



Full wwPDB NMR Structure Validation Report ⓘ

Mar 4, 2026 – 08:24 PM UTC

PDB ID : 2MX0 / pdb_00002mx0
BMRB ID : 25380
Title : Solution structure of HP0268 from Helicobacter pylori
Authors : Lee, K.Y.
Deposited on : 2014-12-05

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

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

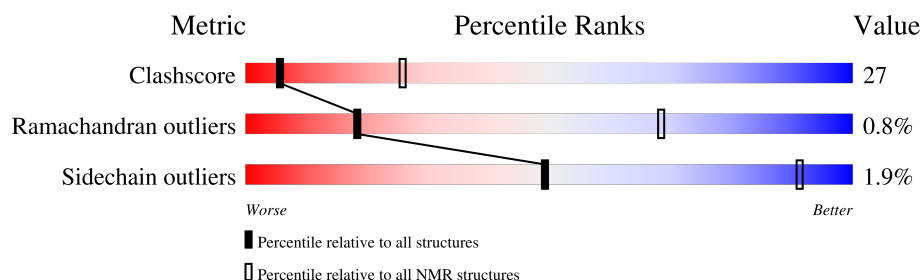
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 75%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	82	30% 54% 5% 11%

2 Ensemble composition and analysis

This entry contains 20 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:4-A:11, A:18-A:82 (73)	0.47	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 2 clusters. No single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1354 atoms, of which 670 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Uncharacterized protein HP_0268.

Mol	Chain	Residues	Atoms						Trace
1	A	82	Total	C	H	N	O	S	0
			1354	438	670	113	131	2	

There are 2 discrepancies between the modelled and reference sequences:

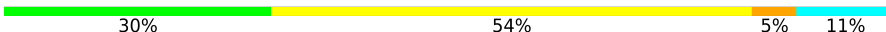
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP O25047
A	2	HIS	-	expression tag	UNP O25047

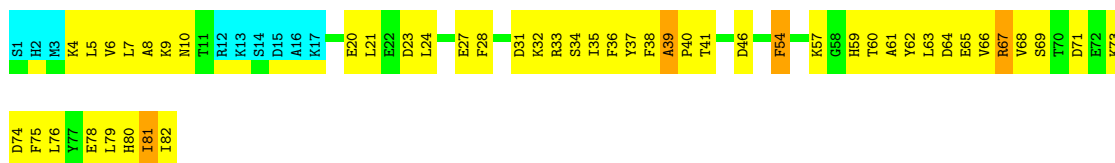
4 Residue-property plots

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: Uncharacterized protein HP_0268

Chain A: 

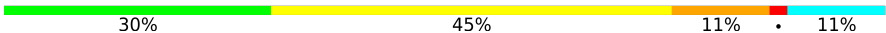


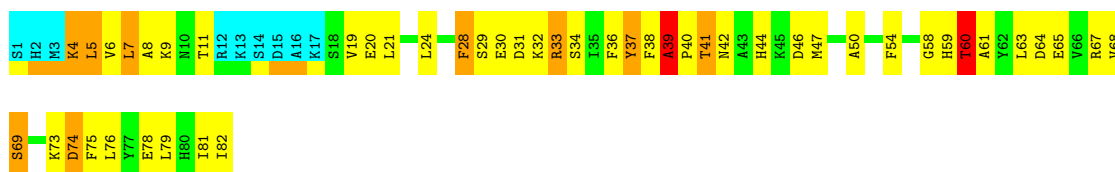
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

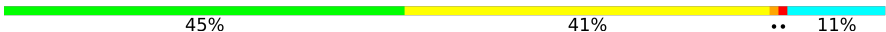
- Molecule 1: Uncharacterized protein HP_0268

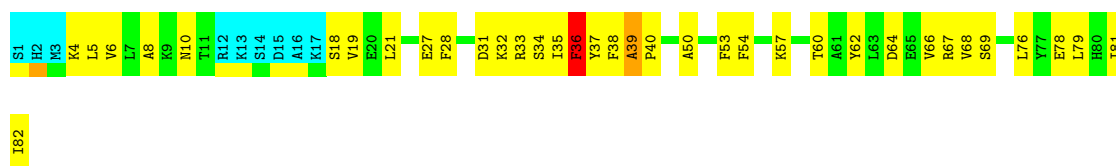
Chain A: 



4.2.2 Score per residue for model 2

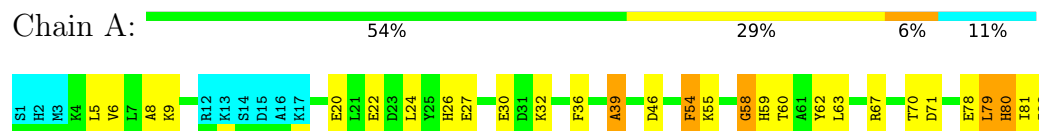
- Molecule 1: Uncharacterized protein HP_0268

Chain A: 



