1:132:A:THR:HG21	2:27:B:SER:H	16	0.83
(1,2061)	1:87:A:PHE:H	1:85:A:VAL:HG21	13	0.82
(1,2017)	1:93:A:GLN:HE22	1:89:A:TYR:HB3	25	0.82
(1,1722)	2:31:B:LEU:HD22	1:128:A:ASN:HB2	1	0.82
(1,1656)	2:37:B:ALA:HB1	2:39:B:TRP:HZ2	21	0.82
(1,1611)	2:39:B:TRP:HZ3	2:39:B:TRP:HB2	12	0.82
(1,1611)	2:39:B:TRP:HZ3	2:39:B:TRP:HB2	23	0.82
(1,1561)	1:57:A:LYS:HD2	1:57:A:LYS:HA	11	0.82
(1,1518)	1:61:A:LEU:HB2	1:61:A:LEU:HD21	5	0.82
(1,1518)	1:61:A:LEU:HB2	1:61:A:LEU:HD22	25	0.82
(1,1341)	1:76:A:MET:HB3	1:73:A:LEU:HA	3	0.82
(1,1261)	1:86:A:PRO:HD2	1:85:A:VAL:HG21	22	0.82
(1,1143)	1:94:A:ARG:HG2	1:94:A:ARG:H	21	0.82
(1,1122)	1:96:A:HIS:HA	1:139:A:ALA:HB1	8	0.82
(1,907)	1:114:A:SER:HB2	1:115:A:ARG:H	8	0.82
(1,907)	1:114:A:SER:HB2	1:115:A:ARG:H	18	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,869)	1:119:A:ARG:HD3	1:119:A:ARG:HB2	1	0.82
(1,868)	1:119:A:ARG:HD2	1:119:A:ARG:HB2	4	0.82
(1,868)	1:119:A:ARG:HD2	1:119:A:ARG:HB2	13	0.82
(1,792)	1:127:A:ILE:HD11	1:124:A:TYR:HD1	8	0.82
(1,563)	1:113:A:LEU:H	1:111:A:ARG:HB2	7	0.82
(1,563)	1:113:A:LEU:H	1:111:A:ARG:HB2	21	0.82
(1,563)	1:134:A:LEU:H	1:135:A:LYS:HB2	23	0.82
(1,530)	1:66:A:LEU:HD22	1:67:A:PHE:H	12	0.82
(1,530)	1:66:A:LEU:HD23	1:67:A:PHE:H	18	0.82
(1,530)	1:66:A:LEU:HD23	1:67:A:PHE:H	20	0.82
(1,529)	1:67:A:PHE:H	1:68:A:GLU:HB3	10	0.82
(1,503)	1:81:A:HIS:H	1:84:A:VAL:HG22	6	0.82
(1,502)	1:81:A:HIS:H	1:82:A:PRO:HB3	16	0.82
(1,465)	1:106:A:CYS:H	1:103:A:ALA:HB3	17	0.82
(1,443)	1:117:A:ARG:H	1:126:A:TYR:HE2	5	0.82
(1,401)	1:113:A:LEU:HD23	1:113:A:LEU:H	8	0.82
(1,401)	1:113:A:LEU:HD22	1:113:A:LEU:H	11	0.82
(1,381)	2:30:B:GLU:HG2	2:31:B:LEU:HB2	6	0.82
(1,381)	2:30:B:GLU:HG2	2:31:B:LEU:HB2	15	0.82
(1,360)	2:27:B:SER:HB3	2:28:B:ASP:HB3	14	0.82
(1,340)	2:31:B:LEU:HD13	1:88:A:LEU:H	24	0.82
(1,323)	1:84:A:VAL:HG22	2:34:B:TYR:HD1	16	0.82
(1,307)	2:39:B:TRP:HE3	2:36:B:THR:HG21	9	0.82
(1,280)	2:31:B:LEU:HG	1:87:A:PHE:HE2	1	0.82
(1,280)	2:31:B:LEU:HG	1:87:A:PHE:HE2	25	0.82
(1,243)	1:62:A:GLU:HG3	1:61:A:LEU:HD23	11	0.82
(1,221)	1:130:A:LEU:HD22	1:70:A:PHE:HZ	22	0.82
(1,218)	1:116:A:ALA:HB3	1:70:A:PHE:HD2	19	0.82
(1,216)	1:113:A:LEU:HD11	1:70:A:PHE:HD2	24	0.82
(1,208)	1:71:A:LEU:HD23	1:88:A:LEU:H	10	0.82
(1,208)	1:71:A:LEU:HD22	1:88:A:LEU:H	11	0.82
(1,208)	1:71:A:LEU:HD21	1:88:A:LEU:H	17	0.82
(1,206)	1:73:A:LEU:HD22	1:117:A:ARG:HD2	19	0.82
(1,203)	1:71:A:LEU:HD11	1:68:A:GLU:H	16	0.82
(1,178)	1:84:A:VAL:HG21	1:78:A:THR:H	3	0.82
(1,153)	1:88:A:LEU:HD22	1:128:A:ASN:HA	5	0.82
(1,153)	1:88:A:LEU:HD23	1:128:A:ASN:HA	9	0.82
(1,153)	1:88:A:LEU:HD22	1:128:A:ASN:HA	12	0.82
(1,153)	1:88:A:LEU:HD22	1:128:A:ASN:HA	17	0.82
(1,136)	1:91:A:ARG:HG3	1:91:A:ARG:H	9	0.82
(1,136)	1:91:A:ARG:HG3	1:91:A:ARG:H	14	0.82
(1,136)	1:91:A:ARG:HG3	1:91:A:ARG:H	16	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,136)	1:91:A:ARG:HG3	1:91:A:ARG:H	18	0.82
(1,16)	1:132:A:THR:HG21	1:133:A:VAL:H	6	0.82
(1,15)	1:132:A:THR:HG21	1:135:A:LYS:H	2	0.82
(1,15)	1:132:A:THR:HG22	1:135:A:LYS:H	5	0.82
(1,9)	1:134:A:LEU:HD23	1:131:A:CYS:HA	6	0.82
(1,2061)	1:87:A:PHE:H	1:85:A:VAL:HG22	10	0.81
(1,1650)	2:37:B:ALA:HB1	1:121:A:ALA:HB1	14	0.81
(1,1611)	2:39:B:TRP:HZ3	2:39:B:TRP:HB2	3	0.81
(1,1611)	2:39:B:TRP:HZ3	2:39:B:TRP:HB2	24	0.81
(1,1456)	1:69:A:GLU:HG2	1:66:A:LEU:HA	10	0.81
(1,1447)	1:69:A:GLU:HA	1:69:A:GLU:HG3	23	0.81
(1,1375)	1:74:A:CYS:HA	1:77:A:GLN:HB3	7	0.81
(1,1375)	1:74:A:CYS:HA	1:77:A:GLN:HB3	13	0.81
(1,1341)	1:76:A:MET:HB3	1:73:A:LEU:HA	21	0.81
(1,1046)	2:30:B:GLU:HG3	2:30:B:GLU:H	1	0.81
(1,907)	1:114:A:SER:HB2	1:115:A:ARG:H	17	0.81
(1,869)	1:119:A:ARG:HD3	1:119:A:ARG:HB2	13	0.81
(1,868)	1:119:A:ARG:HD2	1:119:A:ARG:HB2	14	0.81
(1,793)	1:124:A:TYR:HE2	1:124:A:TYR:H	10	0.81
(1,793)	1:124:A:TYR:HE1	1:124:A:TYR:H	18	0.81
(1,792)	1:127:A:ILE:HD11	1:124:A:TYR:HD1	12	0.81
(1,563)	1:113:A:LEU:H	1:111:A:ARG:HB2	9	0.81
(1,563)	1:113:A:LEU:H	1:111:A:ARG:HB2	15	0.81
(1,563)	1:134:A:LEU:H	1:135:A:LYS:HB2	20	0.81
(1,563)	1:134:A:LEU:H	1:135:A:LYS:HB2	24	0.81
(1,563)	1:134:A:LEU:H	1:135:A:LYS:HB2	25	0.81
(1,530)	1:66:A:LEU:HD21	1:67:A:PHE:H	14	0.81
(1,530)	1:66:A:LEU:HD21	1:67:A:PHE:H	24	0.81
(1,502)	1:81:A:HIS:H	1:82:A:PRO:HB3	5	0.81
(1,498)	1:87:A:PHE:H	1:84:A:VAL:HG13	16	0.81
(1,484)	1:134:A:LEU:HD11	1:94:A:ARG:H	2	0.81
(1,401)	1:113:A:LEU:HD22	1:113:A:LEU:H	7	0.81
(1,381)	2:30:B:GLU:HG2	2:31:B:LEU:HB2	16	0.81
(1,332)	1:127:A:ILE:HG12	1:124:A:TYR:HD2	6	0.81
(1,304)	2:36:B:THR:HG21	2:35:B:PHE:HB2	2	0.81
(1,304)	2:36:B:THR:HG23	2:35:B:PHE:HB2	17	0.81
(1,300)	2:37:B:ALA:HB3	1:123:A:LEU:HB2	19	0.81
(1,263)	1:132:A:THR:HG23	2:28:B:ASP:HB3	22	0.81
(1,208)	1:71:A:LEU:HD23	1:88:A:LEU:H	25	0.81
(1,207)	1:109:A:LEU:HD22	1:113:A:LEU:H	2	0.81
(1,207)	1:109:A:LEU:HD22	1:113:A:LEU:H	9	0.81
(1,207)	1:109:A:LEU:HD21	1:113:A:LEU:H	17	0.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,205)	1:71:A:LEU:HD11	1:75:A:LYS:HE2	15	0.81
(1,203)	1:71:A:LEU:HD13	1:68:A:GLU:H	24	0.81
(1,184)	1:79:A:ALA:HB1	1:75:A:LYS:HA	14	0.81
(1,153)	1:88:A:LEU:HD23	1:128:A:ASN:HA	4	0.81
(1,153)	1:88:A:LEU:HD23	1:128:A:ASN:HA	6	0.81
(1,141)	1:93:A:GLN:HG2	1:89:A:TYR:HD1	20	0.81
(1,136)	1:91:A:ARG:HG3	1:91:A:ARG:H	2	0.81
(1,136)	1:91:A:ARG:HG3	1:91:A:ARG:H	6	0.81
(1,136)	1:91:A:ARG:HG3	1:91:A:ARG:H	20	0.81
(1,136)	1:91:A:ARG:HG3	1:91:A:ARG:H	22	0.81
(1,136)	1:91:A:ARG:HG3	1:91:A:ARG:H	25	0.81
(1,120)	1:95:A:ALA:HB3	1:100:A:LEU:H	12	0.81
(1,39)	1:127:A:ILE:HD12	1:124:A:TYR:HE2	2	0.81
(1,16)	1:132:A:THR:HG22	1:133:A:VAL:H	12	0.81
(1,16)	1:132:A:THR:HG22	1:133:A:VAL:H	22	0.81
(1,16)	1:132:A:THR:HG22	1:133:A:VAL:H	25	0.81
(1,15)	1:132:A:THR:HG22	1:135:A:LYS:H	9	0.81
(1,9)	1:134:A:LEU:HD22	1:131:A:CYS:HA	11	0.81
(1,2119)	1:122:A:LYS:HB3	1:122:A:LYS:H	5	0.8
(1,1722)	2:31:B:LEU:HD21	1:128:A:ASN:HB2	10	0.8
(1,1649)	2:37:B:ALA:HB3	2:38:B:ARG:HB2	21	0.8
(1,1649)	2:37:B:ALA:HB2	2:38:B:ARG:HB2	23	0.8
(1,1611)	2:39:B:TRP:HZ3	2:39:B:TRP:HB2	9	0.8
(1,1611)	2:39:B:TRP:HZ3	2:39:B:TRP:HB2	13	0.8
(1,1611)	2:39:B:TRP:HZ3	2:39:B:TRP:HB2	14	0.8
(1,1447)	1:69:A:GLU:HA	1:69:A:GLU:HG3	14	0.8
(1,1447)	1:69:A:GLU:HA	1:69:A:GLU:HG3	15	0.8
(1,1396)	1:72:A:GLU:HG2	1:72:A:GLU:H	3	0.8
(1,1271)	1:78:A:THR:HG23	1:78:A:THR:HA	2	0.8
(1,1259)	1:85:A:VAL:HG11	1:75:A:LYS:HD2	24	0.8
(1,880)	1:117:A:ARG:HA	1:117:A:ARG:HD2	4	0.8
(1,869)	1:119:A:ARG:HD3	1:119:A:ARG:HB2	14	0.8
(1,793)	1:124:A:TYR:HE2	1:124:A:TYR:H	13	0.8
(1,694)	1:113:A:LEU:HB2	1:114:A:SER:H	1	0.8
(1,577)	1:75:A:LYS:HE2	1:71:A:LEU:HB3	3	0.8
(1,563)	1:134:A:LEU:H	1:135:A:LYS:HB2	18	0.8
(1,533)	1:109:A:LEU:H	1:112:A:VAL:HG21	14	0.8
(1,533)	1:109:A:LEU:H	1:112:A:VAL:HG21	21	0.8
(1,533)	1:109:A:LEU:H	1:112:A:VAL:HG23	24	0.8
(1,530)	1:66:A:LEU:HD22	1:67:A:PHE:H	1	0.8
(1,530)	1:66:A:LEU:HD22	1:67:A:PHE:H	4	0.8
(1,530)	1:66:A:LEU:HD21	1:67:A:PHE:H	7	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,530)	1:66:A:LEU:HD22	1:67:A:PHE:H	9	0.8
(1,530)	1:66:A:LEU:HD23	1:67:A:PHE:H	10	0.8
(1,502)	1:81:A:HIS:H	1:82:A:PRO:HB3	7	0.8
(1,413)	1:131:A:CYS:H	1:130:A:LEU:HD13	4	0.8
(1,413)	1:131:A:CYS:H	1:134:A:LEU:HD13	6	0.8
(1,413)	1:131:A:CYS:H	1:130:A:LEU:HD13	23	0.8
(1,401)	1:113:A:LEU:HD23	1:113:A:LEU:H	13	0.8
(1,332)	1:127:A:ILE:HG12	1:124:A:TYR:HD2	19	0.8
(1,310)	2:35:B:PHE:HD1	1:127:A:ILE:HB	14	0.8
(1,306)	2:36:B:THR:HG21	1:124:A:TYR:HE2	12	0.8
(1,304)	2:36:B:THR:HG21	2:35:B:PHE:HB2	16	0.8
(1,304)	2:36:B:THR:HG22	2:35:B:PHE:HB2	21	0.8
(1,300)	2:37:B:ALA:HB3	1:123:A:LEU:HB2	11	0.8
(1,290)	2:39:B:TRP:HH2	2:36:B:THR:HB	1	0.8
(1,218)	1:116:A:ALA:HB2	1:70:A:PHE:HD2	2	0.8
(1,218)	1:116:A:ALA:HB2	1:70:A:PHE:HD2	21	0.8
(1,207)	1:109:A:LEU:HD21	1:113:A:LEU:H	8	0.8
(1,207)	1:109:A:LEU:HD21	1:113:A:LEU:H	21	0.8
(1,205)	1:71:A:LEU:HD13	1:75:A:LYS:HE2	19	0.8
(1,200)	1:72:A:GLU:HG3	1:71:A:LEU:HD11	10	0.8
(1,200)	1:72:A:GLU:HG2	1:71:A:LEU:HD13	11	0.8
(1,200)	1:72:A:GLU:HG2	1:71:A:LEU:HD11	19	0.8
(1,174)	1:84:A:VAL:HG13	1:124:A:TYR:HA	13	0.8
(1,153)	1:88:A:LEU:HD22	1:128:A:ASN:HA	23	0.8
(1,150)	1:88:A:LEU:HD23	1:128:A:ASN:H	25	0.8
(1,136)	1:91:A:ARG:HG3	1:91:A:ARG:H	7	0.8
(1,136)	1:91:A:ARG:HG3	1:91:A:ARG:H	10	0.8
(1,117)	1:100:A:LEU:HB2	1:100:A:LEU:HD21	4	0.8
(1,117)	1:100:A:LEU:HB2	1:100:A:LEU:HD21	17	0.8
(1,117)	1:100:A:LEU:HB2	1:100:A:LEU:HD23	22	0.8
(1,35)	1:127:A:ILE:HG23	1:88:A:LEU:H	8	0.8
(1,35)	1:127:A:ILE:HG21	1:88:A:LEU:H	24	0.8
(1,15)	1:132:A:THR:HG22	1:135:A:LYS:H	23	0.8
(1,9)	1:134:A:LEU:HD23	1:131:A:CYS:HA	2	0.8
(1,1722)	2:31:B:LEU:HD21	1:128:A:ASN:HB2	13	0.79
(1,1611)	2:39:B:TRP:HZ3	2:39:B:TRP:HB2	4	0.79
(1,1396)	1:72:A:GLU:HG2	1:72:A:GLU:H	16	0.79
(1,1375)	1:74:A:CYS:HA	1:77:A:GLN:HB3	10	0.79
(1,1375)	1:74:A:CYS:HA	1:77:A:GLN:HB3	15	0.79
(1,869)	1:119:A:ARG:HD3	1:119:A:ARG:HB2	4	0.79
(1,792)	1:127:A:ILE:HD13	1:124:A:TYR:HD1	7	0.79
(1,591)	1:138:A:SER:HB3	1:138:A:SER:H	10	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,577)	1:75:A:LYS:HE2	1:71:A:LEU:HB3	13	0.79
(1,577)	1:75:A:LYS:HE2	1:71:A:LEU:HB3	15	0.79
(1,577)	1:75:A:LYS:HE2	1:71:A:LEU:HB3	19	0.79
(1,533)	1:109:A:LEU:H	1:112:A:VAL:HG22	2	0.79
(1,533)	1:109:A:LEU:H	1:112:A:VAL:HG21	8	0.79
(1,533)	1:109:A:LEU:H	1:112:A:VAL:HG22	15	0.79
(1,530)	1:66:A:LEU:HD21	1:67:A:PHE:H	6	0.79
(1,510)	1:73:A:LEU:HD21	1:77:A:GLN:HE22	3	0.79
(1,508)	1:77:A:GLN:HE22	1:76:A:MET:HE2	19	0.79
(1,503)	1:81:A:HIS:H	1:84:A:VAL:HG21	14	0.79
(1,498)	1:87:A:PHE:H	1:84:A:VAL:HG11	8	0.79
(1,443)	1:117:A:ARG:H	1:126:A:TYR:HE2	19	0.79
(1,427)	1:126:A:TYR:H	1:127:A:ILE:HD12	16	0.79
(1,413)	1:131:A:CYS:H	1:130:A:LEU:HD11	8	0.79
(1,413)	1:131:A:CYS:H	1:130:A:LEU:HD11	20	0.79
(1,395)	1:138:A:SER:H	1:95:A:ALA:HB1	15	0.79
(1,369)	2:26:B:ASP:HB2	1:87:A:PHE:HZ	9	0.79
(1,333)	1:127:A:ILE:HG12	1:130:A:LEU:HD23	25	0.79
(1,332)	1:127:A:ILE:HG12	1:124:A:TYR:HD2	3	0.79
(1,321)	2:34:B:TYR:HD1	2:33:B:GLN:HG2	19	0.79
(1,293)	2:39:B:TRP:HD1	2:38:B:ARG:HB3	4	0.79
(1,290)	2:39:B:TRP:HH2	2:36:B:THR:HB	15	0.79
(1,280)	2:31:B:LEU:HG	1:87:A:PHE:HE2	18	0.79
(1,233)	1:66:A:LEU:HD12	1:63:A:ASN:HB3	19	0.79
(1,221)	1:130:A:LEU:HD21	1:70:A:PHE:HZ	25	0.79
(1,218)	1:116:A:ALA:HB1	1:70:A:PHE:HD2	9	0.79
(1,218)	1:116:A:ALA:HB1	1:70:A:PHE:HD2	24	0.79
(1,205)	1:71:A:LEU:HD13	1:75:A:LYS:HE2	3	0.79
(1,200)	1:72:A:GLU:HG2	1:71:A:LEU:HD11	1	0.79
(1,200)	1:72:A:GLU:HG3	1:71:A:LEU:HD11	16	0.79
(1,184)	1:79:A:ALA:HB2	1:75:A:LYS:HA	6	0.79
(1,184)	1:79:A:ALA:HB2	1:75:A:LYS:HA	12	0.79
(1,178)	1:84:A:VAL:HG23	1:78:A:THR:H	11	0.79
(1,170)	1:85:A:VAL:HG11	1:89:A:TYR:H	3	0.79
(1,164)	1:87:A:PHE:HB3	1:87:A:PHE:HE2	24	0.79
(1,153)	1:88:A:LEU:HD23	1:128:A:ASN:HA	15	0.79
(1,136)	1:91:A:ARG:HG3	1:91:A:ARG:H	3	0.79
(1,136)	1:91:A:ARG:HG3	1:91:A:ARG:H	11	0.79
(1,136)	1:91:A:ARG:HG3	1:91:A:ARG:H	23	0.79
(1,128)	1:93:A:GLN:HG2	1:89:A:TYR:HD1	11	0.79
(1,117)	1:100:A:LEU:HB2	1:100:A:LEU:HD23	7	0.79
(1,117)	1:100:A:LEU:HB2	1:100:A:LEU:HD21	10	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,117)	1:100:A:LEU:HB2	1:100:A:LEU:HD21	16	0.79
(1,35)	1:127:A:ILE:HG22	1:88:A:LEU:H	6	0.79
(1,23)	1:130:A:LEU:HD23	1:130:A:LEU:H	3	0.79
(1,1447)	1:69:A:GLU:HA	1:69:A:GLU:HG3	2	0.78
(1,1396)	1:72:A:GLU:HG2	1:72:A:GLU:H	7	0.78
(1,1375)	1:74:A:CYS:HA	1:77:A:GLN:HB3	5	0.78
(1,1071)	1:101:A:ALA:HB2	1:63:A:ASN:HD21	8	0.78
(1,881)	1:117:A:ARG:HD2	1:117:A:ARG:HB2	13	0.78
(1,869)	1:119:A:ARG:HD3	1:119:A:ARG:HB2	15	0.78
(1,869)	1:119:A:ARG:HD3	1:119:A:ARG:HB2	22	0.78
(1,694)	1:113:A:LEU:HB2	1:114:A:SER:H	7	0.78
(1,694)	1:113:A:LEU:HB2	1:114:A:SER:H	13	0.78
(1,591)	1:138:A:SER:HB3	1:138:A:SER:H	8	0.78
(1,577)	1:75:A:LYS:HE2	1:71:A:LEU:HB3	1	0.78
(1,563)	1:113:A:LEU:H	1:111:A:ARG:HB2	10	0.78
(1,563)	1:134:A:LEU:H	1:135:A:LYS:HB2	11	0.78
(1,533)	1:109:A:LEU:H	1:112:A:VAL:HG23	11	0.78
(1,533)	1:109:A:LEU:H	1:112:A:VAL:HG21	18	0.78
(1,530)	1:66:A:LEU:HD21	1:67:A:PHE:H	2	0.78
(1,519)	1:74:A:CYS:H	1:85:A:VAL:HG23	16	0.78
(1,502)	1:81:A:HIS:H	1:82:A:PRO:HB3	13	0.78
(1,502)	1:81:A:HIS:H	1:82:A:PRO:HB3	25	0.78
(1,427)	1:126:A:TYR:H	1:127:A:ILE:HD13	9	0.78
(1,427)	1:126:A:TYR:H	1:127:A:ILE:HD13	10	0.78
(1,395)	1:138:A:SER:H	1:95:A:ALA:HB1	2	0.78
(1,395)	1:138:A:SER:H	1:95:A:ALA:HB3	5	0.78
(1,333)	1:127:A:ILE:HG12	1:130:A:LEU:HD23	11	0.78
(1,332)	1:127:A:ILE:HG12	1:124:A:TYR:HD2	20	0.78
(1,310)	2:35:B:PHE:HD1	1:127:A:ILE:HB	19	0.78
(1,304)	2:36:B:THR:HG22	2:35:B:PHE:HB2	9	0.78
(1,304)	2:36:B:THR:HG21	2:35:B:PHE:HB2	22	0.78
(1,290)	2:39:B:TRP:HH2	2:36:B:THR:HB	18	0.78
(1,233)	1:66:A:LEU:HD13	1:63:A:ASN:HB3	2	0.78
(1,221)	1:112:A:VAL:HG22	1:70:A:PHE:HZ	4	0.78
(1,218)	1:116:A:ALA:HB1	1:70:A:PHE:HD2	5	0.78
(1,207)	1:109:A:LEU:HD22	1:113:A:LEU:H	23	0.78
(1,200)	1:72:A:GLU:HG2	1:71:A:LEU:HD13	22	0.78
(1,200)	1:72:A:GLU:HG2	1:71:A:LEU:HD13	24	0.78
(1,153)	1:88:A:LEU:HD23	1:128:A:ASN:HA	16	0.78
(1,153)	1:88:A:LEU:HD22	1:128:A:ASN:HA	19	0.78
(1,152)	1:67:A:PHE:HE2	1:88:A:LEU:HD11	3	0.78
(1,150)	1:88:A:LEU:HD23	1:128:A:ASN:H	13	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,143)	1:89:A:TYR:HD2	1:86:A:PRO:HB2	21	0.78
(1,136)	1:91:A:ARG:HG3	1:91:A:ARG:H	15	0.78
(1,136)	1:91:A:ARG:HG3	1:91:A:ARG:H	17	0.78
(1,136)	1:91:A:ARG:HG3	1:91:A:ARG:H	19	0.78
(1,136)	1:91:A:ARG:HG3	1:91:A:ARG:H	24	0.78
(1,117)	1:100:A:LEU:HB2	1:100:A:LEU:HD22	23	0.78
(1,117)	1:100:A:LEU:HB2	1:100:A:LEU:HD21	25	0.78
(1,46)	1:126:A:TYR:HE1	1:122:A:LYS:HB3	24	0.78
(1,39)	1:127:A:ILE:HD13	1:124:A:TYR:HE1	4	0.78
(1,35)	1:127:A:ILE:HG22	1:88:A:LEU:H	2	0.78
(1,2274)	2:39:B:TRP:HE1	2:38:B:ARG:HD2	3	0.77
(1,2274)	2:39:B:TRP:HE1	2:38:B:ARG:HD2	18	0.77
(1,1722)	2:31:B:LEU:HD21	1:128:A:ASN:HB2	6	0.77
(1,1649)	2:37:B:ALA:HB2	2:38:B:ARG:HB2	8	0.77
(1,1611)	2:39:B:TRP:HZ3	2:39:B:TRP:HB2	22	0.77
(1,1553)	1:59:A:TYR:HD1	1:57:A:LYS:HB2	2	0.77
(1,1375)	1:74:A:CYS:HA	1:77:A:GLN:HB3	8	0.77
(1,1168)	1:100:A:LEU:HD23	1:92:A:GLN:HG2	8	0.77
(1,907)	1:114:A:SER:HB2	1:115:A:ARG:H	9	0.77
(1,869)	1:119:A:ARG:HD3	1:119:A:ARG:HB2	11	0.77
(1,869)	1:119:A:ARG:HD3	1:119:A:ARG:HB2	20	0.77
(1,869)	1:119:A:ARG:HD3	1:119:A:ARG:HB2	24	0.77
(1,793)	1:124:A:TYR:HE1	1:124:A:TYR:H	8	0.77
(1,791)	1:124:A:TYR:HB2	1:124:A:TYR:HD1	5	0.77
(1,577)	1:75:A:LYS:HE2	1:71:A:LEU:HB3	9	0.77
(1,563)	2:26:B:ASP:H	2:30:B:GLU:HB3	22	0.77
(1,533)	1:109:A:LEU:H	1:112:A:VAL:HG23	22	0.77
(1,502)	1:81:A:HIS:H	1:82:A:PRO:HB3	10	0.77
(1,413)	1:131:A:CYS:H	1:134:A:LEU:HD12	15	0.77
(1,413)	1:131:A:CYS:H	1:134:A:LEU:HD11	19	0.77
(1,413)	1:131:A:CYS:H	1:130:A:LEU:HD12	24	0.77
(1,395)	1:138:A:SER:H	1:95:A:ALA:HB2	20	0.77
(1,333)	1:127:A:ILE:HG12	1:130:A:LEU:HD22	19	0.77
(1,323)	1:84:A:VAL:HG22	2:34:B:TYR:HD1	21	0.77
(1,310)	2:35:B:PHE:HD1	1:127:A:ILE:HB	18	0.77
(1,310)	2:35:B:PHE:HD1	1:127:A:ILE:HB	22	0.77
(1,304)	2:36:B:THR:HG23	2:35:B:PHE:HB2	24	0.77
(1,300)	2:37:B:ALA:HB2	1:123:A:LEU:HB2	12	0.77
(1,293)	2:39:B:TRP:HD1	2:38:B:ARG:HB3	25	0.77
(1,280)	2:31:B:LEU:HG	1:87:A:PHE:HE2	17	0.77
(1,221)	1:130:A:LEU:HD22	1:70:A:PHE:HZ	23	0.77
(1,218)	1:116:A:ALA:HB3	1:70:A:PHE:HD2	4	0.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,208)	1:71:A:LEU:HD23	1:88:A:LEU:H	1	0.77
(1,208)	1:71:A:LEU:HD22	1:88:A:LEU:H	12	0.77
(1,207)	1:109:A:LEU:HD22	1:113:A:LEU:H	3	0.77
(1,207)	1:109:A:LEU:HD22	1:113:A:LEU:H	15	0.77
(1,203)	1:71:A:LEU:HD11	1:68:A:GLU:H	20	0.77
(1,200)	1:72:A:GLU:HG2	1:71:A:LEU:HD13	13	0.77
(1,184)	1:79:A:ALA:HB2	1:75:A:LYS:HA	9	0.77
(1,178)	1:84:A:VAL:HG21	1:78:A:THR:H	1	0.77
(1,178)	1:84:A:VAL:HG23	1:78:A:THR:H	13	0.77
(1,153)	1:88:A:LEU:HD21	1:128:A:ASN:HA	2	0.77
(1,153)	1:88:A:LEU:HD21	1:128:A:ASN:HA	8	0.77
(1,153)	1:88:A:LEU:HD21	1:128:A:ASN:HA	22	0.77
(1,136)	1:91:A:ARG:HG3	1:91:A:ARG:H	21	0.77
(1,39)	1:127:A:ILE:HD12	1:124:A:TYR:HE1	10	0.77
(1,39)	1:127:A:ILE:HD11	1:124:A:TYR:HE1	16	0.77
(1,39)	1:127:A:ILE:HD13	1:124:A:TYR:HE2	17	0.77
(1,39)	1:127:A:ILE:HD12	1:124:A:TYR:HE2	19	0.77
(1,39)	1:127:A:ILE:HD13	1:124:A:TYR:HE1	24	0.77
(1,39)	1:127:A:ILE:HD12	1:124:A:TYR:HE2	25	0.77
(1,16)	1:132:A:THR:HG21	1:133:A:VAL:H	15	0.77
(1,2005)	1:95:A:ALA:H	1:94:A:ARG:HG3	21	0.76
(1,1447)	1:69:A:GLU:HA	1:69:A:GLU:HG3	17	0.76
(1,1341)	1:76:A:MET:HB3	1:73:A:LEU:HA	8	0.76
(1,1328)	1:77:A:GLN:HG2	1:74:A:CYS:HA	1	0.76
(1,1199)	1:89:A:TYR:HE1	1:71:A:LEU:HD12	5	0.76
(1,1098)	1:100:A:LEU:HD23	1:92:A:GLN:HA	8	0.76
(1,868)	1:119:A:ARG:HD2	1:119:A:ARG:HB2	23	0.76
(1,793)	1:124:A:TYR:HE2	1:124:A:TYR:H	16	0.76
(1,793)	1:124:A:TYR:HE1	1:124:A:TYR:H	22	0.76
(1,793)	1:124:A:TYR:HE2	1:124:A:TYR:H	24	0.76
(1,791)	1:124:A:TYR:HB2	1:124:A:TYR:HD1	4	0.76
(1,791)	1:124:A:TYR:HB2	1:124:A:TYR:HD1	10	0.76
(1,791)	1:124:A:TYR:HB2	1:124:A:TYR:HD1	16	0.76
(1,791)	1:124:A:TYR:HB2	1:124:A:TYR:HD1	24	0.76
(1,694)	1:113:A:LEU:HB2	1:114:A:SER:H	24	0.76
(1,619)	1:135:A:LYS:HG2	1:91:A:ARG:HD3	25	0.76
(1,585)	1:139:A:ALA:HB2	1:140:A:LYS:H	5	0.76
(1,585)	1:139:A:ALA:HB2	1:140:A:LYS:H	14	0.76
(1,533)	1:109:A:LEU:H	1:112:A:VAL:HG21	17	0.76
(1,533)	1:109:A:LEU:H	1:112:A:VAL:HG21	25	0.76
(1,530)	1:66:A:LEU:HD22	1:67:A:PHE:H	13	0.76
(1,530)	1:66:A:LEU:HD22	1:67:A:PHE:H	17	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,529)	1:67:A:PHE:H	1:69:A:GLU:HB2	22	0.76
(1,503)	1:81:A:HIS:H	1:84:A:VAL:HG21	19	0.76
(1,502)	1:81:A:HIS:H	1:82:A:PRO:HB3	6	0.76
(1,484)	1:134:A:LEU:HD13	1:94:A:ARG:H	14	0.76
(1,413)	1:131:A:CYS:H	1:134:A:LEU:HD11	17	0.76
(1,413)	1:131:A:CYS:H	1:130:A:LEU:HD13	22	0.76
(1,395)	1:138:A:SER:H	1:95:A:ALA:HB2	13	0.76
(1,369)	2:26:B:ASP:HB2	2:33:B:GLN:HE21	6	0.76
(1,332)	1:127:A:ILE:HG12	1:124:A:TYR:HD2	21	0.76
(1,332)	1:127:A:ILE:HG12	1:124:A:TYR:HD2	23	0.76
(1,310)	2:35:B:PHE:HD1	1:127:A:ILE:HB	21	0.76
(1,304)	2:36:B:THR:HG22	2:35:B:PHE:HB2	13	0.76
(1,293)	2:39:B:TRP:HD1	2:38:B:ARG:HB3	13	0.76
(1,280)	2:31:B:LEU:HG	1:87:A:PHE:HE2	9	0.76
(1,280)	2:31:B:LEU:HG	1:87:A:PHE:HE2	22	0.76
(1,243)	1:62:A:GLU:HG3	1:61:A:LEU:HD22	5	0.76
(1,243)	1:62:A:GLU:HG3	1:61:A:LEU:HD23	10	0.76
(1,221)	1:130:A:LEU:HD22	1:70:A:PHE:HZ	16	0.76
(1,218)	1:116:A:ALA:HB1	1:70:A:PHE:HD2	11	0.76
(1,218)	1:116:A:ALA:HB3	1:70:A:PHE:HD2	13	0.76
(1,218)	1:116:A:ALA:HB2	1:70:A:PHE:HD2	15	0.76
(1,212)	1:71:A:LEU:HD22	1:71:A:LEU:HB2	6	0.76
(1,212)	1:71:A:LEU:HD23	1:71:A:LEU:HB2	11	0.76
(1,211)	1:71:A:LEU:HD23	1:70:A:PHE:HB3	16	0.76
(1,206)	1:71:A:LEU:HD12	1:89:A:TYR:HB2	13	0.76
(1,205)	1:71:A:LEU:HD11	1:75:A:LYS:HE2	5	0.76
(1,205)	1:71:A:LEU:HD13	1:75:A:LYS:HE2	14	0.76
(1,205)	1:71:A:LEU:HD12	1:75:A:LYS:HE2	17	0.76
(1,200)	1:72:A:GLU:HG2	1:71:A:LEU:HD12	2	0.76
(1,200)	1:72:A:GLU:HG2	1:71:A:LEU:HD12	4	0.76
(1,200)	1:72:A:GLU:HG2	1:71:A:LEU:HD12	5	0.76
(1,200)	1:72:A:GLU:HG2	1:71:A:LEU:HD11	18	0.76
(1,200)	1:72:A:GLU:HG2	1:71:A:LEU:HD11	20	0.76
(1,200)	1:72:A:GLU:HG2	1:71:A:LEU:HD11	25	0.76
(1,178)	1:84:A:VAL:HG23	1:78:A:THR:H	9	0.76
(1,150)	1:88:A:LEU:HD23	1:128:A:ASN:H	7	0.76
(1,150)	1:88:A:LEU:HD21	1:128:A:ASN:H	14	0.76
(1,117)	1:100:A:LEU:HD23	1:92:A:GLN:HG2	9	0.76
(1,117)	1:100:A:LEU:HB2	1:100:A:LEU:HD23	15	0.76
(1,117)	1:100:A:LEU:HB2	1:100:A:LEU:HD23	20	0.76
(1,39)	1:127:A:ILE:HD13	1:124:A:TYR:HE2	11	0.76
(1,35)	1:127:A:ILE:HG23	1:88:A:LEU:H	5	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,35)	1:127:A:ILE:HG22	1:88:A:LEU:H	20	0.76
(1,16)	1:132:A:THR:HG22	1:133:A:VAL:H	23	0.76
(1,2005)	1:95:A:ALA:H	1:94:A:ARG:HG3	15	0.75
(1,1611)	2:39:B:TRP:HZ3	2:39:B:TRP:HB2	7	0.75
(1,1477)	1:66:A:LEU:HD23	1:113:A:LEU:HB3	20	0.75
(1,1341)	1:76:A:MET:HB3	1:73:A:LEU:HA	6	0.75
(1,1196)	1:89:A:TYR:HD1	1:71:A:LEU:HD12	7	0.75
(1,1196)	1:89:A:TYR:HD1	1:71:A:LEU:HD12	12	0.75
(1,1071)	1:101:A:ALA:HB2	1:63:A:ASN:HD21	1	0.75
(1,946)	1:110:A:SER:HB2	1:66:A:LEU:HD13	10	0.75
(1,907)	1:114:A:SER:HB2	1:115:A:ARG:H	16	0.75
(1,869)	1:119:A:ARG:HD3	1:119:A:ARG:HB2	17	0.75
(1,792)	1:127:A:ILE:HD13	1:124:A:TYR:HD1	1	0.75
(1,791)	1:124:A:TYR:HB2	1:124:A:TYR:HD1	13	0.75
(1,534)	1:121:A:ALA:H	1:119:A:ARG:HG3	25	0.75
(1,533)	1:109:A:LEU:H	1:112:A:VAL:HG22	1	0.75
(1,530)	1:66:A:LEU:HD21	1:67:A:PHE:H	15	0.75
(1,529)	1:67:A:PHE:H	1:69:A:GLU:HB2	3	0.75
(1,510)	1:73:A:LEU:HD21	1:77:A:GLN:HE22	16	0.75
(1,503)	1:81:A:HIS:H	1:84:A:VAL:HG23	10	0.75
(1,502)	1:81:A:HIS:H	1:82:A:PRO:HB3	19	0.75
(1,484)	1:134:A:LEU:HD11	1:94:A:ARG:H	11	0.75
(1,413)	1:131:A:CYS:H	1:134:A:LEU:HD12	1	0.75
(1,413)	1:131:A:CYS:H	1:134:A:LEU:HD13	7	0.75
(1,413)	1:131:A:CYS:H	1:134:A:LEU:HD11	12	0.75
(1,398)	1:135:A:LYS:HG2	1:136:A:ALA:H	22	0.75
(1,395)	1:138:A:SER:H	1:95:A:ALA:HB1	16	0.75
(1,395)	1:138:A:SER:H	1:95:A:ALA:HB3	19	0.75
(1,395)	1:138:A:SER:H	1:95:A:ALA:HB3	21	0.75
(1,381)	2:30:B:GLU:HG2	2:31:B:LEU:HB2	10	0.75
(1,369)	2:26:B:ASP:HB2	2:33:B:GLN:HE21	20	0.75
(1,359)	2:29:B:SER:HB2	2:26:B:ASP:HB3	6	0.75
(1,333)	1:127:A:ILE:HG12	1:130:A:LEU:HD23	1	0.75
(1,332)	1:127:A:ILE:HG12	1:124:A:TYR:HD1	16	0.75
(1,332)	1:127:A:ILE:HG12	1:124:A:TYR:HD2	22	0.75
(1,323)	1:84:A:VAL:HG23	2:34:B:TYR:HD1	22	0.75
(1,304)	2:36:B:THR:HG23	2:35:B:PHE:HB2	7	0.75
(1,304)	2:36:B:THR:HG21	2:35:B:PHE:HB2	12	0.75
(1,230)	1:66:A:LEU:HA	1:113:A:LEU:HD21	2	0.75
(1,221)	1:130:A:LEU:HD22	1:70:A:PHE:HZ	6	0.75
(1,218)	1:116:A:ALA:HB2	1:70:A:PHE:HD2	20	0.75
(1,216)	1:113:A:LEU:HD11	1:70:A:PHE:HD2	13	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,212)	1:71:A:LEU:HD23	1:71:A:LEU:HB2	7	0.75
(1,212)	1:71:A:LEU:HD23	1:71:A:LEU:HB2	12	0.75
(1,212)	1:71:A:LEU:HD22	1:71:A:LEU:HB2	22	0.75
(1,208)	1:71:A:LEU:HD23	1:88:A:LEU:H	24	0.75
(1,207)	1:109:A:LEU:HD22	1:113:A:LEU:H	11	0.75
(1,205)	1:71:A:LEU:HD13	1:75:A:LYS:HE2	18	0.75
(1,205)	1:71:A:LEU:HD11	1:75:A:LYS:HE2	23	0.75
(1,200)	1:72:A:GLU:HG2	1:71:A:LEU:HD12	8	0.75
(1,200)	1:72:A:GLU:HG2	1:71:A:LEU:HD13	9	0.75
(1,200)	1:72:A:GLU:HG2	1:71:A:LEU:HD13	12	0.75
(1,200)	1:72:A:GLU:HG2	1:71:A:LEU:HD11	14	0.75
(1,200)	1:72:A:GLU:HG2	1:71:A:LEU:HD12	15	0.75
(1,200)	1:72:A:GLU:HG2	1:71:A:LEU:HD13	21	0.75
(1,200)	1:72:A:GLU:HG3	1:71:A:LEU:HD12	23	0.75
(1,178)	1:84:A:VAL:HG23	1:78:A:THR:H	20	0.75
(1,178)	1:84:A:VAL:HG21	1:78:A:THR:H	22	0.75
(1,136)	1:91:A:ARG:HG3	1:91:A:ARG:H	13	0.75
(1,117)	1:100:A:LEU:HD23	1:92:A:GLN:HG2	19	0.75
(1,111)	1:62:A:GLU:HB3	1:59:A:TYR:HD1	5	0.75
(1,111)	1:104:A:GLU:HB3	1:106:A:CYS:H	25	0.75
(1,39)	1:127:A:ILE:HD12	1:124:A:TYR:HE2	9	0.75
(1,39)	1:127:A:ILE:HD12	1:124:A:TYR:HE1	13	0.75
(1,35)	1:127:A:ILE:HG21	1:88:A:LEU:H	22	0.75
(1,17)	1:133:A:VAL:HG12	1:137:A:HIS:HB2	18	0.75
(1,16)	1:132:A:THR:HG23	1:133:A:VAL:H	18	0.75
(1,15)	1:132:A:THR:HG23	1:135:A:LYS:H	10	0.75
(1,2026)	1:67:A:PHE:HD2	1:92:A:GLN:HE21	18	0.74
(1,1976)	1:100:A:LEU:H	1:138:A:SER:HB2	10	0.74
(1,1196)	1:89:A:TYR:HD1	1:71:A:LEU:HD12	10	0.74
(1,1071)	1:101:A:ALA:HB2	1:63:A:ASN:HD21	2	0.74
(1,961)	1:109:A:LEU:HD13	1:109:A:LEU:HA	6	0.74
(1,961)	1:109:A:LEU:HD12	1:109:A:LEU:HA	9	0.74
(1,961)	1:109:A:LEU:HD13	1:109:A:LEU:HA	11	0.74
(1,961)	1:109:A:LEU:HD13	1:109:A:LEU:HA	19	0.74
(1,961)	1:109:A:LEU:HD11	1:109:A:LEU:HA	20	0.74
(1,909)	1:114:A:SER:HB2	1:113:A:LEU:HG	13	0.74
(1,868)	1:119:A:ARG:HD2	1:119:A:ARG:HB2	1	0.74
(1,577)	1:75:A:LYS:HE2	1:71:A:LEU:HB3	11	0.74
(1,533)	1:109:A:LEU:H	1:112:A:VAL:HG22	9	0.74
(1,529)	1:67:A:PHE:H	1:68:A:GLU:HB3	5	0.74
(1,529)	1:67:A:PHE:H	1:68:A:GLU:HB3	25	0.74
(1,498)	1:87:A:PHE:H	1:84:A:VAL:HG12	7	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,484)	1:134:A:LEU:HD12	1:94:A:ARG:H	20	0.74
(1,465)	1:106:A:CYS:H	1:103:A:ALA:HB3	13	0.74
(1,427)	1:126:A:TYR:H	1:127:A:ILE:HD11	3	0.74
(1,333)	1:127:A:ILE:HG12	1:130:A:LEU:HD22	24	0.74
(1,332)	1:127:A:ILE:HG12	1:124:A:TYR:HD2	1	0.74
(1,332)	1:127:A:ILE:HG12	1:124:A:TYR:HD2	2	0.74
(1,332)	1:127:A:ILE:HG12	1:124:A:TYR:HD2	14	0.74
(1,332)	1:127:A:ILE:HG12	1:124:A:TYR:HD1	24	0.74
(1,323)	1:84:A:VAL:HG22	2:34:B:TYR:HD1	19	0.74
(1,218)	1:116:A:ALA:HB2	1:70:A:PHE:HD2	23	0.74
(1,212)	1:71:A:LEU:HD21	1:71:A:LEU:HB2	1	0.74
(1,212)	1:71:A:LEU:HD23	1:71:A:LEU:HB2	14	0.74
(1,212)	1:71:A:LEU:HD21	1:71:A:LEU:HB2	15	0.74
(1,212)	1:71:A:LEU:HD22	1:71:A:LEU:HB2	18	0.74
(1,212)	1:71:A:LEU:HD22	1:71:A:LEU:HB2	23	0.74
(1,212)	1:71:A:LEU:HD21	1:71:A:LEU:HB2	24	0.74
(1,208)	1:71:A:LEU:HD22	1:88:A:LEU:H	7	0.74
(1,207)	1:109:A:LEU:HD23	1:113:A:LEU:H	1	0.74
(1,207)	1:109:A:LEU:HD21	1:113:A:LEU:H	18	0.74
(1,205)	1:71:A:LEU:HD13	1:75:A:LYS:HE2	1	0.74
(1,205)	1:71:A:LEU:HD12	1:75:A:LYS:HE2	22	0.74
(1,200)	1:72:A:GLU:HG2	1:71:A:LEU:HD11	6	0.74
(1,178)	1:84:A:VAL:HG21	1:78:A:THR:H	15	0.74
(1,164)	1:87:A:PHE:HB3	1:87:A:PHE:HE2	13	0.74
(1,153)	1:88:A:LEU:HD23	1:128:A:ASN:HA	13	0.74
(1,153)	1:88:A:LEU:HD23	1:128:A:ASN:HA	25	0.74
(1,141)	1:93:A:GLN:HG2	1:89:A:TYR:HD1	8	0.74
(1,136)	1:91:A:ARG:HG3	1:91:A:ARG:H	8	0.74
(1,132)	1:92:A:GLN:HB3	1:89:A:TYR:HD1	21	0.74
(1,117)	1:100:A:LEU:HB2	1:100:A:LEU:HD23	2	0.74
(1,39)	1:127:A:ILE:HD13	1:124:A:TYR:HE2	3	0.74
(1,39)	1:127:A:ILE:HD12	1:124:A:TYR:HE2	6	0.74
(1,39)	1:127:A:ILE:HD12	1:124:A:TYR:HE2	7	0.74
(1,39)	1:127:A:ILE:HD13	1:124:A:TYR:HE2	15	0.74
(1,39)	1:127:A:ILE:HD11	1:124:A:TYR:HE2	23	0.74
(1,35)	1:127:A:ILE:HG21	1:88:A:LEU:H	11	0.74
(1,17)	1:133:A:VAL:HG12	1:137:A:HIS:HB2	24	0.74
(1,16)	1:132:A:THR:HG22	1:133:A:VAL:H	9	0.74
(1,2274)	2:39:B:TRP:HE1	2:38:B:ARG:HD2	22	0.73
(1,2017)	1:93:A:GLN:HE22	1:89:A:TYR:HB3	5	0.73
(1,1637)	2:38:B:ARG:HD2	2:39:B:TRP:HD1	21	0.73
(1,1611)	2:39:B:TRP:HZ3	2:39:B:TRP:HB2	8	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1375)	1:74:A:CYS:HA	1:77:A:GLN:HB3	6	0.73
(1,1375)	1:74:A:CYS:HA	1:77:A:GLN:HB3	20	0.73
(1,1375)	1:74:A:CYS:HA	1:77:A:GLN:HB3	25	0.73
(1,1341)	1:76:A:MET:HB3	1:73:A:LEU:HA	18	0.73
(1,961)	1:109:A:LEU:HD11	1:109:A:LEU:HA	1	0.73
(1,961)	1:109:A:LEU:HD12	1:109:A:LEU:HA	2	0.73
(1,961)	1:109:A:LEU:HD12	1:109:A:LEU:HA	4	0.73
(1,961)	1:109:A:LEU:HD12	1:109:A:LEU:HA	5	0.73
(1,961)	1:109:A:LEU:HD11	1:109:A:LEU:HA	7	0.73
(1,961)	1:109:A:LEU:HD11	1:109:A:LEU:HA	8	0.73
(1,961)	1:109:A:LEU:HD13	1:109:A:LEU:HA	14	0.73
(1,961)	1:109:A:LEU:HD11	1:109:A:LEU:HA	16	0.73
(1,961)	1:109:A:LEU:HD13	1:109:A:LEU:HA	17	0.73
(1,961)	1:109:A:LEU:HD12	1:109:A:LEU:HA	21	0.73
(1,961)	1:109:A:LEU:HD11	1:109:A:LEU:HA	25	0.73
(1,946)	1:110:A:SER:HB2	1:66:A:LEU:HD11	12	0.73
(1,869)	1:119:A:ARG:HD3	1:119:A:ARG:HB2	10	0.73
(1,868)	1:119:A:ARG:HD2	1:119:A:ARG:HB2	5	0.73
(1,868)	1:119:A:ARG:HD2	1:119:A:ARG:HB2	21	0.73
(1,533)	1:109:A:LEU:H	1:112:A:VAL:HG21	7	0.73
(1,502)	1:81:A:HIS:H	1:82:A:PRO:HB3	14	0.73
(1,498)	1:87:A:PHE:H	1:84:A:VAL:HG13	1	0.73
(1,484)	1:134:A:LEU:HD11	1:94:A:ARG:H	22	0.73
(1,380)	2:27:B:SER:HA	2:30:B:GLU:HB3	11	0.73
(1,369)	2:26:B:ASP:HB2	1:87:A:PHE:HZ	24	0.73
(1,355)	2:29:B:SER:HB3	2:33:B:GLN:H	6	0.73
(1,333)	1:127:A:ILE:HG12	1:130:A:LEU:HD21	20	0.73
(1,332)	1:127:A:ILE:HG12	1:124:A:TYR:HD2	7	0.73
(1,332)	1:127:A:ILE:HG12	1:124:A:TYR:HD2	15	0.73
(1,332)	1:127:A:ILE:HG12	1:124:A:TYR:HD2	25	0.73
(1,323)	1:84:A:VAL:HG23	2:34:B:TYR:HD1	3	0.73
(1,307)	2:39:B:TRP:HE3	2:36:B:THR:HG23	16	0.73
(1,307)	2:39:B:TRP:HE3	2:36:B:THR:HG23	22	0.73
(1,304)	2:36:B:THR:HG21	2:35:B:PHE:HB2	8	0.73
(1,293)	2:39:B:TRP:HD1	2:38:B:ARG:HB3	3	0.73
(1,293)	2:39:B:TRP:HD1	2:38:B:ARG:HB3	6	0.73
(1,293)	2:39:B:TRP:HD1	2:38:B:ARG:HB3	22	0.73
(1,290)	2:39:B:TRP:HH2	2:36:B:THR:HB	9	0.73
(1,290)	2:39:B:TRP:HH2	2:36:B:THR:HA	14	0.73
(1,212)	1:71:A:LEU:HD23	1:71:A:LEU:HB2	4	0.73
(1,212)	1:71:A:LEU:HD21	1:71:A:LEU:HB2	5	0.73
(1,212)	1:71:A:LEU:HD23	1:71:A:LEU:HB2	9	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,212)	1:71:A:LEU:HD23	1:71:A:LEU:HB2	13	0.73
(1,212)	1:71:A:LEU:HD22	1:71:A:LEU:HB2	20	0.73
(1,212)	1:71:A:LEU:HD21	1:71:A:LEU:HB2	25	0.73
(1,207)	1:109:A:LEU:HD21	1:113:A:LEU:H	4	0.73
(1,207)	1:109:A:LEU:HD21	1:113:A:LEU:H	6	0.73
(1,207)	1:109:A:LEU:HD22	1:113:A:LEU:H	14	0.73
(1,206)	1:71:A:LEU:HD12	1:89:A:TYR:HB2	22	0.73
(1,205)	1:71:A:LEU:HD13	1:75:A:LYS:HE2	20	0.73
(1,200)	1:72:A:GLU:HG2	1:71:A:LEU:HD13	17	0.73
(1,184)	1:79:A:ALA:HB3	1:75:A:LYS:HA	3	0.73
(1,178)	1:84:A:VAL:HG23	1:78:A:THR:H	19	0.73
(1,178)	1:84:A:VAL:HG23	1:78:A:THR:H	23	0.73
(1,164)	1:87:A:PHE:HB3	1:87:A:PHE:HE2	10	0.73
(1,136)	1:91:A:ARG:HG3	1:91:A:ARG:H	1	0.73
(1,136)	1:91:A:ARG:HG3	1:91:A:ARG:H	12	0.73
(1,39)	1:127:A:ILE:HD12	1:124:A:TYR:HE2	1	0.73
(1,39)	1:127:A:ILE:HD12	1:124:A:TYR:HE2	18	0.73
(1,39)	1:127:A:ILE:HD12	1:124:A:TYR:HE2	20	0.73
(1,35)	1:127:A:ILE:HG21	1:88:A:LEU:H	3	0.73
(1,35)	1:127:A:ILE:HG21	1:88:A:LEU:H	4	0.73
(1,35)	1:127:A:ILE:HG23	1:88:A:LEU:H	18	0.73
(1,35)	1:127:A:ILE:HG23	1:88:A:LEU:H	23	0.73
(1,17)	1:133:A:VAL:HG11	1:137:A:HIS:HB2	7	0.73
(1,17)	1:133:A:VAL:HG13	1:137:A:HIS:HB2	10	0.73
(1,2114)	1:75:A:LYS:HG2	1:75:A:LYS:H	16	0.72
(1,2017)	1:93:A:GLN:HE22	1:89:A:TYR:HB3	24	0.72
(1,2005)	1:95:A:ALA:H	1:94:A:ARG:HG3	1	0.72
(1,1611)	2:39:B:TRP:HZ3	2:39:B:TRP:HB2	5	0.72
(1,1392)	1:73:A:LEU:HD23	1:117:A:ARG:HD2	25	0.72
(1,1261)	1:86:A:PRO:HD2	1:85:A:VAL:HG22	16	0.72
(1,1071)	1:101:A:ALA:HB3	1:63:A:ASN:HD21	11	0.72
(1,1071)	1:101:A:ALA:HB2	1:63:A:ASN:HD21	18	0.72
(1,1040)	1:62:A:GLU:HB3	1:59:A:TYR:HA	22	0.72
(1,961)	1:109:A:LEU:HD12	1:109:A:LEU:HA	3	0.72
(1,961)	1:109:A:LEU:HD11	1:109:A:LEU:HA	13	0.72
(1,961)	1:109:A:LEU:HD12	1:109:A:LEU:HA	15	0.72
(1,961)	1:109:A:LEU:HD12	1:109:A:LEU:HA	18	0.72
(1,961)	1:109:A:LEU:HD11	1:109:A:LEU:HA	23	0.72
(1,961)	1:109:A:LEU:HD11	1:109:A:LEU:HA	24	0.72
(1,868)	1:119:A:ARG:HD2	1:119:A:ARG:HB2	3	0.72
(1,868)	1:119:A:ARG:HD2	1:119:A:ARG:HB2	8	0.72
(1,868)	1:119:A:ARG:HD2	1:119:A:ARG:HB2	18	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,827)	1:122:A:LYS:HD2	1:122:A:LYS:HA	3	0.72
(1,827)	1:122:A:LYS:HD2	1:122:A:LYS:HA	10	0.72
(1,793)	1:124:A:TYR:HE1	1:124:A:TYR:H	6	0.72
(1,793)	1:124:A:TYR:HE1	1:124:A:TYR:H	21	0.72
(1,792)	1:127:A:ILE:HD13	1:124:A:TYR:HD1	2	0.72
(1,792)	1:127:A:ILE:HD11	1:124:A:TYR:HD1	14	0.72
(1,792)	1:127:A:ILE:HD12	1:124:A:TYR:HD1	23	0.72
(1,563)	1:134:A:LEU:H	1:135:A:LYS:HB2	1	0.72
(1,533)	1:109:A:LEU:H	1:112:A:VAL:HG22	6	0.72
(1,529)	1:67:A:PHE:H	1:69:A:GLU:HB2	12	0.72
(1,503)	1:81:A:HIS:H	1:84:A:VAL:HG21	5	0.72
(1,484)	1:134:A:LEU:HD11	1:94:A:ARG:H	16	0.72
(1,427)	1:126:A:TYR:H	1:127:A:ILE:HD11	24	0.72
(1,413)	1:131:A:CYS:H	1:134:A:LEU:HD11	10	0.72
(1,413)	1:131:A:CYS:H	1:134:A:LEU:HD12	16	0.72
(1,398)	1:135:A:LYS:HG2	1:136:A:ALA:H	1	0.72
(1,395)	1:138:A:SER:H	1:139:A:ALA:HB1	3	0.72
(1,380)	2:27:B:SER:HA	2:30:B:GLU:HB3	9	0.72
(1,333)	1:127:A:ILE:HG12	1:130:A:LEU:HD21	15	0.72
(1,321)	2:34:B:TYR:HD1	2:33:B:GLN:HG2	7	0.72
(1,304)	2:36:B:THR:HG22	2:35:B:PHE:HB2	4	0.72
(1,293)	2:39:B:TRP:HD1	2:38:B:ARG:HB3	9	0.72
(1,293)	2:39:B:TRP:HD1	2:38:B:ARG:HB3	20	0.72
(1,293)	2:39:B:TRP:HD1	2:38:B:ARG:HB3	23	0.72
(1,290)	2:39:B:TRP:HH2	2:36:B:THR:HB	2	0.72
(1,290)	2:39:B:TRP:HH2	2:36:B:THR:HB	23	0.72
(1,280)	2:31:B:LEU:HG	1:87:A:PHE:HD2	10	0.72
(1,221)	1:130:A:LEU:HD22	1:70:A:PHE:HZ	2	0.72
(1,221)	1:130:A:LEU:HD23	1:70:A:PHE:HZ	13	0.72
(1,212)	1:71:A:LEU:HD23	1:71:A:LEU:HB2	8	0.72
(1,189)	1:85:A:VAL:HG11	1:75:A:LYS:HA	23	0.72
(1,187)	1:77:A:GLN:HG3	1:73:A:LEU:HD13	11	0.72
(1,178)	1:84:A:VAL:HG22	1:78:A:THR:H	2	0.72
(1,178)	1:84:A:VAL:HG23	1:78:A:THR:H	5	0.72
(1,178)	1:84:A:VAL:HG21	1:78:A:THR:H	25	0.72
(1,170)	1:85:A:VAL:HG13	1:75:A:LYS:H	8	0.72
(1,153)	1:88:A:LEU:HD22	1:128:A:ASN:HA	1	0.72
(1,153)	1:88:A:LEU:HD21	1:128:A:ASN:HA	14	0.72
(1,153)	1:88:A:LEU:HD23	1:128:A:ASN:HA	20	0.72
(1,153)	1:88:A:LEU:HD23	1:128:A:ASN:HA	24	0.72
(1,42)	1:126:A:TYR:HD1	1:125:A:VAL:HB	15	0.72
(1,39)	1:127:A:ILE:HD13	1:124:A:TYR:HE2	8	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,17)	1:133:A:VAL:HG12	1:137:A:HIS:HB2	2	0.72
(1,2017)	1:93:A:GLN:HE22	1:89:A:TYR:HB3	3	0.71
(1,2017)	1:93:A:GLN:HE22	1:89:A:TYR:HB3	10	0.71
(1,2005)	1:95:A:ALA:H	1:94:A:ARG:HG3	2	0.71
(1,2005)	1:95:A:ALA:H	1:94:A:ARG:HG3	22	0.71
(1,1770)	1:141:A:LYS:HB3	1:141:A:LYS:H	12	0.71
(1,1651)	2:38:B:ARG:HG2	2:37:B:ALA:HB2	25	0.71
(1,1650)	2:37:B:ALA:HB1	1:121:A:ALA:HB3	17	0.71
(1,1447)	1:69:A:GLU:HA	1:69:A:GLU:HG3	6	0.71
(1,1392)	1:73:A:LEU:HD23	1:117:A:ARG:HD2	22	0.71
(1,1341)	1:76:A:MET:HB3	1:73:A:LEU:HA	4	0.71
(1,1071)	1:101:A:ALA:HB1	1:63:A:ASN:HD21	24	0.71
(1,961)	1:109:A:LEU:HD11	1:109:A:LEU:HA	10	0.71
(1,961)	1:109:A:LEU:HD13	1:109:A:LEU:HA	22	0.71
(1,898)	1:115:A:ARG:HA	1:115:A:ARG:HG2	15	0.71
(1,827)	1:122:A:LYS:HD2	1:122:A:LYS:HA	18	0.71
(1,793)	1:124:A:TYR:HE2	1:124:A:TYR:H	5	0.71
(1,793)	1:124:A:TYR:HE1	1:124:A:TYR:H	25	0.71
(1,792)	1:127:A:ILE:HD11	1:124:A:TYR:HD1	15	0.71
(1,792)	1:127:A:ILE:HD13	1:124:A:TYR:HD1	19	0.71
(1,533)	1:109:A:LEU:H	1:112:A:VAL:HG23	4	0.71
(1,533)	1:109:A:LEU:H	1:112:A:VAL:HG22	12	0.71
(1,533)	1:109:A:LEU:H	1:112:A:VAL:HG23	13	0.71
(1,533)	1:109:A:LEU:H	1:112:A:VAL:HG22	20	0.71
(1,533)	1:109:A:LEU:H	1:112:A:VAL:HG21	23	0.71
(1,529)	1:67:A:PHE:H	1:69:A:GLU:HB2	11	0.71
(1,529)	1:67:A:PHE:H	1:69:A:GLU:HB2	13	0.71
(1,510)	1:73:A:LEU:HD21	1:77:A:GLN:HE22	7	0.71
(1,510)	1:73:A:LEU:HD21	1:77:A:GLN:HE22	17	0.71
(1,510)	1:73:A:LEU:HD21	1:77:A:GLN:HE22	24	0.71
(1,502)	1:81:A:HIS:H	1:82:A:PRO:HB3	1	0.71
(1,498)	1:87:A:PHE:H	1:84:A:VAL:HG12	24	0.71
(1,488)	1:92:A:GLN:HE22	1:64:A:GLU:HG3	9	0.71
(1,484)	1:134:A:LEU:HD13	1:94:A:ARG:H	19	0.71
(1,465)	1:108:A:ILE:HD13	1:106:A:CYS:H	12	0.71
(1,401)	1:113:A:LEU:HD23	1:113:A:LEU:H	1	0.71
(1,398)	1:135:A:LYS:HG2	1:136:A:ALA:H	24	0.71
(1,375)	2:27:B:SER:HB2	2:28:B:ASP:HB3	18	0.71
(1,340)	2:31:B:LEU:HD13	1:88:A:LEU:H	2	0.71
(1,332)	1:127:A:ILE:HG12	1:124:A:TYR:HD2	8	0.71
(1,321)	2:34:B:TYR:HD1	1:83:A:GLU:HB3	2	0.71
(1,310)	2:35:B:PHE:HD1	1:127:A:ILE:HB	2	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,307)	2:36:B:THR:HG21	1:128:A:ASN:HD21	3	0.71
(1,300)	2:37:B:ALA:HB2	1:123:A:LEU:HB2	15	0.71
(1,293)	2:39:B:TRP:HD1	2:38:B:ARG:HB3	2	0.71
(1,293)	2:39:B:TRP:HD1	2:38:B:ARG:HB3	8	0.71
(1,290)	2:39:B:TRP:HH2	2:36:B:THR:HB	19	0.71
(1,216)	1:113:A:LEU:HD12	1:70:A:PHE:HD2	2	0.71
(1,216)	1:113:A:LEU:HD13	1:70:A:PHE:HD2	8	0.71
(1,216)	1:113:A:LEU:HD13	1:70:A:PHE:HD2	9	0.71
(1,212)	1:71:A:LEU:HD21	1:71:A:LEU:HB2	10	0.71
(1,212)	1:71:A:LEU:HD22	1:71:A:LEU:HB2	17	0.71
(1,212)	1:71:A:LEU:HD21	1:71:A:LEU:HB2	19	0.71
(1,212)	1:71:A:LEU:HD23	1:71:A:LEU:HB2	21	0.71
(1,207)	1:109:A:LEU:HD21	1:113:A:LEU:H	5	0.71
(1,205)	1:71:A:LEU:HD12	1:75:A:LYS:HE2	11	0.71
(1,170)	1:85:A:VAL:HG12	1:75:A:LYS:H	4	0.71
(1,152)	1:67:A:PHE:HE2	1:88:A:LEU:HD11	13	0.71
(1,128)	1:93:A:GLN:HG2	1:89:A:TYR:HD1	15	0.71
(1,111)	1:104:A:GLU:HB3	1:106:A:CYS:H	20	0.71
(1,35)	1:127:A:ILE:HG21	1:88:A:LEU:H	15	0.71
(1,16)	1:132:A:THR:HG23	1:133:A:VAL:H	1	0.71
(1,2)	1:141:A:LYS:HA	1:141:A:LYS:HB2	18	0.71
(1,2082)	1:81:A:HIS:H	1:79:A:ALA:HB3	5	0.7
(1,2017)	1:93:A:GLN:HE22	1:89:A:TYR:HB3	4	0.7
(1,2017)	1:93:A:GLN:HE22	1:89:A:TYR:HB3	12	0.7
(1,1341)	1:76:A:MET:HB3	1:73:A:LEU:HA	7	0.7
(1,1228)	1:87:A:PHE:HD1	1:88:A:LEU:HD21	7	0.7
(1,1199)	1:89:A:TYR:HE1	1:71:A:LEU:HD11	3	0.7
(1,1071)	1:101:A:ALA:HB1	1:63:A:ASN:HD21	15	0.7
(1,1071)	1:101:A:ALA:HB3	1:63:A:ASN:HD21	20	0.7
(1,1061)	1:103:A:ALA:HB1	1:106:A:CYS:HB3	6	0.7
(1,1004)	1:108:A:ILE:HD13	1:109:A:LEU:H	2	0.7
(1,1004)	1:108:A:ILE:HD13	1:109:A:LEU:H	10	0.7
(1,1004)	1:108:A:ILE:HD13	1:109:A:LEU:H	13	0.7
(1,1004)	1:108:A:ILE:HD12	1:109:A:LEU:H	16	0.7
(1,1004)	1:108:A:ILE:HD12	1:109:A:LEU:H	21	0.7
(1,961)	1:109:A:LEU:HD12	1:109:A:LEU:HA	12	0.7
(1,923)	1:112:A:VAL:HA	1:112:A:VAL:HG21	20	0.7
(1,902)	1:115:A:ARG:HD2	1:115:A:ARG:H	24	0.7
(1,868)	1:119:A:ARG:HD2	1:119:A:ARG:HB2	9	0.7
(1,793)	1:124:A:TYR:HE1	1:124:A:TYR:H	12	0.7
(1,793)	1:124:A:TYR:HE1	1:124:A:TYR:H	23	0.7
(1,661)	1:133:A:VAL:HG13	1:99:A:PHE:HE1	8	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,533)	1:109:A:LEU:H	1:112:A:VAL:HG21	5	0.7
(1,529)	1:67:A:PHE:H	1:69:A:GLU:HB2	24	0.7
(1,519)	1:74:A:CYS:H	1:85:A:VAL:HG22	2	0.7
(1,519)	1:74:A:CYS:H	1:85:A:VAL:HG23	3	0.7
(1,499)	1:85:A:VAL:H	1:74:A:CYS:HB3	3	0.7
(1,498)	1:87:A:PHE:H	1:84:A:VAL:HG12	2	0.7
(1,498)	1:87:A:PHE:H	1:84:A:VAL:HG11	20	0.7
(1,465)	1:108:A:ILE:HD12	1:106:A:CYS:H	4	0.7
(1,465)	1:106:A:CYS:H	1:103:A:ALA:HB3	7	0.7
(1,434)	1:74:A:CYS:H	1:123:A:LEU:HD12	5	0.7
(1,395)	1:138:A:SER:H	1:95:A:ALA:HB3	12	0.7
(1,395)	1:138:A:SER:H	1:95:A:ALA:HB2	18	0.7
(1,380)	2:27:B:SER:HA	2:30:B:GLU:HB3	12	0.7
(1,368)	2:26:B:ASP:HB3	1:87:A:PHE:HZ	23	0.7
(1,333)	1:127:A:ILE:HG12	1:130:A:LEU:HD23	5	0.7
(1,332)	1:127:A:ILE:HG12	1:124:A:TYR:HD2	12	0.7
(1,323)	1:84:A:VAL:HG21	2:34:B:TYR:HD1	17	0.7
(1,323)	1:84:A:VAL:HG21	2:34:B:TYR:HD1	18	0.7
(1,304)	2:36:B:THR:HG23	2:35:B:PHE:HB2	5	0.7
(1,293)	2:39:B:TRP:HD1	2:38:B:ARG:HB3	10	0.7
(1,293)	2:39:B:TRP:HD1	1:121:A:ALA:HB1	12	0.7
(1,293)	2:39:B:TRP:HD1	2:38:B:ARG:HB3	17	0.7
(1,290)	2:39:B:TRP:HH2	2:36:B:THR:HB	20	0.7
(1,265)	1:127:A:ILE:HD13	2:35:B:PHE:HE1	21	0.7
(1,232)	1:66:A:LEU:HD11	1:62:A:GLU:HA	6	0.7
(1,221)	1:112:A:VAL:HG23	1:70:A:PHE:HZ	21	0.7
(1,212)	1:71:A:LEU:HD23	1:74:A:CYS:HG	2	0.7
(1,206)	1:73:A:LEU:HD23	1:117:A:ARG:HD3	11	0.7
(1,187)	1:77:A:GLN:HG3	1:73:A:LEU:HD13	19	0.7
(1,184)	1:79:A:ALA:HB2	1:75:A:LYS:HA	18	0.7
(1,39)	1:127:A:ILE:HD12	1:124:A:TYR:HE1	5	0.7
(1,39)	1:127:A:ILE:HD13	1:124:A:TYR:HE2	12	0.7
(1,39)	1:127:A:ILE:HD13	1:124:A:TYR:HE2	14	0.7
(1,39)	1:127:A:ILE:HD13	1:124:A:TYR:HE2	21	0.7
(1,17)	1:133:A:VAL:HG13	1:137:A:HIS:HB2	12	0.7
(1,17)	1:133:A:VAL:HG11	1:137:A:HIS:HB2	25	0.7
(1,16)	1:132:A:THR:HG23	1:133:A:VAL:H	10	0.7
(1,5)	1:100:A:LEU:HD13	1:100:A:LEU:H	23	0.7
(1,2)	1:141:A:LYS:HA	1:141:A:LYS:HB2	11	0.7
(1,2274)	2:39:B:TRP:HE1	2:38:B:ARG:HD2	9	0.69
(1,1457)	1:68:A:GLU:HB2	1:68:A:GLU:HG2	1	0.69
(1,1457)	1:68:A:GLU:HB2	1:68:A:GLU:HG2	3	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1457)	1:68:A:GLU:HB2	1:68:A:GLU:HG2	5	0.69
(1,1457)	1:68:A:GLU:HB2	1:68:A:GLU:HG2	7	0.69
(1,1457)	1:68:A:GLU:HB2	1:68:A:GLU:HG2	8	0.69
(1,1457)	1:68:A:GLU:HB2	1:68:A:GLU:HG2	10	0.69
(1,1457)	1:68:A:GLU:HB2	1:68:A:GLU:HG2	11	0.69
(1,1457)	1:68:A:GLU:HB2	1:68:A:GLU:HG2	12	0.69
(1,1457)	1:68:A:GLU:HB2	1:68:A:GLU:HG2	16	0.69
(1,1457)	1:68:A:GLU:HB2	1:68:A:GLU:HG2	19	0.69
(1,1457)	1:68:A:GLU:HB2	1:68:A:GLU:HG2	22	0.69
(1,1457)	1:68:A:GLU:HB2	1:68:A:GLU:HG2	24	0.69
(1,1457)	1:68:A:GLU:HB2	1:68:A:GLU:HG2	25	0.69
(1,1447)	1:69:A:GLU:HA	1:69:A:GLU:HG3	21	0.69
(1,1392)	1:73:A:LEU:HD23	1:117:A:ARG:HD2	15	0.69
(1,1341)	1:76:A:MET:HB3	1:73:A:LEU:HA	15	0.69
(1,1071)	1:101:A:ALA:HB2	1:63:A:ASN:HD21	9	0.69
(1,1004)	1:108:A:ILE:HD13	1:109:A:LEU:H	3	0.69
(1,1004)	1:108:A:ILE:HD13	1:109:A:LEU:H	4	0.69
(1,1004)	1:108:A:ILE:HD11	1:109:A:LEU:H	5	0.69
(1,1004)	1:108:A:ILE:HD12	1:109:A:LEU:H	6	0.69
(1,1004)	1:108:A:ILE:HD11	1:109:A:LEU:H	12	0.69
(1,946)	1:110:A:SER:HB2	1:66:A:LEU:HD11	13	0.69
(1,932)	1:112:A:VAL:HG22	1:126:A:TYR:HA	21	0.69
(1,923)	1:112:A:VAL:HA	1:112:A:VAL:HG23	17	0.69
(1,923)	1:112:A:VAL:HA	1:112:A:VAL:HG22	24	0.69
(1,793)	1:124:A:TYR:HE1	1:124:A:TYR:H	9	0.69
(1,585)	1:139:A:ALA:HB1	1:140:A:LYS:H	19	0.69
(1,529)	1:67:A:PHE:H	1:68:A:GLU:HB3	1	0.69
(1,519)	1:74:A:CYS:H	1:85:A:VAL:HG22	22	0.69
(1,510)	1:73:A:LEU:HD23	1:77:A:GLN:HE22	8	0.69
(1,498)	1:87:A:PHE:H	1:84:A:VAL:HG11	3	0.69
(1,498)	1:87:A:PHE:H	1:84:A:VAL:HG12	11	0.69
(1,484)	1:134:A:LEU:HD11	1:94:A:ARG:H	3	0.69
(1,398)	1:135:A:LYS:HG2	1:136:A:ALA:H	12	0.69
(1,333)	1:127:A:ILE:HG12	1:130:A:LEU:HD22	6	0.69
(1,333)	1:127:A:ILE:HG12	1:130:A:LEU:HD21	7	0.69
(1,332)	1:127:A:ILE:HG12	1:124:A:TYR:HD1	10	0.69
(1,323)	1:84:A:VAL:HG23	2:34:B:TYR:HD1	6	0.69
(1,310)	2:35:B:PHE:HD1	1:127:A:ILE:HB	6	0.69
(1,310)	2:35:B:PHE:HD1	1:127:A:ILE:HB	11	0.69
(1,293)	2:39:B:TRP:HD1	2:38:B:ARG:HB3	21	0.69
(1,290)	2:39:B:TRP:HH2	2:36:B:THR:HB	25	0.69
(1,280)	2:31:B:LEU:HG	1:87:A:PHE:HE2	24	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,265)	1:127:A:ILE:HD13	2:35:B:PHE:HE1	14	0.69
(1,230)	1:66:A:LEU:HA	1:113:A:LEU:HD22	9	0.69
(1,221)	1:130:A:LEU:HD21	1:70:A:PHE:HZ	10	0.69
(1,216)	1:113:A:LEU:HD13	1:70:A:PHE:HD2	14	0.69
(1,207)	1:109:A:LEU:HD22	1:113:A:LEU:H	7	0.69
(1,203)	1:71:A:LEU:HD13	1:68:A:GLU:H	11	0.69
(1,203)	1:71:A:LEU:HD13	1:68:A:GLU:H	12	0.69
(1,189)	1:85:A:VAL:HG12	1:75:A:LYS:HA	4	0.69
(1,184)	1:79:A:ALA:HB3	1:75:A:LYS:HA	7	0.69
(1,178)	1:84:A:VAL:HG22	1:78:A:THR:H	10	0.69
(1,152)	1:67:A:PHE:HE1	1:88:A:LEU:HD13	25	0.69
(1,80)	1:94:A:ARG:HD2	1:94:A:ARG:HB2	17	0.69
(1,35)	1:127:A:ILE:HG22	1:88:A:LEU:H	12	0.69
(1,35)	1:127:A:ILE:HG21	1:88:A:LEU:H	13	0.69
(1,5)	1:100:A:LEU:HD11	1:100:A:LEU:H	10	0.69
(1,1650)	2:37:B:ALA:HB1	1:121:A:ALA:HB1	2	0.68
(1,1477)	1:66:A:LEU:HD22	1:113:A:LEU:HB3	2	0.68
(1,1477)	1:66:A:LEU:HD22	1:113:A:LEU:HB3	19	0.68
(1,1457)	1:68:A:GLU:HB2	1:68:A:GLU:HG2	6	0.68
(1,1457)	1:68:A:GLU:HB2	1:68:A:GLU:HG2	17	0.68
(1,1457)	1:68:A:GLU:HB2	1:68:A:GLU:HG2	18	0.68
(1,1457)	1:68:A:GLU:HB2	1:68:A:GLU:HG2	20	0.68
(1,1457)	1:68:A:GLU:HB2	1:68:A:GLU:HG2	21	0.68
(1,1447)	1:69:A:GLU:HA	1:69:A:GLU:HG3	18	0.68
(1,1375)	1:74:A:CYS:HA	1:77:A:GLN:HB3	16	0.68
(1,1375)	1:74:A:CYS:HA	1:77:A:GLN:HB3	22	0.68
(1,1341)	1:76:A:MET:HB3	1:73:A:LEU:HA	5	0.68
(1,1341)	1:76:A:MET:HB3	1:73:A:LEU:HA	14	0.68
(1,1071)	1:101:A:ALA:HB2	1:63:A:ASN:HD21	14	0.68
(1,1071)	1:101:A:ALA:HB3	1:63:A:ASN:HD21	19	0.68
(1,1004)	1:108:A:ILE:HD11	1:109:A:LEU:H	9	0.68
(1,1004)	1:108:A:ILE:HD12	1:109:A:LEU:H	15	0.68
(1,1004)	1:108:A:ILE:HD12	1:109:A:LEU:H	17	0.68
(1,1004)	1:108:A:ILE:HD13	1:109:A:LEU:H	20	0.68
(1,1004)	1:108:A:ILE:HD13	1:109:A:LEU:H	22	0.68
(1,923)	1:112:A:VAL:HA	1:112:A:VAL:HG23	7	0.68
(1,923)	1:112:A:VAL:HA	1:112:A:VAL:HG21	9	0.68
(1,923)	1:112:A:VAL:HA	1:112:A:VAL:HG22	22	0.68
(1,909)	1:114:A:SER:HB2	1:113:A:LEU:HG	24	0.68
(1,792)	1:127:A:ILE:HD13	1:124:A:TYR:HD1	9	0.68
(1,792)	1:127:A:ILE:HD12	1:124:A:TYR:HD1	22	0.68
(1,723)	1:129:A:GLU:HG2	1:125:A:VAL:HG11	16	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,618)	1:56:A:LYS:HG2	1:57:A:LYS:H	23	0.68
(1,563)	2:26:B:ASP:H	2:30:B:GLU:HB3	8	0.68
(1,563)	1:134:A:LEU:H	1:135:A:LYS:HB2	19	0.68
(1,533)	1:109:A:LEU:H	1:112:A:VAL:HG22	3	0.68
(1,533)	1:109:A:LEU:H	1:112:A:VAL:HG21	10	0.68
(1,533)	1:109:A:LEU:H	1:112:A:VAL:HG21	16	0.68
(1,519)	1:74:A:CYS:H	1:85:A:VAL:HG21	18	0.68
(1,519)	1:74:A:CYS:H	1:85:A:VAL:HG22	23	0.68
(1,502)	1:81:A:HIS:H	1:82:A:PRO:HB3	12	0.68
(1,502)	1:81:A:HIS:H	1:82:A:PRO:HB3	24	0.68
(1,499)	1:85:A:VAL:H	1:74:A:CYS:HB3	24	0.68
(1,498)	1:87:A:PHE:H	1:84:A:VAL:HG12	6	0.68
(1,498)	1:87:A:PHE:H	1:84:A:VAL:HG12	10	0.68
(1,484)	1:134:A:LEU:HD12	1:94:A:ARG:H	23	0.68
(1,484)	1:134:A:LEU:HD11	1:94:A:ARG:H	24	0.68
(1,478)	1:95:A:ALA:H	1:91:A:ARG:HD2	7	0.68
(1,427)	1:126:A:TYR:H	1:127:A:ILE:HD11	15	0.68
(1,427)	1:126:A:TYR:H	1:127:A:ILE:HD13	19	0.68
(1,413)	1:131:A:CYS:H	1:134:A:LEU:HD12	11	0.68
(1,407)	1:133:A:VAL:H	1:130:A:LEU:HD13	2	0.68
(1,407)	1:133:A:VAL:H	1:130:A:LEU:HD13	14	0.68
(1,398)	1:135:A:LYS:HG2	1:136:A:ALA:H	16	0.68
(1,333)	1:127:A:ILE:HG12	1:130:A:LEU:HD22	2	0.68
(1,333)	1:127:A:ILE:HG12	1:130:A:LEU:HD22	14	0.68
(1,333)	1:127:A:ILE:HG12	1:130:A:LEU:HD22	22	0.68
(1,332)	1:127:A:ILE:HG12	1:124:A:TYR:HD1	4	0.68
(1,332)	1:127:A:ILE:HG12	1:124:A:TYR:HD1	13	0.68
(1,323)	1:84:A:VAL:HG23	2:34:B:TYR:HD1	15	0.68
(1,321)	2:34:B:TYR:HD1	1:83:A:GLU:HB3	21	0.68
(1,321)	2:34:B:TYR:HD1	1:83:A:GLU:HB3	25	0.68
(1,310)	2:35:B:PHE:HD1	1:127:A:ILE:HB	23	0.68
(1,310)	2:35:B:PHE:HD1	1:127:A:ILE:HB	25	0.68
(1,293)	2:39:B:TRP:HD1	2:38:B:ARG:HB3	1	0.68
(1,293)	2:39:B:TRP:HD1	2:38:B:ARG:HB3	24	0.68
(1,280)	2:31:B:LEU:HG	1:87:A:PHE:HE2	21	0.68
(1,265)	1:127:A:ILE:HD13	2:35:B:PHE:HE1	3	0.68
(1,243)	1:62:A:GLU:HG3	1:61:A:LEU:HD22	22	0.68
(1,232)	1:66:A:LEU:HD13	1:62:A:GLU:HA	13	0.68
(1,221)	1:112:A:VAL:HG21	1:70:A:PHE:HZ	9	0.68
(1,216)	1:113:A:LEU:HD11	1:70:A:PHE:HD2	10	0.68
(1,207)	1:109:A:LEU:HD21	1:113:A:LEU:H	10	0.68
(1,207)	1:109:A:LEU:HD23	1:113:A:LEU:H	12	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,203)	1:71:A:LEU:HD11	1:68:A:GLU:H	10	0.68
(1,203)	1:71:A:LEU:HD13	1:68:A:GLU:H	17	0.68
(1,189)	1:85:A:VAL:HG11	1:75:A:LYS:HA	13	0.68
(1,189)	1:85:A:VAL:HG11	1:75:A:LYS:HA	14	0.68
(1,184)	1:79:A:ALA:HB1	1:75:A:LYS:HA	24	0.68
(1,178)	1:84:A:VAL:HG21	1:78:A:THR:H	4	0.68
(1,178)	1:84:A:VAL:HG23	1:78:A:THR:H	7	0.68
(1,178)	1:84:A:VAL:HG23	1:78:A:THR:H	12	0.68
(1,153)	1:88:A:LEU:HD21	1:128:A:ASN:HA	11	0.68
(1,117)	1:100:A:LEU:HD21	1:92:A:GLN:HG2	24	0.68
(1,111)	1:62:A:GLU:HB3	1:59:A:TYR:HD1	10	0.68
(1,111)	1:104:A:GLU:HB3	1:106:A:CYS:H	11	0.68
(1,39)	1:127:A:ILE:HD11	1:124:A:TYR:HE2	22	0.68
(1,35)	1:127:A:ILE:HG23	1:88:A:LEU:H	14	0.68
(1,2)	1:141:A:LYS:HA	1:141:A:LYS:HB2	12	0.68
(1,2195)	1:56:A:LYS:H	1:56:A:LYS:HG2	25	0.67
(1,2114)	1:75:A:LYS:HG2	1:75:A:LYS:H	19	0.67
(1,2082)	1:81:A:HIS:H	1:79:A:ALA:HB1	23	0.67
(1,2051)	1:89:A:TYR:H	1:90:A:ASN:HB3	23	0.67
(1,2017)	1:93:A:GLN:HE22	1:89:A:TYR:HB3	17	0.67
(1,1996)	1:97:A:SER:H	1:139:A:ALA:HB1	8	0.67
(1,1861)	1:123:A:LEU:HD21	1:123:A:LEU:H	25	0.67
(1,1652)	2:37:B:ALA:HB1	2:38:B:ARG:HD3	14	0.67
(1,1650)	2:37:B:ALA:HB1	1:121:A:ALA:HB1	18	0.67
(1,1644)	2:31:B:LEU:HA	1:128:A:ASN:HD22	24	0.67
(1,1553)	1:59:A:TYR:HD1	1:57:A:LYS:HB2	19	0.67
(1,1489)	1:65:A:LYS:HG2	1:66:A:LEU:H	22	0.67
(1,1341)	1:76:A:MET:HB3	1:73:A:LEU:HA	24	0.67
(1,1259)	1:85:A:VAL:HG11	1:75:A:LYS:HD2	10	0.67
(1,1199)	1:89:A:TYR:HE1	1:71:A:LEU:HD12	23	0.67
(1,1066)	1:101:A:ALA:HA	1:60:A:LYS:HB2	17	0.67
(1,923)	1:112:A:VAL:HA	1:112:A:VAL:HG21	1	0.67
(1,923)	1:112:A:VAL:HA	1:112:A:VAL:HG21	2	0.67
(1,923)	1:112:A:VAL:HA	1:112:A:VAL:HG22	4	0.67
(1,923)	1:112:A:VAL:HA	1:112:A:VAL:HG23	5	0.67
(1,923)	1:112:A:VAL:HA	1:112:A:VAL:HG21	6	0.67
(1,923)	1:112:A:VAL:HA	1:112:A:VAL:HG23	8	0.67
(1,923)	1:112:A:VAL:HA	1:112:A:VAL:HG23	10	0.67
(1,923)	1:112:A:VAL:HA	1:112:A:VAL:HG21	12	0.67
(1,923)	1:112:A:VAL:HA	1:112:A:VAL:HG21	15	0.67
(1,923)	1:112:A:VAL:HA	1:112:A:VAL:HG23	16	0.67
(1,923)	1:112:A:VAL:HA	1:112:A:VAL:HG23	18	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,923)	1:112:A:VAL:HA	1:112:A:VAL:HG23	21	0.67
(1,923)	1:112:A:VAL:HA	1:112:A:VAL:HG23	23	0.67
(1,923)	1:112:A:VAL:HA	1:112:A:VAL:HG23	25	0.67
(1,902)	1:115:A:ARG:HD2	1:115:A:ARG:H	16	0.67
(1,825)	1:122:A:LYS:HG2	1:125:A:VAL:HG22	11	0.67
(1,793)	1:124:A:TYR:HE1	1:124:A:TYR:H	1	0.67
(1,793)	1:124:A:TYR:HE1	1:124:A:TYR:H	20	0.67
(1,723)	1:129:A:GLU:HG2	1:125:A:VAL:HG12	23	0.67
(1,585)	1:139:A:ALA:HB3	1:140:A:LYS:H	22	0.67
(1,577)	1:75:A:LYS:HE2	1:71:A:LEU:HB3	5	0.67
(1,563)	2:26:B:ASP:H	2:30:B:GLU:HB3	3	0.67
(1,519)	1:74:A:CYS:H	1:85:A:VAL:HG23	14	0.67
(1,510)	1:73:A:LEU:HD23	1:77:A:GLN:HE22	18	0.67
(1,503)	1:81:A:HIS:H	1:84:A:VAL:HG21	7	0.67
(1,503)	1:78:A:THR:HG23	1:81:A:HIS:H	9	0.67
(1,499)	1:85:A:VAL:H	1:74:A:CYS:HB3	15	0.67
(1,498)	1:87:A:PHE:H	1:84:A:VAL:HG12	12	0.67
(1,478)	1:95:A:ALA:H	1:91:A:ARG:HD2	20	0.67
(1,434)	1:74:A:CYS:H	1:123:A:LEU:HD13	9	0.67
(1,434)	1:74:A:CYS:H	1:123:A:LEU:HD11	17	0.67
(1,434)	1:74:A:CYS:H	1:123:A:LEU:HD11	20	0.67
(1,434)	1:74:A:CYS:H	1:123:A:LEU:HD12	21	0.67
(1,434)	1:74:A:CYS:H	1:123:A:LEU:HD13	22	0.67
(1,427)	1:126:A:TYR:H	1:127:A:ILE:HD13	2	0.67
(1,427)	1:126:A:TYR:H	1:127:A:ILE:HD11	8	0.67
(1,427)	1:126:A:TYR:H	1:127:A:ILE:HD13	13	0.67
(1,413)	1:131:A:CYS:H	1:134:A:LEU:HD12	5	0.67
(1,407)	1:133:A:VAL:H	1:130:A:LEU:HD12	19	0.67
(1,398)	1:135:A:LYS:HG2	1:136:A:ALA:H	3	0.67
(1,395)	1:138:A:SER:H	1:95:A:ALA:HB2	7	0.67
(1,366)	1:100:A:LEU:HD13	1:138:A:SER:HB3	3	0.67
(1,366)	1:100:A:LEU:HD12	1:138:A:SER:HB3	22	0.67
(1,323)	1:84:A:VAL:HG23	2:34:B:TYR:HD1	1	0.67
(1,323)	1:84:A:VAL:HG22	2:34:B:TYR:HD1	9	0.67
(1,323)	1:84:A:VAL:HG22	2:34:B:TYR:HD1	14	0.67
(1,323)	1:84:A:VAL:HG23	2:34:B:TYR:HD1	25	0.67
(1,319)	2:34:B:TYR:HE1	1:84:A:VAL:HG22	21	0.67
(1,318)	2:34:B:TYR:HE1	1:83:A:GLU:HB3	25	0.67
(1,307)	2:39:B:TRP:HE3	2:36:B:THR:HG23	23	0.67
(1,304)	2:36:B:THR:HG23	2:35:B:PHE:HB2	3	0.67
(1,293)	2:39:B:TRP:HD1	2:38:B:ARG:HB3	18	0.67
(1,281)	2:31:B:LEU:HD21	1:128:A:ASN:H	18	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,253)	1:57:A:LYS:HE3	1:54:A:MET:HG2	1	0.67
(1,230)	1:66:A:LEU:HA	1:113:A:LEU:HD22	10	0.67
(1,216)	1:113:A:LEU:HD12	1:70:A:PHE:HD2	21	0.67
(1,207)	1:109:A:LEU:HD23	1:113:A:LEU:H	24	0.67
(1,199)	1:72:A:GLU:HG2	1:71:A:LEU:HB3	22	0.67
(1,197)	1:73:A:LEU:HD23	1:123:A:LEU:HB2	20	0.67
(1,187)	1:77:A:GLN:HG3	1:73:A:LEU:HD13	1	0.67
(1,170)	1:85:A:VAL:HG13	1:75:A:LYS:H	25	0.67
(1,117)	1:100:A:LEU:HD22	1:92:A:GLN:HG2	1	0.67
(1,35)	1:127:A:ILE:HG22	1:88:A:LEU:H	1	0.67
(1,35)	1:127:A:ILE:HG22	1:88:A:LEU:H	25	0.67
(1,4)	1:130:A:LEU:HD23	1:127:A:ILE:HA	13	0.67
(1,2082)	1:81:A:HIS:H	1:79:A:ALA:HB1	4	0.66
(1,2051)	1:89:A:TYR:H	1:90:A:ASN:HB3	13	0.66
(1,1652)	2:38:B:ARG:HD2	2:37:B:ALA:HB2	5	0.66
(1,1477)	1:66:A:LEU:HD22	1:113:A:LEU:HB3	1	0.66
(1,1477)	1:66:A:LEU:HD22	1:113:A:LEU:HB3	8	0.66
(1,1454)	1:68:A:GLU:HG2	1:69:A:GLU:H	13	0.66
(1,1392)	1:73:A:LEU:HD21	1:117:A:ARG:HD2	5	0.66
(1,1392)	1:73:A:LEU:HD22	1:117:A:ARG:HD2	23	0.66
(1,1341)	1:76:A:MET:HB3	1:73:A:LEU:HA	25	0.66
(1,1122)	1:96:A:HIS:HA	1:139:A:ALA:HB3	16	0.66
(1,1105)	1:134:A:LEU:HD22	1:99:A:PHE:HE1	8	0.66
(1,1062)	1:103:A:ALA:HB2	1:59:A:TYR:HB3	10	0.66
(1,1004)	1:108:A:ILE:HD11	1:109:A:LEU:H	24	0.66
(1,923)	1:112:A:VAL:HA	1:112:A:VAL:HG21	3	0.66
(1,923)	1:112:A:VAL:HA	1:112:A:VAL:HG22	11	0.66
(1,923)	1:112:A:VAL:HA	1:112:A:VAL:HG22	13	0.66
(1,923)	1:112:A:VAL:HA	1:112:A:VAL:HG23	14	0.66
(1,923)	1:112:A:VAL:HA	1:112:A:VAL:HG22	19	0.66
(1,902)	1:115:A:ARG:HD2	1:115:A:ARG:H	10	0.66
(1,902)	1:115:A:ARG:HD2	1:115:A:ARG:H	13	0.66
(1,868)	1:119:A:ARG:HD2	1:119:A:ARG:HB2	12	0.66
(1,793)	1:124:A:TYR:HE1	1:124:A:TYR:H	15	0.66
(1,793)	1:124:A:TYR:HE1	1:124:A:TYR:H	19	0.66
(1,529)	1:67:A:PHE:H	1:68:A:GLU:HB3	16	0.66
(1,519)	1:74:A:CYS:H	1:85:A:VAL:HG23	20	0.66
(1,510)	1:73:A:LEU:HD23	1:77:A:GLN:HE22	6	0.66
(1,503)	1:81:A:HIS:H	1:84:A:VAL:HG21	16	0.66
(1,499)	1:85:A:VAL:H	1:74:A:CYS:HB3	1	0.66
(1,465)	1:106:A:CYS:H	1:103:A:ALA:HB2	21	0.66
(1,434)	1:74:A:CYS:H	1:123:A:LEU:HD13	15	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,427)	1:126:A:TYR:H	1:127:A:ILE:HD13	6	0.66
(1,413)	1:131:A:CYS:H	1:134:A:LEU:HD12	9	0.66
(1,407)	1:133:A:VAL:H	1:130:A:LEU:HD12	11	0.66
(1,407)	1:133:A:VAL:H	1:130:A:LEU:HD11	20	0.66
(1,401)	1:113:A:LEU:HD22	1:113:A:LEU:H	20	0.66
(1,340)	2:31:B:LEU:HD13	1:88:A:LEU:H	9	0.66
(1,319)	2:34:B:TYR:HE1	1:84:A:VAL:HG23	1	0.66
(1,310)	2:35:B:PHE:HD1	1:127:A:ILE:HB	9	0.66
(1,293)	2:39:B:TRP:HD1	2:38:B:ARG:HB3	7	0.66
(1,290)	2:39:B:TRP:HH2	2:36:B:THR:HB	12	0.66
(1,281)	2:31:B:LEU:HD21	1:128:A:ASN:H	22	0.66
(1,265)	1:127:A:ILE:HD12	2:35:B:PHE:HE1	10	0.66
(1,233)	1:66:A:LEU:HD12	1:63:A:ASN:HB3	14	0.66
(1,232)	1:66:A:LEU:HD13	1:62:A:GLU:HA	15	0.66
(1,230)	1:66:A:LEU:HA	1:113:A:LEU:HD22	4	0.66
(1,221)	1:130:A:LEU:HD23	1:70:A:PHE:HZ	3	0.66
(1,206)	1:71:A:LEU:HD13	1:89:A:TYR:HB2	25	0.66
(1,203)	1:71:A:LEU:HD13	1:68:A:GLU:H	9	0.66
(1,189)	1:85:A:VAL:HG12	1:75:A:LYS:HA	3	0.66
(1,184)	1:79:A:ALA:HB2	1:75:A:LYS:HA	20	0.66
(1,178)	1:84:A:VAL:HG23	1:78:A:THR:H	24	0.66
(1,170)	1:85:A:VAL:HG11	1:75:A:LYS:H	7	0.66
(1,170)	1:85:A:VAL:HG11	1:89:A:TYR:H	18	0.66
(1,170)	1:85:A:VAL:HG12	1:75:A:LYS:H	22	0.66
(1,170)	1:85:A:VAL:HG11	1:75:A:LYS:H	23	0.66
(1,153)	1:88:A:LEU:HD23	1:128:A:ASN:HA	7	0.66
(1,152)	1:67:A:PHE:HE1	1:88:A:LEU:HD11	10	0.66
(1,152)	1:67:A:PHE:HE1	1:88:A:LEU:HD13	12	0.66
(1,151)	1:88:A:LEU:HD12	1:70:A:PHE:HD1	3	0.66
(1,80)	1:94:A:ARG:HD3	1:94:A:ARG:HB2	13	0.66
(1,35)	1:127:A:ILE:HG21	1:88:A:LEU:H	7	0.66
(1,35)	1:127:A:ILE:HG21	1:88:A:LEU:H	17	0.66
(1,5)	1:100:A:LEU:HD12	1:100:A:LEU:H	2	0.66
(1,5)	1:100:A:LEU:HD11	1:100:A:LEU:H	5	0.66
(1,2114)	1:75:A:LYS:HG2	1:75:A:LYS:H	1	0.65
(1,2114)	1:75:A:LYS:HG2	1:75:A:LYS:H	5	0.65
(1,2114)	1:75:A:LYS:HG2	1:75:A:LYS:H	11	0.65
(1,2082)	1:81:A:HIS:H	1:79:A:ALA:HB1	8	0.65
(1,2082)	1:81:A:HIS:H	1:79:A:ALA:HB3	19	0.65
(1,2026)	1:67:A:PHE:HD2	1:92:A:GLN:HE22	21	0.65
(1,1861)	1:123:A:LEU:HD22	1:123:A:LEU:H	1	0.65
(1,1760)	2:24:B:GLN:HG2	2:24:B:GLN:HA	6	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1503)	1:64:A:GLU:HB2	1:64:A:GLU:HG2	1	0.65
(1,1503)	1:64:A:GLU:HB2	1:64:A:GLU:HG2	2	0.65
(1,1503)	1:64:A:GLU:HB2	1:64:A:GLU:HG2	4	0.65
(1,1503)	1:64:A:GLU:HB2	1:64:A:GLU:HG2	5	0.65
(1,1503)	1:64:A:GLU:HB2	1:64:A:GLU:HG2	6	0.65
(1,1503)	1:64:A:GLU:HB2	1:64:A:GLU:HG2	9	0.65
(1,1503)	1:64:A:GLU:HB2	1:64:A:GLU:HG2	10	0.65
(1,1503)	1:64:A:GLU:HB2	1:64:A:GLU:HG2	11	0.65
(1,1503)	1:64:A:GLU:HB2	1:64:A:GLU:HG2	13	0.65
(1,1503)	1:64:A:GLU:HB2	1:64:A:GLU:HG2	15	0.65
(1,1503)	1:64:A:GLU:HB2	1:64:A:GLU:HG2	16	0.65
(1,1503)	1:64:A:GLU:HB2	1:64:A:GLU:HG2	17	0.65
(1,1503)	1:64:A:GLU:HB2	1:64:A:GLU:HG2	18	0.65
(1,1503)	1:64:A:GLU:HB2	1:64:A:GLU:HG2	20	0.65
(1,1503)	1:64:A:GLU:HB2	1:64:A:GLU:HG2	21	0.65
(1,1503)	1:64:A:GLU:HB2	1:64:A:GLU:HG2	22	0.65
(1,1503)	1:64:A:GLU:HB2	1:64:A:GLU:HG2	23	0.65
(1,1503)	1:64:A:GLU:HB2	1:64:A:GLU:HG2	24	0.65
(1,1503)	1:64:A:GLU:HB2	1:64:A:GLU:HG2	25	0.65
(1,1489)	1:65:A:LYS:HG2	1:66:A:LEU:H	12	0.65
(1,1421)	1:71:A:LEU:HD23	1:71:A:LEU:H	7	0.65
(1,1375)	1:74:A:CYS:HA	1:77:A:GLN:HB3	17	0.65
(1,1341)	1:76:A:MET:HB3	1:73:A:LEU:HA	9	0.65
(1,1341)	1:76:A:MET:HB3	1:73:A:LEU:HA	22	0.65
(1,1328)	1:77:A:GLN:HG2	1:74:A:CYS:HA	11	0.65
(1,1232)	1:67:A:PHE:HD1	1:67:A:PHE:HB2	22	0.65
(1,1075)	1:101:A:ALA:HB1	1:60:A:LYS:HB2	23	0.65
(1,1062)	1:103:A:ALA:HB2	1:59:A:TYR:HB3	5	0.65
(1,1047)	1:104:A:GLU:HG2	1:105:A:PHE:H	16	0.65
(1,1004)	1:108:A:ILE:HD13	1:109:A:LEU:H	7	0.65
(1,1004)	1:108:A:ILE:HD12	1:109:A:LEU:H	14	0.65
(1,1004)	1:108:A:ILE:HD11	1:109:A:LEU:H	18	0.65
(1,881)	1:117:A:ARG:HD2	1:117:A:ARG:HB2	11	0.65
(1,879)	1:94:A:ARG:HD2	1:90:A:ASN:HD22	7	0.65
(1,827)	1:122:A:LYS:HD2	1:122:A:LYS:HA	20	0.65
(1,793)	1:124:A:TYR:HE2	1:124:A:TYR:H	4	0.65
(1,793)	1:124:A:TYR:HE1	1:124:A:TYR:H	7	0.65
(1,792)	1:127:A:ILE:HD11	1:124:A:TYR:HD1	3	0.65
(1,792)	1:127:A:ILE:HD13	1:124:A:TYR:HD1	20	0.65
(1,619)	1:135:A:LYS:HG2	1:91:A:ARG:HD3	4	0.65
(1,619)	1:135:A:LYS:HG2	1:91:A:ARG:HD3	21	0.65
(1,577)	1:75:A:LYS:HE2	1:71:A:LEU:HB3	12	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,529)	1:67:A:PHE:H	1:69:A:GLU:HB2	8	0.65
(1,529)	1:67:A:PHE:H	1:69:A:GLU:HB2	19	0.65
(1,519)	1:74:A:CYS:H	1:85:A:VAL:HG23	12	0.65
(1,519)	1:74:A:CYS:H	1:85:A:VAL:HG23	15	0.65
(1,510)	1:73:A:LEU:HD21	1:77:A:GLN:HE22	21	0.65
(1,510)	1:73:A:LEU:HD23	1:77:A:GLN:HE22	23	0.65
(1,508)	1:77:A:GLN:HE22	1:120:A:PRO:HG2	11	0.65
(1,484)	1:134:A:LEU:HD11	1:94:A:ARG:H	8	0.65
(1,427)	1:126:A:TYR:H	1:127:A:ILE:HD11	4	0.65
(1,427)	1:126:A:TYR:H	1:127:A:ILE:HD13	20	0.65
(1,413)	1:131:A:CYS:H	1:130:A:LEU:HD23	13	0.65
(1,413)	1:131:A:CYS:H	1:134:A:LEU:HD11	18	0.65
(1,407)	1:133:A:VAL:H	1:130:A:LEU:HD11	8	0.65
(1,407)	1:133:A:VAL:H	1:130:A:LEU:HD11	21	0.65
(1,366)	1:100:A:LEU:HD11	1:138:A:SER:HB3	19	0.65
(1,340)	2:31:B:LEU:HD13	1:88:A:LEU:H	12	0.65
(1,338)	2:31:B:LEU:HD23	2:32:B:GLU:HG3	16	0.65
(1,323)	1:84:A:VAL:HG21	2:34:B:TYR:HD1	2	0.65
(1,323)	1:84:A:VAL:HG22	2:34:B:TYR:HD1	7	0.65
(1,321)	2:34:B:TYR:HD1	1:83:A:GLU:HB3	3	0.65
(1,310)	2:35:B:PHE:HD1	1:127:A:ILE:HB	1	0.65
(1,310)	2:35:B:PHE:HD1	1:127:A:ILE:HB	3	0.65
(1,290)	2:39:B:TRP:HH2	2:36:B:THR:HB	10	0.65
(1,280)	2:31:B:LEU:HG	1:87:A:PHE:HE2	6	0.65
(1,232)	1:66:A:LEU:HD13	1:110:A:SER:HA	7	0.65
(1,232)	1:66:A:LEU:HD11	1:110:A:SER:HA	12	0.65
(1,232)	1:66:A:LEU:HD13	1:62:A:GLU:HA	24	0.65
(1,230)	1:66:A:LEU:HA	1:113:A:LEU:HD21	23	0.65
(1,216)	1:113:A:LEU:HD12	1:70:A:PHE:HD2	3	0.65
(1,216)	1:113:A:LEU:HD13	1:70:A:PHE:HD2	16	0.65
(1,205)	1:71:A:LEU:HD13	1:75:A:LYS:HE2	10	0.65
(1,205)	1:71:A:LEU:HD12	1:75:A:LYS:HE2	24	0.65
(1,178)	1:84:A:VAL:HG22	1:78:A:THR:H	8	0.65
(1,170)	1:85:A:VAL:HG12	1:75:A:LYS:H	5	0.65
(1,170)	1:85:A:VAL:HG12	1:75:A:LYS:H	21	0.65
(1,141)	1:93:A:GLN:HG2	1:89:A:TYR:HD1	7	0.65
(1,30)	1:129:A:GLU:HG3	1:130:A:LEU:H	21	0.65
(1,17)	1:133:A:VAL:HG13	1:137:A:HIS:HB2	13	0.65
(1,17)	1:133:A:VAL:HG13	1:137:A:HIS:HB2	17	0.65
(1,2114)	1:75:A:LYS:HG2	1:75:A:LYS:H	3	0.64
(1,2114)	1:75:A:LYS:HG2	1:75:A:LYS:H	15	0.64
(1,2082)	1:81:A:HIS:H	1:79:A:ALA:HB1	6	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1861)	1:123:A:LEU:HD21	1:123:A:LEU:H	4	0.64
(1,1861)	1:123:A:LEU:HD21	1:123:A:LEU:H	5	0.64
(1,1861)	1:123:A:LEU:HD22	1:123:A:LEU:H	11	0.64
(1,1861)	1:123:A:LEU:HD23	1:123:A:LEU:H	19	0.64
(1,1801)	1:135:A:LYS:H	1:91:A:ARG:HD3	13	0.64
(1,1650)	2:37:B:ALA:HB2	1:121:A:ALA:HB1	1	0.64
(1,1577)	1:77:A:GLN:HG3	1:73:A:LEU:HD13	11	0.64
(1,1503)	1:64:A:GLU:HB2	1:64:A:GLU:HG2	7	0.64
(1,1503)	1:64:A:GLU:HB2	1:64:A:GLU:HG2	8	0.64
(1,1503)	1:64:A:GLU:HB2	1:64:A:GLU:HG2	14	0.64
(1,1503)	1:64:A:GLU:HB2	1:64:A:GLU:HG2	19	0.64
(1,1496)	1:64:A:GLU:HG3	1:64:A:GLU:HA	21	0.64
(1,1489)	1:65:A:LYS:HG2	1:66:A:LEU:H	4	0.64
(1,1484)	1:65:A:LYS:HA	1:65:A:LYS:HG2	10	0.64
(1,1395)	1:116:A:ALA:HB1	1:73:A:LEU:HD22	5	0.64
(1,1341)	1:76:A:MET:HB3	1:73:A:LEU:HA	20	0.64
(1,1232)	1:67:A:PHE:HD1	1:67:A:PHE:HB2	5	0.64
(1,1232)	1:67:A:PHE:HD1	1:67:A:PHE:HB2	7	0.64
(1,1232)	1:67:A:PHE:HD1	1:67:A:PHE:HB2	9	0.64
(1,1232)	1:67:A:PHE:HD1	1:67:A:PHE:HB2	11	0.64
(1,1232)	1:67:A:PHE:HD1	1:67:A:PHE:HB2	24	0.64
(1,1094)	1:100:A:LEU:HD22	1:138:A:SER:HB2	3	0.64
(1,1070)	1:101:A:ALA:HB3	1:102:A:SER:H	14	0.64
(1,1062)	1:103:A:ALA:HB3	1:59:A:TYR:HB3	20	0.64
(1,1004)	1:108:A:ILE:HD11	1:109:A:LEU:H	19	0.64
(1,1004)	1:108:A:ILE:HD11	1:109:A:LEU:H	23	0.64
(1,932)	1:112:A:VAL:HG21	1:126:A:TYR:HA	11	0.64
(1,932)	1:112:A:VAL:HG22	1:126:A:TYR:HA	14	0.64
(1,909)	1:114:A:SER:HB2	1:113:A:LEU:HG	7	0.64
(1,909)	1:114:A:SER:HB2	1:113:A:LEU:HG	20	0.64
(1,825)	1:122:A:LYS:HG2	1:125:A:VAL:HG21	4	0.64
(1,825)	1:122:A:LYS:HG2	1:125:A:VAL:HG21	12	0.64
(1,529)	1:67:A:PHE:H	1:69:A:GLU:HB2	7	0.64
(1,519)	1:74:A:CYS:H	1:85:A:VAL:HG21	4	0.64
(1,519)	1:74:A:CYS:H	1:85:A:VAL:HG21	17	0.64
(1,499)	1:85:A:VAL:H	1:74:A:CYS:HB3	17	0.64
(1,499)	1:85:A:VAL:H	1:74:A:CYS:HB3	22	0.64
(1,498)	1:87:A:PHE:H	1:84:A:VAL:HG13	4	0.64
(1,434)	1:74:A:CYS:H	1:123:A:LEU:HD13	4	0.64
(1,434)	1:74:A:CYS:H	1:123:A:LEU:HD12	11	0.64
(1,434)	1:74:A:CYS:H	1:123:A:LEU:HD11	18	0.64
(1,434)	1:74:A:CYS:H	1:123:A:LEU:HD12	24	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,407)	1:133:A:VAL:H	1:130:A:LEU:HD12	15	0.64
(1,407)	1:133:A:VAL:H	1:130:A:LEU:HD13	16	0.64
(1,395)	1:138:A:SER:H	1:95:A:ALA:HB2	14	0.64
(1,387)	1:141:A:LYS:H	1:141:A:LYS:HG3	6	0.64
(1,366)	1:100:A:LEU:HD11	1:138:A:SER:HB3	15	0.64
(1,333)	1:127:A:ILE:HG12	1:130:A:LEU:HD21	17	0.64
(1,323)	1:84:A:VAL:HG22	2:34:B:TYR:HD1	20	0.64
(1,321)	2:34:B:TYR:HD1	1:83:A:GLU:HB3	16	0.64
(1,319)	2:34:B:TYR:HE1	1:84:A:VAL:HG21	17	0.64
(1,310)	2:35:B:PHE:HD1	1:127:A:ILE:HB	8	0.64
(1,310)	2:35:B:PHE:HD1	1:127:A:ILE:HB	20	0.64
(1,300)	2:37:B:ALA:HB1	1:123:A:LEU:HB2	23	0.64
(1,290)	2:39:B:TRP:HH2	2:36:B:THR:HB	16	0.64
(1,265)	1:127:A:ILE:HD13	2:35:B:PHE:HE1	17	0.64
(1,228)	1:62:A:GLU:HG2	1:66:A:LEU:HD12	10	0.64
(1,207)	1:109:A:LEU:HD23	1:113:A:LEU:H	22	0.64
(1,202)	1:71:A:LEU:HA	1:74:A:CYS:HB2	16	0.64
(1,184)	1:79:A:ALA:HB3	1:75:A:LYS:HA	1	0.64
(1,170)	1:85:A:VAL:HG11	1:75:A:LYS:H	14	0.64
(1,152)	1:67:A:PHE:HE1	1:88:A:LEU:HD12	4	0.64
(1,152)	1:67:A:PHE:HE1	1:88:A:LEU:HD13	17	0.64
(1,144)	1:89:A:TYR:HB2	1:89:A:TYR:HE2	9	0.64
(1,144)	1:89:A:TYR:HB2	1:89:A:TYR:HE2	15	0.64
(1,143)	1:89:A:TYR:HD2	1:86:A:PRO:HB2	10	0.64
(1,134)	1:92:A:GLN:HG2	1:95:A:ALA:H	10	0.64
(1,128)	1:93:A:GLN:HG2	1:89:A:TYR:HD1	4	0.64
(1,97)	1:105:A:PHE:HD1	1:134:A:LEU:HA	1	0.64
(1,80)	1:94:A:ARG:HD2	1:94:A:ARG:HB2	19	0.64
(1,42)	1:126:A:TYR:HD1	1:125:A:VAL:HB	21	0.64
(1,5)	1:100:A:LEU:HD11	1:100:A:LEU:H	20	0.64
(1,2082)	1:81:A:HIS:H	1:79:A:ALA:HB3	10	0.63
(1,2082)	1:81:A:HIS:H	1:79:A:ALA:HB3	14	0.63
(1,2082)	1:81:A:HIS:H	1:79:A:ALA:HB2	16	0.63
(1,2082)	1:81:A:HIS:H	1:79:A:ALA:HB2	21	0.63
(1,1861)	1:123:A:LEU:HD23	1:123:A:LEU:H	10	0.63
(1,1861)	1:123:A:LEU:HD21	1:123:A:LEU:H	16	0.63
(1,1861)	1:123:A:LEU:HD23	1:123:A:LEU:H	18	0.63
(1,1788)	1:139:A:ALA:H	1:135:A:LYS:HD3	5	0.63
(1,1760)	2:24:B:GLN:HG2	2:24:B:GLN:HA	10	0.63
(1,1554)	1:59:A:TYR:HE1	1:57:A:LYS:HB2	15	0.63
(1,1503)	1:64:A:GLU:HB2	1:64:A:GLU:HG2	3	0.63
(1,1489)	1:65:A:LYS:HG2	1:66:A:LEU:H	2	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1477)	1:66:A:LEU:HD21	1:113:A:LEU:HB3	18	0.63
(1,1447)	1:69:A:GLU:HA	1:69:A:GLU:HG3	20	0.63
(1,1232)	1:67:A:PHE:HD1	1:67:A:PHE:HB2	2	0.63
(1,1232)	1:67:A:PHE:HD1	1:67:A:PHE:HB2	6	0.63
(1,1232)	1:67:A:PHE:HD1	1:67:A:PHE:HB2	12	0.63
(1,1232)	1:67:A:PHE:HD1	1:67:A:PHE:HB2	15	0.63
(1,1232)	1:67:A:PHE:HD1	1:67:A:PHE:HB2	16	0.63
(1,1232)	1:67:A:PHE:HD1	1:67:A:PHE:HB2	20	0.63
(1,1199)	1:89:A:TYR:HE1	1:71:A:LEU:HD12	4	0.63
(1,1199)	1:89:A:TYR:HE1	1:71:A:LEU:HD11	14	0.63
(1,1115)	1:98:A:LEU:HD21	1:96:A:HIS:HE1	15	0.63
(1,1004)	1:108:A:ILE:HD12	1:109:A:LEU:H	11	0.63
(1,996)	1:108:A:ILE:HG22	1:112:A:VAL:HG12	24	0.63
(1,946)	1:110:A:SER:HB2	1:66:A:LEU:HD11	4	0.63
(1,932)	1:112:A:VAL:HG22	1:126:A:TYR:HA	25	0.63
(1,848)	1:120:A:PRO:HG3	1:119:A:ARG:HA	1	0.63
(1,825)	1:122:A:LYS:HG2	1:125:A:VAL:HG21	8	0.63
(1,723)	1:129:A:GLU:HG2	1:125:A:VAL:HG11	14	0.63
(1,529)	1:67:A:PHE:H	1:69:A:GLU:HB2	17	0.63
(1,519)	1:74:A:CYS:H	1:85:A:VAL:HG21	5	0.63
(1,519)	1:74:A:CYS:H	1:85:A:VAL:HG21	9	0.63
(1,519)	1:74:A:CYS:H	1:85:A:VAL:HG23	24	0.63
(1,510)	1:73:A:LEU:HD21	1:77:A:GLN:HE22	14	0.63
(1,510)	1:73:A:LEU:HD21	1:77:A:GLN:HE22	22	0.63
(1,510)	1:73:A:LEU:HD21	1:77:A:GLN:HE22	25	0.63
(1,499)	1:85:A:VAL:H	1:74:A:CYS:HB3	8	0.63
(1,499)	1:85:A:VAL:H	1:74:A:CYS:HB3	14	0.63
(1,499)	1:85:A:VAL:H	1:74:A:CYS:HB3	18	0.63
(1,498)	1:87:A:PHE:H	1:84:A:VAL:HG13	14	0.63
(1,498)	1:87:A:PHE:H	1:84:A:VAL:HG12	17	0.63
(1,465)	1:106:A:CYS:H	1:103:A:ALA:HB3	3	0.63
(1,465)	1:106:A:CYS:H	1:103:A:ALA:HB2	22	0.63
(1,454)	1:114:A:SER:H	1:112:A:VAL:HG23	5	0.63
(1,427)	1:126:A:TYR:H	1:127:A:ILE:HD13	7	0.63
(1,427)	1:126:A:TYR:H	1:127:A:ILE:HD11	11	0.63
(1,427)	1:126:A:TYR:H	1:127:A:ILE:HD11	12	0.63
(1,427)	1:126:A:TYR:H	1:127:A:ILE:HD13	18	0.63
(1,407)	1:133:A:VAL:H	1:130:A:LEU:HD13	5	0.63
(1,407)	1:133:A:VAL:H	1:130:A:LEU:HD11	17	0.63
(1,407)	1:133:A:VAL:H	1:130:A:LEU:HD13	25	0.63
(1,395)	1:138:A:SER:H	1:95:A:ALA:HB3	9	0.63
(1,366)	1:100:A:LEU:HD11	1:138:A:SER:HB3	17	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,340)	2:31:B:LEU:HD13	1:88:A:LEU:H	20	0.63
(1,333)	1:127:A:ILE:HG12	1:130:A:LEU:HD21	18	0.63
(1,332)	1:127:A:ILE:HG12	1:124:A:TYR:HD1	5	0.63
(1,323)	1:84:A:VAL:HG22	2:34:B:TYR:HD1	5	0.63
(1,319)	2:34:B:TYR:HE1	1:84:A:VAL:HG23	3	0.63
(1,319)	2:34:B:TYR:HE1	1:84:A:VAL:HG23	6	0.63
(1,319)	2:34:B:TYR:HE1	1:84:A:VAL:HG22	13	0.63
(1,319)	2:34:B:TYR:HE1	1:84:A:VAL:HG22	16	0.63
(1,265)	1:127:A:ILE:HD12	2:35:B:PHE:HE1	1	0.63
(1,265)	1:127:A:ILE:HD13	2:35:B:PHE:HE1	8	0.63
(1,265)	1:127:A:ILE:HD12	2:35:B:PHE:HE1	13	0.63
(1,230)	1:66:A:LEU:HA	1:113:A:LEU:HD21	6	0.63
(1,228)	1:62:A:GLU:HG2	1:66:A:LEU:HD13	4	0.63
(1,228)	1:62:A:GLU:HG2	1:66:A:LEU:HD13	5	0.63
(1,228)	1:62:A:GLU:HG2	1:66:A:LEU:HD12	25	0.63
(1,216)	1:113:A:LEU:HD11	1:70:A:PHE:HD2	18	0.63
(1,212)	1:71:A:LEU:HD22	1:74:A:CYS:HG	3	0.63
(1,195)	1:73:A:LEU:HD23	1:70:A:PHE:HA	15	0.63
(1,170)	1:85:A:VAL:HG12	1:75:A:LYS:H	15	0.63
(1,152)	1:67:A:PHE:HE1	1:88:A:LEU:HD13	18	0.63
(1,144)	1:89:A:TYR:HB2	1:89:A:TYR:HE2	1	0.63
(1,144)	1:89:A:TYR:HB2	1:89:A:TYR:HE2	2	0.63
(1,144)	1:89:A:TYR:HB2	1:89:A:TYR:HE2	3	0.63
(1,144)	1:89:A:TYR:HB2	1:89:A:TYR:HE2	6	0.63
(1,144)	1:89:A:TYR:HB2	1:89:A:TYR:HE2	8	0.63
(1,144)	1:89:A:TYR:HB2	1:89:A:TYR:HE2	13	0.63
(1,144)	1:89:A:TYR:HB2	1:89:A:TYR:HE2	14	0.63
(1,144)	1:89:A:TYR:HB2	1:89:A:TYR:HE2	17	0.63
(1,144)	1:89:A:TYR:HB2	1:89:A:TYR:HE2	19	0.63
(1,144)	1:89:A:TYR:HB2	1:89:A:TYR:HE2	21	0.63
(1,144)	1:89:A:TYR:HB2	1:89:A:TYR:HE2	22	0.63
(1,144)	1:89:A:TYR:HB2	1:89:A:TYR:HE2	24	0.63
(1,123)	1:95:A:ALA:HB2	1:134:A:LEU:HB2	12	0.63
(1,80)	1:94:A:ARG:HD3	1:94:A:ARG:HB2	7	0.63
(1,80)	1:94:A:ARG:HD3	1:94:A:ARG:HB2	8	0.63
(1,44)	1:126:A:TYR:HE2	1:126:A:TYR:HB2	24	0.63
(1,2114)	1:75:A:LYS:HG2	1:75:A:LYS:H	4	0.62
(1,2114)	1:75:A:LYS:HG2	1:75:A:LYS:H	9	0.62
(1,2114)	1:75:A:LYS:HG2	1:75:A:LYS:H	13	0.62
(1,2114)	1:75:A:LYS:HG2	1:75:A:LYS:H	21	0.62
(1,2082)	1:81:A:HIS:H	1:79:A:ALA:HB2	7	0.62
(1,2082)	1:81:A:HIS:H	1:79:A:ALA:HB3	24	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2051)	1:89:A:TYR:H	1:90:A:ASN:HB3	3	0.62
(1,1861)	1:123:A:LEU:HD21	1:123:A:LEU:H	3	0.62
(1,1861)	1:123:A:LEU:HD21	1:123:A:LEU:H	24	0.62
(1,1753)	2:27:B:SER:HB2	2:27:B:SER:HA	21	0.62
(1,1650)	2:37:B:ALA:HB1	1:121:A:ALA:HB3	6	0.62
(1,1633)	2:38:B:ARG:HD2	2:38:B:ARG:HB2	8	0.62
(1,1629)	2:38:B:ARG:HG2	2:38:B:ARG:HA	9	0.62
(1,1577)	1:77:A:GLN:HG3	1:73:A:LEU:HD13	19	0.62
(1,1554)	1:59:A:TYR:HE1	1:57:A:LYS:HB2	2	0.62
(1,1489)	1:65:A:LYS:HG2	1:66:A:LEU:H	7	0.62
(1,1489)	1:65:A:LYS:HG2	1:66:A:LEU:H	15	0.62
(1,1341)	1:76:A:MET:HB3	1:73:A:LEU:HA	13	0.62
(1,1232)	1:67:A:PHE:HD1	1:67:A:PHE:HB2	1	0.62
(1,1232)	1:67:A:PHE:HD1	1:67:A:PHE:HB2	4	0.62
(1,1232)	1:67:A:PHE:HD1	1:67:A:PHE:HB2	8	0.62
(1,1232)	1:67:A:PHE:HD1	1:67:A:PHE:HB2	14	0.62
(1,1232)	1:67:A:PHE:HD1	1:67:A:PHE:HB2	17	0.62
(1,1232)	1:67:A:PHE:HD1	1:67:A:PHE:HB2	18	0.62
(1,1232)	1:67:A:PHE:HD1	1:67:A:PHE:HB2	21	0.62
(1,1232)	1:67:A:PHE:HD1	1:67:A:PHE:HB2	23	0.62
(1,1232)	1:67:A:PHE:HD1	1:67:A:PHE:HB2	25	0.62
(1,1122)	1:96:A:HIS:HA	1:139:A:ALA:HB2	20	0.62
(1,1088)	1:100:A:LEU:HD22	1:105:A:PHE:HD2	19	0.62
(1,1070)	1:101:A:ALA:HB3	1:102:A:SER:H	21	0.62
(1,1070)	1:101:A:ALA:HB3	1:102:A:SER:H	23	0.62
(1,1070)	1:101:A:ALA:HB2	1:102:A:SER:H	24	0.62
(1,1004)	1:108:A:ILE:HD12	1:109:A:LEU:H	1	0.62
(1,1004)	1:108:A:ILE:HD12	1:109:A:LEU:H	25	0.62
(1,932)	1:112:A:VAL:HG21	1:126:A:TYR:HA	4	0.62
(1,932)	1:112:A:VAL:HG21	1:126:A:TYR:HA	13	0.62
(1,932)	1:112:A:VAL:HG22	1:126:A:TYR:HA	23	0.62
(1,909)	1:114:A:SER:HB2	1:113:A:LEU:HG	1	0.62
(1,902)	1:115:A:ARG:HD2	1:115:A:ARG:H	23	0.62
(1,825)	1:122:A:LYS:HG2	1:125:A:VAL:HG23	15	0.62
(1,825)	1:122:A:LYS:HG2	1:125:A:VAL:HG23	19	0.62
(1,766)	1:126:A:TYR:HE1	1:115:A:ARG:HB2	5	0.62
(1,607)	1:136:A:ALA:HB2	1:137:A:HIS:HA	3	0.62
(1,519)	1:74:A:CYS:H	1:85:A:VAL:HG22	1	0.62
(1,519)	1:74:A:CYS:H	1:85:A:VAL:HG22	8	0.62
(1,499)	1:85:A:VAL:H	1:74:A:CYS:HB3	20	0.62
(1,465)	1:106:A:CYS:H	1:103:A:ALA:HB3	16	0.62
(1,451)	1:114:A:SER:H	1:117:A:ARG:HB2	8	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,434)	1:74:A:CYS:H	1:123:A:LEU:HD13	23	0.62
(1,427)	1:126:A:TYR:H	1:127:A:ILE:HD13	1	0.62
(1,427)	1:126:A:TYR:H	1:127:A:ILE:HD11	14	0.62
(1,427)	1:126:A:TYR:H	1:127:A:ILE:HD12	22	0.62
(1,427)	1:126:A:TYR:H	1:127:A:ILE:HD12	23	0.62
(1,413)	1:131:A:CYS:H	1:134:A:LEU:HD11	14	0.62
(1,413)	1:131:A:CYS:H	1:134:A:LEU:HD13	25	0.62
(1,407)	1:133:A:VAL:H	1:130:A:LEU:HD13	3	0.62
(1,407)	1:133:A:VAL:H	1:130:A:LEU:HD13	4	0.62
(1,407)	1:133:A:VAL:H	1:130:A:LEU:HD11	7	0.62
(1,407)	1:133:A:VAL:H	1:130:A:LEU:HD13	9	0.62
(1,380)	2:27:B:SER:HA	2:30:B:GLU:HB3	3	0.62
(1,366)	1:100:A:LEU:HD12	1:138:A:SER:HB3	4	0.62
(1,366)	1:100:A:LEU:HD12	1:138:A:SER:HB3	7	0.62
(1,366)	1:100:A:LEU:HD11	1:138:A:SER:HB3	11	0.62
(1,366)	1:100:A:LEU:HD12	1:138:A:SER:HB3	25	0.62
(1,323)	1:84:A:VAL:HG21	2:34:B:TYR:HD1	10	0.62
(1,323)	1:84:A:VAL:HG22	2:34:B:TYR:HD1	11	0.62
(1,319)	2:34:B:TYR:HE1	1:84:A:VAL:HG21	10	0.62
(1,307)	2:39:B:TRP:HE3	2:36:B:THR:HG22	10	0.62
(1,281)	2:31:B:LEU:HD22	1:128:A:ASN:H	16	0.62
(1,280)	2:31:B:LEU:HG	1:87:A:PHE:HE2	14	0.62
(1,232)	1:66:A:LEU:HD12	1:62:A:GLU:HA	3	0.62
(1,227)	1:62:A:GLU:HG2	1:61:A:LEU:HG	11	0.62
(1,227)	1:62:A:GLU:HG2	1:61:A:LEU:HG	13	0.62
(1,227)	1:62:A:GLU:HG2	1:61:A:LEU:HG	25	0.62
(1,216)	1:113:A:LEU:HD11	1:70:A:PHE:HD2	11	0.62
(1,216)	1:113:A:LEU:HD11	1:70:A:PHE:HD2	12	0.62
(1,207)	1:109:A:LEU:HD23	1:113:A:LEU:H	20	0.62
(1,206)	1:71:A:LEU:HD11	1:89:A:TYR:HB2	4	0.62
(1,199)	1:72:A:GLU:HG2	1:71:A:LEU:HB3	12	0.62
(1,199)	1:72:A:GLU:HG2	1:71:A:LEU:HB3	14	0.62
(1,199)	1:72:A:GLU:HG3	1:71:A:LEU:HB3	16	0.62
(1,189)	1:85:A:VAL:HG11	1:75:A:LYS:HA	9	0.62
(1,170)	1:85:A:VAL:HG11	1:75:A:LYS:H	9	0.62
(1,153)	1:88:A:LEU:HD22	1:128:A:ASN:HA	10	0.62
(1,152)	1:67:A:PHE:HE1	1:88:A:LEU:HD12	1	0.62
(1,152)	1:67:A:PHE:HE1	1:88:A:LEU:HD12	8	0.62
(1,152)	1:67:A:PHE:HE1	1:88:A:LEU:HD13	14	0.62
(1,144)	1:89:A:TYR:HB2	1:89:A:TYR:HE2	4	0.62
(1,144)	1:89:A:TYR:HB2	1:89:A:TYR:HE2	7	0.62
(1,144)	1:59:A:TYR:HE2	1:59:A:TYR:HB2	11	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,144)	1:89:A:TYR:HB2	1:89:A:TYR:HE2	12	0.62
(1,144)	1:89:A:TYR:HB2	1:89:A:TYR:HE2	16	0.62
(1,144)	1:89:A:TYR:HB2	1:89:A:TYR:HE2	18	0.62
(1,144)	1:89:A:TYR:HB2	1:89:A:TYR:HE2	23	0.62
(1,134)	1:92:A:GLN:HG2	1:95:A:ALA:H	9	0.62
(1,80)	1:94:A:ARG:HD2	1:93:A:GLN:HB2	3	0.62
(1,5)	1:100:A:LEU:HD11	1:100:A:LEU:H	14	0.62
(1,5)	1:100:A:LEU:HD13	1:100:A:LEU:H	16	0.62
(1,2114)	1:75:A:LYS:HG2	1:75:A:LYS:H	22	0.61
(1,2082)	1:81:A:HIS:H	1:79:A:ALA:HB3	2	0.61
(1,2082)	1:81:A:HIS:H	1:79:A:ALA:HB1	15	0.61
(1,1861)	1:123:A:LEU:HD23	1:123:A:LEU:H	13	0.61
(1,1861)	1:123:A:LEU:HD21	1:123:A:LEU:H	23	0.61
(1,1798)	1:136:A:ALA:H	1:135:A:LYS:HD3	7	0.61
(1,1772)	1:142:A:LYS:H	1:141:A:LYS:HG3	24	0.61
(1,1753)	2:27:B:SER:HB2	2:27:B:SER:HA	7	0.61
(1,1753)	2:27:B:SER:HB2	2:27:B:SER:HA	14	0.61
(1,1753)	2:27:B:SER:HB2	2:27:B:SER:HA	18	0.61
(1,1738)	2:31:B:LEU:HB3	2:31:B:LEU:HD22	3	0.61
(1,1738)	2:31:B:LEU:HB3	2:31:B:LEU:HD21	4	0.61
(1,1738)	2:31:B:LEU:HB3	2:31:B:LEU:HD22	5	0.61
(1,1738)	2:31:B:LEU:HB3	2:31:B:LEU:HD22	8	0.61
(1,1738)	2:31:B:LEU:HB3	2:31:B:LEU:HD21	9	0.61
(1,1738)	2:31:B:LEU:HB3	2:31:B:LEU:HD22	20	0.61
(1,1642)	2:38:B:ARG:HB3	2:38:B:ARG:HD2	5	0.61
(1,1642)	2:38:B:ARG:HB3	2:38:B:ARG:HD2	12	0.61
(1,1633)	2:38:B:ARG:HD2	2:38:B:ARG:HB2	23	0.61
(1,1629)	2:38:B:ARG:HG2	2:38:B:ARG:HA	3	0.61
(1,1629)	2:38:B:ARG:HG2	2:38:B:ARG:HA	8	0.61
(1,1629)	2:38:B:ARG:HG2	2:38:B:ARG:HA	14	0.61
(1,1576)	1:73:A:LEU:HD13	1:117:A:ARG:H	11	0.61
(1,1501)	1:64:A:GLU:HG2	1:65:A:LYS:H	6	0.61
(1,1501)	1:64:A:GLU:HG2	1:65:A:LYS:H	9	0.61
(1,1501)	1:64:A:GLU:HG2	1:65:A:LYS:H	19	0.61
(1,1496)	1:64:A:GLU:HG3	1:64:A:GLU:HA	19	0.61
(1,1415)	1:71:A:LEU:HB2	1:75:A:LYS:HE2	17	0.61
(1,1232)	1:67:A:PHE:HD1	1:67:A:PHE:HB2	10	0.61
(1,1183)	1:90:A:ASN:HB2	1:87:A:PHE:HD1	12	0.61
(1,1115)	1:98:A:LEU:HD21	1:96:A:HIS:HE1	6	0.61
(1,1070)	1:101:A:ALA:HB3	1:102:A:SER:H	12	0.61
(1,1070)	1:101:A:ALA:HB3	1:102:A:SER:H	25	0.61
(1,1040)	1:62:A:GLU:HB3	1:59:A:TYR:HA	6	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,902)	1:115:A:ARG:HD2	1:115:A:ARG:H	1	0.61
(1,902)	1:115:A:ARG:HD2	1:115:A:ARG:H	4	0.61
(1,902)	1:115:A:ARG:HD2	1:115:A:ARG:H	22	0.61
(1,848)	1:120:A:PRO:HG3	1:119:A:ARG:HA	3	0.61
(1,848)	1:120:A:PRO:HG3	1:119:A:ARG:HA	12	0.61
(1,825)	1:122:A:LYS:HG2	1:125:A:VAL:HG22	14	0.61
(1,825)	1:122:A:LYS:HG2	1:125:A:VAL:HG22	24	0.61
(1,792)	1:127:A:ILE:HD11	1:124:A:TYR:HD1	21	0.61
(1,552)	2:36:B:THR:HA	2:35:B:PHE:H	19	0.61
(1,519)	1:74:A:CYS:H	1:85:A:VAL:HG21	7	0.61
(1,519)	1:74:A:CYS:H	1:85:A:VAL:HG22	13	0.61
(1,519)	1:74:A:CYS:H	1:85:A:VAL:HG21	21	0.61
(1,499)	1:85:A:VAL:H	1:74:A:CYS:HB3	23	0.61
(1,498)	1:87:A:PHE:H	1:84:A:VAL:HG13	5	0.61
(1,498)	1:87:A:PHE:H	1:84:A:VAL:HG12	9	0.61
(1,484)	1:134:A:LEU:HD12	1:94:A:ARG:H	7	0.61
(1,484)	1:134:A:LEU:HD11	1:94:A:ARG:H	9	0.61
(1,478)	1:95:A:ALA:H	1:91:A:ARG:HD2	6	0.61
(1,451)	1:114:A:SER:H	1:117:A:ARG:HB2	12	0.61
(1,434)	1:74:A:CYS:H	1:123:A:LEU:HD13	19	0.61
(1,427)	1:126:A:TYR:H	1:127:A:ILE:HD13	5	0.61
(1,427)	1:126:A:TYR:H	1:127:A:ILE:HD11	21	0.61
(1,407)	1:133:A:VAL:H	1:130:A:LEU:HD12	24	0.61
(1,398)	1:135:A:LYS:HG2	1:136:A:ALA:H	8	0.61
(1,367)	2:26:B:ASP:HB3	2:31:B:LEU:H	21	0.61
(1,340)	2:31:B:LEU:HD13	1:88:A:LEU:H	16	0.61
(1,310)	2:35:B:PHE:HD1	1:127:A:ILE:HB	13	0.61
(1,290)	2:39:B:TRP:HH2	2:36:B:THR:HB	6	0.61
(1,290)	2:39:B:TRP:HH2	2:36:B:THR:HB	21	0.61
(1,281)	2:31:B:LEU:HD22	1:128:A:ASN:H	14	0.61
(1,265)	1:127:A:ILE:HD11	2:35:B:PHE:HE1	16	0.61
(1,263)	1:132:A:THR:HG23	2:28:B:ASP:HB3	19	0.61
(1,243)	1:62:A:GLU:HG3	1:61:A:LEU:HD21	7	0.61
(1,243)	1:62:A:GLU:HG3	1:61:A:LEU:HD23	20	0.61
(1,232)	1:66:A:LEU:HD13	1:62:A:GLU:HA	14	0.61
(1,232)	1:66:A:LEU:HD13	1:110:A:SER:HA	25	0.61
(1,230)	1:66:A:LEU:HA	1:113:A:LEU:HD22	14	0.61
(1,230)	1:66:A:LEU:HA	1:113:A:LEU:HD23	19	0.61
(1,228)	1:62:A:GLU:HG2	1:66:A:LEU:HD11	20	0.61
(1,227)	1:62:A:GLU:HG2	1:61:A:LEU:HG	5	0.61
(1,216)	1:113:A:LEU:HD12	1:70:A:PHE:HD2	17	0.61
(1,216)	1:113:A:LEU:HD11	1:70:A:PHE:HD2	25	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,199)	1:72:A:GLU:HG2	1:71:A:LEU:HB3	5	0.61
(1,199)	1:72:A:GLU:HG2	1:71:A:LEU:HB3	18	0.61
(1,199)	1:72:A:GLU:HG3	1:71:A:LEU:HB3	23	0.61
(1,195)	1:73:A:LEU:HD21	1:70:A:PHE:HA	5	0.61
(1,189)	1:85:A:VAL:HG12	1:75:A:LYS:HA	1	0.61
(1,184)	1:79:A:ALA:HB1	1:75:A:LYS:HA	2	0.61
(1,184)	1:79:A:ALA:HB2	1:75:A:LYS:HA	11	0.61
(1,170)	1:85:A:VAL:HG12	1:75:A:LYS:H	1	0.61
(1,170)	1:85:A:VAL:HG13	1:75:A:LYS:H	6	0.61
(1,170)	1:85:A:VAL:HG11	1:75:A:LYS:H	24	0.61
(1,152)	1:67:A:PHE:HE1	1:88:A:LEU:HD12	7	0.61
(1,152)	1:67:A:PHE:HE1	1:88:A:LEU:HD11	16	0.61
(1,152)	1:67:A:PHE:HE2	1:88:A:LEU:HD11	19	0.61
(1,152)	1:67:A:PHE:HE1	1:88:A:LEU:HD12	23	0.61
(1,151)	1:88:A:LEU:HD12	1:70:A:PHE:HD1	10	0.61
(1,144)	1:59:A:TYR:HE2	1:59:A:TYR:HB2	20	0.61
(1,141)	1:93:A:GLN:HG2	1:89:A:TYR:HD1	1	0.61
(1,141)	1:93:A:GLN:HG2	1:89:A:TYR:HD1	25	0.61
(1,134)	1:92:A:GLN:HG2	1:95:A:ALA:H	1	0.61
(1,134)	1:105:A:PHE:HE2	1:92:A:GLN:HG2	14	0.61
(1,97)	1:105:A:PHE:HD1	1:134:A:LEU:HA	2	0.61
(1,80)	1:94:A:ARG:HD3	1:94:A:ARG:HB2	4	0.61
(1,37)	1:127:A:ILE:HG22	1:128:A:ASN:HD22	24	0.61
(1,5)	1:100:A:LEU:HD13	1:100:A:LEU:H	1	0.61
(1,5)	1:100:A:LEU:HD11	1:100:A:LEU:H	13	0.61
(1,2114)	1:75:A:LYS:HG2	1:75:A:LYS:H	12	0.6
(1,2114)	1:75:A:LYS:HG2	1:75:A:LYS:H	14	0.6
(1,2082)	1:81:A:HIS:H	1:79:A:ALA:HB2	25	0.6
(1,2013)	1:94:A:ARG:H	1:95:A:ALA:HB2	21	0.6
(1,1929)	1:107:A:ASN:HD21	1:103:A:ALA:HB2	14	0.6
(1,1910)	1:109:A:LEU:HD22	1:110:A:SER:H	16	0.6
(1,1753)	2:27:B:SER:HB2	2:27:B:SER:HA	19	0.6
(1,1738)	2:31:B:LEU:HB3	2:31:B:LEU:HD23	2	0.6
(1,1738)	2:31:B:LEU:HB3	2:31:B:LEU:HD21	6	0.6
(1,1738)	2:31:B:LEU:HB3	2:31:B:LEU:HD23	7	0.6
(1,1738)	2:31:B:LEU:HB3	2:31:B:LEU:HD21	10	0.6
(1,1738)	2:31:B:LEU:HB3	2:31:B:LEU:HD21	13	0.6
(1,1738)	2:31:B:LEU:HB3	2:31:B:LEU:HD23	14	0.6
(1,1738)	2:31:B:LEU:HB3	2:31:B:LEU:HD23	17	0.6
(1,1738)	2:31:B:LEU:HB3	2:31:B:LEU:HD23	18	0.6
(1,1738)	2:31:B:LEU:HB3	2:31:B:LEU:HD23	21	0.6
(1,1738)	2:31:B:LEU:HB3	2:31:B:LEU:HD22	22	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1642)	2:38:B:ARG:HB3	2:38:B:ARG:HD2	25	0.6
(1,1629)	2:38:B:ARG:HG2	2:38:B:ARG:HA	13	0.6
(1,1629)	2:38:B:ARG:HG2	2:38:B:ARG:HA	19	0.6
(1,1629)	2:38:B:ARG:HG2	2:38:B:ARG:HA	23	0.6
(1,1576)	1:73:A:LEU:HD12	1:117:A:ARG:H	21	0.6
(1,1557)	1:57:A:LYS:HG3	1:57:A:LYS:HA	3	0.6
(1,1503)	1:64:A:GLU:HB2	1:64:A:GLU:HG2	12	0.6
(1,1496)	1:64:A:GLU:HG3	1:64:A:GLU:HA	3	0.6
(1,1489)	1:65:A:LYS:HG2	1:66:A:LEU:H	11	0.6
(1,1489)	1:65:A:LYS:HG2	1:66:A:LEU:H	16	0.6
(1,1477)	1:66:A:LEU:HD23	1:113:A:LEU:HB3	9	0.6
(1,1421)	1:71:A:LEU:HD22	1:71:A:LEU:H	6	0.6
(1,1395)	1:116:A:ALA:HB2	1:73:A:LEU:HD21	25	0.6
(1,1152)	1:93:A:GLN:HG2	1:93:A:GLN:HE21	20	0.6
(1,1070)	1:101:A:ALA:HB3	1:102:A:SER:H	4	0.6
(1,932)	1:112:A:VAL:HG21	1:126:A:TYR:HA	22	0.6
(1,902)	1:115:A:ARG:HD2	1:115:A:ARG:H	6	0.6
(1,902)	1:115:A:ARG:HD2	1:115:A:ARG:H	11	0.6
(1,827)	1:122:A:LYS:HD2	1:122:A:LYS:HA	2	0.6
(1,825)	1:122:A:LYS:HG2	1:125:A:VAL:HG23	5	0.6
(1,825)	1:122:A:LYS:HG2	1:125:A:VAL:HG22	16	0.6
(1,793)	1:124:A:TYR:HE1	1:124:A:TYR:H	3	0.6
(1,766)	1:126:A:TYR:HE1	1:115:A:ARG:HB2	18	0.6
(1,723)	1:129:A:GLU:HG2	1:125:A:VAL:HG12	1	0.6
(1,723)	1:129:A:GLU:HG2	1:125:A:VAL:HG12	25	0.6
(1,706)	1:85:A:VAL:HG22	1:75:A:LYS:HD2	17	0.6
(1,577)	1:75:A:LYS:HE2	1:71:A:LEU:HB3	22	0.6
(1,577)	1:75:A:LYS:HE2	1:71:A:LEU:HB3	23	0.6
(1,534)	1:121:A:ALA:H	1:119:A:ARG:HG3	7	0.6
(1,519)	1:74:A:CYS:H	1:85:A:VAL:HG23	6	0.6
(1,510)	1:73:A:LEU:HD22	1:77:A:GLN:HE22	12	0.6
(1,499)	1:85:A:VAL:H	1:74:A:CYS:HB3	10	0.6
(1,498)	1:87:A:PHE:H	1:84:A:VAL:HG12	13	0.6
(1,498)	1:87:A:PHE:H	1:84:A:VAL:HG11	18	0.6
(1,498)	1:87:A:PHE:H	1:84:A:VAL:HG11	22	0.6
(1,498)	1:87:A:PHE:H	1:84:A:VAL:HG12	23	0.6
(1,484)	1:134:A:LEU:HD13	1:94:A:ARG:H	12	0.6
(1,454)	1:114:A:SER:H	1:112:A:VAL:HG21	12	0.6
(1,454)	1:114:A:SER:H	1:112:A:VAL:HG22	19	0.6
(1,454)	1:114:A:SER:H	1:112:A:VAL:HG23	21	0.6
(1,407)	1:133:A:VAL:H	1:130:A:LEU:HD12	1	0.6
(1,407)	1:133:A:VAL:H	1:130:A:LEU:HD12	6	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,407)	1:133:A:VAL:H	1:130:A:LEU:HD13	22	0.6
(1,407)	1:133:A:VAL:H	1:130:A:LEU:HD13	23	0.6
(1,366)	1:100:A:LEU:HD13	1:138:A:SER:HB3	21	0.6
(1,338)	2:31:B:LEU:HD21	2:32:B:GLU:HG3	5	0.6
(1,338)	2:31:B:LEU:HD23	2:32:B:GLU:HG3	7	0.6
(1,338)	2:31:B:LEU:HD23	2:32:B:GLU:HG3	24	0.6
(1,333)	1:127:A:ILE:HG12	1:130:A:LEU:HD22	8	0.6
(1,333)	1:127:A:ILE:HG12	1:130:A:LEU:HD22	16	0.6
(1,319)	2:34:B:TYR:HE1	1:84:A:VAL:HG22	14	0.6
(1,319)	2:34:B:TYR:HE1	1:84:A:VAL:HG23	15	0.6
(1,319)	2:34:B:TYR:HE1	1:84:A:VAL:HG22	23	0.6
(1,310)	2:35:B:PHE:HD1	1:127:A:ILE:HB	5	0.6
(1,307)	2:39:B:TRP:HE3	2:36:B:THR:HG23	6	0.6
(1,307)	2:39:B:TRP:HE3	2:36:B:THR:HG23	25	0.6
(1,290)	2:39:B:TRP:HH2	2:36:B:THR:HB	17	0.6
(1,280)	2:31:B:LEU:HG	1:87:A:PHE:HE2	23	0.6
(1,232)	1:66:A:LEU:HD11	1:110:A:SER:HA	4	0.6
(1,232)	1:66:A:LEU:HD13	1:62:A:GLU:HA	11	0.6
(1,230)	1:66:A:LEU:HA	1:113:A:LEU:HD22	3	0.6
(1,230)	1:66:A:LEU:HA	1:113:A:LEU:HD21	15	0.6
(1,203)	1:71:A:LEU:HD11	1:68:A:GLU:H	1	0.6
(1,152)	1:67:A:PHE:HE1	1:88:A:LEU:HD12	5	0.6
(1,152)	1:67:A:PHE:HE1	1:88:A:LEU:HD12	21	0.6
(1,144)	1:59:A:TYR:HE2	1:59:A:TYR:HB2	10	0.6
(1,141)	1:93:A:GLN:HG2	1:89:A:TYR:HD1	3	0.6
(1,141)	1:93:A:GLN:HG2	1:89:A:TYR:HD1	24	0.6
(1,48)	1:126:A:TYR:HE1	1:125:A:VAL:HG12	2	0.6
(1,44)	1:126:A:TYR:HE2	1:126:A:TYR:HB2	11	0.6
(1,44)	1:126:A:TYR:HE2	1:126:A:TYR:HB2	17	0.6
(1,44)	1:126:A:TYR:HE2	1:126:A:TYR:HB2	18	0.6
(1,5)	1:100:A:LEU:HD12	1:100:A:LEU:H	21	0.6
(1,2195)	1:56:A:LYS:H	1:56:A:LYS:HG2	9	0.59
(1,2114)	1:75:A:LYS:HG2	1:75:A:LYS:H	7	0.59
(1,2114)	1:75:A:LYS:HG2	1:75:A:LYS:H	23	0.59
(1,2082)	1:81:A:HIS:H	1:79:A:ALA:HB1	12	0.59
(1,2026)	1:67:A:PHE:HD1	1:92:A:GLN:HE22	13	0.59
(1,2005)	1:95:A:ALA:H	1:94:A:ARG:HG3	6	0.59
(1,1910)	1:109:A:LEU:HD21	1:110:A:SER:H	6	0.59
(1,1910)	1:109:A:LEU:HD22	1:110:A:SER:H	11	0.59
(1,1861)	1:123:A:LEU:HD22	1:123:A:LEU:H	7	0.59
(1,1801)	1:135:A:LYS:H	1:91:A:ARG:HD3	5	0.59
(1,1738)	2:31:B:LEU:HB3	2:31:B:LEU:HD22	11	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1738)	2:31:B:LEU:HB3	2:31:B:LEU:HD23	15	0.59
(1,1738)	2:31:B:LEU:HB3	2:31:B:LEU:HD23	16	0.59
(1,1738)	2:31:B:LEU:HB3	2:31:B:LEU:HD22	23	0.59
(1,1652)	2:38:B:ARG:HD2	2:37:B:ALA:HB3	12	0.59
(1,1633)	2:38:B:ARG:HD2	2:38:B:ARG:HB2	17	0.59
(1,1629)	2:38:B:ARG:HG2	2:38:B:ARG:HA	4	0.59
(1,1629)	2:38:B:ARG:HG2	2:38:B:ARG:HA	22	0.59
(1,1557)	1:57:A:LYS:HG3	1:57:A:LYS:HA	5	0.59
(1,1554)	1:59:A:TYR:HE1	1:57:A:LYS:HB2	19	0.59
(1,1501)	1:64:A:GLU:HG2	1:65:A:LYS:H	15	0.59
(1,1501)	1:64:A:GLU:HG2	1:65:A:LYS:H	18	0.59
(1,1501)	1:64:A:GLU:HG2	1:65:A:LYS:H	20	0.59
(1,1489)	1:65:A:LYS:HG2	1:66:A:LEU:H	9	0.59
(1,1489)	1:65:A:LYS:HG2	1:66:A:LEU:H	24	0.59
(1,1421)	1:71:A:LEU:HD23	1:71:A:LEU:H	2	0.59
(1,1392)	1:73:A:LEU:HD22	1:117:A:ARG:HD3	4	0.59
(1,1341)	1:76:A:MET:HB3	1:73:A:LEU:HA	23	0.59
(1,1338)	1:76:A:MET:HB3	1:76:A:MET:H	5	0.59
(1,1338)	1:76:A:MET:HB3	1:76:A:MET:H	14	0.59
(1,1338)	1:76:A:MET:HB3	1:76:A:MET:H	15	0.59
(1,1123)	1:83:A:GLU:HA	1:83:A:GLU:HG3	6	0.59
(1,1070)	1:101:A:ALA:HB2	1:102:A:SER:H	20	0.59
(1,932)	1:112:A:VAL:HG22	1:126:A:TYR:HA	17	0.59
(1,902)	1:115:A:ARG:HD2	1:115:A:ARG:H	25	0.59
(1,848)	1:120:A:PRO:HG3	1:119:A:ARG:HA	15	0.59
(1,826)	1:117:A:ARG:HG2	1:117:A:ARG:H	11	0.59
(1,825)	1:122:A:LYS:HG2	1:125:A:VAL:HG22	20	0.59
(1,825)	1:122:A:LYS:HG2	1:125:A:VAL:HG21	23	0.59
(1,766)	1:126:A:TYR:HE1	1:115:A:ARG:HB2	2	0.59
(1,723)	1:129:A:GLU:HG2	1:125:A:VAL:HG11	11	0.59
(1,723)	1:129:A:GLU:HG2	1:125:A:VAL:HG13	22	0.59
(1,607)	1:136:A:ALA:HB1	1:137:A:HIS:HA	2	0.59
(1,607)	1:136:A:ALA:HB2	1:137:A:HIS:HA	17	0.59
(1,585)	1:139:A:ALA:HB3	1:140:A:LYS:H	4	0.59
(1,585)	1:139:A:ALA:HB2	1:140:A:LYS:H	6	0.59
(1,577)	1:75:A:LYS:HE2	1:71:A:LEU:HB3	14	0.59
(1,519)	1:74:A:CYS:H	1:85:A:VAL:HG21	11	0.59
(1,519)	1:74:A:CYS:H	1:85:A:VAL:HG22	25	0.59
(1,510)	1:73:A:LEU:HD23	1:77:A:GLN:HE22	4	0.59
(1,510)	1:73:A:LEU:HD23	1:77:A:GLN:HE22	20	0.59
(1,502)	1:81:A:HIS:H	1:82:A:PRO:HB3	2	0.59
(1,499)	1:85:A:VAL:H	1:74:A:CYS:HB3	11	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,499)	1:85:A:VAL:H	1:74:A:CYS:HB3	12	0.59
(1,498)	1:87:A:PHE:H	1:84:A:VAL:HG11	15	0.59
(1,498)	1:87:A:PHE:H	1:84:A:VAL:HG12	19	0.59
(1,484)	1:134:A:LEU:HD12	1:94:A:ARG:H	25	0.59
(1,478)	1:95:A:ALA:H	1:91:A:ARG:HD2	19	0.59
(1,454)	1:114:A:SER:H	1:112:A:VAL:HG23	14	0.59
(1,454)	1:114:A:SER:H	1:112:A:VAL:HG21	15	0.59
(1,451)	1:114:A:SER:H	1:117:A:ARG:HB2	16	0.59
(1,427)	1:126:A:TYR:H	1:127:A:ILE:HD11	17	0.59
(1,407)	1:133:A:VAL:H	1:130:A:LEU:HD13	12	0.59
(1,398)	1:135:A:LYS:HG2	1:136:A:ALA:H	10	0.59
(1,375)	2:29:B:SER:HB2	2:26:B:ASP:HB2	4	0.59
(1,369)	2:26:B:ASP:HB2	2:33:B:GLN:HE21	13	0.59
(1,340)	2:31:B:LEU:HD13	1:88:A:LEU:H	5	0.59
(1,338)	2:31:B:LEU:HD22	2:32:B:GLU:HG3	11	0.59
(1,333)	1:127:A:ILE:HG12	1:130:A:LEU:HD21	12	0.59
(1,333)	1:127:A:ILE:HG12	1:130:A:LEU:HD22	21	0.59
(1,333)	1:127:A:ILE:HG12	1:130:A:LEU:HD22	23	0.59
(1,321)	2:34:B:TYR:HD1	1:83:A:GLU:HB3	5	0.59
(1,319)	2:34:B:TYR:HE1	1:84:A:VAL:HG22	11	0.59
(1,319)	2:34:B:TYR:HE1	1:84:A:VAL:HG22	20	0.59
(1,310)	2:35:B:PHE:HD1	1:127:A:ILE:HB	12	0.59
(1,289)	2:39:B:TRP:HZ3	2:36:B:THR:HB	9	0.59
(1,281)	2:31:B:LEU:HD23	1:128:A:ASN:H	3	0.59
(1,280)	2:31:B:LEU:HG	1:87:A:PHE:HE2	13	0.59
(1,265)	1:127:A:ILE:HD13	2:35:B:PHE:HE1	12	0.59
(1,265)	1:127:A:ILE:HD12	2:35:B:PHE:HE1	20	0.59
(1,265)	1:127:A:ILE:HD11	2:35:B:PHE:HE1	22	0.59
(1,265)	1:127:A:ILE:HD13	2:35:B:PHE:HE1	24	0.59
(1,243)	1:62:A:GLU:HG3	1:61:A:LEU:HD23	24	0.59
(1,232)	1:66:A:LEU:HD11	1:110:A:SER:HA	17	0.59
(1,230)	1:66:A:LEU:HA	1:113:A:LEU:HD21	8	0.59
(1,230)	1:66:A:LEU:HA	1:113:A:LEU:HD22	17	0.59
(1,228)	1:62:A:GLU:HG2	1:66:A:LEU:HD13	16	0.59
(1,216)	1:113:A:LEU:HD11	1:70:A:PHE:HD2	6	0.59
(1,216)	1:113:A:LEU:HD11	1:70:A:PHE:HD2	19	0.59
(1,205)	1:71:A:LEU:HD13	1:75:A:LYS:HE2	16	0.59
(1,203)	1:71:A:LEU:HD12	1:68:A:GLU:H	15	0.59
(1,189)	1:85:A:VAL:HG11	1:75:A:LYS:HA	12	0.59
(1,141)	1:93:A:GLN:HG2	1:89:A:TYR:HD1	19	0.59
(1,89)	1:94:A:ARG:HD2	1:94:A:ARG:HA	6	0.59
(1,44)	1:126:A:TYR:HE2	1:126:A:TYR:HB2	2	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,44)	1:126:A:TYR:HE2	1:126:A:TYR:HB2	3	0.59
(1,44)	1:126:A:TYR:HE2	1:126:A:TYR:HB2	4	0.59
(1,44)	1:126:A:TYR:HE2	1:126:A:TYR:HB2	9	0.59
(1,44)	1:126:A:TYR:HE2	1:126:A:TYR:HB2	19	0.59
(1,44)	1:126:A:TYR:HE2	1:126:A:TYR:HB2	22	0.59
(1,13)	1:133:A:VAL:HG12	1:108:A:ILE:HB	14	0.59
(1,2097)	1:77:A:GLN:HE21	1:77:A:GLN:HA	11	0.58
(1,2082)	1:81:A:HIS:H	1:79:A:ALA:HB2	3	0.58
(1,2013)	1:94:A:ARG:H	1:95:A:ALA:HB2	2	0.58
(1,2012)	1:94:A:ARG:HB3	1:94:A:ARG:H	20	0.58
(1,2012)	1:94:A:ARG:HB3	1:94:A:ARG:H	25	0.58
(1,1910)	1:109:A:LEU:HD22	1:110:A:SER:H	23	0.58
(1,1910)	1:109:A:LEU:HD23	1:110:A:SER:H	24	0.58
(1,1861)	1:123:A:LEU:HD22	1:123:A:LEU:H	8	0.58
(1,1861)	1:123:A:LEU:HD21	1:123:A:LEU:H	15	0.58
(1,1747)	2:26:B:ASP:HB3	2:27:B:SER:HA	1	0.58
(1,1738)	2:31:B:LEU:HB3	2:31:B:LEU:HD22	1	0.58
(1,1738)	2:31:B:LEU:HB3	2:31:B:LEU:HD23	12	0.58
(1,1738)	2:31:B:LEU:HB3	2:31:B:LEU:HD23	19	0.58
(1,1738)	2:31:B:LEU:HB3	2:31:B:LEU:HD23	24	0.58
(1,1738)	2:31:B:LEU:HB3	2:31:B:LEU:HD22	25	0.58
(1,1650)	2:37:B:ALA:HB3	1:121:A:ALA:HB2	3	0.58
(1,1650)	2:37:B:ALA:HB3	1:121:A:ALA:HB2	20	0.58
(1,1649)	2:37:B:ALA:HB2	2:38:B:ARG:HB2	25	0.58
(1,1629)	2:38:B:ARG:HG2	2:38:B:ARG:HA	17	0.58
(1,1577)	1:77:A:GLN:HG3	1:73:A:LEU:HD13	1	0.58
(1,1561)	1:57:A:LYS:HD2	1:57:A:LYS:HA	3	0.58
(1,1554)	1:59:A:TYR:HE1	1:57:A:LYS:HB2	6	0.58
(1,1501)	1:64:A:GLU:HG2	1:65:A:LYS:H	4	0.58
(1,1501)	1:64:A:GLU:HG2	1:65:A:LYS:H	5	0.58
(1,1489)	1:65:A:LYS:HG2	1:66:A:LEU:H	3	0.58
(1,1477)	1:66:A:LEU:HD22	1:113:A:LEU:HB3	11	0.58
(1,1421)	1:71:A:LEU:HD23	1:71:A:LEU:H	8	0.58
(1,1421)	1:71:A:LEU:HD21	1:71:A:LEU:H	25	0.58
(1,1395)	1:116:A:ALA:HB2	1:73:A:LEU:HD23	23	0.58
(1,1368)	1:75:A:LYS:HD3	1:75:A:LYS:HB2	24	0.58
(1,1338)	1:76:A:MET:HB3	1:76:A:MET:H	2	0.58
(1,1338)	1:76:A:MET:HB3	1:76:A:MET:H	4	0.58
(1,1338)	1:76:A:MET:HB3	1:76:A:MET:H	6	0.58
(1,1338)	1:76:A:MET:HB3	1:76:A:MET:H	7	0.58
(1,1338)	1:76:A:MET:HB3	1:76:A:MET:H	9	0.58
(1,1338)	1:76:A:MET:HB3	1:76:A:MET:H	10	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1338)	1:76:A:MET:HB3	1:76:A:MET:H	12	0.58
(1,1338)	1:76:A:MET:HB3	1:76:A:MET:H	18	0.58
(1,1338)	1:76:A:MET:HB3	1:76:A:MET:H	20	0.58
(1,1338)	1:76:A:MET:HB3	1:76:A:MET:H	21	0.58
(1,1338)	1:76:A:MET:HB3	1:76:A:MET:H	23	0.58
(1,1329)	1:77:A:GLN:HG2	1:77:A:GLN:HB3	2	0.58
(1,1329)	1:77:A:GLN:HG2	1:77:A:GLN:HB3	4	0.58
(1,1329)	1:77:A:GLN:HG2	1:77:A:GLN:HB3	7	0.58
(1,1329)	1:77:A:GLN:HG2	1:77:A:GLN:HB3	9	0.58
(1,1329)	1:77:A:GLN:HG2	1:77:A:GLN:HB3	12	0.58
(1,1329)	1:77:A:GLN:HG2	1:77:A:GLN:HB3	13	0.58
(1,1329)	1:77:A:GLN:HG2	1:77:A:GLN:HB3	17	0.58
(1,1329)	1:77:A:GLN:HG2	1:77:A:GLN:HB3	20	0.58
(1,1329)	1:77:A:GLN:HG2	1:77:A:GLN:HB3	23	0.58
(1,1329)	1:77:A:GLN:HG2	1:77:A:GLN:HB3	25	0.58
(1,1199)	1:89:A:TYR:HE1	1:71:A:LEU:HD13	9	0.58
(1,1199)	1:89:A:TYR:HE1	1:71:A:LEU:HD13	11	0.58
(1,1199)	1:89:A:TYR:HE1	1:71:A:LEU:HD13	17	0.58
(1,1183)	1:90:A:ASN:HB2	1:87:A:PHE:HD1	5	0.58
(1,1183)	1:90:A:ASN:HB2	1:87:A:PHE:HD1	22	0.58
(1,1088)	1:100:A:LEU:HD22	1:105:A:PHE:HD2	15	0.58
(1,1075)	1:101:A:ALA:HB2	1:60:A:LYS:HB2	22	0.58
(1,1070)	1:101:A:ALA:HB1	1:102:A:SER:H	7	0.58
(1,932)	1:112:A:VAL:HG23	1:126:A:TYR:HA	1	0.58
(1,932)	1:112:A:VAL:HG22	1:126:A:TYR:HA	5	0.58
(1,932)	1:112:A:VAL:HG23	1:126:A:TYR:HA	6	0.58
(1,932)	1:112:A:VAL:HG21	1:126:A:TYR:HA	19	0.58
(1,932)	1:112:A:VAL:HG23	1:126:A:TYR:HA	20	0.58
(1,902)	1:115:A:ARG:HD2	1:115:A:ARG:H	18	0.58
(1,848)	1:120:A:PRO:HG3	1:119:A:ARG:HA	13	0.58
(1,848)	1:120:A:PRO:HG3	1:119:A:ARG:HA	14	0.58
(1,848)	1:120:A:PRO:HG3	1:119:A:ARG:HA	23	0.58
(1,825)	1:122:A:LYS:HG2	1:125:A:VAL:HG22	25	0.58
(1,790)	1:124:A:TYR:HD1	1:124:A:TYR:HA	25	0.58
(1,723)	1:129:A:GLU:HG2	1:125:A:VAL:HG11	17	0.58
(1,723)	1:129:A:GLU:HG2	1:125:A:VAL:HG12	18	0.58
(1,619)	1:135:A:LYS:HG2	1:91:A:ARG:HD3	10	0.58
(1,607)	1:136:A:ALA:HB1	1:137:A:HIS:HA	5	0.58
(1,607)	1:136:A:ALA:HB1	1:137:A:HIS:HA	12	0.58
(1,607)	1:136:A:ALA:HB3	1:137:A:HIS:HA	25	0.58
(1,552)	2:35:B:PHE:H	2:33:B:GLN:HA	1	0.58
(1,552)	2:35:B:PHE:H	2:33:B:GLN:HA	6	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,534)	1:121:A:ALA:H	1:119:A:ARG:HG3	2	0.58
(1,519)	1:74:A:CYS:H	1:85:A:VAL:HG22	19	0.58
(1,510)	1:73:A:LEU:HD22	1:77:A:GLN:HE22	5	0.58
(1,499)	1:85:A:VAL:H	1:74:A:CYS:HB3	4	0.58
(1,484)	1:134:A:LEU:HD13	1:94:A:ARG:H	4	0.58
(1,484)	1:134:A:LEU:HD12	1:94:A:ARG:H	21	0.58
(1,457)	1:111:A:ARG:H	1:109:A:LEU:HB3	20	0.58
(1,455)	1:112:A:VAL:H	1:113:A:LEU:HB3	12	0.58
(1,454)	1:114:A:SER:H	1:112:A:VAL:HG22	4	0.58
(1,454)	1:114:A:SER:H	1:112:A:VAL:HG23	17	0.58
(1,407)	1:133:A:VAL:H	1:130:A:LEU:HD11	10	0.58
(1,407)	1:133:A:VAL:H	1:130:A:LEU:HD13	18	0.58
(1,395)	1:138:A:SER:H	1:95:A:ALA:HB1	23	0.58
(1,340)	2:31:B:LEU:HD13	1:88:A:LEU:H	7	0.58
(1,338)	2:31:B:LEU:HD22	2:32:B:GLU:HG3	1	0.58
(1,338)	2:31:B:LEU:HD21	2:32:B:GLU:HG3	3	0.58
(1,338)	2:31:B:LEU:HD21	2:32:B:GLU:HG3	10	0.58
(1,338)	2:31:B:LEU:HD23	2:32:B:GLU:HG3	15	0.58
(1,333)	1:127:A:ILE:HG12	1:130:A:LEU:HD22	4	0.58
(1,323)	1:84:A:VAL:HG23	2:34:B:TYR:HD1	4	0.58
(1,323)	1:84:A:VAL:HG22	2:34:B:TYR:HD1	13	0.58
(1,319)	2:34:B:TYR:HE1	1:84:A:VAL:HG22	24	0.58
(1,310)	2:35:B:PHE:HD1	1:127:A:ILE:HB	7	0.58
(1,310)	2:35:B:PHE:HD1	1:127:A:ILE:HB	15	0.58
(1,281)	2:31:B:LEU:HD22	1:128:A:ASN:H	4	0.58
(1,281)	2:31:B:LEU:HD23	1:128:A:ASN:H	10	0.58
(1,280)	2:31:B:LEU:HG	1:87:A:PHE:HE2	19	0.58
(1,265)	1:127:A:ILE:HD12	2:35:B:PHE:HE1	6	0.58
(1,265)	1:127:A:ILE:HD13	2:35:B:PHE:HE1	11	0.58
(1,228)	1:62:A:GLU:HG2	1:66:A:LEU:HD13	23	0.58
(1,227)	1:62:A:GLU:HG2	1:61:A:LEU:HG	10	0.58
(1,206)	1:71:A:LEU:HD11	1:89:A:TYR:HB2	23	0.58
(1,205)	1:71:A:LEU:HD12	1:75:A:LYS:HE2	21	0.58
(1,203)	1:71:A:LEU:HD12	1:68:A:GLU:H	2	0.58
(1,203)	1:71:A:LEU:HD12	1:68:A:GLU:H	5	0.58
(1,199)	1:72:A:GLU:HG3	1:71:A:LEU:HB3	3	0.58
(1,197)	1:73:A:LEU:HD23	1:123:A:LEU:HB2	9	0.58
(1,189)	1:85:A:VAL:HG12	1:75:A:LYS:HA	11	0.58
(1,189)	1:85:A:VAL:HG12	1:75:A:LYS:HA	19	0.58
(1,189)	1:85:A:VAL:HG13	1:75:A:LYS:HA	20	0.58
(1,189)	1:85:A:VAL:HG12	1:75:A:LYS:HA	22	0.58
(1,178)	1:84:A:VAL:HG23	1:78:A:THR:H	16	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,144)	1:59:A:TYR:HE2	1:59:A:TYR:HB2	5	0.58
(1,144)	1:59:A:TYR:HE2	1:59:A:TYR:HB2	25	0.58
(1,141)	1:93:A:GLN:HG2	1:89:A:TYR:HD1	14	0.58
(1,97)	1:105:A:PHE:HD1	1:134:A:LEU:HA	11	0.58
(1,97)	1:105:A:PHE:HD1	1:100:A:LEU:HA	12	0.58
(1,97)	1:105:A:PHE:HD1	1:100:A:LEU:HA	14	0.58
(1,80)	1:94:A:ARG:HD2	1:93:A:GLN:HB2	11	0.58
(1,80)	1:94:A:ARG:HD2	1:93:A:GLN:HB2	18	0.58
(1,44)	1:126:A:TYR:HE2	1:126:A:TYR:HB2	5	0.58
(1,44)	1:126:A:TYR:HE2	1:126:A:TYR:HB2	7	0.58
(1,44)	1:126:A:TYR:HE2	1:126:A:TYR:HB2	8	0.58
(1,44)	1:126:A:TYR:HE2	1:126:A:TYR:HB2	13	0.58
(1,44)	1:126:A:TYR:HE2	1:126:A:TYR:HB2	23	0.58
(1,5)	1:100:A:LEU:HD13	1:100:A:LEU:H	9	0.58
(1,2114)	1:75:A:LYS:HG2	1:75:A:LYS:H	20	0.57
(1,2106)	1:76:A:MET:HB3	1:77:A:GLN:H	2	0.57
(1,2089)	1:79:A:ALA:H	1:78:A:THR:HG23	4	0.57
(1,2037)	1:90:A:ASN:HD21	1:94:A:ARG:HD2	8	0.57
(1,2033)	1:90:A:ASN:HD22	1:94:A:ARG:HG2	2	0.57
(1,2026)	1:67:A:PHE:HD2	1:92:A:GLN:HE21	5	0.57
(1,2026)	1:67:A:PHE:HD2	1:92:A:GLN:HE22	14	0.57
(1,2013)	1:94:A:ARG:H	1:95:A:ALA:HB2	1	0.57
(1,2013)	1:94:A:ARG:H	1:95:A:ALA:HB3	6	0.57
(1,2013)	1:94:A:ARG:H	1:95:A:ALA:HB3	8	0.57
(1,2005)	1:95:A:ALA:H	1:94:A:ARG:HG3	23	0.57
(1,1910)	1:109:A:LEU:HD23	1:110:A:SER:H	1	0.57
(1,1861)	1:123:A:LEU:HD22	1:123:A:LEU:H	2	0.57
(1,1861)	1:123:A:LEU:HD23	1:123:A:LEU:H	6	0.57
(1,1861)	1:123:A:LEU:HD23	1:123:A:LEU:H	14	0.57
(1,1861)	1:123:A:LEU:HD23	1:123:A:LEU:H	21	0.57
(1,1861)	1:123:A:LEU:HD23	1:123:A:LEU:H	22	0.57
(1,1788)	1:139:A:ALA:H	1:135:A:LYS:HD3	25	0.57
(1,1770)	1:141:A:LYS:HB3	1:141:A:LYS:H	18	0.57
(1,1629)	2:38:B:ARG:HG2	2:38:B:ARG:HA	6	0.57
(1,1629)	2:38:B:ARG:HG2	2:38:B:ARG:HA	20	0.57
(1,1576)	1:73:A:LEU:HD13	1:117:A:ARG:H	4	0.57
(1,1501)	1:64:A:GLU:HG2	1:65:A:LYS:H	22	0.57
(1,1496)	1:64:A:GLU:HG3	1:64:A:GLU:HA	6	0.57
(1,1489)	1:65:A:LYS:HG2	1:66:A:LEU:H	17	0.57
(1,1489)	1:65:A:LYS:HG2	1:66:A:LEU:H	21	0.57
(1,1489)	1:65:A:LYS:HG2	1:66:A:LEU:H	23	0.57
(1,1477)	1:66:A:LEU:HD22	1:113:A:LEU:HB3	14	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1421)	1:71:A:LEU:HD23	1:71:A:LEU:H	13	0.57
(1,1395)	1:116:A:ALA:HB1	1:73:A:LEU:HD21	22	0.57
(1,1368)	1:75:A:LYS:HD3	1:75:A:LYS:HB2	10	0.57
(1,1338)	1:76:A:MET:HB3	1:76:A:MET:H	3	0.57
(1,1338)	1:76:A:MET:HB3	1:76:A:MET:H	13	0.57
(1,1338)	1:76:A:MET:HB3	1:76:A:MET:H	16	0.57
(1,1338)	1:76:A:MET:HB3	1:76:A:MET:H	19	0.57
(1,1338)	1:76:A:MET:HB3	1:76:A:MET:H	24	0.57
(1,1338)	1:76:A:MET:HB3	1:76:A:MET:H	25	0.57
(1,1329)	1:77:A:GLN:HG2	1:77:A:GLN:HB3	3	0.57
(1,1329)	1:77:A:GLN:HG2	1:77:A:GLN:HB3	5	0.57
(1,1329)	1:77:A:GLN:HG2	1:77:A:GLN:HB3	6	0.57
(1,1329)	1:77:A:GLN:HG2	1:77:A:GLN:HB3	8	0.57
(1,1329)	1:77:A:GLN:HG2	1:77:A:GLN:HB3	10	0.57
(1,1329)	1:77:A:GLN:HG2	1:77:A:GLN:HB3	14	0.57
(1,1329)	1:77:A:GLN:HG2	1:77:A:GLN:HB3	15	0.57
(1,1329)	1:77:A:GLN:HG2	1:77:A:GLN:HB3	18	0.57
(1,1329)	1:77:A:GLN:HG2	1:77:A:GLN:HB3	21	0.57
(1,1329)	1:77:A:GLN:HG2	1:77:A:GLN:HB3	22	0.57
(1,1329)	1:77:A:GLN:HG2	1:77:A:GLN:HB3	24	0.57
(1,1324)	1:77:A:GLN:HG2	1:77:A:GLN:H	19	0.57
(1,1231)	1:67:A:PHE:HA	1:67:A:PHE:HD1	10	0.57
(1,1199)	1:89:A:TYR:HE1	1:71:A:LEU:HD12	15	0.57
(1,1183)	1:90:A:ASN:HB2	1:87:A:PHE:HD1	3	0.57
(1,1123)	1:83:A:GLU:HA	1:83:A:GLU:HG3	20	0.57
(1,1088)	1:100:A:LEU:HD22	1:105:A:PHE:HD2	14	0.57
(1,1070)	1:101:A:ALA:HB1	1:102:A:SER:H	17	0.57
(1,1070)	1:101:A:ALA:HB2	1:102:A:SER:H	19	0.57
(1,1070)	1:101:A:ALA:HB3	1:102:A:SER:H	22	0.57
(1,932)	1:112:A:VAL:HG23	1:126:A:TYR:HA	12	0.57
(1,902)	1:115:A:ARG:HD2	1:115:A:ARG:H	8	0.57
(1,902)	1:115:A:ARG:HD2	1:115:A:ARG:H	9	0.57
(1,902)	1:115:A:ARG:HD2	1:115:A:ARG:H	19	0.57
(1,848)	1:120:A:PRO:HG3	1:119:A:ARG:HA	2	0.57
(1,826)	1:117:A:ARG:HG2	1:117:A:ARG:H	13	0.57
(1,826)	1:117:A:ARG:HG2	1:117:A:ARG:H	19	0.57
(1,792)	1:127:A:ILE:HD13	1:124:A:TYR:HD1	18	0.57
(1,790)	1:124:A:TYR:HD1	1:124:A:TYR:HA	7	0.57
(1,790)	1:124:A:TYR:HD1	1:124:A:TYR:HA	12	0.57
(1,723)	1:129:A:GLU:HG2	1:125:A:VAL:HG12	15	0.57
(1,723)	1:129:A:GLU:HG2	1:125:A:VAL:HG13	19	0.57
(1,607)	1:136:A:ALA:HB2	1:137:A:HIS:HA	7	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,576)	1:142:A:LYS:HB2	1:142:A:LYS:H	24	0.57
(1,555)	2:36:B:THR:H	2:35:B:PHE:H	1	0.57
(1,552)	2:35:B:PHE:H	2:33:B:GLN:HA	25	0.57
(1,510)	1:73:A:LEU:HD23	1:77:A:GLN:HE22	9	0.57
(1,510)	1:73:A:LEU:HD23	1:77:A:GLN:HE22	13	0.57
(1,499)	1:85:A:VAL:H	1:74:A:CYS:HB3	2	0.57
(1,499)	1:85:A:VAL:H	1:74:A:CYS:HB3	6	0.57
(1,499)	1:85:A:VAL:H	1:74:A:CYS:HB3	9	0.57
(1,499)	1:85:A:VAL:H	1:74:A:CYS:HB3	13	0.57
(1,499)	1:85:A:VAL:H	1:74:A:CYS:HB3	21	0.57
(1,478)	1:95:A:ALA:H	1:91:A:ARG:HD2	1	0.57
(1,457)	1:111:A:ARG:H	1:109:A:LEU:HB3	9	0.57
(1,457)	1:111:A:ARG:H	1:109:A:LEU:HB3	24	0.57
(1,455)	1:112:A:VAL:H	1:113:A:LEU:HB3	3	0.57
(1,455)	1:112:A:VAL:H	1:113:A:LEU:HB3	22	0.57
(1,445)	1:116:A:ALA:H	1:112:A:VAL:HA	6	0.57
(1,444)	1:73:A:LEU:HD13	1:117:A:ARG:H	11	0.57
(1,398)	1:135:A:LYS:HG2	1:136:A:ALA:H	11	0.57
(1,398)	1:135:A:LYS:HG2	1:136:A:ALA:H	15	0.57
(1,395)	1:138:A:SER:H	1:95:A:ALA:HB3	10	0.57
(1,380)	2:27:B:SER:HA	2:30:B:GLU:HB3	16	0.57
(1,361)	2:29:B:SER:HB2	2:32:B:GLU:HG3	1	0.57
(1,340)	2:31:B:LEU:HD12	1:88:A:LEU:H	8	0.57
(1,338)	2:31:B:LEU:HD23	2:32:B:GLU:HG3	21	0.57
(1,338)	2:31:B:LEU:HD22	2:32:B:GLU:HG3	23	0.57
(1,323)	1:84:A:VAL:HG22	2:34:B:TYR:HD1	12	0.57
(1,323)	1:84:A:VAL:HG22	2:34:B:TYR:HD1	23	0.57
(1,319)	2:34:B:TYR:HE1	1:84:A:VAL:HG22	9	0.57
(1,319)	2:34:B:TYR:HE1	1:84:A:VAL:HG22	12	0.57
(1,319)	2:34:B:TYR:HE1	1:84:A:VAL:HG21	18	0.57
(1,293)	2:39:B:TRP:HD1	2:38:B:ARG:HB3	16	0.57
(1,281)	2:31:B:LEU:HD22	1:128:A:ASN:H	9	0.57
(1,265)	1:127:A:ILE:HD12	2:35:B:PHE:HE1	18	0.57
(1,232)	1:66:A:LEU:HD13	1:62:A:GLU:HA	16	0.57
(1,232)	1:66:A:LEU:HD12	1:110:A:SER:HA	21	0.57
(1,228)	1:62:A:GLU:HG2	1:66:A:LEU:HD12	3	0.57
(1,216)	1:113:A:LEU:HD13	1:70:A:PHE:HD2	23	0.57
(1,207)	1:109:A:LEU:HD22	1:113:A:LEU:H	16	0.57
(1,203)	1:71:A:LEU:HD11	1:68:A:GLU:H	6	0.57
(1,199)	1:72:A:GLU:HG2	1:71:A:LEU:HB3	15	0.57
(1,197)	1:73:A:LEU:HD21	1:123:A:LEU:HB2	24	0.57
(1,195)	1:73:A:LEU:HD21	1:70:A:PHE:HA	8	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,189)	1:85:A:VAL:HG12	1:75:A:LYS:HA	21	0.57
(1,170)	1:85:A:VAL:HG12	1:89:A:TYR:H	20	0.57
(1,152)	1:67:A:PHE:HE1	1:88:A:LEU:HD11	2	0.57
(1,152)	1:67:A:PHE:HE1	1:88:A:LEU:HD13	22	0.57
(1,141)	1:93:A:GLN:HG2	1:89:A:TYR:HD1	12	0.57
(1,97)	1:105:A:PHE:HD1	1:134:A:LEU:HA	5	0.57
(1,97)	1:105:A:PHE:HD1	1:134:A:LEU:HA	24	0.57
(1,89)	1:94:A:ARG:HD3	1:94:A:ARG:HA	23	0.57
(1,80)	1:94:A:ARG:HD3	1:94:A:ARG:HB2	10	0.57
(1,56)	1:124:A:TYR:HE2	2:35:B:PHE:HB3	17	0.57
(1,45)	1:59:A:TYR:HE2	1:57:A:LYS:HD3	5	0.57
(1,44)	1:126:A:TYR:HE2	1:126:A:TYR:HB2	6	0.57
(1,44)	1:126:A:TYR:HE2	1:126:A:TYR:HB2	14	0.57
(1,13)	1:133:A:VAL:HG12	1:108:A:ILE:HB	23	0.57
(1,13)	1:133:A:VAL:HG13	1:108:A:ILE:HB	25	0.57
(1,5)	1:100:A:LEU:HD12	1:100:A:LEU:H	3	0.57
(1,2124)	1:73:A:LEU:HD22	1:73:A:LEU:H	16	0.56
(1,2114)	1:75:A:LYS:HG2	1:75:A:LYS:H	6	0.56
(1,2114)	1:75:A:LYS:HG2	1:75:A:LYS:H	18	0.56
(1,2082)	1:81:A:HIS:H	1:79:A:ALA:HB1	13	0.56
(1,2082)	1:81:A:HIS:H	1:79:A:ALA:HB1	20	0.56
(1,2060)	1:86:A:PRO:HB3	1:87:A:PHE:H	21	0.56
(1,2018)	1:93:A:GLN:HE22	1:93:A:GLN:HG3	20	0.56
(1,2017)	1:93:A:GLN:HE22	1:89:A:TYR:HB3	22	0.56
(1,2012)	1:94:A:ARG:HB3	1:94:A:ARG:H	12	0.56
(1,1910)	1:109:A:LEU:HD21	1:110:A:SER:H	4	0.56
(1,1910)	1:109:A:LEU:HD22	1:110:A:SER:H	7	0.56
(1,1910)	1:109:A:LEU:HD21	1:110:A:SER:H	13	0.56
(1,1910)	1:109:A:LEU:HD23	1:110:A:SER:H	22	0.56
(1,1861)	1:123:A:LEU:HD21	1:123:A:LEU:H	9	0.56
(1,1861)	1:123:A:LEU:HD23	1:123:A:LEU:H	20	0.56
(1,1788)	1:139:A:ALA:H	1:135:A:LYS:HD3	17	0.56
(1,1722)	2:31:B:LEU:HD23	1:128:A:ASN:HB2	24	0.56
(1,1716)	2:31:B:LEU:HG	2:32:B:GLU:HG3	24	0.56
(1,1635)	2:39:B:TRP:HA	2:38:B:ARG:HD2	20	0.56
(1,1633)	2:38:B:ARG:HD2	2:38:B:ARG:HB2	3	0.56
(1,1576)	1:73:A:LEU:HD13	1:117:A:ARG:H	18	0.56
(1,1576)	1:73:A:LEU:HD11	1:117:A:ARG:H	23	0.56
(1,1501)	1:64:A:GLU:HG2	1:65:A:LYS:H	1	0.56
(1,1501)	1:64:A:GLU:HG2	1:65:A:LYS:H	2	0.56
(1,1501)	1:64:A:GLU:HG2	1:65:A:LYS:H	11	0.56
(1,1501)	1:64:A:GLU:HG2	1:65:A:LYS:H	14	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1501)	1:64:A:GLU:HG2	1:65:A:LYS:H	16	0.56
(1,1501)	1:64:A:GLU:HG2	1:65:A:LYS:H	24	0.56
(1,1496)	1:64:A:GLU:HG3	1:64:A:GLU:HA	1	0.56
(1,1496)	1:64:A:GLU:HG3	1:64:A:GLU:HA	17	0.56
(1,1489)	1:65:A:LYS:HG2	1:66:A:LEU:H	25	0.56
(1,1421)	1:71:A:LEU:HD21	1:71:A:LEU:H	10	0.56
(1,1421)	1:71:A:LEU:HD23	1:71:A:LEU:H	11	0.56
(1,1421)	1:71:A:LEU:HD21	1:71:A:LEU:H	19	0.56
(1,1421)	1:71:A:LEU:HD22	1:71:A:LEU:H	23	0.56
(1,1395)	1:116:A:ALA:HB3	1:73:A:LEU:HD21	11	0.56
(1,1341)	1:76:A:MET:HB3	1:73:A:LEU:HA	12	0.56
(1,1338)	1:76:A:MET:HB3	1:76:A:MET:H	8	0.56
(1,1338)	1:76:A:MET:HB3	1:76:A:MET:H	11	0.56
(1,1338)	1:76:A:MET:HB3	1:76:A:MET:H	22	0.56
(1,1329)	1:77:A:GLN:HG2	1:77:A:GLN:HB3	16	0.56
(1,1273)	1:85:A:VAL:HG13	1:75:A:LYS:HE2	6	0.56
(1,1183)	1:90:A:ASN:HB2	1:87:A:PHE:HD1	16	0.56
(1,1115)	1:98:A:LEU:HD21	1:96:A:HIS:HE1	20	0.56
(1,1062)	1:103:A:ALA:HB1	1:59:A:TYR:HB3	25	0.56
(1,932)	1:112:A:VAL:HG23	1:126:A:TYR:HA	3	0.56
(1,932)	1:112:A:VAL:HG22	1:126:A:TYR:HA	10	0.56
(1,902)	1:115:A:ARG:HD2	1:115:A:ARG:H	20	0.56
(1,848)	1:120:A:PRO:HG3	1:119:A:ARG:HA	11	0.56
(1,827)	1:122:A:LYS:HD2	1:122:A:LYS:HA	19	0.56
(1,826)	1:117:A:ARG:HG2	1:117:A:ARG:H	4	0.56
(1,825)	1:122:A:LYS:HG2	1:125:A:VAL:HG23	1	0.56
(1,825)	1:122:A:LYS:HG2	1:125:A:VAL:HG22	17	0.56
(1,793)	1:124:A:TYR:HE1	1:124:A:TYR:H	17	0.56
(1,792)	1:127:A:ILE:HD13	1:124:A:TYR:HD1	6	0.56
(1,790)	1:124:A:TYR:HD1	1:124:A:TYR:HA	8	0.56
(1,766)	1:126:A:TYR:HE1	1:115:A:ARG:HB2	9	0.56
(1,577)	1:75:A:LYS:HE2	1:71:A:LEU:HB3	20	0.56
(1,577)	1:75:A:LYS:HE2	1:71:A:LEU:HB3	21	0.56
(1,575)	1:143:A:LEU:HA	1:143:A:LEU:HD21	19	0.56
(1,555)	2:36:B:THR:H	2:37:B:ALA:H	9	0.56
(1,555)	2:36:B:THR:H	2:37:B:ALA:H	17	0.56
(1,552)	2:35:B:PHE:H	2:33:B:GLN:HA	9	0.56
(1,552)	2:35:B:PHE:H	2:33:B:GLN:HA	11	0.56
(1,510)	1:73:A:LEU:HD21	1:77:A:GLN:HE22	15	0.56
(1,498)	1:87:A:PHE:H	1:84:A:VAL:HG13	25	0.56
(1,484)	1:134:A:LEU:HD12	1:94:A:ARG:H	6	0.56
(1,455)	1:112:A:VAL:H	1:113:A:LEU:HB3	4	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,451)	1:114:A:SER:H	1:117:A:ARG:HB2	3	0.56
(1,427)	1:126:A:TYR:H	1:127:A:ILE:HD13	25	0.56
(1,387)	1:141:A:LYS:H	1:141:A:LYS:HG2	1	0.56
(1,366)	1:100:A:LEU:HD12	1:138:A:SER:HB3	24	0.56
(1,361)	2:29:B:SER:HB2	2:32:B:GLU:HG3	15	0.56
(1,338)	2:31:B:LEU:HD21	2:32:B:GLU:HG3	13	0.56
(1,325)	2:33:B:GLN:HG2	2:31:B:LEU:HB2	12	0.56
(1,323)	1:84:A:VAL:HG21	2:34:B:TYR:HD1	8	0.56
(1,319)	2:34:B:TYR:HE1	1:84:A:VAL:HG22	7	0.56
(1,319)	2:34:B:TYR:HE1	1:84:A:VAL:HG21	8	0.56
(1,318)	2:34:B:TYR:HE1	1:83:A:GLU:HB3	2	0.56
(1,318)	2:34:B:TYR:HE1	1:83:A:GLU:HB3	5	0.56
(1,310)	2:35:B:PHE:HD1	1:127:A:ILE:HB	4	0.56
(1,307)	2:39:B:TRP:HE3	2:36:B:THR:HG21	1	0.56
(1,307)	2:39:B:TRP:HE3	2:36:B:THR:HG22	17	0.56
(1,281)	2:31:B:LEU:HD22	1:128:A:ASN:H	7	0.56
(1,265)	1:127:A:ILE:HD12	2:35:B:PHE:HE1	7	0.56
(1,265)	1:127:A:ILE:HD13	2:35:B:PHE:HE1	15	0.56
(1,243)	1:62:A:GLU:HG3	1:61:A:LEU:HD21	16	0.56
(1,232)	1:66:A:LEU:HD11	1:62:A:GLU:HA	9	0.56
(1,230)	1:66:A:LEU:HA	1:113:A:LEU:HD21	1	0.56
(1,230)	1:66:A:LEU:HA	1:113:A:LEU:HD23	18	0.56
(1,228)	1:62:A:GLU:HG2	1:66:A:LEU:HD12	8	0.56
(1,228)	1:62:A:GLU:HG2	1:66:A:LEU:HD13	11	0.56
(1,228)	1:62:A:GLU:HG2	1:66:A:LEU:HD13	13	0.56
(1,227)	1:62:A:GLU:HG2	1:61:A:LEU:HG	20	0.56
(1,216)	1:113:A:LEU:HD13	1:70:A:PHE:HD2	5	0.56
(1,172)	1:85:A:VAL:HG13	1:88:A:LEU:HB2	16	0.56
(1,170)	1:85:A:VAL:HG13	1:89:A:TYR:H	2	0.56
(1,170)	1:85:A:VAL:HG11	1:75:A:LYS:H	13	0.56
(1,170)	1:85:A:VAL:HG12	1:75:A:LYS:H	19	0.56
(1,152)	1:67:A:PHE:HE1	1:88:A:LEU:HD11	9	0.56
(1,152)	1:67:A:PHE:HE1	1:88:A:LEU:HD13	15	0.56
(1,151)	1:88:A:LEU:HD13	1:70:A:PHE:HD1	8	0.56
(1,151)	1:88:A:LEU:HD12	1:70:A:PHE:HD1	13	0.56
(1,134)	1:92:A:GLN:HG2	1:95:A:ALA:H	2	0.56
(1,134)	1:92:A:GLN:HG2	1:95:A:ALA:H	20	0.56
(1,132)	1:67:A:PHE:HE1	1:92:A:GLN:HB3	16	0.56
(1,97)	1:105:A:PHE:HD1	1:134:A:LEU:HA	10	0.56
(1,44)	1:126:A:TYR:HE1	1:112:A:VAL:HA	20	0.56
(1,17)	1:133:A:VAL:HG11	1:137:A:HIS:HB2	5	0.56
(1,5)	1:100:A:LEU:HD11	1:100:A:LEU:H	7	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5)	1:100:A:LEU:HD11	1:100:A:LEU:H	25	0.56
(1,2124)	1:73:A:LEU:HD21	1:73:A:LEU:H	4	0.55
(1,2124)	1:73:A:LEU:HD22	1:73:A:LEU:H	14	0.55
(1,2124)	1:73:A:LEU:HD22	1:73:A:LEU:H	17	0.55
(1,2124)	1:73:A:LEU:HD22	1:73:A:LEU:H	21	0.55
(1,2124)	1:73:A:LEU:HD22	1:73:A:LEU:H	22	0.55
(1,2124)	1:73:A:LEU:HD22	1:73:A:LEU:H	25	0.55
(1,2114)	1:75:A:LYS:HG2	1:75:A:LYS:H	25	0.55
(1,2089)	1:79:A:ALA:H	1:78:A:THR:HG23	10	0.55
(1,2089)	1:79:A:ALA:H	1:78:A:THR:HG21	13	0.55
(1,2082)	1:81:A:HIS:H	1:79:A:ALA:HB1	9	0.55
(1,2082)	1:81:A:HIS:H	1:79:A:ALA:HB1	17	0.55
(1,2013)	1:94:A:ARG:H	1:95:A:ALA:HB1	12	0.55
(1,2011)	1:94:A:ARG:HD2	1:94:A:ARG:H	10	0.55
(1,1986)	1:99:A:PHE:H	1:98:A:LEU:HD22	9	0.55
(1,1910)	1:109:A:LEU:HD21	1:110:A:SER:H	8	0.55
(1,1910)	1:109:A:LEU:HD21	1:110:A:SER:H	18	0.55
(1,1910)	1:109:A:LEU:HD22	1:110:A:SER:H	19	0.55
(1,1910)	1:109:A:LEU:HD22	1:110:A:SER:H	25	0.55
(1,1861)	1:123:A:LEU:HD22	1:123:A:LEU:H	12	0.55
(1,1861)	1:123:A:LEU:HD21	1:123:A:LEU:H	17	0.55
(1,1801)	1:135:A:LYS:H	1:91:A:ARG:HD3	3	0.55
(1,1765)	2:24:B:GLN:HB2	2:24:B:GLN:HG2	5	0.55
(1,1765)	2:24:B:GLN:HB2	2:24:B:GLN:HG2	12	0.55
(1,1765)	2:24:B:GLN:HB2	2:24:B:GLN:HG2	21	0.55
(1,1765)	2:24:B:GLN:HB2	2:24:B:GLN:HG2	24	0.55
(1,1723)	2:31:B:LEU:HD21	2:30:B:GLU:HB2	17	0.55
(1,1629)	2:38:B:ARG:HG3	2:38:B:ARG:HA	5	0.55
(1,1629)	2:38:B:ARG:HG2	2:38:B:ARG:HA	16	0.55
(1,1629)	2:38:B:ARG:HG2	2:38:B:ARG:HA	18	0.55
(1,1629)	2:38:B:ARG:HG3	2:38:B:ARG:HA	25	0.55
(1,1501)	1:64:A:GLU:HG2	1:65:A:LYS:H	25	0.55
(1,1496)	1:64:A:GLU:HG3	1:64:A:GLU:HA	7	0.55
(1,1489)	1:65:A:LYS:HG2	1:66:A:LEU:H	19	0.55
(1,1421)	1:71:A:LEU:HD23	1:71:A:LEU:H	9	0.55
(1,1395)	1:116:A:ALA:HB3	1:73:A:LEU:HD23	4	0.55
(1,1338)	1:76:A:MET:HB3	1:76:A:MET:H	1	0.55
(1,1273)	1:85:A:VAL:HG11	1:75:A:LYS:HE2	7	0.55
(1,1123)	1:83:A:GLU:HA	1:83:A:GLU:HG3	18	0.55
(1,1091)	1:100:A:LEU:HD21	1:92:A:GLN:HE21	6	0.55
(1,1090)	1:100:A:LEU:HD22	1:99:A:PHE:HE1	23	0.55
(1,1062)	1:103:A:ALA:HB1	1:59:A:TYR:HB3	11	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1059)	1:103:A:ALA:HB2	1:104:A:GLU:HA	20	0.55
(1,932)	1:112:A:VAL:HG22	1:126:A:TYR:HA	7	0.55
(1,902)	1:115:A:ARG:HD2	1:115:A:ARG:H	12	0.55
(1,848)	1:120:A:PRO:HG3	1:119:A:ARG:HA	10	0.55
(1,848)	1:120:A:PRO:HG3	1:119:A:ARG:HA	18	0.55
(1,848)	1:120:A:PRO:HG3	1:119:A:ARG:HA	21	0.55
(1,848)	1:120:A:PRO:HG3	1:119:A:ARG:HA	24	0.55
(1,825)	1:122:A:LYS:HG2	1:125:A:VAL:HG22	7	0.55
(1,825)	1:122:A:LYS:HG2	1:125:A:VAL:HG23	10	0.55
(1,723)	1:129:A:GLU:HG2	1:125:A:VAL:HG12	6	0.55
(1,723)	1:129:A:GLU:HG2	1:125:A:VAL:HG11	7	0.55
(1,614)	1:135:A:LYS:HA	1:135:A:LYS:HD2	12	0.55
(1,607)	1:136:A:ALA:HB1	1:137:A:HIS:HA	10	0.55
(1,584)	1:139:A:ALA:HB1	1:96:A:HIS:H	21	0.55
(1,577)	1:75:A:LYS:HE2	1:71:A:LEU:HB3	16	0.55
(1,563)	2:26:B:ASP:H	2:30:B:GLU:HB3	6	0.55
(1,555)	2:36:B:THR:H	2:37:B:ALA:H	10	0.55
(1,555)	2:36:B:THR:H	2:37:B:ALA:H	11	0.55
(1,555)	2:36:B:THR:H	2:37:B:ALA:H	18	0.55
(1,555)	2:36:B:THR:H	2:35:B:PHE:H	22	0.55
(1,555)	2:36:B:THR:H	2:35:B:PHE:H	23	0.55
(1,552)	2:35:B:PHE:H	2:33:B:GLN:HA	14	0.55
(1,529)	1:67:A:PHE:H	1:68:A:GLU:HB2	9	0.55
(1,529)	1:67:A:PHE:H	1:68:A:GLU:HB2	14	0.55
(1,510)	1:73:A:LEU:HD23	1:77:A:GLN:HE22	2	0.55
(1,499)	1:85:A:VAL:H	1:74:A:CYS:HB3	5	0.55
(1,498)	1:87:A:PHE:H	1:84:A:VAL:HG12	21	0.55
(1,478)	1:95:A:ALA:H	1:91:A:ARG:HD2	15	0.55
(1,478)	1:95:A:ALA:H	1:91:A:ARG:HD2	18	0.55
(1,457)	1:111:A:ARG:H	1:109:A:LEU:HB3	15	0.55
(1,457)	1:111:A:ARG:H	1:109:A:LEU:HB3	19	0.55
(1,455)	1:112:A:VAL:H	1:113:A:LEU:HB3	10	0.55
(1,455)	1:112:A:VAL:H	1:113:A:LEU:HB3	11	0.55
(1,454)	1:114:A:SER:H	1:112:A:VAL:HG21	1	0.55
(1,454)	1:114:A:SER:H	1:112:A:VAL:HG22	22	0.55
(1,444)	1:73:A:LEU:HD12	1:117:A:ARG:H	21	0.55
(1,434)	1:74:A:CYS:H	1:123:A:LEU:HD11	10	0.55
(1,434)	1:74:A:CYS:H	1:123:A:LEU:HD12	12	0.55
(1,398)	1:135:A:LYS:HG2	1:136:A:ALA:H	5	0.55
(1,387)	1:141:A:LYS:H	1:141:A:LYS:HG2	2	0.55
(1,367)	2:26:B:ASP:HB3	2:31:B:LEU:H	16	0.55
(1,366)	1:100:A:LEU:HD12	1:138:A:SER:HB3	13	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,361)	2:29:B:SER:HB2	2:30:B:GLU:HG2	19	0.55
(1,356)	2:29:B:SER:HB2	2:31:B:LEU:H	17	0.55
(1,340)	2:31:B:LEU:HD11	1:88:A:LEU:H	6	0.55
(1,340)	2:31:B:LEU:HD11	1:88:A:LEU:H	23	0.55
(1,338)	2:31:B:LEU:HD23	2:32:B:GLU:HG3	2	0.55
(1,338)	2:31:B:LEU:HD21	2:32:B:GLU:HG3	6	0.55
(1,338)	2:31:B:LEU:HD22	2:32:B:GLU:HG3	8	0.55
(1,338)	2:31:B:LEU:HD23	2:32:B:GLU:HG3	12	0.55
(1,338)	2:31:B:LEU:HD22	2:32:B:GLU:HG3	20	0.55
(1,325)	2:33:B:GLN:HG2	2:31:B:LEU:HB2	20	0.55
(1,323)	1:84:A:VAL:HG22	2:34:B:TYR:HD1	24	0.55
(1,307)	2:39:B:TRP:HE3	2:36:B:THR:HG23	2	0.55
(1,289)	2:39:B:TRP:HZ3	2:36:B:THR:HB	10	0.55
(1,232)	1:66:A:LEU:HD12	1:62:A:GLU:HA	8	0.55
(1,232)	1:66:A:LEU:HD12	1:62:A:GLU:HA	10	0.55
(1,228)	1:62:A:GLU:HG2	1:66:A:LEU:HD12	7	0.55
(1,227)	1:62:A:GLU:HG2	1:61:A:LEU:HG	7	0.55
(1,227)	1:62:A:GLU:HG2	1:61:A:LEU:HG	16	0.55
(1,227)	1:62:A:GLU:HG2	1:61:A:LEU:HG	22	0.55
(1,216)	1:113:A:LEU:HD12	1:70:A:PHE:HD2	4	0.55
(1,216)	1:113:A:LEU:HD12	1:70:A:PHE:HD2	15	0.55
(1,207)	1:109:A:LEU:HD21	1:113:A:LEU:H	13	0.55
(1,189)	1:85:A:VAL:HG12	1:75:A:LYS:HA	5	0.55
(1,152)	1:67:A:PHE:HE1	1:88:A:LEU:HD11	11	0.55
(1,152)	1:67:A:PHE:HE1	1:88:A:LEU:HD11	20	0.55
(1,151)	1:88:A:LEU:HD11	1:70:A:PHE:HD1	15	0.55
(1,141)	1:93:A:GLN:HG2	1:89:A:TYR:HD1	6	0.55
(1,134)	1:105:A:PHE:HE2	1:92:A:GLN:HG2	16	0.55
(1,97)	1:105:A:PHE:HD1	1:100:A:LEU:HA	9	0.55
(1,80)	1:94:A:ARG:HD2	1:93:A:GLN:HB2	9	0.55
(1,67)	1:116:A:ALA:HB1	1:120:A:PRO:HA	16	0.55
(1,67)	1:116:A:ALA:HB1	1:120:A:PRO:HA	25	0.55
(1,44)	1:126:A:TYR:HE1	1:112:A:VAL:HA	12	0.55
(1,5)	1:100:A:LEU:HD11	1:100:A:LEU:H	4	0.55
(1,5)	1:100:A:LEU:HD13	1:100:A:LEU:H	12	0.55
(1,2124)	1:73:A:LEU:HD21	1:73:A:LEU:H	2	0.54
(1,2124)	1:73:A:LEU:HD21	1:73:A:LEU:H	23	0.54
(1,2114)	1:75:A:LYS:HG2	1:75:A:LYS:H	8	0.54
(1,2089)	1:79:A:ALA:H	1:78:A:THR:HG21	8	0.54
(1,2089)	1:79:A:ALA:H	1:78:A:THR:HG21	11	0.54
(1,2082)	1:81:A:HIS:H	1:79:A:ALA:HB2	1	0.54
(1,2017)	1:93:A:GLN:HE22	1:89:A:TYR:HB3	8	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2017)	1:93:A:GLN:HE22	1:89:A:TYR:HB3	13	0.54
(1,2012)	1:94:A:ARG:HB3	1:94:A:ARG:H	7	0.54
(1,2012)	1:94:A:ARG:HB3	1:94:A:ARG:H	24	0.54
(1,1910)	1:109:A:LEU:HD22	1:110:A:SER:H	2	0.54
(1,1910)	1:109:A:LEU:HD22	1:110:A:SER:H	3	0.54
(1,1910)	1:109:A:LEU:HD21	1:110:A:SER:H	5	0.54
(1,1910)	1:109:A:LEU:HD22	1:110:A:SER:H	9	0.54
(1,1910)	1:109:A:LEU:HD21	1:110:A:SER:H	10	0.54
(1,1910)	1:109:A:LEU:HD23	1:110:A:SER:H	12	0.54
(1,1910)	1:109:A:LEU:HD22	1:110:A:SER:H	14	0.54
(1,1910)	1:109:A:LEU:HD22	1:110:A:SER:H	15	0.54
(1,1798)	1:136:A:ALA:H	1:135:A:LYS:HD3	4	0.54
(1,1775)	1:143:A:LEU:H	1:141:A:LYS:HG3	18	0.54
(1,1652)	2:38:B:ARG:HD2	2:37:B:ALA:HB2	25	0.54
(1,1633)	2:38:B:ARG:HD2	2:38:B:ARG:HB2	9	0.54
(1,1633)	2:38:B:ARG:HD2	2:38:B:ARG:HB2	18	0.54
(1,1632)	2:38:B:ARG:HG2	2:38:B:ARG:HD2	11	0.54
(1,1629)	2:38:B:ARG:HG2	2:38:B:ARG:HA	2	0.54
(1,1629)	2:38:B:ARG:HG2	2:38:B:ARG:HA	10	0.54
(1,1576)	1:73:A:LEU:HD13	1:117:A:ARG:H	2	0.54
(1,1576)	1:73:A:LEU:HD13	1:117:A:ARG:H	22	0.54
(1,1501)	1:64:A:GLU:HG2	1:65:A:LYS:H	8	0.54
(1,1501)	1:64:A:GLU:HG2	1:65:A:LYS:H	17	0.54
(1,1496)	1:64:A:GLU:HG3	1:64:A:GLU:HA	4	0.54
(1,1496)	1:64:A:GLU:HG3	1:64:A:GLU:HA	20	0.54
(1,1496)	1:64:A:GLU:HG3	1:64:A:GLU:HA	23	0.54
(1,1489)	1:65:A:LYS:HG2	1:66:A:LEU:H	8	0.54
(1,1489)	1:65:A:LYS:HG2	1:66:A:LEU:H	13	0.54
(1,1489)	1:65:A:LYS:HG2	1:66:A:LEU:H	18	0.54
(1,1477)	1:66:A:LEU:HD22	1:113:A:LEU:HB3	6	0.54
(1,1421)	1:71:A:LEU:HD21	1:71:A:LEU:H	15	0.54
(1,1421)	1:71:A:LEU:HD23	1:71:A:LEU:H	21	0.54
(1,1341)	1:76:A:MET:HB3	1:73:A:LEU:HA	2	0.54
(1,1231)	1:67:A:PHE:HA	1:67:A:PHE:HD1	17	0.54
(1,1231)	1:67:A:PHE:HA	1:67:A:PHE:HD1	20	0.54
(1,1183)	1:90:A:ASN:HB2	1:87:A:PHE:HD1	2	0.54
(1,1183)	1:90:A:ASN:HB2	1:87:A:PHE:HD1	8	0.54
(1,1123)	1:83:A:GLU:HA	1:83:A:GLU:HG3	22	0.54
(1,1123)	1:83:A:GLU:HA	1:83:A:GLU:HG3	24	0.54
(1,1115)	1:98:A:LEU:HD23	1:96:A:HIS:HE1	4	0.54
(1,1094)	1:100:A:LEU:HD22	1:138:A:SER:HB2	6	0.54
(1,1070)	1:101:A:ALA:HB1	1:102:A:SER:H	2	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1059)	1:103:A:ALA:HB1	1:104:A:GLU:HA	10	0.54
(1,932)	1:112:A:VAL:HG23	1:126:A:TYR:HA	2	0.54
(1,932)	1:112:A:VAL:HG22	1:126:A:TYR:HA	8	0.54
(1,902)	1:115:A:ARG:HD2	1:115:A:ARG:H	5	0.54
(1,902)	1:115:A:ARG:HD2	1:115:A:ARG:H	7	0.54
(1,902)	1:115:A:ARG:HD2	1:115:A:ARG:H	14	0.54
(1,848)	1:120:A:PRO:HG3	1:119:A:ARG:HA	4	0.54
(1,848)	1:120:A:PRO:HG3	1:119:A:ARG:HA	5	0.54
(1,848)	1:120:A:PRO:HG3	1:119:A:ARG:HA	8	0.54
(1,848)	1:120:A:PRO:HG3	1:119:A:ARG:HA	19	0.54
(1,848)	1:120:A:PRO:HG3	1:119:A:ARG:HA	22	0.54
(1,825)	1:122:A:LYS:HG2	1:125:A:VAL:HG21	2	0.54
(1,825)	1:122:A:LYS:HG2	1:125:A:VAL:HG23	6	0.54
(1,825)	1:122:A:LYS:HG2	1:125:A:VAL:HG23	18	0.54
(1,793)	1:124:A:TYR:HE1	1:124:A:TYR:H	11	0.54
(1,705)	1:130:A:LEU:HD12	1:109:A:LEU:HD13	8	0.54
(1,607)	1:136:A:ALA:HB2	1:137:A:HIS:HA	4	0.54
(1,607)	1:136:A:ALA:HB1	1:137:A:HIS:HA	11	0.54
(1,607)	1:136:A:ALA:HB2	1:137:A:HIS:HA	16	0.54
(1,607)	1:136:A:ALA:HB3	1:137:A:HIS:HA	24	0.54
(1,585)	1:139:A:ALA:HB2	1:140:A:LYS:H	1	0.54
(1,585)	1:139:A:ALA:HB2	1:140:A:LYS:H	24	0.54
(1,575)	1:143:A:LEU:HA	1:143:A:LEU:HD21	3	0.54
(1,555)	2:36:B:THR:H	2:35:B:PHE:H	2	0.54
(1,555)	2:36:B:THR:H	2:35:B:PHE:H	7	0.54
(1,555)	2:36:B:THR:H	2:37:B:ALA:H	8	0.54
(1,555)	2:36:B:THR:H	2:37:B:ALA:H	14	0.54
(1,555)	2:36:B:THR:H	2:37:B:ALA:H	21	0.54
(1,555)	2:36:B:THR:H	2:35:B:PHE:H	25	0.54
(1,552)	2:35:B:PHE:H	2:33:B:GLN:HA	10	0.54
(1,552)	2:35:B:PHE:H	2:33:B:GLN:HA	15	0.54
(1,552)	2:35:B:PHE:H	2:33:B:GLN:HA	16	0.54
(1,552)	2:35:B:PHE:H	2:33:B:GLN:HA	17	0.54
(1,502)	1:81:A:HIS:H	1:82:A:PRO:HB3	22	0.54
(1,484)	1:134:A:LEU:HD13	1:94:A:ARG:H	10	0.54
(1,465)	1:106:A:CYS:H	1:103:A:ALA:HB2	25	0.54
(1,457)	1:111:A:ARG:H	1:109:A:LEU:HB3	2	0.54
(1,455)	1:112:A:VAL:H	1:113:A:LEU:HB3	5	0.54
(1,455)	1:112:A:VAL:H	1:113:A:LEU:HB3	6	0.54
(1,455)	1:112:A:VAL:H	1:113:A:LEU:HB3	17	0.54
(1,454)	1:114:A:SER:H	1:112:A:VAL:HG21	9	0.54
(1,454)	1:114:A:SER:H	1:112:A:VAL:HG23	10	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,451)	1:114:A:SER:H	1:117:A:ARG:HB2	1	0.54
(1,451)	1:114:A:SER:H	1:117:A:ARG:HB2	6	0.54
(1,391)	1:144:A:ASN:H	1:142:A:LYS:HB2	19	0.54
(1,387)	1:141:A:LYS:H	1:141:A:LYS:HG2	4	0.54
(1,387)	1:141:A:LYS:H	1:141:A:LYS:HG3	14	0.54
(1,340)	2:31:B:LEU:HD11	1:88:A:LEU:H	1	0.54
(1,340)	2:31:B:LEU:HD11	1:88:A:LEU:H	18	0.54
(1,338)	2:31:B:LEU:HD23	2:32:B:GLU:HG3	4	0.54
(1,338)	2:31:B:LEU:HD23	2:32:B:GLU:HG3	9	0.54
(1,319)	2:34:B:TYR:HE1	1:84:A:VAL:HG23	4	0.54
(1,310)	2:35:B:PHE:HD1	1:127:A:ILE:HB	10	0.54
(1,281)	2:31:B:LEU:HD22	1:128:A:ASN:H	12	0.54
(1,281)	2:31:B:LEU:HD21	1:128:A:ASN:H	20	0.54
(1,281)	2:31:B:LEU:HD21	1:128:A:ASN:H	25	0.54
(1,265)	1:127:A:ILE:HD12	2:35:B:PHE:HE1	9	0.54
(1,265)	1:127:A:ILE:HD11	2:35:B:PHE:HE1	23	0.54
(1,232)	1:66:A:LEU:HD11	1:110:A:SER:HA	5	0.54
(1,230)	1:66:A:LEU:HA	1:113:A:LEU:HD21	22	0.54
(1,228)	1:62:A:GLU:HG2	1:66:A:LEU:HD13	12	0.54
(1,199)	1:72:A:GLU:HG2	1:71:A:LEU:HB3	13	0.54
(1,195)	1:73:A:LEU:HD21	1:70:A:PHE:HA	13	0.54
(1,195)	1:73:A:LEU:HD22	1:70:A:PHE:HA	14	0.54
(1,195)	1:73:A:LEU:HD22	1:70:A:PHE:HA	17	0.54
(1,194)	1:73:A:LEU:HD22	1:70:A:PHE:HD1	21	0.54
(1,170)	1:85:A:VAL:HG11	1:75:A:LYS:H	12	0.54
(1,151)	1:88:A:LEU:HD13	1:70:A:PHE:HD1	4	0.54
(1,151)	1:88:A:LEU:HD11	1:70:A:PHE:HD1	24	0.54
(1,141)	1:93:A:GLN:HG2	1:89:A:TYR:HD1	16	0.54
(1,141)	1:93:A:GLN:HG2	1:89:A:TYR:HD1	22	0.54
(1,132)	1:92:A:GLN:HB3	1:89:A:TYR:HD1	6	0.54
(1,132)	1:67:A:PHE:HE1	1:92:A:GLN:HB3	10	0.54
(1,97)	1:105:A:PHE:HD1	1:100:A:LEU:HA	19	0.54
(1,15)	1:132:A:THR:HG21	2:27:B:SER:H	14	0.54
(1,6)	1:130:A:LEU:HD23	1:70:A:PHE:HE2	19	0.54
(1,6)	1:130:A:LEU:HD23	1:70:A:PHE:HE2	21	0.54
(1,5)	1:100:A:LEU:HD13	1:100:A:LEU:H	17	0.54
(1,5)	1:100:A:LEU:HD11	1:100:A:LEU:H	22	0.54
(1,2197)	1:55:A:GLY:HA2	1:56:A:LYS:H	9	0.53
(1,2194)	1:56:A:LYS:HB3	1:56:A:LYS:H	2	0.53
(1,2124)	1:73:A:LEU:HD23	1:73:A:LEU:H	5	0.53
(1,2124)	1:73:A:LEU:HD21	1:73:A:LEU:H	6	0.53
(1,2124)	1:73:A:LEU:HD22	1:73:A:LEU:H	7	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2124)	1:73:A:LEU:HD21	1:73:A:LEU:H	9	0.53
(1,2124)	1:73:A:LEU:HD21	1:73:A:LEU:H	13	0.53
(1,2124)	1:73:A:LEU:HD21	1:73:A:LEU:H	20	0.53
(1,2097)	1:77:A:GLN:HE21	1:77:A:GLN:HA	1	0.53
(1,2089)	1:79:A:ALA:H	1:78:A:THR:HG23	1	0.53
(1,2089)	1:79:A:ALA:H	1:78:A:THR:HG23	19	0.53
(1,2089)	1:79:A:ALA:H	1:78:A:THR:HG23	23	0.53
(1,2089)	1:79:A:ALA:H	1:78:A:THR:HG22	25	0.53
(1,2082)	1:81:A:HIS:H	1:79:A:ALA:HB3	22	0.53
(1,2017)	1:93:A:GLN:HE22	1:89:A:TYR:HB3	7	0.53
(1,2013)	1:94:A:ARG:H	1:95:A:ALA:HB1	9	0.53
(1,2013)	1:94:A:ARG:H	1:95:A:ALA:HB3	13	0.53
(1,2013)	1:94:A:ARG:H	1:95:A:ALA:HB2	16	0.53
(1,2013)	1:94:A:ARG:H	1:95:A:ALA:HB1	18	0.53
(1,2013)	1:94:A:ARG:H	1:95:A:ALA:HB3	22	0.53
(1,2012)	1:94:A:ARG:HB3	1:94:A:ARG:H	1	0.53
(1,2012)	1:94:A:ARG:HB3	1:94:A:ARG:H	4	0.53
(1,2012)	1:94:A:ARG:HB3	1:94:A:ARG:H	5	0.53
(1,2012)	1:94:A:ARG:HB3	1:94:A:ARG:H	10	0.53
(1,2012)	1:94:A:ARG:HB3	1:94:A:ARG:H	18	0.53
(1,1996)	1:97:A:SER:H	1:139:A:ALA:HB3	16	0.53
(1,1910)	1:109:A:LEU:HD21	1:110:A:SER:H	17	0.53
(1,1910)	1:109:A:LEU:HD23	1:110:A:SER:H	20	0.53
(1,1910)	1:109:A:LEU:HD21	1:110:A:SER:H	21	0.53
(1,1798)	1:136:A:ALA:H	1:135:A:LYS:HD3	13	0.53
(1,1798)	1:136:A:ALA:H	1:135:A:LYS:HD3	17	0.53
(1,1788)	1:139:A:ALA:H	1:135:A:LYS:HD3	7	0.53
(1,1650)	2:37:B:ALA:HB2	1:121:A:ALA:HB3	4	0.53
(1,1650)	2:37:B:ALA:HB2	1:121:A:ALA:HB2	23	0.53
(1,1633)	2:38:B:ARG:HD2	2:38:B:ARG:HB2	6	0.53
(1,1632)	2:38:B:ARG:HG2	2:38:B:ARG:HD2	15	0.53
(1,1629)	2:38:B:ARG:HG3	2:38:B:ARG:HA	12	0.53
(1,1576)	1:73:A:LEU:HD13	1:117:A:ARG:H	12	0.53
(1,1576)	1:73:A:LEU:HD12	1:117:A:ARG:H	16	0.53
(1,1554)	1:59:A:TYR:HE1	1:57:A:LYS:HB2	25	0.53
(1,1501)	1:64:A:GLU:HG2	1:65:A:LYS:H	10	0.53
(1,1501)	1:64:A:GLU:HG2	1:65:A:LYS:H	13	0.53
(1,1501)	1:64:A:GLU:HG2	1:65:A:LYS:H	23	0.53
(1,1496)	1:64:A:GLU:HG3	1:64:A:GLU:HA	8	0.53
(1,1496)	1:64:A:GLU:HG3	1:64:A:GLU:HA	9	0.53
(1,1496)	1:64:A:GLU:HG3	1:64:A:GLU:HA	14	0.53
(1,1421)	1:71:A:LEU:HD23	1:71:A:LEU:H	14	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1421)	1:71:A:LEU:HD23	1:71:A:LEU:H	16	0.53
(1,1395)	1:116:A:ALA:HB1	1:73:A:LEU:HD21	15	0.53
(1,1231)	1:67:A:PHE:HA	1:67:A:PHE:HD1	1	0.53
(1,1231)	1:67:A:PHE:HA	1:67:A:PHE:HD1	21	0.53
(1,1199)	1:89:A:TYR:HE1	1:71:A:LEU:HD11	1	0.53
(1,1115)	1:98:A:LEU:HD21	1:96:A:HIS:HE1	24	0.53
(1,1070)	1:101:A:ALA:HB2	1:102:A:SER:H	3	0.53
(1,1070)	1:101:A:ALA:HB2	1:102:A:SER:H	10	0.53
(1,996)	1:108:A:ILE:HG21	1:112:A:VAL:HG12	7	0.53
(1,989)	1:108:A:ILE:HG23	1:105:A:PHE:HA	8	0.53
(1,932)	1:112:A:VAL:HG23	1:126:A:TYR:HA	9	0.53
(1,932)	1:112:A:VAL:HG22	1:126:A:TYR:HA	18	0.53
(1,932)	1:112:A:VAL:HG21	1:126:A:TYR:HA	24	0.53
(1,902)	1:115:A:ARG:HD2	1:115:A:ARG:H	2	0.53
(1,902)	1:115:A:ARG:HD2	1:115:A:ARG:H	3	0.53
(1,902)	1:115:A:ARG:HD2	1:115:A:ARG:H	17	0.53
(1,848)	1:120:A:PRO:HG3	1:119:A:ARG:HA	7	0.53
(1,848)	1:120:A:PRO:HG3	1:119:A:ARG:HA	17	0.53
(1,826)	1:117:A:ARG:HG2	1:117:A:ARG:H	5	0.53
(1,826)	1:117:A:ARG:HG2	1:117:A:ARG:H	22	0.53
(1,826)	1:117:A:ARG:HG2	1:117:A:ARG:H	23	0.53
(1,825)	1:122:A:LYS:HG2	1:125:A:VAL:HG23	3	0.53
(1,825)	1:122:A:LYS:HG2	1:125:A:VAL:HG21	13	0.53
(1,792)	1:127:A:ILE:HD11	1:124:A:TYR:HD1	11	0.53
(1,792)	1:127:A:ILE:HD11	1:124:A:TYR:HD1	17	0.53
(1,723)	1:129:A:GLU:HG2	1:125:A:VAL:HG11	3	0.53
(1,723)	1:129:A:GLU:HG2	1:125:A:VAL:HG13	10	0.53
(1,607)	1:136:A:ALA:HB2	1:137:A:HIS:HA	6	0.53
(1,555)	2:36:B:THR:H	2:37:B:ALA:H	3	0.53
(1,555)	2:36:B:THR:H	2:37:B:ALA:H	15	0.53
(1,552)	2:35:B:PHE:H	2:33:B:GLN:HA	8	0.53
(1,552)	2:35:B:PHE:H	2:33:B:GLN:HA	12	0.53
(1,552)	2:35:B:PHE:H	2:33:B:GLN:HA	23	0.53
(1,519)	1:74:A:CYS:H	1:85:A:VAL:HG23	10	0.53
(1,499)	1:85:A:VAL:H	1:74:A:CYS:HB3	7	0.53
(1,484)	1:134:A:LEU:HD13	1:94:A:ARG:H	17	0.53
(1,457)	1:111:A:ARG:H	1:109:A:LEU:HB3	18	0.53
(1,455)	1:112:A:VAL:H	1:113:A:LEU:HB3	21	0.53
(1,454)	1:114:A:SER:H	1:112:A:VAL:HG22	13	0.53
(1,454)	1:114:A:SER:H	1:112:A:VAL:HG21	20	0.53
(1,454)	1:114:A:SER:H	1:112:A:VAL:HG23	23	0.53
(1,444)	1:73:A:LEU:HD13	1:117:A:ARG:H	4	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,434)	1:74:A:CYS:H	1:123:A:LEU:HD11	6	0.53
(1,419)	1:129:A:GLU:H	1:126:A:TYR:H	24	0.53
(1,361)	2:29:B:SER:HB2	2:32:B:GLU:HG3	2	0.53
(1,361)	2:29:B:SER:HB2	2:32:B:GLU:HG3	17	0.53
(1,340)	2:31:B:LEU:HD11	1:88:A:LEU:H	11	0.53
(1,338)	2:31:B:LEU:HD23	2:32:B:GLU:HG3	17	0.53
(1,321)	2:34:B:TYR:HD1	1:83:A:GLU:HB3	15	0.53
(1,289)	2:39:B:TRP:HZ3	2:36:B:THR:HB	18	0.53
(1,281)	2:31:B:LEU:HD21	1:128:A:ASN:H	11	0.53
(1,280)	2:31:B:LEU:HG	1:87:A:PHE:HE2	7	0.53
(1,265)	1:127:A:ILE:HD13	2:35:B:PHE:HE1	4	0.53
(1,249)	1:56:A:LYS:HA	1:57:A:LYS:H	7	0.53
(1,230)	1:66:A:LEU:HA	1:113:A:LEU:HD23	12	0.53
(1,219)	1:70:A:PHE:HD1	1:73:A:LEU:HB3	7	0.53
(1,203)	1:71:A:LEU:HD12	1:68:A:GLU:H	23	0.53
(1,197)	1:73:A:LEU:HD23	1:123:A:LEU:HB2	6	0.53
(1,197)	1:73:A:LEU:HD21	1:123:A:LEU:HB2	17	0.53
(1,195)	1:73:A:LEU:HD23	1:117:A:ARG:HA	24	0.53
(1,194)	1:73:A:LEU:HD21	1:70:A:PHE:HD1	9	0.53
(1,170)	1:85:A:VAL:HG12	1:75:A:LYS:H	11	0.53
(1,170)	1:85:A:VAL:HG12	1:75:A:LYS:H	16	0.53
(1,132)	1:67:A:PHE:HE1	1:92:A:GLN:HB3	8	0.53
(1,132)	1:92:A:GLN:HB3	1:89:A:TYR:HD1	13	0.53
(1,81)	1:116:A:ALA:HB3	1:70:A:PHE:HZ	2	0.53
(1,67)	1:116:A:ALA:HB2	1:120:A:PRO:HA	19	0.53
(1,51)	1:126:A:TYR:HD1	1:125:A:VAL:HG12	21	0.53
(1,48)	1:126:A:TYR:HE1	1:125:A:VAL:HG11	5	0.53
(1,44)	1:126:A:TYR:HE1	1:112:A:VAL:HA	1	0.53
(1,44)	1:126:A:TYR:HE1	1:112:A:VAL:HA	25	0.53
(1,2193)	1:58:A:CYS:H	1:57:A:LYS:HG2	6	0.52
(1,2124)	1:73:A:LEU:HD23	1:73:A:LEU:H	12	0.52
(1,2114)	1:75:A:LYS:HG2	1:75:A:LYS:H	2	0.52
(1,2097)	1:77:A:GLN:HE21	1:77:A:GLN:HA	19	0.52
(1,2089)	1:79:A:ALA:H	1:78:A:THR:HG23	7	0.52
(1,2089)	1:79:A:ALA:H	1:78:A:THR:HG21	17	0.52
(1,2089)	1:79:A:ALA:H	1:78:A:THR:HG22	20	0.52
(1,2089)	1:79:A:ALA:H	1:78:A:THR:HG23	22	0.52
(1,2060)	1:86:A:PRO:HB3	1:87:A:PHE:H	13	0.52
(1,2051)	1:89:A:TYR:H	1:90:A:ASN:HB3	14	0.52
(1,2017)	1:93:A:GLN:HE22	1:89:A:TYR:HB3	6	0.52
(1,2017)	1:93:A:GLN:HE22	1:89:A:TYR:HB3	16	0.52
(1,2013)	1:94:A:ARG:H	1:95:A:ALA:HB1	19	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2012)	1:94:A:ARG:HB3	1:94:A:ARG:H	11	0.52
(1,2012)	1:94:A:ARG:HB3	1:94:A:ARG:H	14	0.52
(1,2012)	1:94:A:ARG:HB3	1:94:A:ARG:H	16	0.52
(1,1986)	1:99:A:PHE:H	1:98:A:LEU:HD22	18	0.52
(1,1968)	1:101:A:ALA:H	1:63:A:ASN:HD22	24	0.52
(1,1929)	1:107:A:ASN:HD21	1:103:A:ALA:HB3	16	0.52
(1,1874)	1:118:A:SER:H	1:117:A:ARG:HG3	14	0.52
(1,1771)	1:142:A:LYS:H	1:142:A:LYS:HD2	3	0.52
(1,1754)	2:30:B:GLU:HG2	2:31:B:LEU:H	25	0.52
(1,1723)	2:31:B:LEU:HD21	2:30:B:GLU:HB2	16	0.52
(1,1670)	2:37:B:ALA:HB3	2:36:B:THR:HA	23	0.52
(1,1633)	2:38:B:ARG:HD2	2:38:B:ARG:HB2	4	0.52
(1,1633)	2:38:B:ARG:HD2	2:38:B:ARG:HB2	22	0.52
(1,1620)	2:39:B:TRP:HD1	2:38:B:ARG:HG2	12	0.52
(1,1576)	1:73:A:LEU:HD11	1:117:A:ARG:H	1	0.52
(1,1576)	1:73:A:LEU:HD11	1:117:A:ARG:H	3	0.52
(1,1496)	1:64:A:GLU:HG3	1:64:A:GLU:HA	10	0.52
(1,1496)	1:64:A:GLU:HG3	1:64:A:GLU:HA	18	0.52
(1,1496)	1:64:A:GLU:HG3	1:64:A:GLU:HA	24	0.52
(1,1481)	1:66:A:LEU:HD21	1:69:A:GLU:H	14	0.52
(1,1475)	1:66:A:LEU:HD23	1:109:A:LEU:HD22	4	0.52
(1,1421)	1:71:A:LEU:HD23	1:71:A:LEU:H	4	0.52
(1,1395)	1:116:A:ALA:HB1	1:73:A:LEU:HD23	20	0.52
(1,1324)	1:77:A:GLN:HG2	1:77:A:GLN:H	1	0.52
(1,1303)	1:137:A:HIS:HE1	1:136:A:ALA:HB1	20	0.52
(1,1123)	1:83:A:GLU:HA	1:83:A:GLU:HG3	2	0.52
(1,1115)	1:98:A:LEU:HD21	1:96:A:HIS:HE1	11	0.52
(1,1094)	1:100:A:LEU:HD21	1:138:A:SER:HB2	15	0.52
(1,1076)	1:101:A:ALA:HB2	1:98:A:LEU:HD21	3	0.52
(1,1076)	1:101:A:ALA:HB1	1:98:A:LEU:HD22	7	0.52
(1,1040)	1:62:A:GLU:HB3	1:59:A:TYR:HA	2	0.52
(1,1004)	1:108:A:ILE:HD13	1:109:A:LEU:H	8	0.52
(1,932)	1:112:A:VAL:HG22	1:126:A:TYR:HA	16	0.52
(1,872)	1:118:A:SER:HB3	1:118:A:SER:H	1	0.52
(1,848)	1:120:A:PRO:HG3	1:119:A:ARG:HA	25	0.52
(1,825)	1:122:A:LYS:HG2	1:125:A:VAL:HG21	9	0.52
(1,766)	1:126:A:TYR:HE1	1:115:A:ARG:HB2	17	0.52
(1,717)	1:129:A:GLU:HB2	1:129:A:GLU:H	13	0.52
(1,705)	1:130:A:LEU:HD11	1:109:A:LEU:HD12	14	0.52
(1,618)	1:56:A:LYS:HG2	1:57:A:LYS:H	4	0.52
(1,607)	1:136:A:ALA:HB2	1:137:A:HIS:HA	20	0.52
(1,555)	2:36:B:THR:H	2:35:B:PHE:H	16	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,555)	2:36:B:THR:H	2:35:B:PHE:H	20	0.52
(1,552)	2:35:B:PHE:H	2:33:B:GLN:HA	21	0.52
(1,529)	1:67:A:PHE:H	1:68:A:GLU:HB2	2	0.52
(1,488)	1:92:A:GLN:HE22	1:64:A:GLU:HG3	22	0.52
(1,484)	1:134:A:LEU:HD13	1:94:A:ARG:H	13	0.52
(1,454)	1:114:A:SER:H	1:112:A:VAL:HG23	7	0.52
(1,454)	1:114:A:SER:H	1:112:A:VAL:HG23	18	0.52
(1,454)	1:114:A:SER:H	1:112:A:VAL:HG23	25	0.52
(1,444)	1:73:A:LEU:HD11	1:117:A:ARG:H	23	0.52
(1,434)	1:74:A:CYS:H	1:123:A:LEU:HD11	25	0.52
(1,398)	1:135:A:LYS:HG2	1:136:A:ALA:H	14	0.52
(1,366)	1:100:A:LEU:HD13	1:138:A:SER:HB3	18	0.52
(1,361)	2:29:B:SER:HB2	2:32:B:GLU:HG3	12	0.52
(1,340)	2:31:B:LEU:HD12	1:88:A:LEU:H	4	0.52
(1,340)	2:31:B:LEU:HD12	1:88:A:LEU:H	15	0.52
(1,340)	2:31:B:LEU:HD11	1:88:A:LEU:H	21	0.52
(1,325)	2:33:B:GLN:HG2	2:31:B:LEU:HB2	4	0.52
(1,325)	2:33:B:GLN:HG2	2:31:B:LEU:HB2	13	0.52
(1,321)	2:34:B:TYR:HD1	1:83:A:GLU:HB3	17	0.52
(1,319)	2:34:B:TYR:HE1	1:84:A:VAL:HG23	22	0.52
(1,318)	2:34:B:TYR:HE1	1:83:A:GLU:HB3	17	0.52
(1,289)	2:39:B:TRP:HZ3	2:36:B:THR:HB	1	0.52
(1,289)	2:39:B:TRP:HZ3	2:36:B:THR:HB	20	0.52
(1,289)	2:39:B:TRP:HZ3	2:36:B:THR:HB	21	0.52
(1,281)	2:31:B:LEU:HD23	1:128:A:ASN:H	13	0.52
(1,281)	2:31:B:LEU:HD22	1:128:A:ASN:H	17	0.52
(1,243)	1:66:A:LEU:HD13	1:62:A:GLU:HG3	19	0.52
(1,230)	1:66:A:LEU:HA	1:113:A:LEU:HD21	21	0.52
(1,228)	1:62:A:GLU:HG2	1:66:A:LEU:HD11	6	0.52
(1,228)	1:62:A:GLU:HG2	1:66:A:LEU:HD13	17	0.52
(1,206)	1:71:A:LEU:HD11	1:89:A:TYR:HB2	5	0.52
(1,206)	1:71:A:LEU:HD11	1:89:A:TYR:HB2	15	0.52
(1,203)	1:71:A:LEU:HD12	1:68:A:GLU:H	4	0.52
(1,197)	1:73:A:LEU:HD21	1:123:A:LEU:HB2	16	0.52
(1,195)	1:73:A:LEU:HD21	1:70:A:PHE:HA	23	0.52
(1,195)	1:73:A:LEU:HD22	1:70:A:PHE:HA	25	0.52
(1,194)	1:73:A:LEU:HD21	1:70:A:PHE:HD1	2	0.52
(1,155)	1:88:A:LEU:HD23	1:131:A:CYS:HB3	6	0.52
(1,152)	1:67:A:PHE:HE1	1:88:A:LEU:HD13	24	0.52
(1,151)	1:88:A:LEU:HD13	1:70:A:PHE:HD1	5	0.52
(1,117)	1:100:A:LEU:HD23	1:92:A:GLN:HG2	13	0.52
(1,80)	1:94:A:ARG:HD2	1:93:A:GLN:HB2	14	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,67)	1:116:A:ALA:HB3	1:120:A:PRO:HA	5	0.52
(1,48)	1:126:A:TYR:HE1	1:125:A:VAL:HG13	13	0.52
(1,48)	1:126:A:TYR:HE1	1:125:A:VAL:HG12	20	0.52
(1,13)	1:133:A:VAL:HG11	1:108:A:ILE:HB	21	0.52
(1,5)	1:100:A:LEU:HD12	1:100:A:LEU:H	18	0.52
(1,5)	1:100:A:LEU:HD13	1:100:A:LEU:H	19	0.52
(1,2197)	1:55:A:GLY:HA2	1:56:A:LYS:H	21	0.51
(1,2173)	1:63:A:ASN:H	1:109:A:LEU:HD11	20	0.51
(1,2124)	1:73:A:LEU:HD22	1:73:A:LEU:H	3	0.51
(1,2124)	1:73:A:LEU:HD21	1:73:A:LEU:H	18	0.51
(1,2106)	1:76:A:MET:HB3	1:77:A:GLN:H	3	0.51
(1,2106)	1:76:A:MET:HB3	1:77:A:GLN:H	22	0.51
(1,2089)	1:79:A:ALA:H	1:78:A:THR:HG22	9	0.51
(1,2089)	1:79:A:ALA:H	1:78:A:THR:HG21	14	0.51
(1,2089)	1:79:A:ALA:H	1:78:A:THR:HG21	15	0.51
(1,2089)	1:79:A:ALA:H	1:78:A:THR:HG21	16	0.51
(1,2089)	1:79:A:ALA:H	1:78:A:THR:HG21	18	0.51
(1,2089)	1:79:A:ALA:H	1:78:A:THR:HG21	21	0.51
(1,2082)	1:81:A:HIS:H	1:79:A:ALA:HB1	11	0.51
(1,2063)	1:85:A:VAL:H	1:71:A:LEU:HD21	16	0.51
(1,2026)	1:67:A:PHE:HD1	1:92:A:GLN:HE22	3	0.51
(1,2013)	1:94:A:ARG:H	1:95:A:ALA:HB2	23	0.51
(1,2012)	1:94:A:ARG:HB3	1:94:A:ARG:H	3	0.51
(1,2011)	1:94:A:ARG:HD2	1:94:A:ARG:H	4	0.51
(1,1986)	1:99:A:PHE:H	1:98:A:LEU:HD23	5	0.51
(1,1986)	1:99:A:PHE:H	1:98:A:LEU:HD23	12	0.51
(1,1986)	1:99:A:PHE:H	1:98:A:LEU:HD22	20	0.51
(1,1983)	1:99:A:PHE:H	1:138:A:SER:HB2	12	0.51
(1,1968)	1:101:A:ALA:H	1:63:A:ASN:HD22	20	0.51
(1,1801)	1:135:A:LYS:H	1:91:A:ARG:HD3	9	0.51
(1,1798)	1:136:A:ALA:H	1:135:A:LYS:HD3	5	0.51
(1,1798)	1:136:A:ALA:H	1:135:A:LYS:HD3	6	0.51
(1,1768)	2:24:B:GLN:HB2	2:24:B:GLN:HG2	6	0.51
(1,1716)	2:31:B:LEU:HG	2:32:B:GLU:HG3	1	0.51
(1,1716)	2:32:B:GLU:HG2	2:31:B:LEU:HG	5	0.51
(1,1650)	2:37:B:ALA:HB2	1:121:A:ALA:HB1	8	0.51
(1,1650)	2:37:B:ALA:HB1	1:121:A:ALA:HB2	9	0.51
(1,1629)	2:38:B:ARG:HG2	2:38:B:ARG:HA	1	0.51
(1,1629)	2:38:B:ARG:HG2	2:38:B:ARG:HA	11	0.51
(1,1576)	1:73:A:LEU:HD13	1:117:A:ARG:H	5	0.51
(1,1496)	1:64:A:GLU:HG3	1:64:A:GLU:HA	2	0.51
(1,1496)	1:64:A:GLU:HG3	1:64:A:GLU:HA	13	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1489)	1:65:A:LYS:HG2	1:66:A:LEU:H	20	0.51
(1,1480)	1:66:A:LEU:HD23	1:63:A:ASN:HA	25	0.51
(1,1421)	1:71:A:LEU:HD21	1:71:A:LEU:H	1	0.51
(1,1421)	1:71:A:LEU:HD21	1:71:A:LEU:H	5	0.51
(1,1393)	1:77:A:GLN:HG3	1:73:A:LEU:HD21	11	0.51
(1,1337)	1:76:A:MET:HA	1:76:A:MET:HG3	10	0.51
(1,1303)	1:137:A:HIS:HE1	1:136:A:ALA:HB1	6	0.51
(1,1231)	1:67:A:PHE:HA	1:67:A:PHE:HD1	18	0.51
(1,1139)	1:134:A:LEU:HD23	1:95:A:ALA:HB3	8	0.51
(1,1115)	1:98:A:LEU:HD23	1:96:A:HIS:HE1	1	0.51
(1,1115)	1:98:A:LEU:HD23	1:96:A:HIS:HE1	3	0.51
(1,1115)	1:98:A:LEU:HD21	1:96:A:HIS:HE1	7	0.51
(1,1115)	1:98:A:LEU:HD22	1:96:A:HIS:HE1	17	0.51
(1,1115)	1:98:A:LEU:HD21	1:96:A:HIS:HE1	22	0.51
(1,1105)	1:134:A:LEU:HD21	1:99:A:PHE:HE1	23	0.51
(1,1076)	1:101:A:ALA:HB1	1:98:A:LEU:HD22	22	0.51
(1,932)	1:112:A:VAL:HG23	1:126:A:TYR:HA	15	0.51
(1,848)	1:120:A:PRO:HG3	1:119:A:ARG:HA	6	0.51
(1,827)	1:122:A:LYS:HD2	1:122:A:LYS:HA	23	0.51
(1,825)	1:122:A:LYS:HG2	1:125:A:VAL:HG23	22	0.51
(1,790)	1:124:A:TYR:HD1	1:124:A:TYR:HA	1	0.51
(1,705)	1:130:A:LEU:HD11	1:109:A:LEU:HD11	9	0.51
(1,618)	1:56:A:LYS:HG2	1:57:A:LYS:H	1	0.51
(1,607)	1:136:A:ALA:HB3	1:137:A:HIS:HA	1	0.51
(1,607)	1:136:A:ALA:HB1	1:137:A:HIS:HA	13	0.51
(1,577)	1:75:A:LYS:HE2	1:71:A:LEU:HB3	18	0.51
(1,561)	2:27:B:SER:H	2:30:B:GLU:HB3	5	0.51
(1,555)	2:36:B:THR:H	2:37:B:ALA:H	6	0.51
(1,555)	2:36:B:THR:H	2:35:B:PHE:H	13	0.51
(1,555)	2:36:B:THR:H	2:37:B:ALA:H	19	0.51
(1,552)	2:35:B:PHE:H	2:33:B:GLN:HA	4	0.51
(1,552)	2:35:B:PHE:H	2:33:B:GLN:HA	18	0.51
(1,520)	1:130:A:LEU:H	1:112:A:VAL:HG22	10	0.51
(1,499)	1:85:A:VAL:H	1:74:A:CYS:HB3	19	0.51
(1,484)	1:134:A:LEU:HD11	1:94:A:ARG:H	5	0.51
(1,457)	1:111:A:ARG:H	1:109:A:LEU:HB3	6	0.51
(1,457)	1:111:A:ARG:H	1:109:A:LEU:HB3	11	0.51
(1,457)	1:111:A:ARG:H	1:109:A:LEU:HB3	12	0.51
(1,455)	1:112:A:VAL:H	1:113:A:LEU:HB3	14	0.51
(1,455)	1:112:A:VAL:H	1:113:A:LEU:HB3	16	0.51
(1,454)	1:114:A:SER:H	1:112:A:VAL:HG23	8	0.51
(1,454)	1:114:A:SER:H	1:112:A:VAL:HG22	11	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,445)	1:116:A:ALA:H	1:112:A:VAL:HA	7	0.51
(1,445)	1:116:A:ALA:H	1:112:A:VAL:HA	20	0.51
(1,444)	1:73:A:LEU:HD13	1:117:A:ARG:H	18	0.51
(1,434)	1:74:A:CYS:H	1:123:A:LEU:HD11	1	0.51
(1,399)	1:135:A:LYS:H	1:133:A:VAL:HA	3	0.51
(1,398)	1:135:A:LYS:HG2	1:136:A:ALA:H	19	0.51
(1,356)	2:29:B:SER:HB2	2:31:B:LEU:H	12	0.51
(1,340)	2:31:B:LEU:HD12	1:88:A:LEU:H	10	0.51
(1,338)	2:31:B:LEU:HD23	2:32:B:GLU:HG3	19	0.51
(1,338)	2:31:B:LEU:HD22	2:32:B:GLU:HG3	22	0.51
(1,321)	2:34:B:TYR:HD1	1:83:A:GLU:HB3	1	0.51
(1,319)	2:34:B:TYR:HE1	1:84:A:VAL:HG21	2	0.51
(1,319)	2:34:B:TYR:HE1	1:84:A:VAL:HG22	5	0.51
(1,319)	2:34:B:TYR:HE1	1:84:A:VAL:HG22	19	0.51
(1,318)	2:34:B:TYR:HE1	1:83:A:GLU:HB3	7	0.51
(1,307)	2:39:B:TRP:HE3	2:36:B:THR:HG22	18	0.51
(1,290)	2:39:B:TRP:HH2	2:36:B:THR:HB	24	0.51
(1,243)	1:66:A:LEU:HD13	1:62:A:GLU:HG3	14	0.51
(1,228)	1:62:A:GLU:HG2	1:66:A:LEU:HD11	9	0.51
(1,228)	1:62:A:GLU:HG2	1:66:A:LEU:HD13	15	0.51
(1,228)	1:62:A:GLU:HG2	1:66:A:LEU:HD13	22	0.51
(1,219)	1:70:A:PHE:HD1	1:73:A:LEU:HB3	2	0.51
(1,203)	1:71:A:LEU:HD11	1:68:A:GLU:H	14	0.51
(1,201)	2:25:B:GLU:HG3	2:25:B:GLU:HB2	23	0.51
(1,199)	1:72:A:GLU:HG2	1:71:A:LEU:HB3	4	0.51
(1,199)	1:72:A:GLU:HG2	1:71:A:LEU:HB3	19	0.51
(1,199)	1:72:A:GLU:HG2	1:71:A:LEU:HB3	20	0.51
(1,199)	1:72:A:GLU:HG2	1:71:A:LEU:HB3	21	0.51
(1,195)	1:73:A:LEU:HD21	1:70:A:PHE:HA	4	0.51
(1,195)	1:73:A:LEU:HD21	1:70:A:PHE:HA	6	0.51
(1,194)	1:73:A:LEU:HD21	1:70:A:PHE:HD1	4	0.51
(1,189)	1:85:A:VAL:HG12	1:75:A:LYS:HA	15	0.51
(1,189)	1:85:A:VAL:HG12	1:75:A:LYS:HA	18	0.51
(1,189)	1:85:A:VAL:HG13	1:75:A:LYS:HA	25	0.51
(1,155)	1:88:A:LEU:HD12	1:74:A:CYS:HB2	10	0.51
(1,152)	1:67:A:PHE:HE1	1:88:A:LEU:HD12	6	0.51
(1,151)	1:88:A:LEU:HD11	1:70:A:PHE:HD1	14	0.51
(1,151)	1:88:A:LEU:HD11	1:70:A:PHE:HD1	18	0.51
(1,132)	1:67:A:PHE:HE1	1:92:A:GLN:HB3	22	0.51
(1,67)	1:116:A:ALA:HB1	1:120:A:PRO:HA	23	0.51
(1,51)	1:126:A:TYR:HD1	1:125:A:VAL:HG13	15	0.51
(1,48)	1:126:A:TYR:HE1	1:125:A:VAL:HG11	7	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,17)	1:133:A:VAL:HG13	1:137:A:HIS:HB2	14	0.51
(1,13)	1:133:A:VAL:HG12	1:108:A:ILE:HB	11	0.51
(1,6)	1:130:A:LEU:HD22	1:70:A:PHE:HE2	15	0.51
(1,6)	1:130:A:LEU:HD22	1:70:A:PHE:HE2	17	0.51
(1,5)	1:100:A:LEU:HD13	1:100:A:LEU:H	15	0.51
(1,5)	1:100:A:LEU:HD11	1:100:A:LEU:H	24	0.51
(1,2274)	2:39:B:TRP:HE1	2:38:B:ARG:HD2	17	0.5
(1,2197)	1:55:A:GLY:HA2	1:56:A:LYS:H	7	0.5
(1,2197)	1:55:A:GLY:HA2	1:56:A:LYS:H	10	0.5
(1,2197)	1:55:A:GLY:HA2	1:56:A:LYS:H	15	0.5
(1,2124)	1:73:A:LEU:HD21	1:73:A:LEU:H	8	0.5
(1,2124)	1:73:A:LEU:HD22	1:73:A:LEU:H	15	0.5
(1,2106)	1:76:A:MET:HB3	1:77:A:GLN:H	14	0.5
(1,2106)	1:76:A:MET:HB3	1:77:A:GLN:H	17	0.5
(1,2106)	1:76:A:MET:HB3	1:77:A:GLN:H	20	0.5
(1,2089)	1:79:A:ALA:H	1:78:A:THR:HG23	5	0.5
(1,2089)	1:79:A:ALA:H	1:78:A:THR:HG21	24	0.5
(1,2060)	1:86:A:PRO:HB3	1:87:A:PHE:H	23	0.5
(1,2051)	1:89:A:TYR:H	1:90:A:ASN:HB3	6	0.5
(1,2051)	1:89:A:TYR:H	1:90:A:ASN:HB3	21	0.5
(1,2037)	1:90:A:ASN:HD21	1:94:A:ARG:HD3	24	0.5
(1,2017)	1:93:A:GLN:HE22	1:89:A:TYR:HB3	9	0.5
(1,2013)	1:94:A:ARG:H	1:95:A:ALA:HB1	10	0.5
(1,2013)	1:94:A:ARG:H	1:95:A:ALA:HB3	14	0.5
(1,2012)	1:94:A:ARG:HB3	1:94:A:ARG:H	8	0.5
(1,2012)	1:94:A:ARG:HB3	1:94:A:ARG:H	9	0.5
(1,2012)	1:94:A:ARG:HB3	1:94:A:ARG:H	17	0.5
(1,1996)	1:97:A:SER:H	1:139:A:ALA:HB1	12	0.5
(1,1986)	1:99:A:PHE:H	1:98:A:LEU:HD21	10	0.5
(1,1986)	1:99:A:PHE:H	1:98:A:LEU:HD23	17	0.5
(1,1983)	1:99:A:PHE:H	1:138:A:SER:HB2	1	0.5
(1,1736)	2:31:B:LEU:HB2	2:31:B:LEU:HD12	2	0.5
(1,1736)	2:31:B:LEU:HB2	2:31:B:LEU:HD11	4	0.5
(1,1736)	2:31:B:LEU:HB2	2:31:B:LEU:HD12	6	0.5
(1,1716)	2:31:B:LEU:HG	2:32:B:GLU:HG3	8	0.5
(1,1649)	2:37:B:ALA:HB3	2:38:B:ARG:HB2	12	0.5
(1,1633)	2:38:B:ARG:HD2	2:38:B:ARG:HB2	13	0.5
(1,1632)	2:38:B:ARG:HG2	2:38:B:ARG:HD2	21	0.5
(1,1629)	2:38:B:ARG:HG2	2:38:B:ARG:HA	7	0.5
(1,1620)	2:39:B:TRP:HD1	2:38:B:ARG:HG2	5	0.5
(1,1576)	1:73:A:LEU:HD12	1:117:A:ARG:H	6	0.5
(1,1576)	1:73:A:LEU:HD12	1:117:A:ARG:H	13	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1576)	1:73:A:LEU:HD13	1:117:A:ARG:H	14	0.5
(1,1576)	1:73:A:LEU:HD12	1:117:A:ARG:H	25	0.5
(1,1501)	1:64:A:GLU:HG2	1:65:A:LYS:H	3	0.5
(1,1501)	1:64:A:GLU:HG2	1:65:A:LYS:H	7	0.5
(1,1496)	1:64:A:GLU:HG3	1:64:A:GLU:HA	5	0.5
(1,1496)	1:64:A:GLU:HG3	1:64:A:GLU:HA	15	0.5
(1,1475)	1:66:A:LEU:HD23	1:109:A:LEU:HD21	1	0.5
(1,1475)	1:66:A:LEU:HD23	1:109:A:LEU:HD23	25	0.5
(1,1447)	1:69:A:GLU:HA	1:69:A:GLU:HG3	9	0.5
(1,1421)	1:71:A:LEU:HD22	1:71:A:LEU:H	3	0.5
(1,1421)	1:71:A:LEU:HD23	1:71:A:LEU:H	12	0.5
(1,1421)	1:71:A:LEU:HD22	1:71:A:LEU:H	20	0.5
(1,1338)	1:76:A:MET:HB3	1:76:A:MET:H	17	0.5
(1,1337)	1:76:A:MET:HA	1:76:A:MET:HG3	5	0.5
(1,1337)	1:76:A:MET:HA	1:76:A:MET:HG3	17	0.5
(1,1303)	1:137:A:HIS:HE1	1:136:A:ALA:HB2	15	0.5
(1,1137)	1:95:A:ALA:HB2	1:91:A:ARG:HD3	21	0.5
(1,1115)	1:98:A:LEU:HD21	1:96:A:HIS:HE1	8	0.5
(1,1098)	1:100:A:LEU:HD22	1:92:A:GLN:HA	17	0.5
(1,1092)	1:100:A:LEU:HD22	1:99:A:PHE:HD2	6	0.5
(1,1076)	1:101:A:ALA:HB1	1:98:A:LEU:HD21	1	0.5
(1,1076)	1:101:A:ALA:HB3	1:98:A:LEU:HD21	4	0.5
(1,1076)	1:101:A:ALA:HB3	1:98:A:LEU:HD22	24	0.5
(1,1070)	1:101:A:ALA:HB2	1:102:A:SER:H	5	0.5
(1,1059)	1:103:A:ALA:HB3	1:104:A:GLU:HA	11	0.5
(1,1059)	1:103:A:ALA:HB3	1:104:A:GLU:HA	25	0.5
(1,946)	1:110:A:SER:HB2	1:66:A:LEU:HD11	17	0.5
(1,946)	1:110:A:SER:HB2	1:66:A:LEU:HD13	25	0.5
(1,901)	1:115:A:ARG:HG2	1:115:A:ARG:H	15	0.5
(1,790)	1:124:A:TYR:HD1	1:124:A:TYR:HA	2	0.5
(1,790)	1:124:A:TYR:HD1	1:124:A:TYR:HA	14	0.5
(1,790)	1:124:A:TYR:HD1	1:124:A:TYR:HA	23	0.5
(1,766)	1:126:A:TYR:HE1	1:115:A:ARG:HB2	14	0.5
(1,723)	1:129:A:GLU:HG2	1:125:A:VAL:HG12	9	0.5
(1,723)	1:129:A:GLU:HG2	1:125:A:VAL:HG12	24	0.5
(1,705)	1:130:A:LEU:HD13	1:109:A:LEU:HD13	1	0.5
(1,670)	1:133:A:VAL:HG23	1:105:A:PHE:HE1	12	0.5
(1,670)	1:133:A:VAL:HG23	1:105:A:PHE:HE1	23	0.5
(1,633)	1:100:A:LEU:HD11	1:92:A:GLN:HE21	6	0.5
(1,607)	1:136:A:ALA:HB3	1:137:A:HIS:HA	22	0.5
(1,576)	1:142:A:LYS:HB2	1:142:A:LYS:H	19	0.5
(1,552)	2:35:B:PHE:H	2:33:B:GLN:HA	20	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,534)	1:121:A:ALA:H	1:119:A:ARG:HG3	6	0.5
(1,529)	1:67:A:PHE:H	1:69:A:GLU:HB2	6	0.5
(1,499)	1:85:A:VAL:H	1:74:A:CYS:HB3	25	0.5
(1,455)	1:112:A:VAL:H	1:113:A:LEU:HB3	18	0.5
(1,454)	1:114:A:SER:H	1:112:A:VAL:HG22	24	0.5
(1,451)	1:114:A:SER:H	1:117:A:ARG:HB2	7	0.5
(1,398)	1:135:A:LYS:HG2	1:136:A:ALA:H	9	0.5
(1,398)	1:135:A:LYS:HG2	1:136:A:ALA:H	23	0.5
(1,376)	2:27:B:SER:HB3	2:26:B:ASP:HB3	6	0.5
(1,366)	1:100:A:LEU:HD12	1:138:A:SER:HB3	20	0.5
(1,338)	2:31:B:LEU:HD22	2:32:B:GLU:HG3	18	0.5
(1,325)	2:33:B:GLN:HG2	2:31:B:LEU:HB2	5	0.5
(1,325)	2:33:B:GLN:HG2	2:31:B:LEU:HB2	9	0.5
(1,325)	2:33:B:GLN:HG2	2:31:B:LEU:HB2	24	0.5
(1,319)	2:34:B:TYR:HE1	1:84:A:VAL:HG23	25	0.5
(1,318)	2:34:B:TYR:HE1	1:83:A:GLU:HB3	13	0.5
(1,293)	2:39:B:TRP:HD1	2:38:B:ARG:HB3	14	0.5
(1,289)	2:39:B:TRP:HZ3	2:36:B:THR:HB	2	0.5
(1,281)	2:31:B:LEU:HD22	1:128:A:ASN:H	15	0.5
(1,280)	2:31:B:LEU:HG	1:87:A:PHE:HE2	11	0.5
(1,265)	1:127:A:ILE:HD12	2:35:B:PHE:HE1	25	0.5
(1,243)	1:66:A:LEU:HD11	1:62:A:GLU:HG3	2	0.5
(1,243)	1:66:A:LEU:HD13	1:62:A:GLU:HG3	18	0.5
(1,243)	1:66:A:LEU:HD11	1:62:A:GLU:HG3	21	0.5
(1,232)	1:66:A:LEU:HD11	1:110:A:SER:HA	23	0.5
(1,228)	1:62:A:GLU:HG2	1:66:A:LEU:HD13	24	0.5
(1,219)	1:70:A:PHE:HD1	1:73:A:LEU:HB3	6	0.5
(1,219)	1:70:A:PHE:HD1	1:73:A:LEU:HB3	10	0.5
(1,219)	1:70:A:PHE:HD1	1:73:A:LEU:HB3	11	0.5
(1,219)	1:70:A:PHE:HD1	1:73:A:LEU:HB3	25	0.5
(1,209)	1:67:A:PHE:HE1	1:71:A:LEU:HD23	24	0.5
(1,203)	1:71:A:LEU:HD13	1:68:A:GLU:H	21	0.5
(1,201)	1:72:A:GLU:HG3	1:72:A:GLU:HB2	5	0.5
(1,201)	2:25:B:GLU:HG3	2:25:B:GLU:HB2	7	0.5
(1,201)	2:25:B:GLU:HG2	2:25:B:GLU:HB2	10	0.5
(1,201)	1:72:A:GLU:HG3	1:72:A:GLU:HB2	15	0.5
(1,199)	1:72:A:GLU:HG2	1:71:A:LEU:HB3	11	0.5
(1,197)	1:73:A:LEU:HD23	1:123:A:LEU:HB2	2	0.5
(1,195)	1:73:A:LEU:HD23	1:70:A:PHE:HA	12	0.5
(1,195)	1:73:A:LEU:HD23	1:70:A:PHE:HA	22	0.5
(1,194)	1:73:A:LEU:HD22	1:70:A:PHE:HD1	14	0.5
(1,189)	1:85:A:VAL:HG13	1:75:A:LYS:HA	8	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,155)	1:88:A:LEU:HD23	1:131:A:CYS:HB3	13	0.5
(1,151)	1:88:A:LEU:HD12	1:70:A:PHE:HD1	2	0.5
(1,151)	1:88:A:LEU:HD13	1:70:A:PHE:HD1	23	0.5
(1,134)	1:92:A:GLN:HG2	1:95:A:ALA:H	15	0.5
(1,134)	1:92:A:GLN:HG2	1:95:A:ALA:H	25	0.5
(1,117)	1:100:A:LEU:HD22	1:92:A:GLN:HG2	21	0.5
(1,81)	1:116:A:ALA:HB3	1:70:A:PHE:HZ	10	0.5
(1,44)	1:126:A:TYR:HE1	1:112:A:VAL:HA	10	0.5
(1,15)	1:132:A:THR:HG21	2:27:B:SER:H	12	0.5
(1,13)	1:133:A:VAL:HG13	1:108:A:ILE:HB	7	0.5
(1,6)	1:130:A:LEU:HD23	1:70:A:PHE:HE2	4	0.5
(1,6)	1:130:A:LEU:HD23	1:70:A:PHE:HE2	8	0.5
(1,6)	1:130:A:LEU:HD21	1:70:A:PHE:HE2	11	0.5
(1,5)	1:100:A:LEU:HD13	1:100:A:LEU:H	11	0.5
(1,2271)	2:25:B:GLU:H	2:25:B:GLU:HG3	10	0.49
(1,2195)	1:56:A:LYS:H	1:56:A:LYS:HG2	20	0.49
(1,2106)	1:76:A:MET:HB3	1:77:A:GLN:H	6	0.49
(1,2106)	1:76:A:MET:HB3	1:77:A:GLN:H	24	0.49
(1,2089)	1:79:A:ALA:H	1:78:A:THR:HG22	12	0.49
(1,2063)	1:85:A:VAL:H	1:71:A:LEU:HD23	20	0.49
(1,2026)	1:67:A:PHE:HD2	1:92:A:GLN:HE22	6	0.49
(1,2017)	1:93:A:GLN:HE22	1:89:A:TYR:HB3	11	0.49
(1,2017)	1:93:A:GLN:HE22	1:89:A:TYR:HB3	15	0.49
(1,2012)	1:94:A:ARG:HB3	1:94:A:ARG:H	19	0.49
(1,1996)	1:97:A:SER:H	1:139:A:ALA:HB3	14	0.49
(1,1986)	1:99:A:PHE:H	1:98:A:LEU:HD21	2	0.49
(1,1986)	1:99:A:PHE:H	1:98:A:LEU:HD21	13	0.49
(1,1986)	1:99:A:PHE:H	1:98:A:LEU:HD23	14	0.49
(1,1986)	1:99:A:PHE:H	1:98:A:LEU:HD23	16	0.49
(1,1986)	1:99:A:PHE:H	1:98:A:LEU:HD23	21	0.49
(1,1986)	1:99:A:PHE:H	1:98:A:LEU:HD21	23	0.49
(1,1874)	1:118:A:SER:H	1:117:A:ARG:HG3	9	0.49
(1,1874)	1:118:A:SER:H	1:117:A:ARG:HG2	21	0.49
(1,1798)	1:136:A:ALA:H	1:135:A:LYS:HD3	25	0.49
(1,1766)	2:24:B:GLN:HG2	2:23:B:SER:HA	10	0.49
(1,1736)	2:31:B:LEU:HB2	2:31:B:LEU:HD11	5	0.49
(1,1736)	2:31:B:LEU:HB2	2:31:B:LEU:HD12	9	0.49
(1,1736)	2:31:B:LEU:HB2	2:31:B:LEU:HD13	11	0.49
(1,1736)	2:31:B:LEU:HB2	2:31:B:LEU:HD11	13	0.49
(1,1736)	2:31:B:LEU:HB2	2:31:B:LEU:HD12	18	0.49
(1,1736)	2:31:B:LEU:HB2	2:31:B:LEU:HD11	20	0.49
(1,1736)	2:31:B:LEU:HB2	2:31:B:LEU:HD12	21	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1736)	2:31:B:LEU:HB2	2:31:B:LEU:HD12	23	0.49
(1,1736)	2:31:B:LEU:HB2	2:31:B:LEU:HD11	24	0.49
(1,1736)	2:31:B:LEU:HB2	2:31:B:LEU:HD11	25	0.49
(1,1716)	2:31:B:LEU:HG	2:32:B:GLU:HG3	2	0.49
(1,1716)	2:31:B:LEU:HG	2:32:B:GLU:HG3	23	0.49
(1,1633)	2:38:B:ARG:HD2	2:38:B:ARG:HB2	2	0.49
(1,1629)	2:38:B:ARG:HG2	2:38:B:ARG:HA	15	0.49
(1,1629)	2:38:B:ARG:HG2	2:38:B:ARG:HA	24	0.49
(1,1576)	1:73:A:LEU:HD11	1:117:A:ARG:H	8	0.49
(1,1576)	1:73:A:LEU:HD13	1:117:A:ARG:H	10	0.49
(1,1576)	1:73:A:LEU:HD13	1:117:A:ARG:H	19	0.49
(1,1576)	1:73:A:LEU:HD13	1:117:A:ARG:H	20	0.49
(1,1501)	1:64:A:GLU:HG2	1:65:A:LYS:H	21	0.49
(1,1496)	1:64:A:GLU:HG3	1:64:A:GLU:HA	16	0.49
(1,1477)	1:66:A:LEU:HD23	1:113:A:LEU:HB3	10	0.49
(1,1475)	1:66:A:LEU:HD23	1:109:A:LEU:HD22	13	0.49
(1,1475)	1:66:A:LEU:HD21	1:109:A:LEU:HD21	20	0.49
(1,1422)	1:71:A:LEU:HD21	1:74:A:CYS:H	10	0.49
(1,1421)	1:71:A:LEU:HD22	1:71:A:LEU:H	17	0.49
(1,1421)	1:71:A:LEU:HD22	1:71:A:LEU:H	22	0.49
(1,1337)	1:76:A:MET:HA	1:76:A:MET:HG3	15	0.49
(1,1331)	1:77:A:GLN:HG2	1:73:A:LEU:HD13	15	0.49
(1,1331)	1:77:A:GLN:HG2	1:73:A:LEU:HD11	25	0.49
(1,1303)	1:137:A:HIS:HE1	1:136:A:ALA:HB1	21	0.49
(1,1183)	1:90:A:ASN:HB2	1:87:A:PHE:HD1	15	0.49
(1,1115)	1:98:A:LEU:HD22	1:96:A:HIS:HE1	12	0.49
(1,1115)	1:98:A:LEU:HD22	1:96:A:HIS:HE1	14	0.49
(1,1115)	1:98:A:LEU:HD21	1:96:A:HIS:HE1	18	0.49
(1,1094)	1:100:A:LEU:HD22	1:138:A:SER:HB2	17	0.49
(1,1094)	1:100:A:LEU:HD21	1:138:A:SER:HB2	23	0.49
(1,1059)	1:103:A:ALA:HB1	1:104:A:GLU:HA	5	0.49
(1,1047)	1:104:A:GLU:HG2	1:105:A:PHE:H	3	0.49
(1,989)	1:108:A:ILE:HG21	1:105:A:PHE:HA	24	0.49
(1,807)	1:123:A:LEU:HD11	1:74:A:CYS:HB2	16	0.49
(1,766)	1:126:A:TYR:HE1	1:115:A:ARG:HB2	4	0.49
(1,723)	1:129:A:GLU:HG2	1:125:A:VAL:HG12	12	0.49
(1,723)	1:129:A:GLU:HG2	1:125:A:VAL:HG12	20	0.49
(1,705)	1:130:A:LEU:HD13	1:109:A:LEU:HD11	6	0.49
(1,705)	1:130:A:LEU:HD13	1:109:A:LEU:HD11	15	0.49
(1,705)	1:130:A:LEU:HD13	1:109:A:LEU:HD12	19	0.49
(1,705)	1:130:A:LEU:HD12	1:109:A:LEU:HD11	21	0.49
(1,575)	1:143:A:LEU:HA	1:143:A:LEU:HD23	6	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,555)	2:36:B:THR:H	2:35:B:PHE:H	5	0.49
(1,552)	2:35:B:PHE:H	2:33:B:GLN:HA	3	0.49
(1,529)	1:67:A:PHE:H	1:68:A:GLU:HB2	4	0.49
(1,488)	1:92:A:GLN:HE22	1:64:A:GLU:HG3	15	0.49
(1,478)	1:95:A:ALA:H	1:91:A:ARG:HD2	11	0.49
(1,457)	1:111:A:ARG:H	1:109:A:LEU:HB3	1	0.49
(1,457)	1:111:A:ARG:H	1:109:A:LEU:HB3	3	0.49
(1,457)	1:111:A:ARG:H	1:109:A:LEU:HB3	7	0.49
(1,457)	1:111:A:ARG:H	1:109:A:LEU:HB3	25	0.49
(1,455)	1:112:A:VAL:H	1:113:A:LEU:HB3	2	0.49
(1,455)	1:112:A:VAL:H	1:113:A:LEU:HB3	8	0.49
(1,455)	1:112:A:VAL:H	1:113:A:LEU:HB3	9	0.49
(1,455)	1:112:A:VAL:H	1:113:A:LEU:HB3	20	0.49
(1,444)	1:73:A:LEU:HD13	1:117:A:ARG:H	2	0.49
(1,444)	1:73:A:LEU:HD12	1:117:A:ARG:H	16	0.49
(1,444)	1:73:A:LEU:HD13	1:117:A:ARG:H	22	0.49
(1,421)	1:72:A:GLU:H	1:70:A:PHE:HD1	5	0.49
(1,398)	1:135:A:LYS:HG2	1:136:A:ALA:H	2	0.49
(1,398)	1:135:A:LYS:HG2	1:136:A:ALA:H	6	0.49
(1,398)	1:135:A:LYS:HG2	1:136:A:ALA:H	20	0.49
(1,379)	2:31:B:LEU:HB2	2:28:B:ASP:HB2	19	0.49
(1,340)	2:31:B:LEU:HD13	1:88:A:LEU:H	13	0.49
(1,340)	2:31:B:LEU:HD13	1:88:A:LEU:H	17	0.49
(1,338)	2:31:B:LEU:HD22	2:32:B:GLU:HG3	25	0.49
(1,325)	2:33:B:GLN:HG2	2:31:B:LEU:HB2	1	0.49
(1,325)	2:33:B:GLN:HG2	2:31:B:LEU:HB2	18	0.49
(1,325)	2:33:B:GLN:HG2	2:31:B:LEU:HB2	21	0.49
(1,324)	2:33:B:GLN:HG2	2:26:B:ASP:HB3	11	0.49
(1,310)	2:35:B:PHE:HD1	1:127:A:ILE:HB	16	0.49
(1,290)	2:39:B:TRP:HH2	2:36:B:THR:HB	4	0.49
(1,289)	2:39:B:TRP:HZ3	2:36:B:THR:HB	7	0.49
(1,289)	2:39:B:TRP:HZ3	2:36:B:THR:HB	11	0.49
(1,289)	2:39:B:TRP:HZ3	2:36:B:THR:HB	15	0.49
(1,289)	2:39:B:TRP:HZ3	2:36:B:THR:HB	16	0.49
(1,289)	2:39:B:TRP:HZ3	2:36:B:THR:HB	23	0.49
(1,281)	2:31:B:LEU:HD21	1:128:A:ASN:H	8	0.49
(1,243)	1:66:A:LEU:HD11	1:62:A:GLU:HG3	1	0.49
(1,230)	1:66:A:LEU:HA	1:113:A:LEU:HD21	13	0.49
(1,228)	1:62:A:GLU:HG2	1:61:A:LEU:HD23	14	0.49
(1,219)	1:70:A:PHE:HD1	1:73:A:LEU:HB3	8	0.49
(1,216)	1:113:A:LEU:HD11	1:70:A:PHE:HD2	22	0.49
(1,201)	2:25:B:GLU:HG3	2:25:B:GLU:HB2	3	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,201)	1:72:A:GLU:HG3	1:72:A:GLU:HB2	12	0.49
(1,201)	1:72:A:GLU:HG3	1:72:A:GLU:HB2	17	0.49
(1,197)	1:73:A:LEU:HD23	1:123:A:LEU:HB2	18	0.49
(1,195)	1:73:A:LEU:HD21	1:70:A:PHE:HA	19	0.49
(1,194)	1:73:A:LEU:HD21	1:70:A:PHE:HD1	18	0.49
(1,186)	1:123:A:LEU:HD21	1:77:A:GLN:HG3	19	0.49
(1,155)	1:88:A:LEU:HD11	1:74:A:CYS:HB2	17	0.49
(1,151)	1:88:A:LEU:HD13	1:70:A:PHE:HD1	6	0.49
(1,151)	1:88:A:LEU:HD12	1:70:A:PHE:HD1	20	0.49
(1,81)	1:116:A:ALA:HB3	1:70:A:PHE:HZ	6	0.49
(1,67)	1:116:A:ALA:HB3	1:120:A:PRO:HA	11	0.49
(1,52)	1:125:A:VAL:HG13	1:128:A:ASN:HB2	2	0.49
(1,48)	1:126:A:TYR:HE1	1:125:A:VAL:HG11	8	0.49
(1,45)	1:59:A:TYR:HE1	1:57:A:LYS:HD3	3	0.49
(1,44)	1:126:A:TYR:HE1	1:112:A:VAL:HA	21	0.49
(1,42)	1:126:A:TYR:HD1	1:125:A:VAL:HB	25	0.49
(1,13)	1:133:A:VAL:HG12	1:108:A:ILE:HB	22	0.49
(1,6)	1:130:A:LEU:HD21	1:70:A:PHE:HE2	1	0.49
(1,6)	1:130:A:LEU:HD23	1:70:A:PHE:HE2	3	0.49
(1,2193)	1:58:A:CYS:H	1:57:A:LYS:HG2	19	0.48
(1,2124)	1:73:A:LEU:HD23	1:73:A:LEU:H	10	0.48
(1,2124)	1:73:A:LEU:HD22	1:73:A:LEU:H	11	0.48
(1,2124)	1:73:A:LEU:HD22	1:73:A:LEU:H	24	0.48
(1,2089)	1:79:A:ALA:H	1:78:A:THR:HG23	6	0.48
(1,2051)	1:89:A:TYR:H	1:90:A:ASN:HB3	20	0.48
(1,2051)	1:89:A:TYR:H	1:90:A:ASN:HB3	25	0.48
(1,2013)	1:94:A:ARG:H	1:95:A:ALA:HB1	5	0.48
(1,2013)	1:94:A:ARG:H	1:95:A:ALA:HB1	17	0.48
(1,2011)	1:94:A:ARG:HD2	1:94:A:ARG:H	7	0.48
(1,1986)	1:99:A:PHE:H	1:98:A:LEU:HD22	24	0.48
(1,1986)	1:99:A:PHE:H	1:98:A:LEU:HD22	25	0.48
(1,1983)	1:99:A:PHE:H	1:138:A:SER:HB2	9	0.48
(1,1929)	1:107:A:ASN:HD21	1:103:A:ALA:HB1	12	0.48
(1,1798)	1:136:A:ALA:H	1:135:A:LYS:HD3	1	0.48
(1,1798)	1:136:A:ALA:H	1:135:A:LYS:HD3	11	0.48
(1,1788)	1:139:A:ALA:H	1:135:A:LYS:HD3	10	0.48
(1,1788)	1:139:A:ALA:H	1:135:A:LYS:HD3	12	0.48
(1,1788)	1:139:A:ALA:H	1:135:A:LYS:HD2	15	0.48
(1,1788)	1:139:A:ALA:H	1:135:A:LYS:HD3	19	0.48
(1,1775)	1:143:A:LEU:H	1:141:A:LYS:HG3	11	0.48
(1,1736)	2:31:B:LEU:HB2	2:31:B:LEU:HD12	1	0.48
(1,1736)	2:31:B:LEU:HB2	2:31:B:LEU:HD13	8	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1736)	2:31:B:LEU:HB2	2:31:B:LEU:HD11	10	0.48
(1,1736)	2:31:B:LEU:HB2	2:31:B:LEU:HD11	12	0.48
(1,1736)	2:31:B:LEU:HB2	2:31:B:LEU:HD11	14	0.48
(1,1736)	2:31:B:LEU:HB2	2:31:B:LEU:HD12	19	0.48
(1,1716)	2:32:B:GLU:HG2	2:31:B:LEU:HG	16	0.48
(1,1649)	2:37:B:ALA:HB2	2:38:B:ARG:HB2	5	0.48
(1,1576)	1:73:A:LEU:HD12	1:117:A:ARG:H	7	0.48
(1,1576)	1:73:A:LEU:HD11	1:117:A:ARG:H	15	0.48
(1,1559)	1:57:A:LYS:HB2	1:57:A:LYS:HG2	12	0.48
(1,1553)	1:59:A:TYR:HD1	1:57:A:LYS:HB2	17	0.48
(1,1496)	1:64:A:GLU:HG3	1:64:A:GLU:HA	11	0.48
(1,1496)	1:64:A:GLU:HG3	1:64:A:GLU:HA	22	0.48
(1,1496)	1:64:A:GLU:HG3	1:64:A:GLU:HA	25	0.48
(1,1481)	1:66:A:LEU:HD21	1:69:A:GLU:H	16	0.48
(1,1481)	1:66:A:LEU:HD23	1:69:A:GLU:H	20	0.48
(1,1475)	1:66:A:LEU:HD22	1:109:A:LEU:HD23	11	0.48
(1,1421)	1:71:A:LEU:HD21	1:71:A:LEU:H	24	0.48
(1,1395)	1:116:A:ALA:HB3	1:73:A:LEU:HD21	24	0.48
(1,1393)	1:77:A:GLN:HG3	1:73:A:LEU:HD23	19	0.48
(1,1337)	1:76:A:MET:HA	1:76:A:MET:HG3	3	0.48
(1,1337)	1:76:A:MET:HA	1:76:A:MET:HG3	8	0.48
(1,1337)	1:76:A:MET:HA	1:76:A:MET:HG3	16	0.48
(1,1337)	1:76:A:MET:HA	1:76:A:MET:HG3	18	0.48
(1,1337)	1:76:A:MET:HA	1:76:A:MET:HG3	22	0.48
(1,1331)	1:77:A:GLN:HG2	1:73:A:LEU:HD11	22	0.48
(1,1326)	1:77:A:GLN:HG2	1:77:A:GLN:HA	12	0.48
(1,1324)	1:77:A:GLN:HG2	1:77:A:GLN:H	11	0.48
(1,1303)	1:137:A:HIS:HE1	1:136:A:ALA:HB1	23	0.48
(1,1283)	1:84:A:VAL:HG23	1:127:A:ILE:HD12	7	0.48
(1,1231)	1:67:A:PHE:HA	1:67:A:PHE:HD1	4	0.48
(1,1199)	1:89:A:TYR:HE1	1:71:A:LEU:HD11	16	0.48
(1,1115)	1:98:A:LEU:HD21	1:96:A:HIS:HE1	25	0.48
(1,1094)	1:100:A:LEU:HD22	1:138:A:SER:HB2	4	0.48
(1,1094)	1:100:A:LEU:HD21	1:138:A:SER:HB2	7	0.48
(1,1076)	1:101:A:ALA:HB1	1:98:A:LEU:HD22	8	0.48
(1,996)	1:108:A:ILE:HG22	1:112:A:VAL:HG13	22	0.48
(1,989)	1:108:A:ILE:HG22	1:105:A:PHE:HA	16	0.48
(1,888)	1:116:A:ALA:HB1	1:123:A:LEU:H	2	0.48
(1,848)	1:120:A:PRO:HG3	1:119:A:ARG:HA	9	0.48
(1,848)	1:120:A:PRO:HG3	1:119:A:ARG:HA	16	0.48
(1,835)	1:120:A:PRO:HB3	1:120:A:PRO:HD2	2	0.48
(1,835)	1:120:A:PRO:HB3	1:120:A:PRO:HD2	3	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,835)	1:120:A:PRO:HB3	1:120:A:PRO:HD2	9	0.48
(1,835)	1:120:A:PRO:HB3	1:120:A:PRO:HD2	12	0.48
(1,835)	1:120:A:PRO:HB3	1:120:A:PRO:HD2	18	0.48
(1,835)	1:120:A:PRO:HB3	1:120:A:PRO:HD2	23	0.48
(1,826)	1:117:A:ARG:HG2	1:117:A:ARG:H	15	0.48
(1,790)	1:124:A:TYR:HD1	1:124:A:TYR:HA	3	0.48
(1,790)	1:124:A:TYR:HD1	1:124:A:TYR:HA	19	0.48
(1,723)	1:129:A:GLU:HG2	1:125:A:VAL:HG11	8	0.48
(1,705)	1:130:A:LEU:HD12	1:109:A:LEU:HD13	7	0.48
(1,705)	1:130:A:LEU:HD13	1:109:A:LEU:HD13	24	0.48
(1,607)	1:136:A:ALA:HB2	1:137:A:HIS:HA	9	0.48
(1,607)	1:136:A:ALA:HB3	1:137:A:HIS:HA	15	0.48
(1,607)	1:136:A:ALA:HB2	1:137:A:HIS:HA	18	0.48
(1,585)	1:139:A:ALA:HB3	1:140:A:LYS:H	23	0.48
(1,555)	2:36:B:THR:H	2:35:B:PHE:H	4	0.48
(1,552)	2:35:B:PHE:H	2:33:B:GLN:HA	7	0.48
(1,552)	2:35:B:PHE:H	2:33:B:GLN:HA	13	0.48
(1,538)	1:63:A:ASN:H	1:61:A:LEU:HA	19	0.48
(1,502)	1:81:A:HIS:H	1:82:A:PRO:HB3	18	0.48
(1,483)	1:93:A:GLN:HG2	1:94:A:ARG:H	25	0.48
(1,465)	1:106:A:CYS:H	1:103:A:ALA:HB3	5	0.48
(1,444)	1:73:A:LEU:HD11	1:117:A:ARG:H	3	0.48
(1,444)	1:73:A:LEU:HD13	1:117:A:ARG:H	12	0.48
(1,399)	1:135:A:LYS:H	1:133:A:VAL:HA	14	0.48
(1,387)	1:141:A:LYS:H	1:141:A:LYS:HG2	10	0.48
(1,380)	2:27:B:SER:HA	2:30:B:GLU:HB3	7	0.48
(1,356)	2:29:B:SER:HB2	2:31:B:LEU:H	15	0.48
(1,340)	2:31:B:LEU:HD12	1:88:A:LEU:H	3	0.48
(1,333)	1:127:A:ILE:HG12	1:130:A:LEU:HD23	10	0.48
(1,325)	2:33:B:GLN:HG2	2:31:B:LEU:HB2	6	0.48
(1,325)	2:33:B:GLN:HG2	2:31:B:LEU:HB2	8	0.48
(1,325)	2:33:B:GLN:HG2	2:31:B:LEU:HB2	10	0.48
(1,325)	2:33:B:GLN:HG2	2:31:B:LEU:HB2	23	0.48
(1,265)	1:127:A:ILE:HD12	2:35:B:PHE:HE1	19	0.48
(1,240)	1:104:A:GLU:HB3	1:105:A:PHE:HA	6	0.48
(1,220)	1:70:A:PHE:HE2	1:113:A:LEU:HB2	1	0.48
(1,219)	1:70:A:PHE:HD1	1:73:A:LEU:HB3	9	0.48
(1,219)	1:70:A:PHE:HD1	1:73:A:LEU:HB3	21	0.48
(1,203)	1:71:A:LEU:HD11	1:68:A:GLU:H	3	0.48
(1,203)	1:71:A:LEU:HD11	1:68:A:GLU:H	25	0.48
(1,201)	1:72:A:GLU:HG3	1:72:A:GLU:HB2	4	0.48
(1,201)	1:72:A:GLU:HG3	1:72:A:GLU:HB2	14	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,199)	1:72:A:GLU:HG3	1:71:A:LEU:HB3	7	0.48
(1,197)	1:73:A:LEU:HD22	1:123:A:LEU:HB2	1	0.48
(1,197)	1:73:A:LEU:HD21	1:123:A:LEU:HB2	14	0.48
(1,195)	1:73:A:LEU:HD23	1:70:A:PHE:HA	10	0.48
(1,155)	1:88:A:LEU:HD12	1:74:A:CYS:HB2	9	0.48
(1,151)	1:88:A:LEU:HD13	1:70:A:PHE:HD1	7	0.48
(1,151)	1:88:A:LEU:HD12	1:70:A:PHE:HD1	9	0.48
(1,134)	1:105:A:PHE:HE2	1:92:A:GLN:HG2	17	0.48
(1,134)	1:92:A:GLN:HG2	1:95:A:ALA:H	19	0.48
(1,134)	1:92:A:GLN:HG2	1:95:A:ALA:H	24	0.48
(1,121)	1:95:A:ALA:HB3	1:134:A:LEU:HA	11	0.48
(1,81)	1:116:A:ALA:HB1	1:70:A:PHE:HZ	3	0.48
(1,81)	1:116:A:ALA:HB3	1:70:A:PHE:HZ	16	0.48
(1,67)	1:116:A:ALA:HB3	1:120:A:PRO:HA	18	0.48
(1,6)	1:130:A:LEU:HD23	1:70:A:PHE:HE2	14	0.48
(1,2086)	1:80:A:ASP:HB2	1:80:A:ASP:H	1	0.47
(1,2086)	1:80:A:ASP:HB2	1:80:A:ASP:H	2	0.47
(1,2063)	1:85:A:VAL:H	1:71:A:LEU:HD23	18	0.47
(1,2063)	1:85:A:VAL:H	1:71:A:LEU:HD22	19	0.47
(1,2063)	1:85:A:VAL:H	1:71:A:LEU:HD21	21	0.47
(1,2063)	1:85:A:VAL:H	1:71:A:LEU:HD23	22	0.47
(1,2060)	1:86:A:PRO:HB3	1:87:A:PHE:H	1	0.47
(1,2060)	1:86:A:PRO:HB3	1:87:A:PHE:H	7	0.47
(1,2060)	1:86:A:PRO:HB3	1:87:A:PHE:H	10	0.47
(1,2037)	1:90:A:ASN:HD21	1:94:A:ARG:HD3	16	0.47
(1,2017)	1:93:A:GLN:HE22	1:89:A:TYR:HB3	14	0.47
(1,2013)	1:94:A:ARG:H	1:95:A:ALA:HB1	11	0.47
(1,2013)	1:94:A:ARG:H	1:95:A:ALA:HB2	15	0.47
(1,2012)	1:94:A:ARG:HB3	1:94:A:ARG:H	13	0.47
(1,2012)	1:94:A:ARG:HB3	1:94:A:ARG:H	21	0.47
(1,2011)	1:94:A:ARG:HD2	1:94:A:ARG:H	8	0.47
(1,1986)	1:99:A:PHE:H	1:98:A:LEU:HD22	6	0.47
(1,1986)	1:99:A:PHE:H	1:98:A:LEU:HD22	11	0.47
(1,1971)	1:100:A:LEU:HD23	1:101:A:ALA:H	25	0.47
(1,1924)	1:108:A:ILE:HG22	1:108:A:ILE:H	8	0.47
(1,1798)	1:136:A:ALA:H	1:135:A:LYS:HD2	24	0.47
(1,1788)	1:139:A:ALA:H	1:135:A:LYS:HD3	6	0.47
(1,1736)	2:31:B:LEU:HB2	2:31:B:LEU:HD11	3	0.47
(1,1736)	2:31:B:LEU:HB2	2:31:B:LEU:HD11	7	0.47
(1,1736)	2:31:B:LEU:HB2	2:31:B:LEU:HD13	15	0.47
(1,1736)	2:31:B:LEU:HB2	2:31:B:LEU:HD11	16	0.47
(1,1736)	2:31:B:LEU:HB2	2:31:B:LEU:HD12	17	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1736)	2:31:B:LEU:HB2	2:31:B:LEU:HD11	22	0.47
(1,1716)	2:31:B:LEU:HG	2:32:B:GLU:HG3	4	0.47
(1,1670)	2:37:B:ALA:HB3	2:36:B:THR:HA	6	0.47
(1,1633)	2:38:B:ARG:HD2	2:38:B:ARG:HB2	10	0.47
(1,1619)	2:39:B:TRP:HD1	2:38:B:ARG:HB2	21	0.47
(1,1576)	1:73:A:LEU:HD12	1:117:A:ARG:H	17	0.47
(1,1554)	1:59:A:TYR:HE1	1:57:A:LYS:HB2	24	0.47
(1,1481)	1:66:A:LEU:HD21	1:69:A:GLU:H	2	0.47
(1,1481)	1:66:A:LEU:HD21	1:69:A:GLU:H	11	0.47
(1,1481)	1:66:A:LEU:HD23	1:69:A:GLU:H	18	0.47
(1,1475)	1:66:A:LEU:HD23	1:109:A:LEU:HD22	8	0.47
(1,1456)	1:69:A:GLU:HG2	1:66:A:LEU:HA	7	0.47
(1,1422)	1:71:A:LEU:HD22	1:74:A:CYS:H	23	0.47
(1,1416)	1:71:A:LEU:HD11	1:71:A:LEU:H	10	0.47
(1,1370)	1:75:A:LYS:HE3	1:72:A:GLU:HB3	17	0.47
(1,1337)	1:76:A:MET:HA	1:76:A:MET:HG3	4	0.47
(1,1331)	1:77:A:GLN:HG2	1:73:A:LEU:HD11	4	0.47
(1,1331)	1:77:A:GLN:HG2	1:73:A:LEU:HD13	13	0.47
(1,1331)	1:77:A:GLN:HG2	1:73:A:LEU:HD12	23	0.47
(1,1326)	1:77:A:GLN:HG2	1:77:A:GLN:HA	2	0.47
(1,1303)	1:137:A:HIS:HE1	1:136:A:ALA:HB1	18	0.47
(1,1303)	1:137:A:HIS:HE1	1:136:A:ALA:HB3	22	0.47
(1,1231)	1:67:A:PHE:HA	1:67:A:PHE:HD1	12	0.47
(1,1231)	1:67:A:PHE:HA	1:67:A:PHE:HD1	25	0.47
(1,1183)	1:90:A:ASN:HB2	1:87:A:PHE:HD1	24	0.47
(1,1137)	1:95:A:ALA:HB2	1:91:A:ARG:HD3	10	0.47
(1,1137)	1:95:A:ALA:HB3	1:91:A:ARG:HD3	15	0.47
(1,1115)	1:98:A:LEU:HD22	1:96:A:HIS:HE1	5	0.47
(1,1094)	1:100:A:LEU:HD21	1:138:A:SER:HB2	11	0.47
(1,1094)	1:100:A:LEU:HD21	1:138:A:SER:HB2	19	0.47
(1,1088)	1:100:A:LEU:HD23	1:105:A:PHE:HD2	22	0.47
(1,1076)	1:101:A:ALA:HB3	1:98:A:LEU:HD22	6	0.47
(1,1076)	1:101:A:ALA:HB2	1:98:A:LEU:HD22	11	0.47
(1,1076)	1:101:A:ALA:HB3	1:98:A:LEU:HD22	15	0.47
(1,1076)	1:101:A:ALA:HB3	1:98:A:LEU:HD22	25	0.47
(1,996)	1:108:A:ILE:HG21	1:112:A:VAL:HG13	17	0.47
(1,917)	1:113:A:LEU:HB2	1:113:A:LEU:HD23	20	0.47
(1,835)	1:120:A:PRO:HB3	1:120:A:PRO:HD2	6	0.47
(1,835)	1:120:A:PRO:HB3	1:120:A:PRO:HD2	7	0.47
(1,835)	1:120:A:PRO:HB3	1:120:A:PRO:HD2	8	0.47
(1,835)	1:120:A:PRO:HB3	1:120:A:PRO:HD2	11	0.47
(1,835)	1:120:A:PRO:HB3	1:120:A:PRO:HD2	14	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,835)	1:120:A:PRO:HB3	1:120:A:PRO:HD2	19	0.47
(1,835)	1:120:A:PRO:HB3	1:120:A:PRO:HD2	21	0.47
(1,835)	1:120:A:PRO:HB3	1:120:A:PRO:HD2	24	0.47
(1,826)	1:117:A:ARG:HG2	1:117:A:ARG:H	25	0.47
(1,790)	1:124:A:TYR:HD1	1:124:A:TYR:HA	9	0.47
(1,790)	1:124:A:TYR:HD1	1:124:A:TYR:HA	15	0.47
(1,790)	1:124:A:TYR:HD1	1:124:A:TYR:HA	20	0.47
(1,766)	1:126:A:TYR:HE1	1:115:A:ARG:HB2	25	0.47
(1,723)	1:129:A:GLU:HG2	1:125:A:VAL:HG13	4	0.47
(1,705)	1:130:A:LEU:HD11	1:109:A:LEU:HD11	2	0.47
(1,705)	1:130:A:LEU:HD11	1:109:A:LEU:HD11	3	0.47
(1,705)	1:130:A:LEU:HD13	1:109:A:LEU:HD12	11	0.47
(1,670)	1:133:A:VAL:HG21	1:105:A:PHE:HE1	14	0.47
(1,670)	1:133:A:VAL:HG23	1:105:A:PHE:HE1	24	0.47
(1,607)	1:136:A:ALA:HB2	1:137:A:HIS:HA	21	0.47
(1,576)	1:142:A:LYS:HB2	1:142:A:LYS:H	17	0.47
(1,538)	1:63:A:ASN:H	1:61:A:LEU:HA	2	0.47
(1,529)	1:67:A:PHE:H	1:68:A:GLU:HB2	15	0.47
(1,502)	1:81:A:HIS:H	1:82:A:PRO:HB3	9	0.47
(1,494)	1:90:A:ASN:H	1:88:A:LEU:HB2	6	0.47
(1,494)	1:90:A:ASN:H	1:88:A:LEU:HB2	19	0.47
(1,492)	1:91:A:ARG:H	1:88:A:LEU:HD23	3	0.47
(1,488)	1:92:A:GLN:HE22	1:64:A:GLU:HG3	24	0.47
(1,478)	1:95:A:ALA:H	1:91:A:ARG:HD2	2	0.47
(1,457)	1:111:A:ARG:H	1:109:A:LEU:HB3	14	0.47
(1,455)	1:112:A:VAL:H	1:113:A:LEU:HB3	13	0.47
(1,455)	1:112:A:VAL:H	1:113:A:LEU:HB3	19	0.47
(1,454)	1:114:A:SER:H	1:112:A:VAL:HG21	2	0.47
(1,444)	1:73:A:LEU:HD11	1:117:A:ARG:H	1	0.47
(1,434)	1:74:A:CYS:H	1:123:A:LEU:HD13	3	0.47
(1,434)	1:74:A:CYS:H	1:123:A:LEU:HD13	13	0.47
(1,421)	1:128:A:ASN:H	1:70:A:PHE:HZ	2	0.47
(1,421)	1:128:A:ASN:H	1:70:A:PHE:HZ	23	0.47
(1,419)	1:129:A:GLU:H	1:126:A:TYR:H	2	0.47
(1,399)	1:135:A:LYS:H	1:133:A:VAL:HA	1	0.47
(1,399)	1:135:A:LYS:H	1:133:A:VAL:HA	8	0.47
(1,399)	1:135:A:LYS:H	1:133:A:VAL:HA	15	0.47
(1,399)	1:135:A:LYS:H	1:133:A:VAL:HA	16	0.47
(1,399)	1:135:A:LYS:H	1:133:A:VAL:HA	24	0.47
(1,362)	2:29:B:SER:HB3	2:32:B:GLU:HG3	16	0.47
(1,333)	1:127:A:ILE:HG12	1:130:A:LEU:HD22	3	0.47
(1,325)	2:33:B:GLN:HG2	2:31:B:LEU:HB2	2	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,325)	2:33:B:GLN:HG2	2:31:B:LEU:HB2	3	0.47
(1,325)	2:33:B:GLN:HG2	2:31:B:LEU:HB2	7	0.47
(1,325)	2:33:B:GLN:HG2	2:31:B:LEU:HB2	14	0.47
(1,325)	2:33:B:GLN:HG2	2:31:B:LEU:HB2	15	0.47
(1,325)	2:33:B:GLN:HG2	2:31:B:LEU:HB2	16	0.47
(1,325)	2:33:B:GLN:HG2	2:31:B:LEU:HB2	17	0.47
(1,325)	2:33:B:GLN:HG2	2:31:B:LEU:HB2	25	0.47
(1,318)	2:34:B:TYR:HE1	1:83:A:GLU:HB3	15	0.47
(1,312)	2:35:B:PHE:HE1	1:124:A:TYR:HA	22	0.47
(1,310)	2:35:B:PHE:HD1	1:127:A:ILE:HB	24	0.47
(1,290)	2:39:B:TRP:HH2	2:36:B:THR:HB	7	0.47
(1,289)	2:39:B:TRP:HZ3	2:36:B:THR:HB	13	0.47
(1,289)	2:39:B:TRP:HZ3	2:36:B:THR:HB	24	0.47
(1,289)	2:39:B:TRP:HZ3	2:36:B:THR:HB	25	0.47
(1,232)	1:66:A:LEU:HD11	1:62:A:GLU:HA	2	0.47
(1,230)	1:66:A:LEU:HA	1:113:A:LEU:HD23	5	0.47
(1,219)	1:70:A:PHE:HD1	1:73:A:LEU:HB3	3	0.47
(1,201)	2:25:B:GLU:HG3	2:25:B:GLU:HB2	16	0.47
(1,201)	1:72:A:GLU:HG3	1:72:A:GLU:HB2	20	0.47
(1,197)	1:73:A:LEU:HD23	1:123:A:LEU:HB2	8	0.47
(1,194)	1:73:A:LEU:HD22	1:70:A:PHE:HD1	17	0.47
(1,155)	1:88:A:LEU:HD13	1:74:A:CYS:HB2	8	0.47
(1,151)	1:88:A:LEU:HD11	1:70:A:PHE:HD1	17	0.47
(1,134)	1:92:A:GLN:HG2	1:95:A:ALA:H	7	0.47
(1,67)	1:116:A:ALA:HB3	1:120:A:PRO:HA	1	0.47
(1,52)	1:125:A:VAL:HG11	1:128:A:ASN:HB2	13	0.47
(1,48)	1:126:A:TYR:HE1	1:125:A:VAL:HG12	6	0.47
(1,42)	1:126:A:TYR:HD1	1:125:A:VAL:HB	14	0.47
(1,13)	1:133:A:VAL:HG12	1:108:A:ILE:HB	17	0.47
(1,6)	1:130:A:LEU:HD22	1:70:A:PHE:HE2	12	0.47
(1,6)	1:130:A:LEU:HD21	1:70:A:PHE:HE2	13	0.47
(1,2197)	1:55:A:GLY:HA2	1:56:A:LYS:H	6	0.46
(1,2197)	1:55:A:GLY:HA2	1:56:A:LYS:H	19	0.46
(1,2124)	1:73:A:LEU:HD23	1:73:A:LEU:H	1	0.46
(1,2124)	1:73:A:LEU:HD21	1:73:A:LEU:H	19	0.46
(1,2106)	1:76:A:MET:HB3	1:77:A:GLN:H	16	0.46
(1,2089)	1:79:A:ALA:H	1:78:A:THR:HG22	3	0.46
(1,2082)	1:81:A:HIS:H	1:79:A:ALA:HB1	18	0.46
(1,2063)	1:85:A:VAL:H	1:71:A:LEU:HD23	3	0.46
(1,2063)	1:85:A:VAL:H	1:71:A:LEU:HD22	5	0.46
(1,2063)	1:85:A:VAL:H	1:71:A:LEU:HD21	9	0.46
(1,2063)	1:85:A:VAL:H	1:71:A:LEU:HD22	24	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2060)	1:86:A:PRO:HB3	1:87:A:PHE:H	15	0.46
(1,2051)	1:89:A:TYR:H	1:90:A:ASN:HB3	10	0.46
(1,2019)	1:93:A:GLN:HE22	1:93:A:GLN:HB3	17	0.46
(1,2012)	1:94:A:ARG:HB3	1:94:A:ARG:H	2	0.46
(1,2012)	1:94:A:ARG:HB3	1:94:A:ARG:H	15	0.46
(1,2012)	1:94:A:ARG:HB3	1:94:A:ARG:H	22	0.46
(1,1986)	1:99:A:PHE:H	1:98:A:LEU:HD21	1	0.46
(1,1986)	1:99:A:PHE:H	1:98:A:LEU:HD21	4	0.46
(1,1971)	1:100:A:LEU:HD23	1:101:A:ALA:H	3	0.46
(1,1874)	1:118:A:SER:H	1:117:A:ARG:HG2	16	0.46
(1,1874)	1:118:A:SER:H	1:117:A:ARG:HG2	20	0.46
(1,1830)	1:128:A:ASN:H	1:128:A:ASN:HB3	2	0.46
(1,1830)	1:128:A:ASN:H	1:128:A:ASN:HB3	5	0.46
(1,1798)	1:136:A:ALA:H	1:135:A:LYS:HD3	19	0.46
(1,1798)	1:136:A:ALA:H	1:135:A:LYS:HD3	20	0.46
(1,1716)	2:31:B:LEU:HG	2:32:B:GLU:HG3	7	0.46
(1,1716)	2:31:B:LEU:HG	2:32:B:GLU:HG3	12	0.46
(1,1629)	2:38:B:ARG:HG2	2:38:B:ARG:HA	21	0.46
(1,1559)	1:57:A:LYS:HB2	1:57:A:LYS:HG2	11	0.46
(1,1422)	1:71:A:LEU:HD23	1:74:A:CYS:H	2	0.46
(1,1422)	1:71:A:LEU:HD22	1:74:A:CYS:H	17	0.46
(1,1393)	1:77:A:GLN:HG3	1:73:A:LEU:HD22	1	0.46
(1,1337)	1:76:A:MET:HA	1:76:A:MET:HG3	12	0.46
(1,1337)	1:76:A:MET:HA	1:76:A:MET:HG3	13	0.46
(1,1337)	1:76:A:MET:HA	1:76:A:MET:HG3	21	0.46
(1,1326)	1:77:A:GLN:HG2	1:77:A:GLN:HA	9	0.46
(1,1303)	1:137:A:HIS:HE1	1:136:A:ALA:HB1	9	0.46
(1,1303)	1:137:A:HIS:HE1	1:136:A:ALA:HB2	19	0.46
(1,1283)	1:84:A:VAL:HG21	1:127:A:ILE:HD12	1	0.46
(1,1231)	1:67:A:PHE:HA	1:67:A:PHE:HD1	2	0.46
(1,1231)	1:67:A:PHE:HA	1:67:A:PHE:HD1	6	0.46
(1,1231)	1:67:A:PHE:HA	1:67:A:PHE:HD1	14	0.46
(1,1231)	1:67:A:PHE:HA	1:67:A:PHE:HD1	16	0.46
(1,1199)	1:89:A:TYR:HE1	1:71:A:LEU:HD11	6	0.46
(1,1183)	1:90:A:ASN:HB2	1:87:A:PHE:HD1	20	0.46
(1,1115)	1:98:A:LEU:HD23	1:96:A:HIS:HE1	2	0.46
(1,1115)	1:98:A:LEU:HD22	1:96:A:HIS:HE1	16	0.46
(1,1094)	1:100:A:LEU:HD21	1:138:A:SER:HB2	13	0.46
(1,1094)	1:100:A:LEU:HD21	1:138:A:SER:HB2	22	0.46
(1,1076)	1:101:A:ALA:HB1	1:98:A:LEU:HD21	2	0.46
(1,1076)	1:101:A:ALA:HB2	1:98:A:LEU:HD21	13	0.46
(1,1070)	1:101:A:ALA:HB2	1:102:A:SER:H	11	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1066)	1:101:A:ALA:HA	1:60:A:LYS:HB2	8	0.46
(1,1059)	1:103:A:ALA:HB2	1:104:A:GLU:HA	1	0.46
(1,1059)	1:103:A:ALA:HB2	1:104:A:GLU:HA	6	0.46
(1,1059)	1:103:A:ALA:HB1	1:104:A:GLU:HA	7	0.46
(1,1059)	1:103:A:ALA:HB1	1:104:A:GLU:HA	9	0.46
(1,1059)	1:103:A:ALA:HB3	1:104:A:GLU:HA	14	0.46
(1,1059)	1:103:A:ALA:HB3	1:104:A:GLU:HA	22	0.46
(1,1040)	1:62:A:GLU:HB3	1:59:A:TYR:HA	14	0.46
(1,1040)	1:62:A:GLU:HB3	1:59:A:TYR:HA	21	0.46
(1,996)	1:108:A:ILE:HG23	1:112:A:VAL:HG12	2	0.46
(1,996)	1:108:A:ILE:HG21	1:112:A:VAL:HG11	6	0.46
(1,996)	1:108:A:ILE:HG21	1:112:A:VAL:HG11	8	0.46
(1,996)	1:108:A:ILE:HG23	1:112:A:VAL:HG12	14	0.46
(1,989)	1:108:A:ILE:HG23	1:105:A:PHE:HA	6	0.46
(1,989)	1:108:A:ILE:HG22	1:105:A:PHE:HA	18	0.46
(1,934)	1:112:A:VAL:HG11	1:126:A:TYR:HB3	25	0.46
(1,888)	1:116:A:ALA:HB1	1:123:A:LEU:H	6	0.46
(1,888)	1:116:A:ALA:HB2	1:123:A:LEU:H	7	0.46
(1,888)	1:116:A:ALA:HB1	1:123:A:LEU:H	10	0.46
(1,848)	1:120:A:PRO:HG3	1:119:A:ARG:HA	20	0.46
(1,835)	1:120:A:PRO:HB3	1:120:A:PRO:HD2	1	0.46
(1,835)	1:120:A:PRO:HB3	1:120:A:PRO:HD2	4	0.46
(1,835)	1:120:A:PRO:HB3	1:120:A:PRO:HD2	5	0.46
(1,835)	1:120:A:PRO:HB3	1:120:A:PRO:HD2	10	0.46
(1,835)	1:120:A:PRO:HB3	1:120:A:PRO:HD2	15	0.46
(1,835)	1:120:A:PRO:HB3	1:120:A:PRO:HD2	16	0.46
(1,835)	1:120:A:PRO:HB3	1:120:A:PRO:HD2	20	0.46
(1,835)	1:120:A:PRO:HB3	1:120:A:PRO:HD2	25	0.46
(1,827)	1:122:A:LYS:HD2	1:122:A:LYS:HA	17	0.46
(1,790)	1:124:A:TYR:HD1	1:124:A:TYR:HA	21	0.46
(1,790)	1:124:A:TYR:HD1	1:124:A:TYR:HA	22	0.46
(1,766)	1:126:A:TYR:HE1	1:115:A:ARG:HB2	13	0.46
(1,723)	1:129:A:GLU:HG2	1:125:A:VAL:HG11	5	0.46
(1,705)	1:130:A:LEU:HD12	1:109:A:LEU:HD12	17	0.46
(1,705)	1:130:A:LEU:HD12	1:109:A:LEU:HD13	20	0.46
(1,670)	1:133:A:VAL:HG21	1:105:A:PHE:HE1	2	0.46
(1,555)	2:36:B:THR:H	2:37:B:ALA:H	12	0.46
(1,555)	2:36:B:THR:H	2:35:B:PHE:H	24	0.46
(1,552)	2:35:B:PHE:H	2:33:B:GLN:HA	5	0.46
(1,541)	1:61:A:LEU:HB3	1:62:A:GLU:H	13	0.46
(1,529)	1:67:A:PHE:H	1:69:A:GLU:HB2	18	0.46
(1,500)	1:85:A:VAL:H	1:83:A:GLU:H	22	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,494)	1:90:A:ASN:H	1:88:A:LEU:HB2	9	0.46
(1,494)	1:90:A:ASN:H	1:88:A:LEU:HB2	16	0.46
(1,494)	1:90:A:ASN:H	1:88:A:LEU:HB2	24	0.46
(1,488)	1:92:A:GLN:HE22	1:64:A:GLU:HG3	19	0.46
(1,483)	1:93:A:GLN:HG2	1:94:A:ARG:H	8	0.46
(1,480)	1:134:A:LEU:HD11	1:95:A:ALA:H	8	0.46
(1,476)	1:96:A:HIS:H	1:95:A:ALA:H	3	0.46
(1,457)	1:111:A:ARG:H	1:109:A:LEU:HB3	4	0.46
(1,457)	1:111:A:ARG:H	1:109:A:LEU:HB3	17	0.46
(1,457)	1:111:A:ARG:H	1:109:A:LEU:HB3	22	0.46
(1,455)	1:112:A:VAL:H	1:113:A:LEU:HB3	1	0.46
(1,455)	1:112:A:VAL:H	1:113:A:LEU:HB3	7	0.46
(1,455)	1:112:A:VAL:H	1:113:A:LEU:HB3	23	0.46
(1,454)	1:114:A:SER:H	1:112:A:VAL:HG21	3	0.46
(1,451)	1:114:A:SER:H	1:117:A:ARG:HB2	9	0.46
(1,445)	1:116:A:ALA:H	1:112:A:VAL:HA	8	0.46
(1,444)	1:73:A:LEU:HD13	1:117:A:ARG:H	5	0.46
(1,444)	1:73:A:LEU:HD12	1:117:A:ARG:H	6	0.46
(1,444)	1:73:A:LEU:HD13	1:117:A:ARG:H	14	0.46
(1,407)	1:133:A:VAL:H	1:130:A:LEU:HD11	13	0.46
(1,399)	1:135:A:LYS:H	1:133:A:VAL:HA	22	0.46
(1,395)	1:138:A:SER:H	1:95:A:ALA:HB2	8	0.46
(1,389)	1:143:A:LEU:H	1:142:A:LYS:HB2	22	0.46
(1,380)	2:27:B:SER:HA	2:25:B:GLU:HB3	22	0.46
(1,366)	1:100:A:LEU:HD11	1:138:A:SER:HB3	16	0.46
(1,343)	2:31:B:LEU:HB2	1:87:A:PHE:HE2	2	0.46
(1,333)	1:127:A:ILE:HG12	1:130:A:LEU:HD23	13	0.46