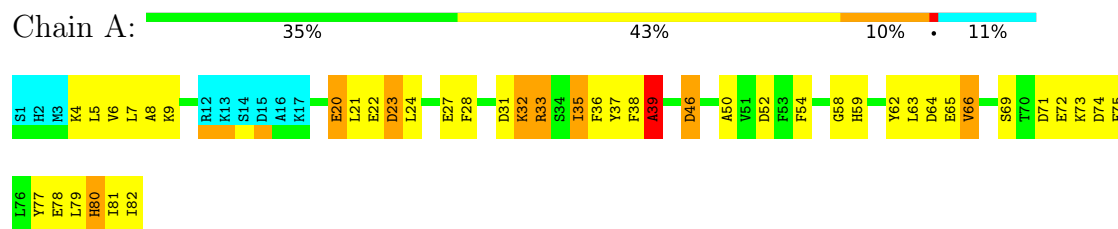
4.2.3 Score per residue for model 3

- Molecule 1: Uncharacterized protein HP_0268



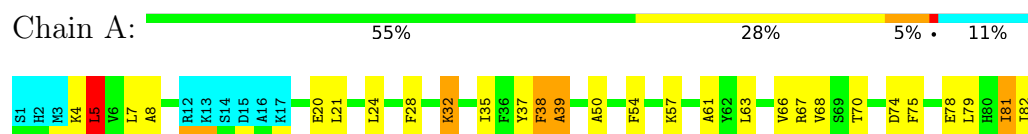
4.2.4 Score per residue for model 4

- Molecule 1: Uncharacterized protein HP_0268



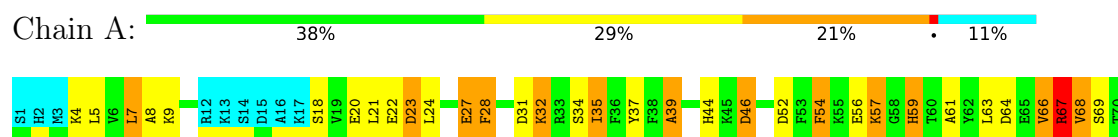
4.2.5 Score per residue for model 5

- Molecule 1: Uncharacterized protein HP_0268



4.2.6 Score per residue for model 6

- Molecule 1: Uncharacterized protein HP_0268





4.2.7 Score per residue for model 7

- Molecule 1: Uncharacterized protein HP_0268



4.2.8 Score per residue for model 8

- Molecule 1: Uncharacterized protein HP_0268



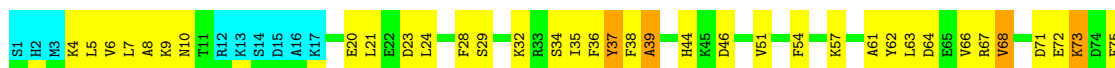
4.2.9 Score per residue for model 9

- Molecule 1: Uncharacterized protein HP_0268



4.2.10 Score per residue for model 10

- Molecule 1: Uncharacterized protein HP_0268

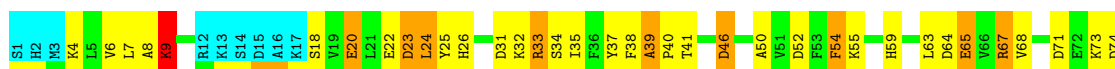




4.2.11 Score per residue for model 11

- Molecule 1: Uncharacterized protein HP_0268

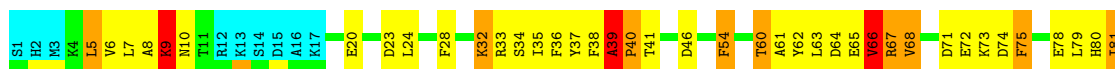
Chain A: 38% 35% 15% • 11%



4.2.12 Score per residue for model 12

- Molecule 1: Uncharacterized protein HP_0268

Chain A: 39% 34% 12% • 11%



4.2.13 Score per residue for model 13

- Molecule 1: Uncharacterized protein HP_0268

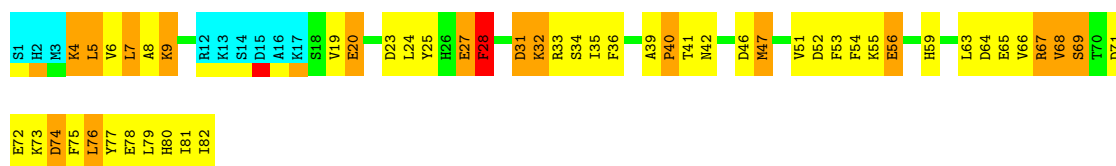
Chain A: 28% 43% 17% • 11%



4.2.14 Score per residue for model 14

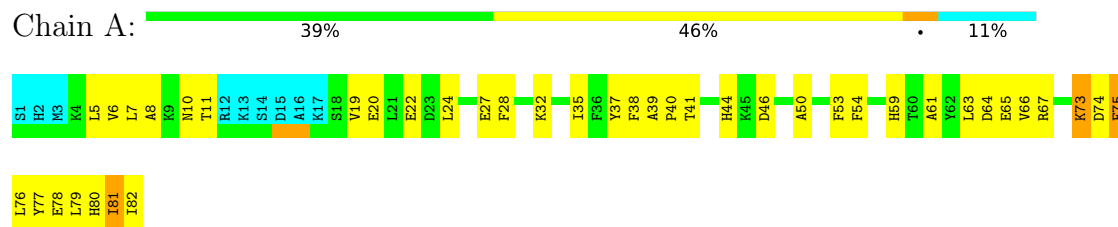
- Molecule 1: Uncharacterized protein HP_0268

Chain A: 27% 41% 20% • 11%



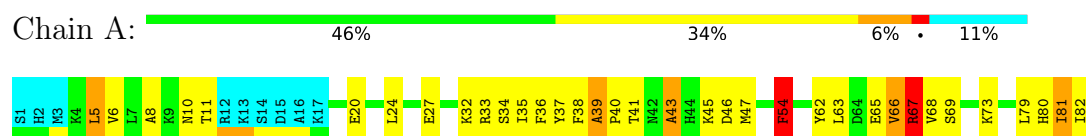
4.2.15 Score per residue for model 15 (medoid)