(1,325)	2:33:B:GLN:HG2	2:31:B:LEU:HB2	22	0.46
(1,318)	2:34:B:TYR:HE1	1:83:A:GLU:HB3	14	0.46
(1,312)	2:35:B:PHE:HE1	2:36:B:THR:HA	14	0.46
(1,312)	2:35:B:PHE:HE1	1:124:A:TYR:HA	15	0.46
(1,307)	2:39:B:TRP:HE3	2:36:B:THR:HG21	20	0.46
(1,289)	2:39:B:TRP:HZ3	2:36:B:THR:HB	3	0.46
(1,265)	1:127:A:ILE:HD12	2:35:B:PHE:HE1	2	0.46
(1,265)	1:127:A:ILE:HD12	2:35:B:PHE:HE1	5	0.46
(1,220)	1:70:A:PHE:HE2	1:113:A:LEU:HB2	13	0.46
(1,219)	1:70:A:PHE:HD1	1:73:A:LEU:HB3	15	0.46
(1,219)	1:70:A:PHE:HD1	1:73:A:LEU:HB3	22	0.46
(1,219)	1:70:A:PHE:HD1	1:73:A:LEU:HB3	23	0.46
(1,201)	1:72:A:GLU:HG3	1:72:A:GLU:HB2	2	0.46
(1,199)	1:72:A:GLU:HG2	1:71:A:LEU:HB3	6	0.46
(1,199)	1:72:A:GLU:HG2	1:71:A:LEU:HB3	8	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,199)	1:72:A:GLU:HG2	1:71:A:LEU:HB3	9	0.46
(1,197)	1:73:A:LEU:HD21	1:123:A:LEU:HB2	21	0.46
(1,195)	1:73:A:LEU:HD22	1:70:A:PHE:HA	16	0.46
(1,195)	1:73:A:LEU:HD22	1:117:A:ARG:HA	18	0.46
(1,191)	1:84:A:VAL:HG11	1:74:A:CYS:HB2	3	0.46
(1,191)	1:84:A:VAL:HG12	1:74:A:CYS:HB2	11	0.46
(1,191)	1:78:A:THR:HG21	1:74:A:CYS:HB2	15	0.46
(1,191)	1:84:A:VAL:HG11	1:74:A:CYS:HB2	20	0.46
(1,189)	1:85:A:VAL:HG11	1:75:A:LYS:HA	24	0.46
(1,151)	1:88:A:LEU:HD13	1:70:A:PHE:HD1	1	0.46
(1,151)	1:88:A:LEU:HD12	1:70:A:PHE:HD1	11	0.46
(1,151)	1:88:A:LEU:HD11	1:70:A:PHE:HD1	12	0.46
(1,151)	1:88:A:LEU:HD12	1:70:A:PHE:HD1	19	0.46
(1,151)	1:88:A:LEU:HD11	1:70:A:PHE:HD1	25	0.46
(1,141)	1:93:A:GLN:HG2	1:89:A:TYR:HD1	9	0.46
(1,134)	1:92:A:GLN:HG2	1:95:A:ALA:H	21	0.46
(1,132)	1:67:A:PHE:HE1	1:92:A:GLN:HB3	11	0.46
(1,122)	1:95:A:ALA:HB2	1:91:A:ARG:HD3	21	0.46
(1,98)	1:105:A:PHE:HD1	1:100:A:LEU:HD23	20	0.46
(1,81)	1:116:A:ALA:HB3	1:70:A:PHE:HZ	21	0.46
(1,80)	1:94:A:ARG:HD3	1:93:A:GLN:HB2	24	0.46
(1,67)	1:116:A:ALA:HB1	1:120:A:PRO:HA	8	0.46
(1,67)	1:116:A:ALA:HB3	1:120:A:PRO:HA	9	0.46
(1,27)	1:130:A:LEU:HD22	1:67:A:PHE:HA	13	0.46
(1,17)	1:133:A:VAL:HG13	1:137:A:HIS:HB2	1	0.46
(1,6)	1:130:A:LEU:HD23	1:70:A:PHE:HE2	22	0.46
(1,2265)	2:26:B:ASP:HB3	2:26:B:ASP:H	19	0.45
(1,2106)	1:76:A:MET:HB3	1:77:A:GLN:H	10	0.45
(1,2106)	1:76:A:MET:HB3	1:77:A:GLN:H	13	0.45
(1,2106)	1:76:A:MET:HB3	1:77:A:GLN:H	18	0.45
(1,2063)	1:85:A:VAL:H	1:71:A:LEU:HD21	11	0.45
(1,2063)	1:85:A:VAL:H	1:71:A:LEU:HD22	15	0.45
(1,2060)	1:86:A:PRO:HB3	1:87:A:PHE:H	4	0.45
(1,2060)	1:86:A:PRO:HB3	1:87:A:PHE:H	19	0.45
(1,2051)	1:89:A:TYR:H	1:90:A:ASN:HB3	18	0.45
(1,2037)	1:90:A:ASN:HD21	1:94:A:ARG:HD2	7	0.45
(1,2019)	1:93:A:GLN:HE22	1:93:A:GLN:HB3	24	0.45
(1,2017)	1:93:A:GLN:HE22	1:89:A:TYR:HB3	19	0.45
(1,2013)	1:94:A:ARG:H	1:95:A:ALA:HB1	20	0.45
(1,1996)	1:97:A:SER:H	1:139:A:ALA:HB1	10	0.45
(1,1986)	1:99:A:PHE:H	1:98:A:LEU:HD22	8	0.45
(1,1971)	1:100:A:LEU:HD21	1:101:A:ALA:H	12	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1929)	1:107:A:ASN:HD21	1:103:A:ALA:HB2	22	0.45
(1,1924)	1:108:A:ILE:HG21	1:108:A:ILE:H	2	0.45
(1,1924)	1:108:A:ILE:HG21	1:108:A:ILE:H	14	0.45
(1,1830)	1:128:A:ASN:H	1:128:A:ASN:HB3	24	0.45
(1,1801)	1:135:A:LYS:H	1:91:A:ARG:HD3	25	0.45
(1,1798)	1:136:A:ALA:H	1:135:A:LYS:HD2	22	0.45
(1,1788)	1:139:A:ALA:H	1:135:A:LYS:HD3	4	0.45
(1,1768)	2:24:B:GLN:HB2	2:24:B:GLN:HG2	10	0.45
(1,1716)	2:31:B:LEU:HG	2:32:B:GLU:HG3	15	0.45
(1,1702)	2:33:B:GLN:HG3	2:34:B:TYR:HE2	16	0.45
(1,1633)	2:38:B:ARG:HD2	2:38:B:ARG:HB2	20	0.45
(1,1477)	1:66:A:LEU:HD21	1:113:A:LEU:HB3	24	0.45
(1,1475)	1:66:A:LEU:HD21	1:109:A:LEU:HD22	10	0.45
(1,1475)	1:66:A:LEU:HD23	1:109:A:LEU:HD23	19	0.45
(1,1475)	1:66:A:LEU:HD22	1:109:A:LEU:HD23	23	0.45
(1,1447)	1:69:A:GLU:HA	1:69:A:GLU:HG3	4	0.45
(1,1431)	1:70:A:PHE:HB2	1:70:A:PHE:HD1	1	0.45
(1,1431)	1:70:A:PHE:HB2	1:70:A:PHE:HD1	5	0.45
(1,1431)	1:70:A:PHE:HB2	1:70:A:PHE:HD1	10	0.45
(1,1431)	1:70:A:PHE:HB2	1:70:A:PHE:HD1	11	0.45
(1,1431)	1:70:A:PHE:HB2	1:70:A:PHE:HD1	12	0.45
(1,1431)	1:70:A:PHE:HB2	1:70:A:PHE:HD1	13	0.45
(1,1431)	1:70:A:PHE:HB2	1:70:A:PHE:HD1	14	0.45
(1,1431)	1:70:A:PHE:HB2	1:70:A:PHE:HD1	15	0.45
(1,1431)	1:70:A:PHE:HB2	1:70:A:PHE:HD1	16	0.45
(1,1431)	1:70:A:PHE:HB2	1:70:A:PHE:HD1	18	0.45
(1,1431)	1:70:A:PHE:HB2	1:70:A:PHE:HD1	20	0.45
(1,1431)	1:70:A:PHE:HB2	1:70:A:PHE:HD1	22	0.45
(1,1431)	1:70:A:PHE:HB2	1:70:A:PHE:HD1	23	0.45
(1,1431)	1:70:A:PHE:HB2	1:70:A:PHE:HD1	24	0.45
(1,1422)	1:71:A:LEU:HD22	1:74:A:CYS:H	3	0.45
(1,1422)	1:71:A:LEU:HD23	1:74:A:CYS:H	4	0.45
(1,1419)	1:71:A:LEU:HD13	1:89:A:TYR:H	19	0.45
(1,1416)	1:71:A:LEU:HD13	1:71:A:LEU:H	17	0.45
(1,1416)	1:71:A:LEU:HD13	1:71:A:LEU:H	21	0.45
(1,1392)	1:73:A:LEU:HD22	1:117:A:ARG:HD2	19	0.45
(1,1385)	1:73:A:LEU:HB2	1:74:A:CYS:H	11	0.45
(1,1345)	1:76:A:MET:HG2	1:77:A:GLN:H	2	0.45
(1,1341)	1:76:A:MET:HB3	1:73:A:LEU:HA	1	0.45
(1,1337)	1:76:A:MET:HA	1:76:A:MET:HG3	6	0.45
(1,1337)	1:76:A:MET:HA	1:76:A:MET:HG3	9	0.45
(1,1337)	1:76:A:MET:HA	1:76:A:MET:HG3	14	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1337)	1:76:A:MET:HA	1:76:A:MET:HG3	20	0.45
(1,1337)	1:76:A:MET:HA	1:76:A:MET:HG3	23	0.45
(1,1337)	1:76:A:MET:HA	1:76:A:MET:HG3	24	0.45
(1,1331)	1:77:A:GLN:HG2	1:73:A:LEU:HD13	7	0.45
(1,1331)	1:77:A:GLN:HG2	1:73:A:LEU:HD11	10	0.45
(1,1326)	1:77:A:GLN:HG2	1:77:A:GLN:HA	7	0.45
(1,1326)	1:77:A:GLN:HG2	1:77:A:GLN:HA	14	0.45
(1,1231)	1:67:A:PHE:HA	1:67:A:PHE:HD1	5	0.45
(1,1231)	1:67:A:PHE:HA	1:67:A:PHE:HD1	8	0.45
(1,1231)	1:67:A:PHE:HA	1:67:A:PHE:HD1	22	0.45
(1,1231)	1:67:A:PHE:HA	1:67:A:PHE:HD1	24	0.45
(1,1088)	1:100:A:LEU:HD21	1:105:A:PHE:HD2	1	0.45
(1,1088)	1:100:A:LEU:HD22	1:105:A:PHE:HD2	9	0.45
(1,1059)	1:103:A:ALA:HB2	1:104:A:GLU:HA	8	0.45
(1,1059)	1:103:A:ALA:HB2	1:104:A:GLU:HA	24	0.45
(1,1040)	1:62:A:GLU:HB3	1:59:A:TYR:HA	24	0.45
(1,989)	1:108:A:ILE:HG22	1:105:A:PHE:HA	3	0.45
(1,989)	1:108:A:ILE:HG22	1:105:A:PHE:HA	13	0.45
(1,989)	1:108:A:ILE:HG22	1:105:A:PHE:HA	19	0.45
(1,960)	1:67:A:PHE:HA	1:109:A:LEU:HD11	2	0.45
(1,888)	1:116:A:ALA:HB3	1:123:A:LEU:H	17	0.45
(1,888)	1:116:A:ALA:HB1	1:123:A:LEU:H	22	0.45
(1,886)	1:116:A:ALA:HA	1:123:A:LEU:HD12	7	0.45
(1,857)	1:119:A:ARG:HB2	1:119:A:ARG:HG3	2	0.45
(1,835)	1:120:A:PRO:HB3	1:120:A:PRO:HD2	13	0.45
(1,835)	1:120:A:PRO:HB3	1:120:A:PRO:HD2	17	0.45
(1,723)	1:129:A:GLU:HG2	1:125:A:VAL:HG11	2	0.45
(1,705)	1:130:A:LEU:HD11	1:109:A:LEU:HD11	12	0.45
(1,705)	1:130:A:LEU:HD12	1:109:A:LEU:HD13	13	0.45
(1,705)	1:130:A:LEU:HD11	1:109:A:LEU:HD11	18	0.45
(1,705)	1:130:A:LEU:HD11	1:109:A:LEU:HD12	25	0.45
(1,670)	1:133:A:VAL:HG23	1:105:A:PHE:HE1	5	0.45
(1,670)	1:133:A:VAL:HG21	1:105:A:PHE:HE1	9	0.45
(1,670)	1:133:A:VAL:HG22	1:105:A:PHE:HE1	10	0.45
(1,670)	1:133:A:VAL:HG21	1:105:A:PHE:HE1	11	0.45
(1,670)	1:133:A:VAL:HG21	1:105:A:PHE:HE1	16	0.45
(1,670)	1:133:A:VAL:HG23	1:105:A:PHE:HE1	18	0.45
(1,661)	1:133:A:VAL:HG13	1:99:A:PHE:HE1	23	0.45
(1,607)	1:136:A:ALA:HB1	1:137:A:HIS:HA	14	0.45
(1,607)	1:136:A:ALA:HB2	1:137:A:HIS:HA	19	0.45
(1,584)	1:139:A:ALA:HB1	1:96:A:HIS:H	12	0.45
(1,552)	2:35:B:PHE:H	2:33:B:GLN:HA	2	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,529)	1:67:A:PHE:H	1:68:A:GLU:HB2	23	0.45
(1,520)	1:130:A:LEU:H	1:112:A:VAL:HG23	3	0.45
(1,502)	1:81:A:HIS:H	1:82:A:PRO:HB3	17	0.45
(1,494)	1:90:A:ASN:H	1:88:A:LEU:HB2	5	0.45
(1,488)	1:92:A:GLN:HE22	1:64:A:GLU:HG3	16	0.45
(1,483)	1:93:A:GLN:HG2	1:94:A:ARG:H	18	0.45
(1,465)	1:108:A:ILE:HD11	1:106:A:CYS:H	23	0.45
(1,457)	1:111:A:ARG:H	1:109:A:LEU:HB3	23	0.45
(1,451)	1:114:A:SER:H	1:117:A:ARG:HB2	17	0.45
(1,445)	1:116:A:ALA:H	1:112:A:VAL:HA	12	0.45
(1,444)	1:73:A:LEU:HD11	1:117:A:ARG:H	8	0.45
(1,444)	1:73:A:LEU:HD12	1:117:A:ARG:H	13	0.45
(1,444)	1:73:A:LEU:HD12	1:117:A:ARG:H	25	0.45
(1,419)	1:129:A:GLU:H	1:126:A:TYR:H	5	0.45
(1,419)	1:129:A:GLU:H	1:126:A:TYR:H	10	0.45
(1,419)	1:129:A:GLU:H	1:126:A:TYR:H	20	0.45
(1,399)	1:135:A:LYS:H	1:133:A:VAL:HA	7	0.45
(1,399)	1:135:A:LYS:H	1:133:A:VAL:HA	12	0.45
(1,399)	1:135:A:LYS:H	1:133:A:VAL:HA	21	0.45
(1,387)	1:141:A:LYS:H	1:141:A:LYS:HG2	5	0.45
(1,387)	1:141:A:LYS:H	1:141:A:LYS:HG2	7	0.45
(1,387)	1:141:A:LYS:H	1:141:A:LYS:HG2	25	0.45
(1,356)	2:29:B:SER:HB2	2:31:B:LEU:H	1	0.45
(1,325)	2:33:B:GLN:HG2	2:31:B:LEU:HB2	11	0.45
(1,318)	2:34:B:TYR:HE1	1:83:A:GLU:HB3	12	0.45
(1,312)	2:35:B:PHE:HE1	1:124:A:TYR:HA	8	0.45
(1,312)	2:35:B:PHE:HE1	1:124:A:TYR:HA	19	0.45
(1,290)	2:39:B:TRP:HH2	2:36:B:THR:HB	3	0.45
(1,290)	2:39:B:TRP:HH2	2:36:B:THR:HB	22	0.45
(1,289)	2:39:B:TRP:HZ3	2:36:B:THR:HB	4	0.45
(1,289)	2:39:B:TRP:HZ3	2:36:B:THR:HB	8	0.45
(1,230)	1:66:A:LEU:HA	1:113:A:LEU:HD23	20	0.45
(1,220)	1:70:A:PHE:HE2	1:113:A:LEU:HB2	5	0.45
(1,220)	1:70:A:PHE:HE2	1:113:A:LEU:HB2	15	0.45
(1,220)	1:70:A:PHE:HE2	1:113:A:LEU:HB2	19	0.45
(1,219)	1:70:A:PHE:HD1	1:73:A:LEU:HB3	5	0.45
(1,219)	1:70:A:PHE:HD1	1:73:A:LEU:HB3	13	0.45
(1,219)	1:70:A:PHE:HD1	1:73:A:LEU:HB3	18	0.45
(1,219)	1:70:A:PHE:HD1	1:73:A:LEU:HB3	24	0.45
(1,201)	1:72:A:GLU:HG3	1:72:A:GLU:HB2	9	0.45
(1,201)	1:72:A:GLU:HG3	1:72:A:GLU:HB2	13	0.45
(1,201)	1:72:A:GLU:HG3	1:72:A:GLU:HB2	18	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,199)	1:72:A:GLU:HG2	1:71:A:LEU:HB3	24	0.45
(1,194)	1:73:A:LEU:HD22	1:70:A:PHE:HD1	16	0.45
(1,194)	1:73:A:LEU:HD22	1:70:A:PHE:HD1	25	0.45
(1,189)	1:85:A:VAL:HG11	1:75:A:LYS:HA	7	0.45
(1,189)	1:85:A:VAL:HG12	1:75:A:LYS:HA	16	0.45
(1,180)	1:82:A:PRO:HA	1:82:A:PRO:HG2	15	0.45
(1,171)	1:84:A:VAL:HG12	1:85:A:VAL:H	10	0.45
(1,155)	1:88:A:LEU:HD22	1:131:A:CYS:HB3	5	0.45
(1,155)	1:88:A:LEU:HD23	1:131:A:CYS:HB3	21	0.45
(1,151)	1:88:A:LEU:HD12	1:70:A:PHE:HD1	16	0.45
(1,151)	1:88:A:LEU:HD13	1:70:A:PHE:HD1	21	0.45
(1,141)	1:93:A:GLN:HG2	1:89:A:TYR:HD1	2	0.45
(1,134)	1:92:A:GLN:HG2	1:95:A:ALA:H	4	0.45
(1,132)	1:67:A:PHE:HE2	1:92:A:GLN:HB3	3	0.45
(1,132)	1:92:A:GLN:HB3	1:89:A:TYR:HD1	14	0.45
(1,97)	1:105:A:PHE:HD1	1:100:A:LEU:HA	13	0.45
(1,52)	1:125:A:VAL:HG11	1:128:A:ASN:HB2	24	0.45
(1,48)	1:126:A:TYR:HE1	1:125:A:VAL:HG13	4	0.45
(1,48)	1:126:A:TYR:HE1	1:125:A:VAL:HG12	12	0.45
(1,36)	1:127:A:ILE:HG21	1:124:A:TYR:HD2	2	0.45
(1,6)	1:130:A:LEU:HD23	1:70:A:PHE:HE2	9	0.45
(1,6)	1:130:A:LEU:HD23	1:70:A:PHE:HE2	16	0.45
(1,6)	1:130:A:LEU:HD23	1:70:A:PHE:HE2	23	0.45
(1,2202)	1:125:A:VAL:H	1:122:A:LYS:HD3	5	0.44
(1,2106)	1:76:A:MET:HB3	1:77:A:GLN:H	4	0.44
(1,2106)	1:76:A:MET:HB3	1:77:A:GLN:H	5	0.44
(1,2106)	1:76:A:MET:HB3	1:77:A:GLN:H	7	0.44
(1,2086)	1:80:A:ASP:HB2	1:80:A:ASP:H	20	0.44
(1,2063)	1:85:A:VAL:H	1:71:A:LEU:HD22	1	0.44
(1,2063)	1:85:A:VAL:H	1:71:A:LEU:HD23	6	0.44
(1,2063)	1:85:A:VAL:H	1:71:A:LEU:HD21	14	0.44
(1,2063)	1:85:A:VAL:H	1:71:A:LEU:HD23	23	0.44
(1,2060)	1:86:A:PRO:HB3	1:87:A:PHE:H	5	0.44
(1,2060)	1:86:A:PRO:HB3	1:87:A:PHE:H	6	0.44
(1,2060)	1:86:A:PRO:HB3	1:87:A:PHE:H	9	0.44
(1,2060)	1:86:A:PRO:HB3	1:87:A:PHE:H	14	0.44
(1,2060)	1:86:A:PRO:HB3	1:87:A:PHE:H	17	0.44
(1,2060)	1:86:A:PRO:HB3	1:87:A:PHE:H	18	0.44
(1,2051)	1:89:A:TYR:H	1:90:A:ASN:HB3	12	0.44
(1,2019)	1:93:A:GLN:HE22	1:93:A:GLN:HB3	22	0.44
(1,1996)	1:97:A:SER:H	1:139:A:ALA:HB3	24	0.44
(1,1986)	1:99:A:PHE:H	1:98:A:LEU:HD22	15	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1986)	1:99:A:PHE:H	1:98:A:LEU:HD22	22	0.44
(1,1971)	1:100:A:LEU:HD22	1:101:A:ALA:H	7	0.44
(1,1924)	1:108:A:ILE:HG23	1:108:A:ILE:H	1	0.44
(1,1924)	1:108:A:ILE:HG23	1:108:A:ILE:H	9	0.44
(1,1924)	1:108:A:ILE:HG21	1:108:A:ILE:H	23	0.44
(1,1788)	1:139:A:ALA:H	1:135:A:LYS:HD2	21	0.44
(1,1768)	2:24:B:GLN:HB2	2:24:B:GLN:HG2	11	0.44
(1,1651)	2:38:B:ARG:HG2	2:37:B:ALA:HB2	5	0.44
(1,1633)	2:38:B:ARG:HD2	2:38:B:ARG:HB2	7	0.44
(1,1576)	1:73:A:LEU:HD11	1:117:A:ARG:H	24	0.44
(1,1561)	1:57:A:LYS:HD2	1:57:A:LYS:HA	5	0.44
(1,1554)	1:59:A:TYR:HE1	1:57:A:LYS:HB2	22	0.44
(1,1485)	1:65:A:LYS:HB2	1:66:A:LEU:H	10	0.44
(1,1481)	1:66:A:LEU:HD21	1:69:A:GLU:H	5	0.44
(1,1480)	1:66:A:LEU:HD22	1:63:A:ASN:HA	11	0.44
(1,1480)	1:66:A:LEU:HD23	1:63:A:ASN:HA	21	0.44
(1,1475)	1:66:A:LEU:HD22	1:109:A:LEU:HD22	6	0.44
(1,1475)	1:66:A:LEU:HD22	1:109:A:LEU:HD23	7	0.44
(1,1475)	1:66:A:LEU:HD23	1:109:A:LEU:HD21	12	0.44
(1,1475)	1:66:A:LEU:HD22	1:109:A:LEU:HD23	16	0.44
(1,1475)	1:66:A:LEU:HD21	1:109:A:LEU:HD22	18	0.44
(1,1447)	1:69:A:GLU:HA	1:69:A:GLU:HG3	13	0.44
(1,1431)	1:70:A:PHE:HB2	1:70:A:PHE:HD1	2	0.44
(1,1431)	1:70:A:PHE:HB2	1:70:A:PHE:HD1	3	0.44
(1,1431)	1:70:A:PHE:HB2	1:70:A:PHE:HD1	4	0.44
(1,1431)	1:70:A:PHE:HB2	1:70:A:PHE:HD1	6	0.44
(1,1431)	1:70:A:PHE:HB2	1:70:A:PHE:HD1	7	0.44
(1,1431)	1:70:A:PHE:HB2	1:70:A:PHE:HD1	8	0.44
(1,1431)	1:70:A:PHE:HB2	1:70:A:PHE:HD1	9	0.44
(1,1431)	1:70:A:PHE:HB2	1:70:A:PHE:HD1	17	0.44
(1,1431)	1:70:A:PHE:HB2	1:70:A:PHE:HD1	19	0.44
(1,1431)	1:70:A:PHE:HB2	1:70:A:PHE:HD1	21	0.44
(1,1431)	1:70:A:PHE:HB2	1:70:A:PHE:HD1	25	0.44
(1,1422)	1:71:A:LEU:HD21	1:74:A:CYS:H	5	0.44
(1,1422)	1:71:A:LEU:HD23	1:74:A:CYS:H	8	0.44
(1,1422)	1:71:A:LEU:HD23	1:74:A:CYS:H	16	0.44
(1,1422)	1:71:A:LEU:HD23	1:74:A:CYS:H	21	0.44
(1,1421)	1:71:A:LEU:HD22	1:71:A:LEU:H	18	0.44
(1,1416)	1:71:A:LEU:HD13	1:71:A:LEU:H	24	0.44
(1,1385)	1:73:A:LEU:HB2	1:74:A:CYS:H	1	0.44
(1,1341)	1:76:A:MET:HB3	1:73:A:LEU:HA	11	0.44
(1,1337)	1:76:A:MET:HA	1:76:A:MET:HG3	7	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1337)	1:76:A:MET:HA	1:76:A:MET:HG3	25	0.44
(1,1326)	1:77:A:GLN:HG2	1:77:A:GLN:HA	25	0.44
(1,1303)	1:137:A:HIS:HE1	1:136:A:ALA:HB3	5	0.44
(1,1303)	1:137:A:HIS:HE1	1:136:A:ALA:HB1	16	0.44
(1,1303)	1:137:A:HIS:HE1	1:136:A:ALA:HB2	25	0.44
(1,1248)	1:85:A:VAL:HA	1:71:A:LEU:HD13	3	0.44
(1,1231)	1:67:A:PHE:HA	1:67:A:PHE:HD1	23	0.44
(1,1183)	1:90:A:ASN:HB2	1:87:A:PHE:HD1	10	0.44
(1,1147)	1:94:A:ARG:HG2	1:94:A:ARG:HA	21	0.44
(1,1139)	1:134:A:LEU:HD22	1:95:A:ALA:HB2	6	0.44
(1,1122)	1:96:A:HIS:HA	1:139:A:ALA:HB3	14	0.44
(1,1098)	1:100:A:LEU:HD21	1:92:A:GLN:HA	13	0.44
(1,1089)	1:105:A:PHE:HZ	1:100:A:LEU:HD22	12	0.44
(1,1076)	1:101:A:ALA:HB1	1:98:A:LEU:HD23	17	0.44
(1,1070)	1:101:A:ALA:HB3	1:102:A:SER:H	15	0.44
(1,1059)	1:103:A:ALA:HB1	1:104:A:GLU:HA	3	0.44
(1,1059)	1:103:A:ALA:HB3	1:104:A:GLU:HA	15	0.44
(1,1059)	1:103:A:ALA:HB1	1:104:A:GLU:HA	16	0.44
(1,1059)	1:103:A:ALA:HB2	1:104:A:GLU:HA	18	0.44
(1,1047)	1:104:A:GLU:HG2	1:105:A:PHE:H	15	0.44
(1,1047)	1:104:A:GLU:HG2	1:105:A:PHE:H	25	0.44
(1,996)	1:108:A:ILE:HG23	1:112:A:VAL:HG13	11	0.44
(1,996)	1:108:A:ILE:HG23	1:112:A:VAL:HG13	19	0.44
(1,989)	1:108:A:ILE:HG21	1:105:A:PHE:HA	1	0.44
(1,989)	1:108:A:ILE:HG22	1:105:A:PHE:HA	15	0.44
(1,989)	1:108:A:ILE:HG21	1:105:A:PHE:HA	22	0.44
(1,888)	1:116:A:ALA:HB3	1:123:A:LEU:H	9	0.44
(1,888)	1:116:A:ALA:HB2	1:123:A:LEU:H	12	0.44
(1,888)	1:116:A:ALA:HB1	1:123:A:LEU:H	15	0.44
(1,888)	1:116:A:ALA:HB3	1:123:A:LEU:H	18	0.44
(1,886)	1:116:A:ALA:HA	1:123:A:LEU:HD13	10	0.44
(1,835)	1:120:A:PRO:HB3	1:120:A:PRO:HD2	22	0.44
(1,790)	1:124:A:TYR:HD1	1:124:A:TYR:HA	6	0.44
(1,766)	1:126:A:TYR:HE1	1:115:A:ARG:HB2	7	0.44
(1,743)	1:127:A:ILE:HG21	1:124:A:TYR:HA	16	0.44
(1,705)	1:130:A:LEU:HD11	1:109:A:LEU:HD12	22	0.44
(1,705)	1:130:A:LEU:HD11	1:109:A:LEU:HD12	23	0.44
(1,670)	1:133:A:VAL:HG21	1:105:A:PHE:HE1	3	0.44
(1,670)	1:133:A:VAL:HG21	1:105:A:PHE:HE1	8	0.44
(1,670)	1:133:A:VAL:HG23	1:105:A:PHE:HE1	17	0.44
(1,552)	2:35:B:PHE:H	2:33:B:GLN:HA	22	0.44
(1,502)	1:81:A:HIS:H	1:82:A:PRO:HB3	21	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,500)	1:85:A:VAL:H	1:83:A:GLU:H	3	0.44
(1,490)	1:91:A:ARG:H	1:94:A:ARG:H	1	0.44
(1,490)	1:91:A:ARG:H	1:94:A:ARG:H	15	0.44
(1,483)	1:93:A:GLN:HG2	1:94:A:ARG:H	9	0.44
(1,465)	1:106:A:CYS:H	1:103:A:ALA:HB1	6	0.44
(1,455)	1:112:A:VAL:H	1:113:A:LEU:HB3	25	0.44
(1,451)	1:114:A:SER:H	1:117:A:ARG:HB2	20	0.44
(1,451)	1:114:A:SER:H	1:117:A:ARG:HB2	21	0.44
(1,444)	1:73:A:LEU:HD12	1:117:A:ARG:H	7	0.44
(1,444)	1:73:A:LEU:HD13	1:117:A:ARG:H	10	0.44
(1,444)	1:73:A:LEU:HD13	1:117:A:ARG:H	19	0.44
(1,444)	1:73:A:LEU:HD13	1:117:A:ARG:H	20	0.44
(1,421)	1:128:A:ASN:H	1:70:A:PHE:HZ	25	0.44
(1,419)	1:129:A:GLU:H	1:126:A:TYR:H	13	0.44
(1,399)	1:135:A:LYS:H	1:133:A:VAL:HA	4	0.44
(1,399)	1:135:A:LYS:H	1:133:A:VAL:HA	13	0.44
(1,399)	1:135:A:LYS:H	1:133:A:VAL:HA	25	0.44
(1,398)	1:135:A:LYS:HG2	1:136:A:ALA:H	4	0.44
(1,380)	2:27:B:SER:HA	2:30:B:GLU:HB3	23	0.44
(1,367)	2:26:B:ASP:HB3	2:31:B:LEU:H	11	0.44
(1,342)	2:31:B:LEU:HD12	1:124:A:TYR:HB3	14	0.44
(1,325)	2:33:B:GLN:HG2	2:31:B:LEU:HB2	19	0.44
(1,290)	2:39:B:TRP:HH2	2:36:B:THR:HB	13	0.44
(1,289)	2:39:B:TRP:HZ3	2:36:B:THR:HB	6	0.44
(1,289)	2:39:B:TRP:HZ3	2:36:B:THR:HB	12	0.44
(1,289)	2:39:B:TRP:HZ3	2:36:B:THR:HB	17	0.44
(1,281)	2:31:B:LEU:HD22	1:128:A:ASN:H	21	0.44
(1,240)	1:104:A:GLU:HB3	1:105:A:PHE:HA	9	0.44
(1,240)	2:33:B:GLN:HB2	2:34:B:TYR:HA	18	0.44
(1,232)	1:66:A:LEU:HD13	1:62:A:GLU:HA	19	0.44
(1,230)	1:66:A:LEU:HA	1:113:A:LEU:HD23	11	0.44
(1,229)	1:105:A:PHE:HE2	1:67:A:PHE:HB2	14	0.44
(1,225)	1:129:A:GLU:HG2	1:125:A:VAL:HG11	16	0.44
(1,219)	1:70:A:PHE:HD1	1:73:A:LEU:HB3	1	0.44
(1,219)	1:70:A:PHE:HD1	1:73:A:LEU:HB3	19	0.44
(1,203)	1:71:A:LEU:HD13	1:68:A:GLU:H	7	0.44
(1,201)	1:72:A:GLU:HG3	1:72:A:GLU:HB2	24	0.44
(1,195)	1:73:A:LEU:HD23	1:70:A:PHE:HA	1	0.44
(1,195)	1:73:A:LEU:HD21	1:70:A:PHE:HA	9	0.44
(1,194)	1:73:A:LEU:HD21	1:70:A:PHE:HD1	6	0.44
(1,194)	1:73:A:LEU:HD21	1:70:A:PHE:HD1	8	0.44
(1,194)	1:73:A:LEU:HD23	1:70:A:PHE:HD1	12	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,194)	1:73:A:LEU:HD21	1:70:A:PHE:HD1	20	0.44
(1,194)	1:73:A:LEU:HD22	1:70:A:PHE:HD1	24	0.44
(1,191)	1:84:A:VAL:HG12	1:74:A:CYS:HB2	6	0.44
(1,191)	1:84:A:VAL:HG13	1:74:A:CYS:HB2	9	0.44
(1,180)	1:82:A:PRO:HA	1:82:A:PRO:HG2	2	0.44
(1,180)	1:82:A:PRO:HA	1:82:A:PRO:HG2	4	0.44
(1,180)	1:82:A:PRO:HA	1:82:A:PRO:HG2	5	0.44
(1,180)	1:82:A:PRO:HA	1:82:A:PRO:HG2	6	0.44
(1,180)	1:82:A:PRO:HA	1:82:A:PRO:HG2	8	0.44
(1,180)	1:82:A:PRO:HA	1:82:A:PRO:HG2	10	0.44
(1,180)	1:82:A:PRO:HA	1:82:A:PRO:HG2	12	0.44
(1,180)	1:82:A:PRO:HA	1:82:A:PRO:HG2	13	0.44
(1,180)	1:82:A:PRO:HA	1:82:A:PRO:HG2	14	0.44
(1,180)	1:82:A:PRO:HA	1:82:A:PRO:HG2	16	0.44
(1,180)	1:82:A:PRO:HA	1:82:A:PRO:HG2	19	0.44
(1,180)	1:82:A:PRO:HA	1:82:A:PRO:HG2	23	0.44
(1,180)	1:82:A:PRO:HA	1:82:A:PRO:HG2	25	0.44
(1,171)	1:84:A:VAL:HG13	1:85:A:VAL:H	4	0.44
(1,171)	1:84:A:VAL:HG11	1:85:A:VAL:H	8	0.44
(1,171)	1:84:A:VAL:HG11	1:85:A:VAL:H	15	0.44
(1,171)	1:84:A:VAL:HG13	1:85:A:VAL:H	25	0.44
(1,170)	1:85:A:VAL:HG11	1:75:A:LYS:H	10	0.44
(1,141)	1:93:A:GLN:HG2	1:89:A:TYR:HD1	23	0.44
(1,87)	1:112:A:VAL:HG12	1:130:A:LEU:H	25	0.44
(1,48)	1:126:A:TYR:HE1	1:125:A:VAL:HG11	3	0.44
(1,48)	1:126:A:TYR:HE1	1:125:A:VAL:HG11	11	0.44
(1,6)	1:130:A:LEU:HD23	1:70:A:PHE:HE2	2	0.44
(1,2271)	2:25:B:GLU:H	2:25:B:GLU:HG2	7	0.43
(1,2136)	1:69:A:GLU:H	1:70:A:PHE:HB2	15	0.43
(1,2063)	1:85:A:VAL:H	1:71:A:LEU:HD21	2	0.43
(1,2063)	1:85:A:VAL:H	1:71:A:LEU:HD21	8	0.43
(1,2063)	1:85:A:VAL:H	1:71:A:LEU:HD22	10	0.43
(1,2060)	1:86:A:PRO:HB3	1:87:A:PHE:H	3	0.43
(1,2060)	1:86:A:PRO:HB3	1:87:A:PHE:H	12	0.43
(1,2060)	1:86:A:PRO:HB3	1:87:A:PHE:H	16	0.43
(1,2060)	1:86:A:PRO:HB3	1:87:A:PHE:H	25	0.43
(1,2019)	1:93:A:GLN:HE22	1:93:A:GLN:HB3	5	0.43
(1,1996)	1:97:A:SER:H	1:139:A:ALA:HB2	23	0.43
(1,1986)	1:99:A:PHE:H	1:98:A:LEU:HD22	7	0.43
(1,1983)	1:99:A:PHE:H	1:138:A:SER:HB2	2	0.43
(1,1983)	1:99:A:PHE:H	1:138:A:SER:HB2	14	0.43
(1,1971)	1:100:A:LEU:HD23	1:101:A:ALA:H	4	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1968)	1:101:A:ALA:H	1:63:A:ASN:HD22	15	0.43
(1,1924)	1:108:A:ILE:HG21	1:108:A:ILE:H	3	0.43
(1,1924)	1:108:A:ILE:HG21	1:108:A:ILE:H	15	0.43
(1,1924)	1:108:A:ILE:HG21	1:108:A:ILE:H	16	0.43
(1,1924)	1:108:A:ILE:HG21	1:108:A:ILE:H	18	0.43
(1,1924)	1:108:A:ILE:HG23	1:108:A:ILE:H	22	0.43
(1,1888)	1:115:A:ARG:H	1:115:A:ARG:HG3	15	0.43
(1,1830)	1:128:A:ASN:H	1:128:A:ASN:HB3	4	0.43
(1,1798)	1:136:A:ALA:H	1:135:A:LYS:HD3	10	0.43
(1,1745)	2:29:B:SER:HB3	2:30:B:GLU:H	6	0.43
(1,1727)	2:31:B:LEU:HD13	2:31:B:LEU:H	10	0.43
(1,1670)	2:37:B:ALA:HB1	2:36:B:THR:HA	12	0.43
(1,1635)	2:39:B:TRP:HA	2:38:B:ARG:HD2	16	0.43
(1,1633)	2:38:B:ARG:HD2	2:38:B:ARG:HB2	1	0.43
(1,1633)	2:38:B:ARG:HD2	2:38:B:ARG:HB2	24	0.43
(1,1622)	2:39:B:TRP:HE3	2:39:B:TRP:HB2	11	0.43
(1,1481)	1:66:A:LEU:HD21	1:69:A:GLU:H	15	0.43
(1,1481)	1:66:A:LEU:HD22	1:69:A:GLU:H	25	0.43
(1,1480)	1:66:A:LEU:HD22	1:63:A:ASN:HA	15	0.43
(1,1480)	1:66:A:LEU:HD22	1:63:A:ASN:HA	16	0.43
(1,1480)	1:66:A:LEU:HD21	1:63:A:ASN:HA	18	0.43
(1,1480)	1:66:A:LEU:HD23	1:63:A:ASN:HA	19	0.43
(1,1477)	1:66:A:LEU:HD21	1:113:A:LEU:HB3	3	0.43
(1,1477)	1:66:A:LEU:HD23	1:113:A:LEU:HB3	13	0.43
(1,1477)	1:66:A:LEU:HD22	1:113:A:LEU:HB3	15	0.43
(1,1475)	1:66:A:LEU:HD21	1:109:A:LEU:HD23	3	0.43
(1,1475)	1:66:A:LEU:HD22	1:109:A:LEU:HD22	5	0.43
(1,1475)	1:66:A:LEU:HD21	1:109:A:LEU:HD21	22	0.43
(1,1422)	1:71:A:LEU:HD23	1:74:A:CYS:H	7	0.43
(1,1422)	1:71:A:LEU:HD23	1:74:A:CYS:H	11	0.43
(1,1422)	1:71:A:LEU:HD23	1:74:A:CYS:H	12	0.43
(1,1422)	1:71:A:LEU:HD23	1:74:A:CYS:H	13	0.43
(1,1422)	1:71:A:LEU:HD23	1:74:A:CYS:H	14	0.43
(1,1422)	1:71:A:LEU:HD21	1:74:A:CYS:H	15	0.43
(1,1422)	1:71:A:LEU:HD21	1:74:A:CYS:H	24	0.43
(1,1419)	1:71:A:LEU:HD12	1:89:A:TYR:H	22	0.43
(1,1416)	1:71:A:LEU:HD11	1:71:A:LEU:H	3	0.43
(1,1416)	1:71:A:LEU:HD13	1:71:A:LEU:H	11	0.43
(1,1416)	1:71:A:LEU:HD11	1:71:A:LEU:H	16	0.43
(1,1416)	1:71:A:LEU:HD11	1:71:A:LEU:H	20	0.43
(1,1395)	1:116:A:ALA:HB3	1:73:A:LEU:HD23	19	0.43
(1,1385)	1:73:A:LEU:HB2	1:74:A:CYS:H	13	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1385)	1:73:A:LEU:HB2	1:74:A:CYS:H	15	0.43
(1,1385)	1:73:A:LEU:HB2	1:74:A:CYS:H	24	0.43
(1,1357)	1:75:A:LYS:HA	1:75:A:LYS:HG3	17	0.43
(1,1341)	1:76:A:MET:HB3	1:73:A:LEU:HA	19	0.43
(1,1331)	1:77:A:GLN:HG2	1:73:A:LEU:HD13	6	0.43
(1,1326)	1:77:A:GLN:HG2	1:77:A:GLN:HA	18	0.43
(1,1303)	1:137:A:HIS:HE1	1:136:A:ALA:HB1	4	0.43
(1,1282)	1:84:A:VAL:HG21	1:85:A:VAL:H	16	0.43
(1,1248)	1:85:A:VAL:HA	1:71:A:LEU:HD11	4	0.43
(1,1248)	1:85:A:VAL:HA	1:71:A:LEU:HD13	16	0.43
(1,1248)	1:85:A:VAL:HA	1:71:A:LEU:HD12	21	0.43
(1,1231)	1:67:A:PHE:HA	1:67:A:PHE:HD1	7	0.43
(1,1231)	1:67:A:PHE:HA	1:67:A:PHE:HD1	9	0.43
(1,1231)	1:67:A:PHE:HA	1:67:A:PHE:HD1	15	0.43
(1,1183)	1:90:A:ASN:HB2	1:87:A:PHE:HD1	14	0.43
(1,1094)	1:100:A:LEU:HD23	1:138:A:SER:HB2	16	0.43
(1,1076)	1:101:A:ALA:HB1	1:98:A:LEU:HD22	9	0.43
(1,1076)	1:101:A:ALA:HB1	1:98:A:LEU:HD23	12	0.43
(1,1076)	1:101:A:ALA:HB1	1:98:A:LEU:HD23	16	0.43
(1,1059)	1:103:A:ALA:HB3	1:104:A:GLU:HA	2	0.43
(1,1059)	1:103:A:ALA:HB1	1:104:A:GLU:HA	13	0.43
(1,1059)	1:103:A:ALA:HB3	1:104:A:GLU:HA	21	0.43
(1,1047)	1:104:A:GLU:HG2	1:105:A:PHE:H	11	0.43
(1,989)	1:108:A:ILE:HG22	1:105:A:PHE:HA	5	0.43
(1,989)	1:108:A:ILE:HG21	1:105:A:PHE:HA	9	0.43
(1,989)	1:108:A:ILE:HG23	1:105:A:PHE:HA	12	0.43
(1,989)	1:108:A:ILE:HG23	1:105:A:PHE:HA	17	0.43
(1,989)	1:108:A:ILE:HG21	1:105:A:PHE:HA	25	0.43
(1,960)	1:67:A:PHE:HA	1:109:A:LEU:HD11	15	0.43
(1,917)	1:113:A:LEU:HB2	1:113:A:LEU:HD21	1	0.43
(1,917)	1:113:A:LEU:HB2	1:113:A:LEU:HD23	7	0.43
(1,888)	1:116:A:ALA:HB2	1:123:A:LEU:H	3	0.43
(1,888)	1:116:A:ALA:HB1	1:123:A:LEU:H	8	0.43
(1,888)	1:116:A:ALA:HB2	1:123:A:LEU:H	13	0.43
(1,888)	1:116:A:ALA:HB3	1:123:A:LEU:H	24	0.43
(1,886)	1:116:A:ALA:HA	1:123:A:LEU:HD13	1	0.43
(1,857)	1:119:A:ARG:HB2	1:119:A:ARG:HG3	19	0.43
(1,766)	1:126:A:TYR:HE1	1:115:A:ARG:HB2	12	0.43
(1,766)	1:126:A:TYR:HE1	1:115:A:ARG:HB2	19	0.43
(1,670)	1:133:A:VAL:HG21	1:105:A:PHE:HE1	20	0.43
(1,670)	1:133:A:VAL:HG23	1:105:A:PHE:HE1	21	0.43
(1,670)	1:133:A:VAL:HG23	1:105:A:PHE:HE1	22	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,585)	1:139:A:ALA:HB3	1:140:A:LYS:H	20	0.43
(1,575)	1:143:A:LEU:HA	1:143:A:LEU:HD23	23	0.43
(1,541)	1:61:A:LEU:HB3	1:62:A:GLU:H	5	0.43
(1,541)	1:61:A:LEU:HB3	1:62:A:GLU:H	10	0.43
(1,541)	1:61:A:LEU:HB3	1:62:A:GLU:H	25	0.43
(1,515)	1:73:A:LEU:HG	1:76:A:MET:H	10	0.43
(1,494)	1:90:A:ASN:H	1:88:A:LEU:HB2	2	0.43
(1,494)	1:90:A:ASN:H	1:88:A:LEU:HB2	11	0.43
(1,494)	1:90:A:ASN:H	1:88:A:LEU:HB2	18	0.43
(1,490)	1:91:A:ARG:H	1:94:A:ARG:H	3	0.43
(1,478)	1:95:A:ALA:H	1:91:A:ARG:HD2	23	0.43
(1,476)	1:96:A:HIS:H	1:95:A:ALA:H	11	0.43
(1,457)	1:111:A:ARG:H	1:109:A:LEU:HB3	8	0.43
(1,457)	1:111:A:ARG:H	1:109:A:LEU:HB3	10	0.43
(1,455)	1:112:A:VAL:H	1:113:A:LEU:HB3	24	0.43
(1,445)	1:116:A:ALA:H	1:112:A:VAL:HA	2	0.43
(1,444)	1:73:A:LEU:HD11	1:117:A:ARG:H	15	0.43
(1,434)	1:74:A:CYS:H	1:123:A:LEU:HD13	7	0.43
(1,434)	1:74:A:CYS:H	1:123:A:LEU:HD12	8	0.43
(1,421)	1:72:A:GLU:H	1:70:A:PHE:HD1	17	0.43
(1,421)	1:128:A:ASN:H	1:70:A:PHE:HZ	22	0.43
(1,419)	1:129:A:GLU:H	1:126:A:TYR:H	21	0.43
(1,399)	1:135:A:LYS:H	1:133:A:VAL:HA	2	0.43
(1,399)	1:135:A:LYS:H	1:133:A:VAL:HA	5	0.43
(1,399)	1:135:A:LYS:H	1:133:A:VAL:HA	11	0.43
(1,399)	1:135:A:LYS:H	1:133:A:VAL:HA	19	0.43
(1,399)	1:135:A:LYS:H	1:133:A:VAL:HA	23	0.43
(1,398)	1:135:A:LYS:HG2	1:136:A:ALA:H	21	0.43
(1,380)	2:27:B:SER:HA	2:30:B:GLU:HB3	6	0.43
(1,379)	2:31:B:LEU:HB2	2:28:B:ASP:HB2	23	0.43
(1,366)	1:100:A:LEU:HD11	1:138:A:SER:HB3	23	0.43
(1,343)	2:31:B:LEU:HB2	1:87:A:PHE:HE2	12	0.43
(1,338)	2:31:B:LEU:HD23	2:32:B:GLU:HG3	14	0.43
(1,321)	2:34:B:TYR:HD1	1:83:A:GLU:HB3	14	0.43
(1,312)	2:35:B:PHE:HE1	1:124:A:TYR:HA	10	0.43
(1,281)	2:31:B:LEU:HD21	1:128:A:ASN:H	23	0.43
(1,253)	1:57:A:LYS:HE2	1:54:A:MET:HG3	11	0.43
(1,244)	1:61:A:LEU:HG	1:61:A:LEU:HA	14	0.43
(1,243)	1:62:A:GLU:HG3	1:61:A:LEU:HD23	15	0.43
(1,240)	1:104:A:GLU:HB3	1:105:A:PHE:HA	5	0.43
(1,240)	1:104:A:GLU:HB3	1:105:A:PHE:HA	19	0.43
(1,240)	2:33:B:GLN:HB2	2:34:B:TYR:HA	22	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,225)	1:129:A:GLU:HG2	1:125:A:VAL:HG12	23	0.43
(1,220)	1:70:A:PHE:HE2	1:113:A:LEU:HB2	7	0.43
(1,220)	1:70:A:PHE:HE2	1:113:A:LEU:HB2	14	0.43
(1,220)	1:70:A:PHE:HE2	1:113:A:LEU:HB2	24	0.43
(1,219)	1:70:A:PHE:HD1	1:73:A:LEU:HB3	4	0.43
(1,219)	1:70:A:PHE:HD1	1:73:A:LEU:HB3	20	0.43
(1,199)	1:72:A:GLU:HG2	1:71:A:LEU:HB3	1	0.43
(1,195)	1:73:A:LEU:HD23	1:70:A:PHE:HA	11	0.43
(1,195)	1:73:A:LEU:HD22	1:70:A:PHE:HA	21	0.43
(1,194)	1:73:A:LEU:HD22	1:70:A:PHE:HD1	3	0.43
(1,194)	1:73:A:LEU:HD23	1:70:A:PHE:HD1	5	0.43
(1,194)	1:73:A:LEU:HD22	1:70:A:PHE:HD1	15	0.43
(1,191)	1:84:A:VAL:HG11	1:74:A:CYS:HB2	5	0.43
(1,191)	1:85:A:VAL:HG13	1:74:A:CYS:HB2	18	0.43
(1,189)	1:85:A:VAL:HG11	1:75:A:LYS:HA	17	0.43
(1,180)	1:82:A:PRO:HA	1:82:A:PRO:HG2	1	0.43
(1,180)	1:82:A:PRO:HA	1:82:A:PRO:HG2	3	0.43
(1,180)	1:82:A:PRO:HA	1:82:A:PRO:HG2	7	0.43
(1,180)	1:82:A:PRO:HA	1:82:A:PRO:HG2	9	0.43
(1,180)	1:82:A:PRO:HA	1:82:A:PRO:HG2	17	0.43
(1,180)	1:82:A:PRO:HA	1:82:A:PRO:HG2	18	0.43
(1,180)	1:82:A:PRO:HA	1:82:A:PRO:HG2	20	0.43
(1,180)	1:82:A:PRO:HA	1:82:A:PRO:HG2	21	0.43
(1,180)	1:82:A:PRO:HA	1:82:A:PRO:HG2	22	0.43
(1,180)	1:82:A:PRO:HA	1:82:A:PRO:HG2	24	0.43
(1,172)	1:85:A:VAL:HG12	1:74:A:CYS:HB3	2	0.43
(1,171)	1:84:A:VAL:HG13	1:85:A:VAL:H	1	0.43
(1,171)	1:84:A:VAL:HG13	1:85:A:VAL:H	5	0.43
(1,171)	1:84:A:VAL:HG12	1:85:A:VAL:H	12	0.43
(1,171)	1:84:A:VAL:HG12	1:85:A:VAL:H	19	0.43
(1,155)	1:88:A:LEU:HD13	1:74:A:CYS:HB2	4	0.43
(1,147)	1:137:A:HIS:HB3	1:138:A:SER:H	6	0.43
(1,122)	1:95:A:ALA:HB2	1:91:A:ARG:HD3	10	0.43
(1,122)	1:95:A:ALA:HB3	1:91:A:ARG:HD3	15	0.43
(1,81)	1:116:A:ALA:HB1	1:70:A:PHE:HZ	7	0.43
(1,67)	1:116:A:ALA:HB2	1:120:A:PRO:HA	3	0.43
(1,56)	1:124:A:TYR:HE2	2:35:B:PHE:HB3	2	0.43
(1,56)	1:124:A:TYR:HE2	2:35:B:PHE:HB3	21	0.43
(1,52)	1:125:A:VAL:HG13	1:128:A:ASN:HB2	3	0.43
(1,52)	1:125:A:VAL:HG11	1:128:A:ASN:HB2	20	0.43
(1,48)	1:126:A:TYR:HE1	1:125:A:VAL:HG12	9	0.43
(1,42)	1:126:A:TYR:HD1	1:125:A:VAL:HB	23	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,30)	1:129:A:GLU:HG3	1:130:A:LEU:H	24	0.43
(1,13)	1:133:A:VAL:HG12	1:108:A:ILE:HB	10	0.43
(1,6)	1:130:A:LEU:HD21	1:70:A:PHE:HE2	10	0.43
(1,2265)	2:26:B:ASP:HB3	2:26:B:ASP:H	9	0.42
(1,2265)	2:26:B:ASP:HB3	2:26:B:ASP:H	17	0.42
(1,2173)	1:63:A:ASN:H	1:109:A:LEU:HD13	9	0.42
(1,2106)	1:76:A:MET:HB3	1:77:A:GLN:H	15	0.42
(1,2063)	1:85:A:VAL:H	1:71:A:LEU:HD21	12	0.42
(1,2063)	1:85:A:VAL:H	1:71:A:LEU:HD21	13	0.42
(1,2063)	1:85:A:VAL:H	1:71:A:LEU:HD23	17	0.42
(1,2060)	1:86:A:PRO:HB3	1:87:A:PHE:H	11	0.42
(1,2051)	1:89:A:TYR:H	1:90:A:ASN:HB3	8	0.42
(1,2051)	1:89:A:TYR:H	1:90:A:ASN:HB3	17	0.42
(1,2037)	1:90:A:ASN:HD21	1:94:A:ARG:HD3	5	0.42
(1,2019)	1:93:A:GLN:HE22	1:93:A:GLN:HB3	7	0.42
(1,2019)	1:93:A:GLN:HE22	1:93:A:GLN:HB3	9	0.42
(1,2019)	1:93:A:GLN:HE22	1:93:A:GLN:HB3	10	0.42
(1,2019)	1:93:A:GLN:HE22	1:93:A:GLN:HB3	16	0.42
(1,2019)	1:93:A:GLN:HE22	1:93:A:GLN:HB3	25	0.42
(1,2013)	1:94:A:ARG:H	1:95:A:ALA:HB1	3	0.42
(1,1986)	1:99:A:PHE:H	1:98:A:LEU:HD21	3	0.42
(1,1971)	1:100:A:LEU:HD23	1:101:A:ALA:H	5	0.42
(1,1971)	1:100:A:LEU:HD22	1:101:A:ALA:H	22	0.42
(1,1924)	1:108:A:ILE:HG21	1:108:A:ILE:H	4	0.42
(1,1924)	1:108:A:ILE:HG21	1:108:A:ILE:H	10	0.42
(1,1924)	1:108:A:ILE:HG21	1:108:A:ILE:H	11	0.42
(1,1924)	1:108:A:ILE:HG22	1:108:A:ILE:H	12	0.42
(1,1924)	1:108:A:ILE:HG22	1:108:A:ILE:H	17	0.42
(1,1924)	1:108:A:ILE:HG23	1:108:A:ILE:H	20	0.42
(1,1924)	1:108:A:ILE:HG22	1:108:A:ILE:H	21	0.42
(1,1874)	1:118:A:SER:H	1:117:A:ARG:HG2	6	0.42
(1,1851)	1:124:A:TYR:HB3	1:124:A:TYR:H	2	0.42
(1,1851)	1:124:A:TYR:HB3	1:124:A:TYR:H	10	0.42
(1,1830)	1:128:A:ASN:H	1:128:A:ASN:HB3	7	0.42
(1,1830)	1:128:A:ASN:H	1:128:A:ASN:HB3	9	0.42
(1,1830)	1:128:A:ASN:H	1:128:A:ASN:HB3	10	0.42
(1,1830)	1:128:A:ASN:H	1:128:A:ASN:HB3	12	0.42
(1,1830)	1:128:A:ASN:H	1:128:A:ASN:HB3	15	0.42
(1,1830)	1:128:A:ASN:H	1:128:A:ASN:HB3	17	0.42
(1,1830)	1:128:A:ASN:H	1:128:A:ASN:HB3	18	0.42
(1,1830)	1:128:A:ASN:H	1:128:A:ASN:HB3	20	0.42
(1,1830)	1:128:A:ASN:H	1:128:A:ASN:HB3	22	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1830)	1:128:A:ASN:H	1:128:A:ASN:HB3	23	0.42
(1,1788)	1:139:A:ALA:H	1:135:A:LYS:HD3	1	0.42
(1,1788)	1:139:A:ALA:H	1:135:A:LYS:HD2	14	0.42
(1,1788)	1:139:A:ALA:H	1:135:A:LYS:HD3	22	0.42
(1,1775)	1:143:A:LEU:H	1:141:A:LYS:HG2	22	0.42
(1,1754)	2:30:B:GLU:HG2	2:31:B:LEU:H	4	0.42
(1,1754)	2:30:B:GLU:HG2	2:31:B:LEU:H	24	0.42
(1,1745)	2:29:B:SER:HB3	2:30:B:GLU:H	14	0.42
(1,1670)	2:37:B:ALA:HB3	2:36:B:THR:HA	17	0.42
(1,1635)	2:39:B:TRP:HA	2:38:B:ARG:HD2	10	0.42
(1,1633)	2:38:B:ARG:HD2	2:38:B:ARG:HB2	16	0.42
(1,1513)	1:62:A:GLU:HA	1:62:A:GLU:HG3	2	0.42
(1,1489)	1:65:A:LYS:HG2	1:66:A:LEU:H	1	0.42
(1,1481)	1:66:A:LEU:HD21	1:69:A:GLU:H	6	0.42
(1,1481)	1:66:A:LEU:HD21	1:69:A:GLU:H	24	0.42
(1,1480)	1:66:A:LEU:HD22	1:63:A:ASN:HA	5	0.42
(1,1475)	1:66:A:LEU:HD23	1:109:A:LEU:HD22	17	0.42
(1,1475)	1:66:A:LEU:HD22	1:109:A:LEU:HD21	24	0.42
(1,1422)	1:71:A:LEU:HD22	1:74:A:CYS:H	6	0.42
(1,1422)	1:71:A:LEU:HD23	1:74:A:CYS:H	9	0.42
(1,1422)	1:71:A:LEU:HD22	1:74:A:CYS:H	18	0.42
(1,1422)	1:71:A:LEU:HD22	1:74:A:CYS:H	20	0.42
(1,1422)	1:71:A:LEU:HD22	1:74:A:CYS:H	22	0.42
(1,1422)	1:71:A:LEU:HD21	1:74:A:CYS:H	25	0.42
(1,1419)	1:71:A:LEU:HD13	1:89:A:TYR:H	2	0.42
(1,1419)	1:71:A:LEU:HD11	1:89:A:TYR:H	5	0.42
(1,1416)	1:71:A:LEU:HD11	1:71:A:LEU:H	1	0.42
(1,1416)	1:71:A:LEU:HD11	1:71:A:LEU:H	18	0.42
(1,1385)	1:73:A:LEU:HB2	1:74:A:CYS:H	12	0.42
(1,1385)	1:73:A:LEU:HB2	1:74:A:CYS:H	16	0.42
(1,1385)	1:73:A:LEU:HB2	1:74:A:CYS:H	19	0.42
(1,1337)	1:76:A:MET:HA	1:76:A:MET:HG3	2	0.42
(1,1337)	1:76:A:MET:HA	1:76:A:MET:HG3	11	0.42
(1,1336)	1:76:A:MET:HA	1:76:A:MET:HB2	11	0.42
(1,1336)	1:76:A:MET:HA	1:76:A:MET:HB2	19	0.42
(1,1331)	1:77:A:GLN:HG2	1:73:A:LEU:HD11	5	0.42
(1,1326)	1:77:A:GLN:HG2	1:77:A:GLN:HA	3	0.42
(1,1326)	1:77:A:GLN:HG2	1:77:A:GLN:HA	4	0.42
(1,1326)	1:77:A:GLN:HG2	1:77:A:GLN:HA	13	0.42
(1,1326)	1:77:A:GLN:HG2	1:77:A:GLN:HA	17	0.42
(1,1326)	1:77:A:GLN:HG2	1:77:A:GLN:HA	20	0.42
(1,1326)	1:77:A:GLN:HG2	1:77:A:GLN:HA	21	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1326)	1:77:A:GLN:HG2	1:77:A:GLN:HA	24	0.42
(1,1303)	1:137:A:HIS:HE1	1:136:A:ALA:HB2	1	0.42
(1,1280)	1:84:A:VAL:HG22	1:81:A:HIS:HB2	4	0.42
(1,1273)	1:85:A:VAL:HG13	1:75:A:LYS:HE2	25	0.42
(1,1248)	1:85:A:VAL:HA	1:71:A:LEU:HD11	5	0.42
(1,1248)	1:85:A:VAL:HA	1:71:A:LEU:HD13	20	0.42
(1,1248)	1:85:A:VAL:HA	1:71:A:LEU:HD12	22	0.42
(1,1248)	1:85:A:VAL:HA	1:71:A:LEU:HD12	24	0.42
(1,1231)	1:67:A:PHE:HA	1:67:A:PHE:HD1	11	0.42
(1,1175)	1:91:A:ARG:HG2	1:134:A:LEU:HB2	17	0.42
(1,1147)	1:94:A:ARG:HG2	1:94:A:ARG:HA	1	0.42
(1,1139)	1:134:A:LEU:HD23	1:95:A:ALA:HB3	18	0.42
(1,1122)	1:96:A:HIS:HA	1:139:A:ALA:HB1	10	0.42
(1,1094)	1:100:A:LEU:HD22	1:138:A:SER:HB2	20	0.42
(1,1088)	1:100:A:LEU:HD22	1:105:A:PHE:HD2	11	0.42
(1,1076)	1:101:A:ALA:HB2	1:98:A:LEU:HD21	10	0.42
(1,1076)	1:101:A:ALA:HB3	1:98:A:LEU:HD21	23	0.42
(1,1059)	1:103:A:ALA:HB1	1:104:A:GLU:HA	17	0.42
(1,1040)	1:62:A:GLU:HB3	1:59:A:TYR:HA	12	0.42
(1,996)	1:108:A:ILE:HG23	1:112:A:VAL:HG13	23	0.42
(1,989)	1:108:A:ILE:HG23	1:105:A:PHE:HA	7	0.42
(1,960)	1:67:A:PHE:HA	1:109:A:LEU:HD12	14	0.42
(1,917)	1:113:A:LEU:HB2	1:113:A:LEU:HD21	13	0.42
(1,888)	1:116:A:ALA:HB2	1:123:A:LEU:H	4	0.42
(1,888)	1:116:A:ALA:HB1	1:123:A:LEU:H	20	0.42
(1,743)	1:127:A:ILE:HG23	1:124:A:TYR:HA	3	0.42
(1,743)	1:127:A:ILE:HG22	1:124:A:TYR:HA	9	0.42
(1,705)	1:130:A:LEU:HD11	1:109:A:LEU:HD11	4	0.42
(1,705)	1:130:A:LEU:HD12	1:109:A:LEU:HD13	10	0.42
(1,705)	1:130:A:LEU:HD11	1:109:A:LEU:HD13	16	0.42
(1,670)	1:133:A:VAL:HG22	1:105:A:PHE:HE1	1	0.42
(1,607)	1:136:A:ALA:HB2	1:137:A:HIS:HA	23	0.42
(1,561)	2:27:B:SER:H	2:30:B:GLU:HB3	25	0.42
(1,538)	1:63:A:ASN:H	1:61:A:LEU:HA	9	0.42
(1,538)	1:63:A:ASN:H	1:61:A:LEU:HA	21	0.42
(1,521)	1:71:A:LEU:H	1:113:A:LEU:HD11	1	0.42
(1,520)	1:130:A:LEU:H	1:112:A:VAL:HG21	13	0.42
(1,500)	1:85:A:VAL:H	1:83:A:GLU:H	18	0.42
(1,494)	1:90:A:ASN:H	1:88:A:LEU:HB2	4	0.42
(1,494)	1:90:A:ASN:H	1:88:A:LEU:HB2	8	0.42
(1,494)	1:90:A:ASN:H	1:88:A:LEU:HB2	14	0.42
(1,494)	1:90:A:ASN:H	1:88:A:LEU:HB2	15	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,494)	1:90:A:ASN:H	1:88:A:LEU:HB2	22	0.42
(1,488)	1:92:A:GLN:HE22	1:64:A:GLU:HG3	7	0.42
(1,488)	1:92:A:GLN:HE22	1:64:A:GLU:HG3	23	0.42
(1,483)	1:93:A:GLN:HG2	1:94:A:ARG:H	1	0.42
(1,483)	1:93:A:GLN:HG2	1:94:A:ARG:H	11	0.42
(1,476)	1:96:A:HIS:H	1:95:A:ALA:H	6	0.42
(1,469)	1:102:A:SER:H	1:104:A:GLU:HB3	24	0.42
(1,465)	1:106:A:CYS:H	1:103:A:ALA:HB3	10	0.42
(1,457)	1:111:A:ARG:H	1:109:A:LEU:HB3	13	0.42
(1,457)	1:111:A:ARG:H	1:109:A:LEU:HB3	16	0.42
(1,457)	1:111:A:ARG:H	1:109:A:LEU:HB3	21	0.42
(1,454)	1:114:A:SER:H	1:112:A:VAL:HG23	16	0.42
(1,451)	1:114:A:SER:H	1:117:A:ARG:HB2	2	0.42
(1,445)	1:116:A:ALA:H	1:112:A:VAL:HA	16	0.42
(1,445)	1:116:A:ALA:H	1:112:A:VAL:HA	18	0.42
(1,445)	1:116:A:ALA:H	1:112:A:VAL:HA	21	0.42
(1,444)	1:73:A:LEU:HD12	1:117:A:ARG:H	17	0.42
(1,421)	1:72:A:GLU:H	1:70:A:PHE:HD1	4	0.42
(1,421)	1:128:A:ASN:H	1:70:A:PHE:HZ	13	0.42
(1,421)	1:128:A:ASN:H	1:70:A:PHE:HZ	18	0.42
(1,399)	1:135:A:LYS:H	1:133:A:VAL:HA	6	0.42
(1,398)	1:135:A:LYS:HG2	1:136:A:ALA:H	7	0.42
(1,398)	1:135:A:LYS:HG2	1:136:A:ALA:H	17	0.42
(1,387)	1:141:A:LYS:H	1:141:A:LYS:HG2	17	0.42
(1,387)	1:141:A:LYS:H	1:139:A:ALA:HB3	20	0.42
(1,387)	1:141:A:LYS:H	1:139:A:ALA:HB3	21	0.42
(1,379)	2:31:B:LEU:HB2	2:28:B:ASP:HB2	15	0.42
(1,375)	2:27:B:SER:HB3	2:28:B:ASP:HB3	11	0.42
(1,367)	2:26:B:ASP:HB3	2:31:B:LEU:H	6	0.42
(1,333)	1:127:A:ILE:HG12	1:130:A:LEU:HD22	9	0.42
(1,312)	2:35:B:PHE:HE1	1:124:A:TYR:HA	1	0.42
(1,312)	2:35:B:PHE:HE1	1:124:A:TYR:HA	7	0.42
(1,312)	2:35:B:PHE:HE1	1:124:A:TYR:HA	11	0.42
(1,312)	2:35:B:PHE:HE1	1:124:A:TYR:HA	20	0.42
(1,307)	2:39:B:TRP:HE3	2:36:B:THR:HG21	15	0.42
(1,232)	1:66:A:LEU:HD11	1:110:A:SER:HA	22	0.42
(1,219)	1:70:A:PHE:HD1	1:73:A:LEU:HB3	17	0.42
(1,201)	1:72:A:GLU:HG3	1:72:A:GLU:HB2	8	0.42
(1,201)	1:72:A:GLU:HG3	1:72:A:GLU:HB2	11	0.42
(1,199)	1:72:A:GLU:HG2	1:71:A:LEU:HB3	2	0.42
(1,199)	1:72:A:GLU:HG3	1:71:A:LEU:HB3	10	0.42
(1,199)	1:72:A:GLU:HG2	1:71:A:LEU:HB3	25	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,197)	1:73:A:LEU:HD22	1:123:A:LEU:HB2	12	0.42
(1,194)	1:73:A:LEU:HD21	1:70:A:PHE:HD1	13	0.42
(1,189)	1:85:A:VAL:HG13	1:75:A:LYS:HA	6	0.42
(1,180)	1:82:A:PRO:HA	1:82:A:PRO:HG2	11	0.42
(1,171)	1:84:A:VAL:HG12	1:85:A:VAL:H	2	0.42
(1,171)	1:84:A:VAL:HG11	1:85:A:VAL:H	3	0.42
(1,171)	1:84:A:VAL:HG12	1:85:A:VAL:H	7	0.42
(1,171)	1:84:A:VAL:HG12	1:85:A:VAL:H	11	0.42
(1,171)	1:84:A:VAL:HG12	1:85:A:VAL:H	13	0.42
(1,171)	1:84:A:VAL:HG13	1:85:A:VAL:H	14	0.42
(1,171)	1:84:A:VAL:HG11	1:85:A:VAL:H	18	0.42
(1,171)	1:84:A:VAL:HG11	1:85:A:VAL:H	22	0.42
(1,171)	1:84:A:VAL:HG12	1:85:A:VAL:H	23	0.42
(1,171)	1:84:A:VAL:HG12	1:85:A:VAL:H	24	0.42
(1,155)	1:88:A:LEU:HD22	1:131:A:CYS:HB3	1	0.42
(1,141)	1:93:A:GLN:HG2	1:89:A:TYR:HD1	5	0.42
(1,141)	1:93:A:GLN:HG2	1:89:A:TYR:HD1	18	0.42
(1,132)	1:92:A:GLN:HB3	1:89:A:TYR:HD1	7	0.42
(1,132)	1:67:A:PHE:HE1	1:92:A:GLN:HB3	17	0.42
(1,128)	1:93:A:GLN:HG2	1:94:A:ARG:H	20	0.42
(1,117)	1:100:A:LEU:HD21	1:92:A:GLN:HG2	5	0.42
(1,98)	1:105:A:PHE:HD1	1:100:A:LEU:HD22	18	0.42
(1,97)	1:105:A:PHE:HD1	1:100:A:LEU:HA	15	0.42
(1,67)	1:116:A:ALA:HB2	1:120:A:PRO:HA	12	0.42
(1,67)	1:116:A:ALA:HB2	1:120:A:PRO:HA	13	0.42
(1,67)	1:116:A:ALA:HB2	1:120:A:PRO:HA	14	0.42
(1,56)	1:124:A:TYR:HE2	2:35:B:PHE:HB3	14	0.42
(1,51)	1:126:A:TYR:HD1	1:125:A:VAL:HG11	11	0.42
(1,48)	1:126:A:TYR:HE1	1:125:A:VAL:HG12	1	0.42
(1,36)	1:127:A:ILE:HG23	1:124:A:TYR:HD2	11	0.42
(1,17)	1:133:A:VAL:HG12	1:137:A:HIS:HB2	4	0.42
(1,17)	1:133:A:VAL:HG11	1:137:A:HIS:HB2	9	0.42
(1,13)	1:133:A:VAL:HG11	1:108:A:ILE:HB	2	0.42
(1,13)	1:133:A:VAL:HG13	1:108:A:ILE:HB	5	0.42
(1,6)	1:130:A:LEU:HD22	1:70:A:PHE:HE2	7	0.42
(1,2265)	2:26:B:ASP:HB3	2:26:B:ASP:H	24	0.41
(1,2202)	1:125:A:VAL:H	1:122:A:LYS:HD2	8	0.41
(1,2173)	1:63:A:ASN:H	1:109:A:LEU:HD12	15	0.41
(1,2106)	1:76:A:MET:HB3	1:77:A:GLN:H	23	0.41
(1,2086)	1:80:A:ASP:HB2	1:80:A:ASP:H	12	0.41
(1,2063)	1:85:A:VAL:H	1:71:A:LEU:HD21	4	0.41
(1,2063)	1:85:A:VAL:H	1:71:A:LEU:HD21	7	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2063)	1:85:A:VAL:H	1:71:A:LEU:HD22	25	0.41
(1,2060)	1:86:A:PRO:HB3	1:87:A:PHE:H	24	0.41
(1,2051)	1:89:A:TYR:H	1:90:A:ASN:HB3	4	0.41
(1,2017)	1:93:A:GLN:HE22	1:89:A:TYR:HB3	2	0.41
(1,2004)	1:95:A:ALA:H	1:94:A:ARG:HB3	12	0.41
(1,2004)	1:95:A:ALA:H	1:94:A:ARG:HB3	25	0.41
(1,1996)	1:97:A:SER:H	1:139:A:ALA:HB3	1	0.41
(1,1996)	1:97:A:SER:H	1:139:A:ALA:HB2	4	0.41
(1,1971)	1:100:A:LEU:HD23	1:101:A:ALA:H	17	0.41
(1,1971)	1:100:A:LEU:HD21	1:101:A:ALA:H	21	0.41
(1,1958)	1:103:A:ALA:H	1:102:A:SER:HB3	20	0.41
(1,1924)	1:108:A:ILE:HG21	1:108:A:ILE:H	5	0.41
(1,1924)	1:108:A:ILE:HG21	1:108:A:ILE:H	13	0.41
(1,1924)	1:108:A:ILE:HG21	1:108:A:ILE:H	19	0.41
(1,1924)	1:108:A:ILE:HG23	1:108:A:ILE:H	25	0.41
(1,1851)	1:124:A:TYR:HB3	1:124:A:TYR:H	3	0.41
(1,1851)	1:124:A:TYR:HB3	1:124:A:TYR:H	7	0.41
(1,1851)	1:124:A:TYR:HB3	1:124:A:TYR:H	16	0.41
(1,1851)	1:124:A:TYR:HB3	1:124:A:TYR:H	17	0.41
(1,1851)	1:124:A:TYR:HB3	1:124:A:TYR:H	19	0.41
(1,1830)	1:128:A:ASN:H	1:128:A:ASN:HB3	1	0.41
(1,1830)	1:128:A:ASN:H	1:128:A:ASN:HB3	3	0.41
(1,1830)	1:128:A:ASN:H	1:128:A:ASN:HB3	6	0.41
(1,1830)	1:128:A:ASN:H	1:128:A:ASN:HB3	8	0.41
(1,1830)	1:128:A:ASN:H	1:128:A:ASN:HB3	13	0.41
(1,1830)	1:128:A:ASN:H	1:128:A:ASN:HB3	14	0.41
(1,1830)	1:128:A:ASN:H	1:128:A:ASN:HB3	25	0.41
(1,1788)	1:139:A:ALA:H	1:135:A:LYS:HD2	2	0.41
(1,1788)	1:139:A:ALA:H	1:135:A:LYS:HD3	11	0.41
(1,1768)	2:24:B:GLN:HG3	2:24:B:GLN:HB2	5	0.41
(1,1755)	2:30:B:GLU:HG2	2:30:B:GLU:HA	9	0.41
(1,1754)	2:30:B:GLU:HG2	2:31:B:LEU:H	8	0.41
(1,1727)	2:31:B:LEU:HD11	2:31:B:LEU:H	16	0.41
(1,1723)	2:31:B:LEU:HD22	2:30:B:GLU:HB2	10	0.41
(1,1720)	2:34:B:TYR:HE1	2:31:B:LEU:HD21	19	0.41
(1,1716)	2:31:B:LEU:HG	2:32:B:GLU:HG3	11	0.41
(1,1650)	2:37:B:ALA:HB3	1:121:A:ALA:HB3	15	0.41
(1,1650)	2:37:B:ALA:HB1	1:121:A:ALA:HB2	19	0.41
(1,1513)	1:62:A:GLU:HA	1:62:A:GLU:HG3	1	0.41
(1,1513)	1:62:A:GLU:HA	1:62:A:GLU:HG3	14	0.41
(1,1513)	1:62:A:GLU:HA	1:62:A:GLU:HG3	18	0.41
(1,1481)	1:66:A:LEU:HD22	1:69:A:GLU:H	1	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1481)	1:66:A:LEU:HD22	1:69:A:GLU:H	8	0.41
(1,1481)	1:66:A:LEU:HD23	1:69:A:GLU:H	10	0.41
(1,1481)	1:66:A:LEU:HD22	1:69:A:GLU:H	13	0.41
(1,1480)	1:66:A:LEU:HD23	1:63:A:ASN:HA	12	0.41
(1,1480)	1:66:A:LEU:HD23	1:63:A:ASN:HA	17	0.41
(1,1480)	1:66:A:LEU:HD21	1:63:A:ASN:HA	22	0.41
(1,1477)	1:66:A:LEU:HD23	1:113:A:LEU:HB3	25	0.41
(1,1475)	1:66:A:LEU:HD23	1:109:A:LEU:HD22	21	0.41
(1,1466)	1:109:A:LEU:HD12	1:66:A:LEU:HG	3	0.41
(1,1466)	1:109:A:LEU:HD12	1:66:A:LEU:HG	4	0.41
(1,1466)	1:109:A:LEU:HD12	1:66:A:LEU:HG	5	0.41
(1,1466)	1:109:A:LEU:HD11	1:66:A:LEU:HG	13	0.41
(1,1466)	1:109:A:LEU:HD13	1:66:A:LEU:HG	17	0.41
(1,1466)	1:109:A:LEU:HD12	1:66:A:LEU:HG	21	0.41
(1,1416)	1:71:A:LEU:HD13	1:71:A:LEU:H	22	0.41
(1,1392)	1:73:A:LEU:HD22	1:117:A:ARG:HD3	13	0.41
(1,1385)	1:73:A:LEU:HB2	1:74:A:CYS:H	2	0.41
(1,1385)	1:73:A:LEU:HB2	1:74:A:CYS:H	3	0.41
(1,1385)	1:73:A:LEU:HB2	1:74:A:CYS:H	9	0.41
(1,1385)	1:73:A:LEU:HB2	1:74:A:CYS:H	10	0.41
(1,1385)	1:73:A:LEU:HB2	1:74:A:CYS:H	20	0.41
(1,1385)	1:73:A:LEU:HB2	1:74:A:CYS:H	23	0.41
(1,1336)	1:76:A:MET:HA	1:76:A:MET:HB2	1	0.41
(1,1336)	1:76:A:MET:HA	1:76:A:MET:HB2	12	0.41
(1,1331)	1:77:A:GLN:HG2	1:73:A:LEU:HD11	14	0.41
(1,1303)	1:137:A:HIS:HE1	1:136:A:ALA:HB3	8	0.41
(1,1303)	1:137:A:HIS:HE1	1:136:A:ALA:HB3	13	0.41
(1,1295)	1:82:A:PRO:HG2	1:81:A:HIS:HA	11	0.41
(1,1280)	1:84:A:VAL:HG22	1:81:A:HIS:HB2	1	0.41
(1,1273)	1:85:A:VAL:HG13	1:75:A:LYS:HE2	8	0.41
(1,1248)	1:85:A:VAL:HA	1:71:A:LEU:HD11	2	0.41
(1,1248)	1:85:A:VAL:HA	1:71:A:LEU:HD13	19	0.41
(1,1199)	1:89:A:TYR:HE1	1:71:A:LEU:HD11	20	0.41
(1,1199)	1:89:A:TYR:HE1	1:71:A:LEU:HD13	24	0.41
(1,1183)	1:90:A:ASN:HB2	1:87:A:PHE:HD1	7	0.41
(1,1183)	1:90:A:ASN:HB2	1:87:A:PHE:HD1	17	0.41
(1,1183)	1:90:A:ASN:HB2	1:87:A:PHE:HD1	18	0.41
(1,1147)	1:94:A:ARG:HG2	1:94:A:ARG:HA	15	0.41
(1,1122)	1:96:A:HIS:HA	1:139:A:ALA:HB3	24	0.41
(1,1115)	1:98:A:LEU:HD21	1:96:A:HIS:HE1	9	0.41
(1,1115)	1:98:A:LEU:HD22	1:96:A:HIS:HE1	21	0.41
(1,1115)	1:98:A:LEU:HD23	1:96:A:HIS:HE1	23	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1094)	1:100:A:LEU:HD23	1:138:A:SER:HB2	12	0.41
(1,1094)	1:100:A:LEU:HD21	1:138:A:SER:HB2	18	0.41
(1,1094)	1:100:A:LEU:HD23	1:138:A:SER:HB2	21	0.41
(1,1088)	1:100:A:LEU:HD23	1:105:A:PHE:HD2	2	0.41
(1,1088)	1:100:A:LEU:HD23	1:105:A:PHE:HD2	7	0.41
(1,1059)	1:103:A:ALA:HB3	1:104:A:GLU:HA	19	0.41
(1,1057)	1:103:A:ALA:HB2	1:59:A:TYR:HD1	16	0.41
(1,960)	1:67:A:PHE:HA	1:109:A:LEU:HD12	9	0.41
(1,917)	1:113:A:LEU:HB2	1:113:A:LEU:HD21	6	0.41
(1,917)	1:113:A:LEU:HB2	1:113:A:LEU:HD23	11	0.41
(1,917)	1:113:A:LEU:HB2	1:113:A:LEU:HD23	25	0.41
(1,888)	1:116:A:ALA:HB1	1:123:A:LEU:H	16	0.41
(1,888)	1:116:A:ALA:HB1	1:123:A:LEU:H	21	0.41
(1,857)	1:119:A:ARG:HB2	1:119:A:ARG:HG3	6	0.41
(1,825)	1:122:A:LYS:HG2	1:125:A:VAL:HG22	21	0.41
(1,790)	1:124:A:TYR:HD1	1:124:A:TYR:HA	11	0.41
(1,790)	1:124:A:TYR:HD1	1:124:A:TYR:HA	18	0.41
(1,743)	1:127:A:ILE:HG23	1:124:A:TYR:HA	10	0.41
(1,743)	1:127:A:ILE:HG21	1:124:A:TYR:HA	12	0.41
(1,743)	1:127:A:ILE:HG22	1:124:A:TYR:HA	18	0.41
(1,670)	1:133:A:VAL:HG22	1:105:A:PHE:HE1	4	0.41
(1,670)	1:133:A:VAL:HG23	1:105:A:PHE:HE1	6	0.41
(1,670)	1:133:A:VAL:HG22	1:105:A:PHE:HE1	7	0.41
(1,670)	1:133:A:VAL:HG23	1:105:A:PHE:HE1	25	0.41
(1,668)	1:133:A:VAL:HG12	1:130:A:LEU:HD13	14	0.41
(1,607)	1:136:A:ALA:HB3	1:137:A:HIS:HA	8	0.41
(1,585)	1:139:A:ALA:HB1	1:140:A:LYS:H	7	0.41
(1,541)	1:61:A:LEU:HB3	1:62:A:GLU:H	11	0.41
(1,541)	1:61:A:LEU:HB3	1:62:A:GLU:H	20	0.41
(1,521)	1:71:A:LEU:H	1:113:A:LEU:HD13	20	0.41
(1,501)	1:80:A:ASP:HB3	1:81:A:HIS:H	2	0.41
(1,501)	1:80:A:ASP:HB3	1:81:A:HIS:H	20	0.41
(1,500)	1:85:A:VAL:H	1:83:A:GLU:H	2	0.41
(1,500)	1:85:A:VAL:H	1:83:A:GLU:H	21	0.41
(1,494)	1:90:A:ASN:H	1:88:A:LEU:HB2	7	0.41
(1,494)	1:90:A:ASN:H	1:88:A:LEU:HB2	17	0.41
(1,494)	1:90:A:ASN:H	1:88:A:LEU:HB2	25	0.41
(1,490)	1:91:A:ARG:H	1:94:A:ARG:H	21	0.41
(1,483)	1:93:A:GLN:HG2	1:94:A:ARG:H	5	0.41
(1,483)	1:93:A:GLN:HG2	1:94:A:ARG:H	14	0.41
(1,483)	1:93:A:GLN:HG2	1:94:A:ARG:H	15	0.41
(1,476)	1:96:A:HIS:H	1:95:A:ALA:H	18	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,457)	1:111:A:ARG:H	1:109:A:LEU:HB3	5	0.41
(1,445)	1:116:A:ALA:H	1:112:A:VAL:HA	3	0.41
(1,428)	1:128:A:ASN:HD22	1:128:A:ASN:HB3	10	0.41
(1,421)	1:128:A:ASN:H	1:70:A:PHE:HZ	9	0.41
(1,421)	1:72:A:GLU:H	1:70:A:PHE:HD1	24	0.41
(1,419)	1:129:A:GLU:H	1:126:A:TYR:H	3	0.41
(1,414)	1:72:A:GLU:H	1:69:A:GLU:HA	14	0.41
(1,399)	1:135:A:LYS:H	1:133:A:VAL:HA	10	0.41
(1,399)	1:135:A:LYS:H	1:133:A:VAL:HA	17	0.41
(1,398)	1:135:A:LYS:HG2	1:136:A:ALA:H	13	0.41
(1,398)	1:135:A:LYS:HG2	1:136:A:ALA:H	25	0.41
(1,392)	1:139:A:ALA:H	1:138:A:SER:H	23	0.41
(1,387)	1:141:A:LYS:H	1:141:A:LYS:HG2	3	0.41
(1,379)	2:31:B:LEU:HB2	2:28:B:ASP:HB2	17	0.41
(1,368)	2:26:B:ASP:HB3	1:87:A:PHE:HZ	6	0.41
(1,356)	2:29:B:SER:HB2	2:31:B:LEU:H	2	0.41
(1,356)	2:29:B:SER:HB2	2:31:B:LEU:H	19	0.41
(1,312)	2:35:B:PHE:HE1	1:124:A:TYR:HA	23	0.41
(1,290)	2:39:B:TRP:HH2	2:36:B:THR:HB	8	0.41
(1,257)	1:113:A:LEU:HD12	1:117:A:ARG:HG2	12	0.41
(1,244)	1:61:A:LEU:HG	1:61:A:LEU:HA	8	0.41
(1,244)	1:61:A:LEU:HG	1:61:A:LEU:HA	21	0.41
(1,236)	1:64:A:GLU:HA	1:67:A:PHE:H	12	0.41
(1,232)	1:66:A:LEU:HD11	1:62:A:GLU:HA	20	0.41
(1,227)	1:62:A:GLU:HG2	1:61:A:LEU:HG	23	0.41
(1,219)	1:70:A:PHE:HD1	1:73:A:LEU:HB3	12	0.41
(1,219)	1:70:A:PHE:HD1	1:73:A:LEU:HB3	14	0.41
(1,219)	1:70:A:PHE:HD1	1:73:A:LEU:HB3	16	0.41
(1,201)	1:72:A:GLU:HG3	1:72:A:GLU:HB2	6	0.41
(1,201)	1:72:A:GLU:HG3	1:72:A:GLU:HB2	25	0.41
(1,197)	1:73:A:LEU:HD21	1:123:A:LEU:HB2	7	0.41
(1,197)	1:73:A:LEU:HD22	1:123:A:LEU:HB2	10	0.41
(1,195)	1:73:A:LEU:HD21	1:70:A:PHE:HA	2	0.41
(1,194)	1:73:A:LEU:HD22	1:70:A:PHE:HD1	7	0.41
(1,194)	1:73:A:LEU:HD23	1:70:A:PHE:HD1	10	0.41
(1,194)	1:73:A:LEU:HD21	1:70:A:PHE:HD1	23	0.41
(1,171)	1:84:A:VAL:HG12	1:85:A:VAL:H	6	0.41
(1,171)	1:84:A:VAL:HG12	1:85:A:VAL:H	9	0.41
(1,155)	1:88:A:LEU:HD12	1:74:A:CYS:HB2	19	0.41
(1,155)	1:88:A:LEU:HD23	1:131:A:CYS:HB3	25	0.41
(1,151)	1:88:A:LEU:HD11	1:70:A:PHE:HD1	22	0.41
(1,140)	2:35:B:PHE:HB3	2:35:B:PHE:HE2	6	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,140)	2:35:B:PHE:HB3	2:35:B:PHE:HE2	8	0.41
(1,140)	2:35:B:PHE:HB3	2:35:B:PHE:HE2	14	0.41
(1,140)	2:35:B:PHE:HB3	2:35:B:PHE:HE2	15	0.41
(1,140)	2:35:B:PHE:HB3	2:35:B:PHE:HE2	19	0.41
(1,132)	1:92:A:GLN:HB3	1:89:A:TYR:HD1	5	0.41
(1,97)	1:105:A:PHE:HD1	1:134:A:LEU:HA	20	0.41
(1,97)	1:105:A:PHE:HD1	1:100:A:LEU:HA	25	0.41
(1,87)	1:112:A:VAL:HG11	1:130:A:LEU:H	12	0.41
(1,87)	1:112:A:VAL:HG12	1:130:A:LEU:H	17	0.41
(1,81)	1:116:A:ALA:HB2	1:70:A:PHE:HZ	9	0.41
(1,80)	1:94:A:ARG:HD3	1:93:A:GLN:HB2	16	0.41
(1,67)	1:116:A:ALA:HB3	1:120:A:PRO:HA	24	0.41
(1,52)	1:125:A:VAL:HG11	1:128:A:ASN:HB2	21	0.41
(1,48)	1:126:A:TYR:HE1	1:125:A:VAL:HG12	21	0.41
(1,45)	1:59:A:TYR:HE2	1:57:A:LYS:HD3	20	0.41
(1,36)	1:127:A:ILE:HG23	1:124:A:TYR:HD2	17	0.41
(1,13)	1:133:A:VAL:HG11	1:108:A:ILE:HB	4	0.41
(1,13)	1:133:A:VAL:HG12	1:108:A:ILE:HB	12	0.41
(1,6)	1:130:A:LEU:HD21	1:70:A:PHE:HE2	5	0.41
(1,2265)	2:26:B:ASP:HB3	2:26:B:ASP:H	10	0.4
(1,2265)	2:26:B:ASP:HB3	2:26:B:ASP:H	13	0.4
(1,2173)	1:63:A:ASN:H	1:109:A:LEU:HD13	4	0.4
(1,2173)	1:63:A:ASN:H	1:109:A:LEU:HD11	7	0.4
(1,2173)	1:63:A:ASN:H	1:109:A:LEU:HD11	11	0.4
(1,2136)	1:69:A:GLU:H	1:70:A:PHE:HB2	2	0.4
(1,2106)	1:76:A:MET:HB3	1:77:A:GLN:H	8	0.4
(1,2106)	1:76:A:MET:HB3	1:77:A:GLN:H	25	0.4
(1,2100)	1:77:A:GLN:HE21	1:76:A:MET:HE1	5	0.4
(1,2060)	1:86:A:PRO:HB3	1:87:A:PHE:H	2	0.4
(1,2037)	1:90:A:ASN:HD21	1:94:A:ARG:HD2	10	0.4
(1,2019)	1:93:A:GLN:HE22	1:93:A:GLN:HB3	13	0.4
(1,2017)	1:93:A:GLN:HE22	1:89:A:TYR:HB3	21	0.4
(1,2017)	1:93:A:GLN:HE22	1:89:A:TYR:HB3	23	0.4
(1,2012)	1:94:A:ARG:HB3	1:94:A:ARG:H	23	0.4
(1,2007)	1:100:A:LEU:HD21	1:95:A:ALA:H	7	0.4
(1,2007)	1:100:A:LEU:HD21	1:95:A:ALA:H	19	0.4
(1,1971)	1:100:A:LEU:HD21	1:101:A:ALA:H	10	0.4
(1,1971)	1:100:A:LEU:HD22	1:101:A:ALA:H	15	0.4
(1,1971)	1:100:A:LEU:HD23	1:101:A:ALA:H	24	0.4
(1,1968)	1:101:A:ALA:H	1:63:A:ASN:HD22	2	0.4
(1,1924)	1:108:A:ILE:HG22	1:108:A:ILE:H	6	0.4
(1,1851)	1:124:A:TYR:HB3	1:124:A:TYR:H	1	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1851)	1:124:A:TYR:HB3	1:124:A:TYR:H	4	0.4
(1,1851)	1:124:A:TYR:HB3	1:124:A:TYR:H	5	0.4
(1,1851)	1:124:A:TYR:HB3	1:124:A:TYR:H	6	0.4
(1,1851)	1:124:A:TYR:HB3	1:124:A:TYR:H	8	0.4
(1,1851)	1:124:A:TYR:HB3	1:124:A:TYR:H	11	0.4
(1,1851)	1:124:A:TYR:HB3	1:124:A:TYR:H	15	0.4
(1,1851)	1:124:A:TYR:HB3	1:124:A:TYR:H	21	0.4
(1,1851)	1:124:A:TYR:HB3	1:124:A:TYR:H	25	0.4
(1,1830)	1:128:A:ASN:H	1:128:A:ASN:HB3	11	0.4
(1,1830)	1:128:A:ASN:H	1:128:A:ASN:HB3	16	0.4
(1,1830)	1:128:A:ASN:H	1:128:A:ASN:HB3	19	0.4
(1,1830)	1:128:A:ASN:H	1:128:A:ASN:HB3	21	0.4
(1,1788)	1:139:A:ALA:H	1:135:A:LYS:HD3	8	0.4
(1,1768)	2:24:B:GLN:HG3	2:24:B:GLN:HB2	21	0.4
(1,1754)	2:30:B:GLU:HG2	2:31:B:LEU:H	18	0.4
(1,1723)	2:31:B:LEU:HD23	2:30:B:GLU:HB2	11	0.4
(1,1716)	2:31:B:LEU:HG	2:32:B:GLU:HG3	3	0.4
(1,1702)	2:33:B:GLN:HG3	2:34:B:TYR:HE2	7	0.4
(1,1622)	2:39:B:TRP:HE3	2:39:B:TRP:HB2	6	0.4
(1,1622)	2:39:B:TRP:HE3	2:39:B:TRP:HB2	15	0.4
(1,1577)	1:77:A:GLN:HG3	1:73:A:LEU:HD13	3	0.4
(1,1481)	1:66:A:LEU:HD22	1:69:A:GLU:H	17	0.4
(1,1481)	1:66:A:LEU:HD22	1:69:A:GLU:H	21	0.4
(1,1481)	1:66:A:LEU:HD21	1:69:A:GLU:H	23	0.4
(1,1480)	1:66:A:LEU:HD22	1:63:A:ASN:HA	2	0.4
(1,1480)	1:66:A:LEU:HD23	1:63:A:ASN:HA	9	0.4
(1,1480)	1:66:A:LEU:HD21	1:63:A:ASN:HA	10	0.4
(1,1477)	1:66:A:LEU:HD23	1:113:A:LEU:HB3	17	0.4
(1,1477)	1:66:A:LEU:HD23	1:113:A:LEU:HB3	21	0.4
(1,1475)	1:66:A:LEU:HD22	1:109:A:LEU:HD23	14	0.4
(1,1466)	1:109:A:LEU:HD13	1:66:A:LEU:HG	22	0.4
(1,1456)	1:69:A:GLU:HG2	1:66:A:LEU:HA	13	0.4
(1,1422)	1:71:A:LEU:HD21	1:74:A:CYS:H	1	0.4
(1,1395)	1:116:A:ALA:HB2	1:73:A:LEU:HD23	13	0.4
(1,1385)	1:73:A:LEU:HB2	1:74:A:CYS:H	4	0.4
(1,1385)	1:73:A:LEU:HB2	1:74:A:CYS:H	18	0.4
(1,1337)	1:76:A:MET:HA	1:76:A:MET:HG3	19	0.4
(1,1336)	1:76:A:MET:HA	1:76:A:MET:HB2	2	0.4
(1,1336)	1:76:A:MET:HA	1:76:A:MET:HB2	4	0.4
(1,1336)	1:76:A:MET:HA	1:76:A:MET:HB2	9	0.4
(1,1336)	1:76:A:MET:HA	1:76:A:MET:HB2	13	0.4
(1,1336)	1:76:A:MET:HA	1:76:A:MET:HB2	14	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1336)	1:76:A:MET:HA	1:76:A:MET:HB2	20	0.4
(1,1336)	1:76:A:MET:HA	1:76:A:MET:HB2	23	0.4
(1,1336)	1:76:A:MET:HA	1:76:A:MET:HB2	24	0.4
(1,1326)	1:77:A:GLN:HG2	1:77:A:GLN:HA	23	0.4
(1,1303)	1:137:A:HIS:HE1	1:136:A:ALA:HB1	3	0.4
(1,1303)	1:137:A:HIS:HE1	1:136:A:ALA:HB3	14	0.4
(1,1280)	1:84:A:VAL:HG21	1:81:A:HIS:HB2	7	0.4
(1,1248)	1:85:A:VAL:HA	1:71:A:LEU:HD13	1	0.4
(1,1248)	1:85:A:VAL:HA	1:71:A:LEU:HD12	9	0.4
(1,1248)	1:85:A:VAL:HA	1:71:A:LEU:HD13	10	0.4
(1,1248)	1:85:A:VAL:HA	1:71:A:LEU:HD12	17	0.4
(1,1248)	1:85:A:VAL:HA	1:71:A:LEU:HD13	18	0.4
(1,1199)	1:89:A:TYR:HE1	1:71:A:LEU:HD11	18	0.4
(1,1199)	1:89:A:TYR:HE1	1:71:A:LEU:HD11	19	0.4
(1,1139)	1:134:A:LEU:HD21	1:95:A:ALA:HB3	20	0.4
(1,1137)	1:95:A:ALA:HB2	1:91:A:ARG:HD3	25	0.4
(1,1122)	1:96:A:HIS:HA	1:139:A:ALA:HB2	4	0.4
(1,1076)	1:101:A:ALA:HB2	1:98:A:LEU:HD23	5	0.4
(1,1070)	1:101:A:ALA:HB1	1:102:A:SER:H	9	0.4
(1,989)	1:108:A:ILE:HG22	1:105:A:PHE:HA	2	0.4
(1,989)	1:108:A:ILE:HG22	1:105:A:PHE:HA	14	0.4
(1,989)	1:108:A:ILE:HG23	1:105:A:PHE:HA	21	0.4
(1,917)	1:113:A:LEU:HB2	1:113:A:LEU:HD21	8	0.4
(1,917)	1:113:A:LEU:HB2	1:113:A:LEU:HD23	19	0.4
(1,917)	1:113:A:LEU:HB2	1:113:A:LEU:HD21	21	0.4
(1,917)	1:113:A:LEU:HB2	1:113:A:LEU:HD22	24	0.4
(1,888)	1:116:A:ALA:HB2	1:123:A:LEU:H	14	0.4
(1,886)	1:116:A:ALA:HA	1:123:A:LEU:HD13	6	0.4
(1,857)	1:119:A:ARG:HB2	1:119:A:ARG:HG3	16	0.4
(1,857)	1:119:A:ARG:HB2	1:119:A:ARG:HG3	25	0.4
(1,809)	1:123:A:LEU:HD11	1:123:A:LEU:HD22	4	0.4
(1,809)	1:123:A:LEU:HD12	1:123:A:LEU:HD21	10	0.4
(1,809)	1:123:A:LEU:HD13	1:123:A:LEU:HD23	15	0.4
(1,809)	1:123:A:LEU:HD11	1:123:A:LEU:HD21	22	0.4
(1,790)	1:124:A:TYR:HD1	1:124:A:TYR:HA	17	0.4
(1,743)	1:127:A:ILE:HG21	1:124:A:TYR:HA	20	0.4
(1,743)	1:127:A:ILE:HG21	1:124:A:TYR:HA	25	0.4
(1,698)	1:98:A:LEU:HG	1:98:A:LEU:HA	19	0.4
(1,697)	1:98:A:LEU:HG	1:98:A:LEU:H	19	0.4
(1,670)	1:133:A:VAL:HG21	1:105:A:PHE:HE1	13	0.4
(1,670)	1:133:A:VAL:HG23	1:105:A:PHE:HE1	15	0.4
(1,670)	1:133:A:VAL:HG22	1:105:A:PHE:HE1	19	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,668)	1:133:A:VAL:HG12	1:130:A:LEU:HD12	11	0.4
(1,668)	1:133:A:VAL:HG12	1:130:A:LEU:HD13	12	0.4
(1,668)	1:133:A:VAL:HG12	1:130:A:LEU:HD13	16	0.4
(1,668)	1:133:A:VAL:HG13	1:130:A:LEU:HD11	20	0.4
(1,561)	2:27:B:SER:H	2:30:B:GLU:HB3	13	0.4
(1,520)	1:130:A:LEU:H	1:112:A:VAL:HG22	25	0.4
(1,500)	1:85:A:VAL:H	1:83:A:GLU:H	6	0.4
(1,500)	1:85:A:VAL:H	1:83:A:GLU:H	11	0.4
(1,500)	1:85:A:VAL:H	1:83:A:GLU:H	17	0.4
(1,500)	1:85:A:VAL:H	1:83:A:GLU:H	20	0.4
(1,494)	1:90:A:ASN:H	1:88:A:LEU:HB2	20	0.4
(1,494)	1:90:A:ASN:H	1:88:A:LEU:HB2	23	0.4
(1,492)	1:91:A:ARG:H	1:88:A:LEU:HD21	7	0.4
(1,492)	1:91:A:ARG:H	1:88:A:LEU:HD23	10	0.4
(1,492)	1:91:A:ARG:H	1:88:A:LEU:HD21	24	0.4
(1,483)	1:93:A:GLN:HG2	1:94:A:ARG:H	12	0.4
(1,483)	1:93:A:GLN:HG2	1:94:A:ARG:H	13	0.4
(1,483)	1:93:A:GLN:HG2	1:94:A:ARG:H	16	0.4
(1,483)	1:93:A:GLN:HG2	1:94:A:ARG:H	17	0.4
(1,476)	1:96:A:HIS:H	1:95:A:ALA:H	14	0.4
(1,476)	1:96:A:HIS:H	1:138:A:SER:H	15	0.4
(1,476)	1:96:A:HIS:H	1:95:A:ALA:H	20	0.4
(1,454)	1:114:A:SER:H	1:112:A:VAL:HG21	6	0.4
(1,445)	1:116:A:ALA:H	1:112:A:VAL:HA	1	0.4
(1,445)	1:116:A:ALA:H	1:112:A:VAL:HA	17	0.4
(1,444)	1:73:A:LEU:HD11	1:117:A:ARG:H	24	0.4
(1,434)	1:74:A:CYS:H	1:123:A:LEU:HD12	14	0.4
(1,428)	1:128:A:ASN:HD22	1:128:A:ASN:HB3	16	0.4
(1,419)	1:129:A:GLU:H	1:126:A:TYR:H	7	0.4
(1,419)	1:129:A:GLU:H	1:126:A:TYR:H	9	0.4
(1,419)	1:129:A:GLU:H	1:126:A:TYR:H	16	0.4
(1,414)	1:72:A:GLU:H	1:68:A:GLU:HA	16	0.4
(1,399)	1:135:A:LYS:H	1:133:A:VAL:HA	9	0.4
(1,399)	1:135:A:LYS:H	1:133:A:VAL:HA	18	0.4
(1,398)	1:135:A:LYS:HG2	1:136:A:ALA:H	18	0.4
(1,395)	1:138:A:SER:H	1:95:A:ALA:HB3	25	0.4
(1,392)	1:139:A:ALA:H	1:138:A:SER:H	13	0.4
(1,392)	1:139:A:ALA:H	1:138:A:SER:H	17	0.4
(1,364)	2:29:B:SER:HB3	2:32:B:GLU:HB2	5	0.4
(1,312)	2:35:B:PHE:HE1	1:124:A:TYR:HA	12	0.4
(1,312)	2:35:B:PHE:HE1	1:124:A:TYR:HA	13	0.4
(1,281)	2:31:B:LEU:HD21	1:128:A:ASN:H	5	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,257)	1:113:A:LEU:HD12	1:117:A:ARG:HG2	10	0.4
(1,244)	1:61:A:LEU:HG	1:61:A:LEU:HA	2	0.4
(1,244)	1:61:A:LEU:HG	1:61:A:LEU:HA	6	0.4
(1,244)	1:61:A:LEU:HG	1:61:A:LEU:HA	17	0.4
(1,244)	1:61:A:LEU:HG	1:61:A:LEU:HA	18	0.4
(1,243)	1:62:A:GLU:HG3	1:61:A:LEU:HD21	8	0.4
(1,232)	1:66:A:LEU:HD11	1:62:A:GLU:HA	1	0.4
(1,230)	1:66:A:LEU:HA	1:113:A:LEU:HD23	7	0.4
(1,230)	1:66:A:LEU:HA	1:113:A:LEU:HD23	25	0.4
(1,210)	1:105:A:PHE:HZ	1:109:A:LEU:HD21	3	0.4
(1,203)	1:71:A:LEU:HD13	1:68:A:GLU:H	13	0.4
(1,191)	1:78:A:THR:HG21	1:74:A:CYS:HB2	14	0.4
(1,191)	1:84:A:VAL:HG13	1:74:A:CYS:HB2	19	0.4
(1,171)	1:84:A:VAL:HG12	1:85:A:VAL:H	17	0.4
(1,171)	1:84:A:VAL:HG11	1:85:A:VAL:H	20	0.4
(1,140)	2:35:B:PHE:HB3	2:35:B:PHE:HE2	1	0.4
(1,140)	2:35:B:PHE:HB3	2:35:B:PHE:HE2	5	0.4
(1,140)	2:35:B:PHE:HB3	2:35:B:PHE:HE2	9	0.4
(1,139)	1:128:A:ASN:HB2	1:128:A:ASN:HD22	5	0.4
(1,117)	1:100:A:LEU:HD21	1:92:A:GLN:HG2	3	0.4
(1,97)	1:105:A:PHE:HD1	1:100:A:LEU:HA	3	0.4
(1,97)	1:105:A:PHE:HD1	1:134:A:LEU:HA	18	0.4
(1,97)	1:105:A:PHE:HD1	1:100:A:LEU:HA	21	0.4
(1,81)	1:116:A:ALA:HB2	1:70:A:PHE:HZ	1	0.4
(1,67)	1:116:A:ALA:HB1	1:120:A:PRO:HA	6	0.4
(1,62)	1:123:A:LEU:HD23	1:70:A:PHE:HE1	5	0.4
(1,56)	1:124:A:TYR:HE2	2:35:B:PHE:HB3	3	0.4
(1,52)	1:125:A:VAL:HG11	1:128:A:ASN:HB2	12	0.4
(1,48)	1:126:A:TYR:HE1	1:125:A:VAL:HG13	15	0.4
(1,48)	1:126:A:TYR:HE1	1:125:A:VAL:HG12	23	0.4
(1,44)	1:126:A:TYR:HE1	1:112:A:VAL:HA	16	0.4
(1,37)	1:127:A:ILE:HG23	1:128:A:ASN:HD22	2	0.4
(1,37)	1:127:A:ILE:HG23	1:128:A:ASN:HD22	12	0.4
(1,30)	1:129:A:GLU:HG3	1:130:A:LEU:H	18	0.4
(1,13)	1:133:A:VAL:HG12	1:108:A:ILE:HB	1	0.4
(1,13)	1:133:A:VAL:HG12	1:108:A:ILE:HB	3	0.4
(1,6)	1:130:A:LEU:HD22	1:70:A:PHE:HE2	18	0.4
(1,6)	1:130:A:LEU:HD22	1:70:A:PHE:HE2	20	0.4
(1,2271)	2:25:B:GLU:H	2:25:B:GLU:HG2	4	0.39
(1,2265)	2:26:B:ASP:HB3	2:26:B:ASP:H	8	0.39
(1,2265)	2:26:B:ASP:HB3	2:26:B:ASP:H	12	0.39
(1,2244)	2:36:B:THR:HG22	2:36:B:THR:H	20	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2197)	1:55:A:GLY:HA2	1:56:A:LYS:H	17	0.39
(1,2173)	1:63:A:ASN:H	1:109:A:LEU:HD11	8	0.39
(1,2142)	1:109:A:LEU:HD23	1:68:A:GLU:H	14	0.39
(1,2136)	1:69:A:GLU:H	1:70:A:PHE:HB2	23	0.39
(1,2060)	1:86:A:PRO:HB3	1:87:A:PHE:H	20	0.39
(1,2019)	1:93:A:GLN:HE22	1:93:A:GLN:HB3	4	0.39
(1,2019)	1:93:A:GLN:HE22	1:93:A:GLN:HB3	14	0.39
(1,2019)	1:93:A:GLN:HE22	1:93:A:GLN:HB3	18	0.39
(1,2019)	1:93:A:GLN:HE22	1:93:A:GLN:HB3	21	0.39
(1,2013)	1:94:A:ARG:H	1:95:A:ALA:HB3	7	0.39
(1,2013)	1:94:A:ARG:H	1:95:A:ALA:HB1	24	0.39
(1,2007)	1:100:A:LEU:HD22	1:95:A:ALA:H	4	0.39
(1,2007)	1:100:A:LEU:HD21	1:95:A:ALA:H	15	0.39
(1,2005)	1:95:A:ALA:H	1:94:A:ARG:HG2	4	0.39
(1,1996)	1:97:A:SER:H	1:139:A:ALA:HB2	2	0.39
(1,1996)	1:97:A:SER:H	1:139:A:ALA:HB1	21	0.39
(1,1983)	1:99:A:PHE:H	1:138:A:SER:HB2	5	0.39
(1,1924)	1:108:A:ILE:HG23	1:108:A:ILE:H	24	0.39
(1,1851)	1:124:A:TYR:HB3	1:124:A:TYR:H	9	0.39
(1,1851)	1:124:A:TYR:HB3	1:124:A:TYR:H	12	0.39
(1,1851)	1:124:A:TYR:HB3	1:124:A:TYR:H	13	0.39
(1,1851)	1:124:A:TYR:HB3	1:124:A:TYR:H	20	0.39
(1,1851)	1:124:A:TYR:HB3	1:124:A:TYR:H	22	0.39
(1,1851)	1:124:A:TYR:HB3	1:124:A:TYR:H	23	0.39
(1,1851)	1:124:A:TYR:HB3	1:124:A:TYR:H	24	0.39
(1,1837)	1:127:A:ILE:H	1:123:A:LEU:HD13	2	0.39
(1,1798)	1:136:A:ALA:H	1:135:A:LYS:HD3	16	0.39
(1,1788)	1:139:A:ALA:H	1:135:A:LYS:HD3	13	0.39
(1,1772)	1:142:A:LYS:H	1:141:A:LYS:HG2	1	0.39
(1,1755)	2:30:B:GLU:HG2	2:30:B:GLU:HA	12	0.39
(1,1754)	2:30:B:GLU:HG2	2:31:B:LEU:H	23	0.39
(1,1745)	2:29:B:SER:HB3	2:30:B:GLU:H	20	0.39
(1,1727)	2:31:B:LEU:HD13	2:31:B:LEU:H	3	0.39
(1,1723)	2:31:B:LEU:HD21	2:30:B:GLU:HB2	7	0.39
(1,1716)	2:31:B:LEU:HG	2:32:B:GLU:HG3	13	0.39
(1,1716)	2:31:B:LEU:HG	2:32:B:GLU:HG3	21	0.39
(1,1670)	2:37:B:ALA:HB3	2:36:B:THR:HA	8	0.39
(1,1633)	2:38:B:ARG:HD2	2:38:B:ARG:HB2	5	0.39
(1,1622)	2:39:B:TRP:HE3	2:39:B:TRP:HB2	25	0.39
(1,1620)	2:39:B:TRP:HD1	2:38:B:ARG:HG2	25	0.39
(1,1619)	2:39:B:TRP:HD1	2:38:B:ARG:HB2	24	0.39
(1,1577)	1:77:A:GLN:HG3	1:73:A:LEU:HD12	2	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1577)	1:77:A:GLN:HG3	1:73:A:LEU:HD12	4	0.39
(1,1568)	1:57:A:LYS:HD2	1:57:A:LYS:HE2	3	0.39
(1,1568)	1:57:A:LYS:HD2	1:57:A:LYS:HE2	5	0.39
(1,1568)	1:57:A:LYS:HD2	1:57:A:LYS:HE2	6	0.39
(1,1481)	1:66:A:LEU:HD21	1:69:A:GLU:H	7	0.39
(1,1481)	1:66:A:LEU:HD22	1:69:A:GLU:H	12	0.39
(1,1481)	1:66:A:LEU:HD22	1:69:A:GLU:H	19	0.39
(1,1481)	1:66:A:LEU:HD23	1:69:A:GLU:H	22	0.39
(1,1480)	1:66:A:LEU:HD22	1:63:A:ASN:HA	6	0.39
(1,1480)	1:66:A:LEU:HD23	1:63:A:ASN:HA	13	0.39
(1,1480)	1:66:A:LEU:HD22	1:63:A:ASN:HA	23	0.39
(1,1477)	1:66:A:LEU:HD22	1:113:A:LEU:HB3	4	0.39
(1,1475)	1:66:A:LEU:HD22	1:109:A:LEU:HD23	2	0.39
(1,1475)	1:66:A:LEU:HD23	1:109:A:LEU:HD23	9	0.39
(1,1470)	1:66:A:LEU:HD13	1:62:A:GLU:HG3	19	0.39
(1,1466)	1:109:A:LEU:HD11	1:66:A:LEU:HG	7	0.39
(1,1466)	1:109:A:LEU:HD12	1:66:A:LEU:HG	12	0.39
(1,1466)	1:109:A:LEU:HD13	1:66:A:LEU:HG	23	0.39
(1,1419)	1:71:A:LEU:HD13	1:89:A:TYR:H	14	0.39
(1,1419)	1:71:A:LEU:HD11	1:89:A:TYR:H	23	0.39
(1,1416)	1:71:A:LEU:HD12	1:71:A:LEU:H	5	0.39
(1,1416)	1:71:A:LEU:HD11	1:71:A:LEU:H	19	0.39
(1,1415)	1:71:A:LEU:HB2	1:75:A:LYS:HE2	24	0.39
(1,1385)	1:73:A:LEU:HB2	1:74:A:CYS:H	8	0.39
(1,1385)	1:73:A:LEU:HB2	1:74:A:CYS:H	14	0.39
(1,1336)	1:76:A:MET:HA	1:76:A:MET:HB2	3	0.39
(1,1336)	1:76:A:MET:HA	1:76:A:MET:HB2	5	0.39
(1,1336)	1:76:A:MET:HA	1:76:A:MET:HB2	6	0.39
(1,1336)	1:76:A:MET:HA	1:76:A:MET:HB2	7	0.39
(1,1336)	1:76:A:MET:HA	1:76:A:MET:HB2	8	0.39
(1,1336)	1:76:A:MET:HA	1:76:A:MET:HB2	10	0.39
(1,1336)	1:76:A:MET:HA	1:76:A:MET:HB2	15	0.39
(1,1336)	1:76:A:MET:HA	1:76:A:MET:HB2	18	0.39
(1,1336)	1:76:A:MET:HA	1:76:A:MET:HB2	22	0.39
(1,1336)	1:76:A:MET:HA	1:76:A:MET:HB2	25	0.39
(1,1331)	1:77:A:GLN:HG2	1:73:A:LEU:HD12	3	0.39
(1,1331)	1:77:A:GLN:HG2	1:73:A:LEU:HD12	8	0.39
(1,1331)	1:77:A:GLN:HG2	1:73:A:LEU:HD13	17	0.39
(1,1303)	1:137:A:HIS:HE1	1:136:A:ALA:HB1	10	0.39
(1,1295)	1:82:A:PRO:HG2	1:81:A:HIS:HA	3	0.39
(1,1282)	1:84:A:VAL:HG22	1:85:A:VAL:H	6	0.39
(1,1282)	1:84:A:VAL:HG21	1:85:A:VAL:H	21	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1248)	1:85:A:VAL:HA	1:71:A:LEU:HD11	15	0.39
(1,1248)	1:85:A:VAL:HA	1:71:A:LEU:HD11	23	0.39
(1,1199)	1:89:A:TYR:HE1	1:71:A:LEU:HD13	22	0.39
(1,1199)	1:89:A:TYR:HE1	1:71:A:LEU:HD11	25	0.39
(1,1147)	1:94:A:ARG:HG2	1:94:A:ARG:HA	22	0.39
(1,1139)	1:134:A:LEU:HD23	1:95:A:ALA:HB1	9	0.39
(1,1137)	1:95:A:ALA:HB3	1:91:A:ARG:HD3	23	0.39
(1,1098)	1:100:A:LEU:HD22	1:92:A:GLN:HA	4	0.39
(1,1088)	1:100:A:LEU:HD21	1:105:A:PHE:HD2	17	0.39
(1,1088)	1:100:A:LEU:HD23	1:105:A:PHE:HD2	20	0.39
(1,1076)	1:101:A:ALA:HB1	1:98:A:LEU:HD23	14	0.39
(1,1059)	1:103:A:ALA:HB2	1:104:A:GLU:HA	4	0.39
(1,1057)	1:103:A:ALA:HB2	1:59:A:TYR:HD1	3	0.39
(1,1047)	1:104:A:GLU:HG2	1:105:A:PHE:H	14	0.39
(1,1040)	1:62:A:GLU:HB3	1:59:A:TYR:HA	19	0.39
(1,1000)	1:108:A:ILE:HD12	1:99:A:PHE:HE1	10	0.39
(1,989)	1:108:A:ILE:HG22	1:105:A:PHE:HA	4	0.39
(1,989)	1:108:A:ILE:HG22	1:105:A:PHE:HA	10	0.39
(1,960)	1:67:A:PHE:HA	1:109:A:LEU:HD11	6	0.39
(1,917)	1:113:A:LEU:HB2	1:113:A:LEU:HD21	23	0.39
(1,888)	1:116:A:ALA:HB3	1:123:A:LEU:H	1	0.39
(1,888)	1:116:A:ALA:HB3	1:123:A:LEU:H	11	0.39
(1,888)	1:116:A:ALA:HB2	1:123:A:LEU:H	19	0.39
(1,888)	1:116:A:ALA:HB1	1:123:A:LEU:H	23	0.39
(1,888)	1:116:A:ALA:HB1	1:123:A:LEU:H	25	0.39
(1,827)	1:122:A:LYS:HD2	1:122:A:LYS:HA	12	0.39
(1,809)	1:123:A:LEU:HD13	1:123:A:LEU:HD23	3	0.39
(1,809)	1:123:A:LEU:HD12	1:123:A:LEU:HD21	6	0.39
(1,809)	1:123:A:LEU:HD13	1:123:A:LEU:HD23	8	0.39
(1,795)	1:127:A:ILE:HD13	1:124:A:TYR:HE1	4	0.39
(1,766)	1:126:A:TYR:HE1	1:115:A:ARG:HB2	8	0.39
(1,766)	1:126:A:TYR:HE1	1:115:A:ARG:HB2	20	0.39
(1,743)	1:127:A:ILE:HG23	1:124:A:TYR:HA	4	0.39
(1,743)	1:127:A:ILE:HG23	1:124:A:TYR:HA	24	0.39
(1,722)	1:129:A:GLU:HG3	1:125:A:VAL:HG12	13	0.39
(1,693)	1:130:A:LEU:HA	1:130:A:LEU:HB3	13	0.39
(1,668)	1:133:A:VAL:HG11	1:130:A:LEU:HD13	2	0.39
(1,668)	1:133:A:VAL:HG12	1:130:A:LEU:HD13	22	0.39
(1,668)	1:133:A:VAL:HG11	1:130:A:LEU:HD12	24	0.39
(1,585)	1:139:A:ALA:HB1	1:140:A:LYS:H	15	0.39
(1,558)	2:32:B:GLU:HA	2:31:B:LEU:H	17	0.39
(1,541)	1:61:A:LEU:HB3	1:62:A:GLU:H	16	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,538)	1:63:A:ASN:H	1:61:A:LEU:HA	17	0.39
(1,522)	1:70:A:PHE:H	1:73:A:LEU:H	8	0.39
(1,521)	1:71:A:LEU:H	1:113:A:LEU:HD11	13	0.39
(1,521)	1:71:A:LEU:H	1:113:A:LEU:HD12	21	0.39
(1,520)	1:130:A:LEU:H	1:112:A:VAL:HG21	4	0.39
(1,515)	1:73:A:LEU:HG	1:76:A:MET:H	8	0.39
(1,515)	1:73:A:LEU:HG	1:76:A:MET:H	16	0.39
(1,502)	1:81:A:HIS:H	1:82:A:PRO:HB3	11	0.39
(1,500)	1:85:A:VAL:H	1:83:A:GLU:H	24	0.39
(1,494)	1:90:A:ASN:H	1:88:A:LEU:HB2	12	0.39
(1,483)	1:93:A:GLN:HG2	1:94:A:ARG:H	6	0.39
(1,483)	1:93:A:GLN:HG2	1:94:A:ARG:H	7	0.39
(1,483)	1:93:A:GLN:HG2	1:94:A:ARG:H	10	0.39
(1,483)	1:93:A:GLN:HG2	1:94:A:ARG:H	23	0.39
(1,478)	1:95:A:ALA:H	1:91:A:ARG:HD2	14	0.39
(1,476)	1:96:A:HIS:H	1:95:A:ALA:H	12	0.39
(1,476)	1:96:A:HIS:H	1:95:A:ALA:H	17	0.39
(1,476)	1:96:A:HIS:H	1:95:A:ALA:H	23	0.39
(1,473)	1:101:A:ALA:H	1:100:A:LEU:HG	18	0.39
(1,465)	1:106:A:CYS:H	1:103:A:ALA:HB3	9	0.39
(1,453)	1:114:A:SER:H	1:113:A:LEU:HD21	10	0.39
(1,448)	1:116:A:ALA:H	1:126:A:TYR:HE2	21	0.39
(1,428)	1:128:A:ASN:HD22	1:128:A:ASN:HB3	3	0.39
(1,428)	1:128:A:ASN:HD22	1:128:A:ASN:HB3	8	0.39
(1,428)	1:128:A:ASN:HD22	1:128:A:ASN:HB3	9	0.39
(1,428)	1:128:A:ASN:HD22	1:128:A:ASN:HB3	11	0.39
(1,428)	1:128:A:ASN:HD22	1:128:A:ASN:HB3	13	0.39
(1,428)	1:128:A:ASN:HD22	1:128:A:ASN:HB3	14	0.39
(1,428)	1:128:A:ASN:HD22	1:128:A:ASN:HB3	20	0.39
(1,428)	1:128:A:ASN:HD22	1:128:A:ASN:HB3	21	0.39
(1,426)	1:125:A:VAL:HG12	1:126:A:TYR:H	18	0.39
(1,426)	1:125:A:VAL:HG12	1:126:A:TYR:H	24	0.39
(1,419)	1:129:A:GLU:H	1:126:A:TYR:H	1	0.39
(1,419)	1:129:A:GLU:H	1:126:A:TYR:H	22	0.39
(1,392)	1:139:A:ALA:H	1:138:A:SER:H	8	0.39
(1,387)	1:141:A:LYS:H	1:141:A:LYS:HG2	19	0.39
(1,379)	2:31:B:LEU:HB2	2:28:B:ASP:HB2	1	0.39
(1,364)	2:29:B:SER:HB3	2:32:B:GLU:HB2	24	0.39
(1,344)	2:31:B:LEU:HB3	1:87:A:PHE:HD2	2	0.39
(1,342)	2:31:B:LEU:HD12	1:124:A:TYR:HB3	16	0.39
(1,318)	2:34:B:TYR:HE1	1:83:A:GLU:HB3	9	0.39
(1,318)	2:34:B:TYR:HE1	1:83:A:GLU:HB3	20	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,293)	2:39:B:TRP:HD1	2:38:B:ARG:HB3	19	0.39
(1,281)	2:31:B:LEU:HD23	1:128:A:ASN:H	6	0.39
(1,281)	2:31:B:LEU:HD23	1:128:A:ASN:H	19	0.39
(1,275)	1:84:A:VAL:HG12	2:35:B:PHE:HE1	16	0.39
(1,240)	1:104:A:GLU:HB3	1:105:A:PHE:HA	12	0.39
(1,236)	1:64:A:GLU:HA	1:67:A:PHE:H	13	0.39
(1,232)	1:66:A:LEU:HD13	1:62:A:GLU:HA	18	0.39
(1,225)	1:129:A:GLU:HG2	1:125:A:VAL:HG11	14	0.39
(1,220)	1:70:A:PHE:HE2	1:113:A:LEU:HB2	4	0.39
(1,220)	1:70:A:PHE:HE2	1:113:A:LEU:HB2	12	0.39
(1,210)	1:105:A:PHE:HZ	1:109:A:LEU:HD23	10	0.39
(1,201)	2:25:B:GLU:HG3	2:25:B:GLU:HB2	21	0.39
(1,194)	1:73:A:LEU:HD23	1:70:A:PHE:HD1	1	0.39
(1,194)	1:73:A:LEU:HD21	1:70:A:PHE:HD1	19	0.39
(1,191)	1:84:A:VAL:HG13	1:74:A:CYS:HB2	13	0.39
(1,155)	1:88:A:LEU:HD21	1:131:A:CYS:HB3	2	0.39
(1,155)	1:88:A:LEU:HD11	1:74:A:CYS:HB2	14	0.39
(1,140)	2:35:B:PHE:HB3	2:35:B:PHE:HE2	2	0.39
(1,132)	1:67:A:PHE:HE1	1:92:A:GLN:HB3	18	0.39
(1,87)	1:112:A:VAL:HG12	1:130:A:LEU:H	23	0.39
(1,81)	1:116:A:ALA:HB2	1:70:A:PHE:HZ	17	0.39
(1,67)	1:116:A:ALA:HB1	1:120:A:PRO:HA	20	0.39
(1,62)	1:123:A:LEU:HD23	1:70:A:PHE:HE1	15	0.39
(1,52)	1:125:A:VAL:HG11	1:128:A:ASN:HB2	6	0.39
(1,52)	1:125:A:VAL:HG11	1:128:A:ASN:HB2	9	0.39
(1,52)	1:125:A:VAL:HG13	1:128:A:ASN:HB2	16	0.39
(1,51)	1:126:A:TYR:HD1	1:125:A:VAL:HG12	14	0.39
(1,48)	1:126:A:TYR:HE1	1:125:A:VAL:HG13	19	0.39
(1,48)	1:126:A:TYR:HE1	1:125:A:VAL:HG11	22	0.39
(1,42)	1:126:A:TYR:HD1	1:125:A:VAL:HB	11	0.39
(1,37)	1:127:A:ILE:HG23	1:128:A:ASN:HD22	1	0.39
(1,37)	1:127:A:ILE:HG22	1:128:A:ASN:HD22	11	0.39
(1,37)	1:127:A:ILE:HG21	1:128:A:ASN:HD22	14	0.39
(1,37)	1:127:A:ILE:HG22	1:128:A:ASN:HD22	15	0.39
(1,37)	1:127:A:ILE:HG23	1:128:A:ASN:HD22	16	0.39
(1,37)	1:127:A:ILE:HG22	1:128:A:ASN:HD22	17	0.39
(1,37)	1:127:A:ILE:HG23	1:128:A:ASN:HD22	19	0.39
(1,37)	1:127:A:ILE:HG22	1:128:A:ASN:HD22	21	0.39
(1,30)	1:129:A:GLU:HG3	1:130:A:LEU:H	25	0.39
(1,13)	1:133:A:VAL:HG11	1:108:A:ILE:HB	6	0.39
(1,13)	1:133:A:VAL:HG11	1:108:A:ILE:HB	15	0.39
(1,13)	1:133:A:VAL:HG12	1:108:A:ILE:HB	16	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6)	1:130:A:LEU:HD21	1:70:A:PHE:HE2	25	0.39
(1,2271)	2:25:B:GLU:H	2:25:B:GLU:HG2	15	0.38
(1,2265)	2:26:B:ASP:HB3	2:26:B:ASP:H	2	0.38
(1,2259)	2:27:B:SER:HB3	2:27:B:SER:H	14	0.38
(1,2197)	1:55:A:GLY:HA2	1:56:A:LYS:H	23	0.38
(1,2173)	1:63:A:ASN:H	1:109:A:LEU:HD12	6	0.38
(1,2173)	1:63:A:ASN:H	1:109:A:LEU:HD13	19	0.38
(1,2173)	1:63:A:ASN:H	1:109:A:LEU:HD11	23	0.38
(1,2173)	1:63:A:ASN:H	1:109:A:LEU:HD12	24	0.38
(1,2142)	1:109:A:LEU:HD22	1:68:A:GLU:H	18	0.38
(1,2142)	1:109:A:LEU:HD21	1:68:A:GLU:H	24	0.38
(1,2106)	1:76:A:MET:HB3	1:77:A:GLN:H	9	0.38
(1,2060)	1:86:A:PRO:HB3	1:87:A:PHE:H	22	0.38
(1,2051)	1:89:A:TYR:H	1:90:A:ASN:HB3	24	0.38
(1,2019)	1:93:A:GLN:HE22	1:93:A:GLN:HB3	2	0.38
(1,2019)	1:93:A:GLN:HE22	1:93:A:GLN:HB3	3	0.38
(1,2019)	1:93:A:GLN:HE22	1:93:A:GLN:HB3	6	0.38
(1,2019)	1:93:A:GLN:HE22	1:93:A:GLN:HB3	19	0.38
(1,2019)	1:93:A:GLN:HE22	1:93:A:GLN:HB3	23	0.38
(1,2011)	1:94:A:ARG:HD2	1:94:A:ARG:H	13	0.38
(1,2011)	1:94:A:ARG:HD2	1:94:A:ARG:H	23	0.38
(1,1971)	1:100:A:LEU:HD22	1:101:A:ALA:H	13	0.38
(1,1968)	1:101:A:ALA:H	1:63:A:ASN:HD22	8	0.38
(1,1874)	1:118:A:SER:H	1:117:A:ARG:HG2	17	0.38
(1,1851)	1:124:A:TYR:HB3	1:124:A:TYR:H	14	0.38
(1,1851)	1:124:A:TYR:HB3	1:124:A:TYR:H	18	0.38
(1,1788)	1:139:A:ALA:H	1:135:A:LYS:HD3	24	0.38
(1,1775)	1:143:A:LEU:H	1:141:A:LYS:HG2	15	0.38
(1,1755)	2:30:B:GLU:HG2	2:30:B:GLU:HA	2	0.38
(1,1755)	2:30:B:GLU:HG2	2:30:B:GLU:HA	13	0.38
(1,1754)	2:30:B:GLU:HG2	2:31:B:LEU:H	5	0.38
(1,1716)	2:31:B:LEU:HG	2:32:B:GLU:HG3	6	0.38
(1,1635)	2:39:B:TRP:HA	2:38:B:ARG:HD2	7	0.38
(1,1633)	2:38:B:ARG:HD2	2:38:B:ARG:HB2	12	0.38
(1,1633)	2:38:B:ARG:HD2	2:38:B:ARG:HB2	25	0.38
(1,1622)	2:39:B:TRP:HE3	2:39:B:TRP:HB2	1	0.38
(1,1619)	2:39:B:TRP:HD1	2:38:B:ARG:HB2	7	0.38
(1,1568)	1:57:A:LYS:HD2	1:57:A:LYS:HE2	2	0.38
(1,1568)	1:57:A:LYS:HD2	1:57:A:LYS:HE2	4	0.38
(1,1568)	1:57:A:LYS:HD2	1:57:A:LYS:HE2	7	0.38
(1,1568)	1:57:A:LYS:HD2	1:57:A:LYS:HE2	8	0.38
(1,1568)	1:57:A:LYS:HD2	1:57:A:LYS:HE2	9	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1568)	1:57:A:LYS:HD2	1:57:A:LYS:HE2	10	0.38
(1,1568)	1:57:A:LYS:HD2	1:57:A:LYS:HE2	11	0.38
(1,1568)	1:57:A:LYS:HD2	1:57:A:LYS:HE2	12	0.38
(1,1568)	1:57:A:LYS:HD2	1:57:A:LYS:HE2	13	0.38
(1,1568)	1:57:A:LYS:HD2	1:57:A:LYS:HE2	16	0.38
(1,1568)	1:57:A:LYS:HD2	1:57:A:LYS:HE2	18	0.38
(1,1568)	1:57:A:LYS:HD2	1:57:A:LYS:HE2	19	0.38
(1,1568)	1:57:A:LYS:HD2	1:57:A:LYS:HE2	21	0.38
(1,1568)	1:57:A:LYS:HD2	1:57:A:LYS:HE2	22	0.38
(1,1568)	1:57:A:LYS:HD2	1:57:A:LYS:HE2	23	0.38
(1,1568)	1:57:A:LYS:HD2	1:57:A:LYS:HE2	25	0.38
(1,1544)	1:103:A:ALA:HA	1:59:A:TYR:HE1	6	0.38
(1,1513)	1:62:A:GLU:HA	1:62:A:GLU:HG3	19	0.38
(1,1480)	1:66:A:LEU:HD21	1:63:A:ASN:HA	3	0.38
(1,1480)	1:66:A:LEU:HD21	1:63:A:ASN:HA	20	0.38
(1,1480)	1:66:A:LEU:HD22	1:63:A:ASN:HA	24	0.38
(1,1477)	1:66:A:LEU:HD22	1:113:A:LEU:HB3	23	0.38
(1,1470)	1:66:A:LEU:HD13	1:62:A:GLU:HG3	14	0.38
(1,1466)	1:109:A:LEU:HD11	1:66:A:LEU:HG	10	0.38
(1,1466)	1:109:A:LEU:HD11	1:66:A:LEU:HG	16	0.38
(1,1419)	1:71:A:LEU:HD11	1:89:A:TYR:H	9	0.38
(1,1419)	1:71:A:LEU:HD13	1:89:A:TYR:H	16	0.38
(1,1419)	1:71:A:LEU:HD11	1:89:A:TYR:H	21	0.38
(1,1416)	1:71:A:LEU:HD12	1:71:A:LEU:H	23	0.38
(1,1395)	1:116:A:ALA:HB1	1:73:A:LEU:HD23	6	0.38
(1,1385)	1:73:A:LEU:HB2	1:74:A:CYS:H	5	0.38
(1,1385)	1:73:A:LEU:HB2	1:74:A:CYS:H	17	0.38
(1,1336)	1:76:A:MET:HA	1:76:A:MET:HB2	16	0.38
(1,1336)	1:76:A:MET:HA	1:76:A:MET:HB2	21	0.38
(1,1326)	1:77:A:GLN:HG2	1:77:A:GLN:HA	6	0.38
(1,1326)	1:77:A:GLN:HG2	1:77:A:GLN:HA	10	0.38
(1,1303)	1:137:A:HIS:HE1	1:136:A:ALA:HB1	7	0.38
(1,1303)	1:137:A:HIS:HE1	1:136:A:ALA:HB3	11	0.38
(1,1303)	1:137:A:HIS:HE1	1:136:A:ALA:HB2	17	0.38
(1,1282)	1:84:A:VAL:HG22	1:85:A:VAL:H	3	0.38
(1,1280)	1:84:A:VAL:HG21	1:81:A:HIS:HB2	5	0.38
(1,1280)	1:84:A:VAL:HG21	1:81:A:HIS:HB2	12	0.38
(1,1280)	1:84:A:VAL:HG21	1:81:A:HIS:HB2	19	0.38
(1,1248)	1:85:A:VAL:HA	1:71:A:LEU:HD12	7	0.38
(1,1248)	1:85:A:VAL:HA	1:71:A:LEU:HD12	11	0.38
(1,1248)	1:85:A:VAL:HA	1:71:A:LEU:HD12	13	0.38
(1,1248)	1:85:A:VAL:HA	1:71:A:LEU:HD13	14	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1137)	1:95:A:ALA:HB1	1:91:A:ARG:HD3	14	0.38
(1,1122)	1:96:A:HIS:HA	1:139:A:ALA:HB3	1	0.38
(1,1098)	1:100:A:LEU:HD22	1:92:A:GLN:HA	5	0.38
(1,1076)	1:101:A:ALA:HB2	1:98:A:LEU:HD22	20	0.38
(1,1074)	1:101:A:ALA:HB1	1:60:A:LYS:HA	23	0.38
(1,1059)	1:103:A:ALA:HB2	1:104:A:GLU:HA	12	0.38
(1,1059)	1:103:A:ALA:HB2	1:104:A:GLU:HA	23	0.38
(1,1040)	1:62:A:GLU:HB3	1:59:A:TYR:HA	15	0.38
(1,1040)	1:62:A:GLU:HB3	1:59:A:TYR:HA	17	0.38
(1,1040)	1:62:A:GLU:HB3	1:59:A:TYR:HA	23	0.38
(1,989)	1:108:A:ILE:HG22	1:105:A:PHE:HA	11	0.38
(1,936)	1:112:A:VAL:HG12	1:112:A:VAL:HG23	3	0.38
(1,934)	1:112:A:VAL:HG11	1:126:A:TYR:HB3	21	0.38
(1,917)	1:113:A:LEU:HB2	1:113:A:LEU:HD22	4	0.38
(1,917)	1:113:A:LEU:HB2	1:113:A:LEU:HD22	9	0.38
(1,917)	1:113:A:LEU:HB2	1:113:A:LEU:HD21	15	0.38
(1,917)	1:113:A:LEU:HB2	1:113:A:LEU:HD22	17	0.38
(1,917)	1:113:A:LEU:HB2	1:113:A:LEU:HD23	18	0.38
(1,886)	1:116:A:ALA:HA	1:123:A:LEU:HD13	2	0.38
(1,886)	1:116:A:ALA:HA	1:123:A:LEU:HD12	3	0.38
(1,879)	1:94:A:ARG:HD3	1:90:A:ASN:HD22	3	0.38
(1,857)	1:119:A:ARG:HB2	1:119:A:ARG:HG3	7	0.38
(1,809)	1:123:A:LEU:HD13	1:123:A:LEU:HD22	13	0.38
(1,809)	1:123:A:LEU:HD11	1:123:A:LEU:HD23	16	0.38
(1,795)	1:127:A:ILE:HD12	1:124:A:TYR:HE1	10	0.38
(1,795)	1:127:A:ILE:HD11	1:124:A:TYR:HE1	16	0.38
(1,795)	1:127:A:ILE:HD13	1:124:A:TYR:HE1	24	0.38
(1,775)	1:126:A:TYR:HE1	1:125:A:VAL:HG12	2	0.38
(1,766)	1:126:A:TYR:HE1	1:115:A:ARG:HB2	23	0.38
(1,743)	1:127:A:ILE:HG21	1:124:A:TYR:HA	1	0.38
(1,743)	1:127:A:ILE:HG22	1:124:A:TYR:HA	8	0.38
(1,743)	1:127:A:ILE:HG23	1:124:A:TYR:HA	11	0.38
(1,743)	1:127:A:ILE:HG23	1:124:A:TYR:HA	13	0.38
(1,743)	1:127:A:ILE:HG23	1:124:A:TYR:HA	15	0.38
(1,693)	1:130:A:LEU:HA	1:130:A:LEU:HB3	1	0.38
(1,693)	1:130:A:LEU:HA	1:130:A:LEU:HB3	6	0.38
(1,693)	1:130:A:LEU:HA	1:130:A:LEU:HB3	7	0.38
(1,693)	1:130:A:LEU:HA	1:130:A:LEU:HB3	8	0.38
(1,693)	1:130:A:LEU:HA	1:130:A:LEU:HB3	9	0.38
(1,693)	1:130:A:LEU:HA	1:130:A:LEU:HB3	10	0.38
(1,693)	1:130:A:LEU:HA	1:130:A:LEU:HB3	11	0.38
(1,693)	1:130:A:LEU:HA	1:130:A:LEU:HB3	12	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,693)	1:130:A:LEU:HA	1:130:A:LEU:HB3	14	0.38
(1,693)	1:130:A:LEU:HA	1:130:A:LEU:HB3	16	0.38
(1,693)	1:130:A:LEU:HA	1:130:A:LEU:HB3	18	0.38
(1,693)	1:130:A:LEU:HA	1:130:A:LEU:HB3	20	0.38
(1,693)	1:130:A:LEU:HA	1:130:A:LEU:HB3	21	0.38
(1,693)	1:130:A:LEU:HA	1:130:A:LEU:HB3	22	0.38
(1,693)	1:130:A:LEU:HA	1:130:A:LEU:HB3	23	0.38
(1,693)	1:130:A:LEU:HA	1:130:A:LEU:HB3	24	0.38
(1,668)	1:133:A:VAL:HG12	1:130:A:LEU:HD11	10	0.38
(1,668)	1:133:A:VAL:HG11	1:130:A:LEU:HD12	15	0.38
(1,668)	1:133:A:VAL:HG11	1:130:A:LEU:HD11	21	0.38
(1,526)	1:69:A:GLU:H	1:113:A:LEU:HD21	21	0.38
(1,508)	1:77:A:GLN:HE22	1:120:A:PRO:HG2	1	0.38
(1,501)	1:80:A:ASP:HB3	1:81:A:HIS:H	1	0.38
(1,494)	1:90:A:ASN:H	1:88:A:LEU:HB2	3	0.38
(1,494)	1:90:A:ASN:H	1:88:A:LEU:HB2	13	0.38
(1,492)	1:91:A:ARG:H	1:88:A:LEU:HD21	15	0.38
(1,492)	1:91:A:ARG:H	1:88:A:LEU:HD21	20	0.38
(1,483)	1:93:A:GLN:HG2	1:94:A:ARG:H	24	0.38
(1,476)	1:96:A:HIS:H	1:95:A:ALA:H	8	0.38
(1,476)	1:96:A:HIS:H	1:95:A:ALA:H	16	0.38
(1,465)	1:106:A:CYS:H	1:103:A:ALA:HB2	2	0.38
(1,455)	1:112:A:VAL:H	1:113:A:LEU:HB3	15	0.38
(1,428)	1:128:A:ASN:HD22	1:128:A:ASN:HB3	1	0.38
(1,428)	1:128:A:ASN:HD22	1:128:A:ASN:HB3	4	0.38
(1,428)	1:128:A:ASN:HD22	1:128:A:ASN:HB3	6	0.38
(1,428)	1:128:A:ASN:HD22	1:128:A:ASN:HB3	7	0.38
(1,428)	1:128:A:ASN:HD22	1:128:A:ASN:HB3	12	0.38
(1,428)	1:128:A:ASN:HD22	1:128:A:ASN:HB3	17	0.38
(1,428)	1:128:A:ASN:HD22	1:128:A:ASN:HB3	18	0.38
(1,428)	1:128:A:ASN:HD22	1:128:A:ASN:HB3	19	0.38
(1,428)	1:128:A:ASN:HD22	1:128:A:ASN:HB3	22	0.38
(1,428)	1:128:A:ASN:HD22	1:128:A:ASN:HB3	25	0.38
(1,419)	1:129:A:GLU:H	1:126:A:TYR:H	11	0.38
(1,419)	1:129:A:GLU:H	1:126:A:TYR:H	12	0.38
(1,419)	1:129:A:GLU:H	1:126:A:TYR:H	17	0.38
(1,399)	1:135:A:LYS:H	1:133:A:VAL:HA	20	0.38
(1,379)	2:31:B:LEU:HB2	2:28:B:ASP:HB2	2	0.38
(1,379)	2:31:B:LEU:HB2	2:28:B:ASP:HB2	22	0.38
(1,340)	2:31:B:LEU:HD13	1:88:A:LEU:H	22	0.38
(1,324)	2:33:B:GLN:HG2	2:26:B:ASP:HB3	21	0.38
(1,321)	2:34:B:TYR:HD1	2:33:B:GLN:HG2	10	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,318)	2:34:B:TYR:HE1	1:83:A:GLU:HB3	3	0.38
(1,318)	2:34:B:TYR:HE1	1:83:A:GLU:HB3	4	0.38
(1,318)	2:34:B:TYR:HE1	1:83:A:GLU:HB3	16	0.38
(1,312)	2:35:B:PHE:HE1	1:124:A:TYR:HA	2	0.38
(1,312)	2:35:B:PHE:HE1	1:124:A:TYR:HA	16	0.38
(1,312)	2:35:B:PHE:HE1	1:124:A:TYR:HA	25	0.38
(1,289)	2:39:B:TRP:HZ3	2:36:B:THR:HB	14	0.38
(1,289)	2:39:B:TRP:HZ3	2:36:B:THR:HB	22	0.38
(1,281)	2:31:B:LEU:HD21	1:128:A:ASN:H	1	0.38
(1,275)	1:84:A:VAL:HG13	2:35:B:PHE:HZ	20	0.38
(1,255)	1:56:A:LYS:HA	1:56:A:LYS:HB3	19	0.38
(1,254)	1:57:A:LYS:HE2	1:54:A:MET:HG3	11	0.38
(1,244)	1:61:A:LEU:HG	1:61:A:LEU:HA	7	0.38
(1,244)	1:111:A:ARG:HA	1:115:A:ARG:HG2	22	0.38
(1,244)	1:61:A:LEU:HG	1:61:A:LEU:HA	23	0.38
(1,240)	1:104:A:GLU:HB3	1:105:A:PHE:HA	24	0.38
(1,230)	1:66:A:LEU:HA	1:113:A:LEU:HD21	16	0.38
(1,227)	1:62:A:GLU:HG2	1:61:A:LEU:HG	24	0.38
(1,220)	1:70:A:PHE:HE2	1:113:A:LEU:HB2	20	0.38
(1,199)	1:72:A:GLU:HG2	1:71:A:LEU:HB3	17	0.38
(1,195)	1:73:A:LEU:HD22	1:70:A:PHE:HA	3	0.38
(1,191)	1:84:A:VAL:HG12	1:74:A:CYS:HB2	12	0.38
(1,186)	1:123:A:LEU:HD23	1:77:A:GLN:HG3	11	0.38
(1,171)	1:84:A:VAL:HG12	1:85:A:VAL:H	21	0.38
(1,163)	1:87:A:PHE:HD1	1:88:A:LEU:HD21	20	0.38
(1,155)	1:88:A:LEU:HD21	1:131:A:CYS:HB3	11	0.38
(1,155)	1:88:A:LEU:HD11	1:74:A:CYS:HB2	18	0.38
(1,140)	1:99:A:PHE:HB3	1:138:A:SER:H	3	0.38
(1,140)	1:99:A:PHE:HB3	1:138:A:SER:H	11	0.38
(1,134)	1:92:A:GLN:HG2	1:95:A:ALA:H	22	0.38
(1,123)	1:95:A:ALA:HB1	1:134:A:LEU:HB2	18	0.38
(1,116)	1:100:A:LEU:HD23	1:105:A:PHE:HE2	11	0.38
(1,87)	1:112:A:VAL:HG13	1:130:A:LEU:H	1	0.38
(1,87)	1:112:A:VAL:HG12	1:130:A:LEU:H	21	0.38
(1,81)	1:116:A:ALA:HB2	1:70:A:PHE:HZ	24	0.38
(1,80)	1:94:A:ARG:HD2	1:93:A:GLN:HB2	12	0.38
(1,67)	1:116:A:ALA:HB1	1:120:A:PRO:HA	21	0.38
(1,67)	1:116:A:ALA:HB1	1:120:A:PRO:HA	22	0.38
(1,62)	1:123:A:LEU:HD22	1:70:A:PHE:HE1	22	0.38
(1,52)	1:125:A:VAL:HG13	1:128:A:ASN:HB2	7	0.38
(1,48)	1:126:A:TYR:HE1	1:125:A:VAL:HG11	17	0.38
(1,42)	1:126:A:TYR:HD1	1:125:A:VAL:HB	22	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,37)	1:127:A:ILE:HG22	1:128:A:ASN:HD22	4	0.38
(1,37)	1:127:A:ILE:HG21	1:128:A:ASN:HD22	5	0.38
(1,37)	1:127:A:ILE:HG21	1:128:A:ASN:HD22	8	0.38
(1,37)	1:127:A:ILE:HG22	1:128:A:ASN:HD22	13	0.38
(1,37)	1:127:A:ILE:HG23	1:128:A:ASN:HD22	20	0.38
(1,36)	1:127:A:ILE:HG21	1:124:A:TYR:HD2	19	0.38
(1,30)	1:129:A:GLU:HG3	1:130:A:LEU:H	8	0.38
(1,27)	1:130:A:LEU:HD21	1:67:A:PHE:HA	9	0.38
(1,24)	1:85:A:VAL:HG22	1:86:A:PRO:HD3	24	0.38
(1,13)	1:133:A:VAL:HG13	1:108:A:ILE:HB	20	0.38
(1,8)	1:134:A:LEU:HD21	1:105:A:PHE:HD1	23	0.38
(1,6)	1:130:A:LEU:HD23	1:70:A:PHE:HE2	24	0.38
(1,2274)	2:39:B:TRP:HE1	2:38:B:ARG:HD2	23	0.37
(1,2265)	2:26:B:ASP:HB3	2:26:B:ASP:H	1	0.37
(1,2265)	2:26:B:ASP:HB3	2:26:B:ASP:H	3	0.37
(1,2265)	2:26:B:ASP:HB3	2:26:B:ASP:H	15	0.37
(1,2265)	2:26:B:ASP:HB3	2:26:B:ASP:H	18	0.37
(1,2265)	2:26:B:ASP:HB3	2:26:B:ASP:H	25	0.37
(1,2228)	2:35:B:PHE:H	2:34:B:TYR:HB3	24	0.37
(1,2188)	1:59:A:TYR:H	1:58:A:CYS:HB2	13	0.37
(1,2173)	1:63:A:ASN:H	1:109:A:LEU:HD13	2	0.37
(1,2142)	1:109:A:LEU:HD22	1:68:A:GLU:H	8	0.37
(1,2136)	1:69:A:GLU:H	1:70:A:PHE:HB2	4	0.37
(1,2136)	1:69:A:GLU:H	1:70:A:PHE:HB2	14	0.37
(1,2060)	1:86:A:PRO:HB3	1:87:A:PHE:H	8	0.37
(1,2019)	1:93:A:GLN:HE22	1:93:A:GLN:HB3	11	0.37
(1,2013)	1:94:A:ARG:H	1:95:A:ALA:HB1	4	0.37
(1,2013)	1:94:A:ARG:H	1:95:A:ALA:HB1	25	0.37
(1,2011)	1:94:A:ARG:HD2	1:94:A:ARG:H	24	0.37
(1,2007)	1:100:A:LEU:HD21	1:95:A:ALA:H	23	0.37
(1,1996)	1:97:A:SER:H	1:139:A:ALA:HB3	13	0.37
(1,1971)	1:100:A:LEU:HD21	1:101:A:ALA:H	16	0.37
(1,1968)	1:101:A:ALA:H	1:63:A:ASN:HD22	14	0.37
(1,1924)	1:108:A:ILE:HG22	1:108:A:ILE:H	7	0.37
(1,1874)	1:118:A:SER:H	1:117:A:ARG:HG2	2	0.37
(1,1874)	1:118:A:SER:H	1:117:A:ARG:HG2	8	0.37
(1,1854)	1:124:A:TYR:H	1:125:A:VAL:HG23	25	0.37
(1,1781)	1:140:A:LYS:H	1:141:A:LYS:HB3	15	0.37
(1,1755)	2:30:B:GLU:HG2	2:30:B:GLU:HA	8	0.37
(1,1755)	2:30:B:GLU:HG2	2:30:B:GLU:HA	23	0.37
(1,1745)	2:29:B:SER:HB3	2:30:B:GLU:H	21	0.37
(1,1727)	2:31:B:LEU:HD12	2:31:B:LEU:H	1	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1650)	2:37:B:ALA:HB3	1:121:A:ALA:HB1	7	0.37
(1,1618)	2:39:B:TRP:HD1	2:39:B:TRP:HB3	19	0.37
(1,1576)	1:73:A:LEU:HD13	1:117:A:ARG:H	9	0.37
(1,1569)	1:57:A:LYS:HE3	1:59:A:TYR:HE1	20	0.37
(1,1568)	1:57:A:LYS:HD2	1:57:A:LYS:HE2	1	0.37
(1,1568)	1:57:A:LYS:HD2	1:57:A:LYS:HE2	15	0.37
(1,1568)	1:57:A:LYS:HD2	1:57:A:LYS:HE2	17	0.37
(1,1568)	1:57:A:LYS:HD2	1:57:A:LYS:HE2	24	0.37
(1,1481)	1:66:A:LEU:HD22	1:69:A:GLU:H	9	0.37
(1,1480)	1:66:A:LEU:HD23	1:63:A:ASN:HA	1	0.37
(1,1480)	1:66:A:LEU:HD22	1:63:A:ASN:HA	14	0.37
(1,1477)	1:66:A:LEU:HD21	1:113:A:LEU:HB3	7	0.37
(1,1475)	1:66:A:LEU:HD22	1:109:A:LEU:HD23	15	0.37
(1,1470)	1:66:A:LEU:HD11	1:62:A:GLU:HG3	2	0.37
(1,1466)	1:109:A:LEU:HD12	1:66:A:LEU:HG	6	0.37
(1,1466)	1:109:A:LEU:HD12	1:66:A:LEU:HG	9	0.37
(1,1466)	1:109:A:LEU:HD13	1:66:A:LEU:HG	25	0.37
(1,1457)	1:68:A:GLU:HB2	1:68:A:GLU:HG2	13	0.37
(1,1456)	1:69:A:GLU:HG2	1:66:A:LEU:HA	3	0.37
(1,1447)	1:69:A:GLU:HA	1:69:A:GLU:HG3	1	0.37
(1,1422)	1:71:A:LEU:HD21	1:74:A:CYS:H	19	0.37
(1,1416)	1:71:A:LEU:HD12	1:71:A:LEU:H	2	0.37
(1,1416)	1:71:A:LEU:HD13	1:71:A:LEU:H	9	0.37
(1,1385)	1:73:A:LEU:HB2	1:74:A:CYS:H	7	0.37
(1,1385)	1:73:A:LEU:HB2	1:74:A:CYS:H	21	0.37
(1,1385)	1:73:A:LEU:HB2	1:74:A:CYS:H	22	0.37
(1,1345)	1:76:A:MET:HG2	1:77:A:GLN:H	1	0.37
(1,1337)	1:76:A:MET:HA	1:76:A:MET:HG3	1	0.37
(1,1336)	1:76:A:MET:HA	1:76:A:MET:HB2	17	0.37
(1,1331)	1:77:A:GLN:HG2	1:73:A:LEU:HD11	2	0.37
(1,1331)	1:77:A:GLN:HG2	1:73:A:LEU:HD12	9	0.37
(1,1303)	1:137:A:HIS:HE1	1:136:A:ALA:HB3	2	0.37
(1,1303)	1:137:A:HIS:HE1	1:136:A:ALA:HB3	24	0.37
(1,1295)	1:82:A:PRO:HG2	1:81:A:HIS:HA	9	0.37
(1,1295)	1:82:A:PRO:HG2	1:81:A:HIS:HA	18	0.37
(1,1282)	1:84:A:VAL:HG23	1:85:A:VAL:H	2	0.37
(1,1282)	1:84:A:VAL:HG21	1:85:A:VAL:H	9	0.37
(1,1282)	1:84:A:VAL:HG23	1:85:A:VAL:H	17	0.37
(1,1280)	1:84:A:VAL:HG23	1:81:A:HIS:HB2	10	0.37
(1,1248)	1:85:A:VAL:HA	1:71:A:LEU:HD13	6	0.37
(1,1248)	1:85:A:VAL:HA	1:71:A:LEU:HD13	25	0.37
(1,1183)	1:90:A:ASN:HB2	1:87:A:PHE:HD1	4	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1139)	1:134:A:LEU:HD22	1:95:A:ALA:HB2	2	0.37
(1,1139)	1:134:A:LEU:HD21	1:95:A:ALA:HB3	7	0.37
(1,1137)	1:95:A:ALA:HB3	1:91:A:ARG:HD3	1	0.37
(1,1126)	1:96:A:HIS:HD2	1:139:A:ALA:HB2	3	0.37
(1,1122)	1:96:A:HIS:HA	1:139:A:ALA:HB2	2	0.37
(1,1076)	1:101:A:ALA:HB3	1:98:A:LEU:HD23	21	0.37
(1,1040)	1:62:A:GLU:HB3	1:59:A:TYR:HA	9	0.37
(1,1000)	1:108:A:ILE:HD13	1:99:A:PHE:HE1	5	0.37
(1,942)	1:111:A:ARG:HB2	1:111:A:ARG:HD2	18	0.37
(1,936)	1:112:A:VAL:HG13	1:112:A:VAL:HG21	4	0.37
(1,936)	1:112:A:VAL:HG11	1:112:A:VAL:HG22	10	0.37
(1,934)	1:112:A:VAL:HG13	1:126:A:TYR:HB3	12	0.37
(1,922)	1:112:A:VAL:HA	1:115:A:ARG:HG3	24	0.37
(1,917)	1:113:A:LEU:HB2	1:113:A:LEU:HD21	2	0.37
(1,917)	1:113:A:LEU:HB2	1:113:A:LEU:HD22	3	0.37
(1,917)	1:113:A:LEU:HB2	1:113:A:LEU:HD23	5	0.37
(1,917)	1:113:A:LEU:HB2	1:113:A:LEU:HD22	14	0.37
(1,886)	1:116:A:ALA:HA	1:123:A:LEU:HD13	16	0.37
(1,809)	1:123:A:LEU:HD13	1:123:A:LEU:HD22	5	0.37
(1,809)	1:123:A:LEU:HD13	1:123:A:LEU:HD21	7	0.37
(1,809)	1:123:A:LEU:HD12	1:123:A:LEU:HD22	17	0.37
(1,809)	1:123:A:LEU:HD12	1:123:A:LEU:HD21	18	0.37
(1,809)	1:123:A:LEU:HD13	1:123:A:LEU:HD21	21	0.37
(1,809)	1:123:A:LEU:HD11	1:123:A:LEU:HD22	23	0.37
(1,809)	1:123:A:LEU:HD12	1:123:A:LEU:HD22	25	0.37
(1,793)	1:124:A:TYR:HE1	1:124:A:TYR:H	2	0.37
(1,743)	1:127:A:ILE:HG21	1:124:A:TYR:HA	6	0.37
(1,743)	1:127:A:ILE:HG23	1:124:A:TYR:HA	7	0.37
(1,743)	1:127:A:ILE:HG23	1:124:A:TYR:HA	17	0.37
(1,743)	1:127:A:ILE:HG23	1:124:A:TYR:HA	21	0.37
(1,743)	1:127:A:ILE:HG23	1:124:A:TYR:HA	22	0.37
(1,743)	1:127:A:ILE:HG22	1:124:A:TYR:HA	23	0.37
(1,693)	1:130:A:LEU:HA	1:130:A:LEU:HB3	2	0.37
(1,693)	1:130:A:LEU:HA	1:130:A:LEU:HB3	4	0.37
(1,693)	1:130:A:LEU:HA	1:130:A:LEU:HB3	5	0.37
(1,693)	1:130:A:LEU:HA	1:130:A:LEU:HB3	15	0.37
(1,693)	1:130:A:LEU:HA	1:130:A:LEU:HB3	17	0.37
(1,693)	1:130:A:LEU:HA	1:130:A:LEU:HB3	19	0.37
(1,693)	1:130:A:LEU:HA	1:130:A:LEU:HB3	25	0.37
(1,668)	1:133:A:VAL:HG13	1:130:A:LEU:HD13	5	0.37
(1,668)	1:133:A:VAL:HG11	1:130:A:LEU:HD12	6	0.37
(1,668)	1:133:A:VAL:HG12	1:130:A:LEU:HD11	8	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,643)	1:134:A:LEU:HD22	1:134:A:LEU:HD12	4	0.37
(1,558)	2:32:B:GLU:HA	2:31:B:LEU:H	22	0.37
(1,541)	1:61:A:LEU:HB3	1:62:A:GLU:H	9	0.37
(1,538)	1:63:A:ASN:H	1:61:A:LEU:HA	1	0.37
(1,538)	1:63:A:ASN:H	1:61:A:LEU:HA	15	0.37
(1,515)	1:73:A:LEU:HG	1:76:A:MET:H	3	0.37
(1,515)	1:73:A:LEU:HG	1:76:A:MET:H	21	0.37
(1,505)	1:79:A:ALA:H	1:76:A:MET:HA	1	0.37
(1,505)	1:79:A:ALA:H	1:76:A:MET:HA	8	0.37
(1,505)	1:79:A:ALA:H	1:76:A:MET:HA	10	0.37
(1,500)	1:85:A:VAL:H	1:83:A:GLU:H	10	0.37
(1,494)	1:90:A:ASN:H	1:88:A:LEU:HB2	1	0.37
(1,494)	1:90:A:ASN:H	1:88:A:LEU:HB2	10	0.37
(1,492)	1:91:A:ARG:H	1:88:A:LEU:HD21	4	0.37
(1,490)	1:91:A:ARG:H	1:94:A:ARG:H	20	0.37
(1,483)	1:93:A:GLN:HG2	1:94:A:ARG:H	3	0.37
(1,483)	1:93:A:GLN:HG2	1:94:A:ARG:H	19	0.37
(1,483)	1:93:A:GLN:HG2	1:94:A:ARG:H	22	0.37
(1,480)	1:134:A:LEU:HD12	1:95:A:ALA:H	6	0.37
(1,476)	1:96:A:HIS:H	1:95:A:ALA:H	1	0.37
(1,476)	1:96:A:HIS:H	1:95:A:ALA:H	4	0.37
(1,476)	1:96:A:HIS:H	1:95:A:ALA:H	7	0.37
(1,476)	1:96:A:HIS:H	1:95:A:ALA:H	13	0.37
(1,465)	1:108:A:ILE:HD11	1:106:A:CYS:H	14	0.37
(1,465)	1:106:A:CYS:H	1:103:A:ALA:HB1	18	0.37
(1,445)	1:116:A:ALA:H	1:112:A:VAL:HA	10	0.37
(1,445)	1:116:A:ALA:H	1:112:A:VAL:HA	22	0.37
(1,445)	1:116:A:ALA:H	1:112:A:VAL:HA	24	0.37
(1,434)	1:74:A:CYS:H	1:123:A:LEU:HD11	2	0.37
(1,428)	1:128:A:ASN:HD22	1:128:A:ASN:HB3	15	0.37
(1,428)	1:128:A:ASN:HD22	1:128:A:ASN:HB3	23	0.37
(1,421)	1:128:A:ASN:H	1:70:A:PHE:HZ	14	0.37
(1,419)	1:129:A:GLU:H	1:126:A:TYR:H	4	0.37
(1,419)	1:129:A:GLU:H	1:126:A:TYR:H	23	0.37
(1,379)	2:31:B:LEU:HB2	2:28:B:ASP:HB2	8	0.37
(1,369)	2:26:B:ASP:HB2	1:87:A:PHE:HZ	12	0.37
(1,368)	2:26:B:ASP:HB3	1:87:A:PHE:HZ	5	0.37
(1,366)	1:100:A:LEU:HD12	1:138:A:SER:HB3	5	0.37
(1,342)	2:31:B:LEU:HD11	1:124:A:TYR:HB3	10	0.37
(1,337)	2:31:B:LEU:HD23	2:28:B:ASP:HB2	2	0.37
(1,318)	2:34:B:TYR:HE1	1:83:A:GLU:HB3	10	0.37
(1,312)	2:35:B:PHE:HE1	2:36:B:THR:HA	6	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,312)	2:35:B:PHE:HE1	1:124:A:TYR:HA	9	0.37
(1,257)	1:113:A:LEU:HD13	1:113:A:LEU:HB2	14	0.37
(1,257)	1:113:A:LEU:HD11	1:113:A:LEU:HB2	24	0.37
(1,255)	1:56:A:LYS:HA	1:56:A:LYS:HB3	22	0.37
(1,240)	1:104:A:GLU:HB3	1:105:A:PHE:HA	1	0.37
(1,240)	1:104:A:GLU:HB3	1:105:A:PHE:HA	20	0.37
(1,236)	1:64:A:GLU:HA	1:67:A:PHE:H	16	0.37
(1,236)	1:64:A:GLU:HA	1:67:A:PHE:H	22	0.37
(1,230)	1:66:A:LEU:HA	1:113:A:LEU:HD22	24	0.37
(1,220)	1:70:A:PHE:HE2	1:113:A:LEU:HB2	11	0.37
(1,209)	1:71:A:LEU:HD21	1:67:A:PHE:HE2	3	0.37
(1,194)	1:73:A:LEU:HD22	1:70:A:PHE:HD1	22	0.37
(1,171)	1:84:A:VAL:HG13	1:85:A:VAL:H	16	0.37
(1,155)	1:88:A:LEU:HD11	1:74:A:CYS:HB2	12	0.37
(1,145)	1:88:A:LEU:HB3	1:85:A:VAL:HA	7	0.37
(1,132)	1:92:A:GLN:HB3	1:89:A:TYR:HD1	1	0.37
(1,121)	1:95:A:ALA:HB3	1:134:A:LEU:HA	17	0.37
(1,98)	1:105:A:PHE:HD1	1:100:A:LEU:HD21	1	0.37
(1,98)	1:105:A:PHE:HD1	1:100:A:LEU:HD23	2	0.37
(1,98)	1:105:A:PHE:HD1	1:100:A:LEU:HD22	19	0.37
(1,87)	1:112:A:VAL:HG13	1:130:A:LEU:H	4	0.37
(1,67)	1:116:A:ALA:HB1	1:120:A:PRO:HA	15	0.37
(1,62)	1:123:A:LEU:HD22	1:70:A:PHE:HE1	10	0.37
(1,56)	1:124:A:TYR:HE2	2:35:B:PHE:HB3	6	0.37
(1,56)	1:124:A:TYR:HE2	2:35:B:PHE:HB3	19	0.37
(1,52)	1:125:A:VAL:HG12	1:128:A:ASN:HB2	4	0.37
(1,52)	1:125:A:VAL:HG13	1:128:A:ASN:HB2	11	0.37
(1,51)	1:126:A:TYR:HD1	1:125:A:VAL:HG11	2	0.37
(1,51)	1:126:A:TYR:HD1	1:125:A:VAL:HG12	20	0.37
(1,51)	1:126:A:TYR:HD1	1:125:A:VAL:HG12	23	0.37
(1,48)	1:126:A:TYR:HE1	1:125:A:VAL:HG11	16	0.37
(1,48)	1:126:A:TYR:HE1	1:125:A:VAL:HG12	18	0.37
(1,48)	1:126:A:TYR:HE1	1:125:A:VAL:HG12	24	0.37
(1,48)	1:126:A:TYR:HE1	1:125:A:VAL:HG13	25	0.37
(1,37)	1:127:A:ILE:HG23	1:128:A:ASN:HD22	6	0.37
(1,37)	1:127:A:ILE:HG22	1:128:A:ASN:HD22	7	0.37
(1,37)	1:127:A:ILE:HG21	1:128:A:ASN:HD22	9	0.37
(1,36)	1:127:A:ILE:HG22	1:124:A:TYR:HD2	18	0.37
(1,36)	1:127:A:ILE:HG21	1:124:A:TYR:HD2	25	0.37
(1,30)	1:129:A:GLU:HG3	1:130:A:LEU:H	3	0.37
(1,30)	1:129:A:GLU:HG3	1:130:A:LEU:H	10	0.37
(1,30)	1:129:A:GLU:HG3	1:130:A:LEU:H	19	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,27)	1:130:A:LEU:HD22	1:67:A:PHE:HA	10	0.37
(1,13)	1:133:A:VAL:HG11	1:108:A:ILE:HB	24	0.37
(1,8)	1:134:A:LEU:HD21	1:67:A:PHE:HZ	17	0.37
(1,6)	1:130:A:LEU:HD23	1:70:A:PHE:HE2	6	0.37
(1,2173)	1:63:A:ASN:H	1:109:A:LEU:HD11	17	0.36
(1,2173)	1:63:A:ASN:H	1:109:A:LEU:HD11	25	0.36
(1,2142)	1:109:A:LEU:HD23	1:68:A:GLU:H	2	0.36
(1,2142)	1:109:A:LEU:HD22	1:68:A:GLU:H	4	0.36
(1,2051)	1:89:A:TYR:H	1:90:A:ASN:HB3	15	0.36
(1,2019)	1:93:A:GLN:HE22	1:93:A:GLN:HB3	15	0.36
(1,2017)	1:93:A:GLN:HE22	1:89:A:TYR:HB3	1	0.36
(1,2007)	1:100:A:LEU:HD21	1:95:A:ALA:H	22	0.36
(1,2005)	1:95:A:ALA:H	1:94:A:ARG:HG2	13	0.36
(1,1996)	1:97:A:SER:H	1:139:A:ALA:HB2	11	0.36
(1,1971)	1:100:A:LEU:HD22	1:101:A:ALA:H	18	0.36
(1,1854)	1:124:A:TYR:H	1:125:A:VAL:HG23	18	0.36
(1,1775)	1:143:A:LEU:H	1:141:A:LYS:HG3	24	0.36
(1,1768)	2:24:B:GLN:HB2	2:24:B:GLN:HG2	7	0.36
(1,1755)	2:30:B:GLU:HG2	2:30:B:GLU:HA	20	0.36
(1,1745)	2:29:B:SER:HB3	2:30:B:GLU:H	22	0.36
(1,1727)	2:31:B:LEU:HD11	2:31:B:LEU:H	20	0.36
(1,1720)	2:34:B:TYR:HE1	2:31:B:LEU:HD23	1	0.36
(1,1720)	2:34:B:TYR:HE1	2:31:B:LEU:HD22	10	0.36
(1,1720)	2:34:B:TYR:HE1	2:31:B:LEU:HD21	21	0.36
(1,1716)	2:31:B:LEU:HG	2:32:B:GLU:HG3	25	0.36
(1,1703)	2:33:B:GLN:HG2	2:31:B:LEU:HD21	24	0.36
(1,1651)	2:38:B:ARG:HG2	2:37:B:ALA:HB3	12	0.36
(1,1648)	2:38:B:ARG:HA	2:37:B:ALA:HB1	18	0.36
(1,1622)	2:39:B:TRP:HE3	2:39:B:TRP:HB2	16	0.36
(1,1622)	2:39:B:TRP:HE3	2:39:B:TRP:HB2	18	0.36
(1,1618)	2:39:B:TRP:HD1	2:39:B:TRP:HB3	1	0.36
(1,1618)	2:39:B:TRP:HD1	2:39:B:TRP:HB3	6	0.36
(1,1618)	2:39:B:TRP:HD1	2:39:B:TRP:HB3	11	0.36
(1,1618)	2:39:B:TRP:HD1	2:39:B:TRP:HB3	15	0.36
(1,1618)	2:39:B:TRP:HD1	2:39:B:TRP:HB3	16	0.36
(1,1618)	2:39:B:TRP:HD1	2:39:B:TRP:HB3	25	0.36
(1,1588)	1:87:A:PHE:HB2	2:31:B:LEU:HD11	24	0.36
(1,1577)	1:77:A:GLN:HG3	1:73:A:LEU:HD11	13	0.36
(1,1577)	1:77:A:GLN:HG3	1:73:A:LEU:HD12	14	0.36
(1,1568)	1:57:A:LYS:HD2	1:57:A:LYS:HE2	14	0.36
(1,1568)	1:57:A:LYS:HD2	1:57:A:LYS:HE2	20	0.36
(1,1538)	1:59:A:TYR:HB3	1:59:A:TYR:HD1	23	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1489)	1:65:A:LYS:HG2	1:66:A:LEU:H	6	0.36
(1,1481)	1:66:A:LEU:HD22	1:69:A:GLU:H	4	0.36
(1,1470)	1:66:A:LEU:HD11	1:62:A:GLU:HG3	1	0.36
(1,1470)	1:66:A:LEU:HD13	1:62:A:GLU:HG3	18	0.36
(1,1470)	1:66:A:LEU:HD11	1:62:A:GLU:HG3	21	0.36
(1,1466)	1:109:A:LEU:HD13	1:66:A:LEU:HG	19	0.36
(1,1416)	1:71:A:LEU:HD12	1:71:A:LEU:H	4	0.36
(1,1416)	1:71:A:LEU:HD13	1:71:A:LEU:H	12	0.36
(1,1385)	1:73:A:LEU:HB2	1:74:A:CYS:H	25	0.36
(1,1345)	1:76:A:MET:HG2	1:77:A:GLN:H	20	0.36
(1,1331)	1:77:A:GLN:HG2	1:73:A:LEU:HD13	16	0.36
(1,1331)	1:77:A:GLN:HG2	1:73:A:LEU:HD13	21	0.36
(1,1326)	1:77:A:GLN:HG2	1:77:A:GLN:HA	8	0.36
(1,1326)	1:77:A:GLN:HG2	1:77:A:GLN:HA	15	0.36
(1,1295)	1:82:A:PRO:HG2	1:81:A:HIS:HA	17	0.36
(1,1295)	1:82:A:PRO:HG2	1:81:A:HIS:HA	21	0.36
(1,1295)	1:82:A:PRO:HG2	1:81:A:HIS:HA	22	0.36
(1,1282)	1:84:A:VAL:HG21	1:85:A:VAL:H	20	0.36
(1,1252)	1:69:A:GLU:HB2	1:69:A:GLU:HG2	10	0.36
(1,1248)	1:85:A:VAL:HA	1:71:A:LEU:HD11	8	0.36
(1,1248)	1:85:A:VAL:HA	1:71:A:LEU:HD12	12	0.36
(1,1228)	1:87:A:PHE:HD1	1:88:A:LEU:HD21	9	0.36
(1,1209)	1:88:A:LEU:HD12	1:70:A:PHE:HE1	12	0.36
(1,1197)	1:89:A:TYR:HD2	1:71:A:LEU:HD21	21	0.36
(1,1185)	1:90:A:ASN:HB2	1:90:A:ASN:HD22	4	0.36
(1,1185)	1:90:A:ASN:HB2	1:90:A:ASN:HD22	14	0.36
(1,1185)	1:90:A:ASN:HB2	1:90:A:ASN:HD22	17	0.36
(1,1185)	1:90:A:ASN:HB2	1:90:A:ASN:HD22	20	0.36
(1,1185)	1:90:A:ASN:HB2	1:90:A:ASN:HD22	24	0.36
(1,1133)	1:95:A:ALA:HB1	1:99:A:PHE:HD2	1	0.36
(1,1098)	1:100:A:LEU:HD22	1:92:A:GLN:HA	3	0.36
(1,1096)	1:100:A:LEU:HD22	1:92:A:GLN:HG3	12	0.36
(1,1094)	1:100:A:LEU:HD22	1:138:A:SER:HB2	25	0.36
(1,1089)	1:105:A:PHE:HZ	1:100:A:LEU:HD22	10	0.36
(1,1088)	1:100:A:LEU:HD23	1:105:A:PHE:HD2	24	0.36
(1,1074)	1:101:A:ALA:HB1	1:60:A:LYS:HA	6	0.36
(1,996)	1:108:A:ILE:HG22	1:112:A:VAL:HG12	20	0.36
(1,989)	1:108:A:ILE:HG21	1:105:A:PHE:HA	20	0.36
(1,936)	1:112:A:VAL:HG11	1:112:A:VAL:HG23	15	0.36
(1,936)	1:112:A:VAL:HG12	1:112:A:VAL:HG22	25	0.36
(1,934)	1:112:A:VAL:HG12	1:126:A:TYR:HB3	1	0.36
(1,934)	1:112:A:VAL:HG11	1:126:A:TYR:HB3	23	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,917)	1:113:A:LEU:HB2	1:113:A:LEU:HD22	10	0.36
(1,917)	1:113:A:LEU:HB2	1:113:A:LEU:HD21	22	0.36
(1,888)	1:116:A:ALA:HB3	1:123:A:LEU:H	5	0.36
(1,886)	1:116:A:ALA:HA	1:123:A:LEU:HD12	19	0.36
(1,886)	1:116:A:ALA:HA	1:123:A:LEU:HD12	22	0.36
(1,875)	1:118:A:SER:HA	1:118:A:SER:HB2	1	0.36
(1,867)	1:119:A:ARG:HD3	1:119:A:ARG:HA	19	0.36
(1,858)	1:119:A:ARG:HG3	1:119:A:ARG:HA	1	0.36
(1,809)	1:123:A:LEU:HD12	1:123:A:LEU:HD23	1	0.36
(1,809)	1:123:A:LEU:HD12	1:123:A:LEU:HD23	2	0.36
(1,809)	1:123:A:LEU:HD11	1:123:A:LEU:HD22	9	0.36
(1,809)	1:123:A:LEU:HD13	1:123:A:LEU:HD23	12	0.36
(1,809)	1:123:A:LEU:HD13	1:123:A:LEU:HD21	14	0.36
(1,809)	1:123:A:LEU:HD12	1:123:A:LEU:HD21	20	0.36
(1,795)	1:127:A:ILE:HD12	1:124:A:TYR:HE1	13	0.36
(1,766)	1:126:A:TYR:HE1	1:115:A:ARG:HB2	1	0.36
(1,743)	1:127:A:ILE:HG22	1:124:A:TYR:HA	5	0.36
(1,743)	1:127:A:ILE:HG21	1:124:A:TYR:HA	19	0.36
(1,693)	1:130:A:LEU:HA	1:130:A:LEU:HB3	3	0.36
(1,668)	1:133:A:VAL:HG12	1:130:A:LEU:HD12	1	0.36
(1,668)	1:133:A:VAL:HG12	1:130:A:LEU:HD13	3	0.36
(1,668)	1:133:A:VAL:HG11	1:130:A:LEU:HD13	4	0.36
(1,668)	1:133:A:VAL:HG13	1:130:A:LEU:HD13	9	0.36
(1,668)	1:133:A:VAL:HG12	1:130:A:LEU:HD11	17	0.36
(1,668)	1:133:A:VAL:HG11	1:130:A:LEU:HD13	18	0.36
(1,668)	1:133:A:VAL:HG13	1:130:A:LEU:HD13	25	0.36
(1,643)	1:134:A:LEU:HD22	1:134:A:LEU:HD12	12	0.36
(1,558)	2:32:B:GLU:HA	2:31:B:LEU:H	18	0.36
(1,558)	2:32:B:GLU:HA	2:31:B:LEU:H	23	0.36
(1,526)	1:69:A:GLU:H	1:113:A:LEU:HD21	15	0.36
(1,521)	1:71:A:LEU:H	1:113:A:LEU:HD11	22	0.36
(1,512)	1:77:A:GLN:H	1:123:A:LEU:HD21	22	0.36
(1,500)	1:85:A:VAL:H	1:83:A:GLU:H	9	0.36
(1,483)	1:93:A:GLN:HG2	1:94:A:ARG:H	21	0.36
(1,476)	1:96:A:HIS:H	1:95:A:ALA:H	2	0.36
(1,476)	1:96:A:HIS:H	1:95:A:ALA:H	9	0.36
(1,465)	1:106:A:CYS:H	1:103:A:ALA:HB1	24	0.36
(1,451)	1:114:A:SER:H	1:117:A:ARG:HB2	14	0.36
(1,445)	1:116:A:ALA:H	1:112:A:VAL:HA	13	0.36
(1,419)	1:129:A:GLU:H	1:126:A:TYR:H	6	0.36
(1,419)	1:129:A:GLU:H	1:126:A:TYR:H	8	0.36
(1,419)	1:129:A:GLU:H	1:126:A:TYR:H	15	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,419)	1:129:A:GLU:H	1:126:A:TYR:H	18	0.36
(1,419)	1:129:A:GLU:H	1:126:A:TYR:H	25	0.36
(1,414)	1:72:A:GLU:H	1:68:A:GLU:HA	2	0.36
(1,414)	1:72:A:GLU:H	1:68:A:GLU:HA	15	0.36
(1,395)	1:138:A:SER:H	1:95:A:ALA:HB3	24	0.36
(1,387)	1:141:A:LYS:H	1:141:A:LYS:HG2	22	0.36
(1,379)	2:31:B:LEU:HB2	2:28:B:ASP:HB2	5	0.36
(1,369)	2:26:B:ASP:HB2	1:87:A:PHE:HZ	7	0.36
(1,356)	2:29:B:SER:HB2	2:33:B:GLN:H	8	0.36
(1,355)	2:29:B:SER:HB3	2:33:B:GLN:H	19	0.36
(1,340)	2:31:B:LEU:HD13	1:88:A:LEU:H	25	0.36
(1,337)	2:31:B:LEU:HD22	2:28:B:ASP:HB3	20	0.36
(1,318)	2:34:B:TYR:HE1	1:83:A:GLU:HB3	23	0.36
(1,289)	2:39:B:TRP:HZ3	2:36:B:THR:HB	5	0.36
(1,281)	2:31:B:LEU:HD22	1:128:A:ASN:H	2	0.36
(1,275)	1:84:A:VAL:HG11	2:35:B:PHE:HE1	2	0.36
(1,257)	1:113:A:LEU:HD13	1:113:A:LEU:HB2	9	0.36
(1,244)	1:61:A:LEU:HG	1:61:A:LEU:HA	13	0.36
(1,244)	1:61:A:LEU:HG	1:61:A:LEU:HA	25	0.36
(1,240)	1:104:A:GLU:HB3	1:99:A:PHE:HA	15	0.36
(1,240)	1:104:A:GLU:HB3	1:105:A:PHE:HA	23	0.36
(1,236)	1:64:A:GLU:HA	1:67:A:PHE:H	25	0.36
(1,225)	1:129:A:GLU:HG2	1:125:A:VAL:HG12	1	0.36
(1,225)	1:129:A:GLU:HG2	1:125:A:VAL:HG12	25	0.36
(1,209)	1:67:A:PHE:HE1	1:71:A:LEU:HD22	7	0.36
(1,191)	1:84:A:VAL:HG12	1:74:A:CYS:HB2	22	0.36
(1,172)	1:85:A:VAL:HG13	1:74:A:CYS:HB3	19	0.36
(1,172)	1:85:A:VAL:HG12	1:74:A:CYS:HB3	23	0.36
(1,163)	1:87:A:PHE:HD1	1:88:A:LEU:HD22	2	0.36
(1,155)	1:88:A:LEU:HD22	1:131:A:CYS:HB3	23	0.36
(1,147)	1:137:A:HIS:HB3	1:138:A:SER:H	9	0.36
(1,132)	1:92:A:GLN:HB3	1:89:A:TYR:HD1	19	0.36
(1,122)	1:95:A:ALA:HB2	1:91:A:ARG:HD3	25	0.36
(1,121)	1:95:A:ALA:HB2	1:134:A:LEU:HA	7	0.36
(1,116)	1:100:A:LEU:HD22	1:105:A:PHE:HE2	1	0.36
(1,98)	1:105:A:PHE:HD1	1:100:A:LEU:HD22	14	0.36
(1,95)	1:107:A:ASN:HB2	1:108:A:ILE:HB	23	0.36
(1,94)	1:90:A:ASN:HA	1:91:A:ARG:H	10	0.36
(1,87)	1:112:A:VAL:HG11	1:130:A:LEU:H	2	0.36
(1,87)	1:112:A:VAL:HG12	1:130:A:LEU:H	24	0.36
(1,54)	1:127:A:ILE:HG23	1:124:A:TYR:HD1	24	0.36
(1,51)	1:126:A:TYR:HD1	1:125:A:VAL:HG12	12	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,42)	1:126:A:TYR:HD1	1:125:A:VAL:HB	1	0.36
(1,37)	1:127:A:ILE:HG21	1:128:A:ASN:HD22	18	0.36
(1,37)	1:127:A:ILE:HG22	1:128:A:ASN:HD22	22	0.36
(1,37)	1:127:A:ILE:HG23	1:128:A:ASN:HD22	25	0.36
(1,36)	1:127:A:ILE:HG22	1:124:A:TYR:HD2	9	0.36
(1,30)	1:129:A:GLU:HG3	1:130:A:LEU:H	17	0.36
(1,24)	1:85:A:VAL:HG22	1:71:A:LEU:HA	8	0.36
(1,24)	1:85:A:VAL:HG22	1:86:A:PRO:HD3	10	0.36
(1,2265)	2:26:B:ASP:HB3	2:26:B:ASP:H	4	0.35
(1,2265)	2:26:B:ASP:HB3	2:26:B:ASP:H	7	0.35
(1,2264)	2:25:B:GLU:HA	2:26:B:ASP:H	9	0.35
(1,2244)	2:36:B:THR:HG21	2:36:B:THR:H	12	0.35
(1,2244)	2:36:B:THR:HG23	2:36:B:THR:H	17	0.35
(1,2142)	1:109:A:LEU:HD23	1:68:A:GLU:H	9	0.35
(1,2142)	1:109:A:LEU:HD21	1:68:A:GLU:H	12	0.35
(1,2142)	1:109:A:LEU:HD22	1:68:A:GLU:H	13	0.35
(1,2142)	1:109:A:LEU:HD23	1:68:A:GLU:H	15	0.35
(1,2142)	1:109:A:LEU:HD23	1:68:A:GLU:H	16	0.35
(1,2142)	1:109:A:LEU:HD21	1:68:A:GLU:H	22	0.35
(1,2100)	1:77:A:GLN:HE21	1:76:A:MET:HE2	22	0.35
(1,2033)	1:90:A:ASN:HD22	1:94:A:ARG:HG2	22	0.35
(1,2019)	1:93:A:GLN:HE22	1:93:A:GLN:HB3	1	0.35
(1,2019)	1:93:A:GLN:HE22	1:93:A:GLN:HB3	8	0.35
(1,2011)	1:94:A:ARG:HD2	1:94:A:ARG:H	5	0.35
(1,2007)	1:100:A:LEU:HD22	1:95:A:ALA:H	3	0.35
(1,1971)	1:100:A:LEU:HD22	1:101:A:ALA:H	19	0.35
(1,1958)	1:103:A:ALA:H	1:102:A:SER:HB3	25	0.35
(1,1854)	1:124:A:TYR:H	1:125:A:VAL:HG21	9	0.35
(1,1854)	1:124:A:TYR:H	1:125:A:VAL:HG21	13	0.35
(1,1854)	1:124:A:TYR:H	1:125:A:VAL:HG23	22	0.35
(1,1772)	1:142:A:LYS:H	1:141:A:LYS:HG2	19	0.35
(1,1768)	2:24:B:GLN:HB2	2:24:B:GLN:HG2	1	0.35
(1,1768)	2:24:B:GLN:HG3	2:24:B:GLN:HB2	8	0.35
(1,1768)	2:24:B:GLN:HG3	2:24:B:GLN:HB2	9	0.35
(1,1768)	2:24:B:GLN:HG3	2:24:B:GLN:HB2	12	0.35
(1,1768)	2:24:B:GLN:HG3	2:24:B:GLN:HB2	16	0.35
(1,1754)	2:30:B:GLU:HG2	2:31:B:LEU:H	20	0.35
(1,1727)	2:31:B:LEU:HD13	2:31:B:LEU:H	15	0.35
(1,1725)	2:31:B:LEU:HD22	1:127:A:ILE:HG23	16	0.35
(1,1720)	2:34:B:TYR:HE1	2:31:B:LEU:HD21	14	0.35
(1,1720)	2:34:B:TYR:HE1	2:31:B:LEU:HD23	25	0.35
(1,1716)	2:31:B:LEU:HG	2:32:B:GLU:HG3	9	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1716)	2:31:B:LEU:HG	2:32:B:GLU:HG3	10	0.35
(1,1716)	2:31:B:LEU:HG	2:32:B:GLU:HG3	20	0.35
(1,1703)	2:33:B:GLN:HG2	2:31:B:LEU:HD21	12	0.35
(1,1670)	2:37:B:ALA:HB1	2:36:B:THR:HA	1	0.35
(1,1648)	2:38:B:ARG:HA	2:37:B:ALA:HB1	11	0.35
(1,1633)	2:38:B:ARG:HD2	2:38:B:ARG:HB2	19	0.35
(1,1622)	2:39:B:TRP:HE3	2:39:B:TRP:HB2	10	0.35
(1,1622)	2:39:B:TRP:HE3	2:39:B:TRP:HB2	19	0.35
(1,1618)	2:39:B:TRP:HD1	2:39:B:TRP:HB3	2	0.35
(1,1618)	2:39:B:TRP:HD1	2:39:B:TRP:HB3	3	0.35
(1,1618)	2:39:B:TRP:HD1	2:39:B:TRP:HB3	10	0.35
(1,1618)	2:39:B:TRP:HD1	2:39:B:TRP:HB3	14	0.35
(1,1618)	2:39:B:TRP:HD1	2:39:B:TRP:HB3	17	0.35
(1,1618)	2:39:B:TRP:HD1	2:39:B:TRP:HB3	20	0.35
(1,1618)	2:39:B:TRP:HD1	2:39:B:TRP:HB3	23	0.35
(1,1567)	1:57:A:LYS:HG3	1:57:A:LYS:HE2	20	0.35
(1,1544)	1:103:A:ALA:HA	1:59:A:TYR:HE1	11	0.35
(1,1538)	1:59:A:TYR:HB3	1:59:A:TYR:HD1	3	0.35
(1,1538)	1:59:A:TYR:HB3	1:59:A:TYR:HD1	12	0.35
(1,1466)	1:109:A:LEU:HD11	1:66:A:LEU:HG	1	0.35
(1,1466)	1:109:A:LEU:HD11	1:66:A:LEU:HG	8	0.35
(1,1447)	1:69:A:GLU:HA	1:69:A:GLU:HG3	24	0.35
(1,1419)	1:71:A:LEU:HD11	1:89:A:TYR:H	15	0.35
(1,1416)	1:71:A:LEU:HD11	1:71:A:LEU:H	14	0.35
(1,1391)	1:74:A:CYS:HA	1:73:A:LEU:HD23	12	0.35
(1,1345)	1:76:A:MET:HG2	1:77:A:GLN:H	14	0.35
(1,1345)	1:76:A:MET:HG2	1:77:A:GLN:H	23	0.35
(1,1345)	1:76:A:MET:HG2	1:77:A:GLN:H	24	0.35
(1,1295)	1:82:A:PRO:HG2	1:81:A:HIS:HA	20	0.35
(1,1282)	1:84:A:VAL:HG21	1:85:A:VAL:H	5	0.35
(1,1282)	1:84:A:VAL:HG21	1:85:A:VAL:H	11	0.35
(1,1282)	1:84:A:VAL:HG21	1:85:A:VAL:H	14	0.35
(1,1282)	1:84:A:VAL:HG22	1:85:A:VAL:H	15	0.35
(1,1282)	1:84:A:VAL:HG23	1:85:A:VAL:H	18	0.35
(1,1282)	1:84:A:VAL:HG22	1:85:A:VAL:H	22	0.35
(1,1252)	1:69:A:GLU:HB2	1:69:A:GLU:HG2	3	0.35
(1,1252)	1:69:A:GLU:HB2	1:69:A:GLU:HG2	4	0.35
(1,1252)	1:69:A:GLU:HB2	1:69:A:GLU:HG2	8	0.35
(1,1252)	1:69:A:GLU:HB2	1:69:A:GLU:HG2	11	0.35
(1,1252)	1:69:A:GLU:HB2	1:69:A:GLU:HG2	16	0.35
(1,1252)	1:69:A:GLU:HB2	1:69:A:GLU:HG2	19	0.35
(1,1252)	1:69:A:GLU:HB2	1:69:A:GLU:HG2	24	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1252)	1:69:A:GLU:HB2	1:69:A:GLU:HG2	25	0.35
(1,1228)	1:87:A:PHE:HD1	1:88:A:LEU:HD21	21	0.35
(1,1185)	1:90:A:ASN:HB2	1:90:A:ASN:HD22	1	0.35
(1,1185)	1:90:A:ASN:HB2	1:90:A:ASN:HD22	3	0.35
(1,1185)	1:90:A:ASN:HB2	1:90:A:ASN:HD22	5	0.35
(1,1185)	1:90:A:ASN:HB2	1:90:A:ASN:HD22	6	0.35
(1,1185)	1:90:A:ASN:HB2	1:90:A:ASN:HD22	13	0.35
(1,1185)	1:90:A:ASN:HB2	1:90:A:ASN:HD22	15	0.35
(1,1185)	1:90:A:ASN:HB2	1:90:A:ASN:HD22	16	0.35
(1,1185)	1:90:A:ASN:HB2	1:90:A:ASN:HD22	18	0.35
(1,1185)	1:90:A:ASN:HB2	1:90:A:ASN:HD22	23	0.35
(1,1185)	1:90:A:ASN:HB2	1:90:A:ASN:HD22	25	0.35
(1,1139)	1:134:A:LEU:HD23	1:95:A:ALA:HB2	16	0.35
(1,1137)	1:95:A:ALA:HB3	1:91:A:ARG:HD3	6	0.35
(1,1133)	1:95:A:ALA:HB2	1:99:A:PHE:HD2	14	0.35
(1,1126)	1:96:A:HIS:HD2	1:139:A:ALA:HB3	24	0.35
(1,1098)	1:100:A:LEU:HD23	1:92:A:GLN:HA	21	0.35
(1,1098)	1:100:A:LEU:HD21	1:92:A:GLN:HA	22	0.35
(1,1088)	1:100:A:LEU:HD21	1:105:A:PHE:HD2	25	0.35
(1,1076)	1:101:A:ALA:HB1	1:98:A:LEU:HD22	18	0.35
(1,960)	1:67:A:PHE:HA	1:109:A:LEU:HD13	8	0.35
(1,942)	1:111:A:ARG:HB2	1:111:A:ARG:HD2	2	0.35
(1,936)	1:112:A:VAL:HG11	1:112:A:VAL:HG23	2	0.35
(1,936)	1:112:A:VAL:HG13	1:112:A:VAL:HG23	6	0.35
(1,936)	1:112:A:VAL:HG12	1:112:A:VAL:HG21	11	0.35
(1,936)	1:112:A:VAL:HG11	1:112:A:VAL:HG23	12	0.35
(1,934)	1:112:A:VAL:HG11	1:126:A:TYR:HB3	11	0.35
(1,934)	1:112:A:VAL:HG11	1:126:A:TYR:HB3	22	0.35
(1,917)	1:113:A:LEU:HB2	1:113:A:LEU:HD21	16	0.35
(1,915)	1:113:A:LEU:HD21	1:69:A:GLU:HB3	13	0.35
(1,886)	1:116:A:ALA:HA	1:123:A:LEU:HD11	21	0.35
(1,881)	1:117:A:ARG:HD2	1:117:A:ARG:HB3	18	0.35
(1,858)	1:119:A:ARG:HG3	1:119:A:ARG:HA	13	0.35
(1,766)	1:126:A:TYR:HE1	1:115:A:ARG:HB2	3	0.35
(1,668)	1:133:A:VAL:HG13	1:130:A:LEU:HD11	7	0.35
(1,668)	1:133:A:VAL:HG13	1:130:A:LEU:HD12	19	0.35
(1,666)	1:134:A:LEU:HD23	1:133:A:VAL:HG12	20	0.35
(1,643)	1:134:A:LEU:HD22	1:134:A:LEU:HD12	10	0.35
(1,643)	1:134:A:LEU:HD22	1:134:A:LEU:HD13	15	0.35
(1,643)	1:134:A:LEU:HD22	1:134:A:LEU:HD13	24	0.35
(1,574)	1:143:A:LEU:HG	1:143:A:LEU:H	17	0.35
(1,558)	2:32:B:GLU:HA	2:31:B:LEU:H	2	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,541)	1:61:A:LEU:HB3	1:62:A:GLU:H	7	0.35
(1,541)	1:61:A:LEU:HB3	1:62:A:GLU:H	14	0.35
(1,538)	1:63:A:ASN:H	1:61:A:LEU:HA	14	0.35
(1,526)	1:69:A:GLU:H	1:113:A:LEU:HD22	14	0.35
(1,521)	1:71:A:LEU:H	1:113:A:LEU:HD11	19	0.35
(1,515)	1:73:A:LEU:HG	1:76:A:MET:H	22	0.35
(1,500)	1:85:A:VAL:H	1:83:A:GLU:H	19	0.35
(1,488)	1:92:A:GLN:HE22	1:64:A:GLU:HG3	17	0.35
(1,483)	1:93:A:GLN:HG2	1:94:A:ARG:H	2	0.35
(1,483)	1:93:A:GLN:HG2	1:94:A:ARG:H	4	0.35
(1,478)	1:95:A:ALA:H	1:91:A:ARG:HD2	8	0.35
(1,476)	1:96:A:HIS:H	1:95:A:ALA:H	10	0.35
(1,476)	1:96:A:HIS:H	1:95:A:ALA:H	19	0.35
(1,473)	1:101:A:ALA:H	1:100:A:LEU:HG	11	0.35
(1,451)	1:114:A:SER:H	1:117:A:ARG:HB2	10	0.35
(1,426)	1:125:A:VAL:HG11	1:126:A:TYR:H	2	0.35
(1,426)	1:125:A:VAL:HG11	1:126:A:TYR:H	3	0.35
(1,421)	1:128:A:ASN:H	1:70:A:PHE:HZ	10	0.35
(1,421)	1:72:A:GLU:H	1:70:A:PHE:HD1	15	0.35
(1,419)	1:129:A:GLU:H	1:126:A:TYR:H	14	0.35
(1,414)	1:72:A:GLU:H	1:68:A:GLU:HA	17	0.35
(1,392)	1:139:A:ALA:H	1:138:A:SER:H	6	0.35
(1,392)	1:139:A:ALA:H	1:138:A:SER:H	25	0.35
(1,387)	1:141:A:LYS:H	1:141:A:LYS:HG2	23	0.35
(1,376)	2:29:B:SER:HB2	2:26:B:ASP:HB3	5	0.35
(1,366)	1:100:A:LEU:HD11	1:138:A:SER:HB3	1	0.35
(1,342)	2:31:B:LEU:HD13	1:124:A:TYR:HB3	6	0.35
(1,337)	2:31:B:LEU:HD22	2:28:B:ASP:HB2	1	0.35
(1,321)	2:34:B:TYR:HD1	1:83:A:GLU:HB3	12	0.35
(1,318)	2:34:B:TYR:HE1	1:83:A:GLU:HB3	1	0.35
(1,318)	2:34:B:TYR:HE1	1:83:A:GLU:HB3	6	0.35
(1,275)	1:84:A:VAL:HG13	2:35:B:PHE:HE1	3	0.35
(1,275)	1:84:A:VAL:HG11	2:35:B:PHE:HZ	6	0.35
(1,275)	1:84:A:VAL:HG11	2:35:B:PHE:HZ	24	0.35
(1,257)	1:113:A:LEU:HD12	1:113:A:LEU:HB2	3	0.35
(1,257)	1:113:A:LEU:HD13	1:113:A:LEU:HB2	8	0.35
(1,244)	1:61:A:LEU:HG	1:61:A:LEU:HA	5	0.35
(1,244)	1:111:A:ARG:HA	1:115:A:ARG:HG2	19	0.35
(1,240)	1:104:A:GLU:HB3	1:105:A:PHE:HA	11	0.35
(1,240)	1:104:A:GLU:HB3	1:105:A:PHE:HA	13	0.35
(1,240)	1:104:A:GLU:HB3	1:105:A:PHE:HA	14	0.35
(1,236)	1:64:A:GLU:HA	1:67:A:PHE:H	5	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,229)	1:105:A:PHE:HE2	1:67:A:PHE:HB2	10	0.35
(1,229)	1:105:A:PHE:HE2	1:67:A:PHE:HB2	15	0.35
(1,228)	1:62:A:GLU:HG2	1:61:A:LEU:HD23	18	0.35
(1,227)	1:62:A:GLU:HG2	1:61:A:LEU:HG	8	0.35
(1,225)	1:129:A:GLU:HG2	1:125:A:VAL:HG11	11	0.35
(1,225)	1:129:A:GLU:HG2	1:125:A:VAL:HG13	22	0.35
(1,209)	1:67:A:PHE:HE1	1:71:A:LEU:HD21	18	0.35
(1,209)	1:67:A:PHE:HE1	1:71:A:LEU:HD23	25	0.35
(1,201)	2:25:B:GLU:HG3	2:25:B:GLU:HB2	1	0.35
(1,197)	1:73:A:LEU:HD21	1:123:A:LEU:HB2	3	0.35
(1,195)	1:73:A:LEU:HD22	1:70:A:PHE:HA	7	0.35
(1,194)	1:73:A:LEU:HD22	1:70:A:PHE:HD1	11	0.35
(1,191)	1:84:A:VAL:HG13	1:74:A:CYS:HB2	1	0.35
(1,191)	1:78:A:THR:HG21	1:74:A:CYS:HB2	8	0.35
(1,172)	1:85:A:VAL:HG13	1:74:A:CYS:HB3	5	0.35
(1,172)	1:85:A:VAL:HG11	1:74:A:CYS:HB3	25	0.35
(1,122)	1:95:A:ALA:HB1	1:91:A:ARG:HD3	14	0.35
(1,122)	1:95:A:ALA:HB3	1:91:A:ARG:HD3	23	0.35
(1,116)	1:100:A:LEU:HD21	1:105:A:PHE:HE2	2	0.35
(1,98)	1:105:A:PHE:HD1	1:100:A:LEU:HD22	9	0.35
(1,98)	1:105:A:PHE:HD1	1:100:A:LEU:HD22	11	0.35
(1,97)	1:105:A:PHE:HD1	1:100:A:LEU:HA	6	0.35
(1,95)	1:107:A:ASN:HB2	1:108:A:ILE:HB	4	0.35
(1,95)	1:107:A:ASN:HB2	1:108:A:ILE:HB	10	0.35
(1,94)	1:107:A:ASN:HA	1:108:A:ILE:H	1	0.35
(1,94)	1:90:A:ASN:HA	1:91:A:ARG:H	2	0.35
(1,94)	1:107:A:ASN:HA	1:108:A:ILE:H	4	0.35
(1,94)	1:107:A:ASN:HA	1:108:A:ILE:H	8	0.35
(1,94)	1:107:A:ASN:HA	1:108:A:ILE:H	12	0.35
(1,94)	1:107:A:ASN:HA	1:108:A:ILE:H	15	0.35
(1,94)	1:90:A:ASN:HA	1:91:A:ARG:H	17	0.35
(1,94)	1:107:A:ASN:HA	1:108:A:ILE:H	19	0.35
(1,94)	1:107:A:ASN:HA	1:108:A:ILE:H	21	0.35
(1,94)	1:107:A:ASN:HA	1:108:A:ILE:H	22	0.35
(1,92)	1:109:A:LEU:HD22	1:67:A:PHE:H	10	0.35
(1,92)	1:109:A:LEU:HD22	1:67:A:PHE:H	13	0.35
(1,87)	1:112:A:VAL:HG12	1:130:A:LEU:H	3	0.35
(1,87)	1:112:A:VAL:HG11	1:130:A:LEU:H	7	0.35
(1,87)	1:112:A:VAL:HG11	1:130:A:LEU:H	10	0.35
(1,87)	1:112:A:VAL:HG11	1:130:A:LEU:H	18	0.35
(1,87)	1:112:A:VAL:HG12	1:130:A:LEU:H	22	0.35
(1,81)	1:116:A:ALA:HB3	1:70:A:PHE:HZ	8	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,81)	1:116:A:ALA:HB3	1:70:A:PHE:HZ	15	0.35
(1,81)	1:116:A:ALA:HB3	1:70:A:PHE:HZ	20	0.35
(1,80)	1:94:A:ARG:HD3	1:93:A:GLN:HB2	5	0.35
(1,52)	1:125:A:VAL:HG11	1:128:A:ASN:HB2	1	0.35
(1,51)	1:126:A:TYR:HD1	1:125:A:VAL:HG13	4	0.35
(1,48)	1:126:A:TYR:HE1	1:125:A:VAL:HG11	10	0.35
(1,30)	1:129:A:GLU:HG3	1:130:A:LEU:H	6	0.35
(1,30)	1:129:A:GLU:HG3	1:130:A:LEU:H	7	0.35
(1,30)	1:129:A:GLU:HG3	1:130:A:LEU:H	12	0.35
(1,30)	1:129:A:GLU:HG3	1:130:A:LEU:H	22	0.35
(1,30)	1:129:A:GLU:HG3	1:130:A:LEU:H	23	0.35
(1,24)	1:85:A:VAL:HG21	1:71:A:LEU:HA	7	0.35
(1,13)	1:133:A:VAL:HG12	1:108:A:ILE:HB	8	0.35
(1,8)	1:134:A:LEU:HD23	1:105:A:PHE:HD1	10	0.35
(1,2265)	2:26:B:ASP:HB3	2:26:B:ASP:H	11	0.34
(1,2244)	2:36:B:THR:HG23	2:36:B:THR:H	18	0.34
(1,2188)	1:59:A:TYR:H	1:58:A:CYS:HB3	18	0.34
(1,2142)	1:109:A:LEU:HD22	1:68:A:GLU:H	6	0.34
(1,2142)	1:109:A:LEU:HD22	1:68:A:GLU:H	10	0.34
(1,2051)	1:89:A:TYR:H	1:90:A:ASN:HB3	1	0.34
(1,2019)	1:93:A:GLN:HE22	1:93:A:GLN:HB3	12	0.34
(1,2011)	1:94:A:ARG:HD2	1:94:A:ARG:H	16	0.34
(1,2006)	1:134:A:LEU:HD21	1:95:A:ALA:H	7	0.34
(1,2006)	1:134:A:LEU:HD21	1:95:A:ALA:H	19	0.34
(1,2006)	1:134:A:LEU:HD21	1:95:A:ALA:H	20	0.34
(1,2004)	1:95:A:ALA:H	1:94:A:ARG:HB3	4	0.34
(1,2004)	1:95:A:ALA:H	1:94:A:ARG:HB3	5	0.34
(1,2004)	1:95:A:ALA:H	1:94:A:ARG:HB3	21	0.34
(1,1996)	1:97:A:SER:H	1:139:A:ALA:HB2	7	0.34
(1,1974)	1:100:A:LEU:HG	1:100:A:LEU:H	6	0.34
(1,1974)	1:100:A:LEU:HG	1:100:A:LEU:H	8	0.34
(1,1971)	1:100:A:LEU:HD22	1:101:A:ALA:H	11	0.34
(1,1854)	1:124:A:TYR:H	1:125:A:VAL:HG23	6	0.34
(1,1854)	1:124:A:TYR:H	1:125:A:VAL:HG23	10	0.34
(1,1854)	1:124:A:TYR:H	1:125:A:VAL:HG22	14	0.34
(1,1854)	1:124:A:TYR:H	1:125:A:VAL:HG23	15	0.34
(1,1854)	1:124:A:TYR:H	1:125:A:VAL:HG23	19	0.34
(1,1798)	1:136:A:ALA:H	1:135:A:LYS:HD3	3	0.34
(1,1770)	1:141:A:LYS:HB3	1:141:A:LYS:H	11	0.34
(1,1768)	2:24:B:GLN:HB2	2:24:B:GLN:HG2	2	0.34
(1,1768)	2:24:B:GLN:HB2	2:24:B:GLN:HG2	13	0.34
(1,1768)	2:24:B:GLN:HG3	2:24:B:GLN:HB2	18	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1768)	2:24:B:GLN:HG3	2:24:B:GLN:HB2	24	0.34
(1,1755)	2:30:B:GLU:HG2	2:30:B:GLU:HA	4	0.34
(1,1755)	2:30:B:GLU:HG2	2:30:B:GLU:HA	5	0.34
(1,1755)	2:30:B:GLU:HG2	2:30:B:GLU:HA	18	0.34
(1,1755)	2:30:B:GLU:HG2	2:30:B:GLU:HA	24	0.34
(1,1727)	2:31:B:LEU:HD11	2:31:B:LEU:H	13	0.34
(1,1727)	2:31:B:LEU:HD11	2:31:B:LEU:H	17	0.34
(1,1720)	2:34:B:TYR:HE1	2:31:B:LEU:HD22	6	0.34
(1,1720)	2:34:B:TYR:HE1	2:31:B:LEU:HD21	15	0.34
(1,1720)	2:34:B:TYR:HE1	2:31:B:LEU:HD23	22	0.34
(1,1670)	2:37:B:ALA:HB1	2:36:B:THR:HA	21	0.34
(1,1648)	2:38:B:ARG:HA	2:37:B:ALA:HB1	15	0.34
(1,1619)	2:39:B:TRP:HD1	2:38:B:ARG:HB2	1	0.34
(1,1619)	2:39:B:TRP:HD1	2:38:B:ARG:HB2	10	0.34
(1,1618)	2:39:B:TRP:HD1	2:39:B:TRP:HB3	4	0.34
(1,1618)	2:39:B:TRP:HD1	2:39:B:TRP:HB3	9	0.34
(1,1618)	2:39:B:TRP:HD1	2:39:B:TRP:HB3	12	0.34
(1,1618)	2:39:B:TRP:HD1	2:39:B:TRP:HB3	13	0.34
(1,1618)	2:39:B:TRP:HD1	2:39:B:TRP:HB3	18	0.34
(1,1618)	2:39:B:TRP:HD1	2:39:B:TRP:HB3	21	0.34
(1,1618)	2:39:B:TRP:HD1	2:39:B:TRP:HB3	22	0.34
(1,1618)	2:39:B:TRP:HD1	2:39:B:TRP:HB3	24	0.34
(1,1577)	1:77:A:GLN:HG3	1:73:A:LEU:HD13	23	0.34
(1,1538)	1:59:A:TYR:HB3	1:59:A:TYR:HD1	4	0.34
(1,1538)	1:59:A:TYR:HB3	1:59:A:TYR:HD1	9	0.34
(1,1538)	1:59:A:TYR:HB3	1:59:A:TYR:HD1	14	0.34
(1,1534)	1:59:A:TYR:HD1	1:59:A:TYR:H	20	0.34
(1,1513)	1:62:A:GLU:HA	1:62:A:GLU:HG3	21	0.34
(1,1501)	1:64:A:GLU:HG2	1:65:A:LYS:H	12	0.34
(1,1481)	1:66:A:LEU:HD23	1:69:A:GLU:H	3	0.34
(1,1477)	1:66:A:LEU:HD23	1:113:A:LEU:HB3	12	0.34
(1,1466)	1:109:A:LEU:HD13	1:66:A:LEU:HG	11	0.34
(1,1466)	1:109:A:LEU:HD13	1:66:A:LEU:HG	14	0.34
(1,1466)	1:109:A:LEU:HD12	1:66:A:LEU:HG	18	0.34
(1,1466)	1:109:A:LEU:HD11	1:66:A:LEU:HG	20	0.34
(1,1466)	1:109:A:LEU:HD11	1:66:A:LEU:HG	24	0.34
(1,1416)	1:71:A:LEU:HD12	1:71:A:LEU:H	15	0.34
(1,1395)	1:116:A:ALA:HB3	1:73:A:LEU:HD23	18	0.34
(1,1392)	1:73:A:LEU:HD23	1:117:A:ARG:HD3	11	0.34
(1,1391)	1:74:A:CYS:HA	1:73:A:LEU:HD22	3	0.34
(1,1385)	1:73:A:LEU:HB2	1:74:A:CYS:H	6	0.34
(1,1361)	1:75:A:LYS:HE2	1:75:A:LYS:HG3	5	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1361)	1:75:A:LYS:HE2	1:75:A:LYS:HG3	12	0.34
(1,1361)	1:75:A:LYS:HE2	1:75:A:LYS:HG3	19	0.34
(1,1345)	1:76:A:MET:HG2	1:77:A:GLN:H	13	0.34
(1,1318)	1:79:A:ALA:HA	1:79:A:ALA:HB2	5	0.34
(1,1318)	1:79:A:ALA:HA	1:79:A:ALA:HB2	14	0.34
(1,1283)	1:84:A:VAL:HG22	1:127:A:ILE:HD12	10	0.34
(1,1282)	1:84:A:VAL:HG21	1:85:A:VAL:H	7	0.34
(1,1282)	1:84:A:VAL:HG21	1:85:A:VAL:H	23	0.34
(1,1282)	1:84:A:VAL:HG22	1:85:A:VAL:H	25	0.34
(1,1280)	1:84:A:VAL:HG21	1:81:A:HIS:HB2	14	0.34
(1,1280)	1:84:A:VAL:HG21	1:81:A:HIS:HB2	23	0.34
(1,1252)	1:69:A:GLU:HB2	1:69:A:GLU:HG2	1	0.34
(1,1252)	1:69:A:GLU:HB2	1:69:A:GLU:HG2	5	0.34
(1,1252)	1:69:A:GLU:HB2	1:69:A:GLU:HG2	7	0.34
(1,1252)	1:69:A:GLU:HB2	1:69:A:GLU:HG2	9	0.34
(1,1252)	1:69:A:GLU:HB2	1:69:A:GLU:HG2	22	0.34
(1,1228)	1:87:A:PHE:HD1	1:88:A:LEU:HD22	11	0.34
(1,1209)	1:88:A:LEU:HD11	1:70:A:PHE:HE1	8	0.34
(1,1185)	1:90:A:ASN:HB2	1:90:A:ASN:HD22	7	0.34
(1,1185)	1:90:A:ASN:HB2	1:90:A:ASN:HD22	8	0.34
(1,1185)	1:90:A:ASN:HB2	1:90:A:ASN:HD22	10	0.34
(1,1185)	1:90:A:ASN:HB2	1:90:A:ASN:HD22	12	0.34
(1,1185)	1:90:A:ASN:HB2	1:90:A:ASN:HD22	21	0.34
(1,1147)	1:94:A:ARG:HG2	1:94:A:ARG:HA	2	0.34
(1,1139)	1:134:A:LEU:HD21	1:95:A:ALA:HB2	11	0.34
(1,1137)	1:95:A:ALA:HB2	1:91:A:ARG:HD3	19	0.34
(1,1122)	1:96:A:HIS:HA	1:139:A:ALA:HB3	9	0.34
(1,1089)	1:105:A:PHE:HZ	1:100:A:LEU:HD21	5	0.34
(1,1088)	1:100:A:LEU:HD22	1:105:A:PHE:HD2	16	0.34
(1,996)	1:108:A:ILE:HG23	1:112:A:VAL:HG11	5	0.34
(1,996)	1:108:A:ILE:HG23	1:112:A:VAL:HG11	18	0.34
(1,960)	1:67:A:PHE:HA	1:109:A:LEU:HD13	24	0.34
(1,936)	1:112:A:VAL:HG13	1:112:A:VAL:HG23	1	0.34
(1,936)	1:112:A:VAL:HG13	1:112:A:VAL:HG22	5	0.34
(1,936)	1:112:A:VAL:HG11	1:112:A:VAL:HG22	7	0.34
(1,936)	1:112:A:VAL:HG11	1:112:A:VAL:HG22	8	0.34
(1,936)	1:112:A:VAL:HG13	1:112:A:VAL:HG22	16	0.34
(1,936)	1:112:A:VAL:HG13	1:112:A:VAL:HG21	19	0.34
(1,936)	1:112:A:VAL:HG12	1:112:A:VAL:HG22	21	0.34
(1,936)	1:112:A:VAL:HG12	1:112:A:VAL:HG22	23	0.34
(1,934)	1:112:A:VAL:HG13	1:126:A:TYR:HB3	15	0.34
(1,917)	1:113:A:LEU:HB2	1:113:A:LEU:HD23	12	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,858)	1:119:A:ARG:HG3	1:119:A:ARG:HA	5	0.34
(1,858)	1:119:A:ARG:HG3	1:119:A:ARG:HA	11	0.34
(1,858)	1:119:A:ARG:HG3	1:119:A:ARG:HA	12	0.34
(1,809)	1:123:A:LEU:HD13	1:123:A:LEU:HD23	11	0.34
(1,809)	1:123:A:LEU:HD13	1:123:A:LEU:HD22	24	0.34
(1,743)	1:127:A:ILE:HG22	1:124:A:TYR:HA	14	0.34
(1,576)	1:142:A:LYS:HB2	1:142:A:LYS:H	8	0.34
(1,558)	2:32:B:GLU:HA	2:31:B:LEU:H	9	0.34
(1,552)	2:35:B:PHE:H	2:33:B:GLN:HA	24	0.34
(1,541)	1:61:A:LEU:HB3	1:62:A:GLU:H	1	0.34
(1,541)	1:61:A:LEU:HB3	1:62:A:GLU:H	8	0.34
(1,541)	1:61:A:LEU:HB3	1:62:A:GLU:H	19	0.34
(1,541)	1:61:A:LEU:HB3	1:62:A:GLU:H	21	0.34
(1,541)	1:61:A:LEU:HB3	1:62:A:GLU:H	24	0.34
(1,538)	1:63:A:ASN:H	1:61:A:LEU:HA	6	0.34
(1,538)	1:63:A:ASN:H	1:61:A:LEU:HA	12	0.34
(1,526)	1:69:A:GLU:H	1:113:A:LEU:HD21	13	0.34
(1,521)	1:71:A:LEU:H	1:113:A:LEU:HD12	4	0.34
(1,521)	1:71:A:LEU:H	1:113:A:LEU:HD13	23	0.34
(1,515)	1:73:A:LEU:HG	1:76:A:MET:H	19	0.34
(1,494)	1:90:A:ASN:H	1:88:A:LEU:HB2	21	0.34
(1,492)	1:91:A:ARG:H	1:88:A:LEU:HD22	2	0.34
(1,492)	1:91:A:ARG:H	1:88:A:LEU:HD22	8	0.34
(1,492)	1:91:A:ARG:H	1:88:A:LEU:HD21	13	0.34
(1,478)	1:95:A:ALA:H	1:91:A:ARG:HD2	24	0.34
(1,476)	1:96:A:HIS:H	1:95:A:ALA:H	25	0.34
(1,445)	1:116:A:ALA:H	1:112:A:VAL:HA	9	0.34
(1,434)	1:74:A:CYS:H	1:123:A:LEU:HD11	16	0.34
(1,426)	1:125:A:VAL:HG11	1:126:A:TYR:H	17	0.34
(1,421)	1:128:A:ASN:H	1:70:A:PHE:HZ	8	0.34
(1,414)	1:72:A:GLU:H	1:68:A:GLU:HA	3	0.34
(1,392)	1:139:A:ALA:H	1:138:A:SER:H	10	0.34
(1,342)	2:31:B:LEU:HD12	1:124:A:TYR:HB3	9	0.34
(1,337)	2:31:B:LEU:HD22	2:28:B:ASP:HB3	18	0.34
(1,240)	1:104:A:GLU:HB3	1:105:A:PHE:HA	2	0.34
(1,240)	1:104:A:GLU:HB3	1:105:A:PHE:HA	4	0.34
(1,240)	1:104:A:GLU:HB3	1:105:A:PHE:HA	21	0.34
(1,236)	1:64:A:GLU:HA	1:67:A:PHE:H	3	0.34
(1,236)	1:64:A:GLU:HA	1:67:A:PHE:H	10	0.34
(1,229)	1:105:A:PHE:HE2	1:67:A:PHE:HB2	11	0.34
(1,225)	1:129:A:GLU:HG2	1:125:A:VAL:HG11	17	0.34
(1,225)	1:129:A:GLU:HG2	1:125:A:VAL:HG12	18	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,210)	1:105:A:PHE:HZ	1:109:A:LEU:HD23	17	0.34
(1,210)	1:105:A:PHE:HZ	1:109:A:LEU:HD22	22	0.34
(1,209)	1:67:A:PHE:HE1	1:71:A:LEU:HD22	12	0.34
(1,201)	2:30:B:GLU:HG3	2:30:B:GLU:HB2	19	0.34
(1,191)	1:84:A:VAL:HG11	1:74:A:CYS:HB2	4	0.34
(1,191)	1:84:A:VAL:HG13	1:74:A:CYS:HB2	10	0.34
(1,172)	1:85:A:VAL:HG13	1:74:A:CYS:HB3	4	0.34
(1,172)	1:85:A:VAL:HG13	1:74:A:CYS:HB3	21	0.34
(1,155)	1:88:A:LEU:HD23	1:131:A:CYS:HB3	7	0.34
(1,140)	1:99:A:PHE:HB3	1:138:A:SER:H	16	0.34
(1,134)	1:105:A:PHE:HE2	1:92:A:GLN:HG2	23	0.34
(1,132)	1:92:A:GLN:HB3	1:89:A:TYR:HD1	20	0.34
(1,121)	1:95:A:ALA:HB3	1:134:A:LEU:HA	19	0.34
(1,121)	1:95:A:ALA:HB3	1:134:A:LEU:HA	25	0.34
(1,116)	1:100:A:LEU:HD23	1:105:A:PHE:HE2	15	0.34
(1,98)	1:105:A:PHE:HD1	1:100:A:LEU:HD23	24	0.34
(1,97)	1:105:A:PHE:HD1	1:100:A:LEU:HA	7	0.34
(1,94)	1:107:A:ASN:HA	1:108:A:ILE:H	3	0.34
(1,94)	1:90:A:ASN:HA	1:91:A:ARG:H	5	0.34
(1,94)	1:107:A:ASN:HA	1:108:A:ILE:H	7	0.34
(1,94)	1:107:A:ASN:HA	1:108:A:ILE:H	11	0.34
(1,94)	1:90:A:ASN:HA	1:91:A:ARG:H	13	0.34
(1,94)	1:90:A:ASN:HA	1:91:A:ARG:H	16	0.34
(1,94)	1:107:A:ASN:HA	1:108:A:ILE:H	25	0.34
(1,87)	1:112:A:VAL:HG13	1:130:A:LEU:H	5	0.34
(1,87)	1:112:A:VAL:HG12	1:130:A:LEU:H	20	0.34
(1,81)	1:116:A:ALA:HB2	1:70:A:PHE:HZ	18	0.34
(1,56)	1:124:A:TYR:HE2	2:35:B:PHE:HB3	18	0.34
(1,52)	1:125:A:VAL:HG13	1:128:A:ASN:HB2	10	0.34
(1,51)	1:126:A:TYR:HD1	1:125:A:VAL:HG11	10	0.34
(1,42)	1:126:A:TYR:HD1	1:125:A:VAL:HB	19	0.34
(1,37)	1:127:A:ILE:HG21	1:128:A:ASN:HD22	23	0.34
(1,36)	1:127:A:ILE:HG23	1:124:A:TYR:HD2	3	0.34
(1,36)	1:127:A:ILE:HG23	1:124:A:TYR:HD1	24	0.34
(1,30)	1:129:A:GLU:HG3	1:130:A:LEU:H	5	0.34
(1,30)	1:129:A:GLU:HG3	1:130:A:LEU:H	9	0.34
(1,30)	1:129:A:GLU:HG3	1:130:A:LEU:H	11	0.34
(1,24)	1:85:A:VAL:HG22	1:71:A:LEU:HA	1	0.34
(1,24)	1:85:A:VAL:HG21	1:71:A:LEU:HA	17	0.34
(1,24)	1:85:A:VAL:HG23	1:86:A:PRO:HD3	18	0.34
(1,8)	1:134:A:LEU:HD21	1:105:A:PHE:HD1	3	0.34
(1,2193)	1:58:A:CYS:H	1:57:A:LYS:HG2	24	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2188)	1:59:A:TYR:H	1:58:A:CYS:HB2	15	0.33
(1,2173)	1:63:A:ASN:H	1:109:A:LEU:HD13	14	0.33
(1,2142)	1:109:A:LEU:HD22	1:68:A:GLU:H	17	0.33
(1,2031)	1:91:A:ARG:H	1:134:A:LEU:HD13	17	0.33
(1,2007)	1:100:A:LEU:HD21	1:95:A:ALA:H	11	0.33
(1,2007)	1:100:A:LEU:HD22	1:95:A:ALA:H	17	0.33
(1,2006)	1:134:A:LEU:HD23	1:95:A:ALA:H	1	0.33
(1,2006)	1:134:A:LEU:HD22	1:95:A:ALA:H	21	0.33
(1,2006)	1:134:A:LEU:HD21	1:95:A:ALA:H	22	0.33
(1,2006)	1:134:A:LEU:HD22	1:95:A:ALA:H	23	0.33
(1,2006)	1:134:A:LEU:HD21	1:95:A:ALA:H	24	0.33
(1,2005)	1:95:A:ALA:H	1:94:A:ARG:HG2	20	0.33
(1,2004)	1:95:A:ALA:H	1:94:A:ARG:HB3	7	0.33
(1,1996)	1:97:A:SER:H	1:139:A:ALA:HB3	18	0.33
(1,1961)	1:102:A:SER:H	1:59:A:TYR:HD1	18	0.33
(1,1874)	1:118:A:SER:H	1:117:A:ARG:HG3	1	0.33
(1,1854)	1:124:A:TYR:H	1:125:A:VAL:HG22	17	0.33
(1,1854)	1:124:A:TYR:H	1:125:A:VAL:HG21	23	0.33
(1,1798)	1:136:A:ALA:H	1:135:A:LYS:HD3	8	0.33
(1,1768)	2:24:B:GLN:HG3	2:24:B:GLN:HB2	19	0.33
(1,1768)	2:24:B:GLN:HB2	2:24:B:GLN:HG2	23	0.33
(1,1755)	2:30:B:GLU:HG2	2:30:B:GLU:HA	25	0.33
(1,1727)	2:31:B:LEU:HD12	2:31:B:LEU:H	21	0.33
(1,1723)	2:31:B:LEU:HD23	2:30:B:GLU:HB2	20	0.33
(1,1720)	2:34:B:TYR:HE1	2:31:B:LEU:HD22	3	0.33
(1,1720)	2:34:B:TYR:HE1	2:31:B:LEU:HD21	4	0.33
(1,1720)	2:34:B:TYR:HE1	2:31:B:LEU:HD23	8	0.33
(1,1720)	2:34:B:TYR:HE1	2:31:B:LEU:HD23	23	0.33
(1,1634)	2:38:B:ARG:HD2	2:37:B:ALA:HB1	14	0.33
(1,1622)	2:39:B:TRP:HE3	2:39:B:TRP:HB2	17	0.33
(1,1619)	2:39:B:TRP:HD1	2:38:B:ARG:HB2	11	0.33
(1,1618)	2:39:B:TRP:HD1	2:39:B:TRP:HB3	7	0.33
(1,1618)	2:39:B:TRP:HD1	2:39:B:TRP:HB3	8	0.33
(1,1591)	1:84:A:VAL:HA	2:31:B:LEU:HD12	24	0.33
(1,1588)	1:87:A:PHE:HB2	2:31:B:LEU:HD11	13	0.33
(1,1577)	1:77:A:GLN:HG3	1:73:A:LEU:HD11	7	0.33
(1,1538)	1:59:A:TYR:HB3	1:59:A:TYR:HD1	1	0.33
(1,1538)	1:59:A:TYR:HB3	1:59:A:TYR:HD1	7	0.33
(1,1538)	1:59:A:TYR:HB3	1:59:A:TYR:HD1	8	0.33
(1,1538)	1:59:A:TYR:HB3	1:59:A:TYR:HD1	15	0.33
(1,1538)	1:59:A:TYR:HB3	1:59:A:TYR:HD1	19	0.33
(1,1538)	1:59:A:TYR:HB3	1:59:A:TYR:HD1	24	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1480)	1:66:A:LEU:HD22	1:63:A:ASN:HA	7	0.33
(1,1477)	1:66:A:LEU:HD22	1:113:A:LEU:HB3	5	0.33
(1,1466)	1:109:A:LEU:HD12	1:66:A:LEU:HG	15	0.33
(1,1447)	1:69:A:GLU:HA	1:69:A:GLU:HG3	12	0.33
(1,1447)	1:69:A:GLU:HA	1:69:A:GLU:HG3	19	0.33
(1,1440)	1:127:A:ILE:HD13	1:70:A:PHE:HZ	2	0.33
(1,1440)	1:127:A:ILE:HD13	1:70:A:PHE:HZ	7	0.33
(1,1440)	1:127:A:ILE:HD13	1:70:A:PHE:HZ	25	0.33
(1,1419)	1:71:A:LEU:HD12	1:89:A:TYR:H	3	0.33
(1,1416)	1:71:A:LEU:HD13	1:71:A:LEU:H	13	0.33
(1,1416)	1:71:A:LEU:HD11	1:71:A:LEU:H	25	0.33
(1,1415)	1:71:A:LEU:HB2	1:75:A:LYS:HE2	10	0.33
(1,1395)	1:116:A:ALA:HB3	1:73:A:LEU:HD21	17	0.33
(1,1395)	1:116:A:ALA:HB1	1:73:A:LEU:HD21	21	0.33
(1,1361)	1:75:A:LYS:HE2	1:75:A:LYS:HG3	1	0.33
(1,1361)	1:75:A:LYS:HE2	1:75:A:LYS:HG3	3	0.33
(1,1361)	1:75:A:LYS:HE2	1:75:A:LYS:HG3	9	0.33
(1,1361)	1:75:A:LYS:HE2	1:75:A:LYS:HG3	11	0.33
(1,1361)	1:75:A:LYS:HE2	1:75:A:LYS:HG3	13	0.33
(1,1361)	1:75:A:LYS:HE2	1:75:A:LYS:HG3	14	0.33
(1,1361)	1:75:A:LYS:HE2	1:75:A:LYS:HG3	15	0.33
(1,1361)	1:75:A:LYS:HE2	1:75:A:LYS:HG3	16	0.33
(1,1361)	1:75:A:LYS:HE2	1:75:A:LYS:HG3	18	0.33
(1,1361)	1:75:A:LYS:HE2	1:75:A:LYS:HG3	21	0.33
(1,1361)	1:75:A:LYS:HE2	1:75:A:LYS:HG3	22	0.33
(1,1345)	1:76:A:MET:HG2	1:77:A:GLN:H	7	0.33
(1,1345)	1:76:A:MET:HG2	1:77:A:GLN:H	11	0.33
(1,1345)	1:76:A:MET:HG2	1:77:A:GLN:H	19	0.33
(1,1326)	1:77:A:GLN:HG2	1:77:A:GLN:HA	16	0.33
(1,1326)	1:77:A:GLN:HG2	1:77:A:GLN:HA	22	0.33
(1,1318)	1:79:A:ALA:HA	1:79:A:ALA:HB1	1	0.33
(1,1318)	1:79:A:ALA:HA	1:79:A:ALA:HB2	2	0.33
(1,1318)	1:79:A:ALA:HA	1:79:A:ALA:HB2	6	0.33
(1,1318)	1:79:A:ALA:HA	1:79:A:ALA:HB2	9	0.33
(1,1318)	1:79:A:ALA:HA	1:79:A:ALA:HB2	10	0.33
(1,1318)	1:79:A:ALA:HA	1:79:A:ALA:HB3	11	0.33
(1,1318)	1:79:A:ALA:HA	1:79:A:ALA:HB1	16	0.33
(1,1318)	1:79:A:ALA:HA	1:79:A:ALA:HB3	18	0.33
(1,1318)	1:79:A:ALA:HA	1:79:A:ALA:HB1	19	0.33
(1,1318)	1:79:A:ALA:HA	1:79:A:ALA:HB3	20	0.33
(1,1318)	1:79:A:ALA:HA	1:79:A:ALA:HB1	21	0.33
(1,1318)	1:79:A:ALA:HA	1:79:A:ALA:HB2	24	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1295)	1:82:A:PRO:HG2	1:81:A:HIS:HA	2	0.33
(1,1282)	1:84:A:VAL:HG22	1:85:A:VAL:H	1	0.33
(1,1282)	1:84:A:VAL:HG22	1:85:A:VAL:H	4	0.33
(1,1282)	1:84:A:VAL:HG21	1:85:A:VAL:H	13	0.33
(1,1282)	1:84:A:VAL:HG21	1:85:A:VAL:H	19	0.33
(1,1280)	1:84:A:VAL:HG21	1:81:A:HIS:HB2	13	0.33
(1,1280)	1:84:A:VAL:HG21	1:81:A:HIS:HB2	16	0.33
(1,1280)	1:84:A:VAL:HG22	1:81:A:HIS:HB2	25	0.33
(1,1252)	1:69:A:GLU:HB2	1:69:A:GLU:HG2	13	0.33
(1,1209)	1:88:A:LEU:HD13	1:70:A:PHE:HE1	20	0.33
(1,1122)	1:96:A:HIS:HA	1:139:A:ALA:HB2	3	0.33
(1,1122)	1:96:A:HIS:HA	1:139:A:ALA:HB2	11	0.33
(1,1072)	1:101:A:ALA:HB2	1:58:A:CYS:HA	25	0.33
(1,1070)	1:101:A:ALA:HB1	1:102:A:SER:H	8	0.33
(1,1066)	1:101:A:ALA:HA	1:60:A:LYS:HB2	22	0.33
(1,1040)	1:62:A:GLU:HB3	1:59:A:TYR:HA	4	0.33
(1,960)	1:67:A:PHE:HA	1:109:A:LEU:HD13	1	0.33
(1,946)	1:110:A:SER:HB2	1:66:A:LEU:HD11	23	0.33
(1,936)	1:112:A:VAL:HG12	1:112:A:VAL:HG23	9	0.33
(1,936)	1:112:A:VAL:HG11	1:112:A:VAL:HG21	13	0.33
(1,936)	1:112:A:VAL:HG11	1:112:A:VAL:HG22	14	0.33
(1,936)	1:112:A:VAL:HG12	1:112:A:VAL:HG21	22	0.33
(1,934)	1:112:A:VAL:HG12	1:126:A:TYR:HB3	6	0.33
(1,934)	1:112:A:VAL:HG11	1:126:A:TYR:HB3	17	0.33
(1,934)	1:112:A:VAL:HG11	1:126:A:TYR:HB3	20	0.33
(1,886)	1:116:A:ALA:HA	1:123:A:LEU:HD11	8	0.33
(1,886)	1:116:A:ALA:HA	1:123:A:LEU:HD11	11	0.33
(1,886)	1:116:A:ALA:HA	1:123:A:LEU:HD12	15	0.33
(1,886)	1:116:A:ALA:HA	1:123:A:LEU:HD13	17	0.33
(1,858)	1:119:A:ARG:HG3	1:119:A:ARG:HA	14	0.33
(1,809)	1:123:A:LEU:HD11	1:123:A:LEU:HD21	19	0.33
(1,778)	1:125:A:VAL:HG22	1:122:A:LYS:HA	21	0.33
(1,643)	1:134:A:LEU:HD21	1:134:A:LEU:HD13	1	0.33
(1,643)	1:134:A:LEU:HD23	1:134:A:LEU:HD13	2	0.33
(1,643)	1:134:A:LEU:HD23	1:134:A:LEU:HD11	6	0.33
(1,643)	1:134:A:LEU:HD22	1:134:A:LEU:HD11	7	0.33
(1,643)	1:134:A:LEU:HD21	1:134:A:LEU:HD13	16	0.33
(1,643)	1:134:A:LEU:HD22	1:134:A:LEU:HD11	20	0.33
(1,643)	1:134:A:LEU:HD23	1:134:A:LEU:HD11	23	0.33
(1,584)	1:139:A:ALA:HB3	1:96:A:HIS:H	18	0.33
(1,561)	2:27:B:SER:H	2:30:B:GLU:HB3	4	0.33
(1,558)	2:32:B:GLU:HA	2:31:B:LEU:H	5	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,558)	2:32:B:GLU:HA	2:31:B:LEU:H	14	0.33
(1,541)	1:61:A:LEU:HB3	1:62:A:GLU:H	3	0.33
(1,541)	1:61:A:LEU:HB3	1:62:A:GLU:H	22	0.33
(1,538)	1:63:A:ASN:H	1:61:A:LEU:HA	18	0.33
(1,529)	1:67:A:PHE:H	1:69:A:GLU:HB2	21	0.33
(1,526)	1:69:A:GLU:H	1:113:A:LEU:HD21	23	0.33
(1,521)	1:71:A:LEU:H	1:113:A:LEU:HD11	24	0.33
(1,515)	1:73:A:LEU:HG	1:76:A:MET:H	1	0.33
(1,505)	1:79:A:ALA:H	1:76:A:MET:HA	2	0.33
(1,502)	1:81:A:HIS:H	1:82:A:PRO:HB3	20	0.33
(1,500)	1:85:A:VAL:H	1:83:A:GLU:H	1	0.33
(1,500)	1:85:A:VAL:H	1:83:A:GLU:H	16	0.33
(1,492)	1:91:A:ARG:H	1:88:A:LEU:HD23	12	0.33
(1,476)	1:96:A:HIS:H	1:95:A:ALA:H	5	0.33
(1,476)	1:96:A:HIS:H	1:95:A:ALA:H	24	0.33
(1,473)	1:101:A:ALA:H	1:100:A:LEU:HG	14	0.33
(1,473)	1:101:A:ALA:H	1:100:A:LEU:HG	15	0.33
(1,473)	1:101:A:ALA:H	1:100:A:LEU:HB3	24	0.33
(1,453)	1:114:A:SER:H	1:113:A:LEU:HD22	12	0.33
(1,444)	1:73:A:LEU:HD13	1:117:A:ARG:H	9	0.33
(1,419)	1:129:A:GLU:H	1:126:A:TYR:H	19	0.33
(1,414)	1:72:A:GLU:H	1:68:A:GLU:HA	10	0.33
(1,414)	1:72:A:GLU:H	1:69:A:GLU:HA	22	0.33
(1,394)	1:137:A:HIS:HB3	1:138:A:SER:H	6	0.33
(1,392)	1:139:A:ALA:H	1:96:A:HIS:HD2	21	0.33
(1,361)	2:29:B:SER:HB2	2:32:B:GLU:HG3	6	0.33
(1,356)	2:29:B:SER:HB2	2:33:B:GLN:H	11	0.33
(1,344)	2:31:B:LEU:HB3	1:87:A:PHE:HD2	12	0.33
(1,342)	2:31:B:LEU:HD11	1:124:A:TYR:HB3	8	0.33
(1,342)	2:31:B:LEU:HD13	1:124:A:TYR:HB3	21	0.33
(1,337)	2:31:B:LEU:HD23	2:28:B:ASP:HB2	24	0.33
(1,321)	2:34:B:TYR:HD1	1:83:A:GLU:HB3	4	0.33
(1,312)	2:35:B:PHE:HE1	1:124:A:TYR:HA	4	0.33
(1,293)	2:39:B:TRP:HD1	1:121:A:ALA:HB2	5	0.33
(1,275)	1:84:A:VAL:HG13	2:35:B:PHE:HE1	8	0.33
(1,275)	1:84:A:VAL:HG13	2:35:B:PHE:HE1	15	0.33
(1,275)	1:84:A:VAL:HG11	2:35:B:PHE:HE1	17	0.33
(1,275)	1:84:A:VAL:HG13	2:35:B:PHE:HE1	22	0.33
(1,257)	1:113:A:LEU:HD11	1:113:A:LEU:HB2	18	0.33
(1,253)	1:57:A:LYS:HE3	1:54:A:MET:HG3	23	0.33
(1,244)	1:111:A:ARG:HA	1:115:A:ARG:HG2	9	0.33
(1,244)	1:111:A:ARG:HA	1:115:A:ARG:HG2	12	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,244)	1:61:A:LEU:HG	1:61:A:LEU:HA	15	0.33
(1,229)	1:105:A:PHE:HE2	1:67:A:PHE:HB2	2	0.33
(1,229)	1:105:A:PHE:HE2	1:67:A:PHE:HB2	7	0.33
(1,225)	1:129:A:GLU:HG2	1:125:A:VAL:HG12	15	0.33
(1,225)	1:129:A:GLU:HG2	1:125:A:VAL:HG13	19	0.33
(1,222)	1:68:A:GLU:HA	1:71:A:LEU:HG	2	0.33
(1,222)	1:68:A:GLU:HA	1:71:A:LEU:HG	9	0.33
(1,222)	1:68:A:GLU:HA	1:71:A:LEU:HG	15	0.33
(1,220)	1:70:A:PHE:HE2	1:113:A:LEU:HB2	10	0.33
(1,220)	1:70:A:PHE:HE2	1:113:A:LEU:HB2	21	0.33
(1,210)	1:105:A:PHE:HZ	1:109:A:LEU:HD21	19	0.33
(1,203)	1:71:A:LEU:HD11	1:68:A:GLU:H	19	0.33
(1,201)	2:30:B:GLU:HG3	2:30:B:GLU:HB2	22	0.33
(1,189)	1:85:A:VAL:HG11	1:75:A:LYS:HA	10	0.33
(1,172)	1:85:A:VAL:HG13	1:74:A:CYS:HB3	11	0.33
(1,172)	1:85:A:VAL:HG13	1:74:A:CYS:HB3	15	0.33
(1,172)	1:85:A:VAL:HG13	1:74:A:CYS:HB3	22	0.33
(1,155)	1:88:A:LEU:HD23	1:131:A:CYS:HB3	15	0.33
(1,155)	1:88:A:LEU:HD23	1:131:A:CYS:HB3	20	0.33
(1,147)	1:137:A:HIS:HB3	1:138:A:SER:H	1	0.33
(1,147)	1:137:A:HIS:HB3	1:138:A:SER:H	2	0.33
(1,147)	1:137:A:HIS:HB3	1:138:A:SER:H	3	0.33
(1,139)	1:128:A:ASN:HB2	1:128:A:ASN:HD22	24	0.33
(1,132)	1:92:A:GLN:HB3	1:89:A:TYR:HD1	2	0.33
(1,132)	1:67:A:PHE:HE1	1:92:A:GLN:HB3	12	0.33
(1,122)	1:95:A:ALA:HB3	1:91:A:ARG:HD3	1	0.33
(1,94)	1:90:A:ASN:HA	1:91:A:ARG:H	6	0.33
(1,94)	1:90:A:ASN:HA	1:91:A:ARG:H	9	0.33
(1,94)	1:90:A:ASN:HA	1:91:A:ARG:H	14	0.33
(1,94)	1:107:A:ASN:HA	1:108:A:ILE:H	18	0.33
(1,94)	1:90:A:ASN:HA	1:91:A:ARG:H	23	0.33
(1,94)	1:107:A:ASN:HA	1:108:A:ILE:H	24	0.33
(1,92)	1:109:A:LEU:HD21	1:67:A:PHE:H	22	0.33
(1,87)	1:112:A:VAL:HG11	1:130:A:LEU:H	8	0.33
(1,81)	1:116:A:ALA:HB1	1:70:A:PHE:HZ	19	0.33
(1,67)	1:116:A:ALA:HB1	1:120:A:PRO:HA	10	0.33
(1,52)	1:125:A:VAL:HG13	1:128:A:ASN:HB2	8	0.33
(1,51)	1:126:A:TYR:HD1	1:125:A:VAL:HG12	1	0.33
(1,51)	1:126:A:TYR:HD1	1:125:A:VAL:HG11	5	0.33
(1,51)	1:126:A:TYR:HD1	1:125:A:VAL:HG11	7	0.33
(1,51)	1:126:A:TYR:HD1	1:125:A:VAL:HG12	13	0.33
(1,51)	1:126:A:TYR:HD1	1:125:A:VAL:HG11	16	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,51)	1:126:A:TYR:HD1	1:125:A:VAL:HG13	25	0.33
(1,48)	1:126:A:TYR:HE1	1:125:A:VAL:HG12	14	0.33
(1,36)	1:127:A:ILE:HG21	1:124:A:TYR:HD2	6	0.33
(1,36)	1:127:A:ILE:HG21	1:124:A:TYR:HD2	20	0.33
(1,30)	1:129:A:GLU:HG3	1:130:A:LEU:H	1	0.33
(1,30)	1:129:A:GLU:HG3	1:130:A:LEU:H	4	0.33
(1,30)	1:129:A:GLU:HG3	1:130:A:LEU:H	14	0.33
(1,30)	1:129:A:GLU:HG3	1:130:A:LEU:H	15	0.33
(1,15)	1:132:A:THR:HG23	2:27:B:SER:H	20	0.33
(1,2244)	2:36:B:THR:HG22	2:36:B:THR:H	1	0.32
(1,2244)	2:36:B:THR:HG22	2:36:B:THR:H	9	0.32
(1,2244)	2:36:B:THR:HG23	2:36:B:THR:H	10	0.32
(1,2228)	2:35:B:PHE:H	2:34:B:TYR:HB3	13	0.32
(1,2179)	1:60:A:LYS:HB3	1:61:A:LEU:H	8	0.32
(1,2173)	1:63:A:ASN:H	1:109:A:LEU:HD11	1	0.32
(1,2173)	1:63:A:ASN:H	1:109:A:LEU:HD12	21	0.32
(1,2142)	1:109:A:LEU:HD23	1:68:A:GLU:H	3	0.32
(1,2138)	1:69:A:GLU:HG3	1:69:A:GLU:H	15	0.32
(1,2138)	1:69:A:GLU:HG3	1:69:A:GLU:H	18	0.32
(1,2136)	1:69:A:GLU:H	1:70:A:PHE:HB2	9	0.32
(1,2106)	1:76:A:MET:HB3	1:77:A:GLN:H	12	0.32
(1,2106)	1:76:A:MET:HB3	1:77:A:GLN:H	21	0.32
(1,2100)	1:77:A:GLN:HE21	1:76:A:MET:HE2	15	0.32
(1,2097)	1:77:A:GLN:HE21	1:77:A:GLN:HA	21	0.32
(1,2051)	1:89:A:TYR:H	1:90:A:ASN:HB3	5	0.32
(1,2007)	1:100:A:LEU:HD22	1:95:A:ALA:H	25	0.32
(1,2006)	1:134:A:LEU:HD22	1:95:A:ALA:H	2	0.32
(1,2005)	1:95:A:ALA:H	1:94:A:ARG:HG2	25	0.32
(1,2004)	1:95:A:ALA:H	1:94:A:ARG:HB3	24	0.32
(1,1996)	1:97:A:SER:H	1:139:A:ALA:HB2	3	0.32
(1,1996)	1:97:A:SER:H	1:139:A:ALA:HB1	6	0.32
(1,1971)	1:100:A:LEU:HD22	1:101:A:ALA:H	23	0.32
(1,1961)	1:102:A:SER:H	1:59:A:TYR:HD1	13	0.32
(1,1854)	1:124:A:TYR:H	1:125:A:VAL:HG22	7	0.32
(1,1854)	1:124:A:TYR:H	1:125:A:VAL:HG21	8	0.32
(1,1854)	1:124:A:TYR:H	1:125:A:VAL:HG22	21	0.32
(1,1837)	1:127:A:ILE:H	1:123:A:LEU:HD12	13	0.32
(1,1801)	1:135:A:LYS:H	1:91:A:ARG:HD3	21	0.32
(1,1798)	1:136:A:ALA:H	1:135:A:LYS:HD2	18	0.32
(1,1792)	1:138:A:SER:H	1:135:A:LYS:HD3	24	0.32
(1,1789)	1:139:A:ALA:H	1:139:A:ALA:HB3	24	0.32
(1,1788)	1:139:A:ALA:H	1:135:A:LYS:HD2	9	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1772)	1:142:A:LYS:H	1:141:A:LYS:HG2	2	0.32
(1,1768)	2:24:B:GLN:HG3	2:24:B:GLN:HB2	20	0.32
(1,1768)	2:24:B:GLN:HG3	2:24:B:GLN:HB2	22	0.32
(1,1768)	2:24:B:GLN:HG3	2:24:B:GLN:HB2	25	0.32
(1,1745)	2:29:B:SER:HB3	2:30:B:GLU:H	19	0.32
(1,1727)	2:31:B:LEU:HD11	2:31:B:LEU:H	7	0.32
(1,1727)	2:31:B:LEU:HD13	2:31:B:LEU:H	8	0.32
(1,1727)	2:31:B:LEU:HD12	2:31:B:LEU:H	11	0.32
(1,1727)	2:31:B:LEU:HD11	2:31:B:LEU:H	12	0.32
(1,1720)	2:34:B:TYR:HE1	2:31:B:LEU:HD22	5	0.32
(1,1720)	2:34:B:TYR:HE1	2:31:B:LEU:HD21	12	0.32
(1,1720)	2:34:B:TYR:HE1	2:31:B:LEU:HD23	18	0.32
(1,1670)	2:37:B:ALA:HB2	2:36:B:THR:HA	24	0.32
(1,1667)	2:36:B:THR:HB	2:36:B:THR:H	3	0.32
(1,1666)	2:36:B:THR:HG21	1:124:A:TYR:H	24	0.32
(1,1650)	2:37:B:ALA:HB1	1:121:A:ALA:HB3	11	0.32
(1,1622)	2:39:B:TRP:HE3	2:39:B:TRP:HB2	20	0.32
(1,1619)	2:39:B:TRP:HD1	2:38:B:ARG:HB2	4	0.32
(1,1619)	2:39:B:TRP:HD1	2:38:B:ARG:HB2	16	0.32
(1,1618)	2:39:B:TRP:HD1	2:39:B:TRP:HB3	5	0.32
(1,1595)	2:31:B:LEU:HD13	1:127:A:ILE:HB	19	0.32
(1,1591)	1:84:A:VAL:HA	2:31:B:LEU:HD12	7	0.32
(1,1549)	1:58:A:CYS:HB2	1:57:A:LYS:HA	21	0.32
(1,1538)	1:59:A:TYR:HB3	1:59:A:TYR:HD1	2	0.32
(1,1538)	1:59:A:TYR:HB3	1:59:A:TYR:HD1	13	0.32
(1,1538)	1:59:A:TYR:HB3	1:59:A:TYR:HD1	17	0.32
(1,1538)	1:59:A:TYR:HB3	1:59:A:TYR:HD1	18	0.32
(1,1538)	1:59:A:TYR:HB3	1:59:A:TYR:HD1	21	0.32
(1,1440)	1:127:A:ILE:HD11	1:70:A:PHE:HZ	14	0.32
(1,1440)	1:127:A:ILE:HD13	1:70:A:PHE:HZ	19	0.32
(1,1416)	1:71:A:LEU:HD11	1:71:A:LEU:H	6	0.32
(1,1416)	1:71:A:LEU:HD13	1:71:A:LEU:H	7	0.32
(1,1395)	1:116:A:ALA:HB1	1:73:A:LEU:HD21	16	0.32
(1,1391)	1:74:A:CYS:HA	1:73:A:LEU:HD22	14	0.32
(1,1370)	1:75:A:LYS:HE3	1:72:A:GLU:HB3	24	0.32
(1,1361)	1:75:A:LYS:HE2	1:75:A:LYS:HG3	20	0.32
(1,1361)	1:75:A:LYS:HE2	1:75:A:LYS:HG3	23	0.32
(1,1345)	1:76:A:MET:HG2	1:77:A:GLN:H	12	0.32
(1,1331)	1:77:A:GLN:HG2	1:73:A:LEU:HD11	20	0.32
(1,1326)	1:77:A:GLN:HG2	1:77:A:GLN:HA	5	0.32
(1,1318)	1:79:A:ALA:HA	1:79:A:ALA:HB3	3	0.32
(1,1318)	1:79:A:ALA:HA	1:79:A:ALA:HB3	4	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1318)	1:79:A:ALA:HA	1:79:A:ALA:HB3	8	0.32
(1,1318)	1:79:A:ALA:HA	1:79:A:ALA:HB2	22	0.32
(1,1303)	1:137:A:HIS:HE1	1:136:A:ALA:HB3	12	0.32
(1,1282)	1:84:A:VAL:HG23	1:85:A:VAL:H	8	0.32
(1,1282)	1:84:A:VAL:HG23	1:85:A:VAL:H	10	0.32
(1,1282)	1:84:A:VAL:HG21	1:85:A:VAL:H	24	0.32
(1,1280)	1:84:A:VAL:HG23	1:81:A:HIS:HB2	8	0.32
(1,1269)	1:84:A:VAL:HG12	1:85:A:VAL:H	10	0.32
(1,1228)	1:87:A:PHE:HD1	1:88:A:LEU:HD21	16	0.32
(1,1209)	1:88:A:LEU:HD13	1:70:A:PHE:HE1	11	0.32
(1,1209)	1:88:A:LEU:HD12	1:70:A:PHE:HE1	15	0.32
(1,1209)	1:88:A:LEU:HD12	1:70:A:PHE:HE1	25	0.32
(1,1168)	1:100:A:LEU:HD23	1:92:A:GLN:HG2	22	0.32
(1,1139)	1:134:A:LEU:HD23	1:95:A:ALA:HB3	14	0.32
(1,1133)	1:95:A:ALA:HB3	1:99:A:PHE:HD2	12	0.32
(1,1126)	1:96:A:HIS:HD2	1:139:A:ALA:HB3	15	0.32
(1,1122)	1:96:A:HIS:HA	1:139:A:ALA:HB1	6	0.32
(1,1074)	1:101:A:ALA:HB3	1:60:A:LYS:HA	3	0.32
(1,1042)	1:62:A:GLU:HB2	1:62:A:GLU:HA	20	0.32
(1,1000)	1:108:A:ILE:HD11	1:99:A:PHE:HE1	14	0.32
(1,996)	1:108:A:ILE:HG21	1:112:A:VAL:HG12	12	0.32
(1,980)	1:108:A:ILE:HA	1:108:A:ILE:HD13	8	0.32
(1,960)	1:67:A:PHE:HA	1:109:A:LEU:HD13	23	0.32
(1,936)	1:112:A:VAL:HG11	1:112:A:VAL:HG22	18	0.32
(1,936)	1:112:A:VAL:HG12	1:112:A:VAL:HG21	24	0.32
(1,934)	1:112:A:VAL:HG13	1:126:A:TYR:HB3	14	0.32
(1,934)	1:112:A:VAL:HG13	1:126:A:TYR:HB3	18	0.32
(1,934)	1:112:A:VAL:HG12	1:126:A:TYR:HB3	19	0.32
(1,858)	1:119:A:ARG:HG3	1:119:A:ARG:HA	15	0.32
(1,858)	1:119:A:ARG:HG3	1:119:A:ARG:HA	23	0.32
(1,778)	1:125:A:VAL:HG23	1:122:A:LYS:HA	22	0.32
(1,766)	1:126:A:TYR:HE1	1:115:A:ARG:HB2	22	0.32
(1,743)	1:127:A:ILE:HG21	1:124:A:TYR:HA	2	0.32
(1,662)	1:133:A:VAL:HA	1:133:A:VAL:HG11	5	0.32
(1,662)	1:133:A:VAL:HA	1:133:A:VAL:HG11	19	0.32
(1,643)	1:134:A:LEU:HD22	1:134:A:LEU:HD13	5	0.32
(1,643)	1:134:A:LEU:HD21	1:134:A:LEU:HD13	8	0.32
(1,643)	1:134:A:LEU:HD21	1:134:A:LEU:HD13	9	0.32
(1,643)	1:134:A:LEU:HD22	1:134:A:LEU:HD13	11	0.32
(1,643)	1:134:A:LEU:HD22	1:134:A:LEU:HD12	13	0.32
(1,643)	1:134:A:LEU:HD22	1:134:A:LEU:HD13	22	0.32
(1,643)	1:134:A:LEU:HD22	1:134:A:LEU:HD11	25	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,633)	1:100:A:LEU:HD11	1:92:A:GLN:HE21	2	0.32
(1,631)	1:73:A:LEU:HD13	1:117:A:ARG:HA	10	0.32
(1,574)	1:143:A:LEU:HG	1:143:A:LEU:H	13	0.32
(1,558)	2:32:B:GLU:HA	2:31:B:LEU:H	6	0.32
(1,558)	2:32:B:GLU:HA	2:31:B:LEU:H	7	0.32
(1,558)	2:32:B:GLU:HA	2:31:B:LEU:H	8	0.32
(1,558)	2:32:B:GLU:HA	2:31:B:LEU:H	11	0.32
(1,558)	2:32:B:GLU:HA	2:31:B:LEU:H	12	0.32
(1,558)	2:32:B:GLU:HA	2:31:B:LEU:H	25	0.32
(1,541)	1:61:A:LEU:HB3	1:62:A:GLU:H	2	0.32
(1,541)	1:61:A:LEU:HB3	1:62:A:GLU:H	6	0.32
(1,521)	1:71:A:LEU:H	1:113:A:LEU:HD12	3	0.32
(1,521)	1:71:A:LEU:H	1:113:A:LEU:HD12	17	0.32
(1,515)	1:73:A:LEU:HG	1:76:A:MET:H	4	0.32
(1,490)	1:91:A:ARG:H	1:94:A:ARG:H	2	0.32
(1,473)	1:101:A:ALA:H	1:100:A:LEU:HG	1	0.32
(1,465)	1:106:A:CYS:H	1:103:A:ALA:HB1	1	0.32
(1,426)	1:125:A:VAL:HG11	1:126:A:TYR:H	7	0.32
(1,426)	1:125:A:VAL:HG11	1:126:A:TYR:H	8	0.32
(1,426)	1:125:A:VAL:HG12	1:126:A:TYR:H	9	0.32
(1,426)	1:125:A:VAL:HG11	1:126:A:TYR:H	10	0.32
(1,426)	1:125:A:VAL:HG12	1:126:A:TYR:H	20	0.32
(1,414)	1:72:A:GLU:H	1:68:A:GLU:HA	9	0.32
(1,414)	1:72:A:GLU:H	1:68:A:GLU:HA	18	0.32
(1,366)	1:100:A:LEU:HD12	1:138:A:SER:HB3	10	0.32
(1,364)	2:29:B:SER:HB3	2:32:B:GLU:HB2	4	0.32
(1,364)	2:29:B:SER:HB3	2:32:B:GLU:HB2	11	0.32
(1,364)	2:29:B:SER:HB3	2:32:B:GLU:HB2	23	0.32
(1,342)	2:31:B:LEU:HD12	1:124:A:TYR:HB3	24	0.32
(1,337)	2:31:B:LEU:HD23	2:28:B:ASP:HB3	4	0.32
(1,324)	2:33:B:GLN:HG2	2:26:B:ASP:HB3	16	0.32
(1,290)	2:39:B:TRP:HH2	2:36:B:THR:HB	5	0.32
(1,286)	2:30:B:GLU:HG2	1:87:A:PHE:HZ	22	0.32
(1,275)	1:84:A:VAL:HG12	2:35:B:PHE:HE1	4	0.32
(1,275)	1:84:A:VAL:HG11	2:35:B:PHE:HZ	12	0.32
(1,275)	1:84:A:VAL:HG11	2:35:B:PHE:HE1	13	0.32
(1,275)	1:84:A:VAL:HG13	2:35:B:PHE:HZ	18	0.32
(1,275)	1:84:A:VAL:HG11	2:35:B:PHE:HZ	21	0.32
(1,275)	1:84:A:VAL:HG11	2:35:B:PHE:HE1	23	0.32
(1,270)	1:88:A:LEU:HD22	2:31:B:LEU:HD12	3	0.32
(1,257)	1:113:A:LEU:HD11	1:113:A:LEU:HB2	1	0.32
(1,257)	1:113:A:LEU:HD11	1:113:A:LEU:HB2	7	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,255)	1:56:A:LYS:HA	1:56:A:LYS:HB3	13	0.32
(1,244)	1:111:A:ARG:HA	1:115:A:ARG:HG2	3	0.32
(1,229)	1:105:A:PHE:HE2	1:67:A:PHE:HB2	4	0.32
(1,228)	1:62:A:GLU:HG2	1:61:A:LEU:HD21	1	0.32
(1,225)	1:129:A:GLU:HG2	1:125:A:VAL:HG12	6	0.32
(1,210)	1:105:A:PHE:HZ	1:109:A:LEU:HD23	5	0.32
(1,210)	1:105:A:PHE:HZ	1:109:A:LEU:HD21	25	0.32
(1,191)	1:85:A:VAL:HG12	1:74:A:CYS:HB2	7	0.32
(1,191)	1:78:A:THR:HG21	1:74:A:CYS:HB2	21	0.32
(1,191)	1:84:A:VAL:HG13	1:74:A:CYS:HB2	24	0.32
(1,172)	1:85:A:VAL:HG13	1:74:A:CYS:HB3	3	0.32
(1,161)	1:87:A:PHE:HE2	2:34:B:TYR:HE1	13	0.32
(1,155)	1:88:A:LEU:HD23	1:131:A:CYS:HB3	16	0.32
(1,147)	1:137:A:HIS:HB3	1:138:A:SER:H	12	0.32
(1,147)	1:137:A:HIS:HB3	1:138:A:SER:H	16	0.32
(1,141)	1:93:A:GLN:HG2	1:89:A:TYR:HD1	11	0.32
(1,122)	1:95:A:ALA:HB3	1:91:A:ARG:HD3	6	0.32
(1,116)	1:100:A:LEU:HD23	1:105:A:PHE:HE2	9	0.32
(1,116)	1:100:A:LEU:HD21	1:105:A:PHE:HE2	20	0.32
(1,98)	1:105:A:PHE:HD1	1:100:A:LEU:HD21	12	0.32
(1,97)	1:105:A:PHE:HD1	1:100:A:LEU:HA	17	0.32
(1,95)	1:107:A:ASN:HB2	1:108:A:ILE:HB	25	0.32
(1,94)	1:90:A:ASN:HA	1:91:A:ARG:H	20	0.32
(1,92)	1:109:A:LEU:HD22	1:67:A:PHE:H	5	0.32
(1,92)	1:109:A:LEU:HD21	1:67:A:PHE:H	12	0.32
(1,87)	1:112:A:VAL:HG11	1:130:A:LEU:H	13	0.32
(1,81)	1:116:A:ALA:HB2	1:70:A:PHE:HZ	11	0.32
(1,81)	1:116:A:ALA:HB1	1:70:A:PHE:HZ	12	0.32
(1,62)	1:123:A:LEU:HD23	1:70:A:PHE:HE1	23	0.32
(1,56)	1:124:A:TYR:HE2	2:35:B:PHE:HB3	22	0.32
(1,54)	1:127:A:ILE:HG23	1:124:A:TYR:HD1	4	0.32
(1,54)	1:127:A:ILE:HG21	1:124:A:TYR:HD1	16	0.32
(1,51)	1:126:A:TYR:HD1	1:125:A:VAL:HG11	22	0.32
(1,37)	1:127:A:ILE:HG22	1:128:A:ASN:HD22	3	0.32
(1,30)	1:129:A:GLU:HG3	1:130:A:LEU:H	2	0.32
(1,30)	1:129:A:GLU:HG3	1:130:A:LEU:H	16	0.32
(1,27)	1:130:A:LEU:HD21	1:67:A:PHE:HA	23	0.32
(1,24)	1:85:A:VAL:HG23	1:71:A:LEU:HA	12	0.32
(1,24)	1:85:A:VAL:HG22	1:86:A:PRO:HD3	20	0.32
(1,24)	1:85:A:VAL:HG22	1:71:A:LEU:HA	25	0.32
(1,17)	1:133:A:VAL:HG13	1:137:A:HIS:HB2	23	0.32
(1,13)	1:133:A:VAL:HG13	1:108:A:ILE:HB	19	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,8)	1:134:A:LEU:HD23	1:105:A:PHE:HD1	13	0.32
(1,2244)	2:36:B:THR:HG21	2:36:B:THR:H	14	0.31
(1,2228)	2:35:B:PHE:H	2:34:B:TYR:HB3	16	0.31
(1,2195)	1:56:A:LYS:H	1:56:A:LYS:HG2	22	0.31
(1,2188)	1:59:A:TYR:H	1:58:A:CYS:HB3	7	0.31
(1,2179)	1:60:A:LYS:HB3	1:61:A:LEU:H	17	0.31
(1,2142)	1:109:A:LEU:HD23	1:68:A:GLU:H	7	0.31
(1,2142)	1:109:A:LEU:HD23	1:68:A:GLU:H	11	0.31
(1,2142)	1:109:A:LEU:HD22	1:68:A:GLU:H	21	0.31
(1,2097)	1:77:A:GLN:HE21	1:77:A:GLN:HA	3	0.31
(1,2071)	1:83:A:GLU:HG3	1:83:A:GLU:H	2	0.31
(1,2071)	1:83:A:GLU:HG3	1:83:A:GLU:H	22	0.31
(1,2007)	1:100:A:LEU:HD23	1:95:A:ALA:H	16	0.31
(1,2006)	1:134:A:LEU:HD21	1:95:A:ALA:H	11	0.31
(1,2006)	1:134:A:LEU:HD21	1:95:A:ALA:H	15	0.31
(1,2006)	1:134:A:LEU:HD23	1:95:A:ALA:H	18	0.31
(1,2004)	1:95:A:ALA:H	1:94:A:ARG:HB3	1	0.31
(1,1968)	1:101:A:ALA:H	1:63:A:ASN:HD22	9	0.31
(1,1906)	1:111:A:ARG:H	1:111:A:ARG:HD2	22	0.31
(1,1886)	1:88:A:LEU:H	1:87:A:PHE:HD1	24	0.31
(1,1854)	1:124:A:TYR:H	1:125:A:VAL:HG23	1	0.31
(1,1854)	1:124:A:TYR:H	1:125:A:VAL:HG23	3	0.31
(1,1854)	1:124:A:TYR:H	1:125:A:VAL:HG22	11	0.31
(1,1854)	1:124:A:TYR:H	1:125:A:VAL:HG22	16	0.31
(1,1788)	1:139:A:ALA:H	1:135:A:LYS:HD2	18	0.31
(1,1788)	1:139:A:ALA:H	1:135:A:LYS:HD2	23	0.31
(1,1768)	2:24:B:GLN:HG3	2:24:B:GLN:HB2	3	0.31
(1,1768)	2:24:B:GLN:HG3	2:24:B:GLN:HB2	15	0.31
(1,1754)	2:30:B:GLU:HG2	2:31:B:LEU:H	13	0.31
(1,1745)	2:29:B:SER:HB3	2:30:B:GLU:H	11	0.31
(1,1727)	2:31:B:LEU:HD11	2:31:B:LEU:H	14	0.31
(1,1720)	2:34:B:TYR:HE1	2:31:B:LEU:HD21	9	0.31
(1,1716)	2:31:B:LEU:HG	2:32:B:GLU:HG3	17	0.31
(1,1713)	2:31:B:LEU:HG	2:31:B:LEU:H	7	0.31
(1,1666)	2:36:B:THR:HG22	1:124:A:TYR:H	16	0.31
(1,1636)	2:35:B:PHE:HB3	2:34:B:TYR:HE1	10	0.31
(1,1622)	2:39:B:TRP:HE3	2:39:B:TRP:HB2	21	0.31
(1,1619)	2:39:B:TRP:HD1	2:38:B:ARG:HB2	2	0.31
(1,1619)	2:39:B:TRP:HD1	2:38:B:ARG:HB2	15	0.31
(1,1592)	1:84:A:VAL:HG22	2:35:B:PHE:HB2	9	0.31
(1,1592)	1:84:A:VAL:HG23	2:35:B:PHE:HB2	25	0.31
(1,1591)	1:84:A:VAL:HA	2:31:B:LEU:HD12	9	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1577)	1:77:A:GLN:HG2	1:73:A:LEU:HD13	24	0.31
(1,1577)	1:77:A:GLN:HG3	1:73:A:LEU:HD11	25	0.31
(1,1570)	1:57:A:LYS:HE2	1:59:A:TYR:HE1	1	0.31
(1,1559)	1:57:A:LYS:HB2	1:57:A:LYS:HG2	25	0.31
(1,1538)	1:59:A:TYR:HB3	1:59:A:TYR:HD1	6	0.31
(1,1538)	1:59:A:TYR:HB3	1:59:A:TYR:HD1	22	0.31
(1,1534)	1:59:A:TYR:HD1	1:59:A:TYR:H	11	0.31
(1,1466)	1:109:A:LEU:HD12	1:66:A:LEU:HG	2	0.31
(1,1456)	1:69:A:GLU:HG2	1:66:A:LEU:HA	24	0.31
(1,1447)	1:69:A:GLU:HA	1:69:A:GLU:HG3	22	0.31
(1,1440)	1:127:A:ILE:HD13	1:70:A:PHE:HZ	6	0.31
(1,1440)	1:127:A:ILE:HD13	1:70:A:PHE:HZ	16	0.31
(1,1419)	1:71:A:LEU:HD11	1:89:A:TYR:H	8	0.31
(1,1416)	1:71:A:LEU:HD12	1:71:A:LEU:H	8	0.31
(1,1395)	1:116:A:ALA:HB3	1:73:A:LEU:HD22	1	0.31
(1,1395)	1:116:A:ALA:HB3	1:73:A:LEU:HD21	14	0.31
(1,1391)	1:74:A:CYS:HA	1:73:A:LEU:HD21	8	0.31
(1,1345)	1:76:A:MET:HG2	1:77:A:GLN:H	4	0.31
(1,1345)	1:76:A:MET:HG2	1:77:A:GLN:H	6	0.31
(1,1345)	1:76:A:MET:HG2	1:77:A:GLN:H	25	0.31
(1,1318)	1:79:A:ALA:HA	1:79:A:ALA:HB1	7	0.31
(1,1318)	1:79:A:ALA:HA	1:79:A:ALA:HB3	13	0.31
(1,1318)	1:79:A:ALA:HA	1:79:A:ALA:HB3	15	0.31
(1,1318)	1:79:A:ALA:HA	1:79:A:ALA:HB3	17	0.31
(1,1318)	1:79:A:ALA:HA	1:79:A:ALA:HB3	23	0.31
(1,1318)	1:79:A:ALA:HA	1:79:A:ALA:HB1	25	0.31
(1,1282)	1:84:A:VAL:HG21	1:85:A:VAL:H	12	0.31
(1,1269)	1:84:A:VAL:HG13	1:85:A:VAL:H	4	0.31
(1,1269)	1:84:A:VAL:HG11	1:85:A:VAL:H	8	0.31
(1,1269)	1:84:A:VAL:HG11	1:85:A:VAL:H	15	0.31
(1,1269)	1:84:A:VAL:HG13	1:85:A:VAL:H	25	0.31
(1,1252)	1:69:A:GLU:HB2	1:69:A:GLU:HG2	12	0.31
(1,1228)	1:87:A:PHE:HD1	1:88:A:LEU:HD21	6	0.31
(1,1228)	1:87:A:PHE:HD1	1:88:A:LEU:HD23	19	0.31
(1,1209)	1:88:A:LEU:HD11	1:70:A:PHE:HE1	5	0.31
(1,1209)	1:88:A:LEU:HD11	1:70:A:PHE:HE1	6	0.31
(1,1209)	1:88:A:LEU:HD13	1:70:A:PHE:HE1	9	0.31
(1,1209)	1:88:A:LEU:HD13	1:70:A:PHE:HE1	16	0.31
(1,1209)	1:88:A:LEU:HD12	1:70:A:PHE:HE1	18	0.31
(1,1209)	1:88:A:LEU:HD13	1:70:A:PHE:HE1	19	0.31
(1,1168)	1:100:A:LEU:HD22	1:92:A:GLN:HG2	10	0.31
(1,1139)	1:134:A:LEU:HD21	1:95:A:ALA:HB1	19	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1139)	1:134:A:LEU:HD22	1:95:A:ALA:HB2	23	0.31
(1,1137)	1:95:A:ALA:HB1	1:91:A:ARG:HD3	7	0.31
(1,1133)	1:95:A:ALA:HB1	1:99:A:PHE:HD2	2	0.31
(1,1133)	1:95:A:ALA:HB3	1:99:A:PHE:HD2	10	0.31
(1,1098)	1:100:A:LEU:HD21	1:92:A:GLN:HA	7	0.31
(1,1094)	1:100:A:LEU:HD22	1:138:A:SER:HB2	24	0.31
(1,1088)	1:100:A:LEU:HD22	1:105:A:PHE:HD2	18	0.31
(1,1074)	1:101:A:ALA:HB2	1:60:A:LYS:HA	22	0.31
(1,1057)	1:103:A:ALA:HB3	1:59:A:TYR:HD1	1	0.31
(1,1057)	1:103:A:ALA:HB2	1:59:A:TYR:HD1	13	0.31
(1,1042)	1:62:A:GLU:HB2	1:62:A:GLU:HA	3	0.31
(1,1042)	1:62:A:GLU:HB2	1:62:A:GLU:HA	8	0.31
(1,1042)	1:62:A:GLU:HB2	1:62:A:GLU:HA	9	0.31
(1,1042)	1:62:A:GLU:HB2	1:62:A:GLU:HA	13	0.31
(1,1000)	1:108:A:ILE:HD13	1:99:A:PHE:HE1	9	0.31
(1,996)	1:108:A:ILE:HG23	1:112:A:VAL:HG13	16	0.31
(1,996)	1:108:A:ILE:HG22	1:112:A:VAL:HG13	25	0.31
(1,960)	1:67:A:PHE:HA	1:109:A:LEU:HD12	19	0.31
(1,936)	1:112:A:VAL:HG12	1:112:A:VAL:HG22	17	0.31
(1,936)	1:112:A:VAL:HG12	1:112:A:VAL:HG23	20	0.31
(1,900)	1:115:A:ARG:HB3	1:115:A:ARG:HG2	2	0.31
(1,900)	1:115:A:ARG:HB3	1:115:A:ARG:HG2	4	0.31
(1,900)	1:115:A:ARG:HB3	1:115:A:ARG:HG2	7	0.31
(1,900)	1:115:A:ARG:HB3	1:115:A:ARG:HG2	9	0.31
(1,900)	1:115:A:ARG:HB3	1:115:A:ARG:HG2	13	0.31
(1,900)	1:115:A:ARG:HB3	1:115:A:ARG:HG2	14	0.31
(1,900)	1:115:A:ARG:HB3	1:115:A:ARG:HG2	18	0.31
(1,900)	1:115:A:ARG:HB3	1:115:A:ARG:HG2	23	0.31
(1,900)	1:115:A:ARG:HB3	1:115:A:ARG:HG2	24	0.31
(1,900)	1:115:A:ARG:HB3	1:115:A:ARG:HG2	25	0.31
(1,886)	1:116:A:ALA:HA	1:123:A:LEU:HD12	13	0.31
(1,886)	1:116:A:ALA:HA	1:123:A:LEU:HD13	18	0.31
(1,867)	1:119:A:ARG:HD3	1:119:A:ARG:HA	6	0.31
(1,795)	1:127:A:ILE:HD12	1:124:A:TYR:HE1	5	0.31
(1,778)	1:125:A:VAL:HG23	1:122:A:LYS:HA	18	0.31
(1,775)	1:126:A:TYR:HE1	1:125:A:VAL:HG11	5	0.31
(1,668)	1:133:A:VAL:HG11	1:130:A:LEU:HD11	13	0.31
(1,666)	1:134:A:LEU:HD23	1:133:A:VAL:HG12	7	0.31
(1,666)	1:134:A:LEU:HD22	1:133:A:VAL:HG13	18	0.31
(1,662)	1:133:A:VAL:HA	1:133:A:VAL:HG12	15	0.31
(1,662)	1:133:A:VAL:HA	1:133:A:VAL:HG12	24	0.31
(1,643)	1:134:A:LEU:HD21	1:134:A:LEU:HD12	18	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,643)	1:134:A:LEU:HD23	1:134:A:LEU:HD11	21	0.31
(1,576)	1:142:A:LYS:HB2	1:142:A:LYS:H	18	0.31
(1,576)	1:142:A:LYS:HB2	1:142:A:LYS:H	25	0.31
(1,562)	2:26:B:ASP:H	2:25:B:GLU:HG3	2	0.31
(1,562)	2:26:B:ASP:H	2:25:B:GLU:HG2	21	0.31
(1,561)	2:27:B:SER:H	2:30:B:GLU:HB3	7	0.31
(1,558)	2:32:B:GLU:HA	2:31:B:LEU:H	4	0.31
(1,558)	2:32:B:GLU:HA	2:31:B:LEU:H	19	0.31
(1,558)	2:32:B:GLU:HA	2:31:B:LEU:H	20	0.31
(1,541)	1:61:A:LEU:HB3	1:62:A:GLU:H	15	0.31
(1,541)	1:61:A:LEU:HB3	1:62:A:GLU:H	17	0.31
(1,541)	1:61:A:LEU:HB3	1:62:A:GLU:H	18	0.31
(1,541)	1:61:A:LEU:HB3	1:62:A:GLU:H	23	0.31
(1,538)	1:63:A:ASN:H	1:61:A:LEU:HA	8	0.31
(1,529)	1:67:A:PHE:H	1:69:A:GLU:HB2	20	0.31
(1,522)	1:70:A:PHE:H	1:73:A:LEU:H	10	0.31
(1,520)	1:130:A:LEU:H	1:112:A:VAL:HG22	17	0.31
(1,515)	1:73:A:LEU:HG	1:76:A:MET:H	5	0.31
(1,515)	1:73:A:LEU:HG	1:76:A:MET:H	13	0.31
(1,515)	1:73:A:LEU:HG	1:76:A:MET:H	23	0.31
(1,505)	1:79:A:ALA:H	1:76:A:MET:HA	4	0.31
(1,505)	1:79:A:ALA:H	1:76:A:MET:HA	22	0.31
(1,505)	1:79:A:ALA:H	1:76:A:MET:HA	25	0.31
(1,500)	1:85:A:VAL:H	1:83:A:GLU:H	7	0.31
(1,492)	1:91:A:ARG:H	1:88:A:LEU:HD21	16	0.31
(1,490)	1:91:A:ARG:H	1:94:A:ARG:H	18	0.31
(1,476)	1:96:A:HIS:H	1:95:A:ALA:H	22	0.31
(1,469)	1:102:A:SER:H	1:100:A:LEU:HB2	19	0.31
(1,445)	1:116:A:ALA:H	1:112:A:VAL:HA	25	0.31
(1,438)	1:66:A:LEU:HD13	1:66:A:LEU:H	23	0.31
(1,426)	1:125:A:VAL:HG12	1:126:A:TYR:H	12	0.31
(1,426)	1:125:A:VAL:HG11	1:126:A:TYR:H	16	0.31
(1,426)	1:125:A:VAL:HG13	1:126:A:TYR:H	19	0.31
(1,426)	1:125:A:VAL:HG11	1:126:A:TYR:H	22	0.31
(1,426)	1:125:A:VAL:HG13	1:126:A:TYR:H	25	0.31
(1,421)	1:128:A:ASN:H	1:70:A:PHE:HZ	12	0.31
(1,421)	1:128:A:ASN:H	1:70:A:PHE:HZ	19	0.31
(1,369)	2:26:B:ASP:HB2	1:87:A:PHE:HZ	15	0.31
(1,355)	2:29:B:SER:HB3	2:31:B:LEU:H	16	0.31
(1,342)	2:31:B:LEU:HD12	1:124:A:TYR:HB3	13	0.31
(1,342)	2:31:B:LEU:HD13	1:124:A:TYR:HB3	18	0.31
(1,337)	2:31:B:LEU:HD21	2:28:B:ASP:HB2	5	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,337)	2:31:B:LEU:HD21	2:28:B:ASP:HB3	10	0.31
(1,321)	2:34:B:TYR:HD1	1:83:A:GLU:HB3	20	0.31
(1,312)	2:35:B:PHE:HE1	2:36:B:THR:HA	3	0.31
(1,307)	2:39:B:TRP:HE3	2:36:B:THR:HG22	11	0.31
(1,275)	1:84:A:VAL:HG11	2:35:B:PHE:HE1	11	0.31
(1,236)	1:64:A:GLU:HA	1:67:A:PHE:H	2	0.31
(1,236)	1:64:A:GLU:HA	1:67:A:PHE:H	7	0.31
(1,236)	1:64:A:GLU:HA	1:67:A:PHE:H	9	0.31
(1,229)	1:105:A:PHE:HE2	1:67:A:PHE:HB2	3	0.31
(1,229)	1:105:A:PHE:HE2	1:67:A:PHE:HB2	23	0.31
(1,225)	1:129:A:GLU:HG2	1:125:A:VAL:HG11	7	0.31
(1,222)	1:68:A:GLU:HA	1:71:A:LEU:HG	4	0.31
(1,210)	1:105:A:PHE:HZ	1:109:A:LEU:HD23	4	0.31
(1,210)	1:105:A:PHE:HZ	1:109:A:LEU:HD23	6	0.31
(1,210)	1:105:A:PHE:HZ	1:109:A:LEU:HD23	13	0.31
(1,210)	1:105:A:PHE:HZ	1:109:A:LEU:HD23	21	0.31
(1,195)	1:73:A:LEU:HD22	1:117:A:ARG:HA	20	0.31
(1,191)	1:84:A:VAL:HG13	1:74:A:CYS:HB2	23	0.31
(1,186)	1:123:A:LEU:HD23	1:77:A:GLN:HG3	1	0.31
(1,172)	1:85:A:VAL:HG12	1:74:A:CYS:HB3	13	0.31
(1,172)	1:85:A:VAL:HG12	1:74:A:CYS:HB3	14	0.31
(1,147)	1:137:A:HIS:HB3	1:138:A:SER:H	5	0.31
(1,145)	1:88:A:LEU:HB3	1:85:A:VAL:HA	1	0.31
(1,116)	1:100:A:LEU:HD23	1:105:A:PHE:HE2	18	0.31
(1,97)	1:105:A:PHE:HD1	1:100:A:LEU:HA	4	0.31
(1,95)	1:107:A:ASN:HB2	1:108:A:ILE:HB	5	0.31
(1,92)	1:109:A:LEU:HD23	1:67:A:PHE:H	3	0.31
(1,87)	1:112:A:VAL:HG12	1:130:A:LEU:H	11	0.31
(1,87)	1:112:A:VAL:HG11	1:130:A:LEU:H	14	0.31
(1,81)	1:116:A:ALA:HB3	1:70:A:PHE:HZ	22	0.31
(1,62)	1:123:A:LEU:HD23	1:70:A:PHE:HE1	4	0.31
(1,51)	1:126:A:TYR:HD1	1:125:A:VAL:HG11	17	0.31
(1,36)	1:127:A:ILE:HG22	1:124:A:TYR:HD2	23	0.31
(1,30)	1:129:A:GLU:HG3	1:130:A:LEU:H	20	0.31
(1,27)	1:130:A:LEU:HD21	1:67:A:PHE:HA	3	0.31
(1,24)	1:85:A:VAL:HG21	1:71:A:LEU:HA	4	0.31
(1,2260)	2:27:B:SER:HB2	2:27:B:SER:H	22	0.3
(1,2244)	2:36:B:THR:HG21	2:36:B:THR:H	8	0.3
(1,2244)	2:36:B:THR:HG21	2:36:B:THR:H	22	0.3
(1,2244)	2:36:B:THR:HG21	2:36:B:THR:H	23	0.3
(1,2228)	2:35:B:PHE:H	2:34:B:TYR:HB3	2	0.3
(1,2197)	1:55:A:GLY:HA2	1:56:A:LYS:H	22	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2193)	1:58:A:CYS:H	1:57:A:LYS:HG2	22	0.3
(1,2173)	1:63:A:ASN:H	1:109:A:LEU:HD13	18	0.3
(1,2142)	1:109:A:LEU:HD22	1:68:A:GLU:H	5	0.3
(1,2142)	1:109:A:LEU:HD21	1:68:A:GLU:H	20	0.3
(1,2142)	1:109:A:LEU:HD23	1:68:A:GLU:H	23	0.3
(1,2138)	1:69:A:GLU:HG3	1:69:A:GLU:H	6	0.3
(1,2097)	1:77:A:GLN:HE21	1:77:A:GLN:HA	7	0.3
(1,2097)	1:77:A:GLN:HE21	1:77:A:GLN:HA	14	0.3
(1,2097)	1:77:A:GLN:HE21	1:77:A:GLN:HA	16	0.3
(1,2017)	1:93:A:GLN:HE22	1:89:A:TYR:HB3	20	0.3
(1,2012)	1:94:A:ARG:HB3	1:94:A:ARG:H	6	0.3
(1,2007)	1:100:A:LEU:HD21	1:95:A:ALA:H	13	0.3
(1,2007)	1:100:A:LEU:HD23	1:95:A:ALA:H	21	0.3
(1,2006)	1:134:A:LEU:HD21	1:95:A:ALA:H	4	0.3
(1,2006)	1:134:A:LEU:HD23	1:95:A:ALA:H	8	0.3
(1,2006)	1:134:A:LEU:HD21	1:95:A:ALA:H	25	0.3
(1,2005)	1:95:A:ALA:H	1:94:A:ARG:HG2	24	0.3
(1,2004)	1:95:A:ALA:H	1:94:A:ARG:HB3	22	0.3
(1,1996)	1:97:A:SER:H	1:139:A:ALA:HB1	22	0.3
(1,1983)	1:99:A:PHE:H	1:138:A:SER:HB2	10	0.3
(1,1968)	1:101:A:ALA:H	1:63:A:ASN:HD22	19	0.3
(1,1961)	1:102:A:SER:H	1:59:A:TYR:HD1	1	0.3
(1,1961)	1:102:A:SER:H	1:59:A:TYR:HD1	8	0.3
(1,1961)	1:102:A:SER:H	1:59:A:TYR:HD1	9	0.3
(1,1854)	1:124:A:TYR:H	1:125:A:VAL:HG21	4	0.3
(1,1854)	1:124:A:TYR:H	1:125:A:VAL:HG22	20	0.3
(1,1801)	1:135:A:LYS:H	1:91:A:ARG:HD3	12	0.3
(1,1768)	2:24:B:GLN:HG3	2:24:B:GLN:HB2	17	0.3
(1,1754)	2:30:B:GLU:HG2	2:31:B:LEU:H	9	0.3
(1,1727)	2:31:B:LEU:HD13	2:31:B:LEU:H	4	0.3
(1,1727)	2:31:B:LEU:HD11	2:31:B:LEU:H	9	0.3
(1,1727)	2:31:B:LEU:HD11	2:31:B:LEU:H	24	0.3
(1,1723)	2:31:B:LEU:HD21	2:30:B:GLU:HB2	14	0.3
(1,1723)	2:31:B:LEU:HD23	2:30:B:GLU:HB2	25	0.3
(1,1720)	2:34:B:TYR:HE1	2:31:B:LEU:HD23	11	0.3
(1,1720)	2:34:B:TYR:HE1	2:31:B:LEU:HD21	17	0.3
(1,1713)	2:31:B:LEU:HG	2:31:B:LEU:H	1	0.3
(1,1713)	2:31:B:LEU:HG	2:31:B:LEU:H	25	0.3
(1,1703)	2:33:B:GLN:HG2	2:31:B:LEU:HD21	17	0.3
(1,1703)	2:33:B:GLN:HG2	2:31:B:LEU:HD23	20	0.3
(1,1666)	2:36:B:THR:HG23	1:124:A:TYR:H	21	0.3
(1,1652)	2:37:B:ALA:HB1	2:38:B:ARG:HD3	15	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1635)	2:39:B:TRP:HA	2:38:B:ARG:HD2	1	0.3
(1,1622)	2:39:B:TRP:HE3	2:39:B:TRP:HB2	2	0.3
(1,1619)	2:39:B:TRP:HD1	2:38:B:ARG:HB2	6	0.3
(1,1592)	1:84:A:VAL:HG21	2:35:B:PHE:HB2	18	0.3
(1,1591)	1:84:A:VAL:HA	2:31:B:LEU:HD11	10	0.3
(1,1591)	1:84:A:VAL:HA	2:31:B:LEU:HD12	12	0.3
(1,1588)	1:87:A:PHE:HB2	2:31:B:LEU:HD11	9	0.3
(1,1577)	1:77:A:GLN:HG3	1:73:A:LEU:HD13	8	0.3
(1,1570)	1:57:A:LYS:HE2	1:59:A:TYR:HE1	17	0.3
(1,1538)	1:59:A:TYR:HB3	1:59:A:TYR:HD1	16	0.3
(1,1534)	1:59:A:TYR:HD1	1:59:A:TYR:H	5	0.3
(1,1534)	1:59:A:TYR:HD1	1:59:A:TYR:H	25	0.3
(1,1496)	1:64:A:GLU:HG3	1:64:A:GLU:HA	12	0.3
(1,1495)	1:64:A:GLU:HA	1:67:A:PHE:HB2	22	0.3
(1,1447)	1:69:A:GLU:HA	1:69:A:GLU:HG3	3	0.3
(1,1419)	1:71:A:LEU:HD12	1:89:A:TYR:H	11	0.3
(1,1391)	1:74:A:CYS:HA	1:73:A:LEU:HD22	17	0.3
(1,1391)	1:74:A:CYS:HA	1:73:A:LEU:HD21	18	0.3
(1,1345)	1:76:A:MET:HG2	1:77:A:GLN:H	3	0.3
(1,1345)	1:76:A:MET:HG2	1:77:A:GLN:H	9	0.3
(1,1345)	1:76:A:MET:HG2	1:77:A:GLN:H	18	0.3
(1,1345)	1:76:A:MET:HG2	1:77:A:GLN:H	22	0.3
(1,1318)	1:79:A:ALA:HA	1:79:A:ALA:HB3	12	0.3
(1,1280)	1:84:A:VAL:HG22	1:81:A:HIS:HB2	15	0.3
(1,1269)	1:84:A:VAL:HG13	1:85:A:VAL:H	1	0.3
(1,1269)	1:84:A:VAL:HG13	1:85:A:VAL:H	5	0.3
(1,1269)	1:84:A:VAL:HG12	1:85:A:VAL:H	7	0.3
(1,1269)	1:84:A:VAL:HG12	1:85:A:VAL:H	12	0.3
(1,1269)	1:84:A:VAL:HG11	1:85:A:VAL:H	18	0.3
(1,1269)	1:84:A:VAL:HG12	1:85:A:VAL:H	19	0.3
(1,1269)	1:84:A:VAL:HG12	1:85:A:VAL:H	24	0.3
(1,1209)	1:88:A:LEU:HD12	1:70:A:PHE:HE1	22	0.3
(1,1199)	1:89:A:TYR:HE1	1:71:A:LEU:HD13	21	0.3
(1,1168)	1:100:A:LEU:HD21	1:92:A:GLN:HG2	4	0.3
(1,1139)	1:134:A:LEU:HD22	1:95:A:ALA:HB1	3	0.3
(1,1115)	1:98:A:LEU:HD23	1:96:A:HIS:HE1	10	0.3
(1,1098)	1:100:A:LEU:HD23	1:92:A:GLN:HA	10	0.3
(1,1089)	1:105:A:PHE:HZ	1:100:A:LEU:HD22	21	0.3
(1,1088)	1:100:A:LEU:HD21	1:105:A:PHE:HD2	4	0.3
(1,1047)	1:104:A:GLU:HG2	1:105:A:PHE:H	22	0.3
(1,1042)	1:62:A:GLU:HB2	1:62:A:GLU:HA	4	0.3
(1,1042)	1:62:A:GLU:HB2	1:62:A:GLU:HA	16	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1042)	1:62:A:GLU:HB2	1:62:A:GLU:HA	23	0.3
(1,1000)	1:108:A:ILE:HD13	1:99:A:PHE:HE1	12	0.3
(1,915)	1:113:A:LEU:HD23	1:69:A:GLU:HB3	24	0.3
(1,900)	1:115:A:ARG:HB3	1:115:A:ARG:HG2	1	0.3
(1,900)	1:115:A:ARG:HB3	1:115:A:ARG:HG2	3	0.3
(1,900)	1:115:A:ARG:HB3	1:115:A:ARG:HG2	5	0.3
(1,900)	1:115:A:ARG:HB3	1:115:A:ARG:HG2	6	0.3
(1,900)	1:115:A:ARG:HB3	1:115:A:ARG:HG2	8	0.3
(1,900)	1:115:A:ARG:HB3	1:115:A:ARG:HG2	10	0.3
(1,900)	1:115:A:ARG:HB3	1:115:A:ARG:HG2	11	0.3
(1,900)	1:115:A:ARG:HB3	1:115:A:ARG:HG2	12	0.3
(1,900)	1:115:A:ARG:HB3	1:115:A:ARG:HG2	16	0.3
(1,900)	1:115:A:ARG:HB3	1:115:A:ARG:HG2	17	0.3
(1,900)	1:115:A:ARG:HB3	1:115:A:ARG:HG2	19	0.3
(1,900)	1:115:A:ARG:HB3	1:115:A:ARG:HG2	20	0.3
(1,900)	1:115:A:ARG:HB3	1:115:A:ARG:HG2	22	0.3
(1,886)	1:116:A:ALA:HA	1:123:A:LEU:HD12	4	0.3
(1,886)	1:116:A:ALA:HA	1:123:A:LEU:HD11	5	0.3
(1,886)	1:116:A:ALA:HA	1:123:A:LEU:HD11	12	0.3
(1,858)	1:119:A:ARG:HG3	1:119:A:ARG:HA	8	0.3
(1,858)	1:119:A:ARG:HG3	1:119:A:ARG:HA	22	0.3
(1,794)	1:124:A:TYR:HE2	1:124:A:TYR:HD2	1	0.3
(1,794)	1:124:A:TYR:HE2	1:124:A:TYR:HD2	2	0.3
(1,794)	1:124:A:TYR:HE2	1:124:A:TYR:HD2	3	0.3
(1,794)	1:124:A:TYR:HD1	1:124:A:TYR:HE1	4	0.3
(1,794)	1:124:A:TYR:HD1	1:124:A:TYR:HE1	5	0.3
(1,794)	1:124:A:TYR:HE2	1:124:A:TYR:HD2	7	0.3
(1,794)	1:124:A:TYR:HE2	1:124:A:TYR:HD2	8	0.3
(1,794)	1:124:A:TYR:HE2	1:124:A:TYR:HD2	9	0.3
(1,794)	1:124:A:TYR:HD1	1:124:A:TYR:HE1	10	0.3
(1,794)	1:124:A:TYR:HE2	1:124:A:TYR:HD2	11	0.3
(1,794)	1:124:A:TYR:HE2	1:124:A:TYR:HD2	12	0.3
(1,794)	1:124:A:TYR:HE2	1:124:A:TYR:HD2	15	0.3
(1,794)	1:124:A:TYR:HD1	1:124:A:TYR:HE1	16	0.3
(1,794)	1:124:A:TYR:HE2	1:124:A:TYR:HD2	17	0.3
(1,794)	1:124:A:TYR:HE2	1:124:A:TYR:HD2	20	0.3
(1,794)	1:124:A:TYR:HE2	1:124:A:TYR:HD2	21	0.3
(1,794)	1:124:A:TYR:HD1	1:124:A:TYR:HE1	24	0.3
(1,794)	1:124:A:TYR:HE2	1:124:A:TYR:HD2	25	0.3
(1,775)	1:126:A:TYR:HE1	1:125:A:VAL:HG13	13	0.3
(1,705)	1:130:A:LEU:HD11	1:109:A:LEU:HD11	5	0.3
(1,668)	1:133:A:VAL:HG12	1:130:A:LEU:HD13	23	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,666)	1:134:A:LEU:HD22	1:133:A:VAL:HG11	1	0.3
(1,666)	1:134:A:LEU:HD23	1:133:A:VAL:HG12	19	0.3
(1,664)	1:133:A:VAL:HG11	1:130:A:LEU:HA	13	0.3
(1,662)	1:133:A:VAL:HA	1:133:A:VAL:HG13	3	0.3
(1,662)	1:133:A:VAL:HA	1:133:A:VAL:HG12	4	0.3
(1,662)	1:133:A:VAL:HA	1:133:A:VAL:HG13	17	0.3
(1,643)	1:134:A:LEU:HD23	1:134:A:LEU:HD13	3	0.3
(1,643)	1:134:A:LEU:HD21	1:134:A:LEU:HD12	14	0.3
(1,643)	1:134:A:LEU:HD21	1:134:A:LEU:HD12	17	0.3
(1,643)	1:134:A:LEU:HD22	1:134:A:LEU:HD12	19	0.3
(1,634)	1:134:A:LEU:HD13	1:134:A:LEU:H	23	0.3
(1,608)	1:136:A:ALA:HA	1:136:A:ALA:HB3	4	0.3
(1,608)	1:136:A:ALA:HA	1:136:A:ALA:HB3	6	0.3
(1,608)	1:136:A:ALA:HA	1:136:A:ALA:HB3	9	0.3
(1,608)	1:136:A:ALA:HA	1:136:A:ALA:HB2	11	0.3
(1,608)	1:136:A:ALA:HA	1:136:A:ALA:HB2	14	0.3
(1,608)	1:136:A:ALA:HA	1:136:A:ALA:HB2	15	0.3
(1,608)	1:136:A:ALA:HA	1:136:A:ALA:HB3	16	0.3
(1,608)	1:136:A:ALA:HA	1:136:A:ALA:HB3	20	0.3
(1,608)	1:136:A:ALA:HA	1:136:A:ALA:HB1	23	0.3
(1,596)	1:137:A:HIS:HA	1:138:A:SER:H	24	0.3
(1,574)	1:143:A:LEU:HG	1:143:A:LEU:H	14	0.3
(1,561)	2:27:B:SER:H	2:30:B:GLU:HB3	18	0.3
(1,558)	2:32:B:GLU:HA	2:31:B:LEU:H	3	0.3
(1,558)	2:32:B:GLU:HA	2:31:B:LEU:H	15	0.3
(1,558)	2:32:B:GLU:HA	2:31:B:LEU:H	21	0.3
(1,551)	2:34:B:TYR:H	2:35:B:PHE:HA	12	0.3
(1,538)	1:63:A:ASN:H	1:61:A:LEU:HA	24	0.3
(1,526)	1:69:A:GLU:H	1:113:A:LEU:HD22	4	0.3
(1,520)	1:130:A:LEU:H	1:112:A:VAL:HG23	12	0.3
(1,515)	1:73:A:LEU:HG	1:76:A:MET:H	11	0.3
(1,512)	1:77:A:GLN:H	1:123:A:LEU:HD22	5	0.3
(1,505)	1:79:A:ALA:H	1:76:A:MET:HA	11	0.3
(1,505)	1:79:A:ALA:H	1:76:A:MET:HA	23	0.3
(1,502)	1:81:A:HIS:H	1:82:A:PRO:HB3	3	0.3
(1,500)	1:85:A:VAL:H	1:83:A:GLU:H	5	0.3
(1,492)	1:91:A:ARG:H	1:88:A:LEU:HD23	5	0.3
(1,488)	1:92:A:GLN:HE22	1:64:A:GLU:HG3	20	0.3
(1,473)	1:101:A:ALA:H	1:100:A:LEU:HG	9	0.3
(1,469)	1:102:A:SER:H	1:100:A:LEU:HB2	2	0.3
(1,453)	1:114:A:SER:H	1:113:A:LEU:HD23	16	0.3
(1,426)	1:125:A:VAL:HG13	1:126:A:TYR:H	4	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,426)	1:125:A:VAL:HG11	1:126:A:TYR:H	11	0.3
(1,421)	1:128:A:ASN:H	1:70:A:PHE:HZ	3	0.3
(1,359)	2:29:B:SER:HB2	2:26:B:ASP:HB3	5	0.3
(1,343)	2:31:B:LEU:HB2	1:87:A:PHE:HE2	5	0.3
(1,342)	2:31:B:LEU:HD12	1:124:A:TYR:HB3	12	0.3
(1,337)	2:31:B:LEU:HD23	2:28:B:ASP:HB2	21	0.3
(1,321)	2:34:B:TYR:HD1	1:83:A:GLU:HB3	6	0.3
(1,321)	2:34:B:TYR:HD1	1:83:A:GLU:HB3	8	0.3
(1,312)	2:35:B:PHE:HE1	1:124:A:TYR:HA	5	0.3
(1,275)	1:84:A:VAL:HG12	2:35:B:PHE:HE1	5	0.3
(1,246)	1:61:A:LEU:HG	1:61:A:LEU:HD21	10	0.3
(1,246)	1:61:A:LEU:HG	1:61:A:LEU:HD21	25	0.3
(1,236)	1:64:A:GLU:HA	1:67:A:PHE:H	15	0.3
(1,236)	1:64:A:GLU:HA	1:67:A:PHE:H	23	0.3
(1,229)	1:105:A:PHE:HE2	1:67:A:PHE:HB2	1	0.3
(1,229)	1:105:A:PHE:HE2	1:67:A:PHE:HB2	9	0.3
(1,229)	1:105:A:PHE:HE2	1:67:A:PHE:HB2	13	0.3
(1,229)	1:105:A:PHE:HE2	1:67:A:PHE:HB2	25	0.3
(1,227)	1:62:A:GLU:HG2	1:61:A:LEU:HG	3	0.3
(1,227)	1:62:A:GLU:HG2	1:61:A:LEU:HG	6	0.3
(1,220)	1:70:A:PHE:HE2	1:113:A:LEU:HB2	3	0.3
(1,220)	1:70:A:PHE:HE2	1:113:A:LEU:HB2	17	0.3
(1,220)	1:70:A:PHE:HE2	1:113:A:LEU:HB2	25	0.3
(1,210)	1:105:A:PHE:HZ	1:109:A:LEU:HD22	1	0.3
(1,209)	1:71:A:LEU:HD22	1:67:A:PHE:HE2	13	0.3
(1,209)	1:71:A:LEU:HD23	1:67:A:PHE:HE2	19	0.3
(1,172)	1:85:A:VAL:HG11	1:74:A:CYS:HB3	8	0.3
(1,163)	1:67:A:PHE:HD1	1:92:A:GLN:HG3	19	0.3
(1,163)	1:67:A:PHE:HD2	1:92:A:GLN:HG3	23	0.3
(1,155)	1:88:A:LEU:HD12	1:74:A:CYS:HB2	3	0.3
(1,145)	1:88:A:LEU:HB3	1:85:A:VAL:HA	25	0.3
(1,132)	1:67:A:PHE:HE1	1:92:A:GLN:HB3	24	0.3
(1,122)	1:95:A:ALA:HB2	1:91:A:ARG:HD3	19	0.3
(1,121)	1:95:A:ALA:HB3	1:134:A:LEU:HA	4	0.3
(1,95)	1:107:A:ASN:HB2	1:108:A:ILE:HB	14	0.3
(1,92)	1:109:A:LEU:HD21	1:67:A:PHE:H	24	0.3
(1,87)	1:112:A:VAL:HG13	1:130:A:LEU:H	6	0.3
(1,87)	1:112:A:VAL:HG11	1:130:A:LEU:H	15	0.3
(1,67)	1:116:A:ALA:HB1	1:120:A:PRO:HA	2	0.3
(1,51)	1:126:A:TYR:HD1	1:125:A:VAL:HG12	6	0.3
(1,51)	1:126:A:TYR:HD1	1:125:A:VAL:HG11	8	0.3
(1,51)	1:126:A:TYR:HD1	1:125:A:VAL:HG13	19	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,36)	1:127:A:ILE:HG23	1:124:A:TYR:HD1	4	0.3
(1,36)	1:127:A:ILE:HG23	1:124:A:TYR:HD2	7	0.3
(1,27)	1:130:A:LEU:HD21	1:67:A:PHE:HA	14	0.3
(1,24)	1:85:A:VAL:HG23	1:71:A:LEU:HA	14	0.3
(1,24)	1:85:A:VAL:HG22	1:71:A:LEU:HA	23	0.3
(1,17)	1:133:A:VAL:HG13	1:137:A:HIS:HB2	16	0.3
(1,14)	1:133:A:VAL:HG22	1:132:A:THR:H	2	0.3
(1,14)	1:133:A:VAL:HG21	1:132:A:THR:H	12	0.3
(1,8)	1:134:A:LEU:HD21	1:67:A:PHE:HZ	8	0.3
(1,1)	1:141:A:LYS:HG3	1:141:A:LYS:HA	21	0.3
(1,2273)	2:25:B:GLU:HB3	2:25:B:GLU:H	6	0.29
(1,2273)	2:25:B:GLU:HB3	2:25:B:GLU:H	18	0.29
(1,2260)	2:27:B:SER:HB2	2:27:B:SER:H	16	0.29
(1,2244)	2:36:B:THR:HG21	2:36:B:THR:H	2	0.29
(1,2244)	2:36:B:THR:HG23	2:36:B:THR:H	3	0.29
(1,2228)	2:35:B:PHE:H	2:34:B:TYR:HB3	21	0.29
(1,2228)	2:35:B:PHE:H	2:34:B:TYR:HB3	22	0.29
(1,2179)	1:60:A:LYS:HB3	1:61:A:LEU:H	25	0.29
(1,2138)	1:69:A:GLU:HG3	1:69:A:GLU:H	17	0.29
(1,2097)	1:77:A:GLN:HE21	1:77:A:GLN:HA	2	0.29
(1,2026)	1:67:A:PHE:HD2	1:92:A:GLN:HE21	8	0.29
(1,2026)	1:67:A:PHE:HD2	1:92:A:GLN:HE21	11	0.29
(1,2006)	1:134:A:LEU:HD21	1:95:A:ALA:H	12	0.29
(1,2006)	1:134:A:LEU:HD23	1:95:A:ALA:H	14	0.29
(1,2006)	1:134:A:LEU:HD23	1:95:A:ALA:H	17	0.29
(1,2004)	1:95:A:ALA:H	1:94:A:ARG:HB3	10	0.29
(1,1987)	1:99:A:PHE:H	1:99:A:PHE:HD2	1	0.29
(1,1975)	1:100:A:LEU:HD11	1:100:A:LEU:H	10	0.29
(1,1975)	1:100:A:LEU:HD13	1:100:A:LEU:H	23	0.29
(1,1971)	1:100:A:LEU:HD22	1:101:A:ALA:H	14	0.29
(1,1968)	1:101:A:ALA:H	1:63:A:ASN:HD22	18	0.29
(1,1874)	1:118:A:SER:H	1:117:A:ARG:HG2	3	0.29
(1,1837)	1:127:A:ILE:H	1:123:A:LEU:HD11	12	0.29
(1,1788)	1:139:A:ALA:H	1:135:A:LYS:HD3	3	0.29
(1,1775)	1:143:A:LEU:H	1:141:A:LYS:HG2	13	0.29
(1,1775)	1:143:A:LEU:H	1:141:A:LYS:HG3	16	0.29
(1,1774)	1:143:A:LEU:HB2	1:143:A:LEU:H	12	0.29
(1,1771)	1:142:A:LYS:H	1:142:A:LYS:HD2	25	0.29
(1,1754)	2:30:B:GLU:HG2	2:31:B:LEU:H	2	0.29
(1,1727)	2:31:B:LEU:HD12	2:31:B:LEU:H	6	0.29
(1,1727)	2:31:B:LEU:HD12	2:31:B:LEU:H	18	0.29
(1,1727)	2:31:B:LEU:HD11	2:31:B:LEU:H	25	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1723)	2:31:B:LEU:HD21	2:30:B:GLU:HB2	15	0.29
(1,1720)	2:34:B:TYR:HE1	2:31:B:LEU:HD22	13	0.29
(1,1720)	2:34:B:TYR:HE1	2:31:B:LEU:HD21	16	0.29
(1,1720)	2:34:B:TYR:HE1	2:31:B:LEU:HD23	20	0.29
(1,1716)	2:31:B:LEU:HG	2:32:B:GLU:HG3	18	0.29
(1,1713)	2:31:B:LEU:HG	2:31:B:LEU:H	12	0.29
(1,1713)	2:31:B:LEU:HG	2:31:B:LEU:H	24	0.29
(1,1670)	2:37:B:ALA:HB3	2:36:B:THR:HA	2	0.29
(1,1666)	2:36:B:THR:HG22	1:124:A:TYR:H	6	0.29
(1,1666)	2:36:B:THR:HG22	1:124:A:TYR:H	14	0.29
(1,1666)	2:36:B:THR:HG21	1:124:A:TYR:H	19	0.29
(1,1648)	2:38:B:ARG:HA	2:37:B:ALA:HB1	9	0.29
(1,1637)	2:38:B:ARG:HD2	2:39:B:TRP:HD1	19	0.29
(1,1636)	2:35:B:PHE:HB3	2:34:B:TYR:HE1	13	0.29
(1,1622)	2:39:B:TRP:HE3	2:39:B:TRP:HB2	3	0.29
(1,1622)	2:39:B:TRP:HE3	2:39:B:TRP:HB2	12	0.29
(1,1622)	2:39:B:TRP:HE3	2:39:B:TRP:HB2	23	0.29
(1,1622)	2:39:B:TRP:HE3	2:39:B:TRP:HB2	24	0.29
(1,1615)	2:39:B:TRP:HE3	2:36:B:THR:HG23	8	0.29
(1,1592)	1:84:A:VAL:HG22	2:35:B:PHE:HB2	5	0.29
(1,1592)	1:84:A:VAL:HG23	2:35:B:PHE:HB2	6	0.29
(1,1592)	1:84:A:VAL:HG22	2:35:B:PHE:HB2	19	0.29
(1,1591)	1:84:A:VAL:HA	2:31:B:LEU:HD11	3	0.29
(1,1591)	1:84:A:VAL:HA	2:31:B:LEU:HD11	15	0.29
(1,1591)	1:84:A:VAL:HA	2:31:B:LEU:HD12	16	0.29
(1,1588)	1:87:A:PHE:HB2	2:31:B:LEU:HD11	7	0.29
(1,1577)	1:77:A:GLN:HG3	1:73:A:LEU:HD13	15	0.29
(1,1570)	1:57:A:LYS:HE2	1:59:A:TYR:HE1	14	0.29
(1,1550)	1:141:A:LYS:HG3	1:141:A:LYS:HA	14	0.29
(1,1549)	1:58:A:CYS:HB2	1:57:A:LYS:HA	15	0.29
(1,1456)	1:69:A:GLU:HG2	1:66:A:LEU:HA	8	0.29
(1,1450)	1:85:A:VAL:HB	1:86:A:PRO:HD3	7	0.29
(1,1450)	1:85:A:VAL:HB	1:86:A:PRO:HD3	10	0.29
(1,1450)	1:85:A:VAL:HB	1:86:A:PRO:HD3	13	0.29
(1,1440)	1:127:A:ILE:HD11	1:70:A:PHE:HZ	8	0.29
(1,1419)	1:71:A:LEU:HD13	1:89:A:TYR:H	4	0.29
(1,1419)	1:71:A:LEU:HD13	1:89:A:TYR:H	18	0.29
(1,1391)	1:74:A:CYS:HA	1:73:A:LEU:HD21	4	0.29
(1,1391)	1:74:A:CYS:HA	1:73:A:LEU:HD22	16	0.29
(1,1361)	1:75:A:LYS:HE2	1:75:A:LYS:HG3	4	0.29
(1,1269)	1:84:A:VAL:HG12	1:85:A:VAL:H	2	0.29
(1,1269)	1:84:A:VAL:HG11	1:85:A:VAL:H	3	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1269)	1:84:A:VAL:HG12	1:85:A:VAL:H	9	0.29
(1,1269)	1:84:A:VAL:HG12	1:85:A:VAL:H	11	0.29
(1,1269)	1:84:A:VAL:HG12	1:85:A:VAL:H	13	0.29
(1,1269)	1:84:A:VAL:HG13	1:85:A:VAL:H	14	0.29
(1,1269)	1:84:A:VAL:HG11	1:85:A:VAL:H	22	0.29
(1,1269)	1:84:A:VAL:HG12	1:85:A:VAL:H	23	0.29
(1,1209)	1:88:A:LEU:HD11	1:70:A:PHE:HE1	7	0.29
(1,1209)	1:88:A:LEU:HD12	1:70:A:PHE:HE1	24	0.29
(1,1183)	1:90:A:ASN:HB2	1:87:A:PHE:HD1	23	0.29
(1,1168)	1:100:A:LEU:HD21	1:92:A:GLN:HG2	17	0.29
(1,1142)	1:94:A:ARG:HD2	1:94:A:ARG:HB2	9	0.29
(1,1137)	1:95:A:ALA:HB2	1:91:A:ARG:HD3	11	0.29
(1,1094)	1:100:A:LEU:HD23	1:138:A:SER:HB2	8	0.29
(1,1074)	1:101:A:ALA:HB1	1:60:A:LYS:HA	4	0.29
(1,1074)	1:101:A:ALA:HB1	1:60:A:LYS:HA	24	0.29
(1,1042)	1:62:A:GLU:HB2	1:62:A:GLU:HA	5	0.29
(1,1042)	1:62:A:GLU:HB2	1:62:A:GLU:HA	6	0.29
(1,1042)	1:62:A:GLU:HB2	1:62:A:GLU:HA	10	0.29
(1,1042)	1:62:A:GLU:HB2	1:62:A:GLU:HA	11	0.29
(1,1042)	1:62:A:GLU:HB2	1:62:A:GLU:HA	12	0.29
(1,1042)	1:62:A:GLU:HB2	1:62:A:GLU:HA	14	0.29
(1,1042)	1:62:A:GLU:HB2	1:62:A:GLU:HA	24	0.29
(1,1040)	1:62:A:GLU:HB3	1:59:A:TYR:HA	3	0.29
(1,1000)	1:108:A:ILE:HD11	1:99:A:PHE:HE1	16	0.29