- Molecule 1: Uncharacterized protein HP_0268



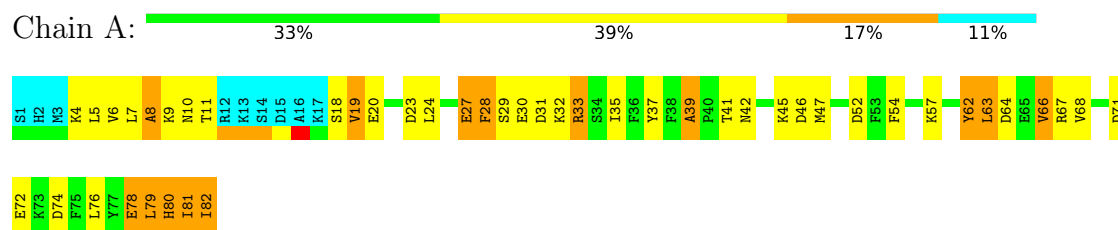
4.2.16 Score per residue for model 16

- Molecule 1: Uncharacterized protein HP_0268



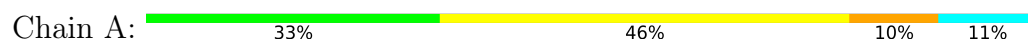
4.2.17 Score per residue for model 17

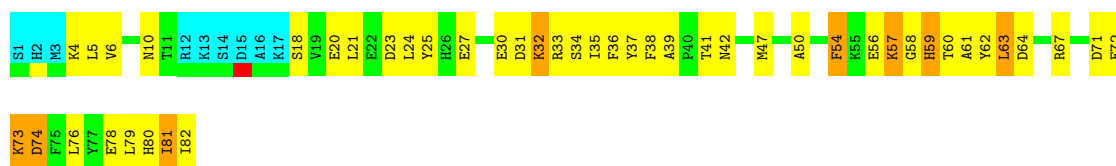
- Molecule 1: Uncharacterized protein HP_0268



4.2.18 Score per residue for model 18

- Molecule 1: Uncharacterized protein HP_0268

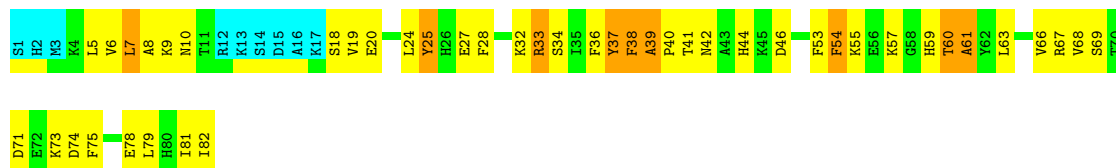




4.2.19 Score per residue for model 19

- Molecule 1: Uncharacterized protein HP_0268

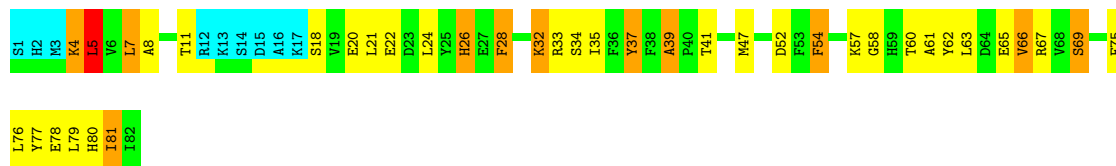
Chain A: 34% 44% 11% 11%



4.2.20 Score per residue for model 20

- Molecule 1: Uncharacterized protein HP_0268

Chain A: 41% 33% 13% 11%



5 Refinement protocol and experimental data overview

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CYANA	structure solution	
CYANA	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	868
Number of shifts mapped to atoms	868
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	75%

6 Model quality i

6.1 Standard geometry i

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.48±0.39	7±7/626 (1.0± 1.1%)	1.91±0.16	18±8/841 (2.1± 0.9%)
All	All	1.53	131/12520 (1.0%)	1.91	361/16820 (2.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	5.8±1.5
All	All	0	117