(1,1000)	1:108:A:ILE:HD12	1:99:A:PHE:HE1	22	0.29
(1,996)	1:108:A:ILE:HG23	1:112:A:VAL:HG12	13	0.29
(1,996)	1:108:A:ILE:HG23	1:112:A:VAL:HG12	15	0.29
(1,942)	1:111:A:ARG:HB2	1:111:A:ARG:HD2	13	0.29
(1,942)	1:111:A:ARG:HB2	1:111:A:ARG:HD2	15	0.29
(1,900)	1:115:A:ARG:HB3	1:115:A:ARG:HG2	21	0.29
(1,886)	1:116:A:ALA:HA	1:123:A:LEU:HD13	25	0.29
(1,867)	1:119:A:ARG:HD3	1:119:A:ARG:HA	2	0.29
(1,858)	1:119:A:ARG:HG3	1:119:A:ARG:HA	10	0.29
(1,811)	1:123:A:LEU:HD23	1:70:A:PHE:HE1	5	0.29
(1,794)	1:124:A:TYR:HE2	1:124:A:TYR:HD2	6	0.29
(1,794)	1:124:A:TYR:HD1	1:124:A:TYR:HE1	13	0.29
(1,794)	1:124:A:TYR:HE2	1:124:A:TYR:HD2	14	0.29
(1,794)	1:124:A:TYR:HE2	1:124:A:TYR:HD2	18	0.29
(1,794)	1:124:A:TYR:HE2	1:124:A:TYR:HD2	19	0.29
(1,794)	1:124:A:TYR:HE2	1:124:A:TYR:HD2	22	0.29
(1,794)	1:124:A:TYR:HE2	1:124:A:TYR:HD2	23	0.29
(1,775)	1:126:A:TYR:HE1	1:125:A:VAL:HG11	7	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,775)	1:126:A:TYR:HE1	1:125:A:VAL:HG12	20	0.29
(1,666)	1:134:A:LEU:HD23	1:133:A:VAL:HG12	5	0.29
(1,666)	1:134:A:LEU:HD23	1:133:A:VAL:HG11	11	0.29
(1,664)	1:133:A:VAL:HG11	1:130:A:LEU:HA	6	0.29
(1,662)	1:133:A:VAL:HA	1:133:A:VAL:HG11	25	0.29
(1,642)	1:134:A:LEU:HD22	1:92:A:GLN:HG3	12	0.29
(1,634)	1:134:A:LEU:HD11	1:134:A:LEU:H	12	0.29
(1,631)	1:73:A:LEU:HD11	1:117:A:ARG:HA	3	0.29
(1,608)	1:136:A:ALA:HA	1:136:A:ALA:HB2	1	0.29
(1,608)	1:136:A:ALA:HA	1:136:A:ALA:HB2	2	0.29
(1,608)	1:136:A:ALA:HA	1:136:A:ALA:HB2	5	0.29
(1,608)	1:136:A:ALA:HA	1:136:A:ALA:HB2	12	0.29
(1,608)	1:136:A:ALA:HA	1:136:A:ALA:HB2	13	0.29
(1,608)	1:136:A:ALA:HA	1:136:A:ALA:HB1	18	0.29
(1,608)	1:136:A:ALA:HA	1:136:A:ALA:HB1	21	0.29
(1,608)	1:136:A:ALA:HA	1:136:A:ALA:HB1	25	0.29
(1,593)	1:138:A:SER:HA	1:138:A:SER:HB2	9	0.29
(1,586)	1:139:A:ALA:HA	1:139:A:ALA:HB1	8	0.29
(1,576)	1:142:A:LYS:HB2	1:142:A:LYS:H	6	0.29
(1,574)	1:143:A:LEU:HG	1:143:A:LEU:H	11	0.29
(1,569)	1:143:A:LEU:HB2	1:144:A:ASN:H	11	0.29
(1,569)	1:143:A:LEU:HB2	1:144:A:ASN:H	14	0.29
(1,561)	2:27:B:SER:H	2:30:B:GLU:HB3	21	0.29
(1,558)	2:32:B:GLU:HA	2:31:B:LEU:H	13	0.29
(1,558)	2:32:B:GLU:HA	2:31:B:LEU:H	24	0.29
(1,551)	2:34:B:TYR:H	2:35:B:PHE:HA	18	0.29
(1,541)	1:61:A:LEU:HB3	1:62:A:GLU:H	12	0.29
(1,540)	1:63:A:ASN:H	1:61:A:LEU:HG	13	0.29
(1,538)	1:63:A:ASN:H	1:61:A:LEU:HA	4	0.29
(1,522)	1:70:A:PHE:H	1:73:A:LEU:H	24	0.29
(1,521)	1:71:A:LEU:H	1:113:A:LEU:HD12	15	0.29
(1,520)	1:130:A:LEU:H	1:112:A:VAL:HG23	9	0.29
(1,515)	1:73:A:LEU:HG	1:76:A:MET:H	6	0.29
(1,515)	1:73:A:LEU:HG	1:76:A:MET:H	14	0.29
(1,515)	1:73:A:LEU:HG	1:76:A:MET:H	15	0.29
(1,515)	1:73:A:LEU:HG	1:76:A:MET:H	25	0.29
(1,505)	1:79:A:ALA:H	1:76:A:MET:HA	13	0.29
(1,492)	1:91:A:ARG:H	1:88:A:LEU:HD23	1	0.29
(1,478)	1:95:A:ALA:H	1:91:A:ARG:HD2	4	0.29
(1,476)	1:96:A:HIS:H	1:95:A:ALA:H	21	0.29
(1,453)	1:114:A:SER:H	1:113:A:LEU:HD22	25	0.29
(1,445)	1:116:A:ALA:H	1:112:A:VAL:HA	14	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,426)	1:125:A:VAL:HG11	1:126:A:TYR:H	5	0.29
(1,426)	1:125:A:VAL:HG12	1:126:A:TYR:H	14	0.29
(1,426)	1:125:A:VAL:HG12	1:126:A:TYR:H	23	0.29
(1,421)	1:128:A:ASN:H	1:70:A:PHE:HZ	20	0.29
(1,392)	1:139:A:ALA:H	1:138:A:SER:H	12	0.29
(1,391)	1:144:A:ASN:H	1:142:A:LYS:HB2	9	0.29
(1,369)	2:26:B:ASP:HB2	1:87:A:PHE:HZ	25	0.29
(1,363)	1:118:A:SER:HB3	1:119:A:ARG:HB2	19	0.29
(1,360)	2:29:B:SER:HB3	2:26:B:ASP:HB3	12	0.29
(1,342)	2:31:B:LEU:HD12	1:124:A:TYR:HB3	25	0.29
(1,340)	2:31:B:LEU:HD11	1:88:A:LEU:H	19	0.29
(1,318)	2:34:B:TYR:HE1	1:83:A:GLU:HB3	8	0.29
(1,312)	2:35:B:PHE:HE1	2:36:B:THR:HA	21	0.29
(1,312)	2:35:B:PHE:HE1	1:124:A:TYR:HA	24	0.29
(1,257)	1:113:A:LEU:HD13	1:117:A:ARG:HG3	21	0.29
(1,246)	1:61:A:LEU:HG	1:61:A:LEU:HD23	5	0.29
(1,246)	1:61:A:LEU:HG	1:61:A:LEU:HD21	13	0.29
(1,246)	1:61:A:LEU:HG	1:61:A:LEU:HD21	20	0.29
(1,243)	1:62:A:GLU:HG3	1:61:A:LEU:HD21	17	0.29
(1,233)	1:62:A:GLU:HG2	1:66:A:LEU:HD11	20	0.29
(1,229)	1:105:A:PHE:HE2	1:67:A:PHE:HB2	16	0.29
(1,227)	1:62:A:GLU:HG2	1:61:A:LEU:HG	15	0.29
(1,225)	1:129:A:GLU:HG2	1:125:A:VAL:HG11	3	0.29
(1,225)	1:129:A:GLU:HG2	1:125:A:VAL:HG13	10	0.29
(1,222)	1:68:A:GLU:HA	1:71:A:LEU:HG	23	0.29
(1,210)	1:105:A:PHE:HZ	1:109:A:LEU:HD21	2	0.29
(1,210)	1:105:A:PHE:HZ	1:109:A:LEU:HD21	7	0.29
(1,210)	1:105:A:PHE:HZ	1:109:A:LEU:HD22	12	0.29
(1,209)	1:67:A:PHE:HE1	1:71:A:LEU:HD21	17	0.29
(1,209)	1:67:A:PHE:HE1	1:71:A:LEU:HD21	20	0.29
(1,191)	1:78:A:THR:HG21	1:74:A:CYS:HB2	17	0.29
(1,191)	1:84:A:VAL:HG11	1:74:A:CYS:HB2	25	0.29
(1,172)	1:85:A:VAL:HG12	1:74:A:CYS:HB3	24	0.29
(1,145)	1:88:A:LEU:HB3	1:85:A:VAL:HA	6	0.29
(1,145)	1:88:A:LEU:HB3	1:85:A:VAL:HA	8	0.29
(1,121)	1:95:A:ALA:HB3	1:134:A:LEU:HA	24	0.29
(1,116)	1:100:A:LEU:HD23	1:105:A:PHE:HE2	14	0.29
(1,116)	1:100:A:LEU:HD23	1:105:A:PHE:HE2	19	0.29
(1,95)	1:107:A:ASN:HB2	1:108:A:ILE:HB	20	0.29
(1,92)	1:109:A:LEU:HD22	1:67:A:PHE:H	4	0.29
(1,92)	1:109:A:LEU:HD22	1:67:A:PHE:H	17	0.29
(1,62)	1:123:A:LEU:HD22	1:70:A:PHE:HE1	20	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,62)	1:123:A:LEU:HD23	1:70:A:PHE:HE1	24	0.29
(1,62)	1:123:A:LEU:HD23	1:70:A:PHE:HE1	25	0.29
(1,54)	1:127:A:ILE:HG22	1:124:A:TYR:HD1	5	0.29
(1,52)	1:125:A:VAL:HG13	1:128:A:ASN:HB2	5	0.29
(1,51)	1:126:A:TYR:HD1	1:125:A:VAL:HG11	3	0.29
(1,42)	1:126:A:TYR:HD1	1:125:A:VAL:HB	10	0.29
(1,42)	1:126:A:TYR:HD1	1:125:A:VAL:HB	13	0.29
(1,36)	1:127:A:ILE:HG21	1:124:A:TYR:HD1	16	0.29
(1,24)	1:85:A:VAL:HG23	1:71:A:LEU:HA	6	0.29
(1,24)	1:85:A:VAL:HG22	1:71:A:LEU:HA	13	0.29
(1,24)	1:85:A:VAL:HG23	1:71:A:LEU:HA	15	0.29
(1,24)	1:85:A:VAL:HG22	1:71:A:LEU:HA	19	0.29
(1,24)	1:85:A:VAL:HG22	1:71:A:LEU:HA	22	0.29
(1,17)	1:133:A:VAL:HG13	1:137:A:HIS:HB2	3	0.29
(1,14)	1:133:A:VAL:HG22	1:132:A:THR:H	14	0.29
(1,14)	1:133:A:VAL:HG22	1:132:A:THR:H	16	0.29
(1,14)	1:133:A:VAL:HG23	1:132:A:THR:H	19	0.29
(1,14)	1:133:A:VAL:HG21	1:132:A:THR:H	24	0.29
(1,13)	1:133:A:VAL:HG13	1:108:A:ILE:HB	9	0.29
(1,13)	1:133:A:VAL:HG11	1:108:A:ILE:HB	13	0.29
(1,2287)	2:33:B:GLN:HE22	2:33:B:GLN:HB3	5	0.28
(1,2274)	2:39:B:TRP:HE1	2:38:B:ARG:HD2	8	0.28
(1,2268)	2:26:B:ASP:H	2:25:B:GLU:HB3	16	0.28
(1,2260)	2:27:B:SER:HB2	2:27:B:SER:H	15	0.28
(1,2244)	2:36:B:THR:HG23	2:36:B:THR:H	7	0.28
(1,2228)	2:35:B:PHE:H	2:34:B:TYR:HB3	5	0.28
(1,2228)	2:35:B:PHE:H	2:34:B:TYR:HB3	7	0.28
(1,2202)	1:125:A:VAL:H	1:122:A:LYS:HD3	12	0.28
(1,2188)	1:59:A:TYR:H	1:58:A:CYS:HB3	10	0.28
(1,2188)	1:59:A:TYR:H	1:58:A:CYS:HB2	21	0.28
(1,2179)	1:60:A:LYS:HB3	1:61:A:LEU:H	22	0.28
(1,2179)	1:60:A:LYS:HB3	1:61:A:LEU:H	23	0.28
(1,2142)	1:109:A:LEU:HD23	1:68:A:GLU:H	19	0.28
(1,2138)	1:69:A:GLU:HG3	1:69:A:GLU:H	14	0.28
(1,2108)	1:77:A:GLN:H	1:78:A:THR:HG23	5	0.28
(1,2097)	1:77:A:GLN:HE21	1:77:A:GLN:HA	4	0.28
(1,2097)	1:77:A:GLN:HE21	1:77:A:GLN:HA	8	0.28
(1,2097)	1:77:A:GLN:HE21	1:77:A:GLN:HA	23	0.28
(1,2071)	1:83:A:GLU:HG3	1:83:A:GLU:H	24	0.28
(1,2006)	1:134:A:LEU:HD22	1:95:A:ALA:H	3	0.28
(1,2006)	1:134:A:LEU:HD23	1:95:A:ALA:H	16	0.28
(1,1968)	1:101:A:ALA:H	1:63:A:ASN:HD22	11	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1906)	1:111:A:ARG:H	1:111:A:ARG:HD2	5	0.28
(1,1886)	1:88:A:LEU:H	1:87:A:PHE:HD2	10	0.28
(1,1854)	1:124:A:TYR:H	1:125:A:VAL:HG21	12	0.28
(1,1798)	1:136:A:ALA:H	1:135:A:LYS:HD2	9	0.28
(1,1789)	1:139:A:ALA:H	1:139:A:ALA:HB3	1	0.28
(1,1772)	1:142:A:LYS:H	1:141:A:LYS:HG2	18	0.28
(1,1768)	2:24:B:GLN:HG3	2:24:B:GLN:HB2	4	0.28
(1,1768)	2:24:B:GLN:HG3	2:24:B:GLN:HB2	14	0.28
(1,1754)	2:30:B:GLU:HG2	2:31:B:LEU:H	12	0.28
(1,1741)	2:29:B:SER:HA	2:30:B:GLU:H	16	0.28
(1,1723)	2:31:B:LEU:HD21	2:30:B:GLU:HB2	9	0.28
(1,1720)	2:34:B:TYR:HE1	2:31:B:LEU:HD21	2	0.28
(1,1720)	2:34:B:TYR:HE1	2:31:B:LEU:HD21	7	0.28
(1,1713)	2:31:B:LEU:HG	2:31:B:LEU:H	10	0.28
(1,1713)	2:31:B:LEU:HG	2:31:B:LEU:H	11	0.28
(1,1713)	2:31:B:LEU:HG	2:31:B:LEU:H	15	0.28
(1,1713)	2:31:B:LEU:HG	2:31:B:LEU:H	16	0.28
(1,1713)	2:31:B:LEU:HG	2:31:B:LEU:H	19	0.28
(1,1708)	2:32:B:GLU:HG2	2:39:B:TRP:HZ2	19	0.28
(1,1703)	2:33:B:GLN:HG2	2:31:B:LEU:HD21	15	0.28
(1,1670)	2:37:B:ALA:HB2	2:36:B:THR:HA	3	0.28
(1,1670)	2:37:B:ALA:HB2	2:36:B:THR:HA	7	0.28
(1,1670)	2:37:B:ALA:HB3	2:36:B:THR:HA	19	0.28
(1,1670)	2:37:B:ALA:HB1	2:36:B:THR:HA	22	0.28
(1,1667)	2:36:B:THR:HB	2:36:B:THR:H	21	0.28
(1,1652)	2:37:B:ALA:HB2	2:38:B:ARG:HD3	11	0.28
(1,1636)	2:35:B:PHE:HB3	2:34:B:TYR:HE1	24	0.28
(1,1627)	2:39:B:TRP:HB2	2:39:B:TRP:HA	6	0.28
(1,1627)	2:39:B:TRP:HB2	2:39:B:TRP:HA	7	0.28
(1,1627)	2:39:B:TRP:HB2	2:39:B:TRP:HA	9	0.28
(1,1627)	2:39:B:TRP:HB2	2:39:B:TRP:HA	12	0.28
(1,1627)	2:39:B:TRP:HB2	2:39:B:TRP:HA	17	0.28
(1,1627)	2:39:B:TRP:HB2	2:39:B:TRP:HA	20	0.28
(1,1627)	2:39:B:TRP:HB2	2:39:B:TRP:HA	22	0.28
(1,1627)	2:39:B:TRP:HB2	2:39:B:TRP:HA	23	0.28
(1,1622)	2:39:B:TRP:HE3	2:39:B:TRP:HB2	9	0.28
(1,1619)	2:39:B:TRP:HD1	2:38:B:ARG:HB2	13	0.28
(1,1619)	2:39:B:TRP:HD1	2:38:B:ARG:HB2	20	0.28
(1,1595)	2:31:B:LEU:HD12	1:127:A:ILE:HB	2	0.28
(1,1592)	1:84:A:VAL:HG23	2:35:B:PHE:HB2	22	0.28
(1,1588)	1:87:A:PHE:HB2	2:31:B:LEU:HD13	8	0.28
(1,1577)	1:77:A:GLN:HG3	1:73:A:LEU:HD12	9	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1577)	1:77:A:GLN:HG3	1:73:A:LEU:HD12	10	0.28
(1,1577)	1:77:A:GLN:HG3	1:73:A:LEU:HD12	12	0.28
(1,1577)	1:77:A:GLN:HG3	1:73:A:LEU:HD11	21	0.28
(1,1570)	1:57:A:LYS:HE2	1:59:A:TYR:HE1	16	0.28
(1,1480)	1:66:A:LEU:HD23	1:63:A:ASN:HA	4	0.28
(1,1480)	1:66:A:LEU:HD23	1:63:A:ASN:HA	8	0.28
(1,1450)	1:85:A:VAL:HB	1:86:A:PRO:HD3	1	0.28
(1,1450)	1:85:A:VAL:HB	1:86:A:PRO:HD3	3	0.28
(1,1450)	1:85:A:VAL:HB	1:86:A:PRO:HD3	14	0.28
(1,1447)	1:69:A:GLU:HA	1:69:A:GLU:HG3	5	0.28
(1,1419)	1:71:A:LEU:HD11	1:89:A:TYR:H	13	0.28
(1,1370)	1:75:A:LYS:HE3	1:72:A:GLU:HB3	14	0.28
(1,1361)	1:75:A:LYS:HE2	1:75:A:LYS:HG3	2	0.28
(1,1280)	1:84:A:VAL:HG21	1:81:A:HIS:HB2	20	0.28
(1,1280)	1:84:A:VAL:HG21	1:81:A:HIS:HB2	24	0.28
(1,1269)	1:84:A:VAL:HG12	1:85:A:VAL:H	6	0.28
(1,1209)	1:88:A:LEU:HD11	1:70:A:PHE:HE1	1	0.28
(1,1209)	1:88:A:LEU:HD13	1:70:A:PHE:HE1	2	0.28
(1,1209)	1:88:A:LEU:HD11	1:70:A:PHE:HE1	23	0.28
(1,1197)	1:89:A:TYR:HD2	1:71:A:LEU:HD23	3	0.28
(1,1183)	1:90:A:ASN:HB2	1:87:A:PHE:HD1	25	0.28
(1,1175)	1:91:A:ARG:HG2	1:134:A:LEU:HB2	25	0.28
(1,1142)	1:94:A:ARG:HD2	1:94:A:ARG:HB2	5	0.28
(1,1142)	1:94:A:ARG:HD2	1:94:A:ARG:HB2	14	0.28
(1,1142)	1:94:A:ARG:HD2	1:94:A:ARG:HB2	16	0.28
(1,1139)	1:134:A:LEU:HD21	1:95:A:ALA:HB1	5	0.28
(1,1137)	1:95:A:ALA:HB1	1:91:A:ARG:HD3	8	0.28
(1,1115)	1:98:A:LEU:HD23	1:96:A:HIS:HE1	13	0.28
(1,1094)	1:100:A:LEU:HD21	1:138:A:SER:HB2	9	0.28
(1,1088)	1:100:A:LEU:HD21	1:105:A:PHE:HD2	21	0.28
(1,1074)	1:101:A:ALA:HB2	1:60:A:LYS:HA	2	0.28
(1,1074)	1:101:A:ALA:HB2	1:60:A:LYS:HA	12	0.28
(1,1074)	1:101:A:ALA:HB3	1:60:A:LYS:HA	13	0.28
(1,1074)	1:101:A:ALA:HB2	1:60:A:LYS:HA	14	0.28
(1,1074)	1:101:A:ALA:HB1	1:60:A:LYS:HA	21	0.28
(1,1072)	1:101:A:ALA:HB1	1:58:A:CYS:HA	10	0.28
(1,1042)	1:62:A:GLU:HB2	1:62:A:GLU:HA	1	0.28
(1,1042)	1:62:A:GLU:HB2	1:62:A:GLU:HA	2	0.28
(1,1042)	1:62:A:GLU:HB2	1:62:A:GLU:HA	7	0.28
(1,1042)	1:62:A:GLU:HB2	1:62:A:GLU:HA	15	0.28
(1,1042)	1:62:A:GLU:HB2	1:62:A:GLU:HA	17	0.28
(1,1042)	1:62:A:GLU:HB2	1:62:A:GLU:HA	18	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1042)	1:62:A:GLU:HB2	1:62:A:GLU:HA	19	0.28
(1,1036)	1:62:A:GLU:HB3	1:62:A:GLU:H	13	0.28
(1,1000)	1:108:A:ILE:HD11	1:99:A:PHE:HE1	25	0.28
(1,996)	1:108:A:ILE:HG23	1:112:A:VAL:HG13	3	0.28
(1,960)	1:67:A:PHE:HA	1:109:A:LEU:HD13	11	0.28
(1,960)	1:67:A:PHE:HA	1:109:A:LEU:HD12	18	0.28
(1,960)	1:67:A:PHE:HA	1:109:A:LEU:HD11	20	0.28
(1,945)	1:110:A:SER:HB2	1:111:A:ARG:H	21	0.28
(1,942)	1:111:A:ARG:HB2	1:111:A:ARG:HD2	19	0.28
(1,886)	1:116:A:ALA:HA	1:123:A:LEU:HD12	9	0.28
(1,886)	1:116:A:ALA:HA	1:123:A:LEU:HD12	23	0.28
(1,878)	1:117:A:ARG:HG2	1:114:A:SER:HA	4	0.28
(1,831)	1:121:A:ALA:HA	1:121:A:ALA:HB2	3	0.28
(1,831)	1:121:A:ALA:HA	1:121:A:ALA:HB3	4	0.28
(1,831)	1:121:A:ALA:HA	1:121:A:ALA:HB2	5	0.28
(1,831)	1:121:A:ALA:HA	1:121:A:ALA:HB1	7	0.28
(1,831)	1:121:A:ALA:HA	1:121:A:ALA:HB2	9	0.28
(1,831)	1:121:A:ALA:HA	1:121:A:ALA:HB1	12	0.28
(1,831)	1:121:A:ALA:HA	1:121:A:ALA:HB1	14	0.28
(1,831)	1:121:A:ALA:HA	1:121:A:ALA:HB3	15	0.28
(1,813)	1:123:A:LEU:HD23	1:124:A:TYR:HE2	10	0.28
(1,811)	1:123:A:LEU:HD23	1:70:A:PHE:HE1	15	0.28
(1,811)	1:123:A:LEU:HD22	1:70:A:PHE:HE1	19	0.28
(1,799)	1:111:A:ARG:HA	1:111:A:ARG:HG3	23	0.28
(1,666)	1:134:A:LEU:HD21	1:133:A:VAL:HG13	2	0.28
(1,666)	1:134:A:LEU:HD22	1:133:A:VAL:HG12	9	0.28
(1,666)	1:134:A:LEU:HD22	1:133:A:VAL:HG11	16	0.28
(1,666)	1:134:A:LEU:HD23	1:133:A:VAL:HG12	25	0.28
(1,662)	1:133:A:VAL:HA	1:133:A:VAL:HG11	7	0.28
(1,662)	1:133:A:VAL:HA	1:133:A:VAL:HG13	8	0.28
(1,662)	1:133:A:VAL:HA	1:133:A:VAL:HG13	10	0.28
(1,662)	1:133:A:VAL:HA	1:133:A:VAL:HG13	16	0.28
(1,608)	1:136:A:ALA:HA	1:136:A:ALA:HB1	3	0.28
(1,608)	1:136:A:ALA:HA	1:136:A:ALA:HB3	7	0.28
(1,608)	1:136:A:ALA:HA	1:136:A:ALA:HB2	8	0.28
(1,608)	1:136:A:ALA:HA	1:136:A:ALA:HB3	10	0.28
(1,608)	1:136:A:ALA:HA	1:136:A:ALA:HB1	17	0.28
(1,608)	1:136:A:ALA:HA	1:136:A:ALA:HB2	22	0.28
(1,586)	1:139:A:ALA:HA	1:139:A:ALA:HB2	9	0.28
(1,586)	1:139:A:ALA:HA	1:139:A:ALA:HB3	12	0.28
(1,586)	1:139:A:ALA:HA	1:139:A:ALA:HB1	14	0.28
(1,586)	1:139:A:ALA:HA	1:139:A:ALA:HB1	18	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,558)	2:32:B:GLU:HA	2:31:B:LEU:H	16	0.28
(1,551)	2:34:B:TYR:H	2:35:B:PHE:HA	22	0.28
(1,541)	1:61:A:LEU:HB3	1:62:A:GLU:H	4	0.28
(1,540)	1:63:A:ASN:H	1:61:A:LEU:HG	10	0.28
(1,526)	1:69:A:GLU:H	1:113:A:LEU:HD23	7	0.28
(1,522)	1:70:A:PHE:H	1:73:A:LEU:H	3	0.28
(1,522)	1:70:A:PHE:H	1:73:A:LEU:H	25	0.28
(1,521)	1:71:A:LEU:H	1:113:A:LEU:HD11	7	0.28
(1,521)	1:71:A:LEU:H	1:113:A:LEU:HD13	14	0.28
(1,520)	1:130:A:LEU:H	1:112:A:VAL:HG22	21	0.28
(1,515)	1:73:A:LEU:HG	1:76:A:MET:H	24	0.28
(1,505)	1:79:A:ALA:H	1:76:A:MET:HA	16	0.28
(1,505)	1:79:A:ALA:H	1:76:A:MET:HA	19	0.28
(1,501)	1:80:A:ASP:HB2	1:81:A:HIS:H	12	0.28
(1,500)	1:85:A:VAL:H	1:83:A:GLU:H	15	0.28
(1,492)	1:91:A:ARG:H	1:88:A:LEU:HD21	25	0.28
(1,490)	1:91:A:ARG:H	1:94:A:ARG:H	5	0.28
(1,473)	1:101:A:ALA:H	1:100:A:LEU:HB3	2	0.28
(1,473)	1:101:A:ALA:H	1:100:A:LEU:HG	19	0.28
(1,466)	1:106:A:CYS:H	1:63:A:ASN:HD21	20	0.28
(1,465)	1:106:A:CYS:H	1:103:A:ALA:HB2	15	0.28
(1,453)	1:114:A:SER:H	1:113:A:LEU:HD21	4	0.28
(1,438)	1:66:A:LEU:HD11	1:66:A:LEU:H	21	0.28
(1,392)	1:139:A:ALA:H	1:96:A:HIS:HD2	2	0.28
(1,392)	1:139:A:ALA:H	1:96:A:HIS:HD2	18	0.28
(1,389)	1:143:A:LEU:H	1:142:A:LYS:HB2	6	0.28
(1,380)	2:27:B:SER:HA	2:30:B:GLU:HB3	4	0.28
(1,380)	2:27:B:SER:HA	2:30:B:GLU:HB3	18	0.28
(1,379)	2:31:B:LEU:HB2	2:28:B:ASP:HB2	21	0.28
(1,367)	2:26:B:ASP:HB3	2:31:B:LEU:H	8	0.28
(1,366)	1:100:A:LEU:HD13	1:138:A:SER:HB3	2	0.28
(1,361)	2:29:B:SER:HB2	2:32:B:GLU:HG3	8	0.28
(1,361)	2:29:B:SER:HB2	2:32:B:GLU:HG3	20	0.28
(1,342)	2:31:B:LEU:HD13	1:124:A:TYR:HB3	1	0.28
(1,342)	2:31:B:LEU:HD12	1:124:A:TYR:HB3	5	0.28
(1,324)	2:33:B:GLN:HG2	2:26:B:ASP:HB3	6	0.28
(1,275)	1:84:A:VAL:HG11	2:35:B:PHE:HZ	9	0.28
(1,258)	1:113:A:LEU:HG	1:113:A:LEU:HD22	1	0.28
(1,258)	1:113:A:LEU:HD13	1:113:A:LEU:HG	2	0.28
(1,258)	1:113:A:LEU:HG	1:113:A:LEU:HD23	10	0.28
(1,258)	1:113:A:LEU:HG	1:113:A:LEU:HD23	16	0.28
(1,258)	1:113:A:LEU:HG	1:113:A:LEU:HD21	20	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,258)	1:113:A:LEU:HD13	1:113:A:LEU:HG	21	0.28
(1,257)	1:113:A:LEU:HD12	1:117:A:ARG:HG2	6	0.28
(1,254)	1:57:A:LYS:HE3	1:54:A:MET:HG3	23	0.28
(1,253)	1:57:A:LYS:HE2	1:54:A:MET:HG3	2	0.28
(1,246)	1:61:A:LEU:HG	1:61:A:LEU:HD22	3	0.28
(1,246)	1:61:A:LEU:HG	1:61:A:LEU:HD22	7	0.28
(1,246)	1:61:A:LEU:HG	1:61:A:LEU:HD22	16	0.28
(1,246)	1:61:A:LEU:HG	1:61:A:LEU:HD22	23	0.28
(1,244)	1:111:A:ARG:HA	1:115:A:ARG:HG2	4	0.28
(1,244)	1:111:A:ARG:HA	1:115:A:ARG:HG2	24	0.28
(1,243)	1:62:A:GLU:HG3	1:61:A:LEU:HD21	6	0.28
(1,240)	1:104:A:GLU:HB3	1:105:A:PHE:HA	16	0.28
(1,229)	1:105:A:PHE:HE2	1:67:A:PHE:HB2	17	0.28
(1,229)	1:105:A:PHE:HE2	1:67:A:PHE:HB2	21	0.28
(1,227)	1:62:A:GLU:HG2	1:61:A:LEU:HG	17	0.28
(1,220)	1:70:A:PHE:HE2	1:113:A:LEU:HB2	8	0.28
(1,220)	1:70:A:PHE:HE2	1:113:A:LEU:HB2	18	0.28
(1,220)	1:70:A:PHE:HE2	1:113:A:LEU:HB2	22	0.28
(1,220)	1:70:A:PHE:HE2	1:113:A:LEU:HB2	23	0.28
(1,210)	1:105:A:PHE:HZ	1:109:A:LEU:HD21	11	0.28
(1,210)	1:105:A:PHE:HZ	1:109:A:LEU:HD21	14	0.28
(1,210)	1:105:A:PHE:HZ	1:109:A:LEU:HD21	16	0.28
(1,209)	1:67:A:PHE:HE1	1:71:A:LEU:HD23	1	0.28
(1,172)	1:85:A:VAL:HG11	1:74:A:CYS:HB3	6	0.28
(1,172)	1:85:A:VAL:HG12	1:74:A:CYS:HB3	9	0.28
(1,172)	1:85:A:VAL:HG12	1:74:A:CYS:HB3	17	0.28
(1,163)	1:67:A:PHE:HD2	1:92:A:GLN:HG3	1	0.28
(1,147)	1:137:A:HIS:HB3	1:138:A:SER:H	8	0.28
(1,147)	1:137:A:HIS:HB3	1:138:A:SER:H	14	0.28
(1,147)	1:137:A:HIS:HB3	1:138:A:SER:H	20	0.28
(1,140)	1:99:A:PHE:HB3	1:138:A:SER:H	22	0.28
(1,122)	1:95:A:ALA:HB1	1:91:A:ARG:HD3	7	0.28
(1,116)	1:100:A:LEU:HD21	1:105:A:PHE:HE2	3	0.28
(1,116)	1:100:A:LEU:HD23	1:105:A:PHE:HE2	7	0.28
(1,111)	1:62:A:GLU:HB3	1:59:A:TYR:HD2	3	0.28
(1,98)	1:105:A:PHE:HD1	1:100:A:LEU:HD23	5	0.28
(1,95)	1:107:A:ASN:HB2	1:108:A:ILE:HB	17	0.28
(1,95)	1:107:A:ASN:HB2	1:108:A:ILE:HB	21	0.28
(1,95)	1:107:A:ASN:HB2	1:108:A:ILE:HB	22	0.28
(1,92)	1:109:A:LEU:HD23	1:67:A:PHE:H	2	0.28
(1,92)	1:109:A:LEU:HD23	1:67:A:PHE:H	14	0.28
(1,92)	1:109:A:LEU:HD23	1:67:A:PHE:H	16	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,87)	1:112:A:VAL:HG12	1:130:A:LEU:H	9	0.28
(1,83)	1:113:A:LEU:HA	1:116:A:ALA:HB3	19	0.28
(1,81)	1:116:A:ALA:HB1	1:70:A:PHE:HZ	13	0.28
(1,80)	1:94:A:ARG:HD2	1:93:A:GLN:HB2	25	0.28
(1,62)	1:123:A:LEU:HD21	1:70:A:PHE:HE1	8	0.28
(1,51)	1:126:A:TYR:HD1	1:125:A:VAL:HG12	18	0.28
(1,36)	1:127:A:ILE:HG21	1:124:A:TYR:HD2	1	0.28
(1,25)	1:85:A:VAL:HG22	1:74:A:CYS:HB2	22	0.28
(1,25)	1:85:A:VAL:HG23	1:74:A:CYS:HB2	24	0.28
(1,24)	1:85:A:VAL:HG23	1:71:A:LEU:HA	3	0.28
(1,24)	1:85:A:VAL:HG21	1:71:A:LEU:HA	9	0.28
(1,24)	1:85:A:VAL:HG21	1:71:A:LEU:HA	21	0.28
(1,14)	1:133:A:VAL:HG21	1:132:A:THR:H	15	0.28
(1,14)	1:133:A:VAL:HG22	1:132:A:THR:H	20	0.28
(1,2287)	2:33:B:GLN:HE22	2:33:B:GLN:HB3	16	0.27
(1,2273)	2:25:B:GLU:HB3	2:25:B:GLU:H	25	0.27
(1,2244)	2:36:B:THR:HG22	2:36:B:THR:H	4	0.27
(1,2228)	2:35:B:PHE:H	2:34:B:TYR:HB3	6	0.27
(1,2228)	2:35:B:PHE:H	2:34:B:TYR:HB3	10	0.27
(1,2202)	1:125:A:VAL:H	1:122:A:LYS:HD3	18	0.27
(1,2173)	1:63:A:ASN:H	1:109:A:LEU:HD13	5	0.27
(1,2142)	1:109:A:LEU:HD21	1:68:A:GLU:H	1	0.27
(1,2138)	1:69:A:GLU:HG3	1:69:A:GLU:H	2	0.27
(1,2108)	1:77:A:GLN:H	1:78:A:THR:HG23	7	0.27
(1,2097)	1:77:A:GLN:HE21	1:77:A:GLN:HA	9	0.27
(1,2097)	1:77:A:GLN:HE21	1:77:A:GLN:HA	10	0.27
(1,2097)	1:77:A:GLN:HE21	1:77:A:GLN:HA	13	0.27
(1,2097)	1:77:A:GLN:HE21	1:77:A:GLN:HA	15	0.27
(1,2097)	1:77:A:GLN:HE21	1:77:A:GLN:HA	24	0.27
(1,2027)	1:92:A:GLN:HE22	1:64:A:GLU:HA	8	0.27
(1,2018)	1:93:A:GLN:HE22	1:93:A:GLN:HG2	1	0.27
(1,2018)	1:93:A:GLN:HE22	1:93:A:GLN:HG2	2	0.27
(1,2018)	1:93:A:GLN:HE22	1:93:A:GLN:HG2	3	0.27
(1,2018)	1:93:A:GLN:HE22	1:93:A:GLN:HG2	6	0.27
(1,2018)	1:93:A:GLN:HE22	1:93:A:GLN:HG2	15	0.27
(1,2018)	1:93:A:GLN:HE22	1:93:A:GLN:HG2	18	0.27
(1,2018)	1:93:A:GLN:HE22	1:93:A:GLN:HG2	19	0.27
(1,2007)	1:100:A:LEU:HD22	1:95:A:ALA:H	2	0.27
(1,2007)	1:100:A:LEU:HD23	1:95:A:ALA:H	10	0.27
(1,2004)	1:95:A:ALA:H	1:94:A:ARG:HB3	19	0.27
(1,2004)	1:95:A:ALA:H	1:94:A:ARG:HB3	20	0.27
(1,1996)	1:97:A:SER:H	1:139:A:ALA:HB2	17	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1971)	1:100:A:LEU:HD21	1:101:A:ALA:H	1	0.27
(1,1971)	1:100:A:LEU:HD22	1:101:A:ALA:H	9	0.27
(1,1874)	1:118:A:SER:H	1:117:A:ARG:HG2	10	0.27
(1,1761)	2:25:B:GLU:HA	2:25:B:GLU:HB2	11	0.27
(1,1761)	2:25:B:GLU:HA	2:25:B:GLU:HB2	13	0.27
(1,1761)	2:25:B:GLU:HA	2:25:B:GLU:HB2	14	0.27
(1,1761)	2:25:B:GLU:HA	2:25:B:GLU:HB2	17	0.27
(1,1761)	2:25:B:GLU:HA	2:25:B:GLU:HB2	21	0.27
(1,1759)	2:30:B:GLU:HA	2:30:B:GLU:HG3	8	0.27
(1,1759)	2:30:B:GLU:HA	2:30:B:GLU:HG3	25	0.27
(1,1747)	2:26:B:ASP:HB3	2:27:B:SER:HA	9	0.27
(1,1727)	2:31:B:LEU:HD11	2:31:B:LEU:H	22	0.27
(1,1716)	2:31:B:LEU:HG	2:32:B:GLU:HG3	19	0.27
(1,1713)	2:31:B:LEU:HG	2:31:B:LEU:H	9	0.27
(1,1713)	2:31:B:LEU:HG	2:31:B:LEU:H	13	0.27
(1,1713)	2:31:B:LEU:HG	2:31:B:LEU:H	23	0.27
(1,1703)	2:33:B:GLN:HG2	2:31:B:LEU:HD22	3	0.27
(1,1703)	2:33:B:GLN:HG2	2:31:B:LEU:HD23	18	0.27
(1,1670)	2:37:B:ALA:HB3	2:36:B:THR:HA	10	0.27
(1,1667)	2:36:B:THR:HB	2:36:B:THR:H	10	0.27
(1,1667)	2:36:B:THR:HB	2:36:B:THR:H	17	0.27
(1,1664)	2:36:B:THR:HG21	2:36:B:THR:HB	11	0.27
(1,1664)	2:36:B:THR:HG21	2:36:B:THR:HB	17	0.27
(1,1664)	2:36:B:THR:HG22	2:36:B:THR:HB	22	0.27
(1,1650)	2:37:B:ALA:HB1	1:121:A:ALA:HB2	10	0.27
(1,1636)	2:35:B:PHE:HB3	2:34:B:TYR:HE1	7	0.27
(1,1627)	2:39:B:TRP:HB2	2:39:B:TRP:HA	1	0.27
(1,1627)	2:39:B:TRP:HB2	2:39:B:TRP:HA	2	0.27
(1,1627)	2:39:B:TRP:HB2	2:39:B:TRP:HA	3	0.27
(1,1627)	2:39:B:TRP:HB2	2:39:B:TRP:HA	5	0.27
(1,1627)	2:39:B:TRP:HB2	2:39:B:TRP:HA	8	0.27
(1,1627)	2:39:B:TRP:HB2	2:39:B:TRP:HA	10	0.27
(1,1627)	2:39:B:TRP:HB2	2:39:B:TRP:HA	11	0.27
(1,1627)	2:39:B:TRP:HB2	2:39:B:TRP:HA	13	0.27
(1,1627)	2:39:B:TRP:HB2	2:39:B:TRP:HA	15	0.27
(1,1627)	2:39:B:TRP:HB2	2:39:B:TRP:HA	16	0.27
(1,1627)	2:39:B:TRP:HB2	2:39:B:TRP:HA	18	0.27
(1,1627)	2:39:B:TRP:HB2	2:39:B:TRP:HA	21	0.27
(1,1627)	2:39:B:TRP:HB2	2:39:B:TRP:HA	24	0.27
(1,1627)	2:39:B:TRP:HB2	2:39:B:TRP:HA	25	0.27
(1,1622)	2:39:B:TRP:HE3	2:39:B:TRP:HB2	13	0.27
(1,1615)	2:39:B:TRP:HE3	2:36:B:THR:HG21	4	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1595)	2:31:B:LEU:HD13	1:127:A:ILE:HB	6	0.27
(1,1592)	1:84:A:VAL:HG21	2:35:B:PHE:HB2	2	0.27
(1,1591)	1:84:A:VAL:HA	2:31:B:LEU:HD12	2	0.27
(1,1591)	1:84:A:VAL:HA	2:31:B:LEU:HD12	13	0.27
(1,1591)	1:84:A:VAL:HA	2:31:B:LEU:HD13	23	0.27
(1,1588)	1:87:A:PHE:HB2	2:31:B:LEU:HD11	2	0.27
(1,1577)	1:77:A:GLN:HG3	1:73:A:LEU:HD11	16	0.27
(1,1549)	1:58:A:CYS:HB2	1:57:A:LYS:HA	13	0.27
(1,1495)	1:64:A:GLU:HA	1:67:A:PHE:HB2	25	0.27
(1,1453)	1:68:A:GLU:HG3	1:69:A:GLU:H	15	0.27
(1,1450)	1:85:A:VAL:HB	1:86:A:PRO:HD3	4	0.27
(1,1450)	1:85:A:VAL:HB	1:86:A:PRO:HD3	8	0.27
(1,1450)	1:85:A:VAL:HB	1:86:A:PRO:HD3	12	0.27
(1,1450)	1:85:A:VAL:HB	1:86:A:PRO:HD3	17	0.27
(1,1450)	1:85:A:VAL:HB	1:86:A:PRO:HD3	21	0.27
(1,1447)	1:69:A:GLU:HA	1:69:A:GLU:HG3	7	0.27
(1,1447)	1:69:A:GLU:HA	1:69:A:GLU:HG3	8	0.27
(1,1419)	1:71:A:LEU:HD13	1:89:A:TYR:H	6	0.27
(1,1391)	1:74:A:CYS:HA	1:73:A:LEU:HD21	9	0.27
(1,1391)	1:74:A:CYS:HA	1:73:A:LEU:HD22	21	0.27
(1,1370)	1:75:A:LYS:HE3	1:72:A:GLU:HB3	5	0.27
(1,1370)	1:75:A:LYS:HE3	1:72:A:GLU:HB3	15	0.27
(1,1345)	1:76:A:MET:HG2	1:77:A:GLN:H	5	0.27
(1,1345)	1:76:A:MET:HG2	1:77:A:GLN:H	15	0.27
(1,1269)	1:84:A:VAL:HG12	1:85:A:VAL:H	17	0.27
(1,1269)	1:84:A:VAL:HG11	1:85:A:VAL:H	20	0.27
(1,1228)	1:87:A:PHE:HD1	1:88:A:LEU:HD21	20	0.27
(1,1228)	1:87:A:PHE:HD1	1:88:A:LEU:HD23	23	0.27
(1,1209)	1:88:A:LEU:HD11	1:70:A:PHE:HE1	4	0.27
(1,1209)	1:88:A:LEU:HD13	1:70:A:PHE:HE1	13	0.27
(1,1209)	1:88:A:LEU:HD12	1:70:A:PHE:HE1	17	0.27
(1,1209)	1:88:A:LEU:HD11	1:70:A:PHE:HE1	21	0.27
(1,1197)	1:89:A:TYR:HD2	1:71:A:LEU:HD22	10	0.27
(1,1168)	1:100:A:LEU:HD22	1:92:A:GLN:HG2	16	0.27
(1,1168)	1:100:A:LEU:HD23	1:92:A:GLN:HG2	23	0.27
(1,1142)	1:94:A:ARG:HD2	1:94:A:ARG:HB2	18	0.27
(1,1142)	1:94:A:ARG:HD2	1:94:A:ARG:HB2	24	0.27
(1,1139)	1:134:A:LEU:HD21	1:95:A:ALA:HB1	10	0.27
(1,1139)	1:134:A:LEU:HD21	1:95:A:ALA:HB2	12	0.27
(1,1126)	1:96:A:HIS:HD2	1:139:A:ALA:HB2	4	0.27
(1,1126)	1:96:A:HIS:HD2	1:139:A:ALA:HB2	7	0.27
(1,1126)	1:96:A:HIS:HD2	1:139:A:ALA:HB2	11	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1126)	1:96:A:HIS:HD2	1:139:A:ALA:HB2	19	0.27
(1,1123)	1:83:A:GLU:HA	1:83:A:GLU:HG3	17	0.27
(1,1098)	1:100:A:LEU:HD22	1:92:A:GLN:HA	25	0.27
(1,1089)	1:105:A:PHE:HZ	1:100:A:LEU:HD23	13	0.27
(1,1074)	1:101:A:ALA:HB2	1:60:A:LYS:HA	7	0.27
(1,1074)	1:101:A:ALA:HB2	1:60:A:LYS:HA	8	0.27
(1,1068)	1:101:A:ALA:HB3	1:59:A:TYR:H	12	0.27
(1,1042)	1:62:A:GLU:HB2	1:62:A:GLU:HA	21	0.27
(1,1040)	1:62:A:GLU:HB3	1:59:A:TYR:HA	18	0.27
(1,1036)	1:62:A:GLU:HB3	1:62:A:GLU:H	8	0.27
(1,1026)	1:109:A:LEU:HD12	1:67:A:PHE:HE1	19	0.27
(1,996)	1:108:A:ILE:HG22	1:112:A:VAL:HG11	1	0.27
(1,942)	1:111:A:ARG:HB2	1:111:A:ARG:HD2	16	0.27
(1,886)	1:116:A:ALA:HA	1:123:A:LEU:HD11	14	0.27
(1,886)	1:116:A:ALA:HA	1:123:A:LEU:HD13	20	0.27
(1,881)	1:117:A:ARG:HD2	1:117:A:ARG:HB2	5	0.27
(1,881)	1:117:A:ARG:HD2	1:117:A:ARG:HB2	22	0.27
(1,831)	1:121:A:ALA:HA	1:121:A:ALA:HB1	1	0.27
(1,831)	1:121:A:ALA:HA	1:121:A:ALA:HB1	2	0.27
(1,831)	1:121:A:ALA:HA	1:121:A:ALA:HB1	8	0.27
(1,831)	1:121:A:ALA:HA	1:121:A:ALA:HB2	10	0.27
(1,831)	1:121:A:ALA:HA	1:121:A:ALA:HB3	13	0.27
(1,831)	1:121:A:ALA:HA	1:121:A:ALA:HB1	18	0.27
(1,831)	1:121:A:ALA:HA	1:121:A:ALA:HB2	19	0.27
(1,831)	1:121:A:ALA:HA	1:121:A:ALA:HB2	20	0.27
(1,831)	1:121:A:ALA:HA	1:121:A:ALA:HB3	22	0.27
(1,831)	1:121:A:ALA:HA	1:121:A:ALA:HB2	23	0.27
(1,831)	1:121:A:ALA:HA	1:121:A:ALA:HB2	24	0.27
(1,811)	1:123:A:LEU:HD22	1:70:A:PHE:HE1	22	0.27
(1,799)	1:111:A:ARG:HA	1:111:A:ARG:HG3	2	0.27
(1,775)	1:126:A:TYR:HE1	1:125:A:VAL:HG11	8	0.27
(1,666)	1:134:A:LEU:HD23	1:133:A:VAL:HG13	24	0.27
(1,664)	1:133:A:VAL:HG12	1:130:A:LEU:HA	1	0.27
(1,664)	1:133:A:VAL:HG12	1:130:A:LEU:HA	8	0.27
(1,664)	1:133:A:VAL:HG11	1:130:A:LEU:HA	18	0.27
(1,662)	1:133:A:VAL:HA	1:133:A:VAL:HG12	2	0.27
(1,662)	1:133:A:VAL:HA	1:133:A:VAL:HG11	9	0.27
(1,662)	1:133:A:VAL:HA	1:133:A:VAL:HG13	11	0.27
(1,662)	1:133:A:VAL:HA	1:133:A:VAL:HG13	12	0.27
(1,662)	1:133:A:VAL:HA	1:133:A:VAL:HG12	18	0.27
(1,662)	1:133:A:VAL:HA	1:133:A:VAL:HG13	22	0.27
(1,662)	1:133:A:VAL:HA	1:133:A:VAL:HG13	23	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,634)	1:134:A:LEU:HD12	1:134:A:LEU:H	3	0.27
(1,634)	1:134:A:LEU:HD11	1:134:A:LEU:H	13	0.27
(1,608)	1:136:A:ALA:HA	1:136:A:ALA:HB1	19	0.27
(1,608)	1:136:A:ALA:HA	1:136:A:ALA:HB2	24	0.27
(1,593)	1:138:A:SER:HA	1:138:A:SER:HB2	14	0.27
(1,586)	1:139:A:ALA:HA	1:139:A:ALA:HB1	1	0.27
(1,586)	1:139:A:ALA:HA	1:139:A:ALA:HB3	2	0.27
(1,586)	1:139:A:ALA:HA	1:139:A:ALA:HB3	3	0.27
(1,586)	1:139:A:ALA:HA	1:139:A:ALA:HB2	10	0.27
(1,586)	1:139:A:ALA:HA	1:139:A:ALA:HB3	13	0.27
(1,586)	1:139:A:ALA:HA	1:139:A:ALA:HB2	22	0.27
(1,586)	1:139:A:ALA:HA	1:139:A:ALA:HB3	23	0.27
(1,561)	2:27:B:SER:H	2:30:B:GLU:HB3	24	0.27
(1,540)	1:63:A:ASN:H	1:61:A:LEU:HG	5	0.27
(1,538)	1:63:A:ASN:H	1:61:A:LEU:HA	7	0.27
(1,538)	1:63:A:ASN:H	1:61:A:LEU:HA	22	0.27
(1,526)	1:69:A:GLU:H	1:113:A:LEU:HD22	17	0.27
(1,522)	1:70:A:PHE:H	1:73:A:LEU:H	7	0.27
(1,521)	1:71:A:LEU:H	1:113:A:LEU:HD11	11	0.27
(1,515)	1:73:A:LEU:HG	1:76:A:MET:H	7	0.27
(1,512)	1:77:A:GLN:H	1:123:A:LEU:HD23	24	0.27
(1,505)	1:79:A:ALA:H	1:76:A:MET:HA	17	0.27
(1,500)	1:85:A:VAL:H	1:83:A:GLU:H	8	0.27
(1,500)	1:85:A:VAL:H	1:83:A:GLU:H	14	0.27
(1,490)	1:91:A:ARG:H	1:94:A:ARG:H	9	0.27
(1,453)	1:114:A:SER:H	1:113:A:LEU:HD22	5	0.27
(1,453)	1:114:A:SER:H	1:113:A:LEU:HD23	8	0.27
(1,445)	1:116:A:ALA:H	1:112:A:VAL:HA	23	0.27
(1,414)	1:72:A:GLU:H	1:68:A:GLU:HA	4	0.27
(1,414)	1:72:A:GLU:H	1:68:A:GLU:HA	23	0.27
(1,392)	1:139:A:ALA:H	1:96:A:HIS:HD2	16	0.27
(1,380)	2:27:B:SER:HA	2:30:B:GLU:HB3	2	0.27
(1,366)	1:100:A:LEU:HD12	1:138:A:SER:HB3	14	0.27
(1,364)	2:29:B:SER:HB3	2:32:B:GLU:HB2	18	0.27
(1,356)	2:29:B:SER:HB2	2:33:B:GLN:H	4	0.27
(1,344)	2:31:B:LEU:HB3	1:87:A:PHE:HE2	5	0.27
(1,324)	2:33:B:GLN:HG2	2:26:B:ASP:HB2	7	0.27
(1,312)	2:35:B:PHE:HE1	2:36:B:THR:HA	18	0.27
(1,289)	2:39:B:TRP:HZ3	2:36:B:THR:HB	19	0.27
(1,275)	1:84:A:VAL:HG11	2:35:B:PHE:HE1	7	0.27
(1,275)	1:84:A:VAL:HG12	2:35:B:PHE:HE1	25	0.27
(1,258)	1:113:A:LEU:HD12	1:113:A:LEU:HG	6	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,258)	1:113:A:LEU:HG	1:113:A:LEU:HD21	7	0.27
(1,258)	1:113:A:LEU:HD12	1:113:A:LEU:HG	12	0.27
(1,258)	1:113:A:LEU:HD11	1:113:A:LEU:HG	14	0.27
(1,258)	1:113:A:LEU:HG	1:113:A:LEU:HD23	24	0.27
(1,246)	1:61:A:LEU:HG	1:61:A:LEU:HD22	1	0.27
(1,246)	1:61:A:LEU:HG	1:61:A:LEU:HD22	8	0.27
(1,246)	1:61:A:LEU:HG	1:61:A:LEU:HD21	11	0.27
(1,246)	1:61:A:LEU:HG	1:61:A:LEU:HD21	15	0.27
(1,246)	1:61:A:LEU:HG	1:61:A:LEU:HD22	17	0.27
(1,246)	1:61:A:LEU:HG	1:61:A:LEU:HD21	18	0.27
(1,246)	1:61:A:LEU:HG	1:61:A:LEU:HD23	22	0.27
(1,240)	1:104:A:GLU:HB3	1:105:A:PHE:HA	3	0.27
(1,240)	1:104:A:GLU:HB3	1:105:A:PHE:HA	7	0.27
(1,220)	1:70:A:PHE:HE2	1:113:A:LEU:HB2	2	0.27
(1,210)	1:105:A:PHE:HZ	1:109:A:LEU:HD21	15	0.27
(1,210)	1:105:A:PHE:HZ	1:109:A:LEU:HD22	20	0.27
(1,210)	1:105:A:PHE:HZ	1:109:A:LEU:HD21	23	0.27
(1,203)	1:71:A:LEU:HD12	1:68:A:GLU:H	8	0.27
(1,172)	1:85:A:VAL:HG12	1:74:A:CYS:HB3	7	0.27
(1,155)	1:88:A:LEU:HD23	1:131:A:CYS:HB3	24	0.27
(1,145)	1:88:A:LEU:HB3	1:85:A:VAL:HA	12	0.27
(1,145)	1:88:A:LEU:HB3	1:85:A:VAL:HA	13	0.27
(1,145)	1:88:A:LEU:HB3	1:85:A:VAL:HA	14	0.27
(1,145)	1:88:A:LEU:HB3	1:85:A:VAL:HA	15	0.27
(1,134)	1:105:A:PHE:HE2	1:92:A:GLN:HG2	5	0.27
(1,134)	1:105:A:PHE:HE2	1:92:A:GLN:HG2	13	0.27
(1,134)	1:105:A:PHE:HE2	1:92:A:GLN:HG2	18	0.27
(1,132)	1:67:A:PHE:HE1	1:92:A:GLN:HB3	25	0.27
(1,116)	1:100:A:LEU:HD23	1:105:A:PHE:HE2	22	0.27
(1,98)	1:105:A:PHE:HD1	1:100:A:LEU:HD22	13	0.27
(1,95)	1:107:A:ASN:HB2	1:108:A:ILE:HB	2	0.27
(1,95)	1:107:A:ASN:HB2	1:108:A:ILE:HB	11	0.27
(1,92)	1:109:A:LEU:HD23	1:67:A:PHE:H	7	0.27
(1,92)	1:109:A:LEU:HD23	1:67:A:PHE:H	9	0.27
(1,92)	1:109:A:LEU:HD22	1:67:A:PHE:H	18	0.27
(1,83)	1:113:A:LEU:HA	1:116:A:ALA:HB3	12	0.27
(1,81)	1:116:A:ALA:HB1	1:70:A:PHE:HZ	4	0.27
(1,81)	1:116:A:ALA:HB3	1:70:A:PHE:HZ	25	0.27
(1,42)	1:126:A:TYR:HD1	1:125:A:VAL:HB	17	0.27
(1,36)	1:127:A:ILE:HG23	1:124:A:TYR:HD2	15	0.27
(1,36)	1:127:A:ILE:HG23	1:124:A:TYR:HD2	22	0.27
(1,27)	1:130:A:LEU:HD21	1:67:A:PHE:HA	2	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,27)	1:130:A:LEU:HD21	1:67:A:PHE:HA	4	0.27
(1,27)	1:130:A:LEU:HD23	1:67:A:PHE:HA	17	0.27
(1,25)	1:85:A:VAL:HG22	1:74:A:CYS:HB2	8	0.27
(1,20)	1:66:A:LEU:HA	1:69:A:GLU:HB2	9	0.27
(1,14)	1:133:A:VAL:HG23	1:132:A:THR:H	1	0.27
(1,14)	1:133:A:VAL:HG23	1:132:A:THR:H	4	0.27
(1,14)	1:133:A:VAL:HG22	1:132:A:THR:H	11	0.27
(1,14)	1:133:A:VAL:HG21	1:132:A:THR:H	25	0.27
(1,8)	1:134:A:LEU:HD22	1:67:A:PHE:HZ	4	0.27
(1,2287)	2:33:B:GLN:HE22	2:33:B:GLN:HB3	2	0.26
(1,2287)	2:33:B:GLN:HE22	2:33:B:GLN:HB3	19	0.26
(1,2287)	2:33:B:GLN:HE22	2:33:B:GLN:HB3	21	0.26
(1,2287)	2:33:B:GLN:HE22	2:33:B:GLN:HB3	22	0.26
(1,2287)	2:33:B:GLN:HE22	2:33:B:GLN:HB3	23	0.26
(1,2273)	2:25:B:GLU:HB3	2:25:B:GLU:H	14	0.26
(1,2244)	2:36:B:THR:HG23	2:36:B:THR:H	5	0.26
(1,2244)	2:36:B:THR:HG23	2:36:B:THR:H	11	0.26
(1,2197)	1:55:A:GLY:HA2	1:56:A:LYS:H	4	0.26
(1,2179)	1:60:A:LYS:HB3	1:61:A:LEU:H	20	0.26
(1,2173)	1:63:A:ASN:H	1:109:A:LEU:HD12	16	0.26
(1,2108)	1:77:A:GLN:H	1:78:A:THR:HG22	25	0.26
(1,2100)	1:77:A:GLN:HE21	1:76:A:MET:HE3	23	0.26
(1,2097)	1:77:A:GLN:HE21	1:77:A:GLN:HA	5	0.26
(1,2097)	1:77:A:GLN:HE21	1:77:A:GLN:HA	6	0.26
(1,2071)	1:83:A:GLU:HG3	1:83:A:GLU:H	18	0.26
(1,2033)	1:90:A:ASN:HD22	1:94:A:ARG:HG2	21	0.26
(1,2032)	1:90:A:ASN:HD22	1:93:A:GLN:HB2	1	0.26
(1,2018)	1:93:A:GLN:HE22	1:93:A:GLN:HG2	4	0.26
(1,2018)	1:93:A:GLN:HE22	1:93:A:GLN:HG2	5	0.26
(1,2018)	1:93:A:GLN:HE22	1:93:A:GLN:HG2	7	0.26
(1,2018)	1:93:A:GLN:HE22	1:93:A:GLN:HG2	9	0.26
(1,2018)	1:93:A:GLN:HE22	1:93:A:GLN:HG2	10	0.26
(1,2018)	1:93:A:GLN:HE22	1:93:A:GLN:HG2	11	0.26
(1,2018)	1:93:A:GLN:HE22	1:93:A:GLN:HG2	12	0.26
(1,2018)	1:93:A:GLN:HE22	1:93:A:GLN:HG2	14	0.26
(1,2018)	1:93:A:GLN:HE22	1:93:A:GLN:HG2	16	0.26
(1,2018)	1:93:A:GLN:HE22	1:93:A:GLN:HG2	21	0.26
(1,2018)	1:93:A:GLN:HE22	1:93:A:GLN:HG2	22	0.26
(1,2018)	1:93:A:GLN:HE22	1:93:A:GLN:HG2	23	0.26
(1,2018)	1:93:A:GLN:HE22	1:93:A:GLN:HG2	25	0.26
(1,2006)	1:134:A:LEU:HD23	1:95:A:ALA:H	9	0.26
(1,2006)	1:134:A:LEU:HD21	1:95:A:ALA:H	13	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1987)	1:99:A:PHE:H	1:99:A:PHE:HD2	6	0.26
(1,1958)	1:103:A:ALA:H	1:102:A:SER:HB3	10	0.26
(1,1906)	1:111:A:ARG:H	1:111:A:ARG:HD2	3	0.26
(1,1854)	1:124:A:TYR:H	1:125:A:VAL:HG21	5	0.26
(1,1798)	1:136:A:ALA:H	1:135:A:LYS:HD2	23	0.26
(1,1789)	1:139:A:ALA:H	1:139:A:ALA:HB3	14	0.26
(1,1789)	1:139:A:ALA:H	1:139:A:ALA:HB3	15	0.26
(1,1781)	1:140:A:LYS:H	1:141:A:LYS:HB3	6	0.26
(1,1771)	1:142:A:LYS:H	1:142:A:LYS:HD2	24	0.26
(1,1761)	2:25:B:GLU:HA	2:25:B:GLU:HB2	6	0.26
(1,1761)	2:25:B:GLU:HA	2:25:B:GLU:HB2	8	0.26
(1,1761)	2:25:B:GLU:HA	2:25:B:GLU:HB2	12	0.26
(1,1761)	2:25:B:GLU:HA	2:25:B:GLU:HB2	20	0.26
(1,1761)	2:25:B:GLU:HA	2:25:B:GLU:HB2	25	0.26
(1,1759)	2:30:B:GLU:HA	2:30:B:GLU:HG3	20	0.26
(1,1746)	1:100:A:LEU:HD11	1:138:A:SER:HB2	12	0.26
(1,1745)	2:29:B:SER:HB3	2:30:B:GLU:H	10	0.26
(1,1741)	2:29:B:SER:HA	2:30:B:GLU:H	24	0.26
(1,1720)	2:34:B:TYR:HE1	2:31:B:LEU:HD21	24	0.26
(1,1713)	2:31:B:LEU:HG	2:31:B:LEU:H	5	0.26
(1,1713)	2:31:B:LEU:HG	2:31:B:LEU:H	6	0.26
(1,1713)	2:31:B:LEU:HG	2:31:B:LEU:H	8	0.26
(1,1703)	2:33:B:GLN:HG2	2:31:B:LEU:HD23	1	0.26
(1,1703)	2:33:B:GLN:HG2	2:31:B:LEU:HD22	13	0.26
(1,1670)	2:37:B:ALA:HB1	2:36:B:THR:HA	4	0.26
(1,1667)	2:36:B:THR:HB	2:36:B:THR:H	9	0.26
(1,1667)	2:36:B:THR:HB	2:36:B:THR:H	18	0.26
(1,1667)	2:36:B:THR:HB	2:36:B:THR:H	24	0.26
(1,1664)	2:36:B:THR:HG23	2:36:B:THR:HB	1	0.26
(1,1664)	2:36:B:THR:HG22	2:36:B:THR:HB	2	0.26
(1,1664)	2:36:B:THR:HG22	2:36:B:THR:HB	14	0.26
(1,1664)	2:36:B:THR:HG23	2:36:B:THR:HB	15	0.26
(1,1664)	2:36:B:THR:HG22	2:36:B:THR:HB	23	0.26
(1,1664)	2:36:B:THR:HG22	2:36:B:THR:HB	25	0.26
(1,1636)	2:35:B:PHE:HB3	2:34:B:TYR:HE1	5	0.26
(1,1627)	2:39:B:TRP:HB2	2:39:B:TRP:HA	4	0.26
(1,1627)	2:39:B:TRP:HB2	2:39:B:TRP:HA	14	0.26
(1,1627)	2:39:B:TRP:HB2	2:39:B:TRP:HA	19	0.26
(1,1622)	2:39:B:TRP:HE3	2:39:B:TRP:HB2	14	0.26
(1,1619)	2:39:B:TRP:HD1	2:38:B:ARG:HB2	17	0.26
(1,1619)	2:39:B:TRP:HD1	2:38:B:ARG:HB2	18	0.26
(1,1619)	2:39:B:TRP:HD1	2:38:B:ARG:HB2	23	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1595)	2:31:B:LEU:HD12	1:127:A:ILE:HB	25	0.26
(1,1592)	1:84:A:VAL:HG22	2:35:B:PHE:HB2	20	0.26
(1,1591)	1:84:A:VAL:HA	2:31:B:LEU:HD12	5	0.26
(1,1591)	1:84:A:VAL:HA	2:31:B:LEU:HD13	6	0.26
(1,1591)	1:84:A:VAL:HA	2:31:B:LEU:HD11	8	0.26
(1,1591)	1:84:A:VAL:HA	2:31:B:LEU:HD13	18	0.26
(1,1570)	1:57:A:LYS:HE2	1:59:A:TYR:HE1	10	0.26
(1,1562)	1:57:A:LYS:HD2	1:57:A:LYS:HG2	1	0.26
(1,1562)	1:57:A:LYS:HD2	1:57:A:LYS:HG2	2	0.26
(1,1562)	1:57:A:LYS:HD2	1:57:A:LYS:HG2	3	0.26
(1,1562)	1:57:A:LYS:HD2	1:57:A:LYS:HG2	6	0.26
(1,1562)	1:57:A:LYS:HD2	1:57:A:LYS:HG2	7	0.26
(1,1562)	1:57:A:LYS:HD2	1:57:A:LYS:HG2	8	0.26
(1,1562)	1:57:A:LYS:HD2	1:57:A:LYS:HG2	9	0.26
(1,1562)	1:57:A:LYS:HD2	1:57:A:LYS:HG2	11	0.26
(1,1562)	1:57:A:LYS:HD2	1:57:A:LYS:HG2	12	0.26
(1,1562)	1:57:A:LYS:HD2	1:57:A:LYS:HG2	13	0.26
(1,1562)	1:57:A:LYS:HD2	1:57:A:LYS:HG2	15	0.26
(1,1562)	1:57:A:LYS:HD2	1:57:A:LYS:HG2	16	0.26
(1,1562)	1:57:A:LYS:HD2	1:57:A:LYS:HG2	18	0.26
(1,1562)	1:57:A:LYS:HD2	1:57:A:LYS:HG2	24	0.26
(1,1542)	1:59:A:TYR:HE2	1:59:A:TYR:HD2	20	0.26
(1,1456)	1:69:A:GLU:HG2	1:66:A:LEU:HA	1	0.26
(1,1450)	1:85:A:VAL:HB	1:86:A:PRO:HD3	5	0.26
(1,1450)	1:85:A:VAL:HB	1:86:A:PRO:HD3	6	0.26
(1,1450)	1:85:A:VAL:HB	1:86:A:PRO:HD3	15	0.26
(1,1450)	1:85:A:VAL:HB	1:86:A:PRO:HD3	19	0.26
(1,1450)	1:85:A:VAL:HB	1:86:A:PRO:HD3	23	0.26
(1,1450)	1:85:A:VAL:HB	1:86:A:PRO:HD3	24	0.26
(1,1450)	1:85:A:VAL:HB	1:86:A:PRO:HD3	25	0.26
(1,1440)	1:127:A:ILE:HD12	1:70:A:PHE:HZ	3	0.26
(1,1395)	1:116:A:ALA:HB1	1:73:A:LEU:HD23	8	0.26
(1,1370)	1:75:A:LYS:HE3	1:72:A:GLU:HB3	12	0.26
(1,1370)	1:75:A:LYS:HE3	1:72:A:GLU:HB3	21	0.26
(1,1228)	1:87:A:PHE:HD1	1:88:A:LEU:HD23	1	0.26
(1,1228)	1:87:A:PHE:HD1	1:88:A:LEU:HD23	5	0.26
(1,1228)	1:87:A:PHE:HD1	1:88:A:LEU:HD22	8	0.26
(1,1228)	1:87:A:PHE:HD1	1:88:A:LEU:HD23	12	0.26
(1,1209)	1:88:A:LEU:HD12	1:70:A:PHE:HE1	14	0.26
(1,1199)	1:89:A:TYR:HE1	1:71:A:LEU:HD12	8	0.26
(1,1197)	1:89:A:TYR:HD2	1:71:A:LEU:HD23	18	0.26
(1,1191)	1:89:A:TYR:HB2	1:89:A:TYR:HE2	1	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1191)	1:89:A:TYR:HB2	1:89:A:TYR:HE2	3	0.26
(1,1191)	1:89:A:TYR:HB2	1:89:A:TYR:HE2	5	0.26
(1,1191)	1:89:A:TYR:HB2	1:89:A:TYR:HE2	6	0.26
(1,1191)	1:89:A:TYR:HB2	1:89:A:TYR:HE2	8	0.26
(1,1191)	1:89:A:TYR:HB2	1:89:A:TYR:HE2	9	0.26
(1,1191)	1:89:A:TYR:HB2	1:89:A:TYR:HE2	11	0.26
(1,1191)	1:89:A:TYR:HB2	1:89:A:TYR:HE2	14	0.26
(1,1191)	1:89:A:TYR:HB2	1:89:A:TYR:HE2	15	0.26
(1,1191)	1:89:A:TYR:HB2	1:89:A:TYR:HE2	17	0.26
(1,1191)	1:89:A:TYR:HB2	1:89:A:TYR:HE2	19	0.26
(1,1191)	1:89:A:TYR:HB2	1:89:A:TYR:HE2	20	0.26
(1,1191)	1:89:A:TYR:HB2	1:89:A:TYR:HE2	22	0.26
(1,1168)	1:100:A:LEU:HD23	1:92:A:GLN:HG2	7	0.26
(1,1142)	1:94:A:ARG:HD2	1:94:A:ARG:HB2	11	0.26
(1,1133)	1:95:A:ALA:HB3	1:99:A:PHE:HD2	5	0.26
(1,1122)	1:96:A:HIS:HA	1:139:A:ALA:HB2	7	0.26
(1,1098)	1:100:A:LEU:HD21	1:92:A:GLN:HA	23	0.26
(1,1089)	1:105:A:PHE:HZ	1:100:A:LEU:HD21	3	0.26
(1,1089)	1:105:A:PHE:HZ	1:100:A:LEU:HD23	18	0.26
(1,1089)	1:105:A:PHE:HZ	1:100:A:LEU:HD23	23	0.26
(1,1089)	1:105:A:PHE:HZ	1:100:A:LEU:HD21	25	0.26
(1,1072)	1:101:A:ALA:HB1	1:58:A:CYS:HA	5	0.26
(1,1057)	1:103:A:ALA:HB3	1:59:A:TYR:HD1	6	0.26
(1,1057)	1:103:A:ALA:HB3	1:59:A:TYR:HD1	8	0.26
(1,1057)	1:103:A:ALA:HB2	1:59:A:TYR:HD1	10	0.26
(1,1057)	1:103:A:ALA:HB3	1:59:A:TYR:HD1	18	0.26
(1,1044)	1:62:A:GLU:HB3	1:62:A:GLU:HG3	3	0.26
(1,1044)	1:62:A:GLU:HB3	1:62:A:GLU:HG3	6	0.26
(1,1044)	1:62:A:GLU:HB3	1:62:A:GLU:HG3	7	0.26
(1,1044)	1:62:A:GLU:HB3	1:62:A:GLU:HG3	12	0.26
(1,1044)	1:62:A:GLU:HB3	1:62:A:GLU:HG3	16	0.26
(1,1042)	1:62:A:GLU:HB2	1:62:A:GLU:HA	25	0.26
(1,1040)	1:62:A:GLU:HB3	1:59:A:TYR:HA	8	0.26
(1,1000)	1:108:A:ILE:HD13	1:99:A:PHE:HE1	24	0.26
(1,996)	1:108:A:ILE:HG22	1:112:A:VAL:HG12	9	0.26
(1,915)	1:113:A:LEU:HD23	1:69:A:GLU:HB3	7	0.26
(1,909)	1:114:A:SER:HB2	1:113:A:LEU:HG	25	0.26
(1,878)	1:117:A:ARG:HG2	1:114:A:SER:HA	5	0.26
(1,858)	1:119:A:ARG:HG3	1:119:A:ARG:HA	3	0.26
(1,858)	1:119:A:ARG:HG3	1:119:A:ARG:HA	17	0.26
(1,831)	1:121:A:ALA:HA	1:121:A:ALA:HB3	6	0.26
(1,831)	1:121:A:ALA:HA	1:121:A:ALA:HB3	17	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,831)	1:121:A:ALA:HA	1:121:A:ALA:HB1	21	0.26
(1,811)	1:123:A:LEU:HD22	1:70:A:PHE:HE1	10	0.26
(1,799)	1:111:A:ARG:HA	1:111:A:ARG:HG3	18	0.26
(1,666)	1:134:A:LEU:HD23	1:133:A:VAL:HG11	12	0.26
(1,666)	1:134:A:LEU:HD22	1:133:A:VAL:HG11	14	0.26
(1,666)	1:134:A:LEU:HD21	1:133:A:VAL:HG13	21	0.26
(1,664)	1:133:A:VAL:HG12	1:130:A:LEU:HA	10	0.26
(1,664)	1:133:A:VAL:HG12	1:130:A:LEU:HA	17	0.26
(1,664)	1:133:A:VAL:HG11	1:130:A:LEU:HA	24	0.26
(1,664)	1:133:A:VAL:HG13	1:130:A:LEU:HA	25	0.26
(1,662)	1:133:A:VAL:HA	1:133:A:VAL:HG13	14	0.26
(1,642)	1:134:A:LEU:HD21	1:92:A:GLN:HG3	8	0.26
(1,634)	1:134:A:LEU:HD12	1:134:A:LEU:H	8	0.26
(1,634)	1:134:A:LEU:HD11	1:134:A:LEU:H	18	0.26
(1,634)	1:134:A:LEU:HD12	1:134:A:LEU:H	24	0.26
(1,614)	1:135:A:LYS:HA	1:135:A:LYS:HD2	1	0.26
(1,596)	1:137:A:HIS:HA	1:138:A:SER:H	25	0.26
(1,586)	1:139:A:ALA:HA	1:139:A:ALA:HB2	4	0.26
(1,586)	1:139:A:ALA:HA	1:139:A:ALA:HB1	6	0.26
(1,586)	1:139:A:ALA:HA	1:139:A:ALA:HB3	7	0.26
(1,586)	1:139:A:ALA:HA	1:139:A:ALA:HB3	15	0.26
(1,586)	1:139:A:ALA:HA	1:139:A:ALA:HB3	17	0.26
(1,586)	1:139:A:ALA:HA	1:139:A:ALA:HB2	19	0.26
(1,586)	1:139:A:ALA:HA	1:139:A:ALA:HB3	20	0.26
(1,586)	1:139:A:ALA:HA	1:139:A:ALA:HB2	21	0.26
(1,561)	2:27:B:SER:H	2:25:B:GLU:HB3	10	0.26
(1,551)	2:34:B:TYR:H	2:35:B:PHE:HA	14	0.26
(1,538)	1:63:A:ASN:H	1:61:A:LEU:HA	20	0.26
(1,526)	1:69:A:GLU:H	1:113:A:LEU:HD23	20	0.26
(1,522)	1:70:A:PHE:H	1:73:A:LEU:H	18	0.26
(1,521)	1:71:A:LEU:H	1:113:A:LEU:HD12	2	0.26
(1,520)	1:130:A:LEU:H	1:112:A:VAL:HG21	22	0.26
(1,512)	1:77:A:GLN:H	1:123:A:LEU:HD22	15	0.26
(1,505)	1:79:A:ALA:H	1:76:A:MET:HA	20	0.26
(1,500)	1:85:A:VAL:H	1:83:A:GLU:H	23	0.26
(1,490)	1:91:A:ARG:H	1:94:A:ARG:H	14	0.26
(1,478)	1:95:A:ALA:H	1:91:A:ARG:HD2	21	0.26
(1,473)	1:101:A:ALA:H	1:100:A:LEU:HB3	20	0.26
(1,465)	1:106:A:CYS:H	1:103:A:ALA:HB2	19	0.26
(1,453)	1:114:A:SER:H	1:113:A:LEU:HD21	3	0.26
(1,453)	1:114:A:SER:H	1:113:A:LEU:HD23	22	0.26
(1,445)	1:116:A:ALA:H	1:112:A:VAL:HA	15	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,445)	1:116:A:ALA:H	1:112:A:VAL:HA	19	0.26
(1,426)	1:125:A:VAL:HG12	1:126:A:TYR:H	1	0.26
(1,394)	1:137:A:HIS:HB3	1:138:A:SER:H	9	0.26
(1,387)	1:141:A:LYS:H	1:141:A:LYS:HG2	15	0.26
(1,380)	2:27:B:SER:HA	2:30:B:GLU:HB3	25	0.26
(1,361)	2:29:B:SER:HB2	2:32:B:GLU:HG3	10	0.26
(1,356)	2:29:B:SER:HB2	2:33:B:GLN:H	24	0.26
(1,342)	2:31:B:LEU:HD13	1:124:A:TYR:HB3	19	0.26
(1,342)	2:31:B:LEU:HD12	1:124:A:TYR:HB3	20	0.26
(1,337)	2:31:B:LEU:HD22	2:28:B:ASP:HB2	8	0.26
(1,258)	1:113:A:LEU:HD13	1:113:A:LEU:HG	3	0.26
(1,258)	1:113:A:LEU:HD11	1:113:A:LEU:HG	8	0.26
(1,258)	1:113:A:LEU:HD11	1:113:A:LEU:HG	9	0.26
(1,258)	1:113:A:LEU:HD13	1:113:A:LEU:HG	17	0.26
(1,257)	1:113:A:LEU:HD11	1:113:A:LEU:HB2	22	0.26
(1,255)	1:56:A:LYS:HA	1:56:A:LYS:HB3	10	0.26
(1,246)	1:61:A:LEU:HG	1:61:A:LEU:HD21	2	0.26
(1,246)	1:61:A:LEU:HG	1:61:A:LEU:HD21	4	0.26
(1,246)	1:61:A:LEU:HG	1:61:A:LEU:HD22	6	0.26
(1,246)	1:61:A:LEU:HG	1:61:A:LEU:HD23	12	0.26
(1,246)	1:61:A:LEU:HG	1:61:A:LEU:HD21	19	0.26
(1,246)	1:61:A:LEU:HG	1:61:A:LEU:HD22	21	0.26
(1,246)	1:61:A:LEU:HG	1:61:A:LEU:HD21	24	0.26
(1,236)	1:64:A:GLU:HA	1:67:A:PHE:H	17	0.26
(1,236)	1:64:A:GLU:HA	1:67:A:PHE:H	24	0.26
(1,229)	1:105:A:PHE:HE2	1:67:A:PHE:HB2	5	0.26
(1,229)	1:105:A:PHE:HE2	1:67:A:PHE:HB2	6	0.26
(1,229)	1:105:A:PHE:HE2	1:67:A:PHE:HB2	18	0.26
(1,225)	1:129:A:GLU:HG2	1:125:A:VAL:HG12	9	0.26
(1,225)	1:129:A:GLU:HG2	1:125:A:VAL:HG12	24	0.26
(1,220)	1:70:A:PHE:HE2	1:113:A:LEU:HB2	16	0.26
(1,210)	1:105:A:PHE:HZ	1:109:A:LEU:HD21	9	0.26
(1,172)	1:85:A:VAL:HG12	1:74:A:CYS:HB3	10	0.26
(1,172)	1:85:A:VAL:HG11	1:74:A:CYS:HB3	20	0.26
(1,160)	1:67:A:PHE:HD1	1:68:A:GLU:H	2	0.26
(1,160)	1:67:A:PHE:HD1	1:68:A:GLU:H	9	0.26
(1,157)	1:130:A:LEU:HD23	1:88:A:LEU:HD11	13	0.26
(1,145)	1:88:A:LEU:HB3	1:85:A:VAL:HA	21	0.26
(1,132)	1:92:A:GLN:HB3	1:89:A:TYR:HD1	4	0.26
(1,116)	1:100:A:LEU:HD22	1:105:A:PHE:HE2	16	0.26
(1,98)	1:105:A:PHE:HD1	1:100:A:LEU:HD22	7	0.26
(1,98)	1:105:A:PHE:HD1	1:100:A:LEU:HD23	17	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,97)	1:105:A:PHE:HD1	1:100:A:LEU:HA	23	0.26
(1,95)	1:107:A:ASN:HB2	1:108:A:ILE:HB	7	0.26
(1,95)	1:107:A:ASN:HB2	1:108:A:ILE:HB	13	0.26
(1,95)	1:107:A:ASN:HB2	1:108:A:ILE:HB	15	0.26
(1,92)	1:109:A:LEU:HD22	1:67:A:PHE:H	8	0.26
(1,92)	1:109:A:LEU:HD22	1:67:A:PHE:H	21	0.26
(1,92)	1:109:A:LEU:HD23	1:67:A:PHE:H	23	0.26
(1,83)	1:113:A:LEU:HA	1:116:A:ALA:HB3	14	0.26
(1,81)	1:116:A:ALA:HB2	1:70:A:PHE:HZ	5	0.26
(1,56)	1:124:A:TYR:HE2	2:35:B:PHE:HB3	1	0.26
(1,56)	1:124:A:TYR:HE2	2:35:B:PHE:HB3	9	0.26
(1,42)	1:126:A:TYR:HD1	1:125:A:VAL:HB	4	0.26
(1,36)	1:127:A:ILE:HG22	1:124:A:TYR:HD1	5	0.26
(1,36)	1:127:A:ILE:HG21	1:124:A:TYR:HD2	12	0.26
(1,24)	1:85:A:VAL:HG21	1:71:A:LEU:HA	11	0.26
(1,17)	1:133:A:VAL:HG13	1:137:A:HIS:HB2	11	0.26
(1,14)	1:133:A:VAL:HG23	1:132:A:THR:H	7	0.26
(1,14)	1:133:A:VAL:HG22	1:132:A:THR:H	8	0.26
(1,14)	1:133:A:VAL:HG21	1:132:A:THR:H	22	0.26
(1,2287)	2:33:B:GLN:HE22	2:33:B:GLN:HB3	4	0.25
(1,2287)	2:33:B:GLN:HE22	2:33:B:GLN:HB3	6	0.25
(1,2287)	2:33:B:GLN:HE22	2:33:B:GLN:HB3	18	0.25
(1,2287)	2:33:B:GLN:HE22	2:33:B:GLN:HB3	24	0.25
(1,2287)	2:33:B:GLN:HE22	2:33:B:GLN:HB3	25	0.25
(1,2267)	2:26:B:ASP:H	2:25:B:GLU:HB2	3	0.25
(1,2244)	2:36:B:THR:HG22	2:36:B:THR:H	15	0.25
(1,2228)	2:35:B:PHE:H	2:34:B:TYR:HB3	11	0.25
(1,2228)	2:35:B:PHE:H	2:34:B:TYR:HB3	25	0.25
(1,2207)	2:38:B:ARG:HB2	2:39:B:TRP:H	11	0.25
(1,2207)	2:38:B:ARG:HB2	2:39:B:TRP:H	15	0.25
(1,2108)	1:77:A:GLN:H	1:78:A:THR:HG21	16	0.25
(1,2097)	1:77:A:GLN:HE21	1:77:A:GLN:HA	18	0.25
(1,2051)	1:89:A:TYR:H	1:90:A:ASN:HB3	16	0.25
(1,2027)	1:92:A:GLN:HE22	1:64:A:GLU:HA	11	0.25
(1,2026)	1:67:A:PHE:HD2	1:92:A:GLN:HE21	12	0.25
(1,2018)	1:93:A:GLN:HE22	1:93:A:GLN:HG2	8	0.25
(1,2018)	1:93:A:GLN:HE22	1:93:A:GLN:HG2	13	0.25
(1,2018)	1:93:A:GLN:HE22	1:93:A:GLN:HG2	17	0.25
(1,2018)	1:93:A:GLN:HE22	1:93:A:GLN:HG2	24	0.25
(1,1996)	1:97:A:SER:H	1:139:A:ALA:HB2	20	0.25
(1,1987)	1:99:A:PHE:H	1:99:A:PHE:HD2	12	0.25
(1,1975)	1:100:A:LEU:HD12	1:100:A:LEU:H	2	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1975)	1:100:A:LEU:HD11	1:100:A:LEU:H	5	0.25
(1,1961)	1:102:A:SER:H	1:59:A:TYR:HD1	15	0.25
(1,1961)	1:102:A:SER:H	1:59:A:TYR:HD1	16	0.25
(1,1961)	1:102:A:SER:H	1:59:A:TYR:HD1	19	0.25
(1,1854)	1:124:A:TYR:H	1:125:A:VAL:HG23	24	0.25
(1,1801)	1:135:A:LYS:H	1:91:A:ARG:HD3	16	0.25
(1,1789)	1:139:A:ALA:H	1:139:A:ALA:HB1	5	0.25
(1,1775)	1:143:A:LEU:H	1:141:A:LYS:HG2	17	0.25
(1,1761)	2:25:B:GLU:HA	2:25:B:GLU:HB2	18	0.25
(1,1761)	2:25:B:GLU:HA	2:25:B:GLU:HB2	24	0.25
(1,1759)	2:30:B:GLU:HA	2:30:B:GLU:HG3	9	0.25
(1,1759)	2:30:B:GLU:HA	2:30:B:GLU:HG3	23	0.25
(1,1745)	2:29:B:SER:HB3	2:30:B:GLU:H	7	0.25
(1,1745)	2:29:B:SER:HB3	2:30:B:GLU:H	8	0.25
(1,1741)	2:29:B:SER:HA	2:30:B:GLU:H	2	0.25
(1,1741)	2:29:B:SER:HA	2:30:B:GLU:H	4	0.25
(1,1741)	2:29:B:SER:HA	2:30:B:GLU:H	5	0.25
(1,1741)	2:29:B:SER:HA	2:30:B:GLU:H	7	0.25
(1,1741)	2:29:B:SER:HA	2:30:B:GLU:H	9	0.25
(1,1741)	2:29:B:SER:HA	2:30:B:GLU:H	18	0.25
(1,1727)	2:31:B:LEU:HD11	2:31:B:LEU:H	2	0.25
(1,1727)	2:31:B:LEU:HD12	2:31:B:LEU:H	23	0.25
(1,1725)	2:31:B:LEU:HD23	1:127:A:ILE:HG22	10	0.25
(1,1725)	2:31:B:LEU:HD21	1:127:A:ILE:HG23	20	0.25
(1,1723)	2:31:B:LEU:HD23	2:30:B:GLU:HB2	1	0.25
(1,1723)	2:31:B:LEU:HD21	2:30:B:GLU:HB2	12	0.25
(1,1713)	2:31:B:LEU:HG	2:31:B:LEU:H	17	0.25
(1,1713)	2:31:B:LEU:HG	2:31:B:LEU:H	18	0.25
(1,1703)	2:33:B:GLN:HG2	2:31:B:LEU:HD21	9	0.25
(1,1670)	2:37:B:ALA:HB3	2:36:B:THR:HA	5	0.25
(1,1670)	2:37:B:ALA:HB1	2:36:B:THR:HA	13	0.25
(1,1667)	2:36:B:THR:HB	2:36:B:THR:H	6	0.25
(1,1667)	2:36:B:THR:HB	2:36:B:THR:H	8	0.25
(1,1667)	2:36:B:THR:HB	2:36:B:THR:H	11	0.25
(1,1667)	2:36:B:THR:HB	2:36:B:THR:H	12	0.25
(1,1667)	2:36:B:THR:HB	2:36:B:THR:H	13	0.25
(1,1667)	2:36:B:THR:HB	2:36:B:THR:H	16	0.25
(1,1667)	2:36:B:THR:HB	2:36:B:THR:H	22	0.25
(1,1664)	2:36:B:THR:HG22	2:36:B:THR:HB	6	0.25
(1,1664)	2:36:B:THR:HG22	2:36:B:THR:HB	10	0.25
(1,1664)	2:36:B:THR:HG22	2:36:B:THR:HB	16	0.25
(1,1664)	2:36:B:THR:HG21	2:36:B:THR:HB	19	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1664)	2:36:B:THR:HG23	2:36:B:THR:HB	21	0.25
(1,1650)	2:37:B:ALA:HB3	1:121:A:ALA:HB2	24	0.25
(1,1648)	2:38:B:ARG:HA	2:37:B:ALA:HB3	20	0.25
(1,1636)	2:35:B:PHE:HB3	2:34:B:TYR:HE1	8	0.25
(1,1622)	2:39:B:TRP:HE3	2:39:B:TRP:HB2	4	0.25
(1,1619)	2:39:B:TRP:HD1	2:38:B:ARG:HB2	8	0.25
(1,1619)	2:39:B:TRP:HD1	2:38:B:ARG:HB2	22	0.25
(1,1595)	2:31:B:LEU:HD12	1:127:A:ILE:HB	5	0.25
(1,1591)	1:84:A:VAL:HA	2:31:B:LEU:HD13	1	0.25
(1,1591)	1:84:A:VAL:HA	2:31:B:LEU:HD11	4	0.25
(1,1591)	1:84:A:VAL:HA	2:31:B:LEU:HD12	20	0.25
(1,1588)	1:87:A:PHE:HB2	2:31:B:LEU:HD12	6	0.25
(1,1588)	1:87:A:PHE:HB2	2:31:B:LEU:HD11	12	0.25
(1,1570)	1:57:A:LYS:HE2	1:59:A:TYR:HE1	21	0.25
(1,1562)	1:57:A:LYS:HD2	1:57:A:LYS:HG2	4	0.25
(1,1562)	1:57:A:LYS:HD2	1:57:A:LYS:HG2	5	0.25
(1,1562)	1:57:A:LYS:HD2	1:57:A:LYS:HG2	10	0.25
(1,1562)	1:57:A:LYS:HD2	1:57:A:LYS:HG2	17	0.25
(1,1562)	1:57:A:LYS:HD2	1:57:A:LYS:HG2	19	0.25
(1,1562)	1:57:A:LYS:HD2	1:57:A:LYS:HG2	21	0.25
(1,1562)	1:57:A:LYS:HD2	1:57:A:LYS:HG2	22	0.25
(1,1562)	1:57:A:LYS:HD2	1:57:A:LYS:HG2	23	0.25
(1,1544)	1:103:A:ALA:HA	1:59:A:TYR:HE1	20	0.25
(1,1542)	1:59:A:TYR:HE2	1:59:A:TYR:HD2	1	0.25
(1,1542)	1:59:A:TYR:HE2	1:59:A:TYR:HD2	2	0.25
(1,1542)	1:59:A:TYR:HD1	1:59:A:TYR:HE1	3	0.25
(1,1542)	1:59:A:TYR:HD1	1:59:A:TYR:HE1	4	0.25
(1,1542)	1:59:A:TYR:HE2	1:59:A:TYR:HD2	6	0.25
(1,1542)	1:59:A:TYR:HE2	1:59:A:TYR:HD2	7	0.25
(1,1542)	1:59:A:TYR:HE2	1:59:A:TYR:HD2	8	0.25
(1,1542)	1:59:A:TYR:HE2	1:59:A:TYR:HD2	9	0.25
(1,1542)	1:59:A:TYR:HD1	1:59:A:TYR:HE1	10	0.25
(1,1542)	1:59:A:TYR:HE2	1:59:A:TYR:HD2	12	0.25
(1,1542)	1:59:A:TYR:HE2	1:59:A:TYR:HD2	13	0.25
(1,1542)	1:59:A:TYR:HD1	1:59:A:TYR:HE1	14	0.25
(1,1542)	1:59:A:TYR:HD1	1:59:A:TYR:HE1	15	0.25
(1,1542)	1:59:A:TYR:HE2	1:59:A:TYR:HD2	16	0.25
(1,1542)	1:59:A:TYR:HE2	1:59:A:TYR:HD2	17	0.25
(1,1542)	1:59:A:TYR:HE2	1:59:A:TYR:HD2	18	0.25
(1,1542)	1:59:A:TYR:HD1	1:59:A:TYR:HE1	19	0.25
(1,1542)	1:59:A:TYR:HE2	1:59:A:TYR:HD2	21	0.25
(1,1542)	1:59:A:TYR:HD1	1:59:A:TYR:HE1	23	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1542)	1:59:A:TYR:HD1	1:59:A:TYR:HE1	24	0.25
(1,1542)	1:59:A:TYR:HE2	1:59:A:TYR:HD2	25	0.25
(1,1539)	1:62:A:GLU:HB3	1:59:A:TYR:HD1	25	0.25
(1,1534)	1:59:A:TYR:HD1	1:59:A:TYR:H	10	0.25
(1,1495)	1:64:A:GLU:HA	1:67:A:PHE:HB2	16	0.25
(1,1457)	1:68:A:GLU:HB2	1:68:A:GLU:HG2	9	0.25
(1,1450)	1:85:A:VAL:HB	1:86:A:PRO:HD3	2	0.25
(1,1450)	1:85:A:VAL:HB	1:86:A:PRO:HD3	9	0.25
(1,1450)	1:85:A:VAL:HB	1:86:A:PRO:HD3	11	0.25
(1,1450)	1:85:A:VAL:HB	1:86:A:PRO:HD3	20	0.25
(1,1447)	1:69:A:GLU:HA	1:69:A:GLU:HG3	25	0.25
(1,1440)	1:127:A:ILE:HD12	1:70:A:PHE:HZ	15	0.25
(1,1440)	1:127:A:ILE:HD11	1:70:A:PHE:HZ	17	0.25
(1,1440)	1:127:A:ILE:HD12	1:70:A:PHE:HZ	23	0.25
(1,1391)	1:74:A:CYS:HA	1:73:A:LEU:HD22	7	0.25
(1,1370)	1:75:A:LYS:HE3	1:72:A:GLU:HB3	22	0.25
(1,1345)	1:76:A:MET:HG2	1:77:A:GLN:H	8	0.25
(1,1269)	1:84:A:VAL:HG12	1:85:A:VAL:H	21	0.25
(1,1228)	1:87:A:PHE:HD1	1:88:A:LEU:HD22	2	0.25
(1,1228)	1:87:A:PHE:HD1	1:88:A:LEU:HD21	15	0.25
(1,1209)	1:88:A:LEU:HD13	1:70:A:PHE:HE1	10	0.25
(1,1199)	1:89:A:TYR:HE1	1:71:A:LEU:HD13	7	0.25
(1,1197)	1:89:A:TYR:HD2	1:71:A:LEU:HD21	8	0.25
(1,1197)	1:89:A:TYR:HD2	1:71:A:LEU:HD21	13	0.25
(1,1197)	1:89:A:TYR:HD2	1:71:A:LEU:HD22	19	0.25
(1,1191)	1:89:A:TYR:HB2	1:89:A:TYR:HE2	2	0.25
(1,1191)	1:89:A:TYR:HB2	1:89:A:TYR:HE2	4	0.25
(1,1191)	1:89:A:TYR:HB2	1:89:A:TYR:HE2	7	0.25
(1,1191)	1:89:A:TYR:HB2	1:89:A:TYR:HE2	10	0.25
(1,1191)	1:89:A:TYR:HB2	1:89:A:TYR:HE2	12	0.25
(1,1191)	1:89:A:TYR:HB2	1:89:A:TYR:HE2	13	0.25
(1,1191)	1:89:A:TYR:HB2	1:89:A:TYR:HE2	16	0.25
(1,1191)	1:89:A:TYR:HB2	1:89:A:TYR:HE2	18	0.25
(1,1191)	1:89:A:TYR:HB2	1:89:A:TYR:HE2	21	0.25
(1,1191)	1:89:A:TYR:HB2	1:89:A:TYR:HE2	23	0.25
(1,1191)	1:89:A:TYR:HB2	1:89:A:TYR:HE2	24	0.25
(1,1191)	1:89:A:TYR:HB2	1:89:A:TYR:HE2	25	0.25
(1,1168)	1:100:A:LEU:HD21	1:92:A:GLN:HG2	2	0.25
(1,1142)	1:94:A:ARG:HD2	1:94:A:ARG:HB2	17	0.25
(1,1139)	1:134:A:LEU:HD23	1:95:A:ALA:HB2	1	0.25
(1,1139)	1:134:A:LEU:HD23	1:95:A:ALA:HB1	17	0.25
(1,1137)	1:95:A:ALA:HB3	1:91:A:ARG:HD3	2	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1137)	1:95:A:ALA:HB1	1:91:A:ARG:HD3	18	0.25
(1,1137)	1:95:A:ALA:HB1	1:91:A:ARG:HD3	20	0.25
(1,1137)	1:95:A:ALA:HB1	1:91:A:ARG:HD3	22	0.25
(1,1133)	1:95:A:ALA:HB3	1:99:A:PHE:HD2	25	0.25
(1,1126)	1:96:A:HIS:HD2	1:139:A:ALA:HB1	22	0.25
(1,1098)	1:100:A:LEU:HD23	1:92:A:GLN:HA	16	0.25
(1,1094)	1:100:A:LEU:HD22	1:138:A:SER:HB2	5	0.25
(1,1091)	1:100:A:LEU:HD22	1:92:A:GLN:HE21	21	0.25
(1,1088)	1:100:A:LEU:HD23	1:105:A:PHE:HD2	23	0.25
(1,1074)	1:101:A:ALA:HB2	1:60:A:LYS:HA	16	0.25
(1,1044)	1:62:A:GLU:HB3	1:62:A:GLU:HG3	4	0.25
(1,1044)	1:62:A:GLU:HB3	1:62:A:GLU:HG3	5	0.25
(1,1044)	1:62:A:GLU:HB3	1:62:A:GLU:HG3	8	0.25
(1,1044)	1:62:A:GLU:HB3	1:62:A:GLU:HG3	9	0.25
(1,1044)	1:62:A:GLU:HB3	1:62:A:GLU:HG3	10	0.25
(1,1044)	1:62:A:GLU:HB3	1:62:A:GLU:HG3	11	0.25
(1,1044)	1:62:A:GLU:HB3	1:62:A:GLU:HG3	13	0.25
(1,1044)	1:62:A:GLU:HB3	1:62:A:GLU:HG3	17	0.25
(1,1044)	1:62:A:GLU:HB3	1:62:A:GLU:HG3	20	0.25
(1,1044)	1:62:A:GLU:HB3	1:62:A:GLU:HG3	23	0.25
(1,1042)	1:62:A:GLU:HB2	1:62:A:GLU:HA	22	0.25
(1,1036)	1:62:A:GLU:HB3	1:62:A:GLU:H	3	0.25
(1,1036)	1:62:A:GLU:HB3	1:62:A:GLU:H	10	0.25
(1,1036)	1:62:A:GLU:HB3	1:62:A:GLU:H	14	0.25
(1,1036)	1:62:A:GLU:HB3	1:62:A:GLU:H	16	0.25
(1,1000)	1:108:A:ILE:HD13	1:99:A:PHE:HE1	18	0.25
(1,942)	1:111:A:ARG:HB2	1:111:A:ARG:HD2	17	0.25
(1,942)	1:111:A:ARG:HB2	1:111:A:ARG:HD2	21	0.25
(1,934)	1:112:A:VAL:HG13	1:126:A:TYR:HB3	7	0.25
(1,913)	1:113:A:LEU:HG	1:113:A:LEU:H	12	0.25
(1,909)	1:114:A:SER:HB2	1:113:A:LEU:HG	2	0.25
(1,886)	1:116:A:ALA:HA	1:123:A:LEU:HD11	24	0.25
(1,868)	1:119:A:ARG:HD2	1:119:A:ARG:HB2	16	0.25
(1,858)	1:119:A:ARG:HG3	1:119:A:ARG:HA	4	0.25
(1,858)	1:119:A:ARG:HG3	1:119:A:ARG:HA	18	0.25
(1,858)	1:119:A:ARG:HG3	1:119:A:ARG:HA	21	0.25
(1,858)	1:119:A:ARG:HG3	1:119:A:ARG:HA	24	0.25
(1,831)	1:121:A:ALA:HA	1:121:A:ALA:HB3	16	0.25
(1,831)	1:121:A:ALA:HA	1:121:A:ALA:HB3	25	0.25
(1,799)	1:111:A:ARG:HA	1:111:A:ARG:HG3	14	0.25
(1,775)	1:126:A:TYR:HE1	1:125:A:VAL:HG12	6	0.25
(1,722)	1:129:A:GLU:HG3	1:125:A:VAL:HG12	21	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,702)	1:85:A:VAL:HG23	1:85:A:VAL:HA	16	0.25
(1,673)	1:133:A:VAL:HG23	1:130:A:LEU:HA	5	0.25
(1,673)	1:133:A:VAL:HG23	1:130:A:LEU:HA	24	0.25
(1,666)	1:134:A:LEU:HD23	1:133:A:VAL:HG13	4	0.25
(1,666)	1:134:A:LEU:HD23	1:133:A:VAL:HG11	10	0.25
(1,666)	1:134:A:LEU:HD23	1:133:A:VAL:HG13	15	0.25
(1,664)	1:133:A:VAL:HG12	1:130:A:LEU:HA	3	0.25
(1,664)	1:133:A:VAL:HG13	1:130:A:LEU:HA	7	0.25
(1,664)	1:133:A:VAL:HG12	1:130:A:LEU:HA	12	0.25
(1,664)	1:133:A:VAL:HG11	1:130:A:LEU:HA	15	0.25
(1,664)	1:133:A:VAL:HG13	1:130:A:LEU:HA	19	0.25
(1,664)	1:133:A:VAL:HG12	1:130:A:LEU:HA	22	0.25
(1,662)	1:133:A:VAL:HA	1:133:A:VAL:HG13	1	0.25
(1,662)	1:133:A:VAL:HA	1:133:A:VAL:HG12	21	0.25
(1,634)	1:134:A:LEU:HD11	1:134:A:LEU:H	10	0.25
(1,618)	1:56:A:LYS:HG2	1:57:A:LYS:H	2	0.25
(1,593)	1:138:A:SER:HA	1:138:A:SER:HB2	1	0.25
(1,593)	1:138:A:SER:HA	1:138:A:SER:HB2	2	0.25
(1,586)	1:139:A:ALA:HA	1:139:A:ALA:HB2	16	0.25
(1,585)	1:139:A:ALA:HB2	1:140:A:LYS:H	16	0.25
(1,570)	1:143:A:LEU:HB2	1:144:A:ASN:HD21	18	0.25
(1,551)	2:34:B:TYR:H	2:35:B:PHE:HA	7	0.25
(1,540)	1:63:A:ASN:H	1:61:A:LEU:HG	16	0.25
(1,538)	1:63:A:ASN:H	1:61:A:LEU:HA	3	0.25
(1,526)	1:69:A:GLU:H	1:113:A:LEU:HD21	2	0.25
(1,522)	1:70:A:PHE:H	1:73:A:LEU:H	6	0.25
(1,522)	1:70:A:PHE:H	1:73:A:LEU:H	13	0.25
(1,521)	1:71:A:LEU:H	1:113:A:LEU:HD11	10	0.25
(1,521)	1:71:A:LEU:H	1:113:A:LEU:HD11	18	0.25
(1,520)	1:130:A:LEU:H	1:112:A:VAL:HG23	2	0.25
(1,520)	1:130:A:LEU:H	1:112:A:VAL:HG22	7	0.25
(1,520)	1:130:A:LEU:H	1:112:A:VAL:HG22	16	0.25
(1,520)	1:130:A:LEU:H	1:112:A:VAL:HG22	23	0.25
(1,515)	1:73:A:LEU:HG	1:76:A:MET:H	20	0.25
(1,512)	1:77:A:GLN:H	1:123:A:LEU:HD22	10	0.25
(1,512)	1:77:A:GLN:H	1:123:A:LEU:HD22	17	0.25
(1,512)	1:77:A:GLN:H	1:123:A:LEU:HD21	20	0.25
(1,492)	1:91:A:ARG:H	1:88:A:LEU:HD21	6	0.25
(1,492)	1:91:A:ARG:H	1:88:A:LEU:HD22	22	0.25
(1,492)	1:91:A:ARG:H	1:88:A:LEU:HD23	23	0.25
(1,490)	1:91:A:ARG:H	1:94:A:ARG:H	23	0.25
(1,488)	1:92:A:GLN:HE22	1:64:A:GLU:HG3	25	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,477)	1:93:A:GLN:HA	1:95:A:ALA:H	23	0.25
(1,473)	1:101:A:ALA:H	1:100:A:LEU:HB3	8	0.25
(1,469)	1:102:A:SER:H	1:104:A:GLU:HB3	14	0.25
(1,466)	1:106:A:CYS:H	1:63:A:ASN:HD21	18	0.25
(1,421)	1:128:A:ASN:H	1:70:A:PHE:HZ	7	0.25
(1,421)	1:128:A:ASN:H	1:70:A:PHE:HZ	11	0.25
(1,414)	1:72:A:GLU:H	1:68:A:GLU:HA	13	0.25
(1,379)	2:31:B:LEU:HB2	2:28:B:ASP:HB2	25	0.25
(1,359)	2:29:B:SER:HB2	2:26:B:ASP:HB3	11	0.25
(1,359)	2:27:B:SER:HB2	2:28:B:ASP:HB3	21	0.25
(1,356)	2:29:B:SER:HB2	2:33:B:GLN:H	5	0.25
(1,342)	2:31:B:LEU:HD11	1:124:A:TYR:HB3	3	0.25
(1,337)	2:31:B:LEU:HD21	2:28:B:ASP:HB2	3	0.25
(1,312)	2:35:B:PHE:HE1	2:36:B:THR:HA	17	0.25
(1,307)	2:39:B:TRP:HE3	2:36:B:THR:HG23	14	0.25
(1,275)	1:84:A:VAL:HG12	2:35:B:PHE:HE1	1	0.25
(1,264)	1:127:A:ILE:HG23	2:35:B:PHE:HE1	3	0.25
(1,264)	1:127:A:ILE:HG23	2:35:B:PHE:HE1	17	0.25
(1,258)	1:113:A:LEU:HD12	1:113:A:LEU:HG	18	0.25
(1,257)	1:113:A:LEU:HD13	1:117:A:ARG:HG2	2	0.25
(1,257)	1:113:A:LEU:HD13	1:117:A:ARG:HG2	17	0.25
(1,244)	1:111:A:ARG:HA	1:115:A:ARG:HG2	16	0.25
(1,233)	1:62:A:GLU:HG2	1:66:A:LEU:HD13	11	0.25
(1,229)	1:105:A:PHE:HE2	1:67:A:PHE:HB2	12	0.25
(1,225)	1:129:A:GLU:HG2	1:125:A:VAL:HG11	8	0.25
(1,225)	1:129:A:GLU:HG2	1:125:A:VAL:HG12	12	0.25
(1,225)	1:129:A:GLU:HG2	1:125:A:VAL:HG12	20	0.25
(1,220)	1:70:A:PHE:HE2	1:113:A:LEU:HB2	9	0.25
(1,210)	1:105:A:PHE:HZ	1:109:A:LEU:HD23	8	0.25
(1,172)	1:85:A:VAL:HG13	1:74:A:CYS:HB3	1	0.25
(1,160)	1:67:A:PHE:HD1	1:68:A:GLU:H	15	0.25
(1,157)	1:130:A:LEU:HD22	1:88:A:LEU:HD11	3	0.25
(1,140)	1:99:A:PHE:HB3	1:138:A:SER:H	20	0.25
(1,132)	1:92:A:GLN:HB3	1:89:A:TYR:HD1	15	0.25
(1,122)	1:95:A:ALA:HB1	1:91:A:ARG:HD3	8	0.25
(1,122)	1:95:A:ALA:HB2	1:91:A:ARG:HD3	11	0.25
(1,116)	1:100:A:LEU:HD23	1:105:A:PHE:HE2	23	0.25
(1,111)	1:62:A:GLU:HB3	1:59:A:TYR:HD2	16	0.25
(1,92)	1:109:A:LEU:HD23	1:67:A:PHE:H	11	0.25
(1,92)	1:109:A:LEU:HD23	1:67:A:PHE:H	15	0.25
(1,92)	1:109:A:LEU:HD21	1:67:A:PHE:H	20	0.25
(1,87)	1:112:A:VAL:HG13	1:130:A:LEU:H	19	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,76)	1:118:A:SER:HA	1:118:A:SER:HB2	2	0.25
(1,67)	1:116:A:ALA:HB2	1:120:A:PRO:HA	4	0.25
(1,62)	1:123:A:LEU:HD22	1:70:A:PHE:HE1	6	0.25
(1,62)	1:123:A:LEU:HD23	1:70:A:PHE:HE1	9	0.25
(1,62)	1:123:A:LEU:HD21	1:70:A:PHE:HE1	12	0.25
(1,62)	1:123:A:LEU:HD23	1:70:A:PHE:HE1	16	0.25
(1,56)	1:124:A:TYR:HE2	2:35:B:PHE:HB3	11	0.25
(1,54)	1:127:A:ILE:HG23	1:124:A:TYR:HD1	10	0.25
(1,42)	1:126:A:TYR:HD1	1:125:A:VAL:HB	6	0.25
(1,27)	1:130:A:LEU:HD23	1:67:A:PHE:HA	12	0.25
(1,27)	1:130:A:LEU:HD21	1:67:A:PHE:HA	16	0.25
(1,27)	1:130:A:LEU:HD21	1:67:A:PHE:HA	22	0.25
(1,25)	1:85:A:VAL:HG22	1:74:A:CYS:HB2	25	0.25
(1,14)	1:133:A:VAL:HG22	1:132:A:THR:H	3	0.25
(1,14)	1:133:A:VAL:HG21	1:132:A:THR:H	5	0.25
(1,14)	1:133:A:VAL:HG21	1:132:A:THR:H	6	0.25
(1,14)	1:133:A:VAL:HG21	1:132:A:THR:H	18	0.25
(1,14)	1:133:A:VAL:HG21	1:132:A:THR:H	23	0.25
(1,2287)	2:33:B:GLN:HE22	2:33:B:GLN:HB3	3	0.24
(1,2287)	2:33:B:GLN:HE22	2:33:B:GLN:HB3	8	0.24
(1,2287)	2:33:B:GLN:HE22	2:33:B:GLN:HB3	9	0.24
(1,2287)	2:33:B:GLN:HE22	2:33:B:GLN:HB3	12	0.24
(1,2287)	2:33:B:GLN:HE22	2:33:B:GLN:HB3	15	0.24
(1,2264)	2:25:B:GLU:HA	2:26:B:ASP:H	12	0.24
(1,2259)	2:27:B:SER:HB3	2:27:B:SER:H	19	0.24
(1,2248)	2:30:B:GLU:HB2	2:31:B:LEU:H	16	0.24
(1,2228)	2:35:B:PHE:H	2:34:B:TYR:HB3	3	0.24
(1,2228)	2:35:B:PHE:H	2:34:B:TYR:HB3	17	0.24
(1,2207)	2:38:B:ARG:HB2	2:39:B:TRP:H	21	0.24
(1,2202)	1:125:A:VAL:H	1:122:A:LYS:HD3	2	0.24
(1,2188)	1:59:A:TYR:H	1:58:A:CYS:HB3	4	0.24
(1,2188)	1:59:A:TYR:H	1:58:A:CYS:HB3	12	0.24
(1,2173)	1:63:A:ASN:H	1:109:A:LEU:HD12	13	0.24
(1,2108)	1:77:A:GLN:H	1:78:A:THR:HG23	4	0.24
(1,2108)	1:77:A:GLN:H	1:78:A:THR:HG23	6	0.24
(1,2108)	1:77:A:GLN:H	1:78:A:THR:HG21	15	0.24
(1,2108)	1:77:A:GLN:H	1:78:A:THR:HG23	19	0.24
(1,2097)	1:77:A:GLN:HE21	1:77:A:GLN:HA	12	0.24
(1,2097)	1:77:A:GLN:HE21	1:77:A:GLN:HA	22	0.24
(1,2006)	1:134:A:LEU:HD21	1:95:A:ALA:H	5	0.24
(1,2006)	1:134:A:LEU:HD22	1:95:A:ALA:H	6	0.24
(1,2005)	1:95:A:ALA:H	1:94:A:ARG:HG2	12	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2005)	1:95:A:ALA:H	1:94:A:ARG:HG2	19	0.24
(1,1971)	1:100:A:LEU:HD23	1:101:A:ALA:H	20	0.24
(1,1854)	1:124:A:TYR:H	1:125:A:VAL:HG21	2	0.24
(1,1837)	1:127:A:ILE:H	1:123:A:LEU:HD12	9	0.24
(1,1803)	1:135:A:LYS:HB3	1:135:A:LYS:H	21	0.24
(1,1798)	1:136:A:ALA:H	1:135:A:LYS:HD2	21	0.24
(1,1789)	1:139:A:ALA:H	1:139:A:ALA:HB2	19	0.24
(1,1789)	1:139:A:ALA:H	1:139:A:ALA:HB1	22	0.24
(1,1741)	2:29:B:SER:HA	2:30:B:GLU:H	3	0.24
(1,1741)	2:29:B:SER:HA	2:30:B:GLU:H	8	0.24
(1,1741)	2:29:B:SER:HA	2:30:B:GLU:H	12	0.24
(1,1741)	2:29:B:SER:HA	2:30:B:GLU:H	19	0.24
(1,1727)	2:31:B:LEU:HD11	2:31:B:LEU:H	5	0.24
(1,1723)	2:31:B:LEU:HD22	2:30:B:GLU:HB2	3	0.24
(1,1713)	2:31:B:LEU:HG	2:31:B:LEU:H	2	0.24
(1,1713)	2:31:B:LEU:HG	2:31:B:LEU:H	3	0.24
(1,1713)	2:31:B:LEU:HG	2:31:B:LEU:H	4	0.24
(1,1713)	2:31:B:LEU:HG	2:31:B:LEU:H	20	0.24
(1,1703)	2:33:B:GLN:HG2	2:31:B:LEU:HD21	2	0.24
(1,1703)	2:33:B:GLN:HG2	2:31:B:LEU:HD21	14	0.24
(1,1667)	2:36:B:THR:HB	2:36:B:THR:H	2	0.24
(1,1667)	2:36:B:THR:HB	2:36:B:THR:H	25	0.24
(1,1664)	2:36:B:THR:HG21	2:36:B:THR:HB	3	0.24
(1,1664)	2:36:B:THR:HG21	2:36:B:THR:HB	5	0.24
(1,1664)	2:36:B:THR:HG21	2:36:B:THR:HB	7	0.24
(1,1664)	2:36:B:THR:HG22	2:36:B:THR:HB	8	0.24
(1,1664)	2:36:B:THR:HG23	2:36:B:THR:HB	9	0.24
(1,1664)	2:36:B:THR:HG22	2:36:B:THR:HB	12	0.24
(1,1664)	2:36:B:THR:HG23	2:36:B:THR:HB	13	0.24
(1,1664)	2:36:B:THR:HG21	2:36:B:THR:HB	18	0.24
(1,1648)	2:38:B:ARG:HA	2:37:B:ALA:HB3	16	0.24
(1,1636)	2:35:B:PHE:HB3	2:34:B:TYR:HE1	1	0.24
(1,1636)	2:35:B:PHE:HB3	2:34:B:TYR:HE1	4	0.24
(1,1636)	2:35:B:PHE:HB3	2:34:B:TYR:HE1	15	0.24
(1,1636)	2:35:B:PHE:HB3	2:34:B:TYR:HE1	23	0.24
(1,1622)	2:39:B:TRP:HE3	2:39:B:TRP:HB2	22	0.24
(1,1595)	2:31:B:LEU:HD12	1:127:A:ILE:HB	17	0.24
(1,1591)	1:84:A:VAL:HA	2:31:B:LEU:HD13	11	0.24
(1,1591)	1:84:A:VAL:HA	2:31:B:LEU:HD12	14	0.24
(1,1591)	1:84:A:VAL:HA	2:31:B:LEU:HD12	17	0.24
(1,1591)	1:84:A:VAL:HA	2:31:B:LEU:HD13	21	0.24
(1,1588)	1:87:A:PHE:HB2	2:31:B:LEU:HD13	15	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1577)	1:77:A:GLN:HG3	1:73:A:LEU:HD11	6	0.24
(1,1577)	1:77:A:GLN:HG3	1:73:A:LEU:HD12	22	0.24
(1,1562)	1:57:A:LYS:HD2	1:57:A:LYS:HG2	25	0.24
(1,1554)	1:59:A:TYR:HE1	1:57:A:LYS:HB2	17	0.24
(1,1545)	1:59:A:TYR:HE1	1:57:A:LYS:HB3	20	0.24
(1,1544)	1:103:A:ALA:HA	1:59:A:TYR:HE1	25	0.24
(1,1542)	1:59:A:TYR:HE2	1:59:A:TYR:HD2	5	0.24
(1,1542)	1:59:A:TYR:HD1	1:59:A:TYR:HE1	11	0.24
(1,1542)	1:59:A:TYR:HD1	1:59:A:TYR:HE1	22	0.24
(1,1477)	1:66:A:LEU:HD21	1:113:A:LEU:HB3	22	0.24
(1,1454)	1:68:A:GLU:HG2	1:69:A:GLU:H	15	0.24
(1,1450)	1:85:A:VAL:HB	1:86:A:PRO:HD3	16	0.24
(1,1450)	1:85:A:VAL:HB	1:86:A:PRO:HD3	18	0.24
(1,1440)	1:127:A:ILE:HD11	1:70:A:PHE:HZ	11	0.24
(1,1440)	1:127:A:ILE:HD11	1:70:A:PHE:HZ	12	0.24
(1,1370)	1:75:A:LYS:HE3	1:72:A:GLU:HB3	1	0.24
(1,1370)	1:75:A:LYS:HE3	1:72:A:GLU:HB3	11	0.24
(1,1370)	1:75:A:LYS:HE3	1:72:A:GLU:HB3	19	0.24
(1,1316)	1:79:A:ALA:HB2	1:79:A:ALA:H	17	0.24
(1,1283)	1:84:A:VAL:HG23	1:127:A:ILE:HD13	24	0.24
(1,1279)	1:84:A:VAL:HG22	1:81:A:HIS:HB3	22	0.24
(1,1269)	1:84:A:VAL:HG13	1:85:A:VAL:H	16	0.24
(1,1228)	1:87:A:PHE:HD1	1:88:A:LEU:HD22	22	0.24
(1,1228)	1:87:A:PHE:HD1	1:88:A:LEU:HD21	25	0.24
(1,1199)	1:89:A:TYR:HE1	1:71:A:LEU:HD13	13	0.24
(1,1197)	1:89:A:TYR:HD2	1:71:A:LEU:HD22	1	0.24
(1,1197)	1:89:A:TYR:HD2	1:71:A:LEU:HD23	17	0.24
(1,1175)	1:91:A:ARG:HG2	1:134:A:LEU:HB2	6	0.24
(1,1171)	1:91:A:ARG:HG2	1:91:A:ARG:HA	1	0.24
(1,1168)	1:100:A:LEU:HD21	1:92:A:GLN:HG2	25	0.24
(1,1142)	1:94:A:ARG:HD2	1:94:A:ARG:HB2	3	0.24
(1,1142)	1:94:A:ARG:HD2	1:94:A:ARG:HB2	25	0.24
(1,1139)	1:134:A:LEU:HD21	1:95:A:ALA:HB3	13	0.24
(1,1126)	1:96:A:HIS:HD2	1:139:A:ALA:HB3	1	0.24
(1,1126)	1:96:A:HIS:HD2	1:139:A:ALA:HB3	14	0.24
(1,1098)	1:100:A:LEU:HD21	1:92:A:GLN:HA	19	0.24
(1,1097)	1:100:A:LEU:HD23	1:100:A:LEU:HD11	1	0.24
(1,1094)	1:100:A:LEU:HD23	1:138:A:SER:HB2	10	0.24
(1,1089)	1:105:A:PHE:HZ	1:100:A:LEU:HD21	4	0.24
(1,1089)	1:105:A:PHE:HZ	1:100:A:LEU:HD21	17	0.24
(1,1074)	1:101:A:ALA:HB1	1:60:A:LYS:HA	25	0.24
(1,1057)	1:103:A:ALA:HB1	1:59:A:TYR:HD1	11	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1044)	1:62:A:GLU:HB3	1:62:A:GLU:HG3	22	0.24
(1,1044)	1:62:A:GLU:HB3	1:62:A:GLU:HG3	24	0.24
(1,1044)	1:62:A:GLU:HB3	1:62:A:GLU:HG3	25	0.24
(1,1040)	1:62:A:GLU:HB3	1:59:A:TYR:HA	7	0.24
(1,1040)	1:62:A:GLU:HB3	1:59:A:TYR:HA	16	0.24
(1,1036)	1:62:A:GLU:HB3	1:62:A:GLU:H	1	0.24
(1,1036)	1:62:A:GLU:HB3	1:62:A:GLU:H	11	0.24
(1,1036)	1:62:A:GLU:HB3	1:62:A:GLU:H	20	0.24
(1,1036)	1:62:A:GLU:HB3	1:62:A:GLU:H	24	0.24
(1,998)	1:108:A:ILE:HD13	1:105:A:PHE:HD1	12	0.24
(1,998)	1:108:A:ILE:HD12	1:105:A:PHE:HD1	13	0.24
(1,996)	1:108:A:ILE:HG23	1:112:A:VAL:HG11	4	0.24
(1,991)	1:108:A:ILE:HA	1:108:A:ILE:HG21	7	0.24
(1,942)	1:111:A:ARG:HB2	1:111:A:ARG:HD2	10	0.24
(1,915)	1:113:A:LEU:HD22	1:69:A:GLU:HB3	1	0.24
(1,913)	1:113:A:LEU:HG	1:113:A:LEU:H	4	0.24
(1,911)	1:113:A:LEU:HB2	1:113:A:LEU:H	20	0.24
(1,904)	1:115:A:ARG:HD3	1:126:A:TYR:HE1	15	0.24
(1,831)	1:121:A:ALA:HA	1:121:A:ALA:HB3	11	0.24
(1,814)	1:123:A:LEU:HD23	1:120:A:PRO:HA	1	0.24
(1,814)	1:123:A:LEU:HD21	1:120:A:PRO:HA	21	0.24
(1,813)	1:123:A:LEU:HD21	1:124:A:TYR:HE2	16	0.24
(1,766)	1:126:A:TYR:HE1	1:115:A:ARG:HB2	11	0.24
(1,766)	1:126:A:TYR:HE1	1:115:A:ARG:HB2	21	0.24
(1,746)	1:127:A:ILE:HD13	1:127:A:ILE:H	9	0.24
(1,746)	1:127:A:ILE:HD12	1:127:A:ILE:H	16	0.24
(1,666)	1:134:A:LEU:HD23	1:133:A:VAL:HG13	13	0.24
(1,666)	1:134:A:LEU:HD22	1:133:A:VAL:HG11	17	0.24
(1,666)	1:134:A:LEU:HD23	1:133:A:VAL:HG11	22	0.24
(1,664)	1:133:A:VAL:HG11	1:130:A:LEU:HA	4	0.24
(1,664)	1:133:A:VAL:HG13	1:130:A:LEU:HA	5	0.24
(1,664)	1:133:A:VAL:HG12	1:130:A:LEU:HA	23	0.24
(1,662)	1:133:A:VAL:HA	1:133:A:VAL:HG12	13	0.24
(1,662)	1:133:A:VAL:HA	1:133:A:VAL:HG11	20	0.24
(1,634)	1:134:A:LEU:HD13	1:134:A:LEU:H	6	0.24
(1,593)	1:138:A:SER:HA	1:138:A:SER:HB2	12	0.24
(1,586)	1:139:A:ALA:HA	1:139:A:ALA:HB2	11	0.24
(1,586)	1:139:A:ALA:HA	1:139:A:ALA:HB3	24	0.24
(1,586)	1:139:A:ALA:HA	1:139:A:ALA:HB3	25	0.24
(1,558)	2:32:B:GLU:HA	2:31:B:LEU:H	1	0.24
(1,551)	2:34:B:TYR:H	2:35:B:PHE:HA	13	0.24
(1,551)	2:34:B:TYR:H	2:35:B:PHE:HA	20	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,540)	1:63:A:ASN:H	1:61:A:LEU:HG	25	0.24
(1,526)	1:69:A:GLU:H	1:113:A:LEU:HD22	9	0.24
(1,521)	1:71:A:LEU:H	1:113:A:LEU:HD13	9	0.24
(1,520)	1:130:A:LEU:H	1:112:A:VAL:HG22	5	0.24
(1,520)	1:130:A:LEU:H	1:112:A:VAL:HG22	14	0.24
(1,515)	1:73:A:LEU:HG	1:76:A:MET:H	18	0.24
(1,505)	1:79:A:ALA:H	1:76:A:MET:HA	14	0.24
(1,490)	1:91:A:ARG:H	1:94:A:ARG:H	4	0.24
(1,490)	1:91:A:ARG:H	1:94:A:ARG:H	10	0.24
(1,490)	1:91:A:ARG:H	1:94:A:ARG:H	13	0.24
(1,478)	1:95:A:ALA:H	1:91:A:ARG:HD2	25	0.24
(1,466)	1:106:A:CYS:H	1:63:A:ASN:HD21	1	0.24
(1,453)	1:114:A:SER:H	1:113:A:LEU:HD23	2	0.24
(1,453)	1:114:A:SER:H	1:113:A:LEU:HD21	9	0.24
(1,453)	1:114:A:SER:H	1:113:A:LEU:HD22	19	0.24
(1,445)	1:116:A:ALA:H	1:112:A:VAL:HA	11	0.24
(1,438)	1:66:A:LEU:HD13	1:66:A:LEU:H	17	0.24
(1,426)	1:125:A:VAL:HG12	1:126:A:TYR:H	6	0.24
(1,421)	1:128:A:ASN:H	1:70:A:PHE:HZ	1	0.24
(1,421)	1:128:A:ASN:H	1:70:A:PHE:HZ	6	0.24
(1,414)	1:72:A:GLU:H	1:69:A:GLU:HA	5	0.24
(1,414)	1:72:A:GLU:H	1:68:A:GLU:HA	25	0.24
(1,392)	1:139:A:ALA:H	1:96:A:HIS:HD2	22	0.24
(1,389)	1:143:A:LEU:H	1:142:A:LYS:HB2	9	0.24
(1,389)	1:143:A:LEU:H	1:142:A:LYS:HD2	21	0.24
(1,364)	2:29:B:SER:HB3	2:32:B:GLU:HB2	3	0.24
(1,363)	1:118:A:SER:HB3	1:119:A:ARG:HB2	2	0.24
(1,361)	2:29:B:SER:HB2	2:32:B:GLU:HG3	9	0.24
(1,361)	2:29:B:SER:HB2	2:32:B:GLU:HG3	21	0.24
(1,340)	2:31:B:LEU:HD13	1:88:A:LEU:H	14	0.24
(1,337)	2:31:B:LEU:HD23	2:28:B:ASP:HB2	7	0.24
(1,318)	2:34:B:TYR:HE1	1:83:A:GLU:HB3	11	0.24
(1,288)	2:32:B:GLU:HA	2:35:B:PHE:HD1	19	0.24
(1,281)	2:31:B:LEU:HD22	1:128:A:ASN:H	24	0.24
(1,264)	1:127:A:ILE:HG21	2:35:B:PHE:HE1	19	0.24
(1,257)	1:113:A:LEU:HD12	1:113:A:LEU:HB2	15	0.24
(1,257)	1:113:A:LEU:HD13	1:113:A:LEU:HB2	23	0.24
(1,246)	1:61:A:LEU:HG	1:61:A:LEU:HD21	9	0.24
(1,246)	1:61:A:LEU:HG	1:61:A:LEU:HD21	14	0.24
(1,243)	1:62:A:GLU:HG3	1:61:A:LEU:HD23	9	0.24
(1,240)	1:104:A:GLU:HB3	1:105:A:PHE:HA	10	0.24
(1,236)	1:64:A:GLU:HA	1:67:A:PHE:H	4	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,233)	1:62:A:GLU:HG2	1:66:A:LEU:HD12	8	0.24
(1,227)	1:62:A:GLU:HG2	1:61:A:LEU:HG	4	0.24
(1,210)	1:105:A:PHE:HZ	1:109:A:LEU:HD23	18	0.24
(1,172)	1:85:A:VAL:HG12	1:74:A:CYS:HB3	12	0.24
(1,160)	1:67:A:PHE:HD1	1:68:A:GLU:H	14	0.24
(1,160)	1:67:A:PHE:HD1	1:68:A:GLU:H	23	0.24
(1,160)	1:67:A:PHE:HD1	1:68:A:GLU:H	25	0.24
(1,155)	1:88:A:LEU:HD21	1:131:A:CYS:HB3	22	0.24
(1,145)	1:88:A:LEU:HB3	1:85:A:VAL:HA	10	0.24
(1,145)	1:88:A:LEU:HB3	1:85:A:VAL:HA	17	0.24
(1,145)	1:88:A:LEU:HB3	1:85:A:VAL:HA	19	0.24
(1,145)	1:88:A:LEU:HB3	1:85:A:VAL:HA	23	0.24
(1,141)	1:93:A:GLN:HG2	1:89:A:TYR:HD1	15	0.24
(1,123)	1:95:A:ALA:HB1	1:134:A:LEU:HB2	20	0.24
(1,117)	1:100:A:LEU:HD23	1:92:A:GLN:HG2	14	0.24
(1,116)	1:100:A:LEU:HD21	1:105:A:PHE:HE2	17	0.24
(1,97)	1:105:A:PHE:HD1	1:100:A:LEU:HA	16	0.24
(1,95)	1:107:A:ASN:HB2	1:108:A:ILE:HB	9	0.24
(1,92)	1:109:A:LEU:HD22	1:67:A:PHE:H	6	0.24
(1,54)	1:127:A:ILE:HG23	1:124:A:TYR:HD1	13	0.24
(1,45)	1:59:A:TYR:HE1	1:57:A:LYS:HD3	25	0.24
(1,37)	1:127:A:ILE:HG22	1:128:A:ASN:HD22	10	0.24
(1,36)	1:127:A:ILE:HG23	1:124:A:TYR:HD2	21	0.24
(1,24)	1:85:A:VAL:HG22	1:71:A:LEU:HA	2	0.24
(1,14)	1:133:A:VAL:HG22	1:132:A:THR:H	9	0.24
(1,2287)	2:33:B:GLN:HE22	2:33:B:GLN:HB3	1	0.23
(1,2287)	2:33:B:GLN:HE22	2:33:B:GLN:HB3	7	0.23
(1,2287)	2:33:B:GLN:HE22	2:33:B:GLN:HB3	14	0.23
(1,2287)	2:33:B:GLN:HE22	2:33:B:GLN:HB3	20	0.23
(1,2265)	2:26:B:ASP:HB3	2:26:B:ASP:H	5	0.23
(1,2228)	2:35:B:PHE:H	2:34:B:TYR:HB3	15	0.23
(1,2228)	2:35:B:PHE:H	2:34:B:TYR:HB3	19	0.23
(1,2202)	1:125:A:VAL:H	1:122:A:LYS:HD3	3	0.23
(1,2202)	1:125:A:VAL:H	1:122:A:LYS:HD3	20	0.23
(1,2197)	1:55:A:GLY:HA2	1:56:A:LYS:H	11	0.23
(1,2142)	1:109:A:LEU:HD23	1:68:A:GLU:H	25	0.23
(1,2138)	1:69:A:GLU:HG3	1:69:A:GLU:H	20	0.23
(1,2138)	1:69:A:GLU:HG3	1:69:A:GLU:H	21	0.23
(1,2138)	1:69:A:GLU:HG3	1:69:A:GLU:H	23	0.23
(1,2108)	1:77:A:GLN:H	1:78:A:THR:HG22	9	0.23
(1,2108)	1:77:A:GLN:H	1:78:A:THR:HG21	13	0.23
(1,2108)	1:77:A:GLN:H	1:78:A:THR:HG22	20	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2106)	1:76:A:MET:HB3	1:77:A:GLN:H	1	0.23
(1,2097)	1:77:A:GLN:HE21	1:77:A:GLN:HA	20	0.23
(1,2094)	1:79:A:ALA:HB1	1:78:A:THR:H	19	0.23
(1,2027)	1:92:A:GLN:HE22	1:64:A:GLU:HA	12	0.23
(1,2007)	1:100:A:LEU:HD22	1:95:A:ALA:H	5	0.23
(1,2007)	1:100:A:LEU:HD23	1:95:A:ALA:H	12	0.23
(1,2007)	1:100:A:LEU:HD21	1:95:A:ALA:H	18	0.23
(1,2005)	1:95:A:ALA:H	1:94:A:ARG:HG2	8	0.23
(1,1987)	1:99:A:PHE:H	1:99:A:PHE:HD2	2	0.23
(1,1987)	1:99:A:PHE:H	1:99:A:PHE:HD2	20	0.23
(1,1975)	1:100:A:LEU:HD11	1:100:A:LEU:H	20	0.23
(1,1971)	1:100:A:LEU:HD23	1:101:A:ALA:H	2	0.23
(1,1961)	1:102:A:SER:H	1:59:A:TYR:HD1	2	0.23
(1,1803)	1:135:A:LYS:HB3	1:135:A:LYS:H	2	0.23
(1,1803)	1:135:A:LYS:HB3	1:135:A:LYS:H	6	0.23
(1,1803)	1:135:A:LYS:HB3	1:135:A:LYS:H	7	0.23
(1,1803)	1:135:A:LYS:HB3	1:135:A:LYS:H	13	0.23
(1,1803)	1:135:A:LYS:HB3	1:135:A:LYS:H	17	0.23
(1,1803)	1:135:A:LYS:HB3	1:135:A:LYS:H	25	0.23
(1,1798)	1:136:A:ALA:H	1:135:A:LYS:HD2	2	0.23
(1,1798)	1:136:A:ALA:H	1:135:A:LYS:HD2	15	0.23
(1,1789)	1:139:A:ALA:H	1:139:A:ALA:HB2	7	0.23
(1,1781)	1:140:A:LYS:H	1:141:A:LYS:HB3	10	0.23
(1,1761)	2:25:B:GLU:HA	2:25:B:GLU:HB2	3	0.23
(1,1761)	2:25:B:GLU:HA	2:25:B:GLU:HB2	16	0.23
(1,1751)	2:27:B:SER:HA	2:28:B:ASP:H	17	0.23
(1,1751)	2:27:B:SER:HA	2:28:B:ASP:H	18	0.23
(1,1747)	2:26:B:ASP:HB3	2:27:B:SER:HA	12	0.23
(1,1741)	2:29:B:SER:HA	2:30:B:GLU:H	11	0.23
(1,1741)	2:29:B:SER:HA	2:30:B:GLU:H	23	0.23
(1,1741)	2:29:B:SER:HA	2:30:B:GLU:H	25	0.23
(1,1713)	2:31:B:LEU:HG	2:31:B:LEU:H	14	0.23
(1,1713)	2:31:B:LEU:HG	2:31:B:LEU:H	22	0.23
(1,1703)	2:33:B:GLN:HG2	2:31:B:LEU:HD23	22	0.23
(1,1703)	2:33:B:GLN:HG2	2:31:B:LEU:HD23	25	0.23
(1,1670)	2:37:B:ALA:HB2	2:36:B:THR:HA	16	0.23
(1,1670)	2:37:B:ALA:HB2	2:36:B:THR:HA	20	0.23
(1,1667)	2:36:B:THR:HB	2:36:B:THR:H	1	0.23
(1,1667)	2:36:B:THR:HB	2:36:B:THR:H	4	0.23
(1,1664)	2:36:B:THR:HG23	2:36:B:THR:HB	4	0.23
(1,1664)	2:36:B:THR:HG21	2:36:B:THR:HB	20	0.23
(1,1664)	2:36:B:THR:HG21	2:36:B:THR:HB	24	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1648)	2:38:B:ARG:HA	2:37:B:ALA:HB1	14	0.23
(1,1636)	2:35:B:PHE:HB3	2:34:B:TYR:HE1	12	0.23
(1,1634)	2:38:B:ARG:HD2	2:37:B:ALA:HB2	5	0.23
(1,1615)	2:39:B:TRP:HE3	2:36:B:THR:HG22	5	0.23
(1,1595)	2:31:B:LEU:HD13	1:127:A:ILE:HB	1	0.23
(1,1595)	2:31:B:LEU:HD13	1:127:A:ILE:HB	11	0.23
(1,1595)	2:31:B:LEU:HD12	1:127:A:ILE:HB	13	0.23
(1,1595)	2:31:B:LEU:HD11	1:127:A:ILE:HB	15	0.23
(1,1595)	2:31:B:LEU:HD13	1:127:A:ILE:HB	21	0.23
(1,1592)	1:84:A:VAL:HG23	2:35:B:PHE:HB2	4	0.23
(1,1592)	1:84:A:VAL:HG23	2:35:B:PHE:HB2	15	0.23
(1,1592)	1:84:A:VAL:HG22	2:35:B:PHE:HB2	21	0.23
(1,1570)	1:57:A:LYS:HE2	1:59:A:TYR:HE1	18	0.23
(1,1562)	1:57:A:LYS:HD2	1:57:A:LYS:HG2	14	0.23
(1,1553)	1:59:A:TYR:HD1	1:57:A:LYS:HB2	9	0.23
(1,1536)	1:59:A:TYR:HD1	1:59:A:TYR:HA	16	0.23
(1,1495)	1:64:A:GLU:HA	1:67:A:PHE:HB2	12	0.23
(1,1477)	1:66:A:LEU:HD22	1:113:A:LEU:HB3	16	0.23
(1,1454)	1:68:A:GLU:HG2	1:69:A:GLU:H	9	0.23
(1,1453)	1:68:A:GLU:HG3	1:69:A:GLU:H	23	0.23
(1,1450)	1:85:A:VAL:HB	1:86:A:PRO:HD3	22	0.23
(1,1370)	1:75:A:LYS:HE3	1:72:A:GLU:HB3	13	0.23
(1,1345)	1:76:A:MET:HG2	1:77:A:GLN:H	10	0.23
(1,1316)	1:79:A:ALA:HB2	1:79:A:ALA:H	1	0.23
(1,1316)	1:79:A:ALA:HB1	1:79:A:ALA:H	20	0.23
(1,1316)	1:79:A:ALA:HB2	1:79:A:ALA:H	25	0.23
(1,1283)	1:84:A:VAL:HG23	1:127:A:ILE:HD13	12	0.23
(1,1279)	1:84:A:VAL:HG23	1:81:A:HIS:HB3	2	0.23
(1,1279)	1:84:A:VAL:HG23	1:81:A:HIS:HB3	17	0.23
(1,1228)	1:87:A:PHE:HD1	1:88:A:LEU:HD21	4	0.23
(1,1228)	1:87:A:PHE:HD1	1:88:A:LEU:HD23	17	0.23
(1,1197)	1:89:A:TYR:HD2	1:71:A:LEU:HD21	16	0.23
(1,1183)	1:90:A:ASN:HB2	1:87:A:PHE:HD1	1	0.23
(1,1171)	1:91:A:ARG:HG2	1:91:A:ARG:HA	8	0.23
(1,1142)	1:94:A:ARG:HD2	1:94:A:ARG:HB2	20	0.23
(1,1126)	1:96:A:HIS:HD2	1:139:A:ALA:HB1	6	0.23
(1,1122)	1:96:A:HIS:HA	1:139:A:ALA:HB2	17	0.23
(1,1122)	1:96:A:HIS:HA	1:139:A:ALA:HB1	22	0.23
(1,1117)	1:98:A:LEU:HG	1:98:A:LEU:HD23	13	0.23
(1,1117)	1:98:A:LEU:HG	1:98:A:LEU:HD22	17	0.23
(1,1117)	1:98:A:LEU:HG	1:98:A:LEU:HD21	20	0.23
(1,1117)	1:98:A:LEU:HG	1:98:A:LEU:HD22	25	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1098)	1:100:A:LEU:HD23	1:92:A:GLN:HA	9	0.23
(1,1098)	1:100:A:LEU:HD21	1:92:A:GLN:HA	15	0.23
(1,1097)	1:100:A:LEU:HD21	1:100:A:LEU:HD11	11	0.23
(1,1097)	1:100:A:LEU:HD21	1:100:A:LEU:HD13	20	0.23
(1,1091)	1:100:A:LEU:HD23	1:92:A:GLN:HE21	14	0.23
(1,1091)	1:100:A:LEU:HD23	1:92:A:GLN:HE21	18	0.23
(1,1088)	1:100:A:LEU:HD23	1:105:A:PHE:HD2	5	0.23
(1,1074)	1:101:A:ALA:HB3	1:60:A:LYS:HA	5	0.23
(1,1074)	1:101:A:ALA:HB2	1:60:A:LYS:HA	17	0.23
(1,1072)	1:101:A:ALA:HB2	1:58:A:CYS:HA	21	0.23
(1,1066)	1:101:A:ALA:HA	1:60:A:LYS:HB2	23	0.23
(1,1044)	1:62:A:GLU:HB3	1:62:A:GLU:HG3	15	0.23
(1,1036)	1:62:A:GLU:HB3	1:62:A:GLU:H	5	0.23
(1,1036)	1:62:A:GLU:HB3	1:62:A:GLU:H	6	0.23
(1,1036)	1:62:A:GLU:HB3	1:62:A:GLU:H	18	0.23
(1,1036)	1:62:A:GLU:HB3	1:62:A:GLU:H	19	0.23
(1,1036)	1:62:A:GLU:HB3	1:62:A:GLU:H	21	0.23
(1,1002)	1:108:A:ILE:HD13	1:104:A:GLU:HG2	24	0.23
(1,998)	1:108:A:ILE:HD12	1:105:A:PHE:HD1	2	0.23
(1,998)	1:108:A:ILE:HD11	1:105:A:PHE:HD1	11	0.23
(1,998)	1:108:A:ILE:HD11	1:105:A:PHE:HD1	16	0.23
(1,998)	1:108:A:ILE:HD11	1:105:A:PHE:HD1	17	0.23
(1,998)	1:108:A:ILE:HD13	1:105:A:PHE:HD1	19	0.23
(1,960)	1:67:A:PHE:HA	1:109:A:LEU:HD11	4	0.23
(1,960)	1:67:A:PHE:HA	1:109:A:LEU:HD11	16	0.23
(1,934)	1:112:A:VAL:HG12	1:126:A:TYR:HB3	5	0.23
(1,922)	1:112:A:VAL:HA	1:115:A:ARG:HG2	15	0.23
(1,913)	1:113:A:LEU:HG	1:113:A:LEU:H	10	0.23
(1,913)	1:113:A:LEU:HG	1:113:A:LEU:H	14	0.23
(1,913)	1:113:A:LEU:HG	1:113:A:LEU:H	16	0.23
(1,909)	1:114:A:SER:HB2	1:113:A:LEU:HG	3	0.23
(1,909)	1:114:A:SER:HB2	1:113:A:LEU:HG	6	0.23
(1,909)	1:114:A:SER:HB2	1:113:A:LEU:HG	22	0.23
(1,878)	1:117:A:ARG:HG2	1:114:A:SER:HA	19	0.23
(1,867)	1:119:A:ARG:HD3	1:119:A:ARG:HA	7	0.23
(1,814)	1:123:A:LEU:HD23	1:120:A:PRO:HA	11	0.23
(1,775)	1:126:A:TYR:HE1	1:125:A:VAL:HG13	4	0.23
(1,775)	1:126:A:TYR:HE1	1:125:A:VAL:HG12	12	0.23
(1,773)	1:125:A:VAL:HA	1:125:A:VAL:HG11	13	0.23
(1,746)	1:127:A:ILE:HD13	1:127:A:ILE:H	10	0.23
(1,719)	1:129:A:GLU:HB2	1:126:A:TYR:HA	13	0.23
(1,708)	1:130:A:LEU:HD23	1:70:A:PHE:HD2	3	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,704)	1:130:A:LEU:HD12	1:109:A:LEU:HD23	13	0.23
(1,673)	1:133:A:VAL:HG21	1:130:A:LEU:HA	3	0.23
(1,672)	1:133:A:VAL:HG22	1:137:A:HIS:HD2	12	0.23
(1,666)	1:134:A:LEU:HD21	1:133:A:VAL:HG13	6	0.23
(1,664)	1:133:A:VAL:HG13	1:130:A:LEU:HA	9	0.23
(1,664)	1:133:A:VAL:HG12	1:130:A:LEU:HA	11	0.23
(1,664)	1:133:A:VAL:HG12	1:130:A:LEU:HA	14	0.23
(1,662)	1:133:A:VAL:HA	1:133:A:VAL:HG12	6	0.23
(1,634)	1:134:A:LEU:HD12	1:134:A:LEU:H	1	0.23
(1,634)	1:134:A:LEU:HD12	1:134:A:LEU:H	15	0.23
(1,634)	1:134:A:LEU:HD12	1:134:A:LEU:H	22	0.23
(1,618)	1:56:A:LYS:HG2	1:57:A:LYS:H	15	0.23
(1,593)	1:138:A:SER:HA	1:138:A:SER:HB2	8	0.23
(1,589)	2:27:B:SER:HA	1:132:A:THR:HG21	19	0.23
(1,586)	1:139:A:ALA:HA	1:139:A:ALA:HB2	5	0.23
(1,569)	1:143:A:LEU:HB2	1:144:A:ASN:H	13	0.23
(1,559)	2:31:B:LEU:H	2:30:B:GLU:HB3	22	0.23
(1,551)	2:34:B:TYR:H	2:35:B:PHE:HA	1	0.23
(1,551)	2:34:B:TYR:H	2:35:B:PHE:HA	3	0.23
(1,551)	2:34:B:TYR:H	2:35:B:PHE:HA	9	0.23
(1,551)	2:34:B:TYR:H	2:35:B:PHE:HA	15	0.23
(1,526)	1:69:A:GLU:H	1:113:A:LEU:HD23	19	0.23
(1,521)	1:71:A:LEU:H	1:113:A:LEU:HD11	25	0.23
(1,515)	1:73:A:LEU:HG	1:76:A:MET:H	9	0.23
(1,505)	1:79:A:ALA:H	1:76:A:MET:HA	3	0.23
(1,500)	1:85:A:VAL:H	1:83:A:GLU:H	4	0.23
(1,500)	1:85:A:VAL:H	1:83:A:GLU:H	25	0.23
(1,492)	1:91:A:ARG:H	1:88:A:LEU:HD22	14	0.23
(1,492)	1:91:A:ARG:H	1:88:A:LEU:HD22	18	0.23
(1,490)	1:91:A:ARG:H	1:94:A:ARG:H	25	0.23
(1,453)	1:114:A:SER:H	1:113:A:LEU:HD22	11	0.23
(1,438)	1:66:A:LEU:HD13	1:66:A:LEU:H	5	0.23
(1,438)	1:66:A:LEU:HD13	1:66:A:LEU:H	14	0.23
(1,414)	1:72:A:GLU:H	1:69:A:GLU:HA	12	0.23
(1,394)	1:137:A:HIS:HB3	1:138:A:SER:H	1	0.23
(1,367)	2:26:B:ASP:HB3	2:31:B:LEU:H	18	0.23
(1,361)	2:29:B:SER:HB2	2:32:B:GLU:HG3	3	0.23
(1,361)	2:29:B:SER:HB2	2:32:B:GLU:HG3	14	0.23
(1,361)	2:29:B:SER:HB2	2:32:B:GLU:HG3	24	0.23
(1,360)	2:27:B:SER:HB3	2:26:B:ASP:HB3	20	0.23
(1,342)	2:31:B:LEU:HD11	1:124:A:TYR:HB3	15	0.23
(1,342)	2:31:B:LEU:HD12	1:124:A:TYR:HB3	22	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,337)	2:31:B:LEU:HD23	2:28:B:ASP:HB2	16	0.23
(1,321)	2:34:B:TYR:HD1	1:83:A:GLU:HB3	11	0.23
(1,293)	2:39:B:TRP:HD1	2:38:B:ARG:HB3	11	0.23
(1,264)	1:127:A:ILE:HG23	2:35:B:PHE:HE1	22	0.23
(1,258)	1:113:A:LEU:HD12	1:113:A:LEU:HG	13	0.23
(1,258)	1:113:A:LEU:HD11	1:113:A:LEU:HG	23	0.23
(1,257)	1:113:A:LEU:HD12	1:113:A:LEU:HB2	4	0.23
(1,257)	1:113:A:LEU:HD13	1:113:A:LEU:HB2	5	0.23
(1,257)	1:113:A:LEU:HD11	1:113:A:LEU:HB2	11	0.23
(1,257)	1:113:A:LEU:HD11	1:113:A:LEU:HB2	19	0.23
(1,257)	1:113:A:LEU:HD11	1:113:A:LEU:HB2	25	0.23
(1,254)	1:57:A:LYS:HE2	1:54:A:MET:HG3	2	0.23
(1,240)	1:104:A:GLU:HB3	1:105:A:PHE:HA	17	0.23
(1,229)	1:105:A:PHE:HE2	1:67:A:PHE:HB2	8	0.23
(1,229)	1:105:A:PHE:HE2	1:67:A:PHE:HB2	19	0.23
(1,229)	1:105:A:PHE:HE2	1:67:A:PHE:HB2	24	0.23
(1,225)	1:129:A:GLU:HG2	1:125:A:VAL:HG13	4	0.23
(1,212)	1:71:A:LEU:HD23	1:74:A:CYS:HG	16	0.23
(1,160)	1:67:A:PHE:HD1	1:68:A:GLU:H	4	0.23
(1,145)	1:88:A:LEU:HB3	1:85:A:VAL:HA	4	0.23
(1,145)	1:88:A:LEU:HB3	1:85:A:VAL:HA	5	0.23
(1,145)	1:88:A:LEU:HB3	1:85:A:VAL:HA	11	0.23
(1,145)	1:88:A:LEU:HB3	1:85:A:VAL:HA	22	0.23
(1,140)	1:99:A:PHE:HB3	1:138:A:SER:H	7	0.23
(1,140)	1:99:A:PHE:HB3	1:138:A:SER:H	18	0.23
(1,123)	1:95:A:ALA:HB1	1:134:A:LEU:HB2	8	0.23
(1,116)	1:100:A:LEU:HD21	1:105:A:PHE:HE2	4	0.23
(1,116)	1:100:A:LEU:HD21	1:105:A:PHE:HE2	25	0.23
(1,98)	1:105:A:PHE:HD1	1:100:A:LEU:HD22	15	0.23
(1,98)	1:105:A:PHE:HD1	1:100:A:LEU:HD22	23	0.23
(1,97)	1:105:A:PHE:HD1	1:100:A:LEU:HA	8	0.23
(1,97)	1:105:A:PHE:HD1	1:100:A:LEU:HA	22	0.23
(1,95)	1:107:A:ASN:HB2	1:108:A:ILE:HB	1	0.23
(1,95)	1:107:A:ASN:HB2	1:108:A:ILE:HB	3	0.23
(1,92)	1:109:A:LEU:HD21	1:67:A:PHE:H	1	0.23
(1,92)	1:109:A:LEU:HD23	1:67:A:PHE:H	25	0.23
(1,87)	1:112:A:VAL:HG13	1:130:A:LEU:H	16	0.23
(1,84)	1:113:A:LEU:HA	1:113:A:LEU:HG	1	0.23
(1,84)	1:113:A:LEU:HA	1:113:A:LEU:HG	13	0.23
(1,84)	1:113:A:LEU:HA	1:113:A:LEU:HG	24	0.23
(1,62)	1:123:A:LEU:HD21	1:70:A:PHE:HE1	7	0.23
(1,56)	1:124:A:TYR:HE2	2:35:B:PHE:HB3	25	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,36)	1:127:A:ILE:HG22	1:124:A:TYR:HD2	8	0.23
(1,27)	1:130:A:LEU:HD23	1:67:A:PHE:HA	18	0.23
(1,25)	1:85:A:VAL:HG23	1:74:A:CYS:HB2	15	0.23
(1,25)	1:85:A:VAL:HG22	1:74:A:CYS:HB2	19	0.23
(1,14)	1:133:A:VAL:HG23	1:132:A:THR:H	10	0.23
(1,14)	1:133:A:VAL:HG21	1:132:A:THR:H	21	0.23
(1,8)	1:134:A:LEU:HD23	1:67:A:PHE:HZ	21	0.23
(1,1)	1:141:A:LYS:HG3	1:141:A:LYS:HA	19	0.23
(1,2287)	2:33:B:GLN:HE22	2:33:B:GLN:HB3	11	0.22
(1,2287)	2:33:B:GLN:HE22	2:33:B:GLN:HB3	17	0.22
(1,2273)	2:25:B:GLU:HB3	2:25:B:GLU:H	3	0.22
(1,2273)	2:25:B:GLU:HB3	2:25:B:GLU:H	16	0.22
(1,2273)	2:25:B:GLU:HB3	2:25:B:GLU:H	24	0.22
(1,2265)	2:26:B:ASP:HB3	2:26:B:ASP:H	23	0.22
(1,2228)	2:35:B:PHE:H	2:34:B:TYR:HB3	1	0.22
(1,2228)	2:35:B:PHE:H	2:34:B:TYR:HB3	4	0.22
(1,2228)	2:35:B:PHE:H	2:34:B:TYR:HB3	14	0.22
(1,2228)	2:35:B:PHE:H	2:34:B:TYR:HB3	20	0.22
(1,2228)	2:35:B:PHE:H	2:34:B:TYR:HB3	23	0.22
(1,2202)	1:125:A:VAL:H	1:122:A:LYS:HD3	10	0.22
(1,2196)	1:56:A:LYS:H	1:56:A:LYS:HB2	16	0.22
(1,2188)	1:59:A:TYR:H	1:58:A:CYS:HB3	2	0.22
(1,2173)	1:63:A:ASN:H	1:109:A:LEU:HD13	12	0.22
(1,2173)	1:63:A:ASN:H	1:109:A:LEU:HD11	22	0.22
(1,2108)	1:77:A:GLN:H	1:78:A:THR:HG23	10	0.22
(1,2108)	1:77:A:GLN:H	1:78:A:THR:HG21	11	0.22
(1,2108)	1:77:A:GLN:H	1:78:A:THR:HG21	18	0.22
(1,2108)	1:77:A:GLN:H	1:78:A:THR:HG21	21	0.22
(1,2107)	1:77:A:GLN:H	1:77:A:GLN:HB3	2	0.22
(1,2051)	1:89:A:TYR:H	1:90:A:ASN:HB3	7	0.22
(1,2032)	1:90:A:ASN:HD22	1:93:A:GLN:HB2	9	0.22
(1,2007)	1:100:A:LEU:HD22	1:95:A:ALA:H	20	0.22
(1,2005)	1:95:A:ALA:H	1:94:A:ARG:HG2	3	0.22
(1,1961)	1:102:A:SER:H	1:59:A:TYR:HD1	6	0.22
(1,1919)	1:109:A:LEU:HB3	1:109:A:LEU:H	9	0.22
(1,1919)	1:109:A:LEU:HB3	1:109:A:LEU:H	16	0.22
(1,1919)	1:109:A:LEU:HB3	1:109:A:LEU:H	24	0.22
(1,1886)	1:88:A:LEU:H	1:87:A:PHE:HD2	13	0.22
(1,1837)	1:127:A:ILE:H	1:123:A:LEU:HD13	17	0.22
(1,1803)	1:135:A:LYS:HB3	1:135:A:LYS:H	4	0.22
(1,1803)	1:135:A:LYS:HB3	1:135:A:LYS:H	9	0.22