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	71	ASP	CG-OD1	-15.66	0.95	1.25	11	3
1	A	33	ARG	CZ-NH1	-14.18	1.12	1.32	4	2
1	A	46	ASP	CG-OD1	-13.78	0.99	1.25	11	3
1	A	74	ASP	CG-OD1	13.76	1.51	1.25	11	5
1	A	52	ASP	CG-OD2	13.72	1.51	1.25	11	3
1	A	74	ASP	CG-OD2	-13.64	0.99	1.25	11	5
1	A	33	ARG	CZ-NH2	-13.51	1.15	1.33	17	2
1	A	23	ASP	CG-OD2	13.47	1.50	1.25	11	5
1	A	52	ASP	CG-OD1	-13.25	1.00	1.25	11	3
1	A	23	ASP	CG-OD1	-13.01	1.00	1.25	11	4
1	A	64	ASP	CG-OD1	12.91	1.49	1.25	17	5
1	A	40	PRO	N-CD	12.54	1.65	1.47	12	2
1	A	31	ASP	CG-OD2	-12.53	1.01	1.25	11	5
1	A	71	ASP	CG-OD2	12.31	1.48	1.25	11	3
1	A	10	ASN	CG-ND2	-12.15	1.07	1.33	17	1
1	A	31	ASP	CG-OD1	12.08	1.48	1.25	17	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	46	ASP	CG-OD2	11.88	1.48	1.25	4	3
1	A	64	ASP	CG-OD2	-11.61	1.03	1.25	17	4
1	A	20	GLU	C-O	-11.43	1.10	1.24	14	2
1	A	82	ILE	C-O	10.06	1.43	1.23	11	4
1	A	20	GLU	CD-OE1	-9.66	1.06	1.25	11	3
1	A	67	ARG	C-O	-9.52	1.10	1.23	7	2
1	A	25	TYR	CZ-OH	-9.43	1.18	1.38	11	1
1	A	41	THR	CB-OG1	-9.20	1.29	1.43	14	4
1	A	22	GLU	CD-OE1	-9.07	1.08	1.25	4	2
1	A	43	ALA	C-O	-8.74	1.12	1.24	13	1
1	A	78	GLU	CD-OE1	-8.67	1.08	1.25	11	1
1	A	40	PRO	C-N	7.95	1.44	1.33	14	1
1	A	55	LYS	C-N	-7.93	1.23	1.33	9	1
1	A	54	PHE	C-O	-7.88	1.14	1.24	7	2
1	A	40	PRO	CA-C	7.68	1.62	1.52	14	1
1	A	82	ILE	C-OXT	-7.58	1.08	1.23	11	2
1	A	67	ARG	CZ-NH1	-7.13	1.22	1.32	13	1
1	A	33	ARG	CD-NE	-6.93	1.36	1.46	17	1
1	A	37	TYR	CA-C	6.93	1.61	1.52	1	1
1	A	72	GLU	CA-C	-6.90	1.43	1.52	4	1
1	A	42	ASN	C-O	-6.88	1.16	1.24	1	1
1	A	32	LYS	C-N	-6.45	1.25	1.33	6	1
1	A	57	LYS	C-O	-6.44	1.15	1.23	17	1
1	A	28	PHE	C-O	6.43	1.31	1.24	14	2
1	A	39	ALA	CA-C	-6.27	1.47	1.52	4	1
1	A	27	GLU	CD-OE1	-6.23	1.13	1.25	17	1
1	A	18	SER	N-CA	6.17	1.53	1.46	11	1
1	A	30	GLU	CD-OE1	-6.17	1.13	1.25	18	1
1	A	22	GLU	CD-OE2	-5.94	1.14	1.25	9	2
1	A	7	LEU	C-O	-5.89	1.16	1.24	1	1
1	A	27	GLU	CA-C	-5.80	1.45	1.52	19	1
1	A	41	THR	N-CA	-5.78	1.39	1.46	14	1
1	A	70	THR	C-O	-5.70	1.17	1.24	13	1
1	A	63	LEU	C-N	5.67	1.40	1.33	17	1
1	A	61	ALA	C-O	-5.64	1.16	1.24	9	1
1	A	36	PHE	C-O	-5.56	1.16	1.24	18	1
1	A	44	HIS	CA-CB	-5.54	1.45	1.53	7	1
1	A	58	GLY	C-O	-5.52	1.17	1.23	4	1
1	A	20	GLU	CD-OE2	5.51	1.35	1.25	9	1
1	A	31	ASP	CA-C	5.50	1.59	1.52	1	1
1	A	32	LYS	C-O	5.45	1.30	1.24	6	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	80	HIS	CA-C	-5.41	1.46	1.52	4	1
1	A	30	GLU	C-N	5.39	1.40	1.33	17	1
1	A	5	LEU	C-O	-5.36	1.17	1.23	13	1
1	A	9	LYS	C-O	-5.30	1.18	1.24	12	2
1	A	71	ASP	C-O	-5.27	1.17	1.24	19	2
1	A	23	ASP	C-O	-5.27	1.17	1.24	17	1
1	A	33	ARG	C-N	-5.24	1.27	1.33	1	1
1	A	27	GLU	CD-OE2	-5.21	1.15	1.25	3	1
1	A	36	PHE	N-CA	5.13	1.52	1.46	10	1
1	A	68	VAL	CA-C	5.12	1.58	1.52	14	1
1	A	56	GLU	CA-C	-5.10	1.46	1.52	7	1
1	A	76	LEU	CA-C	-5.07	1.46	1.52	14	1
1	A	74	ASP	N-CA	5.03	1.52	1.46	14	1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	23	ASP	CA-CB-CG	-14.20	98.40	112.60	4	9
1	A	10	ASN	OD1-CG-ND2	-13.55	109.05	122.60	15	6
1	A	40	PRO	CA-N-CD	-13.22	93.49	112.00	12	1
1	A	39	ALA	O-C-N	11.79	133.27	121.72	12	2
1	A	71	ASP	CA-CB-CG	-11.76	100.84	112.60	11	4
1	A	64	ASP	CA-CB-CG	-11.13	101.47	112.60	11	3
1	A	74	ASP	CA-CB-CG	-11.02	101.58	112.60	4	6
1	A	31	ASP	CA-CB-CG	10.64	123.24	112.60	11	4
1	A	52	ASP	CA-CB-CG	-10.17	102.43	112.60	6	7
1	A	42	ASN	OD1-CG-ND2	-9.59	113.02	122.60	17	2
1	A	36	PHE	CA-CB-CG	9.32	123.12	113.80	2	1
1	A	41	THR	CA-C-N	9.10	132.81	120.44	1	7
1	A	41	THR	C-N-CA	9.10	132.81	120.44	1	7
1	A	54	PHE	N-CA-C	-8.99	100.90	112.23	12	5
1	A	53	PHE	CA-CB-CG	8.88	122.68	113.80	19	2
1	A	61	ALA	N-CA-C	-8.77	102.16	113.12	18	5
1	A	69	SER	N-CA-C	-8.74	101.75	111.28	14	2
1	A	67	ARG	CA-C-N	8.70	133.04	122.26	7	2
1	A	67	ARG	C-N-CA	8.70	133.04	122.26	7	2
1	A	71	ASP	N-CA-C	8.69	122.38	111.69	11	8
1	A	59	HIS	N-CA-C	8.50	120.54	111.28	7	7
1	A	81	ILE	O-C-N	-8.37	112.10	122.57	20	4
1	A	57	LYS	CA-C-O	-8.28	111.40	120.92	6	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	20	GLU	O-C-N	-8.26	113.57	122.07	14	2
1	A	41	THR	N-CA-C	-8.22	102.40	111.36	9	2
1	A	9	LYS	CA-C-N	8.20	131.27	120.28	19	1
1	A	9	LYS	C-N-CA	8.20	131.27	120.28	19	1
1	A	45	LYS	N-CA-C	8.13	119.92	111.14	17	1
1	A	74	ASP	CB-CG-OD1	-8.07	99.83	118.40	11	2
1	A	68	VAL	N-CA-C	-7.80	104.97	111.91	7	5
1	A	40	PRO	N-CD-CG	-7.77	91.55	103.20	12	1
1	A	5	LEU	CA-C-O	-7.76	112.38	121.46	5	2
1	A	55	LYS	CA-C-O	-7.55	112.42	120.42	19	3
1	A	57	LYS	N-CA-C	7.55	119.41	111.03	9	3
1	A	21	LEU	CA-C-N	7.47	130.28	120.28	8	1
1	A	21	LEU	C-N-CA	7.47	130.28	120.28	8	1
1	A	31	ASP	O-C-N	-7.39	115.21	123.48	6	4
1	A	36	PHE	N-CA-C	7.31	120.64	108.73	10	1
1	A	55	LYS	N-CA-C	7.28	119.30	111.36	14	1
1	A	66	VAL	O-C-N	-7.22	114.98	122.63	12	4
1	A	47	MET	N-CA-C	7.18	119.11	111.28	14	2
1	A	60	THR	CA-CB-OG1	-7.14	98.89	109.60	19	2
1	A	23	ASP	OD1-CG-OD2	7.11	139.96	122.90	14	1
1	A	32	LYS	N-CA-C	7.09	119.96	108.41	12	5
1	A	25	TYR	N-CA-C	-7.06	103.51	111.07	14	1
1	A	33	ARG	O-C-N	-7.05	115.71	123.04	1	4
1	A	67	ARG	N-CA-C	6.91	119.99	109.62	12	3
1	A	7	LEU	CA-C-N	6.90	130.67	120.87	6	5
1	A	7	LEU	C-N-CA	6.90	130.67	120.87	6	5
1	A	8	ALA	CA-C-N	6.87	130.76	120.31	17	1
1	A	8	ALA	C-N-CA	6.87	130.76	120.31	17	1
1	A	74	ASP	CB-CG-OD2	-6.86	102.63	118.40	4	3
1	A	40	PRO	N-CA-C	6.84	126.57	112.47	12	1
1	A	29	SER	N-CA-C	6.80	118.77	111.36	17	1
1	A	56	GLU	CA-C-O	-6.76	113.72	120.82	7	2
1	A	66	VAL	CA-C-N	6.72	130.52	120.31	8	3
1	A	66	VAL	C-N-CA	6.72	130.52	120.31	8	3
1	A	54	PHE	CA-C-O	-6.68	113.80	120.82	6	1