(1,1803)	1:135:A:LYS:HB3	1:135:A:LYS:H	14	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1801)	1:135:A:LYS:H	1:91:A:ARG:HD3	10	0.22
(1,1801)	1:135:A:LYS:H	1:91:A:ARG:HD3	24	0.22
(1,1789)	1:139:A:ALA:H	1:139:A:ALA:HB2	2	0.22
(1,1789)	1:139:A:ALA:H	1:139:A:ALA:HB1	10	0.22
(1,1789)	1:139:A:ALA:H	1:139:A:ALA:HB2	25	0.22
(1,1788)	1:139:A:ALA:H	1:135:A:LYS:HD3	16	0.22
(1,1788)	1:139:A:ALA:H	1:135:A:LYS:HD3	20	0.22
(1,1770)	1:141:A:LYS:HB3	1:141:A:LYS:H	24	0.22
(1,1761)	2:25:B:GLU:HA	2:25:B:GLU:HB2	22	0.22
(1,1759)	2:30:B:GLU:HA	2:30:B:GLU:HG3	12	0.22
(1,1759)	2:30:B:GLU:HA	2:30:B:GLU:HG3	18	0.22
(1,1751)	2:27:B:SER:HA	2:28:B:ASP:H	19	0.22
(1,1745)	2:29:B:SER:HB3	2:30:B:GLU:H	23	0.22
(1,1741)	2:29:B:SER:HA	2:30:B:GLU:H	21	0.22
(1,1725)	2:31:B:LEU:HD23	1:127:A:ILE:HG22	3	0.22
(1,1723)	2:31:B:LEU:HD22	2:30:B:GLU:HB2	6	0.22
(1,1723)	2:31:B:LEU:HD21	2:30:B:GLU:HB2	21	0.22
(1,1703)	2:33:B:GLN:HG2	2:31:B:LEU:HD21	4	0.22
(1,1703)	2:33:B:GLN:HG2	2:31:B:LEU:HD21	7	0.22
(1,1667)	2:36:B:THR:HB	2:36:B:THR:H	5	0.22
(1,1667)	2:36:B:THR:HB	2:36:B:THR:H	15	0.22
(1,1666)	2:36:B:THR:HG23	1:124:A:TYR:H	9	0.22
(1,1648)	2:38:B:ARG:HA	2:37:B:ALA:HB1	10	0.22
(1,1636)	2:35:B:PHE:HB3	2:34:B:TYR:HE1	2	0.22
(1,1633)	2:38:B:ARG:HD2	2:38:B:ARG:HB2	21	0.22
(1,1619)	2:39:B:TRP:HD1	2:38:B:ARG:HB2	3	0.22
(1,1595)	2:31:B:LEU:HD13	1:127:A:ILE:HB	23	0.22
(1,1591)	1:84:A:VAL:HA	2:31:B:LEU:HD12	25	0.22
(1,1588)	1:87:A:PHE:HB2	2:31:B:LEU:HD13	10	0.22
(1,1570)	1:57:A:LYS:HE2	1:59:A:TYR:HE1	8	0.22
(1,1552)	1:57:A:LYS:HB2	1:57:A:LYS:HA	20	0.22
(1,1550)	1:141:A:LYS:HG3	1:141:A:LYS:HA	21	0.22
(1,1457)	1:68:A:GLU:HB2	1:68:A:GLU:HG2	2	0.22
(1,1457)	1:68:A:GLU:HB2	1:68:A:GLU:HG2	4	0.22
(1,1457)	1:68:A:GLU:HB2	1:68:A:GLU:HG2	14	0.22
(1,1454)	1:68:A:GLU:HG2	1:69:A:GLU:H	2	0.22
(1,1454)	1:68:A:GLU:HG2	1:69:A:GLU:H	23	0.22
(1,1447)	1:69:A:GLU:HA	1:69:A:GLU:HG3	10	0.22
(1,1440)	1:127:A:ILE:HD13	1:70:A:PHE:HZ	1	0.22
(1,1440)	1:127:A:ILE:HD11	1:70:A:PHE:HZ	18	0.22
(1,1432)	1:70:A:PHE:HA	1:70:A:PHE:HD1	19	0.22
(1,1432)	1:70:A:PHE:HA	1:70:A:PHE:HD1	21	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1391)	1:74:A:CYS:HA	1:73:A:LEU:HD21	2	0.22
(1,1370)	1:75:A:LYS:HE3	1:72:A:GLU:HB3	10	0.22
(1,1356)	1:75:A:LYS:HA	1:75:A:LYS:HG2	6	0.22
(1,1356)	1:75:A:LYS:HA	1:75:A:LYS:HG2	8	0.22
(1,1356)	1:75:A:LYS:HA	1:75:A:LYS:HG2	20	0.22
(1,1345)	1:76:A:MET:HG2	1:77:A:GLN:H	16	0.22
(1,1316)	1:79:A:ALA:HB3	1:79:A:ALA:H	22	0.22
(1,1315)	1:79:A:ALA:HB2	1:80:A:ASP:H	3	0.22
(1,1279)	1:84:A:VAL:HG21	1:81:A:HIS:HB3	21	0.22
(1,1228)	1:87:A:PHE:HD1	1:88:A:LEU:HD23	3	0.22
(1,1228)	1:87:A:PHE:HD1	1:88:A:LEU:HD22	18	0.22
(1,1197)	1:89:A:TYR:HD2	1:71:A:LEU:HD23	20	0.22
(1,1197)	1:89:A:TYR:HD2	1:71:A:LEU:HD23	22	0.22
(1,1183)	1:90:A:ASN:HB2	1:87:A:PHE:HD1	6	0.22
(1,1175)	1:91:A:ARG:HG2	1:134:A:LEU:HB2	9	0.22
(1,1168)	1:100:A:LEU:HD21	1:92:A:GLN:HG2	20	0.22
(1,1142)	1:94:A:ARG:HD3	1:94:A:ARG:HB2	13	0.22
(1,1139)	1:134:A:LEU:HD21	1:95:A:ALA:HB2	15	0.22
(1,1133)	1:95:A:ALA:HB2	1:99:A:PHE:HD2	7	0.22
(1,1126)	1:96:A:HIS:HD2	1:139:A:ALA:HB2	2	0.22
(1,1117)	1:98:A:LEU:HG	1:98:A:LEU:HD22	5	0.22
(1,1117)	1:98:A:LEU:HG	1:98:A:LEU:HD22	9	0.22
(1,1117)	1:98:A:LEU:HG	1:98:A:LEU:HD22	12	0.22
(1,1117)	1:98:A:LEU:HG	1:98:A:LEU:HD22	16	0.22
(1,1117)	1:98:A:LEU:HG	1:98:A:LEU:HD21	18	0.22
(1,1117)	1:98:A:LEU:HG	1:98:A:LEU:HD22	21	0.22
(1,1117)	1:98:A:LEU:HG	1:98:A:LEU:HD21	22	0.22
(1,1098)	1:100:A:LEU:HD22	1:92:A:GLN:HA	20	0.22
(1,1097)	1:100:A:LEU:HD23	1:100:A:LEU:HD11	12	0.22
(1,1097)	1:100:A:LEU:HD23	1:100:A:LEU:HD11	18	0.22
(1,1097)	1:100:A:LEU:HD21	1:100:A:LEU:HD11	23	0.22
(1,1091)	1:100:A:LEU:HD21	1:92:A:GLN:HE21	3	0.22
(1,1091)	1:100:A:LEU:HD21	1:92:A:GLN:HE21	5	0.22
(1,1091)	1:100:A:LEU:HD23	1:92:A:GLN:HE21	13	0.22
(1,1074)	1:101:A:ALA:HB3	1:60:A:LYS:HA	10	0.22
(1,1070)	1:101:A:ALA:HB3	1:102:A:SER:H	6	0.22
(1,1070)	1:101:A:ALA:HB1	1:102:A:SER:H	18	0.22
(1,1040)	1:62:A:GLU:HB3	1:59:A:TYR:HA	1	0.22
(1,1040)	1:62:A:GLU:HB3	1:59:A:TYR:HA	13	0.22
(1,1036)	1:62:A:GLU:HB3	1:62:A:GLU:H	2	0.22
(1,1036)	1:62:A:GLU:HB3	1:62:A:GLU:H	4	0.22
(1,1036)	1:62:A:GLU:HB3	1:62:A:GLU:H	7	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1036)	1:62:A:GLU:HB3	1:62:A:GLU:H	9	0.22
(1,1036)	1:62:A:GLU:HB3	1:62:A:GLU:H	12	0.22
(1,1036)	1:62:A:GLU:HB3	1:62:A:GLU:H	25	0.22
(1,1000)	1:108:A:ILE:HD12	1:99:A:PHE:HE1	3	0.22
(1,1000)	1:108:A:ILE:HD11	1:99:A:PHE:HE1	11	0.22
(1,998)	1:108:A:ILE:HD11	1:105:A:PHE:HD1	1	0.22
(1,998)	1:108:A:ILE:HD12	1:105:A:PHE:HD1	7	0.22
(1,998)	1:108:A:ILE:HD13	1:105:A:PHE:HD1	9	0.22
(1,998)	1:108:A:ILE:HD11	1:105:A:PHE:HD1	15	0.22
(1,998)	1:108:A:ILE:HD12	1:105:A:PHE:HD1	20	0.22
(1,991)	1:108:A:ILE:HA	1:108:A:ILE:HG21	6	0.22
(1,960)	1:67:A:PHE:HA	1:109:A:LEU:HD13	7	0.22
(1,915)	1:113:A:LEU:HD22	1:69:A:GLU:HB3	15	0.22
(1,913)	1:113:A:LEU:HG	1:113:A:LEU:H	3	0.22
(1,913)	1:113:A:LEU:HG	1:113:A:LEU:H	15	0.22
(1,913)	1:113:A:LEU:HG	1:113:A:LEU:H	17	0.22
(1,913)	1:113:A:LEU:HG	1:113:A:LEU:H	21	0.22
(1,913)	1:113:A:LEU:HG	1:113:A:LEU:H	22	0.22
(1,911)	1:113:A:LEU:HB2	1:113:A:LEU:H	1	0.22
(1,868)	1:119:A:ARG:HD2	1:119:A:ARG:HB2	25	0.22
(1,858)	1:119:A:ARG:HG3	1:119:A:ARG:HA	9	0.22
(1,821)	1:122:A:LYS:HG3	1:122:A:LYS:H	11	0.22
(1,775)	1:126:A:TYR:HE1	1:125:A:VAL:HG11	3	0.22
(1,775)	1:126:A:TYR:HE1	1:125:A:VAL:HG11	11	0.22
(1,757)	1:126:A:TYR:HD1	1:126:A:TYR:HB2	3	0.22
(1,757)	1:126:A:TYR:HD1	1:126:A:TYR:HB2	6	0.22
(1,757)	1:126:A:TYR:HD1	1:126:A:TYR:HB2	10	0.22
(1,757)	1:126:A:TYR:HD1	1:126:A:TYR:HB2	13	0.22
(1,757)	1:126:A:TYR:HD1	1:126:A:TYR:HB2	16	0.22
(1,757)	1:126:A:TYR:HD1	1:126:A:TYR:HB2	20	0.22
(1,757)	1:126:A:TYR:HD1	1:126:A:TYR:HB2	21	0.22
(1,757)	1:126:A:TYR:HD1	1:126:A:TYR:HB2	23	0.22
(1,664)	1:133:A:VAL:HG11	1:130:A:LEU:HA	2	0.22
(1,664)	1:133:A:VAL:HG12	1:130:A:LEU:HA	16	0.22
(1,664)	1:133:A:VAL:HG13	1:130:A:LEU:HA	20	0.22
(1,664)	1:133:A:VAL:HG11	1:130:A:LEU:HA	21	0.22
(1,634)	1:134:A:LEU:HD12	1:134:A:LEU:H	5	0.22
(1,634)	1:134:A:LEU:HD12	1:134:A:LEU:H	16	0.22
(1,634)	1:134:A:LEU:HD11	1:134:A:LEU:H	17	0.22
(1,634)	1:134:A:LEU:HD11	1:134:A:LEU:H	19	0.22
(1,634)	1:134:A:LEU:HD13	1:134:A:LEU:H	20	0.22
(1,634)	1:134:A:LEU:HD13	1:134:A:LEU:H	21	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,593)	1:138:A:SER:HA	1:138:A:SER:HB2	10	0.22
(1,589)	2:27:B:SER:HA	1:132:A:THR:HG21	17	0.22
(1,559)	2:31:B:LEU:H	2:30:B:GLU:HB3	19	0.22
(1,551)	2:34:B:TYR:H	2:35:B:PHE:HA	4	0.22
(1,551)	2:34:B:TYR:H	2:35:B:PHE:HA	16	0.22
(1,551)	2:34:B:TYR:H	2:35:B:PHE:HA	24	0.22
(1,522)	1:70:A:PHE:H	1:73:A:LEU:H	5	0.22
(1,522)	1:70:A:PHE:H	1:73:A:LEU:H	14	0.22
(1,522)	1:70:A:PHE:H	1:73:A:LEU:H	19	0.22
(1,522)	1:70:A:PHE:H	1:73:A:LEU:H	21	0.22
(1,505)	1:79:A:ALA:H	1:76:A:MET:HA	15	0.22
(1,490)	1:91:A:ARG:H	1:94:A:ARG:H	24	0.22
(1,488)	1:92:A:GLN:HE22	1:64:A:GLU:HG3	4	0.22
(1,453)	1:114:A:SER:H	1:113:A:LEU:HD21	14	0.22
(1,445)	1:116:A:ALA:H	1:112:A:VAL:HA	5	0.22
(1,438)	1:66:A:LEU:HD13	1:66:A:LEU:H	13	0.22
(1,438)	1:66:A:LEU:HD13	1:66:A:LEU:H	15	0.22
(1,421)	1:128:A:ASN:H	1:70:A:PHE:HZ	21	0.22
(1,394)	1:137:A:HIS:HB3	1:138:A:SER:H	2	0.22
(1,394)	1:137:A:HIS:HB3	1:138:A:SER:H	3	0.22
(1,394)	1:137:A:HIS:HB3	1:138:A:SER:H	12	0.22
(1,394)	1:137:A:HIS:HB3	1:138:A:SER:H	16	0.22
(1,392)	1:139:A:ALA:H	1:138:A:SER:H	5	0.22
(1,389)	1:143:A:LEU:H	1:142:A:LYS:HB2	24	0.22
(1,369)	2:26:B:ASP:HB2	1:87:A:PHE:HZ	23	0.22
(1,367)	2:26:B:ASP:HB3	2:31:B:LEU:H	12	0.22
(1,364)	2:29:B:SER:HB3	2:32:B:GLU:HB2	7	0.22
(1,356)	2:29:B:SER:HB2	2:33:B:GLN:H	7	0.22
(1,343)	2:31:B:LEU:HB2	1:87:A:PHE:HE2	20	0.22
(1,342)	2:31:B:LEU:HD13	1:124:A:TYR:HB3	11	0.22
(1,275)	1:84:A:VAL:HG12	2:35:B:PHE:HE1	14	0.22
(1,264)	1:127:A:ILE:HG22	2:35:B:PHE:HE1	18	0.22
(1,264)	1:127:A:ILE:HG23	2:35:B:PHE:HE1	21	0.22
(1,258)	1:113:A:LEU:HD12	1:113:A:LEU:HG	22	0.22
(1,257)	1:113:A:LEU:HD11	1:113:A:LEU:HB2	13	0.22
(1,249)	1:56:A:LYS:HA	1:57:A:LYS:H	21	0.22
(1,244)	1:111:A:ARG:HA	1:115:A:ARG:HG2	20	0.22
(1,236)	1:64:A:GLU:HA	1:67:A:PHE:H	18	0.22
(1,236)	1:64:A:GLU:HA	1:67:A:PHE:H	21	0.22
(1,229)	1:105:A:PHE:HE2	1:67:A:PHE:HB2	20	0.22
(1,229)	1:105:A:PHE:HE2	1:67:A:PHE:HB2	22	0.22
(1,225)	1:129:A:GLU:HG2	1:125:A:VAL:HG11	5	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,206)	1:73:A:LEU:HD21	1:117:A:ARG:HD3	1	0.22
(1,163)	1:67:A:PHE:HD2	1:92:A:GLN:HG3	16	0.22
(1,160)	1:67:A:PHE:HD1	1:68:A:GLU:H	6	0.22
(1,147)	1:137:A:HIS:HB3	1:138:A:SER:H	13	0.22
(1,145)	1:88:A:LEU:HB3	1:85:A:VAL:HA	2	0.22
(1,145)	1:88:A:LEU:HB3	1:85:A:VAL:HA	9	0.22
(1,140)	1:99:A:PHE:HB3	1:138:A:SER:H	21	0.22
(1,122)	1:95:A:ALA:HB3	1:91:A:ARG:HD3	2	0.22
(1,122)	1:95:A:ALA:HB1	1:91:A:ARG:HD3	20	0.22
(1,84)	1:113:A:LEU:HA	1:113:A:LEU:HG	20	0.22
(1,81)	1:116:A:ALA:HB3	1:70:A:PHE:HZ	23	0.22
(1,76)	1:118:A:SER:HA	1:118:A:SER:HB2	15	0.22
(1,62)	1:123:A:LEU:HD23	1:70:A:PHE:HE1	17	0.22
(1,58)	1:123:A:LEU:HA	1:123:A:LEU:HB3	18	0.22
(1,58)	1:123:A:LEU:HA	1:123:A:LEU:HB3	23	0.22
(1,42)	1:126:A:TYR:HD1	1:125:A:VAL:HB	16	0.22
(1,36)	1:127:A:ILE:HG23	1:124:A:TYR:HD1	10	0.22
(1,36)	1:127:A:ILE:HG23	1:124:A:TYR:HD1	13	0.22
(1,27)	1:130:A:LEU:HD21	1:67:A:PHE:HA	6	0.22
(1,27)	1:130:A:LEU:HD21	1:67:A:PHE:HA	21	0.22
(1,25)	1:85:A:VAL:HG21	1:74:A:CYS:HB2	4	0.22
(1,25)	1:85:A:VAL:HG23	1:74:A:CYS:HB2	10	0.22
(1,17)	1:133:A:VAL:HG13	1:137:A:HIS:HB2	8	0.22
(1,14)	1:133:A:VAL:HG21	1:132:A:THR:H	17	0.22
(1,2248)	2:30:B:GLU:HB2	2:31:B:LEU:H	7	0.21
(1,2248)	2:30:B:GLU:HB2	2:31:B:LEU:H	11	0.21
(1,2244)	2:36:B:THR:HG22	2:36:B:THR:H	21	0.21
(1,2228)	2:35:B:PHE:H	2:34:B:TYR:HB3	8	0.21
(1,2228)	2:35:B:PHE:H	2:34:B:TYR:HB3	18	0.21
(1,2196)	1:56:A:LYS:H	1:56:A:LYS:HB2	18	0.21
(1,2196)	1:56:A:LYS:H	1:56:A:LYS:HB2	25	0.21
(1,2173)	1:63:A:ASN:H	1:109:A:LEU:HD13	3	0.21
(1,2173)	1:63:A:ASN:H	1:109:A:LEU:HD12	10	0.21
(1,2108)	1:77:A:GLN:H	1:78:A:THR:HG23	1	0.21
(1,2108)	1:77:A:GLN:H	1:78:A:THR:HG21	8	0.21
(1,2097)	1:77:A:GLN:HE21	1:77:A:GLN:HA	25	0.21
(1,2094)	1:79:A:ALA:HB1	1:78:A:THR:H	5	0.21
(1,2075)	1:81:A:HIS:H	1:81:A:HIS:HD2	3	0.21
(1,2054)	1:85:A:VAL:HG13	1:89:A:TYR:H	13	0.21
(1,2037)	1:90:A:ASN:HD21	1:94:A:ARG:HD3	9	0.21
(1,2032)	1:90:A:ASN:HD22	1:93:A:GLN:HB2	16	0.21
(1,2005)	1:95:A:ALA:H	1:94:A:ARG:HG2	10	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2004)	1:95:A:ALA:H	1:94:A:ARG:HB3	17	0.21
(1,1996)	1:97:A:SER:H	1:139:A:ALA:HB3	15	0.21
(1,1987)	1:99:A:PHE:H	1:99:A:PHE:HD2	5	0.21
(1,1975)	1:100:A:LEU:HD11	1:100:A:LEU:H	14	0.21
(1,1975)	1:100:A:LEU:HD13	1:100:A:LEU:H	16	0.21
(1,1961)	1:102:A:SER:H	1:59:A:TYR:HD1	3	0.21
(1,1961)	1:102:A:SER:H	1:59:A:TYR:HD1	21	0.21
(1,1919)	1:109:A:LEU:HB3	1:109:A:LEU:H	2	0.21
(1,1919)	1:109:A:LEU:HB3	1:109:A:LEU:H	3	0.21
(1,1919)	1:109:A:LEU:HB3	1:109:A:LEU:H	4	0.21
(1,1919)	1:109:A:LEU:HB3	1:109:A:LEU:H	6	0.21
(1,1919)	1:109:A:LEU:HB3	1:109:A:LEU:H	7	0.21
(1,1919)	1:109:A:LEU:HB3	1:109:A:LEU:H	8	0.21
(1,1919)	1:109:A:LEU:HB3	1:109:A:LEU:H	15	0.21
(1,1919)	1:109:A:LEU:HB3	1:109:A:LEU:H	22	0.21
(1,1919)	1:109:A:LEU:HB3	1:109:A:LEU:H	23	0.21
(1,1798)	1:136:A:ALA:H	1:135:A:LYS:HD2	14	0.21
(1,1781)	1:140:A:LYS:H	1:141:A:LYS:HB3	23	0.21
(1,1751)	2:27:B:SER:HA	2:28:B:ASP:H	13	0.21
(1,1751)	2:27:B:SER:HA	2:28:B:ASP:H	24	0.21
(1,1746)	1:100:A:LEU:HD11	1:138:A:SER:HB2	9	0.21
(1,1745)	2:29:B:SER:HB3	2:30:B:GLU:H	9	0.21
(1,1741)	2:29:B:SER:HA	2:30:B:GLU:H	6	0.21
(1,1741)	2:29:B:SER:HA	2:30:B:GLU:H	14	0.21
(1,1741)	2:29:B:SER:HA	2:30:B:GLU:H	15	0.21
(1,1741)	2:29:B:SER:HA	2:30:B:GLU:H	17	0.21
(1,1741)	2:29:B:SER:HA	2:30:B:GLU:H	22	0.21
(1,1718)	2:31:B:LEU:HD22	2:32:B:GLU:H	18	0.21
(1,1713)	2:31:B:LEU:HG	2:31:B:LEU:H	21	0.21
(1,1667)	2:36:B:THR:HB	2:36:B:THR:H	7	0.21
(1,1667)	2:36:B:THR:HB	2:36:B:THR:H	20	0.21
(1,1648)	2:38:B:ARG:HA	2:37:B:ALA:HB1	2	0.21
(1,1648)	2:38:B:ARG:HA	2:37:B:ALA:HB3	3	0.21
(1,1636)	2:35:B:PHE:HB3	2:34:B:TYR:HE1	3	0.21
(1,1636)	2:35:B:PHE:HB3	2:34:B:TYR:HE1	9	0.21
(1,1636)	2:35:B:PHE:HB3	2:34:B:TYR:HE1	16	0.21
(1,1635)	2:39:B:TRP:HA	2:38:B:ARG:HD2	2	0.21
(1,1635)	2:39:B:TRP:HA	2:38:B:ARG:HD2	13	0.21
(1,1622)	2:39:B:TRP:HE3	2:39:B:TRP:HB2	7	0.21
(1,1615)	2:39:B:TRP:HE3	2:36:B:THR:HG22	7	0.21
(1,1615)	2:39:B:TRP:HE3	2:36:B:THR:HG21	13	0.21
(1,1592)	1:84:A:VAL:HG21	2:35:B:PHE:HB2	8	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1588)	1:87:A:PHE:HB2	2:31:B:LEU:HD11	5	0.21
(1,1577)	1:77:A:GLN:HG3	1:73:A:LEU:HD11	17	0.21
(1,1558)	1:57:A:LYS:HB2	1:57:A:LYS:HG3	2	0.21
(1,1558)	1:57:A:LYS:HB2	1:57:A:LYS:HG3	6	0.21
(1,1558)	1:57:A:LYS:HB2	1:57:A:LYS:HG3	9	0.21
(1,1558)	1:57:A:LYS:HB2	1:57:A:LYS:HG3	15	0.21
(1,1558)	1:57:A:LYS:HB2	1:57:A:LYS:HG3	19	0.21
(1,1558)	1:57:A:LYS:HB2	1:57:A:LYS:HG3	24	0.21
(1,1554)	1:59:A:TYR:HE1	1:57:A:LYS:HB2	9	0.21
(1,1552)	1:57:A:LYS:HB2	1:57:A:LYS:HA	12	0.21
(1,1549)	1:58:A:CYS:HB2	1:57:A:LYS:HA	6	0.21
(1,1536)	1:59:A:TYR:HD1	1:59:A:TYR:HA	6	0.21
(1,1457)	1:68:A:GLU:HB2	1:68:A:GLU:HG2	23	0.21
(1,1454)	1:68:A:GLU:HG2	1:69:A:GLU:H	4	0.21
(1,1453)	1:68:A:GLU:HG3	1:69:A:GLU:H	14	0.21
(1,1440)	1:127:A:ILE:HD11	1:70:A:PHE:HZ	10	0.21
(1,1440)	1:127:A:ILE:HD11	1:70:A:PHE:HZ	21	0.21
(1,1440)	1:127:A:ILE:HD12	1:70:A:PHE:HZ	22	0.21
(1,1432)	1:70:A:PHE:HA	1:70:A:PHE:HD1	2	0.21
(1,1432)	1:70:A:PHE:HA	1:70:A:PHE:HD1	4	0.21
(1,1432)	1:70:A:PHE:HA	1:70:A:PHE:HD1	8	0.21
(1,1419)	1:71:A:LEU:HD12	1:89:A:TYR:H	1	0.21
(1,1391)	1:74:A:CYS:HA	1:73:A:LEU:HD23	1	0.21
(1,1391)	1:74:A:CYS:HA	1:73:A:LEU:HD23	10	0.21
(1,1370)	1:75:A:LYS:HE3	1:72:A:GLU:HB3	18	0.21
(1,1367)	1:75:A:LYS:HD2	1:75:A:LYS:HA	3	0.21
(1,1356)	1:75:A:LYS:HA	1:75:A:LYS:HG2	2	0.21
(1,1356)	1:75:A:LYS:HA	1:75:A:LYS:HG2	15	0.21
(1,1356)	1:75:A:LYS:HA	1:75:A:LYS:HG2	23	0.21
(1,1356)	1:75:A:LYS:HA	1:75:A:LYS:HG2	25	0.21
(1,1345)	1:76:A:MET:HG2	1:77:A:GLN:H	21	0.21
(1,1316)	1:79:A:ALA:HB1	1:79:A:ALA:H	4	0.21
(1,1316)	1:79:A:ALA:HB1	1:79:A:ALA:H	8	0.21
(1,1316)	1:79:A:ALA:HB1	1:79:A:ALA:H	11	0.21
(1,1316)	1:79:A:ALA:HB2	1:79:A:ALA:H	15	0.21
(1,1316)	1:79:A:ALA:HB2	1:79:A:ALA:H	18	0.21
(1,1316)	1:79:A:ALA:HB2	1:79:A:ALA:H	21	0.21
(1,1316)	1:79:A:ALA:HB2	1:79:A:ALA:H	23	0.21
(1,1316)	1:79:A:ALA:HB3	1:79:A:ALA:H	24	0.21
(1,1295)	1:82:A:PRO:HG2	1:81:A:HIS:HA	12	0.21
(1,1295)	1:82:A:PRO:HG2	1:81:A:HIS:HA	13	0.21
(1,1292)	1:129:A:GLU:HG3	1:129:A:GLU:H	21	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1228)	1:87:A:PHE:HD1	1:88:A:LEU:HD22	14	0.21
(1,1209)	1:88:A:LEU:HD13	1:70:A:PHE:HE1	3	0.21
(1,1199)	1:89:A:TYR:HE1	1:71:A:LEU:HD13	12	0.21
(1,1197)	1:89:A:TYR:HD2	1:71:A:LEU:HD21	9	0.21
(1,1197)	1:89:A:TYR:HD2	1:71:A:LEU:HD21	14	0.21
(1,1171)	1:91:A:ARG:HG2	1:91:A:ARG:HA	12	0.21
(1,1142)	1:94:A:ARG:HD2	1:94:A:ARG:HB2	12	0.21
(1,1139)	1:134:A:LEU:HD21	1:95:A:ALA:HB1	25	0.21
(1,1133)	1:95:A:ALA:HB3	1:99:A:PHE:HD2	9	0.21
(1,1133)	1:95:A:ALA:HB3	1:99:A:PHE:HD2	11	0.21
(1,1133)	1:95:A:ALA:HB3	1:99:A:PHE:HD2	24	0.21
(1,1126)	1:96:A:HIS:HD2	1:139:A:ALA:HB1	5	0.21
(1,1117)	1:98:A:LEU:HG	1:98:A:LEU:HD23	1	0.21
(1,1117)	1:98:A:LEU:HG	1:98:A:LEU:HD23	2	0.21
(1,1117)	1:98:A:LEU:HG	1:98:A:LEU:HD21	6	0.21
(1,1117)	1:98:A:LEU:HG	1:98:A:LEU:HD23	10	0.21
(1,1117)	1:98:A:LEU:HG	1:98:A:LEU:HD21	11	0.21
(1,1117)	1:98:A:LEU:HG	1:98:A:LEU:HD22	14	0.21
(1,1117)	1:98:A:LEU:HG	1:98:A:LEU:HD21	15	0.21
(1,1097)	1:100:A:LEU:HD21	1:100:A:LEU:HD11	2	0.21
(1,1097)	1:100:A:LEU:HD23	1:100:A:LEU:HD12	6	0.21
(1,1097)	1:100:A:LEU:HD21	1:100:A:LEU:HD11	9	0.21
(1,1097)	1:100:A:LEU:HD22	1:100:A:LEU:HD12	24	0.21
(1,1089)	1:105:A:PHE:HZ	1:100:A:LEU:HD22	1	0.21
(1,1089)	1:105:A:PHE:HZ	1:100:A:LEU:HD23	7	0.21
(1,1089)	1:105:A:PHE:HZ	1:100:A:LEU:HD22	16	0.21
(1,1088)	1:100:A:LEU:HD21	1:105:A:PHE:HD2	3	0.21
(1,1074)	1:101:A:ALA:HB2	1:60:A:LYS:HA	1	0.21
(1,1057)	1:103:A:ALA:HB3	1:59:A:TYR:HD1	20	0.21
(1,1036)	1:62:A:GLU:HB3	1:62:A:GLU:H	15	0.21
(1,1036)	1:62:A:GLU:HB3	1:62:A:GLU:H	23	0.21
(1,1000)	1:108:A:ILE:HD11	1:99:A:PHE:HE1	1	0.21
(1,1000)	1:108:A:ILE:HD12	1:99:A:PHE:HE1	7	0.21
(1,1000)	1:108:A:ILE:HD11	1:99:A:PHE:HE1	17	0.21
(1,998)	1:108:A:ILE:HD12	1:105:A:PHE:HD1	4	0.21
(1,998)	1:108:A:ILE:HD11	1:105:A:PHE:HD1	6	0.21
(1,998)	1:108:A:ILE:HD12	1:105:A:PHE:HD1	10	0.21
(1,998)	1:108:A:ILE:HD11	1:105:A:PHE:HD1	14	0.21
(1,998)	1:108:A:ILE:HD11	1:105:A:PHE:HD1	21	0.21
(1,995)	1:108:A:ILE:HG23	1:130:A:LEU:HD12	25	0.21
(1,991)	1:108:A:ILE:HA	1:108:A:ILE:HG22	20	0.21
(1,960)	1:67:A:PHE:HA	1:109:A:LEU:HD13	25	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,945)	1:110:A:SER:HB2	1:111:A:ARG:H	5	0.21
(1,934)	1:112:A:VAL:HG13	1:126:A:TYR:HB3	2	0.21
(1,934)	1:112:A:VAL:HG13	1:126:A:TYR:HB3	8	0.21
(1,913)	1:113:A:LEU:HG	1:113:A:LEU:H	5	0.21
(1,913)	1:113:A:LEU:HG	1:113:A:LEU:H	25	0.21
(1,909)	1:114:A:SER:HB2	1:113:A:LEU:HG	21	0.21
(1,878)	1:117:A:ARG:HG2	1:114:A:SER:HA	11	0.21
(1,873)	1:118:A:SER:HB2	1:119:A:ARG:H	22	0.21
(1,868)	1:119:A:ARG:HD2	1:119:A:ARG:HB2	7	0.21
(1,867)	1:119:A:ARG:HD3	1:119:A:ARG:HA	25	0.21
(1,858)	1:119:A:ARG:HG3	1:119:A:ARG:HA	20	0.21
(1,844)	1:120:A:PRO:HB2	1:120:A:PRO:HD2	16	0.21
(1,844)	1:120:A:PRO:HB2	1:120:A:PRO:HD2	22	0.21
(1,844)	1:120:A:PRO:HB2	1:120:A:PRO:HD2	25	0.21
(1,811)	1:123:A:LEU:HD23	1:70:A:PHE:HE1	23	0.21
(1,778)	1:125:A:VAL:HG23	1:122:A:LYS:HA	25	0.21
(1,775)	1:126:A:TYR:HE1	1:125:A:VAL:HG12	9	0.21
(1,757)	1:126:A:TYR:HD1	1:126:A:TYR:HB2	1	0.21
(1,757)	1:126:A:TYR:HD1	1:126:A:TYR:HB2	4	0.21
(1,757)	1:126:A:TYR:HD1	1:126:A:TYR:HB2	7	0.21
(1,757)	1:126:A:TYR:HD1	1:126:A:TYR:HB2	8	0.21
(1,757)	1:126:A:TYR:HD1	1:126:A:TYR:HB2	9	0.21
(1,757)	1:126:A:TYR:HD1	1:126:A:TYR:HB2	11	0.21
(1,757)	1:126:A:TYR:HD1	1:126:A:TYR:HB2	14	0.21
(1,757)	1:126:A:TYR:HD1	1:126:A:TYR:HB2	15	0.21
(1,757)	1:126:A:TYR:HD1	1:126:A:TYR:HB2	19	0.21
(1,757)	1:126:A:TYR:HD1	1:126:A:TYR:HB2	22	0.21
(1,702)	1:85:A:VAL:HG23	1:85:A:VAL:HA	6	0.21
(1,702)	1:85:A:VAL:HG21	1:85:A:VAL:HA	17	0.21
(1,702)	1:85:A:VAL:HG23	1:85:A:VAL:HA	24	0.21
(1,673)	1:133:A:VAL:HG22	1:130:A:LEU:HA	10	0.21
(1,673)	1:133:A:VAL:HG22	1:130:A:LEU:HA	19	0.21
(1,634)	1:134:A:LEU:HD11	1:134:A:LEU:H	4	0.21
(1,619)	1:135:A:LYS:HG2	1:91:A:ARG:HD3	1	0.21
(1,614)	1:135:A:LYS:HA	1:135:A:LYS:HD2	20	0.21
(1,593)	1:138:A:SER:HA	1:138:A:SER:HB2	5	0.21
(1,576)	1:142:A:LYS:HB2	1:142:A:LYS:H	15	0.21
(1,561)	2:27:B:SER:H	2:30:B:GLU:HB3	23	0.21
(1,551)	2:34:B:TYR:H	2:35:B:PHE:HA	11	0.21
(1,551)	2:34:B:TYR:H	2:35:B:PHE:HA	25	0.21
(1,540)	1:63:A:ASN:H	1:61:A:LEU:HG	20	0.21
(1,538)	1:63:A:ASN:H	1:61:A:LEU:HA	23	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,521)	1:71:A:LEU:H	1:113:A:LEU:HD13	8	0.21
(1,520)	1:130:A:LEU:H	1:112:A:VAL:HG21	11	0.21
(1,520)	1:130:A:LEU:H	1:112:A:VAL:HG23	15	0.21
(1,515)	1:73:A:LEU:HG	1:76:A:MET:H	12	0.21
(1,512)	1:77:A:GLN:H	1:123:A:LEU:HD21	18	0.21
(1,505)	1:79:A:ALA:H	1:76:A:MET:HA	24	0.21
(1,492)	1:91:A:ARG:H	1:88:A:LEU:HD23	17	0.21
(1,492)	1:91:A:ARG:H	1:88:A:LEU:HD21	21	0.21
(1,490)	1:91:A:ARG:H	1:94:A:ARG:H	16	0.21
(1,490)	1:91:A:ARG:H	1:94:A:ARG:H	22	0.21
(1,469)	1:102:A:SER:H	1:100:A:LEU:HB2	20	0.21
(1,465)	1:106:A:CYS:H	1:103:A:ALA:HB1	8	0.21
(1,445)	1:116:A:ALA:H	1:112:A:VAL:HA	4	0.21
(1,438)	1:66:A:LEU:HD13	1:66:A:LEU:H	12	0.21
(1,426)	1:125:A:VAL:HG12	1:126:A:TYR:H	21	0.21
(1,414)	1:72:A:GLU:H	1:68:A:GLU:HA	7	0.21
(1,391)	1:144:A:ASN:H	1:142:A:LYS:HB2	6	0.21
(1,379)	2:31:B:LEU:HB2	2:28:B:ASP:HB2	7	0.21
(1,361)	2:29:B:SER:HB2	2:32:B:GLU:HG3	7	0.21
(1,343)	2:31:B:LEU:HB2	1:87:A:PHE:HE2	4	0.21
(1,342)	2:31:B:LEU:HD12	1:124:A:TYR:HB3	7	0.21
(1,342)	2:31:B:LEU:HD13	1:124:A:TYR:HB3	23	0.21
(1,337)	2:31:B:LEU:HD21	2:28:B:ASP:HB3	6	0.21
(1,337)	2:31:B:LEU:HD23	2:28:B:ASP:HB3	14	0.21
(1,337)	2:31:B:LEU:HD23	2:28:B:ASP:HB2	17	0.21
(1,324)	2:33:B:GLN:HG2	2:26:B:ASP:HB3	18	0.21
(1,321)	2:34:B:TYR:HD1	1:83:A:GLU:HB3	22	0.21
(1,264)	1:127:A:ILE:HG23	2:35:B:PHE:HE1	10	0.21
(1,264)	1:127:A:ILE:HG23	2:35:B:PHE:HE1	11	0.21
(1,264)	1:127:A:ILE:HG22	2:35:B:PHE:HE1	14	0.21
(1,258)	1:113:A:LEU:HD12	1:113:A:LEU:HG	11	0.21
(1,258)	1:113:A:LEU:HD13	1:113:A:LEU:HG	15	0.21
(1,258)	1:113:A:LEU:HD12	1:113:A:LEU:HG	19	0.21
(1,258)	1:113:A:LEU:HD12	1:113:A:LEU:HG	25	0.21
(1,253)	1:57:A:LYS:HE3	1:54:A:MET:HG2	16	0.21
(1,243)	1:62:A:GLU:HG3	1:61:A:LEU:HD21	23	0.21
(1,240)	1:104:A:GLU:HB3	1:105:A:PHE:HA	25	0.21
(1,236)	1:64:A:GLU:HA	1:67:A:PHE:H	11	0.21
(1,225)	1:129:A:GLU:HG2	1:125:A:VAL:HG11	2	0.21
(1,209)	1:67:A:PHE:HE1	1:71:A:LEU:HD21	22	0.21
(1,172)	1:85:A:VAL:HG13	1:74:A:CYS:HB3	18	0.21
(1,161)	1:87:A:PHE:HE2	2:34:B:TYR:HE1	5	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,161)	1:87:A:PHE:HE2	2:34:B:TYR:HE1	11	0.21
(1,160)	1:67:A:PHE:HD1	1:68:A:GLU:H	1	0.21
(1,160)	1:67:A:PHE:HD1	1:68:A:GLU:H	16	0.21
(1,147)	1:137:A:HIS:HB3	1:138:A:SER:H	11	0.21
(1,145)	1:88:A:LEU:HB3	1:85:A:VAL:HA	18	0.21
(1,140)	1:99:A:PHE:HB3	1:138:A:SER:H	12	0.21
(1,139)	1:128:A:ASN:HB2	1:128:A:ASN:HD22	12	0.21
(1,139)	1:128:A:ASN:HB2	1:128:A:ASN:HD22	23	0.21
(1,122)	1:95:A:ALA:HB1	1:91:A:ARG:HD3	18	0.21
(1,122)	1:95:A:ALA:HB1	1:91:A:ARG:HD3	22	0.21
(1,114)	1:70:A:PHE:HB3	1:130:A:LEU:HD22	13	0.21
(1,107)	1:69:A:GLU:HA	1:69:A:GLU:HB3	20	0.21
(1,95)	1:107:A:ASN:HB2	1:108:A:ILE:HB	6	0.21
(1,95)	1:107:A:ASN:HB2	1:108:A:ILE:HB	12	0.21
(1,84)	1:113:A:LEU:HA	1:113:A:LEU:HG	25	0.21
(1,83)	1:113:A:LEU:HA	1:116:A:ALA:HB1	1	0.21
(1,76)	1:118:A:SER:HA	1:118:A:SER:HB2	6	0.21
(1,67)	1:116:A:ALA:HB2	1:120:A:PRO:HA	7	0.21
(1,56)	1:124:A:TYR:HE2	2:35:B:PHE:HB3	8	0.21
(1,51)	1:126:A:TYR:HD1	1:125:A:VAL:HG12	9	0.21
(1,42)	1:126:A:TYR:HD1	1:125:A:VAL:HB	12	0.21
(1,27)	1:130:A:LEU:HD21	1:67:A:PHE:HA	8	0.21
(1,24)	1:85:A:VAL:HG21	1:71:A:LEU:HA	5	0.21
(1,2244)	2:36:B:THR:HG21	2:36:B:THR:H	25	0.2
(1,2207)	2:38:B:ARG:HB2	2:39:B:TRP:H	7	0.2
(1,2108)	1:77:A:GLN:H	1:78:A:THR:HG21	17	0.2
(1,2108)	1:77:A:GLN:H	1:78:A:THR:HG23	23	0.2
(1,2100)	1:77:A:GLN:HE21	1:76:A:MET:HE2	12	0.2
(1,2094)	1:79:A:ALA:HB3	1:78:A:THR:H	21	0.2
(1,2032)	1:90:A:ASN:HD22	1:93:A:GLN:HB2	7	0.2
(1,2032)	1:90:A:ASN:HD22	1:93:A:GLN:HB2	11	0.2
(1,2032)	1:90:A:ASN:HD22	1:93:A:GLN:HB2	15	0.2
(1,2032)	1:90:A:ASN:HD22	1:93:A:GLN:HB2	22	0.2
(1,2006)	1:134:A:LEU:HD21	1:95:A:ALA:H	10	0.2
(1,2005)	1:95:A:ALA:H	1:94:A:ARG:HG2	5	0.2
(1,1987)	1:99:A:PHE:H	1:99:A:PHE:HD2	10	0.2
(1,1987)	1:99:A:PHE:H	1:99:A:PHE:HD2	14	0.2
(1,1975)	1:100:A:LEU:HD13	1:100:A:LEU:H	1	0.2
(1,1975)	1:100:A:LEU:HD11	1:100:A:LEU:H	13	0.2
(1,1961)	1:102:A:SER:H	1:59:A:TYR:HD1	7	0.2
(1,1919)	1:109:A:LEU:HB3	1:109:A:LEU:H	1	0.2
(1,1919)	1:109:A:LEU:HB3	1:109:A:LEU:H	5	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1919)	1:109:A:LEU:HB3	1:109:A:LEU:H	11	0.2
(1,1919)	1:109:A:LEU:HB3	1:109:A:LEU:H	12	0.2
(1,1919)	1:109:A:LEU:HB3	1:109:A:LEU:H	13	0.2
(1,1919)	1:109:A:LEU:HB3	1:109:A:LEU:H	18	0.2
(1,1919)	1:109:A:LEU:HB3	1:109:A:LEU:H	19	0.2
(1,1919)	1:109:A:LEU:HB3	1:109:A:LEU:H	20	0.2
(1,1803)	1:135:A:LYS:HB3	1:135:A:LYS:H	8	0.2
(1,1803)	1:135:A:LYS:HB3	1:135:A:LYS:H	18	0.2
(1,1803)	1:135:A:LYS:HB3	1:135:A:LYS:H	23	0.2
(1,1789)	1:139:A:ALA:H	1:139:A:ALA:HB2	3	0.2
(1,1759)	2:30:B:GLU:HA	2:30:B:GLU:HG3	4	0.2
(1,1751)	2:27:B:SER:HA	2:28:B:ASP:H	4	0.2
(1,1751)	2:27:B:SER:HA	2:28:B:ASP:H	9	0.2
(1,1741)	2:29:B:SER:HA	2:30:B:GLU:H	1	0.2
(1,1741)	2:29:B:SER:HA	2:30:B:GLU:H	10	0.2
(1,1741)	2:29:B:SER:HA	2:30:B:GLU:H	13	0.2
(1,1741)	2:29:B:SER:HA	2:30:B:GLU:H	20	0.2
(1,1725)	2:31:B:LEU:HD22	1:127:A:ILE:HG22	24	0.2
(1,1721)	2:31:B:LEU:HD21	2:31:B:LEU:HA	19	0.2
(1,1721)	2:31:B:LEU:HD23	2:31:B:LEU:HA	25	0.2
(1,1718)	2:31:B:LEU:HD21	2:32:B:GLU:H	5	0.2
(1,1667)	2:36:B:THR:HB	2:36:B:THR:H	19	0.2
(1,1667)	2:36:B:THR:HB	2:36:B:THR:H	23	0.2
(1,1648)	2:38:B:ARG:HA	2:37:B:ALA:HB2	1	0.2
(1,1648)	2:38:B:ARG:HA	2:37:B:ALA:HB3	7	0.2
(1,1648)	2:38:B:ARG:HA	2:37:B:ALA:HB2	13	0.2
(1,1648)	2:38:B:ARG:HA	2:37:B:ALA:HB1	19	0.2
(1,1648)	2:38:B:ARG:HA	2:37:B:ALA:HB2	22	0.2
(1,1636)	2:35:B:PHE:HB3	2:34:B:TYR:HE1	11	0.2
(1,1636)	2:35:B:PHE:HB3	2:34:B:TYR:HE1	20	0.2
(1,1636)	2:35:B:PHE:HB3	2:34:B:TYR:HE1	25	0.2
(1,1606)	2:32:B:GLU:HA	2:32:B:GLU:HB2	19	0.2
(1,1595)	2:31:B:LEU:HD11	1:127:A:ILE:HB	4	0.2
(1,1595)	2:31:B:LEU:HD11	1:127:A:ILE:HB	8	0.2
(1,1595)	2:31:B:LEU:HD12	1:127:A:ILE:HB	9	0.2
(1,1595)	2:31:B:LEU:HD12	1:127:A:ILE:HB	20	0.2
(1,1592)	1:84:A:VAL:HG22	2:35:B:PHE:HB2	16	0.2
(1,1588)	1:87:A:PHE:HB2	2:31:B:LEU:HD12	23	0.2
(1,1577)	1:77:A:GLN:HG3	1:73:A:LEU:HD12	20	0.2
(1,1556)	1:57:A:LYS:HG2	1:57:A:LYS:HA	5	0.2
(1,1549)	1:58:A:CYS:HB2	1:57:A:LYS:HA	9	0.2
(1,1545)	1:59:A:TYR:HE1	1:57:A:LYS:HB3	6	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1456)	1:69:A:GLU:HG2	1:66:A:LEU:HA	20	0.2
(1,1454)	1:68:A:GLU:HG2	1:69:A:GLU:H	14	0.2
(1,1453)	1:68:A:GLU:HG3	1:69:A:GLU:H	2	0.2
(1,1453)	1:68:A:GLU:HG3	1:69:A:GLU:H	4	0.2
(1,1453)	1:68:A:GLU:HG3	1:69:A:GLU:H	9	0.2
(1,1447)	1:69:A:GLU:HA	1:69:A:GLU:HG3	11	0.2
(1,1446)	1:69:A:GLU:HG2	1:69:A:GLU:H	11	0.2
(1,1446)	1:69:A:GLU:HG2	1:69:A:GLU:H	16	0.2
(1,1432)	1:70:A:PHE:HA	1:70:A:PHE:HD1	13	0.2
(1,1419)	1:71:A:LEU:HD13	1:89:A:TYR:H	20	0.2
(1,1395)	1:116:A:ALA:HB1	1:73:A:LEU:HD22	10	0.2
(1,1371)	1:75:A:LYS:HE3	1:72:A:GLU:HG2	4	0.2
(1,1370)	1:75:A:LYS:HE3	1:72:A:GLU:HB3	9	0.2
(1,1367)	1:75:A:LYS:HD2	1:75:A:LYS:HA	1	0.2
(1,1356)	1:75:A:LYS:HA	1:75:A:LYS:HG2	5	0.2
(1,1356)	1:75:A:LYS:HA	1:75:A:LYS:HG2	18	0.2
(1,1356)	1:75:A:LYS:HA	1:75:A:LYS:HG2	19	0.2
(1,1356)	1:75:A:LYS:HA	1:75:A:LYS:HG2	21	0.2
(1,1331)	1:77:A:GLN:HG2	1:73:A:LEU:HD11	12	0.2
(1,1319)	1:77:A:GLN:HB3	1:78:A:THR:H	3	0.2
(1,1317)	1:79:A:ALA:HB1	1:76:A:MET:HA	10	0.2
(1,1316)	1:79:A:ALA:HB3	1:79:A:ALA:H	7	0.2
(1,1316)	1:79:A:ALA:HB3	1:79:A:ALA:H	10	0.2
(1,1316)	1:79:A:ALA:HB2	1:79:A:ALA:H	13	0.2
(1,1316)	1:79:A:ALA:HB3	1:79:A:ALA:H	14	0.2
(1,1316)	1:79:A:ALA:HB2	1:79:A:ALA:H	16	0.2
(1,1295)	1:82:A:PRO:HG2	1:81:A:HIS:HA	6	0.2
(1,1295)	1:82:A:PRO:HG2	1:81:A:HIS:HA	24	0.2
(1,1279)	1:84:A:VAL:HG21	1:81:A:HIS:HB3	9	0.2
(1,1275)	1:78:A:THR:HG21	1:77:A:GLN:HB3	14	0.2
(1,1199)	1:89:A:TYR:HE1	1:71:A:LEU:HD11	10	0.2
(1,1197)	1:89:A:TYR:HD2	1:71:A:LEU:HD23	6	0.2
(1,1197)	1:89:A:TYR:HD2	1:71:A:LEU:HD22	25	0.2
(1,1142)	1:94:A:ARG:HD2	1:94:A:ARG:HB2	19	0.2
(1,1117)	1:98:A:LEU:HG	1:98:A:LEU:HD23	4	0.2
(1,1117)	1:98:A:LEU:HG	1:98:A:LEU:HD21	7	0.2
(1,1117)	1:98:A:LEU:HG	1:98:A:LEU:HD21	8	0.2
(1,1117)	1:98:A:LEU:HG	1:98:A:LEU:HD22	19	0.2
(1,1117)	1:98:A:LEU:HG	1:98:A:LEU:HD23	23	0.2
(1,1117)	1:98:A:LEU:HG	1:98:A:LEU:HD21	24	0.2
(1,1097)	1:100:A:LEU:HD22	1:100:A:LEU:HD12	5	0.2
(1,1097)	1:100:A:LEU:HD23	1:100:A:LEU:HD12	8	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1096)	1:100:A:LEU:HD23	1:92:A:GLN:HG3	11	0.2
(1,1094)	1:100:A:LEU:HD21	1:138:A:SER:HB2	14	0.2
(1,1091)	1:100:A:LEU:HD21	1:92:A:GLN:HE21	4	0.2
(1,1089)	1:105:A:PHE:HZ	1:100:A:LEU:HD21	2	0.2
(1,1089)	1:105:A:PHE:HZ	1:100:A:LEU:HD23	11	0.2
(1,1072)	1:101:A:ALA:HB1	1:58:A:CYS:HA	19	0.2
(1,1072)	1:101:A:ALA:HB3	1:58:A:CYS:HA	22	0.2
(1,1070)	1:101:A:ALA:HB2	1:102:A:SER:H	13	0.2
(1,1068)	1:101:A:ALA:HB2	1:59:A:TYR:H	21	0.2
(1,1057)	1:103:A:ALA:HB3	1:59:A:TYR:HD1	4	0.2
(1,1057)	1:103:A:ALA:HB1	1:59:A:TYR:HD1	25	0.2
(1,1026)	1:109:A:LEU:HD11	1:67:A:PHE:HE1	3	0.2
(1,1026)	1:109:A:LEU:HD13	1:67:A:PHE:HE1	13	0.2
(1,1002)	1:108:A:ILE:HD12	1:104:A:GLU:HG2	20	0.2
(1,999)	1:108:A:ILE:HD12	1:99:A:PHE:HZ	8	0.2
(1,998)	1:108:A:ILE:HD13	1:105:A:PHE:HD1	5	0.2
(1,998)	1:108:A:ILE:HD13	1:105:A:PHE:HD1	24	0.2
(1,998)	1:108:A:ILE:HD11	1:105:A:PHE:HD1	25	0.2
(1,991)	1:108:A:ILE:HA	1:108:A:ILE:HG23	19	0.2
(1,944)	1:110:A:SER:HB2	1:110:A:SER:H	15	0.2
(1,934)	1:112:A:VAL:HG12	1:126:A:TYR:HB3	4	0.2
(1,913)	1:113:A:LEU:HG	1:113:A:LEU:H	6	0.2
(1,913)	1:113:A:LEU:HG	1:113:A:LEU:H	19	0.2
(1,913)	1:113:A:LEU:HG	1:113:A:LEU:H	23	0.2
(1,911)	1:113:A:LEU:HB2	1:113:A:LEU:H	13	0.2
(1,909)	1:114:A:SER:HB2	1:113:A:LEU:HG	23	0.2
(1,881)	1:117:A:ARG:HD2	1:117:A:ARG:HB2	15	0.2
(1,873)	1:118:A:SER:HB2	1:119:A:ARG:H	3	0.2
(1,873)	1:118:A:SER:HB2	1:119:A:ARG:H	23	0.2
(1,844)	1:120:A:PRO:HB2	1:120:A:PRO:HD2	4	0.2
(1,844)	1:120:A:PRO:HB2	1:120:A:PRO:HD2	5	0.2
(1,844)	1:120:A:PRO:HB2	1:120:A:PRO:HD2	6	0.2
(1,844)	1:120:A:PRO:HB2	1:120:A:PRO:HD2	7	0.2
(1,844)	1:120:A:PRO:HB2	1:120:A:PRO:HD2	8	0.2
(1,844)	1:120:A:PRO:HB2	1:120:A:PRO:HD2	9	0.2
(1,844)	1:120:A:PRO:HB2	1:120:A:PRO:HD2	10	0.2
(1,844)	1:120:A:PRO:HB2	1:120:A:PRO:HD2	11	0.2
(1,844)	1:120:A:PRO:HB2	1:120:A:PRO:HD2	13	0.2
(1,844)	1:120:A:PRO:HB2	1:120:A:PRO:HD2	14	0.2
(1,844)	1:120:A:PRO:HB2	1:120:A:PRO:HD2	15	0.2
(1,844)	1:120:A:PRO:HB2	1:120:A:PRO:HD2	17	0.2
(1,844)	1:120:A:PRO:HB2	1:120:A:PRO:HD2	19	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,844)	1:120:A:PRO:HB2	1:120:A:PRO:HD2	20	0.2
(1,844)	1:120:A:PRO:HB2	1:120:A:PRO:HD2	21	0.2
(1,844)	1:120:A:PRO:HB2	1:120:A:PRO:HD2	24	0.2
(1,813)	1:123:A:LEU:HD21	1:124:A:TYR:HE2	4	0.2
(1,811)	1:123:A:LEU:HD23	1:70:A:PHE:HE1	4	0.2
(1,775)	1:126:A:TYR:HE1	1:125:A:VAL:HG12	1	0.2
(1,771)	1:125:A:VAL:HA	1:128:A:ASN:HD21	2	0.2
(1,757)	1:126:A:TYR:HD1	1:126:A:TYR:HB2	2	0.2
(1,757)	1:126:A:TYR:HD1	1:126:A:TYR:HB2	5	0.2
(1,757)	1:126:A:TYR:HD1	1:126:A:TYR:HB2	12	0.2
(1,757)	1:126:A:TYR:HD1	1:126:A:TYR:HB2	17	0.2
(1,746)	1:127:A:ILE:HD11	1:127:A:ILE:H	3	0.2
(1,702)	1:85:A:VAL:HG22	1:85:A:VAL:HA	1	0.2
(1,702)	1:85:A:VAL:HG23	1:85:A:VAL:HA	14	0.2
(1,702)	1:85:A:VAL:HG23	1:85:A:VAL:HA	15	0.2
(1,702)	1:85:A:VAL:HG21	1:85:A:VAL:HA	18	0.2
(1,702)	1:85:A:VAL:HG21	1:85:A:VAL:HA	21	0.2
(1,702)	1:85:A:VAL:HG22	1:85:A:VAL:HA	22	0.2
(1,673)	1:133:A:VAL:HG23	1:130:A:LEU:HA	12	0.2
(1,673)	1:133:A:VAL:HG23	1:130:A:LEU:HA	15	0.2
(1,673)	1:133:A:VAL:HG23	1:130:A:LEU:HA	25	0.2
(1,634)	1:134:A:LEU:HD12	1:134:A:LEU:H	2	0.2
(1,633)	1:100:A:LEU:HD12	1:92:A:GLN:HE21	1	0.2
(1,633)	1:100:A:LEU:HD12	1:92:A:GLN:HE21	15	0.2
(1,633)	1:100:A:LEU:HD13	1:92:A:GLN:HE21	25	0.2
(1,614)	1:135:A:LYS:HA	1:135:A:LYS:HD2	11	0.2
(1,582)	1:139:A:ALA:HA	1:96:A:HIS:HB2	18	0.2
(1,558)	2:32:B:GLU:HA	2:31:B:LEU:H	10	0.2
(1,551)	2:34:B:TYR:H	2:35:B:PHE:HA	8	0.2
(1,551)	2:34:B:TYR:H	2:35:B:PHE:HA	17	0.2
(1,540)	1:63:A:ASN:H	1:61:A:LEU:HG	6	0.2
(1,540)	1:63:A:ASN:H	1:61:A:LEU:HG	23	0.2
(1,522)	1:70:A:PHE:H	1:73:A:LEU:H	4	0.2
(1,522)	1:70:A:PHE:H	1:73:A:LEU:H	11	0.2
(1,522)	1:70:A:PHE:H	1:73:A:LEU:H	12	0.2
(1,522)	1:70:A:PHE:H	1:73:A:LEU:H	17	0.2
(1,521)	1:71:A:LEU:H	1:113:A:LEU:HD11	6	0.2
(1,520)	1:130:A:LEU:H	1:112:A:VAL:HG23	1	0.2
(1,465)	1:106:A:CYS:H	1:103:A:ALA:HB2	11	0.2
(1,453)	1:114:A:SER:H	1:113:A:LEU:HD22	18	0.2
(1,438)	1:66:A:LEU:HD11	1:66:A:LEU:H	6	0.2
(1,438)	1:66:A:LEU:HD12	1:66:A:LEU:H	7	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,438)	1:66:A:LEU:HD13	1:66:A:LEU:H	22	0.2
(1,410)	1:134:A:LEU:H	1:132:A:THR:H	3	0.2
(1,394)	1:137:A:HIS:HB3	1:138:A:SER:H	5	0.2
(1,391)	1:144:A:ASN:H	1:142:A:LYS:HB2	1	0.2
(1,391)	1:144:A:ASN:H	1:142:A:LYS:HB2	11	0.2
(1,380)	2:27:B:SER:HA	2:30:B:GLU:HB3	8	0.2
(1,361)	2:29:B:SER:HB2	2:32:B:GLU:HG3	11	0.2
(1,356)	2:29:B:SER:HB2	2:33:B:GLN:H	23	0.2
(1,342)	2:31:B:LEU:HD11	1:124:A:TYR:HB3	4	0.2
(1,337)	2:31:B:LEU:HD23	2:28:B:ASP:HB2	19	0.2
(1,321)	2:34:B:TYR:HD1	1:83:A:GLU:HB3	9	0.2
(1,293)	2:39:B:TRP:HD1	2:38:B:ARG:HB3	15	0.2
(1,285)	2:31:B:LEU:HD13	1:127:A:ILE:HB	19	0.2
(1,264)	1:127:A:ILE:HG21	2:35:B:PHE:HE1	20	0.2
(1,264)	1:127:A:ILE:HG21	2:35:B:PHE:HE1	25	0.2
(1,258)	1:113:A:LEU:HD13	1:113:A:LEU:HG	4	0.2
(1,258)	1:113:A:LEU:HD11	1:113:A:LEU:HG	5	0.2
(1,236)	1:64:A:GLU:HA	1:67:A:PHE:H	14	0.2
(1,233)	1:62:A:GLU:HG2	1:66:A:LEU:HD11	9	0.2
(1,233)	1:62:A:GLU:HG2	1:66:A:LEU:HD13	15	0.2
(1,228)	1:62:A:GLU:HG2	1:61:A:LEU:HD23	2	0.2
(1,160)	1:67:A:PHE:HD1	1:68:A:GLU:H	11	0.2
(1,157)	1:130:A:LEU:HD23	1:88:A:LEU:HD11	10	0.2
(1,157)	1:130:A:LEU:HD22	1:88:A:LEU:HD13	14	0.2
(1,157)	1:130:A:LEU:HD21	1:88:A:LEU:HD13	18	0.2
(1,157)	1:130:A:LEU:HD22	1:88:A:LEU:HD13	24	0.2
(1,147)	1:137:A:HIS:HB3	1:138:A:SER:H	15	0.2
(1,139)	1:128:A:ASN:HB2	1:128:A:ASN:HD22	4	0.2
(1,139)	1:128:A:ASN:HB2	1:128:A:ASN:HD22	6	0.2
(1,139)	1:128:A:ASN:HB2	1:128:A:ASN:HD22	7	0.2
(1,139)	1:128:A:ASN:HB2	1:128:A:ASN:HD22	8	0.2
(1,139)	1:128:A:ASN:HB2	1:128:A:ASN:HD22	15	0.2
(1,139)	1:128:A:ASN:HB2	1:128:A:ASN:HD22	17	0.2
(1,109)	1:64:A:GLU:HB3	1:65:A:LYS:H	19	0.2
(1,98)	1:105:A:PHE:HD1	1:100:A:LEU:HD22	22	0.2
(1,92)	1:109:A:LEU:HD23	1:67:A:PHE:H	19	0.2
(1,84)	1:113:A:LEU:HA	1:113:A:LEU:HG	2	0.2
(1,83)	1:113:A:LEU:HA	1:116:A:ALA:HB2	15	0.2
(1,81)	1:116:A:ALA:HB1	1:70:A:PHE:HZ	14	0.2
(1,76)	1:118:A:SER:HA	1:118:A:SER:HB2	11	0.2
(1,76)	1:118:A:SER:HA	1:118:A:SER:HB2	25	0.2
(1,56)	1:124:A:TYR:HE2	2:35:B:PHE:HB3	23	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,55)	1:124:A:TYR:HE2	2:35:B:PHE:HB3	14	0.2
(1,51)	1:126:A:TYR:HD1	1:125:A:VAL:HG12	24	0.2
(1,42)	1:126:A:TYR:HD1	1:125:A:VAL:HB	18	0.2
(1,27)	1:130:A:LEU:HD22	1:67:A:PHE:HA	5	0.2
(1,27)	1:130:A:LEU:HD23	1:67:A:PHE:HA	15	0.2
(1,25)	1:85:A:VAL:HG23	1:74:A:CYS:HB2	3	0.2
(1,2273)	2:25:B:GLU:HB3	2:25:B:GLU:H	13	0.19
(1,2228)	2:35:B:PHE:H	2:34:B:TYR:HB3	9	0.19
(1,2228)	2:35:B:PHE:H	2:34:B:TYR:HB3	12	0.19
(1,2202)	1:125:A:VAL:H	1:122:A:LYS:HD2	9	0.19
(1,2151)	1:65:A:LYS:HG3	1:66:A:LEU:H	1	0.19
(1,2151)	1:65:A:LYS:HG3	1:66:A:LEU:H	6	0.19
(1,2108)	1:77:A:GLN:H	1:78:A:THR:HG23	22	0.19
(1,2100)	1:77:A:GLN:HE21	1:76:A:MET:HE1	20	0.19
(1,2097)	1:77:A:GLN:HE21	1:77:A:GLN:HA	17	0.19
(1,2094)	1:79:A:ALA:HB2	1:78:A:THR:H	9	0.19
(1,2007)	1:100:A:LEU:HD22	1:95:A:ALA:H	24	0.19
(1,2005)	1:95:A:ALA:H	1:94:A:ARG:HG2	14	0.19
(1,1987)	1:99:A:PHE:H	1:99:A:PHE:HD2	18	0.19
(1,1975)	1:100:A:LEU:HD12	1:100:A:LEU:H	21	0.19
(1,1968)	1:101:A:ALA:H	1:63:A:ASN:HD22	1	0.19
(1,1961)	1:102:A:SER:H	1:59:A:TYR:HD1	12	0.19
(1,1961)	1:102:A:SER:H	1:59:A:TYR:HD1	17	0.19
(1,1961)	1:102:A:SER:H	1:59:A:TYR:HD1	23	0.19
(1,1919)	1:109:A:LEU:HB3	1:109:A:LEU:H	10	0.19
(1,1919)	1:109:A:LEU:HB3	1:109:A:LEU:H	14	0.19
(1,1919)	1:109:A:LEU:HB3	1:109:A:LEU:H	17	0.19
(1,1919)	1:109:A:LEU:HB3	1:109:A:LEU:H	21	0.19
(1,1919)	1:109:A:LEU:HB3	1:109:A:LEU:H	25	0.19
(1,1803)	1:135:A:LYS:HB3	1:135:A:LYS:H	5	0.19
(1,1803)	1:135:A:LYS:HB3	1:135:A:LYS:H	15	0.19
(1,1771)	1:142:A:LYS:H	1:142:A:LYS:HD2	16	0.19
(1,1754)	2:30:B:GLU:HG2	2:31:B:LEU:H	19	0.19
(1,1753)	2:27:B:SER:HB2	2:27:B:SER:HA	24	0.19
(1,1751)	2:27:B:SER:HA	2:28:B:ASP:H	7	0.19
(1,1751)	2:27:B:SER:HA	2:28:B:ASP:H	10	0.19
(1,1751)	2:27:B:SER:HA	2:28:B:ASP:H	22	0.19
(1,1751)	2:27:B:SER:HA	2:28:B:ASP:H	25	0.19
(1,1746)	1:100:A:LEU:HD12	1:138:A:SER:HB2	5	0.19
(1,1721)	2:31:B:LEU:HD23	2:31:B:LEU:HA	23	0.19
(1,1718)	2:31:B:LEU:HD23	2:32:B:GLU:H	7	0.19
(1,1718)	2:31:B:LEU:HD22	2:32:B:GLU:H	22	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1703)	2:33:B:GLN:HG2	2:31:B:LEU:HD22	5	0.19
(1,1702)	2:33:B:GLN:HG3	2:34:B:TYR:HE2	19	0.19
(1,1670)	2:37:B:ALA:HB3	2:36:B:THR:HA	14	0.19
(1,1622)	2:39:B:TRP:HE3	2:39:B:TRP:HB2	8	0.19
(1,1606)	2:32:B:GLU:HA	2:32:B:GLU:HB2	10	0.19
(1,1606)	2:32:B:GLU:HA	2:32:B:GLU:HB2	12	0.19
(1,1606)	2:32:B:GLU:HA	2:32:B:GLU:HB2	14	0.19
(1,1606)	2:32:B:GLU:HA	2:32:B:GLU:HB2	20	0.19
(1,1606)	2:32:B:GLU:HA	2:32:B:GLU:HB2	22	0.19
(1,1606)	2:32:B:GLU:HA	2:32:B:GLU:HB2	25	0.19
(1,1595)	2:31:B:LEU:HD12	1:127:A:ILE:HB	14	0.19
(1,1592)	1:84:A:VAL:HG21	2:35:B:PHE:HB2	17	0.19
(1,1577)	1:77:A:GLN:HG3	1:73:A:LEU:HD12	5	0.19
(1,1570)	1:57:A:LYS:HE2	1:59:A:TYR:HE1	23	0.19
(1,1569)	1:57:A:LYS:HE3	1:59:A:TYR:HE1	25	0.19
(1,1558)	1:57:A:LYS:HB2	1:57:A:LYS:HG3	22	0.19
(1,1549)	1:58:A:CYS:HB2	1:57:A:LYS:HA	14	0.19
(1,1539)	1:62:A:GLU:HB3	1:59:A:TYR:HD1	20	0.19
(1,1486)	1:65:A:LYS:HA	1:65:A:LYS:HB2	11	0.19
(1,1486)	1:65:A:LYS:HA	1:65:A:LYS:HB2	21	0.19
(1,1486)	1:65:A:LYS:HA	1:65:A:LYS:HB2	24	0.19
(1,1456)	1:69:A:GLU:HG2	1:66:A:LEU:HA	9	0.19
(1,1440)	1:127:A:ILE:HD12	1:70:A:PHE:HZ	4	0.19
(1,1440)	1:127:A:ILE:HD12	1:70:A:PHE:HZ	24	0.19
(1,1432)	1:70:A:PHE:HA	1:70:A:PHE:HD1	9	0.19
(1,1432)	1:70:A:PHE:HA	1:70:A:PHE:HD1	14	0.19
(1,1432)	1:70:A:PHE:HA	1:70:A:PHE:HD1	17	0.19
(1,1419)	1:71:A:LEU:HD11	1:89:A:TYR:H	24	0.19
(1,1356)	1:75:A:LYS:HA	1:75:A:LYS:HG2	7	0.19
(1,1356)	1:75:A:LYS:HA	1:75:A:LYS:HG2	9	0.19
(1,1356)	1:75:A:LYS:HA	1:75:A:LYS:HG2	11	0.19
(1,1356)	1:75:A:LYS:HA	1:75:A:LYS:HG2	12	0.19
(1,1356)	1:75:A:LYS:HA	1:75:A:LYS:HG2	13	0.19
(1,1356)	1:75:A:LYS:HA	1:75:A:LYS:HG2	14	0.19
(1,1356)	1:75:A:LYS:HA	1:75:A:LYS:HG2	22	0.19
(1,1346)	1:76:A:MET:HG2	1:73:A:LEU:HA	10	0.19
(1,1316)	1:79:A:ALA:HB3	1:79:A:ALA:H	5	0.19
(1,1316)	1:79:A:ALA:HB3	1:79:A:ALA:H	19	0.19
(1,1295)	1:82:A:PRO:HG2	1:81:A:HIS:HA	4	0.19
(1,1295)	1:82:A:PRO:HG2	1:81:A:HIS:HA	19	0.19
(1,1283)	1:84:A:VAL:HG22	1:127:A:ILE:HD13	8	0.19
(1,1283)	1:84:A:VAL:HG23	1:127:A:ILE:HD11	16	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1280)	1:84:A:VAL:HG21	1:81:A:HIS:HB2	9	0.19
(1,1257)	1:85:A:VAL:HG13	1:71:A:LEU:HA	16	0.19
(1,1197)	1:89:A:TYR:HD2	1:71:A:LEU:HD21	11	0.19
(1,1197)	1:89:A:TYR:HD2	1:71:A:LEU:HD22	24	0.19
(1,1175)	1:91:A:ARG:HG2	1:134:A:LEU:HB2	13	0.19
(1,1171)	1:91:A:ARG:HG2	1:91:A:ARG:HA	15	0.19
(1,1147)	1:94:A:ARG:HG2	1:94:A:ARG:HA	25	0.19
(1,1142)	1:94:A:ARG:HD3	1:94:A:ARG:HB2	7	0.19
(1,1142)	1:94:A:ARG:HD3	1:94:A:ARG:HB2	8	0.19
(1,1132)	1:95:A:ALA:HB2	1:96:A:HIS:H	8	0.19
(1,1132)	1:95:A:ALA:HB3	1:96:A:HIS:H	21	0.19
(1,1118)	1:98:A:LEU:HB3	1:98:A:LEU:HD22	3	0.19
(1,1117)	1:98:A:LEU:HG	1:98:A:LEU:HD23	3	0.19
(1,1097)	1:100:A:LEU:HD23	1:100:A:LEU:HD12	10	0.19
(1,1097)	1:100:A:LEU:HD23	1:100:A:LEU:HD13	21	0.19
(1,1089)	1:105:A:PHE:HZ	1:100:A:LEU:HD23	14	0.19
(1,1089)	1:105:A:PHE:HZ	1:100:A:LEU:HD21	20	0.19
(1,1088)	1:100:A:LEU:HD23	1:105:A:PHE:HD2	13	0.19
(1,1070)	1:101:A:ALA:HB1	1:102:A:SER:H	1	0.19
(1,1068)	1:101:A:ALA:HB3	1:59:A:TYR:H	17	0.19
(1,1057)	1:103:A:ALA:HB2	1:59:A:TYR:HD1	5	0.19
(1,1027)	1:67:A:PHE:HE1	1:109:A:LEU:HD21	19	0.19
(1,999)	1:108:A:ILE:HD13	1:99:A:PHE:HZ	23	0.19
(1,996)	1:108:A:ILE:HG21	1:112:A:VAL:HG13	21	0.19
(1,991)	1:108:A:ILE:HA	1:108:A:ILE:HG23	4	0.19
(1,991)	1:108:A:ILE:HA	1:108:A:ILE:HG23	5	0.19
(1,991)	1:108:A:ILE:HA	1:108:A:ILE:HG23	10	0.19
(1,991)	1:108:A:ILE:HA	1:108:A:ILE:HG23	11	0.19
(1,991)	1:108:A:ILE:HA	1:108:A:ILE:HG21	12	0.19
(1,991)	1:108:A:ILE:HA	1:108:A:ILE:HG23	16	0.19
(1,991)	1:108:A:ILE:HA	1:108:A:ILE:HG21	17	0.19
(1,991)	1:108:A:ILE:HA	1:108:A:ILE:HG21	21	0.19
(1,991)	1:108:A:ILE:HA	1:108:A:ILE:HG22	24	0.19
(1,989)	1:108:A:ILE:HG22	1:105:A:PHE:HA	23	0.19
(1,963)	1:109:A:LEU:HD12	1:63:A:ASN:HB2	1	0.19
(1,944)	1:110:A:SER:HB2	1:110:A:SER:H	8	0.19
(1,944)	1:110:A:SER:HB2	1:110:A:SER:H	13	0.19
(1,944)	1:110:A:SER:HB2	1:110:A:SER:H	18	0.19
(1,913)	1:113:A:LEU:HG	1:113:A:LEU:H	9	0.19
(1,909)	1:114:A:SER:HB2	1:113:A:LEU:HG	4	0.19
(1,909)	1:114:A:SER:HB2	1:113:A:LEU:HG	14	0.19
(1,909)	1:114:A:SER:HB2	1:113:A:LEU:HG	15	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,909)	1:114:A:SER:HB2	1:113:A:LEU:HG	16	0.19
(1,909)	1:114:A:SER:HB2	1:113:A:LEU:HG	17	0.19
(1,881)	1:117:A:ARG:HD2	1:117:A:ARG:HB2	25	0.19
(1,879)	1:94:A:ARG:HD3	1:90:A:ASN:HD22	9	0.19
(1,873)	1:118:A:SER:HB2	1:119:A:ARG:H	5	0.19
(1,873)	1:118:A:SER:HB2	1:119:A:ARG:H	13	0.19
(1,873)	1:118:A:SER:HB2	1:119:A:ARG:H	14	0.19
(1,867)	1:119:A:ARG:HD3	1:119:A:ARG:HA	16	0.19
(1,844)	1:120:A:PRO:HB2	1:120:A:PRO:HD2	1	0.19
(1,844)	1:120:A:PRO:HB2	1:120:A:PRO:HD2	2	0.19
(1,844)	1:120:A:PRO:HB2	1:120:A:PRO:HD2	3	0.19
(1,844)	1:120:A:PRO:HB2	1:120:A:PRO:HD2	12	0.19
(1,844)	1:120:A:PRO:HB2	1:120:A:PRO:HD2	18	0.19
(1,844)	1:120:A:PRO:HB2	1:120:A:PRO:HD2	23	0.19
(1,812)	1:123:A:LEU:HD22	1:77:A:GLN:HE21	25	0.19
(1,811)	1:123:A:LEU:HD23	1:70:A:PHE:HE1	24	0.19
(1,775)	1:126:A:TYR:HE1	1:125:A:VAL:HG12	21	0.19
(1,773)	1:125:A:VAL:HA	1:125:A:VAL:HG13	2	0.19
(1,771)	1:125:A:VAL:HA	1:128:A:ASN:HD21	5	0.19
(1,766)	1:126:A:TYR:HE1	1:115:A:ARG:HB2	10	0.19
(1,757)	1:126:A:TYR:HD1	1:126:A:TYR:HB2	18	0.19
(1,757)	1:126:A:TYR:HD1	1:126:A:TYR:HB2	25	0.19
(1,702)	1:85:A:VAL:HG21	1:85:A:VAL:HA	4	0.19
(1,702)	1:85:A:VAL:HG21	1:85:A:VAL:HA	7	0.19
(1,702)	1:85:A:VAL:HG22	1:85:A:VAL:HA	8	0.19
(1,702)	1:85:A:VAL:HG21	1:85:A:VAL:HA	9	0.19
(1,702)	1:85:A:VAL:HG23	1:85:A:VAL:HA	10	0.19
(1,702)	1:85:A:VAL:HG21	1:85:A:VAL:HA	11	0.19
(1,702)	1:85:A:VAL:HG23	1:85:A:VAL:HA	12	0.19
(1,702)	1:85:A:VAL:HG22	1:85:A:VAL:HA	13	0.19
(1,702)	1:85:A:VAL:HG22	1:85:A:VAL:HA	19	0.19
(1,702)	1:85:A:VAL:HG22	1:85:A:VAL:HA	23	0.19
(1,672)	1:133:A:VAL:HG23	1:137:A:HIS:HD2	13	0.19
(1,672)	1:133:A:VAL:HG22	1:137:A:HIS:HD2	18	0.19
(1,634)	1:134:A:LEU:HD12	1:134:A:LEU:H	9	0.19
(1,618)	1:56:A:LYS:HG2	1:57:A:LYS:H	21	0.19
(1,596)	1:137:A:HIS:HA	1:138:A:SER:H	7	0.19
(1,551)	2:34:B:TYR:H	2:35:B:PHE:HA	5	0.19
(1,551)	2:34:B:TYR:H	2:35:B:PHE:HA	10	0.19
(1,551)	2:34:B:TYR:H	2:35:B:PHE:HA	21	0.19
(1,542)	1:61:A:LEU:HG	1:61:A:LEU:H	4	0.19
(1,542)	1:61:A:LEU:HG	1:61:A:LEU:H	9	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,540)	1:63:A:ASN:H	1:61:A:LEU:HG	3	0.19
(1,532)	1:66:A:LEU:H	1:64:A:GLU:HB2	19	0.19
(1,522)	1:70:A:PHE:H	1:73:A:LEU:H	2	0.19
(1,522)	1:70:A:PHE:H	1:73:A:LEU:H	16	0.19
(1,522)	1:70:A:PHE:H	1:73:A:LEU:H	22	0.19
(1,506)	1:78:A:THR:H	1:74:A:CYS:HB3	19	0.19
(1,505)	1:79:A:ALA:H	1:76:A:MET:HA	12	0.19
(1,490)	1:91:A:ARG:H	1:94:A:ARG:H	6	0.19
(1,477)	1:93:A:GLN:HA	1:95:A:ALA:H	14	0.19
(1,456)	1:112:A:VAL:H	1:108:A:ILE:HG23	11	0.19
(1,456)	1:112:A:VAL:H	1:108:A:ILE:HG22	25	0.19
(1,453)	1:114:A:SER:H	1:113:A:LEU:HD23	15	0.19
(1,438)	1:66:A:LEU:HD11	1:66:A:LEU:H	2	0.19
(1,438)	1:66:A:LEU:HD13	1:66:A:LEU:H	16	0.19
(1,438)	1:66:A:LEU:HD13	1:66:A:LEU:H	18	0.19
(1,414)	1:72:A:GLU:H	1:68:A:GLU:HA	24	0.19
(1,410)	1:134:A:LEU:H	1:132:A:THR:H	1	0.19
(1,410)	1:134:A:LEU:H	1:132:A:THR:H	6	0.19
(1,379)	2:31:B:LEU:HB2	2:28:B:ASP:HB2	11	0.19
(1,369)	2:26:B:ASP:HB2	1:87:A:PHE:HZ	2	0.19
(1,368)	2:26:B:ASP:HB3	1:87:A:PHE:HZ	14	0.19
(1,367)	2:26:B:ASP:HB3	2:31:B:LEU:H	1	0.19
(1,361)	2:29:B:SER:HB2	2:32:B:GLU:HG3	4	0.19
(1,356)	2:29:B:SER:HB2	2:33:B:GLN:H	3	0.19
(1,337)	2:31:B:LEU:HD23	2:28:B:ASP:HB2	15	0.19
(1,288)	2:32:B:GLU:HA	2:35:B:PHE:HD1	25	0.19
(1,264)	1:127:A:ILE:HG22	2:35:B:PHE:HE1	9	0.19
(1,264)	1:127:A:ILE:HG21	2:35:B:PHE:HE1	12	0.19
(1,262)	1:80:A:ASP:HB3	1:81:A:HIS:HD2	18	0.19
(1,236)	1:64:A:GLU:HA	1:67:A:PHE:H	19	0.19
(1,236)	1:64:A:GLU:HA	1:67:A:PHE:H	20	0.19
(1,209)	1:67:A:PHE:HE1	1:71:A:LEU:HD21	6	0.19
(1,197)	1:73:A:LEU:HD23	1:117:A:ARG:HB2	15	0.19
(1,197)	1:73:A:LEU:HD22	1:117:A:ARG:HB2	19	0.19
(1,191)	1:78:A:THR:HG21	1:74:A:CYS:HB2	2	0.19
(1,160)	1:67:A:PHE:HD1	1:68:A:GLU:H	10	0.19
(1,160)	1:67:A:PHE:HD2	1:68:A:GLU:H	13	0.19
(1,157)	1:130:A:LEU:HD21	1:88:A:LEU:HD11	20	0.19
(1,157)	1:130:A:LEU:HD22	1:88:A:LEU:HD13	22	0.19
(1,147)	1:137:A:HIS:HB3	1:138:A:SER:H	10	0.19
(1,145)	1:88:A:LEU:HB3	1:85:A:VAL:HA	24	0.19
(1,139)	1:128:A:ASN:HB2	1:128:A:ASN:HD22	1	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,139)	1:128:A:ASN:HB2	1:128:A:ASN:HD22	18	0.19
(1,139)	1:128:A:ASN:HB2	1:128:A:ASN:HD22	20	0.19
(1,139)	1:128:A:ASN:HB2	1:128:A:ASN:HD22	21	0.19
(1,139)	1:128:A:ASN:HB2	1:128:A:ASN:HD22	25	0.19
(1,133)	1:105:A:PHE:HE2	1:92:A:GLN:HG3	2	0.19
(1,121)	1:95:A:ALA:HB2	1:134:A:LEU:HA	22	0.19
(1,116)	1:100:A:LEU:HD22	1:105:A:PHE:HE2	21	0.19
(1,111)	1:62:A:GLU:HB3	1:59:A:TYR:HD2	15	0.19
(1,107)	1:69:A:GLU:HA	1:69:A:GLU:HB3	12	0.19
(1,98)	1:105:A:PHE:HD1	1:100:A:LEU:HD21	16	0.19
(1,98)	1:105:A:PHE:HD1	1:100:A:LEU:HD23	25	0.19
(1,84)	1:113:A:LEU:HA	1:113:A:LEU:HG	7	0.19
(1,84)	1:113:A:LEU:HA	1:113:A:LEU:HG	22	0.19
(1,83)	1:113:A:LEU:HA	1:116:A:ALA:HB2	20	0.19
(1,76)	1:118:A:SER:HA	1:118:A:SER:HB2	12	0.19
(1,76)	1:118:A:SER:HA	1:118:A:SER:HB2	16	0.19
(1,62)	1:123:A:LEU:HD22	1:70:A:PHE:HE1	13	0.19
(1,56)	1:124:A:TYR:HE2	2:35:B:PHE:HB3	20	0.19
(1,25)	1:85:A:VAL:HG21	1:74:A:CYS:HB2	5	0.19
(1,25)	1:85:A:VAL:HG22	1:74:A:CYS:HB2	23	0.19
(1,1)	1:141:A:LYS:HG3	1:141:A:LYS:HA	16	0.19
(1,2287)	2:33:B:GLN:HE22	2:33:B:GLN:HB3	10	0.18
(1,2287)	2:33:B:GLN:HE22	2:33:B:GLN:HB3	13	0.18
(1,2272)	2:25:B:GLU:H	2:25:B:GLU:HB2	5	0.18
(1,2207)	2:38:B:ARG:HB2	2:39:B:TRP:H	16	0.18
(1,2202)	1:125:A:VAL:H	1:122:A:LYS:HD2	4	0.18
(1,2202)	1:125:A:VAL:H	1:122:A:LYS:HD3	23	0.18
(1,2202)	1:125:A:VAL:H	1:122:A:LYS:HD2	25	0.18
(1,2136)	1:69:A:GLU:H	1:70:A:PHE:HB2	13	0.18
(1,2136)	1:69:A:GLU:H	1:70:A:PHE:HB3	21	0.18
(1,2107)	1:77:A:GLN:H	1:77:A:GLN:HB3	14	0.18
(1,2107)	1:77:A:GLN:H	1:77:A:GLN:HB3	20	0.18
(1,2106)	1:76:A:MET:HB3	1:77:A:GLN:H	11	0.18
(1,2100)	1:77:A:GLN:HE21	1:76:A:MET:HE1	10	0.18
(1,2095)	1:77:A:GLN:HG2	1:77:A:GLN:HE22	11	0.18
(1,2075)	1:81:A:HIS:H	1:81:A:HIS:HD2	21	0.18
(1,2071)	1:83:A:GLU:HG3	1:83:A:GLU:H	20	0.18
(1,2051)	1:89:A:TYR:H	1:90:A:ASN:HB3	22	0.18
(1,2032)	1:90:A:ASN:HD22	1:93:A:GLN:HB2	5	0.18
(1,2031)	1:91:A:ARG:H	1:134:A:LEU:HD12	24	0.18
(1,2007)	1:100:A:LEU:HD23	1:95:A:ALA:H	1	0.18
(1,2005)	1:95:A:ALA:H	1:94:A:ARG:HG2	9	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1961)	1:102:A:SER:H	1:59:A:TYR:HD1	14	0.18
(1,1803)	1:135:A:LYS:HB3	1:135:A:LYS:H	19	0.18
(1,1759)	2:30:B:GLU:HA	2:30:B:GLU:HG3	2	0.18
(1,1753)	2:27:B:SER:HB2	2:27:B:SER:HA	17	0.18
(1,1751)	2:27:B:SER:HA	2:28:B:ASP:H	2	0.18
(1,1751)	2:27:B:SER:HA	2:28:B:ASP:H	23	0.18
(1,1745)	2:29:B:SER:HB3	2:30:B:GLU:H	13	0.18
(1,1727)	2:31:B:LEU:HD12	2:31:B:LEU:H	19	0.18
(1,1725)	2:31:B:LEU:HD22	1:127:A:ILE:HG22	7	0.18
(1,1725)	2:31:B:LEU:HD22	1:127:A:ILE:HG23	12	0.18
(1,1723)	2:31:B:LEU:HD23	2:30:B:GLU:HB2	8	0.18
(1,1721)	2:31:B:LEU:HD22	2:31:B:LEU:HA	5	0.18
(1,1721)	2:31:B:LEU:HD21	2:31:B:LEU:HA	12	0.18
(1,1718)	2:31:B:LEU:HD23	2:32:B:GLU:H	9	0.18
(1,1705)	2:33:B:GLN:HA	2:34:B:TYR:H	7	0.18
(1,1705)	2:33:B:GLN:HA	2:34:B:TYR:H	12	0.18
(1,1705)	2:33:B:GLN:HA	2:34:B:TYR:H	22	0.18
(1,1705)	2:33:B:GLN:HA	2:34:B:TYR:H	24	0.18
(1,1703)	2:33:B:GLN:HG2	2:31:B:LEU:HD23	8	0.18
(1,1703)	2:33:B:GLN:HG2	2:31:B:LEU:HD23	23	0.18
(1,1670)	2:37:B:ALA:HB3	2:36:B:THR:HA	9	0.18
(1,1648)	2:38:B:ARG:HA	2:37:B:ALA:HB2	4	0.18
(1,1648)	2:38:B:ARG:HA	2:37:B:ALA:HB3	24	0.18
(1,1636)	2:35:B:PHE:HB3	2:34:B:TYR:HE1	6	0.18
(1,1636)	2:35:B:PHE:HB3	2:34:B:TYR:HE1	21	0.18
(1,1635)	2:39:B:TRP:HA	2:38:B:ARG:HD2	9	0.18
(1,1622)	2:39:B:TRP:HE3	2:39:B:TRP:HB2	5	0.18
(1,1619)	2:39:B:TRP:HD1	2:38:B:ARG:HB2	9	0.18
(1,1606)	2:32:B:GLU:HA	2:32:B:GLU:HB2	1	0.18
(1,1606)	2:32:B:GLU:HA	2:32:B:GLU:HB2	2	0.18
(1,1606)	2:32:B:GLU:HA	2:32:B:GLU:HB2	3	0.18
(1,1606)	2:32:B:GLU:HA	2:32:B:GLU:HB2	4	0.18
(1,1606)	2:32:B:GLU:HA	2:32:B:GLU:HB2	5	0.18
(1,1606)	2:32:B:GLU:HA	2:32:B:GLU:HB2	6	0.18
(1,1606)	2:32:B:GLU:HA	2:32:B:GLU:HB2	7	0.18
(1,1606)	2:32:B:GLU:HA	2:32:B:GLU:HB2	9	0.18
(1,1606)	2:32:B:GLU:HA	2:32:B:GLU:HB2	11	0.18
(1,1606)	2:32:B:GLU:HA	2:32:B:GLU:HB2	13	0.18
(1,1606)	2:32:B:GLU:HA	2:32:B:GLU:HB2	15	0.18
(1,1606)	2:32:B:GLU:HA	2:32:B:GLU:HB2	16	0.18
(1,1606)	2:32:B:GLU:HA	2:32:B:GLU:HB2	17	0.18
(1,1606)	2:32:B:GLU:HA	2:32:B:GLU:HB2	21	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1606)	2:32:B:GLU:HA	2:32:B:GLU:HB2	23	0.18
(1,1606)	2:32:B:GLU:HA	2:32:B:GLU:HB2	24	0.18
(1,1595)	2:31:B:LEU:HD11	1:127:A:ILE:HB	3	0.18
(1,1595)	2:31:B:LEU:HD12	1:127:A:ILE:HB	12	0.18
(1,1592)	1:84:A:VAL:HG23	2:35:B:PHE:HB2	3	0.18
(1,1577)	1:77:A:GLN:HG2	1:73:A:LEU:HD12	18	0.18
(1,1570)	1:57:A:LYS:HE2	1:59:A:TYR:HE1	4	0.18
(1,1570)	1:57:A:LYS:HE2	1:59:A:TYR:HE1	7	0.18
(1,1561)	1:57:A:LYS:HD2	1:57:A:LYS:HA	20	0.18
(1,1552)	1:57:A:LYS:HB2	1:57:A:LYS:HA	4	0.18
(1,1552)	1:57:A:LYS:HB2	1:57:A:LYS:HA	14	0.18
(1,1549)	1:58:A:CYS:HB2	1:57:A:LYS:HA	5	0.18
(1,1539)	1:62:A:GLU:HB3	1:59:A:TYR:HD1	5	0.18
(1,1512)	1:62:A:GLU:HG2	1:62:A:GLU:H	22	0.18
(1,1495)	1:64:A:GLU:HA	1:67:A:PHE:HB2	13	0.18
(1,1486)	1:65:A:LYS:HA	1:65:A:LYS:HB2	2	0.18
(1,1486)	1:65:A:LYS:HA	1:65:A:LYS:HB2	3	0.18
(1,1486)	1:65:A:LYS:HA	1:65:A:LYS:HB2	4	0.18
(1,1486)	1:65:A:LYS:HA	1:65:A:LYS:HB2	7	0.18
(1,1486)	1:65:A:LYS:HA	1:65:A:LYS:HB2	8	0.18
(1,1486)	1:65:A:LYS:HA	1:65:A:LYS:HB2	9	0.18
(1,1486)	1:65:A:LYS:HA	1:65:A:LYS:HB2	12	0.18
(1,1486)	1:65:A:LYS:HA	1:65:A:LYS:HB2	13	0.18
(1,1486)	1:65:A:LYS:HA	1:65:A:LYS:HB2	15	0.18
(1,1486)	1:65:A:LYS:HA	1:65:A:LYS:HB2	16	0.18
(1,1486)	1:65:A:LYS:HA	1:65:A:LYS:HB2	17	0.18
(1,1486)	1:65:A:LYS:HA	1:65:A:LYS:HB2	18	0.18
(1,1486)	1:65:A:LYS:HA	1:65:A:LYS:HB2	19	0.18
(1,1486)	1:65:A:LYS:HA	1:65:A:LYS:HB2	20	0.18
(1,1486)	1:65:A:LYS:HA	1:65:A:LYS:HB2	22	0.18
(1,1486)	1:65:A:LYS:HA	1:65:A:LYS:HB2	23	0.18
(1,1486)	1:65:A:LYS:HA	1:65:A:LYS:HB2	25	0.18
(1,1457)	1:68:A:GLU:HB2	1:68:A:GLU:HG2	15	0.18
(1,1447)	1:69:A:GLU:HA	1:69:A:GLU:HG3	16	0.18
(1,1432)	1:70:A:PHE:HA	1:70:A:PHE:HD1	1	0.18
(1,1432)	1:70:A:PHE:HA	1:70:A:PHE:HD1	3	0.18
(1,1432)	1:70:A:PHE:HA	1:70:A:PHE:HD1	6	0.18
(1,1432)	1:70:A:PHE:HA	1:70:A:PHE:HD1	10	0.18
(1,1432)	1:70:A:PHE:HA	1:70:A:PHE:HD1	15	0.18
(1,1432)	1:70:A:PHE:HA	1:70:A:PHE:HD1	23	0.18
(1,1432)	1:70:A:PHE:HA	1:70:A:PHE:HD1	25	0.18
(1,1391)	1:74:A:CYS:HA	1:73:A:LEU:HD21	20	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1367)	1:75:A:LYS:HD2	1:75:A:LYS:HA	22	0.18
(1,1356)	1:75:A:LYS:HA	1:75:A:LYS:HG2	1	0.18
(1,1356)	1:75:A:LYS:HA	1:75:A:LYS:HG2	16	0.18
(1,1346)	1:76:A:MET:HG2	1:73:A:LEU:HA	20	0.18
(1,1329)	1:77:A:GLN:HG2	1:77:A:GLN:HB3	1	0.18
(1,1317)	1:79:A:ALA:HB1	1:76:A:MET:HA	2	0.18
(1,1317)	1:79:A:ALA:HB2	1:76:A:MET:HA	8	0.18
(1,1316)	1:79:A:ALA:HB1	1:79:A:ALA:H	2	0.18
(1,1316)	1:79:A:ALA:HB1	1:79:A:ALA:H	9	0.18
(1,1315)	1:79:A:ALA:HB3	1:80:A:ASP:H	2	0.18
(1,1315)	1:79:A:ALA:HB2	1:80:A:ASP:H	25	0.18
(1,1295)	1:82:A:PRO:HG2	1:81:A:HIS:HA	1	0.18
(1,1295)	1:82:A:PRO:HG2	1:81:A:HIS:HA	14	0.18
(1,1283)	1:84:A:VAL:HG23	1:127:A:ILE:HD13	11	0.18
(1,1171)	1:91:A:ARG:HG2	1:91:A:ARG:HA	13	0.18
(1,1171)	1:91:A:ARG:HG2	1:91:A:ARG:HA	19	0.18
(1,1139)	1:134:A:LEU:HD21	1:95:A:ALA:HB3	22	0.18
(1,1139)	1:134:A:LEU:HD21	1:95:A:ALA:HB1	24	0.18
(1,1132)	1:95:A:ALA:HB3	1:96:A:HIS:H	10	0.18
(1,1122)	1:96:A:HIS:HA	1:139:A:ALA:HB3	15	0.18
(1,1118)	1:98:A:LEU:HB3	1:98:A:LEU:HD22	4	0.18
(1,1097)	1:100:A:LEU:HD21	1:100:A:LEU:HD12	14	0.18
(1,1097)	1:100:A:LEU:HD23	1:100:A:LEU:HD11	16	0.18
(1,1097)	1:100:A:LEU:HD22	1:100:A:LEU:HD11	17	0.18
(1,1094)	1:100:A:LEU:HD22	1:138:A:SER:HB2	2	0.18
(1,1091)	1:100:A:LEU:HD22	1:92:A:GLN:HE21	16	0.18
(1,1091)	1:100:A:LEU:HD21	1:92:A:GLN:HE21	17	0.18
(1,1091)	1:100:A:LEU:HD23	1:92:A:GLN:HE21	22	0.18
(1,1072)	1:101:A:ALA:HB1	1:58:A:CYS:HA	3	0.18
(1,1072)	1:101:A:ALA:HB2	1:58:A:CYS:HA	23	0.18
(1,1068)	1:101:A:ALA:HB2	1:59:A:TYR:H	23	0.18
(1,1061)	1:103:A:ALA:HB1	1:106:A:CYS:HB3	12	0.18
(1,1036)	1:62:A:GLU:HB3	1:62:A:GLU:H	17	0.18
(1,1036)	1:62:A:GLU:HB3	1:62:A:GLU:H	22	0.18
(1,1027)	1:67:A:PHE:HE1	1:109:A:LEU:HD23	13	0.18
(1,998)	1:108:A:ILE:HD12	1:105:A:PHE:HD1	3	0.18
(1,998)	1:108:A:ILE:HD13	1:105:A:PHE:HD1	18	0.18
(1,991)	1:108:A:ILE:HA	1:108:A:ILE:HG23	13	0.18
(1,991)	1:108:A:ILE:HA	1:108:A:ILE:HG22	22	0.18
(1,991)	1:108:A:ILE:HA	1:108:A:ILE:HG22	25	0.18
(1,960)	1:67:A:PHE:HA	1:109:A:LEU:HD11	21	0.18
(1,944)	1:110:A:SER:HB2	1:110:A:SER:H	1	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,944)	1:110:A:SER:HB2	1:110:A:SER:H	4	0.18
(1,944)	1:110:A:SER:HB2	1:110:A:SER:H	10	0.18
(1,944)	1:110:A:SER:HB2	1:110:A:SER:H	11	0.18
(1,944)	1:110:A:SER:HB2	1:110:A:SER:H	12	0.18
(1,944)	1:110:A:SER:HB2	1:110:A:SER:H	19	0.18
(1,944)	1:110:A:SER:HB2	1:110:A:SER:H	20	0.18
(1,944)	1:110:A:SER:HB2	1:110:A:SER:H	25	0.18
(1,913)	1:113:A:LEU:HG	1:113:A:LEU:H	2	0.18
(1,873)	1:118:A:SER:HB2	1:119:A:ARG:H	8	0.18
(1,873)	1:118:A:SER:HB2	1:119:A:ARG:H	15	0.18
(1,873)	1:118:A:SER:HB2	1:119:A:ARG:H	17	0.18
(1,873)	1:118:A:SER:HB2	1:119:A:ARG:H	18	0.18
(1,873)	1:118:A:SER:HB2	1:119:A:ARG:H	24	0.18
(1,827)	1:122:A:LYS:HD2	1:122:A:LYS:HA	11	0.18
(1,813)	1:123:A:LEU:HD21	1:124:A:TYR:HE2	24	0.18
(1,812)	1:123:A:LEU:HD21	1:77:A:GLN:HE21	13	0.18
(1,811)	1:123:A:LEU:HD22	1:70:A:PHE:HE1	20	0.18
(1,811)	1:123:A:LEU:HD23	1:70:A:PHE:HE1	25	0.18
(1,789)	1:124:A:TYR:HD1	1:124:A:TYR:HE1	12	0.18
(1,789)	1:124:A:TYR:HD1	1:124:A:TYR:HE1	14	0.18
(1,789)	1:124:A:TYR:HD1	1:124:A:TYR:HE1	15	0.18
(1,789)	1:124:A:TYR:HD1	1:124:A:TYR:HE1	23	0.18
(1,778)	1:125:A:VAL:HG22	1:122:A:LYS:HA	14	0.18
(1,775)	1:126:A:TYR:HE1	1:125:A:VAL:HG13	15	0.18
(1,775)	1:126:A:TYR:HE1	1:125:A:VAL:HG12	23	0.18
(1,746)	1:127:A:ILE:HD11	1:127:A:ILE:H	24	0.18
(1,702)	1:85:A:VAL:HG22	1:85:A:VAL:HA	2	0.18
(1,702)	1:85:A:VAL:HG23	1:85:A:VAL:HA	3	0.18
(1,702)	1:85:A:VAL:HG21	1:85:A:VAL:HA	5	0.18
(1,702)	1:85:A:VAL:HG23	1:85:A:VAL:HA	20	0.18
(1,702)	1:85:A:VAL:HG22	1:85:A:VAL:HA	25	0.18
(1,672)	1:133:A:VAL:HG23	1:137:A:HIS:HD2	2	0.18
(1,672)	1:133:A:VAL:HG21	1:137:A:HIS:HD2	7	0.18
(1,672)	1:133:A:VAL:HG22	1:137:A:HIS:HD2	24	0.18
(1,634)	1:134:A:LEU:HD12	1:134:A:LEU:H	11	0.18
(1,634)	1:134:A:LEU:HD11	1:134:A:LEU:H	14	0.18
(1,618)	1:56:A:LYS:HG2	1:57:A:LYS:H	14	0.18
(1,596)	1:137:A:HIS:HA	1:138:A:SER:H	4	0.18
(1,596)	1:137:A:HIS:HA	1:138:A:SER:H	21	0.18
(1,551)	2:34:B:TYR:H	2:35:B:PHE:HA	2	0.18
(1,551)	2:34:B:TYR:H	2:35:B:PHE:HA	19	0.18
(1,551)	2:34:B:TYR:H	2:35:B:PHE:HA	23	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,540)	1:63:A:ASN:H	1:61:A:LEU:HG	7	0.18
(1,540)	1:63:A:ASN:H	1:61:A:LEU:HG	9	0.18
(1,540)	1:63:A:ASN:H	1:61:A:LEU:HG	11	0.18
(1,540)	1:63:A:ASN:H	1:61:A:LEU:HG	12	0.18
(1,522)	1:70:A:PHE:H	1:73:A:LEU:H	1	0.18
(1,522)	1:70:A:PHE:H	1:73:A:LEU:H	15	0.18
(1,521)	1:71:A:LEU:H	1:113:A:LEU:HD13	16	0.18
(1,520)	1:130:A:LEU:H	1:112:A:VAL:HG22	8	0.18
(1,509)	1:77:A:GLN:HE22	1:73:A:LEU:HG	16	0.18
(1,505)	1:79:A:ALA:H	1:76:A:MET:HA	9	0.18
(1,505)	1:79:A:ALA:H	1:76:A:MET:HA	21	0.18
(1,490)	1:91:A:ARG:H	1:94:A:ARG:H	12	0.18
(1,475)	1:98:A:LEU:HD22	1:98:A:LEU:H	20	0.18
(1,438)	1:66:A:LEU:HD11	1:66:A:LEU:H	1	0.18
(1,438)	1:66:A:LEU:HD12	1:66:A:LEU:H	3	0.18
(1,438)	1:66:A:LEU:HD11	1:66:A:LEU:H	9	0.18
(1,414)	1:72:A:GLU:H	1:68:A:GLU:HA	21	0.18
(1,410)	1:134:A:LEU:H	1:132:A:THR:H	13	0.18
(1,410)	1:134:A:LEU:H	1:132:A:THR:H	14	0.18
(1,410)	1:134:A:LEU:H	1:132:A:THR:H	22	0.18
(1,394)	1:137:A:HIS:HB3	1:138:A:SER:H	14	0.18
(1,394)	1:137:A:HIS:HB3	1:138:A:SER:H	20	0.18
(1,392)	1:139:A:ALA:H	1:96:A:HIS:HD2	4	0.18
(1,374)	2:28:B:ASP:HB3	1:128:A:ASN:HA	20	0.18
(1,369)	2:26:B:ASP:HB2	2:33:B:GLN:HE21	8	0.18
(1,367)	2:26:B:ASP:HB3	2:31:B:LEU:H	20	0.18
(1,361)	2:29:B:SER:HB2	2:32:B:GLU:HG3	13	0.18
(1,361)	2:29:B:SER:HB2	2:32:B:GLU:HG3	18	0.18
(1,361)	2:29:B:SER:HB2	2:32:B:GLU:HG3	22	0.18
(1,337)	2:31:B:LEU:HD21	2:28:B:ASP:HB2	13	0.18
(1,337)	2:31:B:LEU:HD22	2:28:B:ASP:HB2	22	0.18
(1,313)	2:35:B:PHE:HE2	1:81:A:HIS:HB3	11	0.18
(1,288)	2:32:B:GLU:HA	2:35:B:PHE:HD1	2	0.18
(1,275)	1:84:A:VAL:HG11	2:35:B:PHE:HE1	10	0.18
(1,274)	1:87:A:PHE:HD2	2:34:B:TYR:HE1	10	0.18
(1,264)	1:127:A:ILE:HG21	2:35:B:PHE:HE1	1	0.18
(1,264)	1:127:A:ILE:HG21	2:35:B:PHE:HE1	2	0.18
(1,264)	1:127:A:ILE:HG21	2:35:B:PHE:HE1	6	0.18
(1,264)	1:127:A:ILE:HG22	2:35:B:PHE:HE1	8	0.18
(1,264)	1:127:A:ILE:HG22	2:35:B:PHE:HE1	23	0.18
(1,262)	1:80:A:ASP:HB2	1:81:A:HIS:HD2	2	0.18
(1,253)	1:57:A:LYS:HE2	1:54:A:MET:HG3	24	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,244)	1:111:A:ARG:HA	1:115:A:ARG:HG2	10	0.18
(1,233)	1:62:A:GLU:HG2	1:66:A:LEU:HD13	24	0.18
(1,157)	1:130:A:LEU:HD21	1:88:A:LEU:HD13	17	0.18
(1,147)	1:137:A:HIS:HB3	1:138:A:SER:H	18	0.18
(1,145)	1:88:A:LEU:HB3	1:85:A:VAL:HA	3	0.18
(1,141)	1:93:A:GLN:HG2	1:89:A:TYR:HD1	4	0.18
(1,139)	1:128:A:ASN:HB2	1:128:A:ASN:HD22	3	0.18
(1,139)	1:128:A:ASN:HB2	1:128:A:ASN:HD22	13	0.18
(1,111)	1:62:A:GLU:HB3	1:59:A:TYR:HD2	6	0.18
(1,107)	1:69:A:GLU:HA	1:69:A:GLU:HB3	18	0.18
(1,95)	1:107:A:ASN:HB2	1:108:A:ILE:HB	19	0.18
(1,83)	1:113:A:LEU:HA	1:116:A:ALA:HB3	7	0.18
(1,76)	1:118:A:SER:HA	1:118:A:SER:HB2	10	0.18
(1,76)	1:118:A:SER:HA	1:118:A:SER:HB2	19	0.18
(1,62)	1:123:A:LEU:HD22	1:70:A:PHE:HE1	18	0.18
(1,52)	1:125:A:VAL:HG11	1:128:A:ASN:HB2	14	0.18
(1,36)	1:127:A:ILE:HG22	1:124:A:TYR:HD2	14	0.18
(1,2244)	2:36:B:THR:HG22	2:36:B:THR:H	13	0.17
(1,2244)	2:36:B:THR:HG23	2:36:B:THR:H	19	0.17
(1,2207)	2:38:B:ARG:HB2	2:39:B:TRP:H	24	0.17
(1,2194)	1:56:A:LYS:HB3	1:56:A:LYS:H	3	0.17
(1,2108)	1:77:A:GLN:H	1:78:A:THR:HG22	12	0.17
(1,2107)	1:77:A:GLN:H	1:77:A:GLN:HB3	6	0.17
(1,2107)	1:77:A:GLN:H	1:77:A:GLN:HB3	18	0.17
(1,2107)	1:77:A:GLN:H	1:77:A:GLN:HB3	22	0.17
(1,2107)	1:77:A:GLN:H	1:77:A:GLN:HB3	24	0.17
(1,2106)	1:76:A:MET:HB3	1:77:A:GLN:H	19	0.17
(1,2100)	1:77:A:GLN:HE21	1:76:A:MET:HE2	13	0.17
(1,2075)	1:81:A:HIS:H	1:81:A:HIS:HD2	22	0.17
(1,2032)	1:90:A:ASN:HD22	1:93:A:GLN:HB2	10	0.17
(1,1987)	1:99:A:PHE:H	1:99:A:PHE:HD2	11	0.17
(1,1987)	1:99:A:PHE:H	1:99:A:PHE:HD2	21	0.17
(1,1975)	1:100:A:LEU:HD13	1:100:A:LEU:H	9	0.17
(1,1837)	1:127:A:ILE:H	1:123:A:LEU:HD13	20	0.17
(1,1803)	1:135:A:LYS:HB3	1:135:A:LYS:H	10	0.17
(1,1803)	1:135:A:LYS:HB3	1:135:A:LYS:H	20	0.17
(1,1789)	1:139:A:ALA:H	1:139:A:ALA:HB2	11	0.17
(1,1781)	1:140:A:LYS:H	1:141:A:LYS:HB3	5	0.17
(1,1781)	1:140:A:LYS:H	1:141:A:LYS:HB3	22	0.17
(1,1771)	1:142:A:LYS:H	1:142:A:LYS:HD2	7	0.17
(1,1759)	2:30:B:GLU:HA	2:30:B:GLU:HG3	24	0.17
(1,1753)	2:27:B:SER:HB2	2:27:B:SER:HA	8	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1753)	2:27:B:SER:HB2	2:27:B:SER:HA	25	0.17
(1,1751)	2:27:B:SER:HA	2:28:B:ASP:H	15	0.17
(1,1745)	2:29:B:SER:HB3	2:30:B:GLU:H	5	0.17
(1,1725)	2:31:B:LEU:HD22	1:127:A:ILE:HG21	9	0.17
(1,1721)	2:31:B:LEU:HD21	2:31:B:LEU:HA	2	0.17
(1,1721)	2:31:B:LEU:HD21	2:31:B:LEU:HA	4	0.17
(1,1721)	2:31:B:LEU:HD22	2:31:B:LEU:HA	6	0.17
(1,1718)	2:31:B:LEU:HD22	2:32:B:GLU:H	11	0.17
(1,1708)	2:32:B:GLU:HG2	2:39:B:TRP:HZ2	11	0.17
(1,1705)	2:33:B:GLN:HA	2:34:B:TYR:H	1	0.17
(1,1705)	2:33:B:GLN:HA	2:34:B:TYR:H	3	0.17
(1,1705)	2:33:B:GLN:HA	2:34:B:TYR:H	11	0.17
(1,1705)	2:33:B:GLN:HA	2:34:B:TYR:H	13	0.17
(1,1705)	2:33:B:GLN:HA	2:34:B:TYR:H	14	0.17
(1,1705)	2:33:B:GLN:HA	2:34:B:TYR:H	15	0.17
(1,1705)	2:33:B:GLN:HA	2:34:B:TYR:H	20	0.17
(1,1703)	2:33:B:GLN:HG2	2:31:B:LEU:HD23	11	0.17
(1,1702)	2:33:B:GLN:HG3	2:34:B:TYR:HE2	3	0.17
(1,1702)	2:33:B:GLN:HG3	2:34:B:TYR:HE2	24	0.17
(1,1670)	2:37:B:ALA:HB3	2:36:B:THR:HA	18	0.17
(1,1666)	2:36:B:THR:HG21	1:124:A:TYR:H	11	0.17
(1,1666)	2:36:B:THR:HG21	1:124:A:TYR:H	18	0.17
(1,1666)	2:36:B:THR:HG22	1:124:A:TYR:H	25	0.17
(1,1648)	2:38:B:ARG:HA	2:37:B:ALA:HB1	6	0.17
(1,1636)	2:35:B:PHE:HB3	2:34:B:TYR:HE1	17	0.17
(1,1636)	2:35:B:PHE:HB3	2:34:B:TYR:HE1	22	0.17
(1,1634)	2:38:B:ARG:HD2	2:37:B:ALA:HB3	12	0.17
(1,1606)	2:32:B:GLU:HA	2:32:B:GLU:HB2	8	0.17
(1,1606)	2:32:B:GLU:HA	2:32:B:GLU:HB2	18	0.17
(1,1595)	2:31:B:LEU:HD12	1:127:A:ILE:HB	7	0.17
(1,1592)	1:84:A:VAL:HG22	2:35:B:PHE:HB2	23	0.17
(1,1591)	1:84:A:VAL:HA	2:31:B:LEU:HD12	22	0.17
(1,1588)	1:87:A:PHE:HB2	2:31:B:LEU:HD11	16	0.17
(1,1558)	1:57:A:LYS:HB2	1:57:A:LYS:HG3	20	0.17
(1,1554)	1:59:A:TYR:HE1	1:57:A:LYS:HB2	11	0.17
(1,1549)	1:58:A:CYS:HB2	1:57:A:LYS:HA	11	0.17
(1,1486)	1:65:A:LYS:HA	1:65:A:LYS:HB2	1	0.17
(1,1486)	1:65:A:LYS:HA	1:65:A:LYS:HB2	6	0.17
(1,1456)	1:69:A:GLU:HG2	1:66:A:LEU:HA	19	0.17
(1,1440)	1:127:A:ILE:HD13	1:70:A:PHE:HZ	5	0.17
(1,1432)	1:70:A:PHE:HA	1:70:A:PHE:HD1	11	0.17
(1,1395)	1:116:A:ALA:HB3	1:73:A:LEU:HD23	9	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1391)	1:74:A:CYS:HA	1:73:A:LEU:HD22	24	0.17
(1,1367)	1:75:A:LYS:HD2	1:75:A:LYS:HA	12	0.17
(1,1367)	1:75:A:LYS:HD2	1:75:A:LYS:HA	14	0.17
(1,1350)	1:76:A:MET:HB3	1:76:A:MET:HG3	1	0.17
(1,1350)	1:76:A:MET:HB3	1:76:A:MET:HG3	3	0.17
(1,1350)	1:76:A:MET:HB3	1:76:A:MET:HG3	4	0.17
(1,1350)	1:76:A:MET:HB3	1:76:A:MET:HG3	5	0.17
(1,1350)	1:76:A:MET:HB3	1:76:A:MET:HG3	6	0.17
(1,1350)	1:76:A:MET:HB3	1:76:A:MET:HG3	7	0.17
(1,1350)	1:76:A:MET:HB3	1:76:A:MET:HG3	8	0.17
(1,1350)	1:76:A:MET:HB3	1:76:A:MET:HG3	9	0.17
(1,1350)	1:76:A:MET:HB3	1:76:A:MET:HG3	13	0.17
(1,1350)	1:76:A:MET:HB3	1:76:A:MET:HG3	14	0.17
(1,1350)	1:76:A:MET:HB3	1:76:A:MET:HG3	16	0.17
(1,1350)	1:76:A:MET:HB3	1:76:A:MET:HG3	17	0.17
(1,1350)	1:76:A:MET:HB3	1:76:A:MET:HG3	18	0.17
(1,1350)	1:76:A:MET:HB3	1:76:A:MET:HG3	19	0.17
(1,1350)	1:76:A:MET:HB3	1:76:A:MET:HG3	20	0.17
(1,1350)	1:76:A:MET:HB3	1:76:A:MET:HG3	21	0.17
(1,1350)	1:76:A:MET:HB3	1:76:A:MET:HG3	23	0.17
(1,1350)	1:76:A:MET:HB3	1:76:A:MET:HG3	24	0.17
(1,1350)	1:76:A:MET:HB3	1:76:A:MET:HG3	25	0.17
(1,1346)	1:76:A:MET:HG2	1:73:A:LEU:HA	14	0.17
(1,1346)	1:76:A:MET:HG2	1:73:A:LEU:HA	21	0.17
(1,1346)	1:76:A:MET:HG2	1:73:A:LEU:HA	23	0.17
(1,1329)	1:77:A:GLN:HG2	1:77:A:GLN:HB3	11	0.17
(1,1319)	1:77:A:GLN:HB3	1:78:A:THR:H	11	0.17
(1,1319)	1:77:A:GLN:HB3	1:78:A:THR:H	14	0.17
(1,1317)	1:79:A:ALA:HB1	1:76:A:MET:HA	19	0.17
(1,1317)	1:79:A:ALA:HB3	1:76:A:MET:HA	21	0.17
(1,1317)	1:79:A:ALA:HB2	1:76:A:MET:HA	23	0.17
(1,1316)	1:79:A:ALA:HB2	1:79:A:ALA:H	12	0.17
(1,1283)	1:84:A:VAL:HG21	1:127:A:ILE:HD13	3	0.17
(1,1283)	1:84:A:VAL:HG23	1:127:A:ILE:HD12	13	0.17
(1,1275)	1:78:A:THR:HG21	1:77:A:GLN:HB3	21	0.17
(1,1247)	1:88:A:LEU:HD12	1:85:A:VAL:HA	11	0.17
(1,1171)	1:91:A:ARG:HG2	1:91:A:ARG:HA	11	0.17
(1,1171)	1:91:A:ARG:HG2	1:91:A:ARG:HA	24	0.17
(1,1142)	1:94:A:ARG:HD3	1:94:A:ARG:HB2	4	0.17
(1,1133)	1:95:A:ALA:HB1	1:99:A:PHE:HD2	15	0.17
(1,1133)	1:95:A:ALA:HB3	1:99:A:PHE:HD2	19	0.17
(1,1118)	1:98:A:LEU:HB3	1:98:A:LEU:HD23	7	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1118)	1:98:A:LEU:HB3	1:98:A:LEU:HD23	8	0.17
(1,1118)	1:98:A:LEU:HB3	1:98:A:LEU:HD23	22	0.17
(1,1097)	1:100:A:LEU:HD22	1:100:A:LEU:HD12	4	0.17
(1,1097)	1:100:A:LEU:HD21	1:100:A:LEU:HD12	13	0.17
(1,1097)	1:100:A:LEU:HD21	1:100:A:LEU:HD12	22	0.17
(1,1097)	1:100:A:LEU:HD22	1:100:A:LEU:HD12	25	0.17
(1,1091)	1:100:A:LEU:HD23	1:92:A:GLN:HE21	15	0.17
(1,1074)	1:101:A:ALA:HB2	1:60:A:LYS:HA	18	0.17
(1,1072)	1:101:A:ALA:HB1	1:58:A:CYS:HA	20	0.17
(1,1068)	1:101:A:ALA:HB2	1:59:A:TYR:H	4	0.17
(1,1061)	1:103:A:ALA:HB1	1:106:A:CYS:HB3	23	0.17
(1,1027)	1:67:A:PHE:HE1	1:109:A:LEU:HD21	3	0.17
(1,1000)	1:108:A:ILE:HD12	1:99:A:PHE:HE1	2	0.17
(1,996)	1:108:A:ILE:HG23	1:112:A:VAL:HG12	10	0.17
(1,995)	1:108:A:ILE:HG22	1:130:A:LEU:HD13	7	0.17
(1,991)	1:108:A:ILE:HA	1:108:A:ILE:HG23	2	0.17
(1,991)	1:108:A:ILE:HA	1:108:A:ILE:HG22	9	0.17
(1,991)	1:108:A:ILE:HA	1:108:A:ILE:HG23	15	0.17
(1,991)	1:108:A:ILE:HA	1:108:A:ILE:HG23	18	0.17
(1,944)	1:110:A:SER:HB2	1:110:A:SER:H	17	0.17
(1,930)	1:126:A:TYR:HD1	1:112:A:VAL:HG13	14	0.17
(1,930)	1:126:A:TYR:HD1	1:112:A:VAL:HG11	17	0.17
(1,922)	1:112:A:VAL:HA	1:115:A:ARG:HG3	25	0.17
(1,913)	1:113:A:LEU:HG	1:113:A:LEU:H	11	0.17
(1,913)	1:113:A:LEU:HG	1:113:A:LEU:H	18	0.17
(1,911)	1:113:A:LEU:HB2	1:113:A:LEU:H	11	0.17
(1,909)	1:114:A:SER:HB2	1:113:A:LEU:HG	8	0.17
(1,909)	1:114:A:SER:HB2	1:113:A:LEU:HG	10	0.17
(1,904)	1:115:A:ARG:HD3	1:126:A:TYR:HE1	21	0.17
(1,881)	1:117:A:ARG:HD2	1:117:A:ARG:HB3	24	0.17
(1,878)	1:117:A:ARG:HG2	1:114:A:SER:HA	22	0.17
(1,873)	1:118:A:SER:HB2	1:119:A:ARG:H	10	0.17
(1,814)	1:123:A:LEU:HD21	1:120:A:PRO:HA	14	0.17
(1,812)	1:123:A:LEU:HD23	1:77:A:GLN:HE21	2	0.17
(1,812)	1:123:A:LEU:HD21	1:77:A:GLN:HE21	20	0.17
(1,811)	1:123:A:LEU:HD21	1:70:A:PHE:HE1	8	0.17
(1,789)	1:124:A:TYR:HD1	1:124:A:TYR:HE1	1	0.17
(1,789)	1:124:A:TYR:HD1	1:124:A:TYR:HE1	2	0.17
(1,789)	1:124:A:TYR:HD1	1:124:A:TYR:HE1	3	0.17
(1,789)	1:124:A:TYR:HD1	1:124:A:TYR:HE1	6	0.17
(1,789)	1:124:A:TYR:HD1	1:124:A:TYR:HE1	7	0.17
(1,789)	1:124:A:TYR:HD1	1:124:A:TYR:HE1	8	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,789)	1:124:A:TYR:HD1	1:124:A:TYR:HE1	9	0.17
(1,789)	1:124:A:TYR:HD1	1:124:A:TYR:HE1	11	0.17
(1,789)	1:124:A:TYR:HD1	1:124:A:TYR:HE1	17	0.17
(1,789)	1:124:A:TYR:HD1	1:124:A:TYR:HE1	18	0.17
(1,789)	1:124:A:TYR:HD1	1:124:A:TYR:HE1	19	0.17
(1,789)	1:124:A:TYR:HD1	1:124:A:TYR:HE1	20	0.17
(1,789)	1:124:A:TYR:HD1	1:124:A:TYR:HE1	21	0.17
(1,789)	1:124:A:TYR:HD1	1:124:A:TYR:HE1	22	0.17
(1,789)	1:124:A:TYR:HD1	1:124:A:TYR:HE1	25	0.17
(1,775)	1:126:A:TYR:HE1	1:125:A:VAL:HG13	19	0.17
(1,775)	1:126:A:TYR:HE1	1:125:A:VAL:HG11	22	0.17
(1,773)	1:125:A:VAL:HA	1:125:A:VAL:HG11	6	0.17
(1,757)	1:126:A:TYR:HD1	1:126:A:TYR:HB2	24	0.17
(1,706)	1:85:A:VAL:HG21	1:75:A:LYS:HD2	15	0.17
(1,704)	1:130:A:LEU:HD12	1:109:A:LEU:HD23	10	0.17
(1,704)	1:130:A:LEU:HD11	1:109:A:LEU:HD21	14	0.17
(1,704)	1:130:A:LEU:HD11	1:109:A:LEU:HD21	23	0.17
(1,672)	1:133:A:VAL:HG22	1:137:A:HIS:HD2	17	0.17
(1,634)	1:134:A:LEU:HD13	1:134:A:LEU:H	7	0.17
(1,619)	1:135:A:LYS:HG2	1:91:A:ARG:HD3	18	0.17
(1,604)	1:136:A:ALA:HB1	1:136:A:ALA:H	11	0.17
(1,604)	1:136:A:ALA:HB1	1:136:A:ALA:H	13	0.17
(1,604)	1:136:A:ALA:HB1	1:136:A:ALA:H	14	0.17
(1,604)	1:136:A:ALA:HB2	1:136:A:ALA:H	23	0.17
(1,601)	1:137:A:HIS:HB3	1:137:A:HIS:H	3	0.17
(1,599)	1:137:A:HIS:HA	1:137:A:HIS:HB2	6	0.17
(1,596)	1:137:A:HIS:HA	1:138:A:SER:H	17	0.17
(1,589)	2:27:B:SER:HA	1:132:A:THR:HG21	25	0.17
(1,585)	1:139:A:ALA:HB3	1:140:A:LYS:H	21	0.17
(1,582)	1:139:A:ALA:HA	1:96:A:HIS:HB2	12	0.17
(1,574)	1:143:A:LEU:HG	1:143:A:LEU:H	9	0.17
(1,542)	1:61:A:LEU:HG	1:61:A:LEU:H	17	0.17
(1,542)	1:61:A:LEU:HG	1:61:A:LEU:H	19	0.17
(1,542)	1:61:A:LEU:HG	1:61:A:LEU:H	21	0.17
(1,526)	1:69:A:GLU:H	1:113:A:LEU:HD21	6	0.17
(1,522)	1:70:A:PHE:H	1:73:A:LEU:H	9	0.17
(1,522)	1:70:A:PHE:H	1:73:A:LEU:H	20	0.17
(1,522)	1:70:A:PHE:H	1:73:A:LEU:H	23	0.17
(1,521)	1:71:A:LEU:H	1:113:A:LEU:HD13	5	0.17
(1,512)	1:77:A:GLN:H	1:123:A:LEU:HD22	4	0.17
(1,509)	1:77:A:GLN:HE22	1:73:A:LEU:HG	18	0.17
(1,505)	1:79:A:ALA:H	1:76:A:MET:HA	6	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,505)	1:79:A:ALA:H	1:76:A:MET:HA	7	0.17
(1,505)	1:79:A:ALA:H	1:76:A:MET:HA	18	0.17
(1,500)	1:85:A:VAL:H	1:83:A:GLU:H	12	0.17
(1,492)	1:91:A:ARG:H	1:88:A:LEU:HD22	11	0.17
(1,490)	1:91:A:ARG:H	1:94:A:ARG:H	8	0.17
(1,480)	1:100:A:LEU:HD12	1:95:A:ALA:H	13	0.17
(1,475)	1:98:A:LEU:HD22	1:98:A:LEU:H	8	0.17
(1,469)	1:102:A:SER:H	1:100:A:LEU:HB2	9	0.17
(1,456)	1:112:A:VAL:H	1:108:A:ILE:HG23	4	0.17
(1,456)	1:112:A:VAL:H	1:108:A:ILE:HG22	24	0.17
(1,453)	1:114:A:SER:H	1:113:A:LEU:HD21	17	0.17
(1,448)	1:116:A:ALA:H	1:126:A:TYR:HE2	14	0.17
(1,426)	1:125:A:VAL:HG13	1:126:A:TYR:H	15	0.17
(1,394)	1:137:A:HIS:HB3	1:138:A:SER:H	8	0.17
(1,363)	1:118:A:SER:HB3	1:119:A:ARG:HB2	15	0.17
(1,361)	2:29:B:SER:HB2	2:32:B:GLU:HG3	5	0.17
(1,356)	2:29:B:SER:HB2	2:33:B:GLN:H	9	0.17
(1,343)	2:31:B:LEU:HB2	1:87:A:PHE:HE2	15	0.17
(1,288)	2:32:B:GLU:HA	2:35:B:PHE:HD1	4	0.17
(1,288)	2:32:B:GLU:HA	2:35:B:PHE:HD1	6	0.17
(1,288)	2:32:B:GLU:HA	2:35:B:PHE:HD1	15	0.17
(1,270)	1:88:A:LEU:HD23	2:31:B:LEU:HD12	4	0.17
(1,264)	1:127:A:ILE:HG23	2:35:B:PHE:HE1	4	0.17
(1,264)	1:127:A:ILE:HG23	2:35:B:PHE:HE1	7	0.17
(1,264)	1:127:A:ILE:HG23	2:35:B:PHE:HE1	13	0.17
(1,264)	1:127:A:ILE:HG21	2:35:B:PHE:HE1	16	0.17
(1,262)	1:80:A:ASP:HB2	1:81:A:HIS:HD2	1	0.17
(1,262)	1:80:A:ASP:HB3	1:81:A:HIS:HD2	3	0.17
(1,256)	1:142:A:LYS:HA	1:142:A:LYS:HD2	11	0.17
(1,253)	1:57:A:LYS:HE3	1:54:A:MET:HG2	6	0.17
(1,233)	1:66:A:LEU:HD11	1:63:A:ASN:HB3	10	0.17
(1,210)	1:105:A:PHE:HZ	1:109:A:LEU:HD22	24	0.17
(1,209)	1:67:A:PHE:HE1	1:71:A:LEU:HD22	21	0.17
(1,206)	1:73:A:LEU:HD22	1:117:A:ARG:HD3	9	0.17
(1,198)	2:30:B:GLU:HG3	1:87:A:PHE:HZ	22	0.17
(1,163)	1:67:A:PHE:HD2	1:92:A:GLN:HG3	22	0.17
(1,160)	1:67:A:PHE:HD1	1:68:A:GLU:H	5	0.17
(1,160)	1:67:A:PHE:HD1	1:68:A:GLU:H	7	0.17
(1,160)	1:67:A:PHE:HD1	1:68:A:GLU:H	18	0.17
(1,160)	1:67:A:PHE:HD1	1:68:A:GLU:H	22	0.17
(1,160)	1:67:A:PHE:HD1	1:68:A:GLU:H	24	0.17
(1,157)	1:130:A:LEU:HD22	1:88:A:LEU:HD12	6	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,157)	1:130:A:LEU:HD23	1:88:A:LEU:HD11	11	0.17
(1,157)	1:130:A:LEU:HD21	1:88:A:LEU:HD13	12	0.17
(1,157)	1:130:A:LEU:HD23	1:88:A:LEU:HD13	25	0.17
(1,139)	1:128:A:ASN:HB2	1:128:A:ASN:HD22	14	0.17
(1,139)	1:128:A:ASN:HB2	1:128:A:ASN:HD22	16	0.17
(1,134)	1:105:A:PHE:HE2	1:92:A:GLN:HG2	6	0.17
(1,123)	1:95:A:ALA:HB2	1:134:A:LEU:HB2	5	0.17
(1,123)	1:95:A:ALA:HB2	1:134:A:LEU:HB2	11	0.17
(1,123)	1:95:A:ALA:HB3	1:134:A:LEU:HB2	16	0.17
(1,116)	1:100:A:LEU:HD22	1:105:A:PHE:HE2	10	0.17
(1,116)	1:100:A:LEU:HD23	1:105:A:PHE:HE2	13	0.17
(1,107)	1:69:A:GLU:HA	1:69:A:GLU:HB3	21	0.17
(1,100)	1:67:A:PHE:HE2	1:88:A:LEU:HD11	13	0.17
(1,98)	1:105:A:PHE:HD1	1:100:A:LEU:HD23	4	0.17
(1,98)	1:105:A:PHE:HD1	1:100:A:LEU:HD21	10	0.17
(1,95)	1:107:A:ASN:HB2	1:108:A:ILE:HB	8	0.17
(1,95)	1:107:A:ASN:HB2	1:108:A:ILE:HB	24	0.17
(1,83)	1:113:A:LEU:HA	1:116:A:ALA:HB3	13	0.17
(1,76)	1:118:A:SER:HA	1:118:A:SER:HB2	13	0.17
(1,76)	1:118:A:SER:HA	1:118:A:SER:HB2	22	0.17
(1,66)	1:80:A:ASP:HA	1:80:A:ASP:H	5	0.17
(1,56)	1:124:A:TYR:HE1	2:35:B:PHE:HB3	10	0.17
(1,52)	1:125:A:VAL:HG13	1:128:A:ASN:HB2	17	0.17
(1,52)	1:125:A:VAL:HG12	1:128:A:ASN:HB2	25	0.17
(1,45)	1:59:A:TYR:HE1	1:57:A:LYS:HD2	22	0.17
(1,27)	1:130:A:LEU:HD22	1:67:A:PHE:HA	11	0.17
(1,27)	1:130:A:LEU:HD22	1:67:A:PHE:HA	25	0.17
(1,25)	1:85:A:VAL:HG21	1:74:A:CYS:HB2	18	0.17
(1,25)	1:85:A:VAL:HG21	1:74:A:CYS:HB2	21	0.17
(1,20)	1:61:A:LEU:HA	1:64:A:GLU:HB2	1	0.17
(1,17)	1:133:A:VAL:HG13	1:137:A:HIS:HB2	22	0.17
(1,2196)	1:56:A:LYS:H	1:56:A:LYS:HB2	8	0.16
(1,2188)	1:59:A:TYR:H	1:58:A:CYS:HB3	24	0.16
(1,2153)	1:109:A:LEU:HD11	1:66:A:LEU:H	20	0.16
(1,2136)	1:69:A:GLU:H	1:70:A:PHE:HB2	17	0.16
(1,2107)	1:77:A:GLN:H	1:77:A:GLN:HB3	1	0.16
(1,2107)	1:77:A:GLN:H	1:77:A:GLN:HB3	3	0.16
(1,2107)	1:77:A:GLN:H	1:77:A:GLN:HB3	4	0.16
(1,2107)	1:77:A:GLN:H	1:77:A:GLN:HB3	5	0.16
(1,2107)	1:77:A:GLN:H	1:77:A:GLN:HB3	7	0.16
(1,2107)	1:77:A:GLN:H	1:77:A:GLN:HB3	13	0.16
(1,2107)	1:77:A:GLN:H	1:77:A:GLN:HB3	15	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2107)	1:77:A:GLN:H	1:77:A:GLN:HB3	23	0.16
(1,2107)	1:77:A:GLN:H	1:77:A:GLN:HB3	25	0.16
(1,2080)	1:81:A:HIS:H	1:81:A:HIS:HB3	17	0.16
(1,2080)	1:81:A:HIS:H	1:81:A:HIS:HB3	20	0.16
(1,2054)	1:85:A:VAL:HG13	1:89:A:TYR:H	14	0.16
(1,2032)	1:90:A:ASN:HD22	1:93:A:GLN:HB2	8	0.16
(1,2032)	1:90:A:ASN:HD22	1:93:A:GLN:HB2	12	0.16
(1,2032)	1:90:A:ASN:HD22	1:93:A:GLN:HB2	24	0.16
(1,2031)	1:91:A:ARG:H	1:134:A:LEU:HD13	13	0.16
(1,2005)	1:95:A:ALA:H	1:94:A:ARG:HG2	18	0.16
(1,2004)	1:95:A:ALA:H	1:94:A:ARG:HB3	16	0.16
(1,1987)	1:99:A:PHE:H	1:99:A:PHE:HD2	9	0.16
(1,1987)	1:99:A:PHE:H	1:99:A:PHE:HD2	16	0.16
(1,1975)	1:100:A:LEU:HD12	1:100:A:LEU:H	3	0.16
(1,1967)	1:102:A:SER:H	1:101:A:ALA:H	22	0.16
(1,1961)	1:102:A:SER:H	1:59:A:TYR:HD1	4	0.16
(1,1837)	1:127:A:ILE:H	1:123:A:LEU:HD12	3	0.16
(1,1837)	1:127:A:ILE:H	1:123:A:LEU:HD12	4	0.16
(1,1837)	1:127:A:ILE:H	1:123:A:LEU:HD11	14	0.16
(1,1803)	1:135:A:LYS:HB3	1:135:A:LYS:H	3	0.16
(1,1803)	1:135:A:LYS:HB3	1:135:A:LYS:H	11	0.16
(1,1803)	1:135:A:LYS:HB3	1:135:A:LYS:H	16	0.16
(1,1781)	1:140:A:LYS:H	1:141:A:LYS:HB3	4	0.16
(1,1781)	1:140:A:LYS:H	1:141:A:LYS:HB3	19	0.16
(1,1769)	2:26:B:ASP:HB3	2:30:B:GLU:HG3	9	0.16
(1,1745)	2:29:B:SER:HB3	2:30:B:GLU:H	3	0.16
(1,1725)	2:31:B:LEU:HD21	1:127:A:ILE:HG21	18	0.16
(1,1721)	2:31:B:LEU:HD21	2:31:B:LEU:HA	7	0.16
(1,1721)	2:31:B:LEU:HD23	2:31:B:LEU:HA	8	0.16
(1,1721)	2:31:B:LEU:HD21	2:31:B:LEU:HA	9	0.16
(1,1721)	2:31:B:LEU:HD22	2:31:B:LEU:HA	13	0.16
(1,1721)	2:31:B:LEU:HD23	2:31:B:LEU:HA	22	0.16
(1,1718)	2:31:B:LEU:HD22	2:32:B:GLU:H	8	0.16
(1,1718)	2:31:B:LEU:HD23	2:32:B:GLU:H	16	0.16
(1,1705)	2:33:B:GLN:HA	2:34:B:TYR:H	4	0.16
(1,1705)	2:33:B:GLN:HA	2:34:B:TYR:H	5	0.16
(1,1705)	2:33:B:GLN:HA	2:34:B:TYR:H	8	0.16
(1,1705)	2:33:B:GLN:HA	2:34:B:TYR:H	9	0.16
(1,1705)	2:33:B:GLN:HA	2:34:B:TYR:H	10	0.16
(1,1705)	2:33:B:GLN:HA	2:34:B:TYR:H	16	0.16
(1,1705)	2:33:B:GLN:HA	2:34:B:TYR:H	18	0.16
(1,1705)	2:33:B:GLN:HA	2:34:B:TYR:H	25	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1667)	2:36:B:THR:HB	2:36:B:THR:H	14	0.16
(1,1636)	2:35:B:PHE:HB3	2:34:B:TYR:HE1	14	0.16
(1,1636)	2:35:B:PHE:HB3	2:34:B:TYR:HE1	19	0.16
(1,1635)	2:39:B:TRP:HA	2:38:B:ARG:HD2	24	0.16
(1,1617)	2:39:B:TRP:HD1	2:38:B:ARG:HA	5	0.16
(1,1615)	2:39:B:TRP:HE3	2:36:B:THR:HG22	3	0.16
(1,1595)	2:31:B:LEU:HD13	1:127:A:ILE:HB	18	0.16
(1,1595)	2:31:B:LEU:HD12	1:127:A:ILE:HB	22	0.16
(1,1595)	2:31:B:LEU:HD12	1:127:A:ILE:HB	24	0.16
(1,1591)	1:84:A:VAL:HA	2:31:B:LEU:HD13	19	0.16
(1,1588)	1:87:A:PHE:HB2	2:31:B:LEU:HD12	11	0.16
(1,1556)	1:57:A:LYS:HG2	1:57:A:LYS:HA	25	0.16
(1,1553)	1:59:A:TYR:HD1	1:57:A:LYS:HB2	5	0.16
(1,1552)	1:57:A:LYS:HB2	1:57:A:LYS:HA	7	0.16
(1,1552)	1:57:A:LYS:HB2	1:57:A:LYS:HA	11	0.16
(1,1552)	1:57:A:LYS:HB2	1:57:A:LYS:HA	16	0.16
(1,1552)	1:57:A:LYS:HB2	1:57:A:LYS:HA	17	0.16
(1,1552)	1:57:A:LYS:HB2	1:57:A:LYS:HA	21	0.16
(1,1550)	1:141:A:LYS:HG2	1:141:A:LYS:HA	24	0.16
(1,1549)	1:58:A:CYS:HB2	1:57:A:LYS:HA	24	0.16
(1,1536)	1:59:A:TYR:HD1	1:59:A:TYR:HA	1	0.16
(1,1536)	1:59:A:TYR:HD1	1:59:A:TYR:HA	18	0.16
(1,1512)	1:62:A:GLU:HG2	1:62:A:GLU:H	7	0.16
(1,1486)	1:65:A:LYS:HA	1:65:A:LYS:HB2	5	0.16
(1,1486)	1:65:A:LYS:HA	1:65:A:LYS:HB2	14	0.16
(1,1456)	1:69:A:GLU:HG2	1:66:A:LEU:HA	4	0.16
(1,1446)	1:69:A:GLU:HG2	1:69:A:GLU:H	12	0.16
(1,1440)	1:127:A:ILE:HD13	1:70:A:PHE:HZ	20	0.16
(1,1432)	1:70:A:PHE:HA	1:70:A:PHE:HD1	5	0.16
(1,1432)	1:70:A:PHE:HA	1:70:A:PHE:HD1	7	0.16
(1,1423)	1:71:A:LEU:HD22	1:70:A:PHE:HD1	3	0.16
(1,1395)	1:116:A:ALA:HB2	1:73:A:LEU:HD21	7	0.16
(1,1391)	1:74:A:CYS:HA	1:73:A:LEU:HD21	6	0.16
(1,1391)	1:74:A:CYS:HA	1:73:A:LEU:HD22	25	0.16
(1,1371)	1:75:A:LYS:HE3	1:72:A:GLU:HG2	2	0.16
(1,1367)	1:75:A:LYS:HD2	1:75:A:LYS:HA	13	0.16
(1,1367)	1:75:A:LYS:HD2	1:75:A:LYS:HA	19	0.16
(1,1356)	1:75:A:LYS:HA	1:75:A:LYS:HG2	3	0.16
(1,1356)	1:75:A:LYS:HA	1:75:A:LYS:HG2	4	0.16
(1,1350)	1:76:A:MET:HB3	1:76:A:MET:HG3	2	0.16
(1,1350)	1:76:A:MET:HB3	1:76:A:MET:HG3	10	0.16
(1,1350)	1:76:A:MET:HB3	1:76:A:MET:HG3	11	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1350)	1:76:A:MET:HB3	1:76:A:MET:HG3	12	0.16
(1,1350)	1:76:A:MET:HB3	1:76:A:MET:HG3	15	0.16
(1,1350)	1:76:A:MET:HB3	1:76:A:MET:HG3	22	0.16
(1,1346)	1:76:A:MET:HG2	1:73:A:LEU:HA	3	0.16
(1,1346)	1:76:A:MET:HG2	1:73:A:LEU:HA	6	0.16
(1,1346)	1:76:A:MET:HG2	1:73:A:LEU:HA	12	0.16
(1,1346)	1:76:A:MET:HG2	1:73:A:LEU:HA	18	0.16
(1,1346)	1:76:A:MET:HG2	1:73:A:LEU:HA	22	0.16
(1,1346)	1:76:A:MET:HG2	1:73:A:LEU:HA	24	0.16
(1,1346)	1:76:A:MET:HG2	1:73:A:LEU:HA	25	0.16
(1,1345)	1:76:A:MET:HG2	1:77:A:GLN:H	17	0.16
(1,1343)	1:76:A:MET:HG2	1:76:A:MET:H	1	0.16
(1,1343)	1:76:A:MET:HG2	1:76:A:MET:H	2	0.16
(1,1343)	1:76:A:MET:HG2	1:76:A:MET:H	19	0.16
(1,1319)	1:77:A:GLN:HB3	1:78:A:THR:H	17	0.16
(1,1319)	1:77:A:GLN:HB3	1:78:A:THR:H	18	0.16
(1,1319)	1:77:A:GLN:HB3	1:78:A:THR:H	21	0.16
(1,1319)	1:77:A:GLN:HB3	1:78:A:THR:H	25	0.16
(1,1316)	1:79:A:ALA:HB2	1:79:A:ALA:H	3	0.16
(1,1316)	1:79:A:ALA:HB1	1:79:A:ALA:H	6	0.16
(1,1315)	1:79:A:ALA:HB2	1:80:A:ASP:H	1	0.16
(1,1315)	1:79:A:ALA:HB1	1:80:A:ASP:H	8	0.16
(1,1315)	1:79:A:ALA:HB2	1:80:A:ASP:H	16	0.16
(1,1295)	1:82:A:PRO:HG2	1:81:A:HIS:HA	16	0.16
(1,1197)	1:89:A:TYR:HD2	1:71:A:LEU:HD21	12	0.16
(1,1175)	1:91:A:ARG:HG2	1:134:A:LEU:HB2	2	0.16
(1,1175)	1:91:A:ARG:HG2	1:134:A:LEU:HB2	5	0.16
(1,1175)	1:91:A:ARG:HG2	1:134:A:LEU:HB2	14	0.16
(1,1175)	1:91:A:ARG:HG2	1:134:A:LEU:HB2	18	0.16
(1,1171)	1:91:A:ARG:HG2	1:91:A:ARG:HA	23	0.16
(1,1133)	1:95:A:ALA:HB3	1:99:A:PHE:HD2	17	0.16
(1,1133)	1:95:A:ALA:HB2	1:99:A:PHE:HD2	22	0.16
(1,1118)	1:98:A:LEU:HB3	1:98:A:LEU:HD22	1	0.16
(1,1118)	1:98:A:LEU:HB3	1:98:A:LEU:HD21	14	0.16
(1,1118)	1:98:A:LEU:HB3	1:98:A:LEU:HD22	23	0.16
(1,1098)	1:100:A:LEU:HD23	1:92:A:GLN:HA	12	0.16
(1,1088)	1:100:A:LEU:HD22	1:105:A:PHE:HD2	10	0.16
(1,1072)	1:101:A:ALA:HB2	1:58:A:CYS:HA	24	0.16
(1,1057)	1:103:A:ALA:HB1	1:59:A:TYR:HD1	15	0.16
(1,1035)	1:62:A:GLU:HA	1:65:A:LYS:H	20	0.16
(1,1003)	1:108:A:ILE:HB	1:108:A:ILE:HD12	22	0.16
(1,995)	1:108:A:ILE:HG21	1:130:A:LEU:HD12	3	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,995)	1:108:A:ILE:HG22	1:130:A:LEU:HD13	17	0.16
(1,995)	1:108:A:ILE:HG22	1:130:A:LEU:HD13	21	0.16
(1,991)	1:108:A:ILE:HA	1:108:A:ILE:HG22	1	0.16
(1,960)	1:67:A:PHE:HA	1:109:A:LEU:HD12	17	0.16
(1,937)	1:112:A:VAL:HG23	1:113:A:LEU:HA	17	0.16
(1,934)	1:112:A:VAL:HG11	1:126:A:TYR:HB3	24	0.16
(1,930)	1:126:A:TYR:HD1	1:112:A:VAL:HG13	2	0.16
(1,930)	1:126:A:TYR:HD1	1:112:A:VAL:HG13	13	0.16
(1,913)	1:113:A:LEU:HG	1:113:A:LEU:H	8	0.16
(1,911)	1:113:A:LEU:HB2	1:113:A:LEU:H	7	0.16
(1,909)	1:114:A:SER:HB2	1:113:A:LEU:HG	19	0.16
(1,878)	1:117:A:ARG:HG2	1:114:A:SER:HA	13	0.16
(1,878)	1:117:A:ARG:HG2	1:114:A:SER:HA	23	0.16
(1,873)	1:118:A:SER:HB2	1:119:A:ARG:H	11	0.16
(1,873)	1:118:A:SER:HB2	1:119:A:ARG:H	12	0.16
(1,873)	1:118:A:SER:HB2	1:119:A:ARG:H	19	0.16
(1,873)	1:118:A:SER:HB2	1:119:A:ARG:H	20	0.16
(1,873)	1:118:A:SER:HB2	1:119:A:ARG:H	21	0.16
(1,870)	1:118:A:SER:HA	1:119:A:ARG:H	6	0.16
(1,870)	1:118:A:SER:HA	1:119:A:ARG:H	7	0.16
(1,870)	1:118:A:SER:HA	1:119:A:ARG:H	16	0.16
(1,827)	1:122:A:LYS:HD2	1:122:A:LYS:HA	5	0.16
(1,821)	1:122:A:LYS:HG3	1:122:A:LYS:H	5	0.16
(1,812)	1:123:A:LEU:HD22	1:77:A:GLN:HE21	9	0.16
(1,807)	1:123:A:LEU:HD11	1:74:A:CYS:HB2	18	0.16
(1,807)	1:123:A:LEU:HD13	1:74:A:CYS:HB2	22	0.16
(1,778)	1:125:A:VAL:HG21	1:122:A:LYS:HA	9	0.16
(1,775)	1:126:A:TYR:HE1	1:125:A:VAL:HG11	17	0.16
(1,716)	1:129:A:GLU:HA	1:133:A:VAL:HG22	13	0.16
(1,634)	1:134:A:LEU:HD13	1:134:A:LEU:H	25	0.16
(1,633)	1:100:A:LEU:HD13	1:92:A:GLN:HE21	10	0.16
(1,633)	1:100:A:LEU:HD13	1:92:A:GLN:HE21	24	0.16
(1,631)	1:73:A:LEU:HD12	1:117:A:ARG:HA	7	0.16
(1,619)	1:135:A:LYS:HG2	1:91:A:ARG:HD3	8	0.16
(1,604)	1:136:A:ALA:HB1	1:136:A:ALA:H	1	0.16
(1,604)	1:136:A:ALA:HB1	1:136:A:ALA:H	2	0.16
(1,604)	1:136:A:ALA:HB2	1:136:A:ALA:H	4	0.16
(1,604)	1:136:A:ALA:HB1	1:136:A:ALA:H	5	0.16
(1,604)	1:136:A:ALA:HB3	1:136:A:ALA:H	9	0.16
(1,604)	1:136:A:ALA:HB3	1:136:A:ALA:H	15	0.16
(1,604)	1:136:A:ALA:HB3	1:136:A:ALA:H	16	0.16
(1,604)	1:136:A:ALA:HB3	1:136:A:ALA:H	21	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,604)	1:136:A:ALA:HB3	1:136:A:ALA:H	25	0.16
(1,596)	1:137:A:HIS:HA	1:138:A:SER:H	22	0.16
(1,582)	1:139:A:ALA:HA	1:96:A:HIS:HB2	9	0.16
(1,542)	1:61:A:LEU:HG	1:61:A:LEU:H	1	0.16
(1,542)	1:61:A:LEU:HG	1:61:A:LEU:H	2	0.16
(1,542)	1:61:A:LEU:HG	1:61:A:LEU:H	3	0.16
(1,542)	1:61:A:LEU:HG	1:61:A:LEU:H	8	0.16
(1,542)	1:61:A:LEU:HG	1:61:A:LEU:H	12	0.16
(1,542)	1:61:A:LEU:HG	1:61:A:LEU:H	18	0.16
(1,540)	1:63:A:ASN:H	1:61:A:LEU:HG	22	0.16
(1,537)	1:63:A:ASN:H	1:61:A:LEU:H	6	0.16
(1,520)	1:130:A:LEU:H	1:112:A:VAL:HG23	6	0.16
(1,520)	1:130:A:LEU:H	1:112:A:VAL:HG23	20	0.16
(1,509)	1:77:A:GLN:HE22	1:73:A:LEU:HG	3	0.16
(1,509)	1:77:A:GLN:HE22	1:73:A:LEU:HG	10	0.16
(1,490)	1:91:A:ARG:H	1:94:A:ARG:H	17	0.16
(1,475)	1:98:A:LEU:HD22	1:98:A:LEU:H	6	0.16
(1,466)	1:106:A:CYS:H	1:63:A:ASN:HD21	19	0.16
(1,456)	1:112:A:VAL:H	1:108:A:ILE:HG21	7	0.16
(1,456)	1:112:A:VAL:H	1:108:A:ILE:HG22	22	0.16
(1,456)	1:112:A:VAL:H	1:108:A:ILE:HG23	23	0.16
(1,453)	1:114:A:SER:H	1:113:A:LEU:HD23	6	0.16
(1,453)	1:114:A:SER:H	1:113:A:LEU:HD23	23	0.16
(1,438)	1:66:A:LEU:HD13	1:66:A:LEU:H	4	0.16
(1,438)	1:66:A:LEU:HD12	1:66:A:LEU:H	10	0.16
(1,438)	1:66:A:LEU:HD13	1:66:A:LEU:H	11	0.16
(1,438)	1:66:A:LEU:HD13	1:66:A:LEU:H	24	0.16
(1,438)	1:66:A:LEU:HD12	1:66:A:LEU:H	25	0.16
(1,428)	1:128:A:ASN:HD22	1:128:A:ASN:HB3	5	0.16
(1,414)	1:72:A:GLU:H	1:68:A:GLU:HA	11	0.16
(1,410)	1:134:A:LEU:H	1:132:A:THR:H	4	0.16
(1,410)	1:134:A:LEU:H	1:132:A:THR:H	18	0.16
(1,410)	1:134:A:LEU:H	1:132:A:THR:H	23	0.16
(1,389)	1:143:A:LEU:H	1:142:A:LYS:HD2	5	0.16
(1,380)	2:27:B:SER:HA	2:30:B:GLU:HB3	24	0.16
(1,366)	1:100:A:LEU:HD11	1:138:A:SER:HB3	9	0.16
(1,361)	2:29:B:SER:HB2	2:32:B:GLU:HG3	23	0.16
(1,361)	2:29:B:SER:HB2	2:32:B:GLU:HG3	25	0.16
(1,324)	2:33:B:GLN:HG2	2:26:B:ASP:HB2	3	0.16
(1,324)	2:33:B:GLN:HG2	2:26:B:ASP:HB3	24	0.16
(1,288)	2:32:B:GLU:HA	2:35:B:PHE:HD1	5	0.16
(1,285)	2:31:B:LEU:HD12	1:127:A:ILE:HB	2	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,244)	1:111:A:ARG:HA	1:115:A:ARG:HG2	1	0.16
(1,227)	1:62:A:GLU:HG2	1:61:A:LEU:HG	9	0.16
(1,161)	1:87:A:PHE:HE2	2:34:B:TYR:HE1	12	0.16
(1,160)	1:67:A:PHE:HD1	1:68:A:GLU:H	17	0.16
(1,160)	1:67:A:PHE:HD1	1:68:A:GLU:H	21	0.16
(1,157)	1:130:A:LEU:HD22	1:88:A:LEU:HD11	16	0.16
(1,147)	1:137:A:HIS:HB3	1:138:A:SER:H	17	0.16
(1,145)	1:88:A:LEU:HB3	1:85:A:VAL:HA	20	0.16
(1,140)	1:99:A:PHE:HB3	1:138:A:SER:H	10	0.16
(1,139)	1:128:A:ASN:HB2	1:128:A:ASN:HD22	10	0.16
(1,111)	1:62:A:GLU:HB3	1:59:A:TYR:HD2	4	0.16
(1,107)	1:69:A:GLU:HA	1:69:A:GLU:HB3	6	0.16
(1,98)	1:105:A:PHE:HD1	1:100:A:LEU:HD23	3	0.16
(1,95)	1:107:A:ASN:HB2	1:108:A:ILE:HB	16	0.16
(1,84)	1:113:A:LEU:HA	1:113:A:LEU:HG	6	0.16
(1,84)	1:114:A:SER:HB2	1:113:A:LEU:HG	14	0.16
(1,84)	1:114:A:SER:HB2	1:113:A:LEU:HG	16	0.16
(1,84)	1:114:A:SER:HB2	1:113:A:LEU:HG	17	0.16
(1,84)	1:114:A:SER:HB2	1:113:A:LEU:HG	23	0.16
(1,76)	1:118:A:SER:HA	1:118:A:SER:HB3	1	0.16
(1,76)	1:118:A:SER:HA	1:118:A:SER:HB2	7	0.16
(1,76)	1:118:A:SER:HA	1:118:A:SER:HB2	17	0.16