1	A	42	ASN	N-CA-C	6.66	118.54	111.28	14	3
1	A	18	SER	CA-C-N	6.65	129.87	120.42	18	3
1	A	18	SER	C-N-CA	6.65	129.87	120.42	18	3
1	A	36	PHE	CA-C-N	6.62	131.24	122.30	7	1
1	A	36	PHE	C-N-CA	6.62	131.24	122.30	7	1
1	A	23	ASP	CB-CG-OD1	6.59	133.55	118.40	11	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	59	HIS	CA-C-O	-6.57	112.41	119.97	6	1
1	A	11	THR	CA-CB-OG1	-6.56	99.76	109.60	15	2
1	A	73	LYS	CA-C-O	-6.55	113.99	121.65	8	1
1	A	75	PHE	N-CA-C	6.55	119.58	107.99	12	2
1	A	60	THR	O-C-N	-6.51	113.93	122.59	1	2
1	A	72	GLU	N-CA-C	-6.47	105.03	113.12	14	2
1	A	31	ASP	OD1-CG-OD2	6.46	138.42	122.90	14	1
1	A	33	ARG	N-CA-C	6.43	116.95	107.88	19	1
1	A	21	LEU	CA-C-O	-6.41	114.09	120.82	6	1
1	A	27	GLU	CA-C-N	6.40	128.76	120.44	18	2
1	A	27	GLU	C-N-CA	6.40	128.76	120.44	18	2
1	A	23	ASP	CB-CG-OD2	-6.40	103.69	118.40	11	2
1	A	37	TYR	CD1-CE1-CZ	6.36	131.05	119.60	20	1
1	A	11	THR	N-CA-C	6.26	118.19	111.36	7	3
1	A	58	GLY	CA-C-N	6.22	129.12	120.29	18	3
1	A	58	GLY	C-N-CA	6.22	129.12	120.29	18	3
1	A	19	VAL	N-CA-C	6.22	116.39	110.42	14	2
1	A	73	LYS	O-C-N	-6.21	114.85	122.55	13	2
1	A	18	SER	N-CA-C	6.19	120.67	113.18	17	2
1	A	66	VAL	CA-C-O	-6.16	113.97	120.57	9	2
1	A	25	TYR	CE1-CZ-CE2	6.16	132.63	120.30	9	1
1	A	22	GLU	O-C-N	6.12	128.60	122.12	6	1
1	A	26	HIS	N-CA-C	6.11	117.74	111.14	20	1
1	A	39	ALA	CA-C-N	-6.09	113.51	119.78	7	2
1	A	39	ALA	C-N-CA	-6.09	113.51	119.78	7	2
1	A	52	ASP	CB-CG-OD1	6.08	132.38	118.40	11	1
1	A	73	LYS	N-CA-C	6.06	119.79	111.54	15	4
1	A	41	THR	N-CA-CB	6.04	119.11	110.16	9	1
1	A	46	ASP	CA-CB-CG	-6.04	106.56	112.60	4	1
1	A	64	ASP	O-C-N	-6.03	116.72	123.48	6	3
1	A	4	LYS	N-CA-CB	-6.02	102.87	111.84	5	1
1	A	52	ASP	CB-CG-OD2	6.01	132.23	118.40	17	2
1	A	29	SER	O-C-N	5.97	128.22	122.07	7	2
1	A	33	ARG	NE-CZ-NH2	5.94	124.55	119.20	1	1
1	A	72	GLU	CA-C-N	5.92	130.54	122.07	12	4
1	A	72	GLU	C-N-CA	5.92	130.54	122.07	12	4
1	A	70	THR	N-CA-C	-5.91	104.84	111.28	3	1
1	A	54	PHE	CA-C-N	5.90	128.47	120.44	16	4
1	A	54	PHE	C-N-CA	5.90	128.47	120.44	16	4
1	A	64	ASP	N-CA-C	5.89	118.14	109.24	2	2
1	A	73	LYS	CA-C-N	5.87	130.77	121.44	7	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	73	LYS	C-N-CA	5.87	130.77	121.44	7	1
1	A	4	LYS	N-CA-C	-5.85	105.96	112.57	13	5
1	A	43	ALA	CA-C-N	5.83	130.41	122.07	16	1
1	A	43	ALA	C-N-CA	5.83	130.41	122.07	16	1
1	A	80	HIS	ND1-CE1-NE2	5.81	114.21	108.40	17	1
1	A	21	LEU	N-CA-C	5.81	117.28	111.07	4	1
1	A	54	PHE	CA-CB-CG	5.80	119.60	113.80	8	1
1	A	37	TYR	O-C-N	-5.78	116.49	123.13	7	1
1	A	37	TYR	N-CA-C	5.75	117.67	108.41	1	1
1	A	66	VAL	N-CA-C	5.75	116.58	108.36	9	1
1	A	9	LYS	O-C-N	-5.75	116.15	122.07	12	1
1	A	22	GLU	CA-C-O	-5.73	114.34	120.42	11	2
1	A	29	SER	CA-C-N	5.72	128.22	120.44	17	1
1	A	29	SER	C-N-CA	5.72	128.22	120.44	17	1
1	A	46	ASP	O-C-N	-5.71	116.06	122.12	6	1
1	A	42	ASN	CB-CG-ND2	5.69	124.94	116.40	17	1
1	A	6	VAL	N-CA-C	5.68	116.05	107.75	7	1
1	A	51	VAL	N-CA-C	-5.67	104.98	110.42	14	2
1	A	25	TYR	CE1-CZ-OH	-5.66	102.91	119.90	19	1
1	A	22	GLU	N-CA-C	5.66	117.53	111.36	3	1
1	A	31	ASP	N-CA-C	5.65	116.85	108.60	9	1
1	A	53	PHE	N-CA-C	5.64	117.51	111.36	14	1
1	A	56	GLU	N-CA-C	5.64	118.97	111.75	14	1
1	A	72	GLU	O-C-N	-5.63	116.61	121.85	17	1
1	A	80	HIS	CA-CB-CG	5.59	119.39	113.80	11	1
1	A	46	ASP	CB-CG-OD1	5.59	131.25	118.40	4	1
1	A	24	LEU	O-C-N	5.55	129.97	122.59	11	1
1	A	20	GLU	CA-C-O	-5.50	115.05	120.82	8	1
1	A	70	THR	CA-C-N	5.48	128.07	120.29	8	1
1	A	70	THR	C-N-CA	5.48	128.07	120.29	8	1
1	A	10	ASN	N-CA-C	-5.48	105.31	111.28	10	3
1	A	41	THR	CA-CB-OG1	5.47	117.81	109.60	15	1
1	A	71	ASP	CA-C-O	-5.43	114.21	120.24	11	2
1	A	26	HIS	CE1-NE2-CD2	-5.43	103.56	109.00	11	1
1	A	41	THR	O-C-N	5.42	127.86	122.12	1	1
1	A	56	GLU	O-C-N	5.41	127.71	122.09	6	2
1	A	53	PHE	O-C-N	5.37	128.27	122.15	14	1
1	A	10	ASN	CA-C-N	5.37	127.91	120.29	8	1
1	A	10	ASN	C-N-CA	5.37	127.91	120.29	8	1
1	A	27	GLU	N-CA-CB	5.37	117.79	110.01	19	1
1	A	37	TYR	CA-C-N	5.32	130.84	122.34	8	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	37	TYR	C-N-CA	5.32	130.84	122.34	8	2
1	A	61	ALA	CA-C-N	5.31	130.58	121.87	12	1
1	A	61	ALA	C-N-CA	5.31	130.58	121.87	12	1
1	A	68	VAL	CA-C-N	5.30	127.82	120.29	9	4
1	A	68	VAL	C-N-CA	5.30	127.82	120.29	9	4
1	A	65	GLU	N-CA-C	5.30	116.92	110.41	11	1
1	A	80	HIS	CA-C-O	-5.29	114.50	120.32	4	1
1	A	70	THR	O-C-N	5.26	127.70	122.12	5	1
1	A	61	ALA	O-C-N	5.26	129.59	122.59	12	1
1	A	62	TYR	N-CA-C	5.25	116.82	108.79	18	1
1	A	71	ASP	CB-CG-OD1	5.23	130.42	118.40	11	1
1	A	67	ARG	O-C-N	-5.21	115.73	122.61	9	1
1	A	49	LYS	N-CA-C	5.19	117.84	111.82	7	1
1	A	27	GLU	CA-C-O	-5.17	115.07	120.55	6	1
1	A	78	GLU	O-C-N	-5.15	117.29	123.31	6	1
1	A	71	ASP	CB-CG-OD2	5.14	130.23	118.40	17	1
1	A	64	ASP	OD1-CG-OD2	5.14	135.23	122.90	14	1
1	A	79	LEU	CA-C-O	-5.11	114.84	120.36	6	1
1	A	81	ILE	CA-C-O	-5.10	114.40	120.78	16	1
1	A	27	GLU	N-CA-C	-5.09	105.62	111.07	14	2
1	A	50	ALA	N-CA-C	5.08	116.82	111.28	4	1
1	A	65	GLU	CA-C-N	-5.07	116.54	122.93	7	1
1	A	65	GLU	C-N-CA	-5.07	116.54	122.93	7	1
1	A	32	LYS	CA-C-O	-5.06	114.90	120.36	8	1
1	A	59	HIS	ND1-CE1-NE2	5.05	113.45	108.40	13	1
1	A	42	ASN	N-CA-CB	-5.05	102.69	110.16	18	1
1	A	80	HIS	ND1-CG-CD2	5.05	111.15	106.10	3	1
1	A	67	ARG	NE-CZ-NH2	5.04	123.74	119.20	6	1
1	A	29	SER	CA-CB-OG	-5.03	101.03	111.10	10	1
1	A	67	ARG	CA-C-O	-5.03	116.15	122.63	7	1
1	A	58	GLY	N-CA-C	5.00	120.17	114.67	7	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	32	LYS	Peptide	20
1	A	39	ALA	Peptide	20
1	A	67	ARG	Peptide	17
1	A	65	GLU	Peptide	8