(1,76)	1:118:A:SER:HA	1:118:A:SER:HB2	20	0.16
(1,76)	1:118:A:SER:HA	1:118:A:SER:HB2	21	0.16
(1,76)	1:118:A:SER:HA	1:118:A:SER:HB2	23	0.16
(1,67)	1:116:A:ALA:HB3	1:120:A:PRO:HA	17	0.16
(1,56)	1:124:A:TYR:HE1	2:35:B:PHE:HB3	13	0.16
(1,56)	1:124:A:TYR:HE1	2:35:B:PHE:HB3	16	0.16
(1,52)	1:125:A:VAL:HG12	1:128:A:ASN:HB2	15	0.16
(1,52)	1:125:A:VAL:HG11	1:128:A:ASN:HB2	23	0.16
(1,45)	1:59:A:TYR:HE1	1:57:A:LYS:HD2	9	0.16
(1,24)	1:85:A:VAL:HG22	1:86:A:PRO:HD3	16	0.16
(1,19)	1:133:A:VAL:HG23	1:130:A:LEU:HA	5	0.16
(1,19)	1:133:A:VAL:HG23	1:130:A:LEU:HA	24	0.16
(1,13)	1:133:A:VAL:HG11	1:108:A:ILE:HB	18	0.16
(1,2268)	2:26:B:ASP:H	2:25:B:GLU:HB3	12	0.15
(1,2248)	2:30:B:GLU:HB2	2:31:B:LEU:H	10	0.15
(1,2248)	2:30:B:GLU:HB2	2:31:B:LEU:H	17	0.15
(1,2202)	1:125:A:VAL:H	1:122:A:LYS:HD2	7	0.15
(1,2153)	1:109:A:LEU:HD11	1:66:A:LEU:H	1	0.15
(1,2153)	1:109:A:LEU:HD13	1:66:A:LEU:H	14	0.15
(1,2108)	1:77:A:GLN:H	1:78:A:THR:HG21	24	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2107)	1:77:A:GLN:H	1:77:A:GLN:HB3	8	0.15
(1,2107)	1:77:A:GLN:H	1:77:A:GLN:HB3	9	0.15
(1,2107)	1:77:A:GLN:H	1:77:A:GLN:HB3	10	0.15
(1,2107)	1:77:A:GLN:H	1:77:A:GLN:HB3	11	0.15
(1,2107)	1:77:A:GLN:H	1:77:A:GLN:HB3	12	0.15
(1,2107)	1:77:A:GLN:H	1:77:A:GLN:HB3	16	0.15
(1,2107)	1:77:A:GLN:H	1:77:A:GLN:HB3	17	0.15
(1,2107)	1:77:A:GLN:H	1:77:A:GLN:HB3	19	0.15
(1,2100)	1:77:A:GLN:HE21	1:76:A:MET:HE1	2	0.15
(1,2095)	1:77:A:GLN:HG2	1:77:A:GLN:HE22	1	0.15
(1,2095)	1:77:A:GLN:HG2	1:77:A:GLN:HE22	5	0.15
(1,2095)	1:77:A:GLN:HG2	1:77:A:GLN:HE22	9	0.15
(1,2095)	1:77:A:GLN:HG2	1:77:A:GLN:HE22	19	0.15
(1,2095)	1:77:A:GLN:HG2	1:77:A:GLN:HE22	20	0.15
(1,2080)	1:81:A:HIS:H	1:81:A:HIS:HB3	2	0.15
(1,2075)	1:81:A:HIS:H	1:81:A:HIS:HD2	11	0.15
(1,2054)	1:85:A:VAL:HG12	1:89:A:TYR:H	6	0.15
(1,2054)	1:85:A:VAL:HG13	1:89:A:TYR:H	9	0.15
(1,2054)	1:85:A:VAL:HG11	1:89:A:TYR:H	19	0.15
(1,2007)	1:100:A:LEU:HD21	1:95:A:ALA:H	14	0.15
(1,2005)	1:95:A:ALA:H	1:94:A:ARG:HG2	7	0.15
(1,2004)	1:95:A:ALA:H	1:94:A:ARG:HB3	11	0.15
(1,1996)	1:97:A:SER:H	1:139:A:ALA:HB1	5	0.15
(1,1975)	1:100:A:LEU:HD11	1:100:A:LEU:H	7	0.15
(1,1975)	1:100:A:LEU:HD11	1:100:A:LEU:H	25	0.15
(1,1837)	1:127:A:ILE:H	1:123:A:LEU:HD12	15	0.15
(1,1837)	1:127:A:ILE:H	1:123:A:LEU:HD13	18	0.15
(1,1837)	1:127:A:ILE:H	1:123:A:LEU:HD11	24	0.15
(1,1790)	1:139:A:ALA:H	1:138:A:SER:H	24	0.15
(1,1781)	1:140:A:LYS:H	1:141:A:LYS:HB3	3	0.15
(1,1781)	1:140:A:LYS:H	1:141:A:LYS:HB3	21	0.15
(1,1781)	1:140:A:LYS:H	1:141:A:LYS:HB3	25	0.15
(1,1777)	1:144:A:ASN:HB3	1:144:A:ASN:H	22	0.15
(1,1775)	1:143:A:LEU:H	1:141:A:LYS:HG3	1	0.15
(1,1771)	1:142:A:LYS:H	1:142:A:LYS:HD2	14	0.15
(1,1759)	2:30:B:GLU:HA	2:30:B:GLU:HG3	5	0.15
(1,1753)	2:27:B:SER:HB2	2:27:B:SER:HA	13	0.15
(1,1751)	2:27:B:SER:HA	2:28:B:ASP:H	5	0.15
(1,1745)	2:29:B:SER:HB3	2:30:B:GLU:H	4	0.15
(1,1725)	2:31:B:LEU:HD22	1:127:A:ILE:HG22	4	0.15
(1,1725)	2:31:B:LEU:HD21	1:127:A:ILE:HG22	11	0.15
(1,1723)	2:31:B:LEU:HD22	2:30:B:GLU:HB2	13	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1723)	2:31:B:LEU:HD23	2:30:B:GLU:HB2	18	0.15
(1,1721)	2:31:B:LEU:HD23	2:31:B:LEU:HA	1	0.15
(1,1721)	2:31:B:LEU:HD21	2:31:B:LEU:HA	14	0.15
(1,1721)	2:31:B:LEU:HD21	2:31:B:LEU:HA	15	0.15
(1,1721)	2:31:B:LEU:HD23	2:31:B:LEU:HA	18	0.15
(1,1721)	2:31:B:LEU:HD23	2:31:B:LEU:HA	20	0.15
(1,1721)	2:31:B:LEU:HD21	2:31:B:LEU:HA	24	0.15
(1,1718)	2:31:B:LEU:HD21	2:32:B:GLU:H	13	0.15
(1,1718)	2:31:B:LEU:HD23	2:32:B:GLU:H	19	0.15
(1,1716)	2:31:B:LEU:HG	2:32:B:GLU:HG3	22	0.15
(1,1705)	2:33:B:GLN:HA	2:34:B:TYR:H	2	0.15
(1,1705)	2:33:B:GLN:HA	2:34:B:TYR:H	17	0.15
(1,1705)	2:33:B:GLN:HA	2:34:B:TYR:H	19	0.15
(1,1705)	2:33:B:GLN:HA	2:34:B:TYR:H	21	0.15
(1,1705)	2:33:B:GLN:HA	2:34:B:TYR:H	23	0.15
(1,1703)	2:33:B:GLN:HG2	2:31:B:LEU:HD22	6	0.15
(1,1703)	2:33:B:GLN:HG2	2:31:B:LEU:HD21	21	0.15
(1,1648)	2:38:B:ARG:HA	2:37:B:ALA:HB1	17	0.15
(1,1639)	2:38:B:ARG:HD2	2:38:B:ARG:H	4	0.15
(1,1595)	2:31:B:LEU:HD11	1:127:A:ILE:HB	10	0.15
(1,1592)	1:84:A:VAL:HG22	2:35:B:PHE:HB2	14	0.15
(1,1588)	1:87:A:PHE:HB2	2:31:B:LEU:HD12	1	0.15
(1,1556)	1:57:A:LYS:HG2	1:57:A:LYS:HA	3	0.15
(1,1556)	1:57:A:LYS:HG2	1:57:A:LYS:HA	22	0.15
(1,1553)	1:59:A:TYR:HD1	1:57:A:LYS:HB2	3	0.15
(1,1552)	1:57:A:LYS:HB2	1:57:A:LYS:HA	8	0.15
(1,1552)	1:57:A:LYS:HB2	1:57:A:LYS:HA	13	0.15
(1,1549)	1:58:A:CYS:HB2	1:57:A:LYS:HA	19	0.15
(1,1539)	1:62:A:GLU:HB3	1:59:A:TYR:HD1	11	0.15
(1,1529)	1:59:A:TYR:HB2	1:59:A:TYR:HD1	5	0.15
(1,1529)	1:59:A:TYR:HB2	1:59:A:TYR:HD1	20	0.15
(1,1529)	1:59:A:TYR:HB2	1:59:A:TYR:HD1	25	0.15
(1,1512)	1:62:A:GLU:HG2	1:62:A:GLU:H	17	0.15
(1,1491)	1:65:A:LYS:HB2	1:65:A:LYS:HG2	2	0.15
(1,1491)	1:65:A:LYS:HB2	1:65:A:LYS:HG2	3	0.15
(1,1491)	1:65:A:LYS:HB2	1:65:A:LYS:HG2	4	0.15
(1,1491)	1:65:A:LYS:HB2	1:65:A:LYS:HG2	7	0.15
(1,1491)	1:65:A:LYS:HB2	1:65:A:LYS:HG2	8	0.15
(1,1491)	1:65:A:LYS:HB2	1:65:A:LYS:HG2	9	0.15
(1,1491)	1:65:A:LYS:HB2	1:65:A:LYS:HG2	11	0.15
(1,1491)	1:65:A:LYS:HB2	1:65:A:LYS:HG2	12	0.15
(1,1491)	1:65:A:LYS:HB2	1:65:A:LYS:HG2	15	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1491)	1:65:A:LYS:HB2	1:65:A:LYS:HG2	16	0.15
(1,1491)	1:65:A:LYS:HB2	1:65:A:LYS:HG2	17	0.15
(1,1491)	1:65:A:LYS:HB2	1:65:A:LYS:HG2	18	0.15
(1,1491)	1:65:A:LYS:HB2	1:65:A:LYS:HG2	19	0.15
(1,1491)	1:65:A:LYS:HB2	1:65:A:LYS:HG2	20	0.15
(1,1491)	1:65:A:LYS:HB2	1:65:A:LYS:HG2	21	0.15
(1,1491)	1:65:A:LYS:HB2	1:65:A:LYS:HG2	22	0.15
(1,1491)	1:65:A:LYS:HB2	1:65:A:LYS:HG2	23	0.15
(1,1491)	1:65:A:LYS:HB2	1:65:A:LYS:HG2	25	0.15
(1,1446)	1:69:A:GLU:HG2	1:69:A:GLU:H	7	0.15
(1,1446)	1:69:A:GLU:HG2	1:69:A:GLU:H	10	0.15
(1,1432)	1:70:A:PHE:HA	1:70:A:PHE:HD1	12	0.15
(1,1432)	1:70:A:PHE:HA	1:70:A:PHE:HD1	18	0.15
(1,1432)	1:70:A:PHE:HA	1:70:A:PHE:HD1	20	0.15
(1,1432)	1:70:A:PHE:HA	1:70:A:PHE:HD1	22	0.15
(1,1432)	1:70:A:PHE:HA	1:70:A:PHE:HD1	24	0.15
(1,1371)	1:75:A:LYS:HE3	1:72:A:GLU:HG2	9	0.15
(1,1370)	1:75:A:LYS:HE3	1:72:A:GLU:HB3	2	0.15
(1,1370)	1:75:A:LYS:HE3	1:72:A:GLU:HB3	20	0.15
(1,1367)	1:75:A:LYS:HD2	1:75:A:LYS:HA	4	0.15
(1,1367)	1:75:A:LYS:HD2	1:75:A:LYS:HA	5	0.15
(1,1346)	1:76:A:MET:HG2	1:73:A:LEU:HA	4	0.15
(1,1346)	1:76:A:MET:HG2	1:73:A:LEU:HA	5	0.15
(1,1346)	1:76:A:MET:HG2	1:73:A:LEU:HA	8	0.15
(1,1346)	1:76:A:MET:HG2	1:73:A:LEU:HA	13	0.15
(1,1346)	1:76:A:MET:HG2	1:73:A:LEU:HA	15	0.15
(1,1346)	1:76:A:MET:HG2	1:73:A:LEU:HA	16	0.15
(1,1343)	1:76:A:MET:HG2	1:76:A:MET:H	11	0.15
(1,1317)	1:79:A:ALA:HB3	1:76:A:MET:HA	3	0.15
(1,1317)	1:79:A:ALA:HB2	1:76:A:MET:HA	18	0.15
(1,1295)	1:82:A:PRO:HG2	1:81:A:HIS:HA	10	0.15
(1,1295)	1:82:A:PRO:HG2	1:81:A:HIS:HA	15	0.15
(1,1295)	1:82:A:PRO:HG2	1:81:A:HIS:HA	25	0.15
(1,1283)	1:84:A:VAL:HG23	1:127:A:ILE:HD12	5	0.15
(1,1283)	1:84:A:VAL:HG23	1:127:A:ILE:HD12	19	0.15
(1,1283)	1:84:A:VAL:HG23	1:127:A:ILE:HD11	23	0.15
(1,1279)	1:84:A:VAL:HG21	1:81:A:HIS:HB3	24	0.15
(1,1212)	1:88:A:LEU:HB2	1:88:A:LEU:HD12	16	0.15
(1,1171)	1:91:A:ARG:HG2	1:91:A:ARG:HA	17	0.15
(1,1139)	1:134:A:LEU:HD21	1:95:A:ALA:HB1	4	0.15
(1,1118)	1:98:A:LEU:HB3	1:98:A:LEU:HD23	6	0.15
(1,1118)	1:98:A:LEU:HB3	1:98:A:LEU:HD23	11	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1118)	1:98:A:LEU:HB3	1:98:A:LEU:HD21	12	0.15
(1,1118)	1:98:A:LEU:HB3	1:98:A:LEU:HD23	15	0.15
(1,1118)	1:98:A:LEU:HB3	1:98:A:LEU:HD23	25	0.15
(1,1091)	1:100:A:LEU:HD23	1:92:A:GLN:HE21	9	0.15
(1,1091)	1:100:A:LEU:HD21	1:92:A:GLN:HE21	25	0.15
(1,1089)	1:105:A:PHE:HZ	1:100:A:LEU:HD23	22	0.15
(1,1075)	1:101:A:ALA:HB2	1:60:A:LYS:HB2	6	0.15
(1,1072)	1:101:A:ALA:HB1	1:58:A:CYS:HA	11	0.15
(1,1056)	1:103:A:ALA:HB1	1:104:A:GLU:H	10	0.15
(1,999)	1:108:A:ILE:HD11	1:99:A:PHE:HZ	25	0.15
(1,991)	1:108:A:ILE:HA	1:108:A:ILE:HG23	3	0.15
(1,991)	1:108:A:ILE:HA	1:108:A:ILE:HG23	14	0.15
(1,991)	1:108:A:ILE:HA	1:108:A:ILE:HG23	23	0.15
(1,937)	1:112:A:VAL:HG21	1:113:A:LEU:HA	2	0.15
(1,937)	1:112:A:VAL:HG21	1:113:A:LEU:HA	3	0.15
(1,937)	1:112:A:VAL:HG21	1:113:A:LEU:HA	6	0.15
(1,930)	1:126:A:TYR:HD1	1:112:A:VAL:HG11	25	0.15
(1,915)	1:113:A:LEU:HD23	1:69:A:GLU:HB3	17	0.15
(1,913)	1:113:A:LEU:HG	1:113:A:LEU:H	7	0.15
(1,913)	1:113:A:LEU:HG	1:113:A:LEU:H	24	0.15
(1,911)	1:113:A:LEU:HB2	1:113:A:LEU:H	8	0.15
(1,911)	1:113:A:LEU:HB2	1:113:A:LEU:H	24	0.15
(1,909)	1:114:A:SER:HB2	1:113:A:LEU:HG	11	0.15
(1,897)	1:115:A:ARG:HA	1:115:A:ARG:HD3	15	0.15
(1,878)	1:117:A:ARG:HG2	1:114:A:SER:HA	25	0.15
(1,873)	1:118:A:SER:HB2	1:119:A:ARG:H	4	0.15
(1,860)	1:119:A:ARG:HG2	1:119:A:ARG:H	6	0.15
(1,860)	1:119:A:ARG:HG2	1:119:A:ARG:H	7	0.15
(1,860)	1:119:A:ARG:HG2	1:119:A:ARG:H	25	0.15
(1,812)	1:123:A:LEU:HD22	1:77:A:GLN:HE21	5	0.15
(1,812)	1:123:A:LEU:HD22	1:77:A:GLN:HE21	17	0.15
(1,811)	1:123:A:LEU:HD23	1:70:A:PHE:HE1	16	0.15
(1,779)	1:125:A:VAL:HB	1:125:A:VAL:HG13	4	0.15
(1,779)	1:125:A:VAL:HB	1:125:A:VAL:HG12	6	0.15
(1,779)	1:125:A:VAL:HB	1:125:A:VAL:HG11	8	0.15
(1,779)	1:125:A:VAL:HB	1:125:A:VAL:HG12	9	0.15
(1,779)	1:125:A:VAL:HB	1:125:A:VAL:HG13	20	0.15
(1,775)	1:126:A:TYR:HE1	1:125:A:VAL:HG11	16	0.15
(1,775)	1:126:A:TYR:HE1	1:125:A:VAL:HG12	18	0.15
(1,775)	1:126:A:TYR:HE1	1:125:A:VAL:HG12	24	0.15
(1,775)	1:126:A:TYR:HE1	1:125:A:VAL:HG13	25	0.15
(1,773)	1:125:A:VAL:HA	1:125:A:VAL:HG12	4	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,773)	1:125:A:VAL:HA	1:125:A:VAL:HG13	7	0.15
(1,773)	1:125:A:VAL:HA	1:125:A:VAL:HG11	9	0.15
(1,766)	1:126:A:TYR:HE1	1:115:A:ARG:HB2	6	0.15
(1,708)	1:130:A:LEU:HD21	1:70:A:PHE:HD2	10	0.15
(1,673)	1:133:A:VAL:HG21	1:130:A:LEU:HA	2	0.15
(1,673)	1:133:A:VAL:HG21	1:130:A:LEU:HA	11	0.15
(1,673)	1:133:A:VAL:HG21	1:130:A:LEU:HA	14	0.15
(1,642)	1:134:A:LEU:HD22	1:92:A:GLN:HG3	11	0.15
(1,619)	1:135:A:LYS:HG2	1:91:A:ARG:HD3	19	0.15
(1,618)	1:56:A:LYS:HG2	1:57:A:LYS:H	11	0.15
(1,604)	1:136:A:ALA:HB3	1:136:A:ALA:H	3	0.15
(1,604)	1:136:A:ALA:HB2	1:136:A:ALA:H	7	0.15
(1,604)	1:136:A:ALA:HB2	1:136:A:ALA:H	10	0.15
(1,604)	1:136:A:ALA:HB2	1:136:A:ALA:H	12	0.15
(1,604)	1:136:A:ALA:HB3	1:136:A:ALA:H	20	0.15
(1,596)	1:137:A:HIS:HA	1:138:A:SER:H	18	0.15
(1,596)	1:137:A:HIS:HA	1:138:A:SER:H	19	0.15
(1,591)	1:138:A:SER:HB3	1:138:A:SER:H	19	0.15
(1,591)	1:138:A:SER:HB3	1:138:A:SER:H	22	0.15
(1,591)	1:138:A:SER:HB3	1:138:A:SER:H	25	0.15
(1,569)	1:143:A:LEU:HB2	1:144:A:ASN:H	9	0.15
(1,551)	2:34:B:TYR:H	2:35:B:PHE:HA	6	0.15
(1,549)	2:39:B:TRP:HE1	1:78:A:THR:HG21	19	0.15
(1,542)	1:61:A:LEU:HG	1:61:A:LEU:H	6	0.15
(1,542)	1:61:A:LEU:HG	1:61:A:LEU:H	14	0.15
(1,542)	1:61:A:LEU:HG	1:61:A:LEU:H	15	0.15
(1,542)	1:61:A:LEU:HG	1:61:A:LEU:H	22	0.15
(1,542)	1:61:A:LEU:HG	1:61:A:LEU:H	23	0.15
(1,542)	1:61:A:LEU:HG	1:61:A:LEU:H	24	0.15
(1,540)	1:63:A:ASN:H	1:61:A:LEU:HG	4	0.15
(1,540)	1:63:A:ASN:H	1:61:A:LEU:HG	17	0.15
(1,540)	1:63:A:ASN:H	1:61:A:LEU:HG	21	0.15
(1,538)	1:63:A:ASN:H	1:61:A:LEU:HA	11	0.15
(1,538)	1:63:A:ASN:H	1:61:A:LEU:HA	16	0.15
(1,520)	1:130:A:LEU:H	1:112:A:VAL:HG22	18	0.15
(1,509)	1:77:A:GLN:HE22	1:73:A:LEU:HG	8	0.15
(1,500)	1:85:A:VAL:H	1:83:A:GLU:H	13	0.15
(1,490)	1:91:A:ARG:H	1:94:A:ARG:H	7	0.15
(1,475)	1:98:A:LEU:HD22	1:98:A:LEU:H	18	0.15
(1,464)	1:107:A:ASN:H	1:108:A:ILE:HB	8	0.15
(1,456)	1:112:A:VAL:H	1:108:A:ILE:HG23	14	0.15
(1,456)	1:112:A:VAL:H	1:108:A:ILE:HG22	20	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,438)	1:66:A:LEU:HD11	1:66:A:LEU:H	20	0.15
(1,410)	1:134:A:LEU:H	1:132:A:THR:H	7	0.15
(1,410)	1:134:A:LEU:H	1:132:A:THR:H	9	0.15
(1,410)	1:134:A:LEU:H	1:132:A:THR:H	16	0.15
(1,410)	1:134:A:LEU:H	1:132:A:THR:H	20	0.15
(1,388)	1:57:A:LYS:HA	1:57:A:LYS:H	6	0.15
(1,388)	1:57:A:LYS:HA	1:57:A:LYS:H	15	0.15
(1,375)	2:27:B:SER:HB3	2:28:B:ASP:HB3	5	0.15
(1,369)	2:26:B:ASP:HB2	2:33:B:GLN:HE21	22	0.15
(1,367)	2:26:B:ASP:HB3	2:31:B:LEU:H	14	0.15
(1,367)	2:26:B:ASP:HB3	2:31:B:LEU:H	19	0.15
(1,344)	2:31:B:LEU:HB3	1:87:A:PHE:HE2	4	0.15
(1,288)	2:32:B:GLU:HA	2:35:B:PHE:HD1	1	0.15
(1,288)	2:32:B:GLU:HA	2:35:B:PHE:HD1	7	0.15
(1,288)	2:32:B:GLU:HA	2:35:B:PHE:HD1	16	0.15
(1,285)	2:31:B:LEU:HD13	1:127:A:ILE:HB	6	0.15
(1,279)	1:84:A:VAL:HG22	2:35:B:PHE:HZ	24	0.15
(1,264)	1:127:A:ILE:HG22	2:35:B:PHE:HE1	5	0.15
(1,244)	1:111:A:ARG:HA	1:115:A:ARG:HG2	11	0.15
(1,238)	1:66:A:LEU:HD13	1:62:A:GLU:HA	17	0.15
(1,228)	1:62:A:GLU:HG2	1:61:A:LEU:HD21	21	0.15
(1,220)	1:70:A:PHE:HE2	1:113:A:LEU:HB2	6	0.15
(1,209)	1:67:A:PHE:HE1	1:71:A:LEU:HD22	4	0.15
(1,209)	1:67:A:PHE:HE1	1:71:A:LEU:HD22	8	0.15
(1,209)	1:67:A:PHE:HE1	1:71:A:LEU:HD22	11	0.15
(1,198)	2:30:B:GLU:HG3	1:87:A:PHE:HZ	19	0.15
(1,163)	1:67:A:PHE:HD2	1:92:A:GLN:HG3	17	0.15
(1,160)	1:67:A:PHE:HD1	1:68:A:GLU:H	8	0.15
(1,160)	1:67:A:PHE:HD2	1:68:A:GLU:H	19	0.15
(1,160)	1:67:A:PHE:HD1	1:68:A:GLU:H	20	0.15
(1,157)	1:130:A:LEU:HD22	1:88:A:LEU:HD11	2	0.15
(1,147)	1:137:A:HIS:HB3	1:138:A:SER:H	19	0.15
(1,140)	1:99:A:PHE:HB3	1:138:A:SER:H	4	0.15
(1,123)	1:95:A:ALA:HB2	1:134:A:LEU:HB2	25	0.15
(1,121)	1:95:A:ALA:HB1	1:134:A:LEU:HA	15	0.15
(1,116)	1:100:A:LEU:HD21	1:105:A:PHE:HE2	24	0.15
(1,113)	1:93:A:GLN:HA	1:94:A:ARG:H	21	0.15
(1,98)	1:105:A:PHE:HD1	1:100:A:LEU:HD21	21	0.15
(1,84)	1:113:A:LEU:HA	1:113:A:LEU:HG	3	0.15
(1,84)	1:114:A:SER:HB2	1:113:A:LEU:HG	4	0.15
(1,84)	1:113:A:LEU:HA	1:113:A:LEU:HG	15	0.15
(1,84)	1:113:A:LEU:HA	1:113:A:LEU:HG	21	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,83)	1:113:A:LEU:HA	1:116:A:ALA:HB1	5	0.15
(1,83)	1:113:A:LEU:HA	1:116:A:ALA:HB2	8	0.15
(1,79)	1:117:A:ARG:HD3	1:117:A:ARG:HG2	1	0.15
(1,76)	1:118:A:SER:HA	1:118:A:SER:HB2	4	0.15
(1,76)	1:118:A:SER:HA	1:118:A:SER:HB2	9	0.15
(1,76)	1:118:A:SER:HA	1:118:A:SER:HB2	14	0.15
(1,66)	1:121:A:ALA:HA	1:121:A:ALA:H	10	0.15
(1,66)	1:121:A:ALA:HA	1:121:A:ALA:H	16	0.15
(1,66)	1:121:A:ALA:HA	1:121:A:ALA:H	25	0.15
(1,27)	1:130:A:LEU:HD23	1:67:A:PHE:HA	7	0.15
(1,26)	1:134:A:LEU:HD13	1:67:A:PHE:HE2	2	0.15
(1,25)	1:85:A:VAL:HG23	1:74:A:CYS:HB2	6	0.15
(1,25)	1:85:A:VAL:HG21	1:74:A:CYS:HB2	11	0.15
(1,25)	1:85:A:VAL:HG23	1:74:A:CYS:HB2	14	0.15
(1,25)	1:85:A:VAL:HG21	1:74:A:CYS:HB2	17	0.15
(1,2268)	2:26:B:ASP:H	2:25:B:GLU:HB3	2	0.14
(1,2267)	2:26:B:ASP:H	2:25:B:GLU:HB2	16	0.14
(1,2248)	2:30:B:GLU:HB2	2:31:B:LEU:H	9	0.14
(1,2207)	2:38:B:ARG:HB2	2:39:B:TRP:H	1	0.14
(1,2165)	1:63:A:ASN:HD22	1:63:A:ASN:HD21	13	0.14
(1,2107)	1:77:A:GLN:H	1:77:A:GLN:HB3	21	0.14
(1,2100)	1:77:A:GLN:HE21	1:76:A:MET:HE3	8	0.14
(1,2095)	1:77:A:GLN:HG2	1:77:A:GLN:HE22	2	0.14
(1,2095)	1:77:A:GLN:HG2	1:77:A:GLN:HE22	6	0.14
(1,2095)	1:77:A:GLN:HG2	1:77:A:GLN:HE22	7	0.14
(1,2095)	1:77:A:GLN:HG2	1:77:A:GLN:HE22	8	0.14
(1,2095)	1:77:A:GLN:HG2	1:77:A:GLN:HE22	12	0.14
(1,2095)	1:77:A:GLN:HG2	1:77:A:GLN:HE22	13	0.14
(1,2095)	1:77:A:GLN:HG2	1:77:A:GLN:HE22	15	0.14
(1,2095)	1:77:A:GLN:HG2	1:77:A:GLN:HE22	18	0.14
(1,2095)	1:77:A:GLN:HG2	1:77:A:GLN:HE22	21	0.14
(1,2095)	1:77:A:GLN:HG2	1:77:A:GLN:HE22	22	0.14
(1,2095)	1:77:A:GLN:HG2	1:77:A:GLN:HE22	23	0.14
(1,2095)	1:77:A:GLN:HG2	1:77:A:GLN:HE22	24	0.14
(1,2095)	1:77:A:GLN:HG2	1:77:A:GLN:HE22	25	0.14
(1,2075)	1:81:A:HIS:H	1:81:A:HIS:HD2	9	0.14
(1,2054)	1:85:A:VAL:HG13	1:89:A:TYR:H	17	0.14
(1,2007)	1:100:A:LEU:HD21	1:95:A:ALA:H	9	0.14
(1,1975)	1:100:A:LEU:HD11	1:100:A:LEU:H	4	0.14
(1,1975)	1:100:A:LEU:HD13	1:100:A:LEU:H	12	0.14
(1,1961)	1:102:A:SER:H	1:59:A:TYR:HD1	24	0.14
(1,1874)	1:118:A:SER:H	1:117:A:ARG:HG2	12	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1801)	1:135:A:LYS:H	1:91:A:ARG:HD3	4	0.14
(1,1781)	1:140:A:LYS:H	1:141:A:LYS:HB3	8	0.14
(1,1781)	1:140:A:LYS:H	1:141:A:LYS:HB3	14	0.14
(1,1764)	2:24:B:GLN:HB3	2:24:B:GLN:HG3	4	0.14
(1,1764)	2:24:B:GLN:HB3	2:24:B:GLN:HG3	14	0.14
(1,1754)	2:30:B:GLU:HG2	2:31:B:LEU:H	22	0.14
(1,1753)	2:27:B:SER:HB2	2:27:B:SER:HA	3	0.14
(1,1746)	1:100:A:LEU:HD13	1:138:A:SER:HB2	2	0.14
(1,1746)	1:100:A:LEU:HD11	1:138:A:SER:HB2	23	0.14
(1,1745)	2:29:B:SER:HB3	2:30:B:GLU:H	25	0.14
(1,1721)	2:31:B:LEU:HD21	2:31:B:LEU:HA	17	0.14
(1,1718)	2:31:B:LEU:HD21	2:32:B:GLU:H	3	0.14
(1,1718)	2:31:B:LEU:HD23	2:32:B:GLU:H	4	0.14
(1,1718)	2:31:B:LEU:HD21	2:32:B:GLU:H	10	0.14
(1,1718)	2:31:B:LEU:HD23	2:32:B:GLU:H	17	0.14
(1,1718)	2:31:B:LEU:HD23	2:32:B:GLU:H	21	0.14
(1,1718)	2:31:B:LEU:HD22	2:32:B:GLU:H	23	0.14
(1,1705)	2:33:B:GLN:HA	2:34:B:TYR:H	6	0.14
(1,1650)	2:37:B:ALA:HB3	1:121:A:ALA:HB1	12	0.14
(1,1644)	2:31:B:LEU:HA	1:128:A:ASN:HD22	2	0.14
(1,1636)	2:35:B:PHE:HB3	2:34:B:TYR:HE1	18	0.14
(1,1608)	2:32:B:GLU:HA	2:33:B:GLN:H	2	0.14
(1,1603)	2:33:B:GLN:HG2	2:33:B:GLN:HB2	10	0.14
(1,1556)	1:57:A:LYS:HG2	1:57:A:LYS:HA	20	0.14
(1,1552)	1:57:A:LYS:HB2	1:57:A:LYS:HA	1	0.14
(1,1550)	1:141:A:LYS:HG3	1:141:A:LYS:HA	19	0.14
(1,1549)	1:58:A:CYS:HB2	1:57:A:LYS:HA	25	0.14
(1,1529)	1:59:A:TYR:HB2	1:59:A:TYR:HD1	10	0.14
(1,1495)	1:64:A:GLU:HA	1:67:A:PHE:HB2	5	0.14
(1,1491)	1:65:A:LYS:HB2	1:65:A:LYS:HG2	13	0.14
(1,1491)	1:65:A:LYS:HB2	1:65:A:LYS:HG2	24	0.14
(1,1488)	1:65:A:LYS:HG3	1:65:A:LYS:H	5	0.14
(1,1484)	1:65:A:LYS:HA	1:65:A:LYS:HG2	14	0.14
(1,1440)	1:127:A:ILE:HD11	1:70:A:PHE:HZ	9	0.14
(1,1432)	1:70:A:PHE:HA	1:70:A:PHE:HD1	16	0.14
(1,1423)	1:71:A:LEU:HD22	1:70:A:PHE:HD1	18	0.14
(1,1423)	1:71:A:LEU:HD23	1:70:A:PHE:HD1	21	0.14
(1,1419)	1:71:A:LEU:HD11	1:89:A:TYR:H	17	0.14
(1,1419)	1:71:A:LEU:HD13	1:89:A:TYR:H	25	0.14
(1,1411)	1:71:A:LEU:HD23	1:71:A:LEU:HB2	16	0.14
(1,1367)	1:75:A:LYS:HD2	1:75:A:LYS:HA	9	0.14
(1,1367)	1:75:A:LYS:HD2	1:75:A:LYS:HA	15	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1367)	1:75:A:LYS:HD2	1:75:A:LYS:HA	16	0.14
(1,1346)	1:76:A:MET:HG2	1:73:A:LEU:HA	2	0.14
(1,1346)	1:76:A:MET:HG2	1:73:A:LEU:HA	7	0.14
(1,1346)	1:76:A:MET:HG2	1:73:A:LEU:HA	9	0.14
(1,1329)	1:77:A:GLN:HG2	1:77:A:GLN:HB3	19	0.14
(1,1319)	1:77:A:GLN:HB3	1:78:A:THR:H	2	0.14
(1,1319)	1:77:A:GLN:HB3	1:78:A:THR:H	4	0.14
(1,1317)	1:79:A:ALA:HB3	1:76:A:MET:HA	16	0.14
(1,1317)	1:79:A:ALA:HB1	1:76:A:MET:HA	22	0.14
(1,1315)	1:79:A:ALA:HB2	1:80:A:ASP:H	7	0.14
(1,1315)	1:79:A:ALA:HB3	1:80:A:ASP:H	10	0.14
(1,1315)	1:79:A:ALA:HB1	1:80:A:ASP:H	11	0.14
(1,1315)	1:79:A:ALA:HB1	1:80:A:ASP:H	12	0.14
(1,1315)	1:79:A:ALA:HB3	1:80:A:ASP:H	14	0.14
(1,1315)	1:79:A:ALA:HB1	1:80:A:ASP:H	20	0.14
(1,1295)	1:82:A:PRO:HG2	1:81:A:HIS:HA	23	0.14
(1,1283)	1:84:A:VAL:HG22	1:127:A:ILE:HD12	2	0.14
(1,1283)	1:84:A:VAL:HG22	1:127:A:ILE:HD13	17	0.14
(1,1247)	1:88:A:LEU:HD13	1:85:A:VAL:HA	6	0.14
(1,1247)	1:88:A:LEU:HD12	1:85:A:VAL:HA	9	0.14
(1,1197)	1:89:A:TYR:HD2	1:71:A:LEU:HD21	7	0.14
(1,1171)	1:91:A:ARG:HG2	1:91:A:ARG:HA	3	0.14
(1,1171)	1:91:A:ARG:HG2	1:91:A:ARG:HA	7	0.14
(1,1171)	1:91:A:ARG:HG2	1:91:A:ARG:HA	16	0.14
(1,1118)	1:98:A:LEU:HB3	1:98:A:LEU:HD22	2	0.14
(1,1118)	1:98:A:LEU:HB3	1:98:A:LEU:HD21	5	0.14
(1,1118)	1:98:A:LEU:HB3	1:98:A:LEU:HD22	10	0.14
(1,1118)	1:98:A:LEU:HB3	1:98:A:LEU:HD21	16	0.14
(1,1118)	1:98:A:LEU:HB3	1:98:A:LEU:HD21	17	0.14
(1,1118)	1:98:A:LEU:HB3	1:98:A:LEU:HD23	18	0.14
(1,1118)	1:98:A:LEU:HB3	1:98:A:LEU:HD23	24	0.14
(1,1097)	1:100:A:LEU:HD22	1:100:A:LEU:HD13	3	0.14
(1,1091)	1:100:A:LEU:HD23	1:92:A:GLN:HE21	7	0.14
(1,1089)	1:105:A:PHE:HZ	1:100:A:LEU:HD23	15	0.14
(1,1074)	1:101:A:ALA:HB1	1:60:A:LYS:HA	15	0.14
(1,1057)	1:103:A:ALA:HB3	1:59:A:TYR:HD1	23	0.14
(1,1014)	1:74:A:CYS:HA	1:78:A:THR:HG23	4	0.14
(1,1003)	1:108:A:ILE:HB	1:108:A:ILE:HD12	7	0.14
(1,1003)	1:108:A:ILE:HB	1:108:A:ILE:HD13	19	0.14
(1,999)	1:108:A:ILE:HD12	1:99:A:PHE:HZ	7	0.14
(1,999)	1:108:A:ILE:HD12	1:99:A:PHE:HZ	13	0.14
(1,999)	1:108:A:ILE:HD12	1:99:A:PHE:HZ	22	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,998)	1:108:A:ILE:HD12	1:105:A:PHE:HD1	22	0.14
(1,995)	1:108:A:ILE:HG21	1:130:A:LEU:HD12	14	0.14
(1,995)	1:108:A:ILE:HG21	1:130:A:LEU:HD12	23	0.14
(1,963)	1:109:A:LEU:HD13	1:63:A:ASN:HB2	2	0.14
(1,937)	1:112:A:VAL:HG23	1:113:A:LEU:HA	8	0.14
(1,937)	1:112:A:VAL:HG22	1:113:A:LEU:HA	11	0.14
(1,937)	1:112:A:VAL:HG23	1:113:A:LEU:HA	14	0.14
(1,937)	1:112:A:VAL:HG23	1:113:A:LEU:HA	16	0.14
(1,937)	1:112:A:VAL:HG22	1:113:A:LEU:HA	19	0.14
(1,937)	1:112:A:VAL:HG22	1:113:A:LEU:HA	24	0.14
(1,934)	1:112:A:VAL:HG12	1:126:A:TYR:HB3	16	0.14
(1,930)	1:126:A:TYR:HD1	1:112:A:VAL:HG13	8	0.14
(1,930)	1:126:A:TYR:HD1	1:112:A:VAL:HG13	18	0.14
(1,930)	1:126:A:TYR:HD1	1:112:A:VAL:HG11	22	0.14
(1,930)	1:126:A:TYR:HD1	1:112:A:VAL:HG11	23	0.14
(1,922)	1:112:A:VAL:HA	1:115:A:ARG:HG3	9	0.14
(1,915)	1:113:A:LEU:HD23	1:69:A:GLU:HB3	14	0.14
(1,873)	1:118:A:SER:HB2	1:119:A:ARG:H	2	0.14
(1,873)	1:118:A:SER:HB2	1:119:A:ARG:H	9	0.14
(1,870)	1:118:A:SER:HA	1:119:A:ARG:H	9	0.14
(1,870)	1:118:A:SER:HA	1:119:A:ARG:H	19	0.14
(1,870)	1:118:A:SER:HA	1:119:A:ARG:H	25	0.14
(1,830)	1:121:A:ALA:HB1	1:122:A:LYS:H	16	0.14
(1,827)	1:122:A:LYS:HD2	1:122:A:LYS:HA	8	0.14
(1,811)	1:123:A:LEU:HD22	1:70:A:PHE:HE1	6	0.14
(1,811)	1:123:A:LEU:HD23	1:70:A:PHE:HE1	9	0.14
(1,811)	1:123:A:LEU:HD21	1:70:A:PHE:HE1	12	0.14
(1,807)	1:123:A:LEU:HD12	1:74:A:CYS:HB2	11	0.14
(1,807)	1:123:A:LEU:HD13	1:74:A:CYS:HB2	15	0.14
(1,807)	1:123:A:LEU:HD11	1:74:A:CYS:HB2	17	0.14
(1,807)	1:123:A:LEU:HD12	1:74:A:CYS:HB2	21	0.14
(1,779)	1:125:A:VAL:HB	1:125:A:VAL:HG11	7	0.14
(1,778)	1:125:A:VAL:HG23	1:122:A:LYS:HA	1	0.14
(1,773)	1:125:A:VAL:HA	1:125:A:VAL:HG11	1	0.14
(1,773)	1:125:A:VAL:HA	1:125:A:VAL:HG13	5	0.14
(1,773)	1:125:A:VAL:HA	1:125:A:VAL:HG13	8	0.14
(1,773)	1:125:A:VAL:HA	1:125:A:VAL:HG12	19	0.14
(1,773)	1:125:A:VAL:HA	1:125:A:VAL:HG11	20	0.14
(1,746)	1:127:A:ILE:HD13	1:127:A:ILE:H	2	0.14
(1,746)	1:127:A:ILE:HD13	1:127:A:ILE:H	6	0.14
(1,746)	1:127:A:ILE:HD13	1:127:A:ILE:H	7	0.14
(1,746)	1:127:A:ILE:HD11	1:127:A:ILE:H	8	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,746)	1:127:A:ILE:HD13	1:127:A:ILE:H	20	0.14
(1,706)	1:85:A:VAL:HG22	1:75:A:LYS:HD2	5	0.14
(1,673)	1:133:A:VAL:HG21	1:130:A:LEU:HA	9	0.14
(1,673)	1:133:A:VAL:HG21	1:130:A:LEU:HA	16	0.14
(1,672)	1:133:A:VAL:HG21	1:137:A:HIS:HD2	10	0.14
(1,672)	1:133:A:VAL:HG22	1:137:A:HIS:HD2	25	0.14
(1,636)	1:134:A:LEU:HD23	1:134:A:LEU:H	19	0.14
(1,618)	1:56:A:LYS:HG2	1:57:A:LYS:H	3	0.14
(1,618)	1:56:A:LYS:HG2	1:57:A:LYS:H	24	0.14
(1,614)	1:135:A:LYS:HA	1:135:A:LYS:HD2	25	0.14
(1,604)	1:136:A:ALA:HB2	1:136:A:ALA:H	6	0.14
(1,604)	1:136:A:ALA:HB3	1:136:A:ALA:H	18	0.14
(1,601)	1:137:A:HIS:HB3	1:137:A:HIS:H	17	0.14
(1,599)	1:137:A:HIS:HA	1:137:A:HIS:HB2	1	0.14
(1,599)	1:137:A:HIS:HA	1:137:A:HIS:HB2	2	0.14
(1,599)	1:137:A:HIS:HA	1:137:A:HIS:HB2	3	0.14
(1,599)	1:137:A:HIS:HA	1:137:A:HIS:HB2	5	0.14
(1,599)	1:137:A:HIS:HA	1:137:A:HIS:HB2	7	0.14
(1,599)	1:137:A:HIS:HA	1:137:A:HIS:HB2	8	0.14
(1,599)	1:137:A:HIS:HA	1:137:A:HIS:HB2	9	0.14
(1,599)	1:137:A:HIS:HA	1:137:A:HIS:HB2	10	0.14
(1,599)	1:137:A:HIS:HA	1:137:A:HIS:HB2	11	0.14
(1,599)	1:137:A:HIS:HA	1:137:A:HIS:HB2	12	0.14
(1,599)	1:137:A:HIS:HA	1:137:A:HIS:HB2	13	0.14
(1,599)	1:137:A:HIS:HA	1:137:A:HIS:HB2	14	0.14
(1,599)	1:137:A:HIS:HA	1:137:A:HIS:HB2	15	0.14
(1,599)	1:137:A:HIS:HA	1:137:A:HIS:HB2	16	0.14
(1,599)	1:137:A:HIS:HA	1:137:A:HIS:HB2	17	0.14
(1,599)	1:137:A:HIS:HA	1:137:A:HIS:HB2	18	0.14
(1,599)	1:137:A:HIS:HA	1:137:A:HIS:HB2	19	0.14
(1,599)	1:137:A:HIS:HA	1:137:A:HIS:HB2	20	0.14
(1,599)	1:137:A:HIS:HA	1:137:A:HIS:HB2	22	0.14
(1,599)	1:137:A:HIS:HA	1:137:A:HIS:HB2	23	0.14
(1,596)	1:137:A:HIS:HA	1:138:A:SER:H	15	0.14
(1,596)	1:137:A:HIS:HA	1:138:A:SER:H	23	0.14
(1,594)	1:95:A:ALA:HB1	1:138:A:SER:HB3	15	0.14
(1,594)	1:95:A:ALA:HB3	1:138:A:SER:HB3	19	0.14
(1,591)	1:138:A:SER:HB3	1:138:A:SER:H	17	0.14
(1,582)	1:139:A:ALA:HA	1:96:A:HIS:HB2	16	0.14
(1,576)	1:142:A:LYS:HB2	1:142:A:LYS:H	7	0.14
(1,572)	1:143:A:LEU:HB2	1:143:A:LEU:HD12	16	0.14
(1,572)	1:143:A:LEU:HB2	1:143:A:LEU:HD11	25	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,562)	2:26:B:ASP:H	2:25:B:GLU:HG2	12	0.14
(1,549)	2:39:B:TRP:HE1	1:127:A:ILE:HG13	2	0.14
(1,537)	1:63:A:ASN:H	1:61:A:LEU:H	21	0.14
(1,523)	1:70:A:PHE:H	1:69:A:GLU:HB3	4	0.14
(1,520)	1:130:A:LEU:H	1:112:A:VAL:HG21	24	0.14
(1,512)	1:77:A:GLN:H	1:123:A:LEU:HD22	25	0.14
(1,509)	1:77:A:GLN:HE22	1:73:A:LEU:HG	5	0.14
(1,509)	1:77:A:GLN:HE22	1:73:A:LEU:HG	24	0.14
(1,480)	1:100:A:LEU:HD11	1:95:A:ALA:H	23	0.14
(1,477)	1:93:A:GLN:HA	1:95:A:ALA:H	8	0.14
(1,475)	1:98:A:LEU:HD23	1:98:A:LEU:H	16	0.14
(1,469)	1:102:A:SER:H	1:100:A:LEU:HB2	12	0.14
(1,466)	1:106:A:CYS:H	1:63:A:ASN:HD21	2	0.14
(1,464)	1:107:A:ASN:H	1:108:A:ILE:HB	16	0.14
(1,456)	1:112:A:VAL:H	1:108:A:ILE:HG21	8	0.14
(1,456)	1:112:A:VAL:H	1:108:A:ILE:HG23	15	0.14
(1,438)	1:66:A:LEU:HD12	1:66:A:LEU:H	8	0.14
(1,428)	1:128:A:ASN:HD22	1:128:A:ASN:HB3	2	0.14
(1,410)	1:134:A:LEU:H	1:132:A:THR:H	15	0.14
(1,388)	1:57:A:LYS:HA	1:57:A:LYS:H	13	0.14
(1,388)	1:57:A:LYS:HA	1:57:A:LYS:H	14	0.14
(1,388)	1:57:A:LYS:HA	1:57:A:LYS:H	22	0.14
(1,379)	2:31:B:LEU:HB2	2:28:B:ASP:HB2	13	0.14
(1,367)	2:26:B:ASP:HB3	2:31:B:LEU:H	9	0.14
(1,364)	2:29:B:SER:HB3	2:32:B:GLU:HB2	25	0.14
(1,356)	2:29:B:SER:HB2	2:33:B:GLN:H	18	0.14
(1,356)	2:29:B:SER:HB2	2:33:B:GLN:H	21	0.14
(1,344)	2:31:B:LEU:HB3	1:87:A:PHE:HD2	20	0.14
(1,337)	2:31:B:LEU:HD22	2:28:B:ASP:HB2	11	0.14
(1,321)	2:34:B:TYR:HD1	1:83:A:GLU:HB3	13	0.14
(1,305)	2:36:B:THR:HG23	2:35:B:PHE:HD1	19	0.14
(1,288)	2:32:B:GLU:HA	2:35:B:PHE:HD1	8	0.14
(1,288)	2:32:B:GLU:HA	2:35:B:PHE:HD1	12	0.14
(1,288)	2:32:B:GLU:HA	2:35:B:PHE:HD1	23	0.14
(1,288)	2:32:B:GLU:HA	2:35:B:PHE:HD1	24	0.14
(1,285)	2:31:B:LEU:HD12	1:127:A:ILE:HB	25	0.14
(1,264)	1:127:A:ILE:HG23	2:35:B:PHE:HE1	24	0.14
(1,262)	1:80:A:ASP:HB3	1:81:A:HIS:HD2	9	0.14
(1,253)	1:57:A:LYS:HE2	1:54:A:MET:HG3	5	0.14
(1,243)	1:62:A:GLU:HG3	1:61:A:LEU:HD21	3	0.14
(1,238)	1:66:A:LEU:HD11	1:62:A:GLU:HA	21	0.14
(1,236)	1:64:A:GLU:HA	1:67:A:PHE:H	1	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,227)	1:62:A:GLU:HG2	1:61:A:LEU:HG	12	0.14
(1,209)	1:67:A:PHE:HE1	1:71:A:LEU:HD22	9	0.14
(1,163)	1:67:A:PHE:HD2	1:92:A:GLN:HG3	10	0.14
(1,160)	1:67:A:PHE:HD2	1:68:A:GLU:H	3	0.14
(1,160)	1:67:A:PHE:HD1	1:68:A:GLU:H	12	0.14
(1,157)	1:130:A:LEU:HD23	1:88:A:LEU:HD12	5	0.14
(1,157)	1:130:A:LEU:HD21	1:88:A:LEU:HD12	7	0.14
(1,157)	1:130:A:LEU:HD22	1:88:A:LEU:HD11	9	0.14
(1,157)	1:130:A:LEU:HD21	1:88:A:LEU:HD13	15	0.14
(1,157)	1:130:A:LEU:HD22	1:88:A:LEU:HD11	19	0.14
(1,147)	1:137:A:HIS:HB3	1:138:A:SER:H	7	0.14
(1,147)	1:137:A:HIS:HB3	1:138:A:SER:H	21	0.14
(1,147)	1:137:A:HIS:HB3	1:138:A:SER:H	23	0.14
(1,140)	1:99:A:PHE:HB3	1:138:A:SER:H	17	0.14
(1,132)	1:92:A:GLN:HB3	1:89:A:TYR:HD1	23	0.14
(1,121)	1:95:A:ALA:HB3	1:134:A:LEU:HA	3	0.14
(1,109)	1:64:A:GLU:HB3	1:65:A:LYS:H	4	0.14
(1,100)	1:67:A:PHE:HE1	1:88:A:LEU:HD13	25	0.14
(1,95)	1:107:A:ASN:HB2	1:108:A:ILE:HB	18	0.14
(1,89)	1:94:A:ARG:HD2	1:94:A:ARG:HA	2	0.14
(1,83)	1:113:A:LEU:HA	1:116:A:ALA:HB1	11	0.14
(1,79)	1:117:A:ARG:HD3	1:117:A:ARG:HG2	9	0.14
(1,76)	1:118:A:SER:HA	1:118:A:SER:HB2	3	0.14
(1,76)	1:118:A:SER:HA	1:118:A:SER:HB2	18	0.14
(1,66)	1:121:A:ALA:HA	1:121:A:ALA:H	3	0.14
(1,66)	1:121:A:ALA:HA	1:121:A:ALA:H	11	0.14
(1,66)	1:121:A:ALA:HA	1:121:A:ALA:H	12	0.14
(1,66)	1:121:A:ALA:HA	1:121:A:ALA:H	15	0.14
(1,61)	1:61:A:LEU:HD22	1:59:A:TYR:HA	16	0.14
(1,56)	1:124:A:TYR:HE1	2:35:B:PHE:HB3	5	0.14
(1,55)	1:124:A:TYR:HE2	1:81:A:HIS:HB3	2	0.14
(1,55)	1:124:A:TYR:HE2	2:35:B:PHE:HB3	19	0.14
(1,25)	1:85:A:VAL:HG22	1:74:A:CYS:HB2	1	0.14
(1,25)	1:85:A:VAL:HG21	1:74:A:CYS:HB2	7	0.14
(1,25)	1:85:A:VAL:HG23	1:74:A:CYS:HB2	20	0.14
(1,20)	1:66:A:LEU:HA	1:69:A:GLU:HB2	2	0.14
(1,20)	1:66:A:LEU:HA	1:69:A:GLU:HB2	14	0.14
(1,20)	1:66:A:LEU:HA	1:69:A:GLU:HB2	15	0.14
(1,19)	1:133:A:VAL:HG21	1:130:A:LEU:HA	3	0.14
(1,17)	1:133:A:VAL:HG11	1:137:A:HIS:HB2	20	0.14
(1,8)	1:134:A:LEU:HD22	1:67:A:PHE:HZ	12	0.14
(1,8)	1:134:A:LEU:HD21	1:67:A:PHE:HZ	14	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1)	1:141:A:LYS:HG3	1:141:A:LYS:HA	8	0.14
(1,1)	1:141:A:LYS:HG3	1:141:A:LYS:HA	23	0.14
(1,2272)	2:25:B:GLU:H	2:25:B:GLU:HB2	1	0.13
(1,2255)	2:28:B:ASP:H	2:27:B:SER:HB2	3	0.13
(1,2248)	2:30:B:GLU:HB2	2:31:B:LEU:H	25	0.13
(1,2244)	2:36:B:THR:HG23	2:36:B:THR:H	24	0.13
(1,2202)	1:125:A:VAL:H	1:122:A:LYS:HD2	14	0.13
(1,2195)	1:56:A:LYS:H	1:56:A:LYS:HG2	15	0.13
(1,2194)	1:56:A:LYS:HB3	1:56:A:LYS:H	11	0.13
(1,2185)	1:59:A:TYR:HE1	1:59:A:TYR:H	20	0.13
(1,2183)	1:60:A:LYS:H	1:60:A:LYS:HG2	17	0.13
(1,2165)	1:63:A:ASN:HD22	1:63:A:ASN:HD21	3	0.13
(1,2165)	1:63:A:ASN:HD22	1:63:A:ASN:HD21	4	0.13
(1,2165)	1:63:A:ASN:HD22	1:63:A:ASN:HD21	5	0.13
(1,2165)	1:63:A:ASN:HD22	1:63:A:ASN:HD21	6	0.13
(1,2165)	1:63:A:ASN:HD22	1:63:A:ASN:HD21	7	0.13
(1,2165)	1:63:A:ASN:HD22	1:63:A:ASN:HD21	10	0.13
(1,2165)	1:63:A:ASN:HD22	1:63:A:ASN:HD21	12	0.13
(1,2165)	1:63:A:ASN:HD22	1:63:A:ASN:HD21	16	0.13
(1,2165)	1:63:A:ASN:HD22	1:63:A:ASN:HD21	17	0.13
(1,2165)	1:63:A:ASN:HD22	1:63:A:ASN:HD21	21	0.13
(1,2165)	1:63:A:ASN:HD22	1:63:A:ASN:HD21	22	0.13
(1,2165)	1:63:A:ASN:HD22	1:63:A:ASN:HD21	23	0.13
(1,2161)	1:64:A:GLU:HB3	1:64:A:GLU:H	19	0.13
(1,2161)	1:64:A:GLU:HB3	1:64:A:GLU:H	21	0.13
(1,2151)	1:65:A:LYS:HG3	1:66:A:LEU:H	7	0.13
(1,2151)	1:65:A:LYS:HG3	1:66:A:LEU:H	13	0.13
(1,2151)	1:65:A:LYS:HG3	1:66:A:LEU:H	16	0.13
(1,2095)	1:77:A:GLN:HG2	1:77:A:GLN:HE22	4	0.13
(1,2095)	1:77:A:GLN:HG2	1:77:A:GLN:HE22	10	0.13
(1,2095)	1:77:A:GLN:HG2	1:77:A:GLN:HE22	14	0.13
(1,2095)	1:77:A:GLN:HG2	1:77:A:GLN:HE22	16	0.13
(1,2095)	1:77:A:GLN:HG2	1:77:A:GLN:HE22	17	0.13
(1,2080)	1:81:A:HIS:H	1:81:A:HIS:HB3	21	0.13
(1,1989)	1:98:A:LEU:H	1:138:A:SER:HB2	21	0.13
(1,1987)	1:99:A:PHE:H	1:99:A:PHE:HD2	24	0.13
(1,1975)	1:100:A:LEU:HD13	1:100:A:LEU:H	17	0.13
(1,1975)	1:100:A:LEU:HD11	1:100:A:LEU:H	22	0.13
(1,1961)	1:102:A:SER:H	1:59:A:TYR:HD1	22	0.13
(1,1958)	1:103:A:ALA:H	1:102:A:SER:HB3	3	0.13
(1,1893)	1:115:A:ARG:HD3	1:115:A:ARG:H	21	0.13
(1,1776)	1:144:A:ASN:HA	1:144:A:ASN:H	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1776)	1:144:A:ASN:HA	1:144:A:ASN:H	16	0.13
(1,1776)	1:144:A:ASN:HA	1:144:A:ASN:H	21	0.13
(1,1776)	1:144:A:ASN:HA	1:144:A:ASN:H	24	0.13
(1,1776)	1:144:A:ASN:HA	1:144:A:ASN:H	25	0.13
(1,1775)	1:143:A:LEU:H	1:141:A:LYS:HG2	5	0.13
(1,1771)	1:142:A:LYS:H	1:142:A:LYS:HD2	1	0.13
(1,1765)	2:24:B:GLN:HB2	2:24:B:GLN:HG2	6	0.13
(1,1764)	2:24:B:GLN:HB3	2:24:B:GLN:HG3	17	0.13
(1,1753)	2:27:B:SER:HB2	2:27:B:SER:HA	4	0.13
(1,1751)	2:27:B:SER:HA	2:28:B:ASP:H	8	0.13
(1,1745)	2:29:B:SER:HB3	2:30:B:GLU:H	18	0.13
(1,1721)	2:31:B:LEU:HD23	2:31:B:LEU:HA	11	0.13
(1,1718)	2:31:B:LEU:HD23	2:32:B:GLU:H	2	0.13
(1,1718)	2:31:B:LEU:HD21	2:32:B:GLU:H	6	0.13
(1,1718)	2:31:B:LEU:HD23	2:32:B:GLU:H	14	0.13
(1,1718)	2:31:B:LEU:HD23	2:32:B:GLU:H	15	0.13
(1,1718)	2:31:B:LEU:HD23	2:32:B:GLU:H	24	0.13
(1,1708)	2:32:B:GLU:HG2	2:39:B:TRP:HZ2	1	0.13
(1,1703)	2:33:B:GLN:HG2	2:31:B:LEU:HD21	19	0.13
(1,1653)	2:37:B:ALA:HB1	2:37:B:ALA:HA	1	0.13
(1,1653)	2:37:B:ALA:HB1	2:37:B:ALA:HA	2	0.13
(1,1653)	2:37:B:ALA:HB3	2:37:B:ALA:HA	10	0.13
(1,1653)	2:37:B:ALA:HB3	2:37:B:ALA:HA	16	0.13
(1,1653)	2:37:B:ALA:HB3	2:37:B:ALA:HA	20	0.13
(1,1639)	2:38:B:ARG:HD2	2:38:B:ARG:H	22	0.13
(1,1617)	2:39:B:TRP:HD1	2:38:B:ARG:HA	4	0.13
(1,1617)	2:39:B:TRP:HD1	2:38:B:ARG:HA	14	0.13
(1,1617)	2:39:B:TRP:HD1	2:38:B:ARG:HA	22	0.13
(1,1608)	2:32:B:GLU:HA	2:33:B:GLN:H	3	0.13
(1,1608)	2:32:B:GLU:HA	2:33:B:GLN:H	6	0.13
(1,1608)	2:32:B:GLU:HA	2:33:B:GLN:H	7	0.13
(1,1608)	2:32:B:GLU:HA	2:33:B:GLN:H	11	0.13
(1,1608)	2:32:B:GLU:HA	2:33:B:GLN:H	12	0.13
(1,1608)	2:32:B:GLU:HA	2:33:B:GLN:H	13	0.13
(1,1608)	2:32:B:GLU:HA	2:33:B:GLN:H	15	0.13
(1,1608)	2:32:B:GLU:HA	2:33:B:GLN:H	24	0.13
(1,1608)	2:32:B:GLU:HA	2:33:B:GLN:H	25	0.13
(1,1552)	1:57:A:LYS:HB2	1:57:A:LYS:HA	18	0.13
(1,1549)	1:58:A:CYS:HB2	1:57:A:LYS:HA	10	0.13
(1,1543)	1:59:A:TYR:HE1	1:103:A:ALA:H	11	0.13
(1,1540)	1:59:A:TYR:HD1	1:57:A:LYS:HB3	25	0.13
(1,1536)	1:59:A:TYR:HD1	1:59:A:TYR:HA	13	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1491)	1:65:A:LYS:HB2	1:65:A:LYS:HG2	1	0.13
(1,1491)	1:65:A:LYS:HB2	1:65:A:LYS:HG2	10	0.13
(1,1446)	1:69:A:GLU:HG2	1:69:A:GLU:H	25	0.13
(1,1423)	1:71:A:LEU:HD23	1:70:A:PHE:HD1	14	0.13
(1,1423)	1:71:A:LEU:HD22	1:70:A:PHE:HD1	17	0.13
(1,1391)	1:74:A:CYS:HA	1:73:A:LEU:HD21	13	0.13
(1,1367)	1:75:A:LYS:HD2	1:75:A:LYS:HA	21	0.13
(1,1346)	1:76:A:MET:HG2	1:73:A:LEU:HA	17	0.13
(1,1319)	1:77:A:GLN:HB3	1:78:A:THR:H	12	0.13
(1,1317)	1:79:A:ALA:HB2	1:76:A:MET:HA	4	0.13
(1,1317)	1:79:A:ALA:HB1	1:76:A:MET:HA	14	0.13
(1,1315)	1:79:A:ALA:HB1	1:80:A:ASP:H	4	0.13
(1,1315)	1:79:A:ALA:HB3	1:80:A:ASP:H	24	0.13
(1,1295)	1:82:A:PRO:HG2	1:81:A:HIS:HA	5	0.13
(1,1295)	1:82:A:PRO:HG2	1:81:A:HIS:HA	7	0.13
(1,1283)	1:84:A:VAL:HG23	1:127:A:ILE:HD13	14	0.13
(1,1257)	1:85:A:VAL:HG13	1:71:A:LEU:HA	3	0.13
(1,1257)	1:85:A:VAL:HG13	1:71:A:LEU:HA	15	0.13
(1,1247)	1:88:A:LEU:HD13	1:85:A:VAL:HA	1	0.13
(1,1247)	1:88:A:LEU:HD13	1:85:A:VAL:HA	7	0.13
(1,1247)	1:88:A:LEU:HD11	1:85:A:VAL:HA	12	0.13
(1,1197)	1:89:A:TYR:HD2	1:71:A:LEU:HD23	23	0.13
(1,1175)	1:91:A:ARG:HG2	1:134:A:LEU:HB2	7	0.13
(1,1171)	1:91:A:ARG:HG2	1:91:A:ARG:HA	22	0.13
(1,1147)	1:94:A:ARG:HG2	1:94:A:ARG:HA	12	0.13
(1,1147)	1:94:A:ARG:HG2	1:94:A:ARG:HA	20	0.13
(1,1144)	1:111:A:ARG:HG2	1:107:A:ASN:HA	8	0.13
(1,1142)	1:94:A:ARG:HD3	1:94:A:ARG:HB2	10	0.13
(1,1133)	1:95:A:ALA:HB3	1:99:A:PHE:HD2	3	0.13
(1,1133)	1:95:A:ALA:HB3	1:99:A:PHE:HD2	4	0.13
(1,1132)	1:95:A:ALA:HB1	1:96:A:HIS:H	2	0.13
(1,1126)	1:96:A:HIS:HD2	1:139:A:ALA:HB1	10	0.13
(1,1118)	1:98:A:LEU:HB3	1:98:A:LEU:HD21	21	0.13
(1,1109)	1:98:A:LEU:HB3	1:98:A:LEU:H	7	0.13
(1,1109)	1:98:A:LEU:HB3	1:98:A:LEU:H	11	0.13
(1,1109)	1:98:A:LEU:HB3	1:98:A:LEU:H	15	0.13
(1,1109)	1:98:A:LEU:HB3	1:98:A:LEU:H	17	0.13
(1,1109)	1:98:A:LEU:HB3	1:98:A:LEU:H	25	0.13
(1,1097)	1:100:A:LEU:HD21	1:100:A:LEU:HD12	7	0.13
(1,1091)	1:100:A:LEU:HD23	1:92:A:GLN:HE21	23	0.13
(1,1068)	1:101:A:ALA:HB3	1:59:A:TYR:H	22	0.13
(1,1067)	1:101:A:ALA:HB3	1:60:A:LYS:H	12	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1028)	1:67:A:PHE:HE1	1:88:A:LEU:HB3	8	0.13
(1,1014)	1:74:A:CYS:HA	1:78:A:THR:HG21	24	0.13
(1,1003)	1:108:A:ILE:HB	1:108:A:ILE:HD11	14	0.13
(1,999)	1:108:A:ILE:HD12	1:99:A:PHE:HZ	4	0.13
(1,995)	1:108:A:ILE:HG22	1:130:A:LEU:HD11	6	0.13
(1,995)	1:108:A:ILE:HG21	1:130:A:LEU:HD11	11	0.13
(1,963)	1:109:A:LEU:HD11	1:63:A:ASN:HB2	19	0.13
(1,963)	1:109:A:LEU:HD12	1:63:A:ASN:HB2	20	0.13
(1,942)	1:111:A:ARG:HB2	1:111:A:ARG:HD2	14	0.13
(1,937)	1:112:A:VAL:HG23	1:113:A:LEU:HA	5	0.13
(1,937)	1:112:A:VAL:HG21	1:113:A:LEU:HA	9	0.13
(1,937)	1:112:A:VAL:HG23	1:113:A:LEU:HA	10	0.13
(1,937)	1:112:A:VAL:HG21	1:113:A:LEU:HA	15	0.13
(1,937)	1:112:A:VAL:HG23	1:113:A:LEU:HA	18	0.13
(1,937)	1:112:A:VAL:HG23	1:113:A:LEU:HA	21	0.13
(1,937)	1:112:A:VAL:HG22	1:113:A:LEU:HA	22	0.13
(1,937)	1:112:A:VAL:HG23	1:113:A:LEU:HA	25	0.13
(1,934)	1:112:A:VAL:HG11	1:126:A:TYR:HB3	3	0.13
(1,934)	1:112:A:VAL:HG13	1:126:A:TYR:HB3	10	0.13
(1,931)	1:112:A:VAL:HG11	1:126:A:TYR:HA	21	0.13
(1,930)	1:126:A:TYR:HD1	1:112:A:VAL:HG12	6	0.13
(1,930)	1:126:A:TYR:HD1	1:112:A:VAL:HG11	24	0.13
(1,915)	1:113:A:LEU:HD21	1:69:A:GLU:HB3	5	0.13
(1,915)	1:113:A:LEU:HD21	1:69:A:GLU:HB3	20	0.13
(1,913)	1:113:A:LEU:HG	1:113:A:LEU:H	13	0.13
(1,911)	1:113:A:LEU:HB2	1:113:A:LEU:H	5	0.13
(1,911)	1:113:A:LEU:HB2	1:113:A:LEU:H	6	0.13
(1,911)	1:113:A:LEU:HB2	1:113:A:LEU:H	18	0.13
(1,911)	1:113:A:LEU:HB2	1:113:A:LEU:H	22	0.13
(1,911)	1:113:A:LEU:HB2	1:113:A:LEU:H	23	0.13
(1,909)	1:114:A:SER:HB2	1:113:A:LEU:HG	5	0.13
(1,909)	1:114:A:SER:HB2	1:113:A:LEU:HG	9	0.13
(1,909)	1:114:A:SER:HB2	1:113:A:LEU:HG	18	0.13
(1,897)	1:115:A:ARG:HA	1:115:A:ARG:HD3	24	0.13
(1,870)	1:118:A:SER:HA	1:119:A:ARG:H	2	0.13
(1,870)	1:118:A:SER:HA	1:119:A:ARG:H	4	0.13
(1,870)	1:118:A:SER:HA	1:119:A:ARG:H	8	0.13
(1,870)	1:118:A:SER:HA	1:119:A:ARG:H	14	0.13
(1,870)	1:118:A:SER:HA	1:119:A:ARG:H	17	0.13
(1,870)	1:118:A:SER:HA	1:119:A:ARG:H	18	0.13
(1,870)	1:118:A:SER:HA	1:119:A:ARG:H	20	0.13
(1,870)	1:118:A:SER:HA	1:119:A:ARG:H	21	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,870)	1:118:A:SER:HA	1:119:A:ARG:H	24	0.13
(1,821)	1:122:A:LYS:HG3	1:122:A:LYS:H	12	0.13
(1,814)	1:123:A:LEU:HD21	1:120:A:PRO:HA	13	0.13
(1,812)	1:123:A:LEU:HD22	1:77:A:GLN:HE21	15	0.13
(1,807)	1:123:A:LEU:HD11	1:74:A:CYS:HB2	2	0.13
(1,807)	1:123:A:LEU:HD12	1:74:A:CYS:HB2	5	0.13
(1,807)	1:123:A:LEU:HD13	1:74:A:CYS:HB2	9	0.13
(1,789)	1:124:A:TYR:HD1	1:124:A:TYR:HE1	4	0.13
(1,789)	1:124:A:TYR:HD1	1:124:A:TYR:HE1	5	0.13
(1,789)	1:124:A:TYR:HD1	1:124:A:TYR:HE1	10	0.13
(1,789)	1:124:A:TYR:HD1	1:124:A:TYR:HE1	13	0.13
(1,789)	1:124:A:TYR:HD1	1:124:A:TYR:HE1	16	0.13
(1,789)	1:124:A:TYR:HD1	1:124:A:TYR:HE1	24	0.13
(1,779)	1:125:A:VAL:HB	1:125:A:VAL:HG11	5	0.13
(1,779)	1:125:A:VAL:HB	1:125:A:VAL:HG12	12	0.13
(1,775)	1:126:A:TYR:HE1	1:125:A:VAL:HG11	10	0.13
(1,773)	1:125:A:VAL:HA	1:125:A:VAL:HG11	12	0.13
(1,773)	1:125:A:VAL:HA	1:125:A:VAL:HG12	15	0.13
(1,773)	1:125:A:VAL:HA	1:125:A:VAL:HG11	18	0.13
(1,773)	1:125:A:VAL:HA	1:125:A:VAL:HG12	25	0.13
(1,746)	1:127:A:ILE:HD11	1:127:A:ILE:H	4	0.13
(1,746)	1:127:A:ILE:HD11	1:127:A:ILE:H	15	0.13
(1,746)	1:127:A:ILE:HD13	1:127:A:ILE:H	19	0.13
(1,718)	1:129:A:GLU:HB3	1:126:A:TYR:HA	13	0.13
(1,704)	1:130:A:LEU:HD11	1:109:A:LEU:HD21	3	0.13
(1,704)	1:130:A:LEU:HD11	1:109:A:LEU:HD21	25	0.13
(1,673)	1:133:A:VAL:HG23	1:130:A:LEU:HA	18	0.13
(1,638)	1:134:A:LEU:HD23	1:99:A:PHE:HE2	10	0.13
(1,633)	1:100:A:LEU:HD12	1:92:A:GLN:HE21	17	0.13
(1,633)	1:100:A:LEU:HD12	1:92:A:GLN:HE21	19	0.13
(1,614)	1:135:A:LYS:HA	1:135:A:LYS:HD2	19	0.13
(1,604)	1:136:A:ALA:HB1	1:136:A:ALA:H	8	0.13
(1,604)	1:136:A:ALA:HB3	1:136:A:ALA:H	17	0.13
(1,604)	1:136:A:ALA:HB1	1:136:A:ALA:H	24	0.13
(1,601)	1:137:A:HIS:HB3	1:137:A:HIS:H	12	0.13
(1,601)	1:137:A:HIS:HB3	1:137:A:HIS:H	25	0.13
(1,599)	1:137:A:HIS:HA	1:137:A:HIS:HB2	4	0.13
(1,599)	1:137:A:HIS:HA	1:137:A:HIS:HB2	21	0.13
(1,599)	1:137:A:HIS:HA	1:137:A:HIS:HB2	24	0.13
(1,599)	1:137:A:HIS:HA	1:137:A:HIS:HB2	25	0.13
(1,596)	1:137:A:HIS:HA	1:138:A:SER:H	13	0.13
(1,583)	1:139:A:ALA:HA	1:96:A:HIS:HB2	18	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,582)	1:139:A:ALA:HA	1:96:A:HIS:HB2	21	0.13
(1,578)	1:57:A:LYS:HA	1:57:A:LYS:H	11	0.13
(1,572)	1:143:A:LEU:HB2	1:143:A:LEU:HD13	2	0.13
(1,561)	2:27:B:SER:H	2:30:B:GLU:HB3	3	0.13
(1,537)	1:63:A:ASN:H	1:61:A:LEU:H	12	0.13
(1,532)	1:66:A:LEU:H	1:64:A:GLU:HB2	21	0.13
(1,526)	1:69:A:GLU:H	1:113:A:LEU:HD21	1	0.13
(1,526)	1:69:A:GLU:H	1:113:A:LEU:HD22	3	0.13
(1,515)	1:73:A:LEU:HG	1:76:A:MET:H	2	0.13
(1,512)	1:77:A:GLN:H	1:123:A:LEU:HD21	6	0.13
(1,512)	1:77:A:GLN:H	1:123:A:LEU:HD22	23	0.13
(1,509)	1:77:A:GLN:HE22	1:73:A:LEU:HG	12	0.13
(1,509)	1:77:A:GLN:HE22	1:73:A:LEU:HG	15	0.13
(1,509)	1:77:A:GLN:HE22	1:73:A:LEU:HG	20	0.13
(1,509)	1:77:A:GLN:HE22	1:73:A:LEU:HG	22	0.13
(1,509)	1:77:A:GLN:HE22	1:73:A:LEU:HG	23	0.13
(1,492)	1:91:A:ARG:H	1:88:A:LEU:HD23	19	0.13
(1,490)	1:91:A:ARG:H	1:94:A:ARG:H	11	0.13
(1,490)	1:91:A:ARG:H	1:94:A:ARG:H	19	0.13
(1,475)	1:98:A:LEU:HD23	1:98:A:LEU:H	12	0.13
(1,466)	1:106:A:CYS:H	1:63:A:ASN:HD21	14	0.13
(1,464)	1:107:A:ASN:H	1:108:A:ILE:HB	3	0.13
(1,464)	1:107:A:ASN:H	1:108:A:ILE:HB	9	0.13
(1,464)	1:107:A:ASN:H	1:108:A:ILE:HB	19	0.13
(1,464)	1:107:A:ASN:H	1:108:A:ILE:HB	22	0.13
(1,459)	1:111:A:ARG:HB2	1:110:A:SER:H	7	0.13
(1,459)	1:111:A:ARG:HB2	1:110:A:SER:H	20	0.13
(1,430)	1:123:A:LEU:H	1:126:A:TYR:HD2	24	0.13
(1,410)	1:134:A:LEU:H	1:132:A:THR:H	2	0.13
(1,410)	1:134:A:LEU:H	1:132:A:THR:H	8	0.13
(1,410)	1:134:A:LEU:H	1:132:A:THR:H	19	0.13
(1,391)	1:144:A:ASN:H	1:142:A:LYS:HB2	2	0.13
(1,379)	2:31:B:LEU:HB2	2:28:B:ASP:HB2	3	0.13
(1,376)	2:27:B:SER:HB3	2:28:B:ASP:HB3	21	0.13
(1,343)	2:31:B:LEU:HB2	1:87:A:PHE:HE2	24	0.13
(1,342)	2:31:B:LEU:HD12	1:124:A:TYR:HB3	17	0.13
(1,288)	2:32:B:GLU:HA	2:35:B:PHE:HD1	9	0.13
(1,285)	2:31:B:LEU:HD12	1:127:A:ILE:HB	5	0.13
(1,270)	1:88:A:LEU:HD21	2:31:B:LEU:HD11	18	0.13
(1,264)	1:127:A:ILE:HG23	2:35:B:PHE:HE1	15	0.13
(1,262)	1:80:A:ASP:HB3	1:81:A:HIS:HD2	11	0.13
(1,254)	1:57:A:LYS:HE2	1:54:A:MET:HG3	24	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,242)	1:62:A:GLU:HG3	1:61:A:LEU:HG	18	0.13
(1,238)	1:66:A:LEU:HD13	1:62:A:GLU:HA	22	0.13
(1,222)	1:68:A:GLU:HA	1:71:A:LEU:HG	14	0.13
(1,211)	1:71:A:LEU:HD21	1:74:A:CYS:HB2	10	0.13
(1,197)	1:73:A:LEU:HD23	1:117:A:ARG:HB2	11	0.13
(1,161)	1:87:A:PHE:HE2	2:34:B:TYR:HE1	18	0.13
(1,157)	1:130:A:LEU:HD23	1:88:A:LEU:HD12	1	0.13
(1,157)	1:130:A:LEU:HD22	1:88:A:LEU:HD12	4	0.13
(1,157)	1:130:A:LEU:HD22	1:88:A:LEU:HD12	21	0.13
(1,157)	1:130:A:LEU:HD22	1:88:A:LEU:HD12	23	0.13
(1,156)	1:88:A:LEU:HB3	1:88:A:LEU:HD11	3	0.13
(1,147)	1:137:A:HIS:HB3	1:138:A:SER:H	4	0.13
(1,147)	1:137:A:HIS:HB3	1:138:A:SER:H	22	0.13
(1,123)	1:95:A:ALA:HB2	1:134:A:LEU:HB2	21	0.13
(1,111)	1:62:A:GLU:HB3	1:59:A:TYR:HD2	18	0.13
(1,109)	1:64:A:GLU:HB3	1:65:A:LYS:H	6	0.13
(1,107)	1:69:A:GLU:HA	1:69:A:GLU:HB3	2	0.13
(1,107)	1:69:A:GLU:HA	1:69:A:GLU:HB3	7	0.13
(1,107)	1:69:A:GLU:HA	1:69:A:GLU:HB3	11	0.13
(1,107)	1:69:A:GLU:HA	1:69:A:GLU:HB3	22	0.13
(1,84)	1:114:A:SER:HB2	1:113:A:LEU:HG	8	0.13
(1,84)	1:114:A:SER:HB2	1:113:A:LEU:HG	10	0.13
(1,83)	1:113:A:LEU:HA	1:116:A:ALA:HB2	21	0.13
(1,78)	1:118:A:SER:HB3	1:119:A:ARG:HG3	6	0.13
(1,78)	1:118:A:SER:HB3	1:119:A:ARG:HG3	25	0.13
(1,76)	1:118:A:SER:HA	1:118:A:SER:HB2	5	0.13
(1,66)	1:121:A:ALA:HA	1:121:A:ALA:H	7	0.13
(1,66)	1:121:A:ALA:HA	1:121:A:ALA:H	18	0.13
(1,61)	1:123:A:LEU:HD13	1:120:A:PRO:HA	11	0.13
(1,56)	1:124:A:TYR:HE2	2:35:B:PHE:HB3	15	0.13
(1,52)	1:125:A:VAL:HG11	1:128:A:ASN:HB2	18	0.13
(1,45)	1:59:A:TYR:HE1	1:57:A:LYS:HD2	2	0.13
(1,42)	1:126:A:TYR:HD1	1:125:A:VAL:HB	8	0.13
(1,27)	1:130:A:LEU:HD22	1:67:A:PHE:HA	1	0.13
(1,25)	1:85:A:VAL:HG22	1:74:A:CYS:HB2	13	0.13
(1,19)	1:133:A:VAL:HG22	1:130:A:LEU:HA	19	0.13
(1,2268)	2:26:B:ASP:H	2:25:B:GLU:HB3	19	0.12
(1,2267)	2:26:B:ASP:H	2:25:B:GLU:HB2	22	0.12
(1,2265)	2:26:B:ASP:HB3	2:26:B:ASP:H	22	0.12
(1,2259)	2:27:B:SER:HB3	2:27:B:SER:H	7	0.12
(1,2248)	2:30:B:GLU:HB2	2:31:B:LEU:H	1	0.12
(1,2207)	2:38:B:ARG:HB2	2:39:B:TRP:H	10	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2202)	1:125:A:VAL:H	1:122:A:LYS:HD2	1	0.12
(1,2202)	1:125:A:VAL:H	1:122:A:LYS:HD3	19	0.12
(1,2202)	1:125:A:VAL:H	1:122:A:LYS:HD2	21	0.12
(1,2202)	1:125:A:VAL:H	1:122:A:LYS:HD2	22	0.12
(1,2202)	1:125:A:VAL:H	1:122:A:LYS:HD2	24	0.12
(1,2185)	1:59:A:TYR:HE1	1:59:A:TYR:H	25	0.12
(1,2165)	1:63:A:ASN:HD22	1:63:A:ASN:HD21	1	0.12
(1,2165)	1:63:A:ASN:HD22	1:63:A:ASN:HD21	2	0.12
(1,2165)	1:63:A:ASN:HD22	1:63:A:ASN:HD21	8	0.12
(1,2165)	1:63:A:ASN:HD22	1:63:A:ASN:HD21	9	0.12
(1,2165)	1:63:A:ASN:HD22	1:63:A:ASN:HD21	11	0.12
(1,2165)	1:63:A:ASN:HD22	1:63:A:ASN:HD21	14	0.12
(1,2165)	1:63:A:ASN:HD22	1:63:A:ASN:HD21	15	0.12
(1,2165)	1:63:A:ASN:HD22	1:63:A:ASN:HD21	18	0.12
(1,2165)	1:63:A:ASN:HD22	1:63:A:ASN:HD21	19	0.12
(1,2165)	1:63:A:ASN:HD22	1:63:A:ASN:HD21	20	0.12
(1,2165)	1:63:A:ASN:HD22	1:63:A:ASN:HD21	24	0.12
(1,2165)	1:63:A:ASN:HD22	1:63:A:ASN:HD21	25	0.12
(1,2161)	1:64:A:GLU:HB3	1:64:A:GLU:H	6	0.12
(1,2161)	1:64:A:GLU:HB3	1:64:A:GLU:H	9	0.12
(1,2161)	1:64:A:GLU:HB3	1:64:A:GLU:H	17	0.12
(1,2153)	1:109:A:LEU:HD12	1:66:A:LEU:H	2	0.12
(1,2153)	1:109:A:LEU:HD11	1:66:A:LEU:H	7	0.12
(1,2151)	1:65:A:LYS:HG3	1:66:A:LEU:H	8	0.12
(1,2151)	1:65:A:LYS:HG3	1:66:A:LEU:H	11	0.12
(1,2151)	1:65:A:LYS:HG3	1:66:A:LEU:H	15	0.12
(1,2136)	1:69:A:GLU:H	1:70:A:PHE:HB2	18	0.12
(1,2100)	1:77:A:GLN:HE21	1:76:A:MET:HE2	9	0.12
(1,2095)	1:77:A:GLN:HG2	1:77:A:GLN:HE22	3	0.12
(1,2094)	1:79:A:ALA:HB2	1:78:A:THR:H	6	0.12
(1,2094)	1:79:A:ALA:HB2	1:78:A:THR:H	13	0.12
(1,2094)	1:79:A:ALA:HB1	1:78:A:THR:H	14	0.12
(1,2071)	1:83:A:GLU:HG3	1:83:A:GLU:H	6	0.12
(1,1927)	1:107:A:ASN:HD22	1:107:A:ASN:HB2	24	0.12
(1,1837)	1:127:A:ILE:H	1:123:A:LEU:HD11	8	0.12
(1,1789)	1:139:A:ALA:H	1:139:A:ALA:HB2	17	0.12
(1,1777)	1:144:A:ASN:HB3	1:144:A:ASN:H	18	0.12
(1,1776)	1:144:A:ASN:HA	1:144:A:ASN:H	10	0.12
(1,1776)	1:144:A:ASN:HA	1:144:A:ASN:H	12	0.12
(1,1776)	1:144:A:ASN:HA	1:144:A:ASN:H	15	0.12
(1,1776)	1:144:A:ASN:HA	1:144:A:ASN:H	18	0.12
(1,1776)	1:144:A:ASN:HA	1:144:A:ASN:H	20	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1776)	1:144:A:ASN:HA	1:144:A:ASN:H	22	0.12
(1,1771)	1:142:A:LYS:H	1:142:A:LYS:HD2	5	0.12
(1,1764)	2:24:B:GLN:HB3	2:24:B:GLN:HG3	20	0.12
(1,1746)	1:100:A:LEU:HD11	1:138:A:SER:HB2	1	0.12
(1,1746)	1:100:A:LEU:HD12	1:138:A:SER:HB2	10	0.12
(1,1746)	1:100:A:LEU:HD12	1:138:A:SER:HB2	14	0.12
(1,1725)	2:31:B:LEU:HD22	1:127:A:ILE:HG22	17	0.12
(1,1725)	2:31:B:LEU:HD21	1:127:A:ILE:HG22	22	0.12
(1,1723)	2:31:B:LEU:HD23	2:30:B:GLU:HB2	23	0.12
(1,1721)	2:31:B:LEU:HD22	2:31:B:LEU:HA	3	0.12
(1,1721)	2:31:B:LEU:HD21	2:31:B:LEU:HA	21	0.12
(1,1718)	2:31:B:LEU:HD23	2:32:B:GLU:H	12	0.12
(1,1718)	2:31:B:LEU:HD22	2:32:B:GLU:H	20	0.12
(1,1718)	2:31:B:LEU:HD22	2:32:B:GLU:H	25	0.12
(1,1708)	2:32:B:GLU:HG2	2:39:B:TRP:HZ2	6	0.12
(1,1708)	2:32:B:GLU:HG2	2:39:B:TRP:HZ2	23	0.12
(1,1702)	2:33:B:GLN:HG3	2:34:B:TYR:HE2	1	0.12
(1,1653)	2:37:B:ALA:HB1	2:37:B:ALA:HA	9	0.12
(1,1653)	2:37:B:ALA:HB1	2:37:B:ALA:HA	19	0.12
(1,1617)	2:39:B:TRP:HD1	2:38:B:ARG:HA	12	0.12
(1,1608)	2:32:B:GLU:HA	2:33:B:GLN:H	1	0.12
(1,1608)	2:32:B:GLU:HA	2:33:B:GLN:H	4	0.12
(1,1608)	2:32:B:GLU:HA	2:33:B:GLN:H	5	0.12
(1,1608)	2:32:B:GLU:HA	2:33:B:GLN:H	8	0.12
(1,1608)	2:32:B:GLU:HA	2:33:B:GLN:H	16	0.12
(1,1608)	2:32:B:GLU:HA	2:33:B:GLN:H	17	0.12
(1,1608)	2:32:B:GLU:HA	2:33:B:GLN:H	19	0.12
(1,1608)	2:32:B:GLU:HA	2:33:B:GLN:H	20	0.12
(1,1608)	2:32:B:GLU:HA	2:33:B:GLN:H	23	0.12
(1,1603)	2:33:B:GLN:HG2	2:33:B:GLN:HB2	7	0.12
(1,1603)	2:33:B:GLN:HG2	2:33:B:GLN:HB2	11	0.12
(1,1603)	2:33:B:GLN:HG2	2:33:B:GLN:HB2	17	0.12
(1,1592)	1:84:A:VAL:HG22	2:35:B:PHE:HB2	11	0.12
(1,1570)	1:57:A:LYS:HE2	1:59:A:TYR:HE1	12	0.12
(1,1562)	1:57:A:LYS:HD2	1:57:A:LYS:HG2	20	0.12
(1,1549)	1:58:A:CYS:HB2	1:57:A:LYS:HA	22	0.12
(1,1539)	1:62:A:GLU:HB3	1:59:A:TYR:HD1	10	0.12
(1,1536)	1:59:A:TYR:HD1	1:59:A:TYR:HA	17	0.12
(1,1536)	1:59:A:TYR:HD1	1:59:A:TYR:HA	22	0.12
(1,1529)	1:59:A:TYR:HB2	1:59:A:TYR:HD1	11	0.12
(1,1512)	1:62:A:GLU:HG2	1:62:A:GLU:H	23	0.12
(1,1491)	1:65:A:LYS:HB2	1:65:A:LYS:HG2	6	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1473)	1:66:A:LEU:HD12	1:109:A:LEU:HD12	4	0.12
(1,1423)	1:71:A:LEU:HD23	1:70:A:PHE:HD1	2	0.12
(1,1423)	1:71:A:LEU:HD23	1:70:A:PHE:HD1	4	0.12
(1,1423)	1:71:A:LEU:HD21	1:70:A:PHE:HD1	5	0.12
(1,1423)	1:71:A:LEU:HD23	1:70:A:PHE:HD1	12	0.12
(1,1419)	1:71:A:LEU:HD12	1:89:A:TYR:H	7	0.12
(1,1419)	1:71:A:LEU:HD12	1:89:A:TYR:H	10	0.12
(1,1411)	1:71:A:LEU:HD22	1:71:A:LEU:HB2	3	0.12
(1,1411)	1:71:A:LEU:HD22	1:71:A:LEU:HB2	6	0.12
(1,1411)	1:71:A:LEU:HD23	1:71:A:LEU:HB2	11	0.12
(1,1371)	1:75:A:LYS:HE3	1:72:A:GLU:HG2	7	0.12
(1,1369)	1:75:A:LYS:HE3	1:72:A:GLU:HA	15	0.12
(1,1367)	1:75:A:LYS:HD2	1:75:A:LYS:HA	11	0.12
(1,1367)	1:75:A:LYS:HD2	1:75:A:LYS:HA	18	0.12
(1,1346)	1:76:A:MET:HG2	1:73:A:LEU:HA	19	0.12
(1,1319)	1:77:A:GLN:HB3	1:78:A:THR:H	6	0.12
(1,1319)	1:77:A:GLN:HB3	1:78:A:THR:H	19	0.12
(1,1319)	1:77:A:GLN:HB3	1:78:A:THR:H	20	0.12
(1,1317)	1:79:A:ALA:HB3	1:76:A:MET:HA	1	0.12
(1,1317)	1:79:A:ALA:HB1	1:76:A:MET:HA	5	0.12
(1,1317)	1:79:A:ALA:HB3	1:76:A:MET:HA	25	0.12
(1,1315)	1:79:A:ALA:HB3	1:80:A:ASP:H	19	0.12
(1,1283)	1:84:A:VAL:HG21	1:127:A:ILE:HD13	15	0.12
(1,1280)	1:84:A:VAL:HG23	1:81:A:HIS:HB2	18	0.12
(1,1279)	1:84:A:VAL:HG21	1:81:A:HIS:HB3	20	0.12
(1,1275)	1:78:A:THR:HG22	1:77:A:GLN:HB3	3	0.12
(1,1257)	1:85:A:VAL:HG11	1:71:A:LEU:HA	6	0.12
(1,1247)	1:88:A:LEU:HD12	1:85:A:VAL:HA	19	0.12
(1,1225)	1:87:A:PHE:HB2	1:87:A:PHE:HD1	3	0.12
(1,1212)	1:88:A:LEU:HB2	1:88:A:LEU:HD12	19	0.12
(1,1212)	1:88:A:LEU:HB2	1:88:A:LEU:HD13	21	0.12
(1,1186)	1:90:A:ASN:HB3	1:90:A:ASN:HA	19	0.12
(1,1183)	1:90:A:ASN:HB2	1:87:A:PHE:HD1	9	0.12
(1,1171)	1:91:A:ARG:HG2	1:91:A:ARG:HA	18	0.12
(1,1144)	1:111:A:ARG:HG2	1:107:A:ASN:HA	14	0.12
(1,1132)	1:95:A:ALA:HB3	1:96:A:HIS:H	5	0.12
(1,1118)	1:98:A:LEU:HB3	1:98:A:LEU:HD22	13	0.12
(1,1118)	1:98:A:LEU:HB3	1:98:A:LEU:HD23	20	0.12
(1,1109)	1:98:A:LEU:HB3	1:98:A:LEU:H	1	0.12
(1,1109)	1:98:A:LEU:HB3	1:98:A:LEU:H	3	0.12
(1,1109)	1:98:A:LEU:HB3	1:98:A:LEU:H	10	0.12
(1,1109)	1:98:A:LEU:HB3	1:98:A:LEU:H	13	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1109)	1:98:A:LEU:HB3	1:98:A:LEU:H	18	0.12
(1,1109)	1:98:A:LEU:HB3	1:98:A:LEU:H	21	0.12
(1,1109)	1:98:A:LEU:HB3	1:98:A:LEU:H	22	0.12
(1,1098)	1:100:A:LEU:HD23	1:92:A:GLN:HA	11	0.12
(1,1097)	1:100:A:LEU:HD21	1:100:A:LEU:HD11	15	0.12
(1,1097)	1:100:A:LEU:HD21	1:100:A:LEU:HD11	19	0.12
(1,1094)	1:100:A:LEU:HD23	1:138:A:SER:HB2	1	0.12
(1,1072)	1:101:A:ALA:HB2	1:58:A:CYS:HA	4	0.12
(1,1057)	1:103:A:ALA:HB2	1:59:A:TYR:HD1	7	0.12
(1,1014)	1:74:A:CYS:HA	1:78:A:THR:HG22	25	0.12
(1,1003)	1:108:A:ILE:HB	1:108:A:ILE:HD11	1	0.12
(1,1003)	1:108:A:ILE:HB	1:108:A:ILE:HD12	4	0.12
(1,1003)	1:108:A:ILE:HB	1:108:A:ILE:HD11	11	0.12
(1,999)	1:108:A:ILE:HD11	1:99:A:PHE:HZ	17	0.12
(1,995)	1:108:A:ILE:HG21	1:130:A:LEU:HD12	5	0.12
(1,995)	1:108:A:ILE:HG21	1:130:A:LEU:HD13	10	0.12
(1,991)	1:108:A:ILE:HA	1:108:A:ILE:HG21	8	0.12
(1,963)	1:109:A:LEU:HD13	1:63:A:ASN:HB2	18	0.12
(1,960)	1:67:A:PHE:HA	1:109:A:LEU:HD13	13	0.12
(1,940)	1:111:A:ARG:HB3	1:111:A:ARG:H	7	0.12
(1,940)	1:111:A:ARG:HB3	1:111:A:ARG:H	11	0.12
(1,940)	1:111:A:ARG:HB3	1:111:A:ARG:H	20	0.12
(1,940)	1:111:A:ARG:HB3	1:111:A:ARG:H	25	0.12
(1,937)	1:112:A:VAL:HG22	1:113:A:LEU:HA	4	0.12
(1,937)	1:112:A:VAL:HG23	1:113:A:LEU:HA	23	0.12
(1,931)	1:112:A:VAL:HG11	1:126:A:TYR:HA	23	0.12
(1,930)	1:126:A:TYR:HD1	1:112:A:VAL:HG11	3	0.12
(1,930)	1:126:A:TYR:HD1	1:112:A:VAL:HG12	4	0.12
(1,930)	1:126:A:TYR:HD1	1:112:A:VAL:HG12	5	0.12
(1,930)	1:126:A:TYR:HD1	1:112:A:VAL:HG13	7	0.12
(1,924)	1:112:A:VAL:HA	1:115:A:ARG:HB3	16	0.12
(1,922)	1:112:A:VAL:HA	1:115:A:ARG:HG3	23	0.12
(1,915)	1:113:A:LEU:HD22	1:69:A:GLU:HB3	16	0.12
(1,915)	1:113:A:LEU:HD21	1:69:A:GLU:HB3	25	0.12
(1,911)	1:113:A:LEU:HB2	1:113:A:LEU:H	2	0.12
(1,911)	1:113:A:LEU:HB2	1:113:A:LEU:H	19	0.12
(1,909)	1:114:A:SER:HB2	1:113:A:LEU:HG	12	0.12
(1,881)	1:117:A:ARG:HD2	1:117:A:ARG:HB2	23	0.12
(1,870)	1:118:A:SER:HA	1:119:A:ARG:H	1	0.12
(1,870)	1:118:A:SER:HA	1:119:A:ARG:H	3	0.12
(1,870)	1:118:A:SER:HA	1:119:A:ARG:H	5	0.12
(1,870)	1:118:A:SER:HA	1:119:A:ARG:H	10	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,870)	1:118:A:SER:HA	1:119:A:ARG:H	11	0.12
(1,870)	1:118:A:SER:HA	1:119:A:ARG:H	12	0.12
(1,860)	1:119:A:ARG:HG2	1:119:A:ARG:H	2	0.12
(1,860)	1:119:A:ARG:HG2	1:119:A:ARG:H	16	0.12
(1,859)	1:119:A:ARG:HG2	1:119:A:ARG:HA	2	0.12
(1,859)	1:119:A:ARG:HG2	1:119:A:ARG:HA	19	0.12
(1,837)	1:120:A:PRO:HD2	1:119:A:ARG:H	16	0.12
(1,821)	1:122:A:LYS:HG3	1:122:A:LYS:H	15	0.12
(1,811)	1:123:A:LEU:HD21	1:70:A:PHE:HE1	7	0.12
(1,807)	1:123:A:LEU:HD13	1:74:A:CYS:HB2	19	0.12
(1,807)	1:123:A:LEU:HD11	1:74:A:CYS:HB2	20	0.12
(1,807)	1:123:A:LEU:HD13	1:74:A:CYS:HB2	23	0.12
(1,779)	1:125:A:VAL:HB	1:125:A:VAL:HG12	1	0.12
(1,779)	1:125:A:VAL:HB	1:125:A:VAL:HG12	2	0.12
(1,779)	1:125:A:VAL:HB	1:125:A:VAL:HG11	3	0.12
(1,778)	1:125:A:VAL:HG21	1:122:A:LYS:HA	4	0.12
(1,778)	1:125:A:VAL:HG23	1:122:A:LYS:HA	19	0.12
(1,773)	1:125:A:VAL:HA	1:125:A:VAL:HG13	11	0.12
(1,773)	1:125:A:VAL:HA	1:125:A:VAL:HG11	14	0.12
(1,773)	1:125:A:VAL:HA	1:125:A:VAL:HG13	17	0.12
(1,711)	1:130:A:LEU:HD21	1:109:A:LEU:HD21	9	0.12
(1,673)	1:133:A:VAL:HG23	1:130:A:LEU:HA	17	0.12
(1,673)	1:133:A:VAL:HG21	1:130:A:LEU:HA	20	0.12
(1,601)	1:137:A:HIS:HB3	1:137:A:HIS:H	2	0.12
(1,601)	1:137:A:HIS:HB3	1:137:A:HIS:H	5	0.12
(1,601)	1:137:A:HIS:HB3	1:137:A:HIS:H	6	0.12
(1,601)	1:137:A:HIS:HB3	1:137:A:HIS:H	16	0.12
(1,596)	1:137:A:HIS:HA	1:138:A:SER:H	10	0.12
(1,596)	1:137:A:HIS:HA	1:138:A:SER:H	11	0.12
(1,594)	1:95:A:ALA:HB2	1:138:A:SER:HB3	22	0.12
(1,578)	1:57:A:LYS:HA	1:57:A:LYS:H	6	0.12
(1,578)	1:57:A:LYS:HA	1:57:A:LYS:H	20	0.12
(1,553)	2:29:B:SER:HB2	2:30:B:GLU:H	10	0.12
(1,538)	1:63:A:ASN:H	1:61:A:LEU:HA	13	0.12
(1,537)	1:63:A:ASN:H	1:61:A:LEU:H	3	0.12
(1,537)	1:63:A:ASN:H	1:61:A:LEU:H	17	0.12
(1,532)	1:66:A:LEU:H	1:64:A:GLU:HB2	6	0.12
(1,526)	1:69:A:GLU:H	1:113:A:LEU:HD22	24	0.12
(1,521)	1:71:A:LEU:H	1:113:A:LEU:HD11	12	0.12
(1,509)	1:77:A:GLN:HE22	1:73:A:LEU:HG	9	0.12
(1,509)	1:77:A:GLN:HE22	1:73:A:LEU:HG	17	0.12
(1,505)	1:79:A:ALA:H	1:76:A:MET:HA	5	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,492)	1:91:A:ARG:H	1:88:A:LEU:HD21	9	0.12
(1,475)	1:98:A:LEU:HD23	1:98:A:LEU:H	5	0.12
(1,456)	1:112:A:VAL:H	1:108:A:ILE:HG21	12	0.12
(1,456)	1:112:A:VAL:H	1:108:A:ILE:HG21	17	0.12
(1,456)	1:112:A:VAL:H	1:108:A:ILE:HG23	19	0.12
(1,453)	1:114:A:SER:H	1:113:A:LEU:HD23	21	0.12
(1,448)	1:116:A:ALA:H	1:126:A:TYR:HE2	15	0.12
(1,438)	1:66:A:LEU:HD13	1:66:A:LEU:H	19	0.12
(1,420)	1:129:A:GLU:H	1:125:A:VAL:HG12	21	0.12
(1,414)	1:72:A:GLU:H	1:68:A:GLU:HA	8	0.12
(1,410)	1:134:A:LEU:H	1:132:A:THR:H	21	0.12
(1,397)	1:137:A:HIS:H	1:134:A:LEU:HA	23	0.12
(1,394)	1:137:A:HIS:HB3	1:138:A:SER:H	13	0.12
(1,392)	1:139:A:ALA:H	1:96:A:HIS:HD2	3	0.12
(1,392)	1:139:A:ALA:H	1:96:A:HIS:HD2	9	0.12
(1,380)	2:27:B:SER:HA	2:30:B:GLU:HB3	10	0.12
(1,379)	2:31:B:LEU:HB2	2:28:B:ASP:HB2	24	0.12
(1,376)	2:27:B:SER:HB3	2:26:B:ASP:HB3	11	0.12
(1,369)	2:26:B:ASP:HB2	1:87:A:PHE:HZ	3	0.12
(1,367)	2:26:B:ASP:HB3	2:31:B:LEU:H	17	0.12
(1,356)	2:29:B:SER:HB2	2:33:B:GLN:H	25	0.12
(1,353)	2:27:B:SER:HB2	2:27:B:SER:H	13	0.12
(1,343)	2:31:B:LEU:HB2	1:87:A:PHE:HE2	16	0.12
(1,337)	2:31:B:LEU:HD23	2:28:B:ASP:HB3	12	0.12
(1,288)	2:32:B:GLU:HA	2:35:B:PHE:HD1	3	0.12
(1,288)	2:32:B:GLU:HA	2:35:B:PHE:HD1	11	0.12
(1,285)	2:31:B:LEU:HD12	1:127:A:ILE:HB	17	0.12
(1,257)	1:113:A:LEU:HD11	1:117:A:ARG:HG3	16	0.12
(1,236)	1:64:A:GLU:HA	1:67:A:PHE:H	8	0.12
(1,209)	1:67:A:PHE:HE1	1:71:A:LEU:HD23	5	0.12
(1,163)	1:67:A:PHE:HD2	1:92:A:GLN:HG3	7	0.12
(1,157)	1:130:A:LEU:HD22	1:88:A:LEU:HD12	8	0.12
(1,156)	1:88:A:LEU:HB3	1:88:A:LEU:HD11	13	0.12
(1,121)	1:95:A:ALA:HB1	1:138:A:SER:HB3	1	0.12
(1,116)	1:100:A:LEU:HD21	1:105:A:PHE:HE2	5	0.12
(1,107)	1:69:A:GLU:HA	1:69:A:GLU:HB3	23	0.12
(1,100)	1:67:A:PHE:HE1	1:88:A:LEU:HD11	10	0.12
(1,84)	1:114:A:SER:HB2	1:113:A:LEU:HG	19	0.12
(1,80)	1:94:A:ARG:HD2	1:93:A:GLN:HB2	20	0.12
(1,79)	1:117:A:ARG:HD3	1:117:A:ARG:HG2	2	0.12
(1,79)	1:117:A:ARG:HD3	1:117:A:ARG:HG2	3	0.12
(1,79)	1:111:A:ARG:HD3	1:111:A:ARG:HG2	22	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,78)	1:118:A:SER:HB3	1:119:A:ARG:HG3	7	0.12
(1,78)	1:118:A:SER:HB3	1:119:A:ARG:HG3	16	0.12
(1,76)	1:118:A:SER:HA	1:118:A:SER:HB2	8	0.12
(1,76)	1:118:A:SER:HA	1:118:A:SER:HB2	24	0.12
(1,66)	1:121:A:ALA:HA	1:121:A:ALA:H	1	0.12
(1,66)	1:121:A:ALA:HA	1:121:A:ALA:H	9	0.12
(1,66)	1:121:A:ALA:HA	1:121:A:ALA:H	19	0.12
(1,66)	1:121:A:ALA:HA	1:121:A:ALA:H	24	0.12
(1,61)	1:123:A:LEU:HD12	1:120:A:PRO:HA	10	0.12
(1,56)	1:124:A:TYR:HE2	2:35:B:PHE:HB3	7	0.12
(1,56)	1:124:A:TYR:HE2	2:35:B:PHE:HB3	12	0.12
(1,42)	1:126:A:TYR:HD1	1:125:A:VAL:HB	5	0.12
(1,42)	1:126:A:TYR:HD1	1:125:A:VAL:HB	7	0.12
(1,25)	1:85:A:VAL:HG23	1:74:A:CYS:HB2	12	0.12
(1,20)	1:66:A:LEU:HA	1:69:A:GLU:HB2	12	0.12
(1,19)	1:133:A:VAL:HG22	1:130:A:LEU:HA	10	0.12
(1,2286)	2:33:B:GLN:HG2	2:33:B:GLN:HE22	13	0.11
(1,2248)	2:30:B:GLU:HB2	2:31:B:LEU:H	3	0.11
(1,2248)	2:30:B:GLU:HB2	2:31:B:LEU:H	8	0.11
(1,2248)	2:30:B:GLU:HB2	2:31:B:LEU:H	15	0.11
(1,2244)	2:36:B:THR:HG21	2:36:B:THR:H	6	0.11
(1,2244)	2:36:B:THR:HG21	2:36:B:THR:H	16	0.11
(1,2197)	1:55:A:GLY:HA2	1:56:A:LYS:H	1	0.11
(1,2194)	1:56:A:LYS:HB3	1:56:A:LYS:H	24	0.11
(1,2185)	1:59:A:TYR:HE1	1:59:A:TYR:H	5	0.11
(1,2161)	1:64:A:GLU:HB3	1:64:A:GLU:H	1	0.11
(1,2161)	1:64:A:GLU:HB3	1:64:A:GLU:H	2	0.11
(1,2161)	1:64:A:GLU:HB3	1:64:A:GLU:H	4	0.11
(1,2161)	1:64:A:GLU:HB3	1:64:A:GLU:H	14	0.11
(1,2161)	1:64:A:GLU:HB3	1:64:A:GLU:H	18	0.11
(1,2161)	1:64:A:GLU:HB3	1:64:A:GLU:H	20	0.11
(1,2161)	1:64:A:GLU:HB3	1:64:A:GLU:H	23	0.11
(1,2153)	1:109:A:LEU:HD11	1:66:A:LEU:H	8	0.11
(1,2153)	1:109:A:LEU:HD12	1:66:A:LEU:H	9	0.11
(1,2153)	1:109:A:LEU:HD11	1:66:A:LEU:H	24	0.11
(1,2151)	1:65:A:LYS:HG3	1:66:A:LEU:H	20	0.11
(1,2151)	1:65:A:LYS:HG3	1:66:A:LEU:H	22	0.11
(1,2151)	1:65:A:LYS:HG3	1:66:A:LEU:H	24	0.11
(1,2136)	1:69:A:GLU:H	1:70:A:PHE:HB2	6	0.11
(1,2136)	1:69:A:GLU:H	1:70:A:PHE:HB3	19	0.11
(1,2136)	1:69:A:GLU:H	1:70:A:PHE:HB2	20	0.11
(1,2108)	1:77:A:GLN:H	1:78:A:THR:HG21	14	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2094)	1:79:A:ALA:HB3	1:78:A:THR:H	1	0.11
(1,2094)	1:79:A:ALA:HB2	1:78:A:THR:H	23	0.11
(1,2080)	1:81:A:HIS:H	1:81:A:HIS:HB3	3	0.11
(1,2080)	1:81:A:HIS:H	1:81:A:HIS:HB3	24	0.11
(1,2004)	1:95:A:ALA:H	1:94:A:ARG:HB3	15	0.11
(1,1989)	1:98:A:LEU:H	1:138:A:SER:HB2	18	0.11
(1,1987)	1:99:A:PHE:H	1:99:A:PHE:HD2	13	0.11
(1,1975)	1:100:A:LEU:HD12	1:100:A:LEU:H	18	0.11
(1,1975)	1:100:A:LEU:HD13	1:100:A:LEU:H	19	0.11
(1,1958)	1:103:A:ALA:H	1:102:A:SER:HB3	21	0.11
(1,1950)	1:104:A:GLU:H	1:102:A:SER:HA	4	0.11
(1,1837)	1:127:A:ILE:H	1:123:A:LEU:HD11	5	0.11
(1,1803)	1:135:A:LYS:HB3	1:135:A:LYS:H	24	0.11
(1,1792)	1:138:A:SER:H	1:135:A:LYS:HD3	13	0.11
(1,1781)	1:140:A:LYS:H	1:141:A:LYS:HB3	13	0.11
(1,1777)	1:144:A:ASN:HB3	1:144:A:ASN:H	15	0.11
(1,1777)	1:144:A:ASN:HB3	1:144:A:ASN:H	21	0.11
(1,1776)	1:144:A:ASN:HA	1:144:A:ASN:H	1	0.11
(1,1776)	1:144:A:ASN:HA	1:144:A:ASN:H	5	0.11
(1,1776)	1:144:A:ASN:HA	1:144:A:ASN:H	7	0.11
(1,1776)	1:144:A:ASN:HA	1:144:A:ASN:H	9	0.11
(1,1776)	1:144:A:ASN:HA	1:144:A:ASN:H	11	0.11
(1,1772)	1:142:A:LYS:H	1:141:A:LYS:HG2	11	0.11
(1,1769)	2:26:B:ASP:HB3	2:30:B:GLU:HG2	8	0.11
(1,1764)	2:24:B:GLN:HB3	2:24:B:GLN:HG3	3	0.11
(1,1764)	2:24:B:GLN:HB3	2:24:B:GLN:HG3	15	0.11
(1,1764)	2:24:B:GLN:HB3	2:24:B:GLN:HG3	22	0.11
(1,1759)	2:30:B:GLU:HA	2:30:B:GLU:HG3	13	0.11
(1,1740)	2:31:B:LEU:HA	2:32:B:GLU:H	3	0.11
(1,1725)	2:31:B:LEU:HD23	1:127:A:ILE:HG22	13	0.11
(1,1724)	2:31:B:LEU:HG	2:31:B:LEU:HD22	2	0.11
(1,1724)	2:31:B:LEU:HG	2:31:B:LEU:HD21	3	0.11
(1,1724)	2:31:B:LEU:HG	2:31:B:LEU:HD23	6	0.11
(1,1724)	2:31:B:LEU:HG	2:31:B:LEU:HD23	7	0.11
(1,1724)	2:31:B:LEU:HG	2:31:B:LEU:HD22	8	0.11
(1,1724)	2:31:B:LEU:HG	2:31:B:LEU:HD22	11	0.11
(1,1724)	2:31:B:LEU:HG	2:31:B:LEU:HD22	12	0.11
(1,1724)	2:31:B:LEU:HG	2:31:B:LEU:HD22	14	0.11
(1,1724)	2:31:B:LEU:HG	2:31:B:LEU:HD22	15	0.11
(1,1724)	2:31:B:LEU:HG	2:31:B:LEU:HD22	16	0.11
(1,1724)	2:31:B:LEU:HG	2:31:B:LEU:HD22	20	0.11
(1,1724)	2:31:B:LEU:HG	2:31:B:LEU:HD22	23	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1724)	2:31:B:LEU:HG	2:31:B:LEU:HD22	24	0.11
(1,1723)	2:31:B:LEU:HD21	2:30:B:GLU:HB2	4	0.11
(1,1721)	2:31:B:LEU:HD21	2:31:B:LEU:HA	16	0.11
(1,1715)	2:31:B:LEU:HG	2:31:B:LEU:HA	3	0.11
(1,1715)	2:31:B:LEU:HG	2:31:B:LEU:HA	4	0.11
(1,1715)	2:31:B:LEU:HG	2:31:B:LEU:HA	14	0.11
(1,1715)	2:31:B:LEU:HG	2:31:B:LEU:HA	20	0.11
(1,1708)	2:32:B:GLU:HG2	2:39:B:TRP:HZ2	14	0.11
(1,1708)	2:32:B:GLU:HG2	2:39:B:TRP:HZ2	16	0.11
(1,1707)	2:33:B:GLN:HB2	2:33:B:GLN:HA	1	0.11
(1,1707)	2:33:B:GLN:HB2	2:33:B:GLN:HA	2	0.11
(1,1707)	2:33:B:GLN:HB2	2:33:B:GLN:HA	3	0.11
(1,1707)	2:33:B:GLN:HB2	2:33:B:GLN:HA	4	0.11
(1,1707)	2:33:B:GLN:HB2	2:33:B:GLN:HA	5	0.11
(1,1707)	2:33:B:GLN:HB2	2:33:B:GLN:HA	6	0.11
(1,1707)	2:33:B:GLN:HB2	2:33:B:GLN:HA	7	0.11
(1,1707)	2:33:B:GLN:HB2	2:33:B:GLN:HA	8	0.11
(1,1707)	2:33:B:GLN:HB2	2:33:B:GLN:HA	9	0.11
(1,1707)	2:33:B:GLN:HB2	2:33:B:GLN:HA	10	0.11
(1,1707)	2:33:B:GLN:HB2	2:33:B:GLN:HA	11	0.11
(1,1707)	2:33:B:GLN:HB2	2:33:B:GLN:HA	12	0.11
(1,1707)	2:33:B:GLN:HB2	2:33:B:GLN:HA	13	0.11
(1,1707)	2:33:B:GLN:HB2	2:33:B:GLN:HA	14	0.11
(1,1707)	2:33:B:GLN:HB2	2:33:B:GLN:HA	16	0.11
(1,1707)	2:33:B:GLN:HB2	2:33:B:GLN:HA	17	0.11
(1,1707)	2:33:B:GLN:HB2	2:33:B:GLN:HA	18	0.11
(1,1707)	2:33:B:GLN:HB2	2:33:B:GLN:HA	20	0.11
(1,1707)	2:33:B:GLN:HB2	2:33:B:GLN:HA	21	0.11
(1,1707)	2:33:B:GLN:HB2	2:33:B:GLN:HA	22	0.11
(1,1707)	2:33:B:GLN:HB2	2:33:B:GLN:HA	23	0.11
(1,1707)	2:33:B:GLN:HB2	2:33:B:GLN:HA	25	0.11
(1,1703)	2:33:B:GLN:HG2	2:31:B:LEU:HD22	10	0.11
(1,1703)	2:33:B:GLN:HG2	2:31:B:LEU:HD21	16	0.11
(1,1702)	2:33:B:GLN:HG3	2:34:B:TYR:HE2	22	0.11
(1,1690)	2:34:B:TYR:HE1	2:34:B:TYR:HD1	10	0.11
(1,1653)	2:37:B:ALA:HB2	2:37:B:ALA:HA	3	0.11
(1,1653)	2:37:B:ALA:HB1	2:37:B:ALA:HA	13	0.11
(1,1653)	2:37:B:ALA:HB1	2:37:B:ALA:HA	14	0.11
(1,1653)	2:37:B:ALA:HB1	2:37:B:ALA:HA	22	0.11
(1,1653)	2:37:B:ALA:HB2	2:37:B:ALA:HA	24	0.11
(1,1639)	2:38:B:ARG:HD2	2:38:B:ARG:H	9	0.11
(1,1634)	2:38:B:ARG:HD2	2:37:B:ALA:HB2	25	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1617)	2:39:B:TRP:HD1	2:38:B:ARG:HA	8	0.11
(1,1615)	2:39:B:TRP:HE3	2:36:B:THR:HG23	12	0.11
(1,1608)	2:32:B:GLU:HA	2:33:B:GLN:H	9	0.11
(1,1608)	2:32:B:GLU:HA	2:33:B:GLN:H	18	0.11
(1,1608)	2:32:B:GLU:HA	2:33:B:GLN:H	22	0.11
(1,1603)	2:33:B:GLN:HG2	2:33:B:GLN:HB2	6	0.11
(1,1603)	2:33:B:GLN:HG2	2:33:B:GLN:HB2	8	0.11
(1,1603)	2:33:B:GLN:HG2	2:33:B:GLN:HB2	13	0.11
(1,1603)	2:33:B:GLN:HG2	2:33:B:GLN:HB2	14	0.11
(1,1603)	2:33:B:GLN:HG2	2:33:B:GLN:HB2	20	0.11
(1,1603)	2:33:B:GLN:HG2	2:33:B:GLN:HB2	25	0.11
(1,1595)	2:31:B:LEU:HD12	1:127:A:ILE:HB	16	0.11
(1,1588)	1:87:A:PHE:HB2	2:31:B:LEU:HD13	4	0.11
(1,1567)	1:57:A:LYS:HG3	1:57:A:LYS:HE2	22	0.11
(1,1550)	1:141:A:LYS:HG3	1:141:A:LYS:HA	16	0.11
(1,1545)	1:59:A:TYR:HE1	1:57:A:LYS:HB2	5	0.11
(1,1544)	1:103:A:ALA:HA	1:59:A:TYR:HE1	15	0.11
(1,1536)	1:59:A:TYR:HD1	1:59:A:TYR:HA	21	0.11
(1,1536)	1:59:A:TYR:HD1	1:59:A:TYR:HA	24	0.11
(1,1512)	1:62:A:GLU:HG2	1:62:A:GLU:H	6	0.11
(1,1512)	1:62:A:GLU:HG2	1:62:A:GLU:H	12	0.11
(1,1512)	1:62:A:GLU:HG2	1:62:A:GLU:H	16	0.11
(1,1495)	1:64:A:GLU:HA	1:67:A:PHE:HB2	7	0.11
(1,1430)	1:88:A:LEU:HD12	1:70:A:PHE:HD1	3	0.11
(1,1423)	1:71:A:LEU:HD21	1:70:A:PHE:HD1	1	0.11
(1,1423)	1:71:A:LEU:HD23	1:70:A:PHE:HD1	8	0.11
(1,1423)	1:71:A:LEU:HD23	1:70:A:PHE:HD1	9	0.11
(1,1423)	1:71:A:LEU:HD23	1:70:A:PHE:HD1	13	0.11
(1,1423)	1:71:A:LEU:HD21	1:70:A:PHE:HD1	15	0.11
(1,1423)	1:71:A:LEU:HD23	1:70:A:PHE:HD1	16	0.11
(1,1423)	1:71:A:LEU:HD21	1:70:A:PHE:HD1	19	0.11
(1,1423)	1:71:A:LEU:HD22	1:70:A:PHE:HD1	20	0.11
(1,1423)	1:71:A:LEU:HD22	1:70:A:PHE:HD1	22	0.11
(1,1423)	1:71:A:LEU:HD22	1:70:A:PHE:HD1	23	0.11
(1,1411)	1:71:A:LEU:HD23	1:71:A:LEU:HB2	2	0.11
(1,1411)	1:71:A:LEU:HD23	1:71:A:LEU:HB2	7	0.11
(1,1411)	1:71:A:LEU:HD23	1:71:A:LEU:HB2	12	0.11
(1,1411)	1:71:A:LEU:HD22	1:71:A:LEU:HB2	22	0.11
(1,1391)	1:74:A:CYS:HA	1:73:A:LEU:HD21	23	0.11
(1,1371)	1:75:A:LYS:HE3	1:72:A:GLU:HG2	13	0.11
(1,1371)	1:75:A:LYS:HE3	1:72:A:GLU:HG2	18	0.11
(1,1369)	1:75:A:LYS:HE3	1:72:A:GLU:HA	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1369)	1:75:A:LYS:HE3	1:72:A:GLU:HA	3	0.11
(1,1369)	1:75:A:LYS:HE3	1:72:A:GLU:HA	14	0.11
(1,1369)	1:75:A:LYS:HE3	1:72:A:GLU:HA	16	0.11
(1,1369)	1:75:A:LYS:HE3	1:72:A:GLU:HA	21	0.11
(1,1360)	1:75:A:LYS:HG3	1:75:A:LYS:H	15	0.11
(1,1346)	1:76:A:MET:HG2	1:73:A:LEU:HA	11	0.11
(1,1343)	1:76:A:MET:HG2	1:76:A:MET:H	12	0.11
(1,1343)	1:76:A:MET:HG2	1:76:A:MET:H	14	0.11
(1,1331)	1:77:A:GLN:HG2	1:73:A:LEU:HD13	24	0.11
(1,1319)	1:77:A:GLN:HB3	1:78:A:THR:H	7	0.11
(1,1319)	1:77:A:GLN:HB3	1:78:A:THR:H	9	0.11
(1,1319)	1:77:A:GLN:HB3	1:78:A:THR:H	10	0.11
(1,1319)	1:77:A:GLN:HB3	1:78:A:THR:H	16	0.11
(1,1319)	1:77:A:GLN:HB3	1:78:A:THR:H	24	0.11
(1,1317)	1:79:A:ALA:HB2	1:76:A:MET:HA	11	0.11
(1,1317)	1:79:A:ALA:HB2	1:76:A:MET:HA	13	0.11
(1,1257)	1:85:A:VAL:HG11	1:71:A:LEU:HA	8	0.11
(1,1257)	1:85:A:VAL:HG12	1:71:A:LEU:HA	9	0.11
(1,1257)	1:85:A:VAL:HG12	1:71:A:LEU:HA	14	0.11
(1,1257)	1:85:A:VAL:HG13	1:71:A:LEU:HA	18	0.11
(1,1257)	1:85:A:VAL:HG12	1:71:A:LEU:HA	24	0.11
(1,1247)	1:88:A:LEU:HD13	1:85:A:VAL:HA	21	0.11
(1,1247)	1:88:A:LEU:HD11	1:85:A:VAL:HA	24	0.11
(1,1247)	1:88:A:LEU:HD11	1:85:A:VAL:HA	25	0.11
(1,1197)	1:89:A:TYR:HD2	1:71:A:LEU:HD21	4	0.11
(1,1186)	1:90:A:ASN:HB3	1:90:A:ASN:HA	1	0.11
(1,1186)	1:90:A:ASN:HB3	1:90:A:ASN:HA	2	0.11
(1,1186)	1:90:A:ASN:HB3	1:90:A:ASN:HA	5	0.11
(1,1186)	1:90:A:ASN:HB3	1:90:A:ASN:HA	7	0.11
(1,1186)	1:90:A:ASN:HB3	1:90:A:ASN:HA	9	0.11
(1,1186)	1:90:A:ASN:HB3	1:90:A:ASN:HA	10	0.11
(1,1186)	1:90:A:ASN:HB3	1:90:A:ASN:HA	11	0.11
(1,1186)	1:90:A:ASN:HB3	1:90:A:ASN:HA	15	0.11
(1,1186)	1:90:A:ASN:HB3	1:90:A:ASN:HA	16	0.11
(1,1186)	1:90:A:ASN:HB3	1:90:A:ASN:HA	22	0.11
(1,1186)	1:90:A:ASN:HB3	1:90:A:ASN:HA	24	0.11
(1,1183)	1:90:A:ASN:HB2	1:87:A:PHE:HD1	11	0.11
(1,1175)	1:91:A:ARG:HG2	1:134:A:LEU:HB2	21	0.11
(1,1171)	1:91:A:ARG:HG2	1:91:A:ARG:HA	6	0.11
(1,1171)	1:91:A:ARG:HG2	1:91:A:ARG:HA	9	0.11
(1,1171)	1:91:A:ARG:HG2	1:91:A:ARG:HA	14	0.11
(1,1147)	1:94:A:ARG:HG2	1:94:A:ARG:HA	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1147)	1:94:A:ARG:HG2	1:94:A:ARG:HA	7	0.11
(1,1147)	1:94:A:ARG:HG2	1:94:A:ARG:HA	16	0.11
(1,1139)	1:134:A:LEU:HD22	1:95:A:ALA:HB1	21	0.11
(1,1132)	1:95:A:ALA:HB3	1:96:A:HIS:H	24	0.11
(1,1123)	1:83:A:GLU:HA	1:83:A:GLU:HG3	21	0.11
(1,1109)	1:98:A:LEU:HB3	1:98:A:LEU:H	2	0.11
(1,1109)	1:98:A:LEU:HB3	1:98:A:LEU:H	4	0.11
(1,1109)	1:98:A:LEU:HB3	1:98:A:LEU:H	5	0.11
(1,1109)	1:98:A:LEU:HB3	1:98:A:LEU:H	14	0.11
(1,1109)	1:98:A:LEU:HB3	1:98:A:LEU:H	23	0.11
(1,1109)	1:98:A:LEU:HB3	1:98:A:LEU:H	24	0.11
(1,1077)	1:101:A:ALA:HB1	1:98:A:LEU:HA	12	0.11
(1,1077)	1:101:A:ALA:HB1	1:98:A:LEU:HA	16	0.11
(1,1056)	1:103:A:ALA:HB1	1:104:A:GLU:H	13	0.11
(1,1049)	1:108:A:ILE:HD13	1:104:A:GLU:HG2	24	0.11
(1,1048)	1:104:A:GLU:HG2	1:99:A:PHE:HE1	3	0.11
(1,1045)	1:62:A:GLU:HB2	1:59:A:TYR:HD1	5	0.11
(1,1003)	1:108:A:ILE:HB	1:108:A:ILE:HD12	3	0.11
(1,1003)	1:108:A:ILE:HB	1:108:A:ILE:HD13	12	0.11
(1,1003)	1:108:A:ILE:HB	1:108:A:ILE:HD11	16	0.11
(1,1003)	1:108:A:ILE:HB	1:108:A:ILE:HD11	17	0.11
(1,1003)	1:108:A:ILE:HB	1:108:A:ILE:HD13	18	0.11
(1,1003)	1:108:A:ILE:HB	1:108:A:ILE:HD11	21	0.11
(1,1003)	1:108:A:ILE:HB	1:108:A:ILE:HD13	24	0.11
(1,1003)	1:108:A:ILE:HB	1:108:A:ILE:HD11	25	0.11
(1,995)	1:108:A:ILE:HG21	1:130:A:LEU:HD12	4	0.11
(1,995)	1:108:A:ILE:HG23	1:130:A:LEU:HD12	22	0.11
(1,994)	1:108:A:ILE:HG12	1:108:A:ILE:HG23	23	0.11
(1,960)	1:67:A:PHE:HA	1:109:A:LEU:HD12	12	0.11
(1,940)	1:111:A:ARG:HB3	1:111:A:ARG:H	6	0.11
(1,940)	1:111:A:ARG:HB3	1:111:A:ARG:H	9	0.11
(1,940)	1:111:A:ARG:HB3	1:111:A:ARG:H	12	0.11
(1,940)	1:111:A:ARG:HB3	1:111:A:ARG:H	18	0.11
(1,940)	1:111:A:ARG:HB3	1:111:A:ARG:H	24	0.11
(1,937)	1:112:A:VAL:HG21	1:113:A:LEU:HA	1	0.11
(1,937)	1:112:A:VAL:HG23	1:113:A:LEU:HA	7	0.11
(1,937)	1:112:A:VAL:HG21	1:113:A:LEU:HA	12	0.11
(1,937)	1:112:A:VAL:HG22	1:113:A:LEU:HA	13	0.11
(1,937)	1:112:A:VAL:HG21	1:113:A:LEU:HA	20	0.11
(1,930)	1:126:A:TYR:HD1	1:112:A:VAL:HG11	9	0.11
(1,930)	1:126:A:TYR:HD1	1:112:A:VAL:HG11	11	0.11
(1,930)	1:126:A:TYR:HD1	1:112:A:VAL:HG13	12	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,911)	1:113:A:LEU:HB2	1:113:A:LEU:H	21	0.11
(1,911)	1:113:A:LEU:HB2	1:113:A:LEU:H	25	0.11
(1,898)	1:115:A:ARG:HA	1:115:A:ARG:HG2	3	0.11
(1,898)	1:115:A:ARG:HA	1:115:A:ARG:HG2	8	0.11
(1,870)	1:118:A:SER:HA	1:119:A:ARG:H	13	0.11
(1,870)	1:118:A:SER:HA	1:119:A:ARG:H	15	0.11
(1,870)	1:118:A:SER:HA	1:119:A:ARG:H	22	0.11
(1,870)	1:118:A:SER:HA	1:119:A:ARG:H	23	0.11
(1,837)	1:120:A:PRO:HD2	1:119:A:ARG:H	25	0.11
(1,830)	1:121:A:ALA:HB3	1:122:A:LYS:H	5	0.11
(1,830)	1:121:A:ALA:HB3	1:122:A:LYS:H	10	0.11
(1,829)	1:121:A:ALA:HB3	1:121:A:ALA:H	5	0.11
(1,821)	1:122:A:LYS:HG3	1:122:A:LYS:H	17	0.11
(1,814)	1:123:A:LEU:HD22	1:120:A:PRO:HA	3	0.11
(1,811)	1:123:A:LEU:HD23	1:70:A:PHE:HE1	17	0.11
(1,807)	1:123:A:LEU:HD13	1:74:A:CYS:HB2	3	0.11
(1,807)	1:123:A:LEU:HD13	1:74:A:CYS:HB2	4	0.11
(1,807)	1:123:A:LEU:HD12	1:74:A:CYS:HB2	12	0.11
(1,779)	1:125:A:VAL:HB	1:125:A:VAL:HG11	11	0.11
(1,779)	1:125:A:VAL:HB	1:125:A:VAL:HG13	13	0.11
(1,779)	1:125:A:VAL:HB	1:125:A:VAL:HG13	19	0.11
(1,775)	1:126:A:TYR:HE1	1:125:A:VAL:HG12	14	0.11
(1,773)	1:125:A:VAL:HA	1:125:A:VAL:HG11	21	0.11
(1,773)	1:125:A:VAL:HA	1:125:A:VAL:HG13	22	0.11
(1,773)	1:125:A:VAL:HA	1:125:A:VAL:HG11	23	0.11
(1,751)	1:127:A:ILE:HG23	1:127:A:ILE:HD13	17	0.11
(1,751)	1:127:A:ILE:HG21	1:127:A:ILE:HD12	25	0.11
(1,746)	1:127:A:ILE:HD11	1:127:A:ILE:H	12	0.11
(1,746)	1:127:A:ILE:HD13	1:127:A:ILE:H	18	0.11
(1,711)	1:130:A:LEU:HD21	1:109:A:LEU:HD21	19	0.11
(1,706)	1:85:A:VAL:HG23	1:75:A:LYS:HD2	1	0.11
(1,704)	1:130:A:LEU:HD12	1:109:A:LEU:HD23	17	0.11
(1,673)	1:133:A:VAL:HG22	1:130:A:LEU:HA	4	0.11
(1,673)	1:133:A:VAL:HG22	1:130:A:LEU:HA	7	0.11
(1,673)	1:133:A:VAL:HG23	1:130:A:LEU:HA	22	0.11
(1,638)	1:134:A:LEU:HD23	1:99:A:PHE:HE2	5	0.11
(1,636)	1:134:A:LEU:HD23	1:134:A:LEU:H	20	0.11
(1,619)	1:135:A:LYS:HG2	1:91:A:ARG:HD3	7	0.11
(1,619)	1:135:A:LYS:HG2	1:91:A:ARG:HD3	11	0.11
(1,619)	1:135:A:LYS:HG2	1:91:A:ARG:HD3	23	0.11
(1,604)	1:136:A:ALA:HB3	1:136:A:ALA:H	19	0.11
(1,604)	1:136:A:ALA:HB1	1:136:A:ALA:H	22	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,601)	1:137:A:HIS:HB3	1:137:A:HIS:H	4	0.11
(1,601)	1:137:A:HIS:HB3	1:137:A:HIS:H	7	0.11
(1,601)	1:137:A:HIS:HB3	1:137:A:HIS:H	11	0.11
(1,601)	1:137:A:HIS:HB3	1:137:A:HIS:H	13	0.11
(1,601)	1:137:A:HIS:HB3	1:137:A:HIS:H	20	0.11
(1,601)	1:137:A:HIS:HB3	1:137:A:HIS:H	24	0.11
(1,594)	1:95:A:ALA:HB2	1:138:A:SER:HB3	7	0.11
(1,591)	1:138:A:SER:HB3	1:138:A:SER:H	15	0.11
(1,578)	1:57:A:LYS:HA	1:57:A:LYS:H	2	0.11
(1,578)	1:57:A:LYS:HA	1:57:A:LYS:H	10	0.11
(1,578)	1:57:A:LYS:HA	1:57:A:LYS:H	13	0.11
(1,578)	1:57:A:LYS:HA	1:57:A:LYS:H	15	0.11
(1,572)	1:143:A:LEU:HB2	1:143:A:LEU:HD13	5	0.11
(1,572)	1:143:A:LEU:HB2	1:143:A:LEU:HD13	9	0.11
(1,572)	1:143:A:LEU:HB2	1:143:A:LEU:HD11	10	0.11
(1,572)	1:143:A:LEU:HB2	1:143:A:LEU:HD12	11	0.11
(1,572)	1:143:A:LEU:HB2	1:143:A:LEU:HD12	12	0.11
(1,572)	1:143:A:LEU:HB2	1:143:A:LEU:HD13	20	0.11
(1,562)	2:26:B:ASP:H	2:25:B:GLU:HG3	24	0.11
(1,561)	2:27:B:SER:H	2:30:B:GLU:HB3	2	0.11
(1,553)	2:29:B:SER:HB2	2:30:B:GLU:H	11	0.11
(1,553)	2:29:B:SER:HB2	2:30:B:GLU:H	13	0.11
(1,553)	2:29:B:SER:HB2	2:30:B:GLU:H	14	0.11
(1,540)	1:63:A:ASN:H	1:61:A:LEU:HG	19	0.11
(1,537)	1:63:A:ASN:H	1:61:A:LEU:H	7	0.11
(1,532)	1:66:A:LEU:H	1:64:A:GLU:HB2	4	0.11
(1,520)	1:130:A:LEU:H	1:112:A:VAL:HG21	19	0.11
(1,477)	1:93:A:GLN:HA	1:95:A:ALA:H	3	0.11
(1,474)	1:101:A:ALA:H	1:98:A:LEU:HD23	19	0.11
(1,464)	1:107:A:ASN:H	1:108:A:ILE:HB	5	0.11
(1,464)	1:107:A:ASN:H	1:108:A:ILE:HB	21	0.11
(1,459)	1:111:A:ARG:HB2	1:110:A:SER:H	24	0.11
(1,459)	1:111:A:ARG:HB2	1:110:A:SER:H	25	0.11
(1,456)	1:112:A:VAL:H	1:108:A:ILE:HG23	2	0.11
(1,456)	1:112:A:VAL:H	1:108:A:ILE:HG23	5	0.11
(1,441)	1:116:A:ALA:HA	1:119:A:ARG:H	1	0.11
(1,410)	1:134:A:LEU:H	1:132:A:THR:H	17	0.11
(1,394)	1:137:A:HIS:HB3	1:138:A:SER:H	11	0.11
(1,392)	1:139:A:ALA:H	1:96:A:HIS:HD2	7	0.11
(1,369)	2:26:B:ASP:HB2	1:87:A:PHE:HZ	19	0.11
(1,367)	2:26:B:ASP:HB3	2:31:B:LEU:H	15	0.11
(1,360)	2:27:B:SER:HB3	2:26:B:ASP:HB3	6	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,288)	2:32:B:GLU:HA	2:35:B:PHE:HD1	10	0.11
(1,288)	2:32:B:GLU:HA	2:35:B:PHE:HD1	13	0.11
(1,285)	2:31:B:LEU:HD13	1:127:A:ILE:HB	1	0.11
(1,285)	2:31:B:LEU:HD13	1:127:A:ILE:HB	11	0.11
(1,285)	2:31:B:LEU:HD12	1:127:A:ILE:HB	13	0.11
(1,285)	2:31:B:LEU:HD11	1:127:A:ILE:HB	15	0.11
(1,285)	2:31:B:LEU:HD13	1:127:A:ILE:HB	21	0.11
(1,270)	1:88:A:LEU:HD23	2:31:B:LEU:HD13	24	0.11
(1,209)	1:67:A:PHE:HE1	1:71:A:LEU:HD23	15	0.11
(1,197)	1:73:A:LEU:HD22	1:117:A:ARG:HB2	23	0.11
(1,176)	1:84:A:VAL:HG13	1:127:A:ILE:HG12	10	0.11
(1,163)	1:67:A:PHE:HD2	1:92:A:GLN:HG3	9	0.11
(1,139)	1:90:A:ASN:HB2	1:90:A:ASN:HD22	19	0.11
(1,132)	1:92:A:GLN:HB3	1:89:A:TYR:HD1	9	0.11
(1,123)	1:95:A:ALA:HB1	1:134:A:LEU:HB2	7	0.11
(1,123)	1:95:A:ALA:HB1	1:134:A:LEU:HB2	22	0.11
(1,107)	1:69:A:GLU:HA	1:69:A:GLU:HB3	5	0.11
(1,107)	1:69:A:GLU:HA	1:69:A:GLU:HB3	14	0.11
(1,107)	1:69:A:GLU:HA	1:69:A:GLU:HB3	17	0.11
(1,107)	1:69:A:GLU:HA	1:69:A:GLU:HB3	25	0.11
(1,89)	1:94:A:ARG:HD2	1:94:A:ARG:HA	1	0.11
(1,84)	1:114:A:SER:HB2	1:113:A:LEU:HG	11	0.11
(1,83)	1:113:A:LEU:HA	1:116:A:ALA:HB1	17	0.11
(1,83)	1:113:A:LEU:HA	1:116:A:ALA:HB2	22	0.11
(1,83)	1:113:A:LEU:HA	1:116:A:ALA:HB1	24	0.11
(1,79)	1:117:A:ARG:HD3	1:117:A:ARG:HG2	10	0.11
(1,79)	1:117:A:ARG:HD3	1:117:A:ARG:HG2	14	0.11
(1,79)	1:117:A:ARG:HD3	1:117:A:ARG:HG2	25	0.11
(1,78)	1:118:A:SER:HB3	1:119:A:ARG:HG3	2	0.11
(1,75)	1:119:A:ARG:HG2	1:119:A:ARG:HD3	7	0.11
(1,75)	1:119:A:ARG:HG2	1:119:A:ARG:HD3	16	0.11
(1,66)	1:121:A:ALA:HA	1:121:A:ALA:H	6	0.11
(1,66)	1:121:A:ALA:HA	1:121:A:ALA:H	8	0.11
(1,66)	1:121:A:ALA:HA	1:121:A:ALA:H	13	0.11
(1,66)	1:121:A:ALA:HA	1:121:A:ALA:H	14	0.11
(1,66)	1:121:A:ALA:HA	1:121:A:ALA:H	20	0.11
(1,52)	1:125:A:VAL:HG12	1:128:A:ASN:HB2	19	0.11
(1,43)	1:126:A:TYR:HD1	1:125:A:VAL:HG12	21	0.11
(1,27)	1:130:A:LEU:HD23	1:67:A:PHE:HA	20	0.11
(1,25)	1:85:A:VAL:HG21	1:74:A:CYS:HB2	9	0.11
(1,19)	1:133:A:VAL:HG23	1:130:A:LEU:HA	12	0.11
(1,19)	1:133:A:VAL:HG23	1:130:A:LEU:HA	15	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,19)	1:133:A:VAL:HG23	1:130:A:LEU:HA	25	0.11
(1,17)	1:133:A:VAL:HG11	1:137:A:HIS:HB2	19	0.11
(1,14)	1:133:A:VAL:HG22	1:132:A:THR:H	13	0.11
(1,8)	1:134:A:LEU:HD22	1:67:A:PHE:HZ	25	0.11
(1,1)	1:141:A:LYS:HG3	1:141:A:LYS:HA	7	0.11
(1,1)	1:141:A:LYS:HG3	1:141:A:LYS:HA	22	0.11
(1,1)	1:141:A:LYS:HG3	1:141:A:LYS:HA	25	0.11
(1,2286)	2:33:B:GLN:HG2	2:33:B:GLN:HE22	1	0.1
(1,2286)	2:33:B:GLN:HG2	2:33:B:GLN:HE22	10	0.1
(1,2286)	2:33:B:GLN:HG2	2:33:B:GLN:HE22	12	0.1
(1,2286)	2:33:B:GLN:HG2	2:33:B:GLN:HE22	15	0.1
(1,2286)	2:33:B:GLN:HG2	2:33:B:GLN:HE22	17	0.1
(1,2286)	2:33:B:GLN:HG2	2:33:B:GLN:HE22	25	0.1
(1,2273)	2:25:B:GLU:HB3	2:25:B:GLU:H	20	0.1
(1,2255)	2:28:B:ASP:H	2:27:B:SER:HB2	7	0.1
(1,2197)	1:55:A:GLY:HA2	1:56:A:LYS:H	12	0.1
(1,2194)	1:56:A:LYS:HB3	1:56:A:LYS:H	9	0.1
(1,2194)	1:56:A:LYS:HB3	1:56:A:LYS:H	15	0.1
(1,2161)	1:64:A:GLU:HB3	1:64:A:GLU:H	15	0.1
(1,2161)	1:64:A:GLU:HB3	1:64:A:GLU:H	24	0.1
(1,2100)	1:77:A:GLN:HE21	1:76:A:MET:HE1	24	0.1
(1,2094)	1:79:A:ALA:HB1	1:78:A:THR:H	10	0.1
(1,2094)	1:79:A:ALA:HB3	1:78:A:THR:H	25	0.1
(1,2080)	1:81:A:HIS:H	1:81:A:HIS:HB3	9	0.1
(1,2054)	1:85:A:VAL:HG12	1:89:A:TYR:H	8	0.1
(1,1975)	1:100:A:LEU:HD13	1:100:A:LEU:H	15	0.1
(1,1975)	1:100:A:LEU:HD11	1:100:A:LEU:H	24	0.1
(1,1837)	1:127:A:ILE:H	1:123:A:LEU:HD12	23	0.1
(1,1781)	1:140:A:LYS:H	1:141:A:LYS:HB3	2	0.1
(1,1764)	2:24:B:GLN:HB3	2:24:B:GLN:HG2	12	0.1
(1,1764)	2:24:B:GLN:HB3	2:24:B:GLN:HG3	19	0.1
(1,1764)	2:24:B:GLN:HB3	2:24:B:GLN:HG3	25	0.1
(1,1740)	2:31:B:LEU:HA	2:32:B:GLU:H	1	0.1
(1,1740)	2:31:B:LEU:HA	2:32:B:GLU:H	2	0.1
(1,1740)	2:31:B:LEU:HA	2:32:B:GLU:H	17	0.1
(1,1740)	2:31:B:LEU:HA	2:32:B:GLU:H	18	0.1
(1,1740)	2:31:B:LEU:HA	2:32:B:GLU:H	23	0.1
(1,1724)	2:31:B:LEU:HG	2:31:B:LEU:HD23	10	0.1
(1,1724)	2:31:B:LEU:HG	2:31:B:LEU:HD21	13	0.1
(1,1724)	2:31:B:LEU:HG	2:31:B:LEU:HD22	21	0.1
(1,1724)	2:31:B:LEU:HG	2:31:B:LEU:HD21	25	0.1
(1,1718)	2:31:B:LEU:HD22	2:32:B:GLU:H	1	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1715)	2:31:B:LEU:HG	2:31:B:LEU:HA	10	0.1
(1,1715)	2:31:B:LEU:HG	2:31:B:LEU:HA	17	0.1
(1,1715)	2:31:B:LEU:HG	2:31:B:LEU:HA	18	0.1
(1,1708)	2:32:B:GLU:HG2	2:39:B:TRP:HZ2	2	0.1
(1,1708)	2:32:B:GLU:HG2	2:39:B:TRP:HZ2	3	0.1
(1,1708)	2:32:B:GLU:HG2	2:39:B:TRP:HZ2	15	0.1
(1,1707)	2:33:B:GLN:HB2	2:33:B:GLN:HA	15	0.1
(1,1707)	2:33:B:GLN:HB2	2:33:B:GLN:HA	19	0.1
(1,1707)	2:33:B:GLN:HB2	2:33:B:GLN:HA	24	0.1
(1,1690)	2:34:B:TYR:HE1	2:34:B:TYR:HD1	3	0.1
(1,1690)	2:34:B:TYR:HE1	2:34:B:TYR:HD1	6	0.1
(1,1690)	2:34:B:TYR:HE1	2:34:B:TYR:HD1	7	0.1
(1,1690)	2:34:B:TYR:HE1	2:34:B:TYR:HD1	13	0.1
(1,1690)	2:34:B:TYR:HE1	2:34:B:TYR:HD1	14	0.1
(1,1690)	2:34:B:TYR:HE1	2:34:B:TYR:HD1	16	0.1
(1,1690)	2:34:B:TYR:HE1	2:34:B:TYR:HD1	19	0.1
(1,1690)	2:34:B:TYR:HE1	2:34:B:TYR:HD1	21	0.1
(1,1690)	2:34:B:TYR:HE1	2:34:B:TYR:HD1	24	0.1
(1,1648)	2:38:B:ARG:HA	2:37:B:ALA:HB2	23	0.1
(1,1639)	2:38:B:ARG:HD2	2:38:B:ARG:H	3	0.1
(1,1608)	2:32:B:GLU:HA	2:33:B:GLN:H	14	0.1
(1,1608)	2:32:B:GLU:HA	2:33:B:GLN:H	21	0.1
(1,1603)	2:33:B:GLN:HG2	2:33:B:GLN:HB2	1	0.1
(1,1603)	2:33:B:GLN:HG2	2:33:B:GLN:HB2	3	0.1
(1,1603)	2:33:B:GLN:HG2	2:33:B:GLN:HB2	4	0.1
(1,1603)	2:33:B:GLN:HG2	2:33:B:GLN:HB2	15	0.1
(1,1603)	2:33:B:GLN:HG2	2:33:B:GLN:HB2	18	0.1
(1,1603)	2:33:B:GLN:HG2	2:33:B:GLN:HB2	19	0.1
(1,1603)	2:33:B:GLN:HG2	2:33:B:GLN:HB2	21	0.1
(1,1603)	2:33:B:GLN:HG2	2:33:B:GLN:HB2	23	0.1
(1,1603)	2:33:B:GLN:HG2	2:33:B:GLN:HB2	24	0.1
(1,1592)	1:84:A:VAL:HG22	2:35:B:PHE:HB2	13	0.1
(1,1588)	1:87:A:PHE:HB2	2:31:B:LEU:HD11	20	0.1
(1,1569)	1:57:A:LYS:HE3	1:59:A:TYR:HE1	11	0.1
(1,1556)	1:57:A:LYS:HG2	1:57:A:LYS:HA	19	0.1
(1,1553)	1:59:A:TYR:HD1	1:57:A:LYS:HB2	4	0.1
(1,1552)	1:57:A:LYS:HB2	1:57:A:LYS:HA	23	0.1
(1,1549)	1:58:A:CYS:HB2	1:57:A:LYS:HA	8	0.1
(1,1536)	1:59:A:TYR:HD1	1:59:A:TYR:HA	15	0.1
(1,1514)	1:62:A:GLU:HG2	1:62:A:GLU:HA	19	0.1
(1,1512)	1:62:A:GLU:HG2	1:62:A:GLU:H	20	0.1
(1,1488)	1:65:A:LYS:HG3	1:65:A:LYS:H	14	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1484)	1:65:A:LYS:HA	1:65:A:LYS:HG2	5	0.1
(1,1452)	1:68:A:GLU:HG2	1:68:A:GLU:H	13	0.1
(1,1446)	1:69:A:GLU:HG2	1:69:A:GLU:H	22	0.1
(1,1423)	1:71:A:LEU:HD21	1:70:A:PHE:HD1	10	0.1
(1,1423)	1:71:A:LEU:HD21	1:70:A:PHE:HD1	24	0.1
(1,1391)	1:74:A:CYS:HA	1:73:A:LEU:HD21	19	0.1
(1,1386)	1:73:A:LEU:HB2	1:73:A:LEU:HD22	19	0.1
(1,1369)	1:75:A:LYS:HE3	1:72:A:GLU:HA	12	0.1
(1,1369)	1:75:A:LYS:HE3	1:72:A:GLU:HA	13	0.1
(1,1319)	1:77:A:GLN:HB3	1:78:A:THR:H	8	0.1
(1,1283)	1:84:A:VAL:HG21	1:127:A:ILE:HD12	6	0.1
(1,1280)	1:84:A:VAL:HG22	1:81:A:HIS:HB2	22	0.1
(1,1279)	1:84:A:VAL:HG23	1:81:A:HIS:HB3	18	0.1
(1,1257)	1:85:A:VAL:HG12	1:71:A:LEU:HA	2	0.1
(1,1257)	1:85:A:VAL:HG11	1:71:A:LEU:HA	20	0.1
(1,1212)	1:88:A:LEU:HB2	1:88:A:LEU:HD13	6	0.1
(1,1186)	1:90:A:ASN:HB3	1:90:A:ASN:HA	4	0.1
(1,1186)	1:90:A:ASN:HB3	1:90:A:ASN:HA	8	0.1
(1,1186)	1:90:A:ASN:HB3	1:90:A:ASN:HA	12	0.1
(1,1186)	1:90:A:ASN:HB3	1:90:A:ASN:HA	17	0.1
(1,1186)	1:90:A:ASN:HB3	1:90:A:ASN:HA	21	0.1
(1,1151)	1:93:A:GLN:HG2	1:93:A:GLN:H	20	0.1
(1,1147)	1:94:A:ARG:HG2	1:94:A:ARG:HA	24	0.1
(1,1122)	1:96:A:HIS:HA	1:139:A:ALA:HB1	5	0.1
(1,1118)	1:98:A:LEU:HB3	1:98:A:LEU:HD23	9	0.1
(1,1109)	1:98:A:LEU:HB3	1:98:A:LEU:H	9	0.1
(1,1109)	1:98:A:LEU:HB3	1:98:A:LEU:H	16	0.1
(1,1109)	1:98:A:LEU:HB3	1:98:A:LEU:H	20	0.1
(1,1089)	1:105:A:PHE:HZ	1:100:A:LEU:HD21	24	0.1
(1,1028)	1:67:A:PHE:HE1	1:88:A:LEU:HB3	14	0.1
(1,1014)	1:74:A:CYS:HA	1:78:A:THR:HG23	10	0.1
(1,1003)	1:108:A:ILE:HB	1:108:A:ILE:HD13	5	0.1
(1,1003)	1:108:A:ILE:HB	1:108:A:ILE:HD13	8	0.1
(1,1003)	1:108:A:ILE:HB	1:108:A:ILE:HD11	15	0.1
(1,995)	1:108:A:ILE:HG21	1:130:A:LEU:HD11	19	0.1
(1,995)	1:108:A:ILE:HG23	1:130:A:LEU:HD11	24	0.1
(1,960)	1:67:A:PHE:HA	1:109:A:LEU:HD13	10	0.1
(1,940)	1:111:A:ARG:HB3	1:111:A:ARG:H	2	0.1
(1,940)	1:111:A:ARG:HB3	1:111:A:ARG:H	3	0.1
(1,940)	1:111:A:ARG:HB3	1:111:A:ARG:H	4	0.1
(1,940)	1:111:A:ARG:HB3	1:111:A:ARG:H	17	0.1
(1,931)	1:112:A:VAL:HG13	1:126:A:TYR:HA	13	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,924)	1:112:A:VAL:HA	1:115:A:ARG:HB3	6	0.1
(1,911)	1:113:A:LEU:HB2	1:113:A:LEU:H	9	0.1
(1,898)	1:115:A:ARG:HA	1:115:A:ARG:HG2	11	0.1
(1,837)	1:120:A:PRO:HD2	1:119:A:ARG:H	5	0.1
(1,837)	1:120:A:PRO:HD2	1:119:A:ARG:H	6	0.1
(1,837)	1:120:A:PRO:HD2	1:119:A:ARG:H	19	0.1
(1,811)	1:123:A:LEU:HD21	1:70:A:PHE:HE1	1	0.1
(1,811)	1:123:A:LEU:HD21	1:70:A:PHE:HE1	11	0.1
(1,779)	1:125:A:VAL:HB	1:125:A:VAL:HG12	18	0.1
(1,766)	1:126:A:TYR:HE1	1:115:A:ARG:HB2	15	0.1
(1,746)	1:127:A:ILE:HD11	1:127:A:ILE:H	21	0.1
(1,746)	1:127:A:ILE:HD12	1:127:A:ILE:H	23	0.1
(1,704)	1:130:A:LEU:HD13	1:109:A:LEU:HD22	1	0.1
(1,636)	1:134:A:LEU:HD23	1:134:A:LEU:H	12	0.1
(1,619)	1:135:A:LYS:HG2	1:91:A:ARG:HD3	15	0.1
(1,601)	1:137:A:HIS:HB3	1:137:A:HIS:H	22	0.1
(1,578)	1:57:A:LYS:HA	1:57:A:LYS:H	14	0.1
(1,578)	1:57:A:LYS:HA	1:57:A:LYS:H	22	0.1
(1,578)	1:57:A:LYS:HA	1:57:A:LYS:H	24	0.1
(1,553)	2:29:B:SER:HB2	2:30:B:GLU:H	22	0.1
(1,537)	1:63:A:ASN:H	1:61:A:LEU:H	16	0.1
(1,512)	1:77:A:GLN:H	1:123:A:LEU:HD23	7	0.1
(1,509)	1:77:A:GLN:HE22	1:73:A:LEU:HG	6	0.1
(1,509)	1:77:A:GLN:HE22	1:73:A:LEU:HG	21	0.1
(1,488)	1:92:A:GLN:HE22	1:64:A:GLU:HG3	12	0.1
(1,466)	1:106:A:CYS:H	1:63:A:ASN:HD21	8	0.1
(1,466)	1:106:A:CYS:H	1:63:A:ASN:HD21	11	0.1
(1,464)	1:107:A:ASN:H	1:108:A:ILE:HB	6	0.1
(1,464)	1:107:A:ASN:H	1:108:A:ILE:HB	17	0.1
(1,410)	1:134:A:LEU:H	1:132:A:THR:H	11	0.1
(1,389)	1:143:A:LEU:H	1:142:A:LYS:HB2	7	0.1
(1,353)	2:29:B:SER:HB2	2:29:B:SER:H	22	0.1
(1,353)	2:29:B:SER:HB2	2:29:B:SER:H	24	0.1
(1,245)	1:61:A:LEU:HG	1:62:A:GLU:HA	25	0.1
(1,148)	1:88:A:LEU:HD23	1:88:A:LEU:H	3	0.1
(1,123)	1:95:A:ALA:HB2	1:134:A:LEU:HB2	19	0.1
(1,113)	1:93:A:GLN:HA	1:94:A:ARG:H	23	0.1
(1,111)	1:62:A:GLU:HB3	1:59:A:TYR:HD2	1	0.1
(1,107)	1:69:A:GLU:HA	1:69:A:GLU:HB3	16	0.1
(1,79)	1:117:A:ARG:HD3	1:117:A:ARG:HG2	18	0.1
(1,66)	1:121:A:ALA:HA	1:121:A:ALA:H	23	0.1
(1,52)	1:125:A:VAL:HG13	1:128:A:ASN:HB2	22	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,44)	1:126:A:TYR:HE1	1:112:A:VAL:HA	15	0.1
(1,42)	1:126:A:TYR:HD1	1:125:A:VAL:HB	20	0.1
(1,26)	1:134:A:LEU:HD13	1:67:A:PHE:HE1	3	0.1

10 Dihedral-angle violation analysis

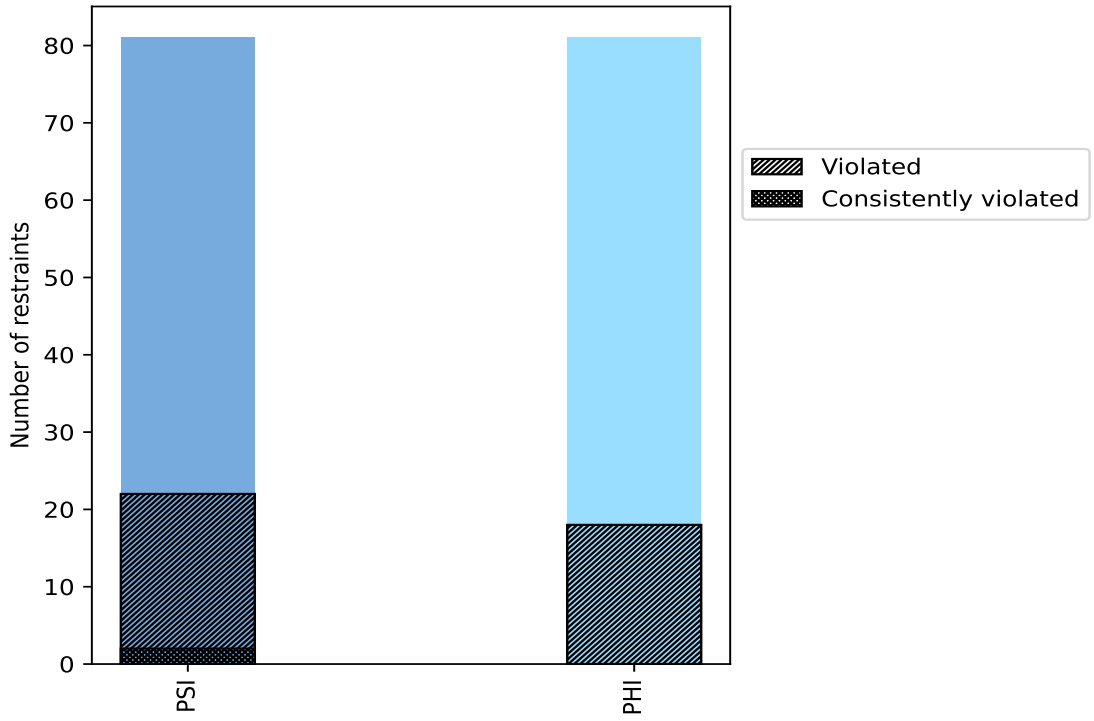
10.1 Summary of dihedral-angle violations

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	81	50.0	22	27.2	13.6	2	2.5	1.2
PHI	81	50.0	18	22.2	11.1	0	0.0	0.0
Total	162	100.0	40	24.7	24.7	2	1.2	1.2

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

10.1.1 Bar chart : Distribution of dihedral-angles and violations



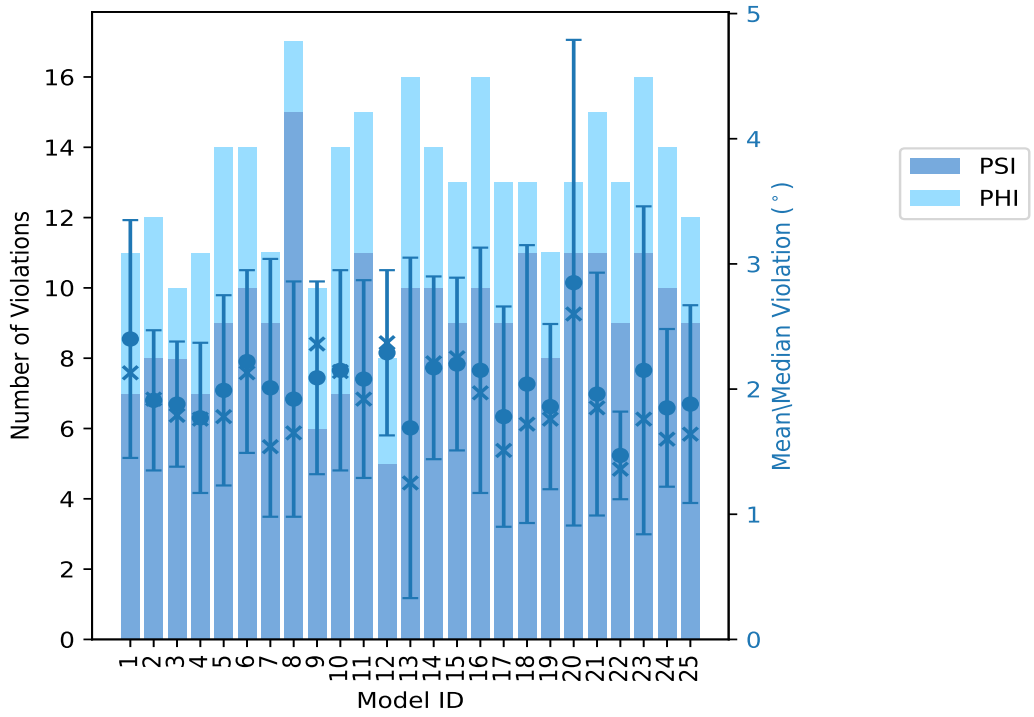
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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	7	4	11	2.4	4.04	0.95	2.13
2	8	4	12	1.91	2.85	0.56	1.92
3	8	2	10	1.88	2.99	0.5	1.79
4	7	4	11	1.77	2.72	0.6	1.76
5	9	5	14	1.99	4.13	0.76	1.78
6	10	4	14	2.22	3.63	0.73	2.13
7	9	2	11	2.01	4.78	1.03	1.54
8	15	2	17	1.92	4.69	0.94	1.65
9	6	4	10	2.09	3.15	0.77	2.36
10	7	7	14	2.15	3.63	0.8	2.14
11	11	4	15	2.08	4.22	0.79	1.92
12	5	3	8	2.29	3.33	0.66	2.37
13	10	6	16	1.69	6.8	1.36	1.25
14	10	4	14	2.17	3.19	0.73	2.21
15	9	4	13	2.2	3.02	0.69	2.25
16	10	6	16	2.15	4.84	0.98	1.97
17	9	4	13	1.78	4.66	0.88	1.51
18	11	2	13	2.04	5.01	1.11	1.72
19	8	3	11	1.86	3.13	0.66	1.76
20	11	2	13	2.85	7.01	1.94	2.6
21	11	4	15	1.96	4.74	0.97	1.85
22	9	4	13	1.47	2.11	0.35	1.36
23	11	5	16	2.15	6.68	1.31	1.76
24	10	4	14	1.85	2.99	0.63	1.6
25	9	3	12	1.88	3.89	0.79	1.64

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]	%
4	4	8	1	4.0
1	4	5	2	8.0
0	1	1	3	12.0
1	4	5	4	16.0
1	0	1	5	20.0
2	1	3	6	24.0
0	1	1	7	28.0
1	0	1	8	32.0
3	0	3	9	36.0
1	0	1	10	40.0
0	0	0	11	44.0

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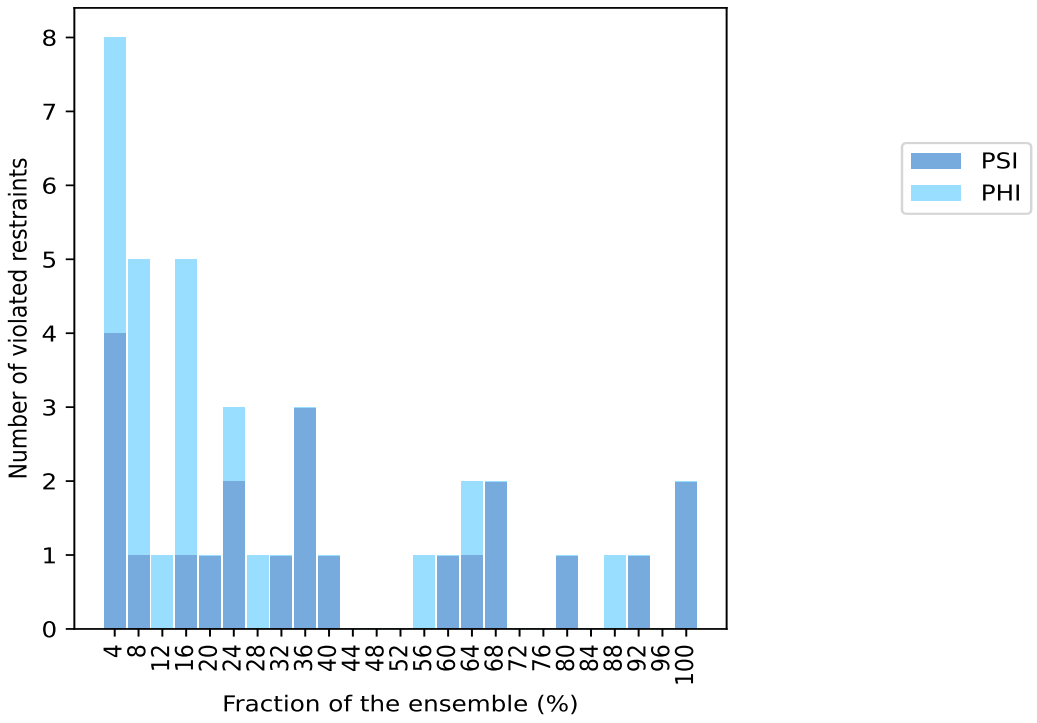
Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count[1]	%
0	0	0	12	48.0
0	0	0	13	52.0
0	1	1	14	56.0
1	0	1	15	60.0
1	1	2	16	64.0
2	0	2	17	68.0
0	0	0	18	72.0
0	0	0	19	76.0
1	0	1	20	80.0
0	0	0	21	84.0
0	1	1	22	88.0
1	0	1	23	92.0
0	0	0	24	96.0
2	0	2	25	100.0

[1] Number of models with violations

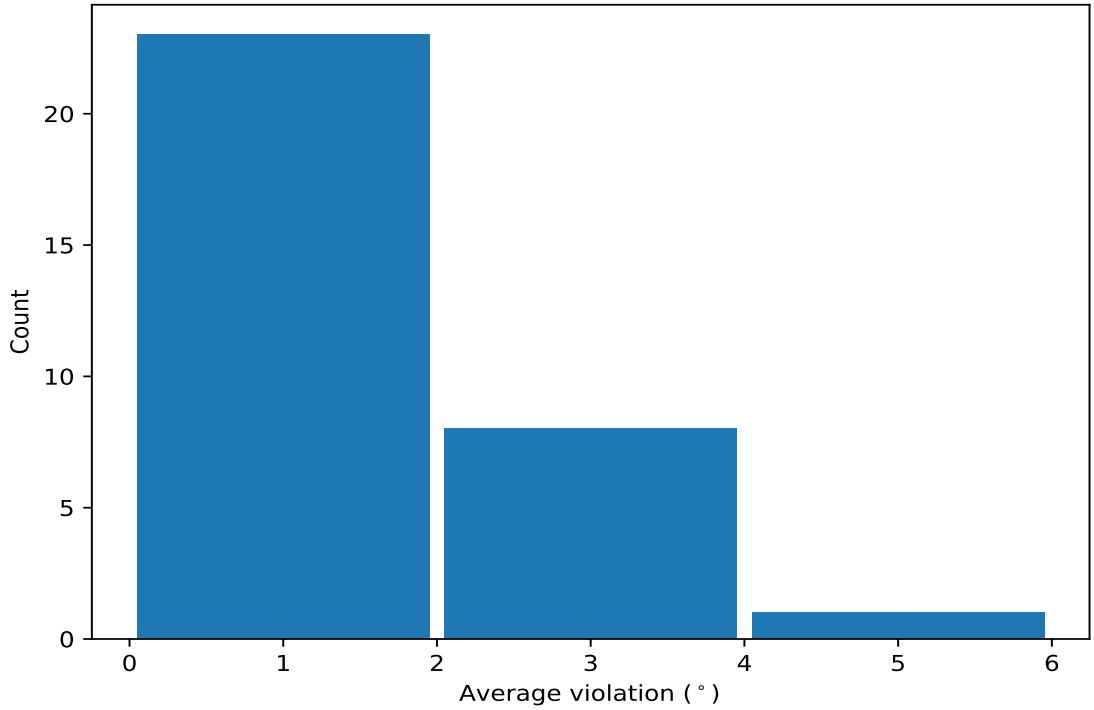
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble



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
(1,89)	1:72:A:GLU:N	1:72:A:GLU:CA	1:72:A:GLU:C	1:73:A:LEU:N	25	2.86	0.86	2.63
(1,98)	1:84:A:VAL:N	1:84:A:VAL:CA	1:84:A:VAL:C	1:85:A:VAL:N	25	2.12	0.49	2.16
(1,140)	1:129:A:GLU:N	1:129:A:GLU:CA	1:129:A:GLU:C	1:130:A:LEU:N	23	2.49	0.49	2.61
(1,72)	1:134:A:LEU:C	1:135:A:LYS:N	1:135:A:LYS:CA	1:135:A:LYS:C	22	1.92	0.63	1.9
(1,103)	1:89:A:TYR:N	1:89:A:TYR:CA	1:89:A:TYR:C	1:90:A:ASN:N	20	1.67	0.68	1.5
(1,79)	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1:63:A:ASN:N	17	2.43	0.77	2.33
(1,145)	1:134:A:LEU:N	1:134:A:LEU:CA	1:134:A:LEU:C	1:135:A:LYS:N	17	1.85	0.44	1.92
(1,123)	1:111:A:ARG:N	1:111:A:ARG:CA	1:111:A:ARG:C	1:112:A:VAL:N	16	1.99	0.92	1.75
(1,23)	1:82:A:PRO:C	1:83:A:GLU:N	1:83:A:GLU:CA	1:83:A:GLU:C	16	1.44	0.41	1.32
(1,146)	1:135:A:LYS:N	1:135:A:LYS:CA	1:135:A:LYS:C	1:136:A:ALA:N	15	1.81	0.73	1.46
(1,46)	1:107:A:ASN:C	1:108:A:ILE:N	1:108:A:ILE:CA	1:108:A:ILE:C	14	1.7	0.38	1.76
(1,76)	1:58:A:CYS:N	1:58:A:CYS:CA	1:58:A:CYS:C	1:59:A:TYR:N	10	3.19	1.66	3.05
(1,148)	1:138:A:SER:N	1:138:A:SER:CA	1:138:A:SER:C	1:139:A:ALA:N	9	4.68	1.82	4.74

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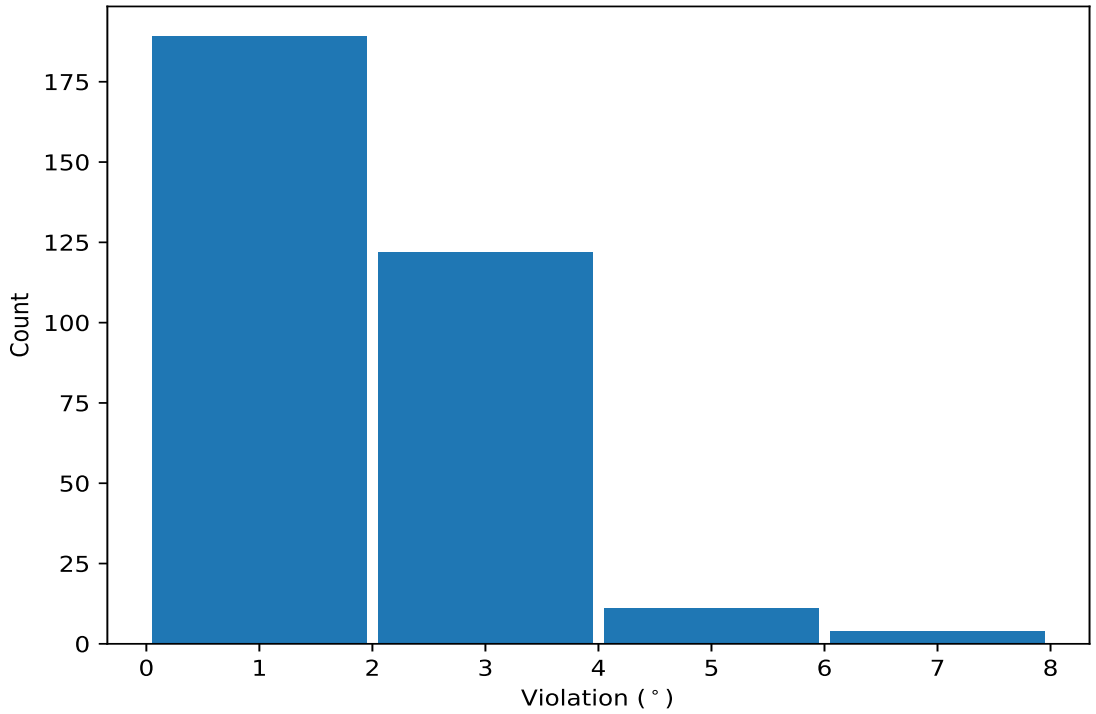
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,106)	1:92:A:GLN:N	1:92:A:GLN:CA	1:92:A:GLN:C	1:93:A:GLN:N	9	1.38	0.29	1.27
(1,121)	1:109:A:LEU:N	1:109:A:LEU:CA	1:109:A:LEU:C	1:110:A:SER:N	9	1.3	0.16	1.27
(1,94)	1:77:A:GLN:N	1:77:A:GLN:CA	1:77:A:GLN:C	1:78:A:THR:N	8	1.27	0.23	1.23
(1,18)	1:74:A:CYS:C	1:75:A:LYS:N	1:75:A:LYS:CA	1:75:A:LYS:C	7	1.3	0.25	1.2
(1,12)	1:68:A:GLU:C	1:69:A:GLU:N	1:69:A:GLU:CA	1:69:A:GLU:C	6	2.45	0.41	2.58
(1,114)	1:100:A:LEU:N	1:100:A:LEU:CA	1:100:A:LEU:C	1:101:A:ALA:N	6	2.0	0.56	2.17
(1,120)	1:108:A:ILE:N	1:108:A:ILE:CA	1:108:A:ILE:C	1:109:A:LEU:N	6	1.42	0.3	1.35
(1,85)	1:68:A:GLU:N	1:68:A:GLU:CA	1:68:A:GLU:C	1:69:A:GLU:N	5	1.59	0.35	1.52
(1,149)	2:23:B:SER:C	2:24:B:GLN:N	2:24:B:GLN:CA	2:24:B:GLN:C	4	1.87	0.7	1.76
(1,81)	1:64:A:GLU:N	1:64:A:GLU:CA	1:64:A:GLU:C	1:65:A:LYS:N	4	1.76	0.91	1.28
(1,8)	1:64:A:GLU:C	1:65:A:LYS:N	1:65:A:LYS:CA	1:65:A:LYS:C	4	1.75	0.7	1.62
(1,5)	1:61:A:LEU:C	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	4	1.6	0.25	1.65
(1,70)	1:132:A:THR:C	1:133:A:VAL:N	1:133:A:VAL:CA	1:133:A:VAL:C	4	1.25	0.18	1.21
(1,63)	1:125:A:VAL:C	1:126:A:TYR:N	1:126:A:TYR:CA	1:126:A:TYR:C	3	1.38	0.38	1.16
(1,1)	1:56:A:LYS:C	1:57:A:LYS:N	1:57:A:LYS:CA	1:57:A:LYS:C	2	2.5	0.36	2.5
(1,158)	2:29:B:SER:N	2:29:B:SER:CA	2:29:B:SER:C	2:30:B:GLU:N	2	1.56	0.29	1.56
(1,67)	1:129:A:GLU:C	1:130:A:LEU:N	1:130:A:LEU:CA	1:130:A:LEU:C	2	1.44	0.34	1.44
(1,2)	1:57:A:LYS:C	1:58:A:CYS:N	1:58:A:CYS:CA	1:58:A:CYS:C	2	1.42	0.21	1.42
(1,54)	1:115:A:ARG:C	1:116:A:ALA:N	1:116:A:ALA:CA	1:116:A:ALA:C	2	1.06	0.01	1.06

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

10.5 All violated dihedral-angle restraints (i)

10.5.1 Histogram : Distribution of violations (i)

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



10.5.2 Table: All violated dihedral-angle restraints

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,76)	1:58:A:CYS:N	1:58:A:CYS:CA	1:58:A:CYS:C	1:59:A:TYR:N	20	7.01
(1,148)	1:138:A:SER:N	1:138:A:SER:CA	1:138:A:SER:C	1:139:A:ALA:N	13	6.8
(1,148)	1:138:A:SER:N	1:138:A:SER:CA	1:138:A:SER:C	1:139:A:ALA:N	20	6.72
(1,148)	1:138:A:SER:N	1:138:A:SER:CA	1:138:A:SER:C	1:139:A:ALA:N	23	6.68
(1,148)	1:138:A:SER:N	1:138:A:SER:CA	1:138:A:SER:C	1:139:A:ALA:N	18	5.01
(1,89)	1:72:A:GLU:N	1:72:A:GLU:CA	1:72:A:GLU:C	1:73:A:LEU:N	16	4.84
(1,89)	1:72:A:GLU:N	1:72:A:GLU:CA	1:72:A:GLU:C	1:73:A:LEU:N	7	4.78
(1,148)	1:138:A:SER:N	1:138:A:SER:CA	1:138:A:SER:C	1:139:A:ALA:N	21	4.74
(1,148)	1:138:A:SER:N	1:138:A:SER:CA	1:138:A:SER:C	1:139:A:ALA:N	8	4.69
(1,89)	1:72:A:GLU:N	1:72:A:GLU:CA	1:72:A:GLU:C	1:73:A:LEU:N	17	4.66
(1,76)	1:58:A:CYS:N	1:58:A:CYS:CA	1:58:A:CYS:C	1:59:A:TYR:N	11	4.22
(1,76)	1:58:A:CYS:N	1:58:A:CYS:CA	1:58:A:CYS:C	1:59:A:TYR:N	5	4.13
(1,103)	1:89:A:TYR:N	1:89:A:TYR:CA	1:89:A:TYR:C	1:90:A:ASN:N	20	4.1
(1,79)	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1:63:A:ASN:N	1	4.04
(1,123)	1:111:A:ARG:N	1:111:A:ARG:CA	1:111:A:ARG:C	1:112:A:VAL:N	1	4.01
(1,76)	1:58:A:CYS:N	1:58:A:CYS:CA	1:58:A:CYS:C	1:59:A:TYR:N	25	3.89
(1,79)	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1:63:A:ASN:N	18	3.78
(1,148)	1:138:A:SER:N	1:138:A:SER:CA	1:138:A:SER:C	1:139:A:ALA:N	16	3.65
(1,89)	1:72:A:GLU:N	1:72:A:GLU:CA	1:72:A:GLU:C	1:73:A:LEU:N	6	3.63
(1,76)	1:58:A:CYS:N	1:58:A:CYS:CA	1:58:A:CYS:C	1:59:A:TYR:N	10	3.63
(1,89)	1:72:A:GLU:N	1:72:A:GLU:CA	1:72:A:GLU:C	1:73:A:LEU:N	10	3.41

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,140)	1:129:A:GLU:N	1:129:A:GLU:CA	1:129:A:GLU:C	1:130:A:LEU:N	20	3.34
(1,146)	1:135:A:LYS:N	1:135:A:LYS:CA	1:135:A:LYS:C	1:136:A:ALA:N	8	3.33
(1,81)	1:64:A:GLU:N	1:64:A:GLU:CA	1:64:A:GLU:C	1:65:A:LYS:N	12	3.33
(1,72)	1:134:A:LEU:C	1:135:A:LYS:N	1:135:A:LYS:CA	1:135:A:LYS:C	6	3.27
(1,123)	1:111:A:ARG:N	1:111:A:ARG:CA	1:111:A:ARG:C	1:112:A:VAL:N	10	3.26
(1,140)	1:129:A:GLU:N	1:129:A:GLU:CA	1:129:A:GLU:C	1:130:A:LEU:N	21	3.2
(1,146)	1:135:A:LYS:N	1:135:A:LYS:CA	1:135:A:LYS:C	1:136:A:ALA:N	14	3.19
(1,79)	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1:63:A:ASN:N	14	3.16
(1,89)	1:72:A:GLU:N	1:72:A:GLU:CA	1:72:A:GLU:C	1:73:A:LEU:N	9	3.15
(1,79)	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1:63:A:ASN:N	19	3.13
(1,72)	1:134:A:LEU:C	1:135:A:LYS:N	1:135:A:LYS:CA	1:135:A:LYS:C	14	3.13
(1,89)	1:72:A:GLU:N	1:72:A:GLU:CA	1:72:A:GLU:C	1:73:A:LEU:N	23	3.11
(1,123)	1:111:A:ARG:N	1:111:A:ARG:CA	1:111:A:ARG:C	1:112:A:VAL:N	11	3.03
(1,123)	1:111:A:ARG:N	1:111:A:ARG:CA	1:111:A:ARG:C	1:112:A:VAL:N	15	3.02
(1,98)	1:84:A:VAL:N	1:84:A:VAL:CA	1:84:A:VAL:C	1:85:A:VAL:N	1	3.0
(1,98)	1:84:A:VAL:N	1:84:A:VAL:CA	1:84:A:VAL:C	1:85:A:VAL:N	24	2.99
(1,89)	1:72:A:GLU:N	1:72:A:GLU:CA	1:72:A:GLU:C	1:73:A:LEU:N	3	2.99
(1,140)	1:129:A:GLU:N	1:129:A:GLU:CA	1:129:A:GLU:C	1:130:A:LEU:N	15	2.98
(1,89)	1:72:A:GLU:N	1:72:A:GLU:CA	1:72:A:GLU:C	1:73:A:LEU:N	25	2.97
(1,140)	1:129:A:GLU:N	1:129:A:GLU:CA	1:129:A:GLU:C	1:130:A:LEU:N	6	2.96
(1,140)	1:129:A:GLU:N	1:129:A:GLU:CA	1:129:A:GLU:C	1:130:A:LEU:N	23	2.94
(1,89)	1:72:A:GLU:N	1:72:A:GLU:CA	1:72:A:GLU:C	1:73:A:LEU:N	15	2.94
(1,149)	2:23:B:SER:C	2:24:B:GLN:N	2:24:B:GLN:CA	2:24:B:GLN:C	14	2.87
(1,72)	1:134:A:LEU:C	1:135:A:LYS:N	1:135:A:LYS:CA	1:135:A:LYS:C	9	2.87
(1,1)	1:56:A:LYS:C	1:57:A:LYS:N	1:57:A:LYS:CA	1:57:A:LYS:C	2	2.85
(1,140)	1:129:A:GLU:N	1:129:A:GLU:CA	1:129:A:GLU:C	1:130:A:LEU:N	2	2.83
(1,89)	1:72:A:GLU:N	1:72:A:GLU:CA	1:72:A:GLU:C	1:73:A:LEU:N	12	2.82
(1,12)	1:68:A:GLU:C	1:69:A:GLU:N	1:69:A:GLU:CA	1:69:A:GLU:C	15	2.82
(1,140)	1:129:A:GLU:N	1:129:A:GLU:CA	1:129:A:GLU:C	1:130:A:LEU:N	1	2.81
(1,89)	1:72:A:GLU:N	1:72:A:GLU:CA	1:72:A:GLU:C	1:73:A:LEU:N	19	2.81
(1,12)	1:68:A:GLU:C	1:69:A:GLU:N	1:69:A:GLU:CA	1:69:A:GLU:C	9	2.8
(1,98)	1:84:A:VAL:N	1:84:A:VAL:CA	1:84:A:VAL:C	1:85:A:VAL:N	16	2.79
(1,79)	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1:63:A:ASN:N	20	2.79
(1,72)	1:134:A:LEU:C	1:135:A:LYS:N	1:135:A:LYS:CA	1:135:A:LYS:C	16	2.79
(1,140)	1:129:A:GLU:N	1:129:A:GLU:CA	1:129:A:GLU:C	1:130:A:LEU:N	12	2.75
(1,140)	1:129:A:GLU:N	1:129:A:GLU:CA	1:129:A:GLU:C	1:130:A:LEU:N	4	2.72
(1,140)	1:129:A:GLU:N	1:129:A:GLU:CA	1:129:A:GLU:C	1:130:A:LEU:N	24	2.72
(1,8)	1:64:A:GLU:C	1:65:A:LYS:N	1:65:A:LYS:CA	1:65:A:LYS:C	6	2.71
(1,98)	1:84:A:VAL:N	1:84:A:VAL:CA	1:84:A:VAL:C	1:85:A:VAL:N	7	2.68
(1,123)	1:111:A:ARG:N	1:111:A:ARG:CA	1:111:A:ARG:C	1:112:A:VAL:N	16	2.63
(1,89)	1:72:A:GLU:N	1:72:A:GLU:CA	1:72:A:GLU:C	1:73:A:LEU:N	1	2.63
(1,79)	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1:63:A:ASN:N	9	2.63
(1,12)	1:68:A:GLU:C	1:69:A:GLU:N	1:69:A:GLU:CA	1:69:A:GLU:C	23	2.63
(1,145)	1:134:A:LEU:N	1:134:A:LEU:CA	1:134:A:LEU:C	1:135:A:LYS:N	15	2.62
(1,140)	1:129:A:GLU:N	1:129:A:GLU:CA	1:129:A:GLU:C	1:130:A:LEU:N	11	2.62
(1,89)	1:72:A:GLU:N	1:72:A:GLU:CA	1:72:A:GLU:C	1:73:A:LEU:N	4	2.62
(1,89)	1:72:A:GLU:N	1:72:A:GLU:CA	1:72:A:GLU:C	1:73:A:LEU:N	20	2.62
(1,140)	1:129:A:GLU:N	1:129:A:GLU:CA	1:129:A:GLU:C	1:130:A:LEU:N	7	2.61
(1,98)	1:84:A:VAL:N	1:84:A:VAL:CA	1:84:A:VAL:C	1:85:A:VAL:N	20	2.6
(1,79)	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1:63:A:ASN:N	15	2.6
(1,114)	1:100:A:LEU:N	1:100:A:LEU:CA	1:100:A:LEU:C	1:101:A:ALA:N	5	2.59

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,89)	1:72:A:GLU:N	1:72:A:GLU:CA	1:72:A:GLU:C	1:73:A:LEU:N	8	2.58
(1,140)	1:129:A:GLU:N	1:129:A:GLU:CA	1:129:A:GLU:C	1:130:A:LEU:N	5	2.57
(1,145)	1:134:A:LEU:N	1:134:A:LEU:CA	1:134:A:LEU:C	1:135:A:LYS:N	24	2.56
(1,114)	1:100:A:LEU:N	1:100:A:LEU:CA	1:100:A:LEU:C	1:101:A:ALA:N	21	2.55
(1,12)	1:68:A:GLU:C	1:69:A:GLU:N	1:69:A:GLU:CA	1:69:A:GLU:C	4	2.54
(1,148)	1:138:A:SER:N	1:138:A:SER:CA	1:138:A:SER:C	1:139:A:ALA:N	6	2.52
(1,89)	1:72:A:GLU:N	1:72:A:GLU:CA	1:72:A:GLU:C	1:73:A:LEU:N	14	2.52
(1,140)	1:129:A:GLU:N	1:129:A:GLU:CA	1:129:A:GLU:C	1:130:A:LEU:N	9	2.51
(1,98)	1:84:A:VAL:N	1:84:A:VAL:CA	1:84:A:VAL:C	1:85:A:VAL:N	10	2.51
(1,89)	1:72:A:GLU:N	1:72:A:GLU:CA	1:72:A:GLU:C	1:73:A:LEU:N	5	2.51
(1,146)	1:135:A:LYS:N	1:135:A:LYS:CA	1:135:A:LYS:C	1:136:A:ALA:N	24	2.5
(1,98)	1:84:A:VAL:N	1:84:A:VAL:CA	1:84:A:VAL:C	1:85:A:VAL:N	12	2.5
(1,23)	1:82:A:PRO:C	1:83:A:GLU:N	1:83:A:GLU:CA	1:83:A:GLU:C	11	2.49
(1,76)	1:58:A:CYS:N	1:58:A:CYS:CA	1:58:A:CYS:C	1:59:A:TYR:N	8	2.47
(1,140)	1:129:A:GLU:N	1:129:A:GLU:CA	1:129:A:GLU:C	1:130:A:LEU:N	8	2.42
(1,89)	1:72:A:GLU:N	1:72:A:GLU:CA	1:72:A:GLU:C	1:73:A:LEU:N	21	2.42
(1,79)	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1:63:A:ASN:N	2	2.42
(1,98)	1:84:A:VAL:N	1:84:A:VAL:CA	1:84:A:VAL:C	1:85:A:VAL:N	18	2.38
(1,140)	1:129:A:GLU:N	1:129:A:GLU:CA	1:129:A:GLU:C	1:130:A:LEU:N	14	2.35
(1,114)	1:100:A:LEU:N	1:100:A:LEU:CA	1:100:A:LEU:C	1:101:A:ALA:N	10	2.34
(1,89)	1:72:A:GLU:N	1:72:A:GLU:CA	1:72:A:GLU:C	1:73:A:LEU:N	24	2.34
(1,103)	1:89:A:TYR:N	1:89:A:TYR:CA	1:89:A:TYR:C	1:90:A:ASN:N	18	2.33
(1,79)	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1:63:A:ASN:N	3	2.33
(1,146)	1:135:A:LYS:N	1:135:A:LYS:CA	1:135:A:LYS:C	1:136:A:ALA:N	11	2.32
(1,123)	1:111:A:ARG:N	1:111:A:ARG:CA	1:111:A:ARG:C	1:112:A:VAL:N	19	2.31
(1,79)	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1:63:A:ASN:N	11	2.31
(1,79)	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1:63:A:ASN:N	6	2.29
(1,72)	1:134:A:LEU:C	1:135:A:LYS:N	1:135:A:LYS:CA	1:135:A:LYS:C	10	2.29
(1,12)	1:68:A:GLU:C	1:69:A:GLU:N	1:69:A:GLU:CA	1:69:A:GLU:C	14	2.29
(1,145)	1:134:A:LEU:N	1:134:A:LEU:CA	1:134:A:LEU:C	1:135:A:LYS:N	21	2.27
(1,140)	1:129:A:GLU:N	1:129:A:GLU:CA	1:129:A:GLU:C	1:130:A:LEU:N	16	2.26
(1,146)	1:135:A:LYS:N	1:135:A:LYS:CA	1:135:A:LYS:C	1:136:A:ALA:N	15	2.25
(1,98)	1:84:A:VAL:N	1:84:A:VAL:CA	1:84:A:VAL:C	1:85:A:VAL:N	11	2.25
(1,23)	1:82:A:PRO:C	1:83:A:GLU:N	1:83:A:GLU:CA	1:83:A:GLU:C	12	2.23
(1,98)	1:84:A:VAL:N	1:84:A:VAL:CA	1:84:A:VAL:C	1:85:A:VAL:N	23	2.22
(1,98)	1:84:A:VAL:N	1:84:A:VAL:CA	1:84:A:VAL:C	1:85:A:VAL:N	15	2.21
(1,46)	1:107:A:ASN:C	1:108:A:ILE:N	1:108:A:ILE:CA	1:108:A:ILE:C	25	2.21
(1,98)	1:84:A:VAL:N	1:84:A:VAL:CA	1:84:A:VAL:C	1:85:A:VAL:N	9	2.2
(1,85)	1:68:A:GLU:N	1:68:A:GLU:CA	1:68:A:GLU:C	1:69:A:GLU:N	19	2.19
(1,103)	1:89:A:TYR:N	1:89:A:TYR:CA	1:89:A:TYR:C	1:90:A:ASN:N	17	2.18
(1,149)	2:23:B:SER:C	2:24:B:GLN:N	2:24:B:GLN:CA	2:24:B:GLN:C	6	2.17
(1,72)	1:134:A:LEU:C	1:135:A:LYS:N	1:135:A:LYS:CA	1:135:A:LYS:C	5	2.17
(1,98)	1:84:A:VAL:N	1:84:A:VAL:CA	1:84:A:VAL:C	1:85:A:VAL:N	8	2.16
(1,46)	1:107:A:ASN:C	1:108:A:ILE:N	1:108:A:ILE:CA	1:108:A:ILE:C	10	2.15
(1,72)	1:134:A:LEU:C	1:135:A:LYS:N	1:135:A:LYS:CA	1:135:A:LYS:C	3	2.14
(1,1)	1:56:A:LYS:C	1:57:A:LYS:N	1:57:A:LYS:CA	1:57:A:LYS:C	10	2.14
(1,145)	1:134:A:LEU:N	1:134:A:LEU:CA	1:134:A:LEU:C	1:135:A:LYS:N	14	2.13
(1,8)	1:64:A:GLU:C	1:65:A:LYS:N	1:65:A:LYS:CA	1:65:A:LYS:C	1	2.13
(1,145)	1:134:A:LEU:N	1:134:A:LEU:CA	1:134:A:LEU:C	1:135:A:LYS:N	22	2.11
(1,46)	1:107:A:ASN:C	1:108:A:ILE:N	1:108:A:ILE:CA	1:108:A:ILE:C	7	2.11
(1,98)	1:84:A:VAL:N	1:84:A:VAL:CA	1:84:A:VAL:C	1:85:A:VAL:N	6	2.1

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,103)	1:89:A:TYR:N	1:89:A:TYR:CA	1:89:A:TYR:C	1:90:A:ASN:N	16	2.09
(1,72)	1:134:A:LEU:C	1:135:A:LYS:N	1:135:A:LYS:CA	1:135:A:LYS:C	1	2.09
(1,72)	1:134:A:LEU:C	1:135:A:LYS:N	1:135:A:LYS:CA	1:135:A:LYS:C	2	2.08
(1,140)	1:129:A:GLU:N	1:129:A:GLU:CA	1:129:A:GLU:C	1:130:A:LEU:N	17	2.07
(1,146)	1:135:A:LYS:N	1:135:A:LYS:CA	1:135:A:LYS:C	1:136:A:ALA:N	2	2.06
(1,145)	1:134:A:LEU:N	1:134:A:LEU:CA	1:134:A:LEU:C	1:135:A:LYS:N	7	2.06
(1,89)	1:72:A:GLU:N	1:72:A:GLU:CA	1:72:A:GLU:C	1:73:A:LEU:N	18	2.06
(1,46)	1:107:A:ASN:C	1:108:A:ILE:N	1:108:A:ILE:CA	1:108:A:ILE:C	6	2.06
(1,72)	1:134:A:LEU:C	1:135:A:LYS:N	1:135:A:LYS:CA	1:135:A:LYS:C	15	2.05
(1,123)	1:111:A:ARG:N	1:111:A:ARG:CA	1:111:A:ARG:C	1:112:A:VAL:N	24	2.04
(1,145)	1:134:A:LEU:N	1:134:A:LEU:CA	1:134:A:LEU:C	1:135:A:LYS:N	16	2.03
(1,103)	1:89:A:TYR:N	1:89:A:TYR:CA	1:89:A:TYR:C	1:90:A:ASN:N	3	2.02
(1,114)	1:100:A:LEU:N	1:100:A:LEU:CA	1:100:A:LEU:C	1:101:A:ALA:N	25	2.01
(1,72)	1:134:A:LEU:C	1:135:A:LYS:N	1:135:A:LYS:CA	1:135:A:LYS:C	12	2.0
(1,46)	1:107:A:ASN:C	1:108:A:ILE:N	1:108:A:ILE:CA	1:108:A:ILE:C	13	1.99
(1,89)	1:72:A:GLU:N	1:72:A:GLU:CA	1:72:A:GLU:C	1:73:A:LEU:N	2	1.98
(1,140)	1:129:A:GLU:N	1:129:A:GLU:CA	1:129:A:GLU:C	1:130:A:LEU:N	22	1.97
(1,98)	1:84:A:VAL:N	1:84:A:VAL:CA	1:84:A:VAL:C	1:85:A:VAL:N	13	1.96
(1,120)	1:108:A:ILE:N	1:108:A:ILE:CA	1:108:A:ILE:C	1:109:A:LEU:N	8	1.95
(1,145)	1:134:A:LEU:N	1:134:A:LEU:CA	1:134:A:LEU:C	1:135:A:LYS:N	25	1.94
(1,79)	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1:63:A:ASN:N	23	1.94
(1,98)	1:84:A:VAL:N	1:84:A:VAL:CA	1:84:A:VAL:C	1:85:A:VAL:N	4	1.93
(1,145)	1:134:A:LEU:N	1:134:A:LEU:CA	1:134:A:LEU:C	1:135:A:LYS:N	11	1.92
(1,103)	1:89:A:TYR:N	1:89:A:TYR:CA	1:89:A:TYR:C	1:90:A:ASN:N	6	1.92
(1,98)	1:84:A:VAL:N	1:84:A:VAL:CA	1:84:A:VAL:C	1:85:A:VAL:N	14	1.92
(1,79)	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1:63:A:ASN:N	21	1.92
(1,63)	1:125:A:VAL:C	1:126:A:TYR:N	1:126:A:TYR:CA	1:126:A:TYR:C	21	1.92
(1,76)	1:58:A:CYS:N	1:58:A:CYS:CA	1:58:A:CYS:C	1:59:A:TYR:N	16	1.91
(1,46)	1:107:A:ASN:C	1:108:A:ILE:N	1:108:A:ILE:CA	1:108:A:ILE:C	23	1.9
(1,98)	1:84:A:VAL:N	1:84:A:VAL:CA	1:84:A:VAL:C	1:85:A:VAL:N	19	1.87
(1,145)	1:134:A:LEU:N	1:134:A:LEU:CA	1:134:A:LEU:C	1:135:A:LYS:N	4	1.86
(1,89)	1:72:A:GLU:N	1:72:A:GLU:CA	1:72:A:GLU:C	1:73:A:LEU:N	13	1.86
(1,5)	1:61:A:LEU:C	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	10	1.86
(1,158)	2:29:B:SER:N	2:29:B:SER:CA	2:29:B:SER:C	2:30:B:GLU:N	14	1.85
(1,145)	1:134:A:LEU:N	1:134:A:LEU:CA	1:134:A:LEU:C	1:135:A:LYS:N	2	1.85
(1,106)	1:92:A:GLN:N	1:92:A:GLN:CA	1:92:A:GLN:C	1:93:A:GLN:N	21	1.85
(1,76)	1:58:A:CYS:N	1:58:A:CYS:CA	1:58:A:CYS:C	1:59:A:TYR:N	6	1.84
(1,46)	1:107:A:ASN:C	1:108:A:ILE:N	1:108:A:ILE:CA	1:108:A:ILE:C	16	1.82
(1,98)	1:84:A:VAL:N	1:84:A:VAL:CA	1:84:A:VAL:C	1:85:A:VAL:N	5	1.81
(1,98)	1:84:A:VAL:N	1:84:A:VAL:CA	1:84:A:VAL:C	1:85:A:VAL:N	22	1.81
(1,72)	1:134:A:LEU:C	1:135:A:LYS:N	1:135:A:LYS:CA	1:135:A:LYS:C	23	1.81
(1,5)	1:61:A:LEU:C	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	5	1.81
(1,98)	1:84:A:VAL:N	1:84:A:VAL:CA	1:84:A:VAL:C	1:85:A:VAL:N	3	1.8
(1,145)	1:134:A:LEU:N	1:134:A:LEU:CA	1:134:A:LEU:C	1:135:A:LYS:N	3	1.78
(1,67)	1:129:A:GLU:C	1:130:A:LEU:N	1:130:A:LEU:CA	1:130:A:LEU:C	3	1.78
(1,140)	1:129:A:GLU:N	1:129:A:GLU:CA	1:129:A:GLU:C	1:130:A:LEU:N	19	1.76
(1,123)	1:111:A:ARG:N	1:111:A:ARG:CA	1:111:A:ARG:C	1:112:A:VAL:N	4	1.76
(1,23)	1:82:A:PRO:C	1:83:A:GLU:N	1:83:A:GLU:CA	1:83:A:GLU:C	5	1.75
(1,123)	1:111:A:ARG:N	1:111:A:ARG:CA	1:111:A:ARG:C	1:112:A:VAL:N	18	1.74
(1,103)	1:89:A:TYR:N	1:89:A:TYR:CA	1:89:A:TYR:C	1:90:A:ASN:N	11	1.74
(1,79)	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1:63:A:ASN:N	8	1.73

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,140)	1:129:A:GLU:N	1:129:A:GLU:CA	1:129:A:GLU:C	1:130:A:LEU:N	18	1.72
(1,94)	1:77:A:GLN:N	1:77:A:GLN:CA	1:77:A:GLN:C	1:78:A:THR:N	23	1.72
(1,18)	1:74:A:CYS:C	1:75:A:LYS:N	1:75:A:LYS:CA	1:75:A:LYS:C	19	1.72
(1,89)	1:72:A:GLU:N	1:72:A:GLU:CA	1:72:A:GLU:C	1:73:A:LEU:N	22	1.71
(1,46)	1:107:A:ASN:C	1:108:A:ILE:N	1:108:A:ILE:CA	1:108:A:ILE:C	21	1.71
(1,103)	1:89:A:TYR:N	1:89:A:TYR:CA	1:89:A:TYR:C	1:90:A:ASN:N	14	1.69
(1,72)	1:134:A:LEU:C	1:135:A:LYS:N	1:135:A:LYS:CA	1:135:A:LYS:C	22	1.69
(1,85)	1:68:A:GLU:N	1:68:A:GLU:CA	1:68:A:GLU:C	1:69:A:GLU:N	20	1.68
(1,66)	1:128:A:ASN:C	1:129:A:GLU:N	1:129:A:GLU:CA	1:129:A:GLU:C	24	1.68
(1,106)	1:92:A:GLN:N	1:92:A:GLN:CA	1:92:A:GLN:C	1:93:A:GLN:N	23	1.67
(1,23)	1:82:A:PRO:C	1:83:A:GLU:N	1:83:A:GLU:CA	1:83:A:GLU:C	17	1.67
(1,120)	1:108:A:ILE:N	1:108:A:ILE:CA	1:108:A:ILE:C	1:109:A:LEU:N	2	1.65
(1,72)	1:134:A:LEU:C	1:135:A:LYS:N	1:135:A:LYS:CA	1:135:A:LYS:C	8	1.65
(1,140)	1:129:A:GLU:N	1:129:A:GLU:CA	1:129:A:GLU:C	1:130:A:LEU:N	25	1.64
(1,103)	1:89:A:TYR:N	1:89:A:TYR:CA	1:89:A:TYR:C	1:90:A:ASN:N	25	1.64
(1,46)	1:107:A:ASN:C	1:108:A:ILE:N	1:108:A:ILE:CA	1:108:A:ILE:C	5	1.64
(1,2)	1:57:A:LYS:C	1:58:A:CYS:N	1:58:A:CYS:CA	1:58:A:CYS:C	17	1.64
(1,106)	1:92:A:GLN:N	1:92:A:GLN:CA	1:92:A:GLN:C	1:93:A:GLN:N	11	1.63
(1,23)	1:82:A:PRO:C	1:83:A:GLU:N	1:83:A:GLU:CA	1:83:A:GLU:C	15	1.63
(1,106)	1:92:A:GLN:N	1:92:A:GLN:CA	1:92:A:GLN:C	1:93:A:GLN:N	17	1.62
(1,12)	1:68:A:GLU:C	1:69:A:GLU:N	1:69:A:GLU:CA	1:69:A:GLU:C	2	1.62
(1,140)	1:129:A:GLU:N	1:129:A:GLU:CA	1:129:A:GLU:C	1:130:A:LEU:N	10	1.61
(1,79)	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1:63:A:ASN:N	13	1.61
(1,77)	1:60:A:LYS:N	1:60:A:LYS:CA	1:60:A:LYS:C	1:61:A:LEU:N	16	1.6
(1,18)	1:74:A:CYS:C	1:75:A:LYS:N	1:75:A:LYS:CA	1:75:A:LYS:C	5	1.6
(1,122)	1:110:A:SER:N	1:110:A:SER:CA	1:110:A:SER:C	1:111:A:ARG:N	5	1.58
(1,146)	1:135:A:LYS:N	1:135:A:LYS:CA	1:135:A:LYS:C	1:136:A:ALA:N	22	1.57
(1,89)	1:72:A:GLU:N	1:72:A:GLU:CA	1:72:A:GLU:C	1:73:A:LEU:N	11	1.56
(1,76)	1:58:A:CYS:N	1:58:A:CYS:CA	1:58:A:CYS:C	1:59:A:TYR:N	1	1.55
(1,72)	1:134:A:LEU:C	1:135:A:LYS:N	1:135:A:LYS:CA	1:135:A:LYS:C	7	1.54
(1,70)	1:132:A:THR:C	1:133:A:VAL:N	1:133:A:VAL:CA	1:133:A:VAL:C	23	1.53
(1,103)	1:89:A:TYR:N	1:89:A:TYR:CA	1:89:A:TYR:C	1:90:A:ASN:N	12	1.52
(1,85)	1:68:A:GLU:N	1:68:A:GLU:CA	1:68:A:GLU:C	1:69:A:GLU:N	24	1.52
(1,121)	1:109:A:LEU:N	1:109:A:LEU:CA	1:109:A:LEU:C	1:110:A:SER:N	17	1.51
(1,145)	1:134:A:LEU:N	1:134:A:LEU:CA	1:134:A:LEU:C	1:135:A:LYS:N	18	1.5
(1,103)	1:89:A:TYR:N	1:89:A:TYR:CA	1:89:A:TYR:C	1:90:A:ASN:N	23	1.49
(1,5)	1:61:A:LEU:C	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	11	1.49
(1,85)	1:68:A:GLU:N	1:68:A:GLU:CA	1:68:A:GLU:C	1:69:A:GLU:N	3	1.48
(1,146)	1:135:A:LYS:N	1:135:A:LYS:CA	1:135:A:LYS:C	1:136:A:ALA:N	4	1.46
(1,121)	1:109:A:LEU:N	1:109:A:LEU:CA	1:109:A:LEU:C	1:110:A:SER:N	8	1.46
(1,94)	1:77:A:GLN:N	1:77:A:GLN:CA	1:77:A:GLN:C	1:78:A:THR:N	8	1.46
(1,98)	1:84:A:VAL:N	1:84:A:VAL:CA	1:84:A:VAL:C	1:85:A:VAL:N	25	1.45
(1,49)	1:110:A:SER:C	1:111:A:ARG:N	1:111:A:ARG:CA	1:111:A:ARG:C	23	1.45
(1,146)	1:135:A:LYS:N	1:135:A:LYS:CA	1:135:A:LYS:C	1:136:A:ALA:N	13	1.44
(1,121)	1:109:A:LEU:N	1:109:A:LEU:CA	1:109:A:LEU:C	1:110:A:SER:N	5	1.44
(1,120)	1:108:A:ILE:N	1:108:A:ILE:CA	1:108:A:ILE:C	1:109:A:LEU:N	20	1.44
(1,103)	1:89:A:TYR:N	1:89:A:TYR:CA	1:89:A:TYR:C	1:90:A:ASN:N	13	1.44
(1,46)	1:107:A:ASN:C	1:108:A:ILE:N	1:108:A:ILE:CA	1:108:A:ILE:C	11	1.44
(1,121)	1:109:A:LEU:N	1:109:A:LEU:CA	1:109:A:LEU:C	1:110:A:SER:N	1	1.42
(1,94)	1:77:A:GLN:N	1:77:A:GLN:CA	1:77:A:GLN:C	1:78:A:THR:N	7	1.42
(1,81)	1:64:A:GLU:N	1:64:A:GLU:CA	1:64:A:GLU:C	1:65:A:LYS:N	7	1.41

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,23)	1:82:A:PRO:C	1:83:A:GLU:N	1:83:A:GLU:CA	1:83:A:GLU:C	1	1.41
(1,145)	1:134:A:LEU:N	1:134:A:LEU:CA	1:134:A:LEU:C	1:135:A:LYS:N	17	1.4
(1,146)	1:135:A:LYS:N	1:135:A:LYS:CA	1:135:A:LYS:C	1:136:A:ALA:N	3	1.38
(1,98)	1:84:A:VAL:N	1:84:A:VAL:CA	1:84:A:VAL:C	1:85:A:VAL:N	17	1.38
(1,126)	1:114:A:SER:N	1:114:A:SER:CA	1:114:A:SER:C	1:115:A:ARG:N	7	1.37
(1,149)	2:23:B:SER:C	2:24:B:GLN:N	2:24:B:GLN:CA	2:24:B:GLN:C	25	1.36
(1,72)	1:134:A:LEU:C	1:135:A:LYS:N	1:135:A:LYS:CA	1:135:A:LYS:C	20	1.36
(1,23)	1:82:A:PRO:C	1:83:A:GLU:N	1:83:A:GLU:CA	1:83:A:GLU:C	22	1.36
(1,98)	1:84:A:VAL:N	1:84:A:VAL:CA	1:84:A:VAL:C	1:85:A:VAL:N	21	1.35
(1,148)	1:138:A:SER:N	1:138:A:SER:CA	1:138:A:SER:C	1:139:A:ALA:N	9	1.34
(1,103)	1:89:A:TYR:N	1:89:A:TYR:CA	1:89:A:TYR:C	1:90:A:ASN:N	24	1.34
(1,79)	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1:63:A:ASN:N	24	1.34
(1,18)	1:74:A:CYS:C	1:75:A:LYS:N	1:75:A:LYS:CA	1:75:A:LYS:C	17	1.34
(1,23)	1:82:A:PRO:C	1:83:A:GLU:N	1:83:A:GLU:CA	1:83:A:GLU:C	16	1.33
(1,114)	1:100:A:LEU:N	1:100:A:LEU:CA	1:100:A:LEU:C	1:101:A:ALA:N	18	1.32
(1,24)	1:83:A:GLU:C	1:84:A:VAL:N	1:84:A:VAL:CA	1:84:A:VAL:C	10	1.31
(1,76)	1:58:A:CYS:N	1:58:A:CYS:CA	1:58:A:CYS:C	1:59:A:TYR:N	13	1.3
(1,23)	1:82:A:PRO:C	1:83:A:GLU:N	1:83:A:GLU:CA	1:83:A:GLU:C	24	1.3
(1,123)	1:111:A:ARG:N	1:111:A:ARG:CA	1:111:A:ARG:C	1:112:A:VAL:N	6	1.29
(1,123)	1:111:A:ARG:N	1:111:A:ARG:CA	1:111:A:ARG:C	1:112:A:VAL:N	8	1.29
(1,70)	1:132:A:THR:C	1:133:A:VAL:N	1:133:A:VAL:CA	1:133:A:VAL:C	10	1.28
(1,46)	1:107:A:ASN:C	1:108:A:ILE:N	1:108:A:ILE:CA	1:108:A:ILE:C	1	1.28
(1,158)	2:29:B:SER:N	2:29:B:SER:CA	2:29:B:SER:C	2:30:B:GLU:N	22	1.27
(1,121)	1:109:A:LEU:N	1:109:A:LEU:CA	1:109:A:LEU:C	1:110:A:SER:N	19	1.27
(1,106)	1:92:A:GLN:N	1:92:A:GLN:CA	1:92:A:GLN:C	1:93:A:GLN:N	16	1.27
(1,72)	1:134:A:LEU:C	1:135:A:LYS:N	1:135:A:LYS:CA	1:135:A:LYS:C	24	1.27
(1,46)	1:107:A:ASN:C	1:108:A:ILE:N	1:108:A:ILE:CA	1:108:A:ILE:C	17	1.27
(1,120)	1:108:A:ILE:N	1:108:A:ILE:CA	1:108:A:ILE:C	1:109:A:LEU:N	18	1.26
(1,72)	1:134:A:LEU:C	1:135:A:LYS:N	1:135:A:LYS:CA	1:135:A:LYS:C	25	1.26
(1,103)	1:89:A:TYR:N	1:89:A:TYR:CA	1:89:A:TYR:C	1:90:A:ASN:N	22	1.25
(1,123)	1:111:A:ARG:N	1:111:A:ARG:CA	1:111:A:ARG:C	1:112:A:VAL:N	9	1.24
(1,121)	1:109:A:LEU:N	1:109:A:LEU:CA	1:109:A:LEU:C	1:110:A:SER:N	10	1.24
(1,103)	1:89:A:TYR:N	1:89:A:TYR:CA	1:89:A:TYR:C	1:90:A:ASN:N	15	1.24
(1,5)	1:61:A:LEU:C	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	16	1.24
(1,94)	1:77:A:GLN:N	1:77:A:GLN:CA	1:77:A:GLN:C	1:78:A:THR:N	24	1.23
(1,79)	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1:63:A:ASN:N	17	1.23
(1,72)	1:134:A:LEU:C	1:135:A:LYS:N	1:135:A:LYS:CA	1:135:A:LYS:C	4	1.23
(1,72)	1:134:A:LEU:C	1:135:A:LYS:N	1:135:A:LYS:CA	1:135:A:LYS:C	21	1.23
(1,145)	1:134:A:LEU:N	1:134:A:LEU:CA	1:134:A:LEU:C	1:135:A:LYS:N	6	1.22
(1,123)	1:111:A:ARG:N	1:111:A:ARG:CA	1:111:A:ARG:C	1:112:A:VAL:N	5	1.22
(1,121)	1:109:A:LEU:N	1:109:A:LEU:CA	1:109:A:LEU:C	1:110:A:SER:N	23	1.22
(1,106)	1:92:A:GLN:N	1:92:A:GLN:CA	1:92:A:GLN:C	1:93:A:GLN:N	15	1.22
(1,94)	1:77:A:GLN:N	1:77:A:GLN:CA	1:77:A:GLN:C	1:78:A:THR:N	2	1.22
(1,23)	1:82:A:PRO:C	1:83:A:GLU:N	1:83:A:GLU:CA	1:83:A:GLU:C	18	1.22
(1,146)	1:135:A:LYS:N	1:135:A:LYS:CA	1:135:A:LYS:C	1:136:A:ALA:N	25	1.21
(1,2)	1:57:A:LYS:C	1:58:A:CYS:N	1:58:A:CYS:CA	1:58:A:CYS:C	13	1.21
(1,145)	1:134:A:LEU:N	1:134:A:LEU:CA	1:134:A:LEU:C	1:135:A:LYS:N	20	1.2
(1,103)	1:89:A:TYR:N	1:89:A:TYR:CA	1:89:A:TYR:C	1:90:A:ASN:N	4	1.2
(1,46)	1:107:A:ASN:C	1:108:A:ILE:N	1:108:A:ILE:CA	1:108:A:ILE:C	12	1.2
(1,18)	1:74:A:CYS:C	1:75:A:LYS:N	1:75:A:LYS:CA	1:75:A:LYS:C	16	1.2
(1,72)	1:134:A:LEU:C	1:135:A:LYS:N	1:135:A:LYS:CA	1:135:A:LYS:C	19	1.19

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,23)	1:82:A:PRO:C	1:83:A:GLU:N	1:83:A:GLU:CA	1:83:A:GLU:C	2	1.19
(1,114)	1:100:A:LEU:N	1:100:A:LEU:CA	1:100:A:LEU:C	1:101:A:ALA:N	11	1.18
(1,98)	1:84:A:VAL:N	1:84:A:VAL:CA	1:84:A:VAL:C	1:85:A:VAL:N	2	1.16
(1,81)	1:64:A:GLU:N	1:64:A:GLU:CA	1:64:A:GLU:C	1:65:A:LYS:N	14	1.16
(1,63)	1:125:A:VAL:C	1:126:A:TYR:N	1:126:A:TYR:CA	1:126:A:TYR:C	14	1.16
(1,146)	1:135:A:LYS:N	1:135:A:LYS:CA	1:135:A:LYS:C	1:136:A:ALA:N	18	1.14
(1,81)	1:64:A:GLU:N	1:64:A:GLU:CA	1:64:A:GLU:C	1:65:A:LYS:N	8	1.14
(1,70)	1:132:A:THR:C	1:133:A:VAL:N	1:133:A:VAL:CA	1:133:A:VAL:C	9	1.14
(1,120)	1:108:A:ILE:N	1:108:A:ILE:CA	1:108:A:ILE:C	1:109:A:LEU:N	3	1.13
(1,106)	1:92:A:GLN:N	1:92:A:GLN:CA	1:92:A:GLN:C	1:93:A:GLN:N	7	1.13
(1,83)	1:66:A:LEU:N	1:66:A:LEU:CA	1:66:A:LEU:C	1:67:A:PHE:N	22	1.13
(1,23)	1:82:A:PRO:C	1:83:A:GLU:N	1:83:A:GLU:CA	1:83:A:GLU:C	19	1.13
(1,146)	1:135:A:LYS:N	1:135:A:LYS:CA	1:135:A:LYS:C	1:136:A:ALA:N	17	1.12
(1,146)	1:135:A:LYS:N	1:135:A:LYS:CA	1:135:A:LYS:C	1:136:A:ALA:N	21	1.12
(1,72)	1:134:A:LEU:C	1:135:A:LYS:N	1:135:A:LYS:CA	1:135:A:LYS:C	13	1.11
(1,23)	1:82:A:PRO:C	1:83:A:GLU:N	1:83:A:GLU:CA	1:83:A:GLU:C	20	1.11
(1,8)	1:64:A:GLU:C	1:65:A:LYS:N	1:65:A:LYS:CA	1:65:A:LYS:C	4	1.11
(1,120)	1:108:A:ILE:N	1:108:A:ILE:CA	1:108:A:ILE:C	1:109:A:LEU:N	23	1.1
(1,103)	1:89:A:TYR:N	1:89:A:TYR:CA	1:89:A:TYR:C	1:90:A:ASN:N	19	1.1
(1,85)	1:68:A:GLU:N	1:68:A:GLU:CA	1:68:A:GLU:C	1:69:A:GLU:N	8	1.1
(1,18)	1:74:A:CYS:C	1:75:A:LYS:N	1:75:A:LYS:CA	1:75:A:LYS:C	22	1.1
(1,149)	2:23:B:SER:C	2:24:B:GLN:N	2:24:B:GLN:CA	2:24:B:GLN:C	24	1.09
(1,67)	1:129:A:GLU:C	1:130:A:LEU:N	1:130:A:LEU:CA	1:130:A:LEU:C	10	1.09
(1,18)	1:74:A:CYS:C	1:75:A:LYS:N	1:75:A:LYS:CA	1:75:A:LYS:C	21	1.09
(1,121)	1:109:A:LEU:N	1:109:A:LEU:CA	1:109:A:LEU:C	1:110:A:SER:N	21	1.08
(1,145)	1:134:A:LEU:N	1:134:A:LEU:CA	1:134:A:LEU:C	1:135:A:LYS:N	13	1.07
(1,63)	1:125:A:VAL:C	1:126:A:TYR:N	1:126:A:TYR:CA	1:126:A:TYR:C	11	1.07
(1,106)	1:92:A:GLN:N	1:92:A:GLN:CA	1:92:A:GLN:C	1:93:A:GLN:N	8	1.06
(1,103)	1:89:A:TYR:N	1:89:A:TYR:CA	1:89:A:TYR:C	1:90:A:ASN:N	8	1.06
(1,94)	1:77:A:GLN:N	1:77:A:GLN:CA	1:77:A:GLN:C	1:78:A:THR:N	13	1.06
(1,70)	1:132:A:THR:C	1:133:A:VAL:N	1:133:A:VAL:CA	1:133:A:VAL:C	13	1.06
(1,54)	1:115:A:ARG:C	1:116:A:ALA:N	1:116:A:ALA:CA	1:116:A:ALA:C	13	1.06
(1,23)	1:82:A:PRO:C	1:83:A:GLU:N	1:83:A:GLU:CA	1:83:A:GLU:C	4	1.06
(1,54)	1:115:A:ARG:C	1:116:A:ALA:N	1:116:A:ALA:CA	1:116:A:ALA:C	22	1.05
(1,46)	1:107:A:ASN:C	1:108:A:ILE:N	1:108:A:ILE:CA	1:108:A:ILE:C	8	1.05
(1,23)	1:82:A:PRO:C	1:83:A:GLU:N	1:83:A:GLU:CA	1:83:A:GLU:C	9	1.05
(1,121)	1:109:A:LEU:N	1:109:A:LEU:CA	1:109:A:LEU:C	1:110:A:SER:N	25	1.04
(1,94)	1:77:A:GLN:N	1:77:A:GLN:CA	1:77:A:GLN:C	1:78:A:THR:N	6	1.04
(1,94)	1:77:A:GLN:N	1:77:A:GLN:CA	1:77:A:GLN:C	1:78:A:THR:N	22	1.04
(1,8)	1:64:A:GLU:C	1:65:A:LYS:N	1:65:A:LYS:CA	1:65:A:LYS:C	18	1.04
(1,123)	1:111:A:ARG:N	1:111:A:ARG:CA	1:111:A:ARG:C	1:112:A:VAL:N	20	1.03
(1,23)	1:82:A:PRO:C	1:83:A:GLU:N	1:83:A:GLU:CA	1:83:A:GLU:C	13	1.03
(1,18)	1:74:A:CYS:C	1:75:A:LYS:N	1:75:A:LYS:CA	1:75:A:LYS:C	15	1.03
(1,146)	1:135:A:LYS:N	1:135:A:LYS:CA	1:135:A:LYS:C	1:136:A:ALA:N	23	1.02
(1,123)	1:111:A:ARG:N	1:111:A:ARG:CA	1:111:A:ARG:C	1:112:A:VAL:N	21	1.02
(1,62)	1:124:A:TYR:C	1:125:A:VAL:N	1:125:A:VAL:CA	1:125:A:VAL:C	16	1.02
(1,123)	1:111:A:ARG:N	1:111:A:ARG:CA	1:111:A:ARG:C	1:112:A:VAL:N	13	1.0
(1,106)	1:92:A:GLN:N	1:92:A:GLN:CA	1:92:A:GLN:C	1:93:A:GLN:N	14	1.0
(1,103)	1:89:A:TYR:N	1:89:A:TYR:CA	1:89:A:TYR:C	1:90:A:ASN:N	5	1.0
(1,103)	1:89:A:TYR:N	1:89:A:TYR:CA	1:89:A:TYR:C	1:90:A:ASN:N	7	1.0