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	60	THR	Peptide	5
1	A	74	ASP	Peptide	5
1	A	9	LYS	Peptide	5
1	A	54	PHE	Sidechain	4
1	A	66	VAL	Peptide	4
1	A	35	ILE	Peptide	3
1	A	59	HIS	Peptide	2
1	A	58	GLY	Peptide	2
1	A	73	LYS	Peptide	2
1	A	25	TYR	Sidechain	2
1	A	69	SER	Peptide	2
1	A	62	TYR	Sidechain	2
1	A	30	GLU	Sidechain	1
1	A	36	PHE	Sidechain	1
1	A	68	VAL	Peptide	1
1	A	75	PHE	Peptide	1
1	A	80	HIS	Peptide	1
1	A	33	ARG	Peptide	1
1	A	34	SER	Peptide	1
1	A	43	ALA	Peptide	1
1	A	44	HIS	Peptide	1
1	A	5	LEU	Peptide	1
1	A	72	GLU	Peptide	1
1	A	37	TYR	Peptide	1
1	A	38	PHE	Peptide	1
1	A	18	SER	Peptide	1

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	612	594	594	33±9
All	All	12240	11880	11880	662

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 27.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:6:VAL:HG23	1:A:35:ILE:HD11	1.11	1.21	17	2
1:A:21:LEU:HD22	1:A:57:LYS:HE3	1.02	1.32	9	3
1:A:79:LEU:HD13	1:A:82:ILE:HD12	1.01	1.28	14	4
1:A:20:GLU:O	1:A:24:LEU:HD13	0.98	1.56	14	6
1:A:79:LEU:HD13	1:A:82:ILE:CD1	0.97	1.89	19	4
1:A:61:ALA:CB	1:A:82:ILE:HG22	0.95	1.91	5	4
1:A:47:MET:HG3	1:A:76:LEU:HD11	0.95	1.38	14	5
1:A:54:PHE:CD2	1:A:63:LEU:HD22	0.93	1.98	20	9
1:A:54:PHE:HD2	1:A:63:LEU:HD22	0.92	1.24	13	13
1:A:79:LEU:HD23	1:A:82:ILE:CD1	0.90	1.96	9	2
1:A:6:VAL:HG21	1:A:20:GLU:OE1	0.89	1.67	4	9
1:A:79:LEU:CD1	1:A:82:ILE:HD12	0.88	1.99	18	4
1:A:79:LEU:HD13	1:A:82:ILE:HD13	0.86	1.47	19	1
1:A:81:ILE:O	1:A:82:ILE:HG22	0.86	1.70	12	2
1:A:79:LEU:CD2	1:A:82:ILE:HD12	0.86	2.01	15	2
1:A:82:ILE:O	1:A:82:ILE:HD13	0.85	1.72	12	1
1:A:6:VAL:CG2	1:A:35:ILE:HD11	0.85	2.01	2	2
1:A:6:VAL:HG11	1:A:20:GLU:HB3	0.84	1.50	14	2
1:A:79:LEU:HD23	1:A:82:ILE:HD12	0.84	1.48	15	2
1:A:66:VAL:HG12	1:A:68:VAL:H	0.83	1.32	12	9
1:A:34:SER:CB	1:A:79:LEU:HD23	0.83	2.04	14	5
1:A:5:LEU:C	1:A:5:LEU:HD12	0.83	1.98	14	3
1:A:5:LEU:O	1:A:5:LEU:HD12	0.82	1.74	1	7
1:A:79:LEU:HD23	1:A:82:ILE:HD13	0.82	1.49	9	2
1:A:8:ALA:HB1	1:A:46:ASP:OD2	0.82	1.74	4	14
1:A:24:LEU:HD23	1:A:80:HIS:NE2	0.81	1.88	3	2
1:A:54:PHE:HD2	1:A:63:LEU:HD13	0.81	1.33	5	2
1:A:66:VAL:HG23	1:A:69:SER:H	0.80	1.36	8	1
1:A:27:GLU:HB3	1:A:33:ARG:HD3	0.80	1.51	14	4
1:A:27:GLU:OE1	1:A:35:ILE:HD11	0.80	1.77	15	3
1:A:61:ALA:HB1	1:A:82:ILE:HG22	0.79	1.54	5	4
1:A:63:LEU:C	1:A:63:LEU:HD23	0.79	2.03	1	4
1:A:28:PHE:CZ	1:A:81:ILE:HD11	0.79	2.12	1	2
1:A:5:LEU:HD12	1:A:5:LEU:O	0.79	1.76	14	3
1:A:5:LEU:HD23	1:A:38:PHE:CE1	0.78	2.13	18	1
1:A:6:VAL:HG13	1:A:19:VAL:CG1	0.77	2.09	2	3
1:A:21:LEU:HD22	1:A:57:LYS:HD2	0.77	1.57	5	5
1:A:6:VAL:HG11	1:A:20:GLU:HB2	0.77	1.57	10	6
1:A:79:LEU:HD22	1:A:82:ILE:HD12	0.76	1.55	5	4
1:A:34:SER:HB2	1:A:79:LEU:HD23	0.76	1.57	18	6
1:A:28:PHE:CE1	1:A:81:ILE:HD11	0.75	2.16	1	1
1:A:9:LYS:HD3	1:A:9:LYS:H	0.75	1.42	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:54:PHE:CD2	1:A:63:LEU:HD12	0.75	2.16	1	4
1:A:63:LEU:HD13	1:A:78:GLU:OE1	0.74	1.82	11	1
1:A:28:PHE:HD1	1:A:28:PHE:C	0.74	1.91	14	1
1:A:28:PHE:C	1:A:28:PHE:CD1	0.73	2.66	14	11
1:A:40:PRO:HD3	1:A:46:ASP:HB2	0.73	1.59	19	9
1:A:81:ILE:HG22	1:A:81:ILE:O	0.73	1.81	14	9
1:A:79:LEU:HD12	1:A:82:ILE:CB	0.73	2.14	12	1
1:A:24:LEU:HD23	1:A:80:HIS:CE1	0.73	2.18	15	6
1:A:62:TYR:HB2	1:A:79:LEU:HD21	0.73	1.59	12	3
1:A:6:VAL:HG13	1:A:19:VAL:HG13	0.72	1.59	19	3
1:A:5:LEU:HD23	1:A:38:PHE:HE1	0.71	1.44	18	1
1:A:61:ALA:HB2	1:A:81:ILE:HA	0.71	1.61	10	2
1:A:81:ILE:O	1:A:81:ILE:HG23	0.71	1.86	7	1
1:A:79:LEU:N	1:A:79:LEU:HD23	0.71	2.00	17	1
1:A:79:LEU:H	1:A:79:LEU:HD23	0.71	1.44	12	1
1:A:35:ILE:CD1	1:A:37:TYR:HE1	0.71	1.99	20	1
1:A:8:ALA:CB	1:A:40:PRO:HD2	0.70	2.16	12	1
1:A:35:ILE:C	1:A:35:ILE:HD12	0.70	2.10	4	1
1:A:7:LEU:HD23	1:A:38:PHE:HB3	0.70	1.62	13	4
1:A:54:PHE:CD2	1:A:63:LEU:CD1	0.70	2.74	12	4
1:A:5:LEU:HD12	1:A:5:LEU:C	0.70	2.11	5	7
1:A:78:GLU:C	1:A:79:LEU:HD12	0.70	2.11	10	10
1:A:79:LEU:HD12	1:A:82:ILE:HB	0.70	1.64	12	2
1:A:20:GLU:HG2	1:A:54:PHE:CE1	0.70	2.21	16	6
1:A:35:ILE:HD12	1:A:80:HIS:ND1	0.70	2.02	11	1
1:A:6:VAL:HG23	1:A:35:ILE:CD1	0.69	2.11	17	2
1:A:66:VAL:HG12	1:A:68:VAL:N	0.69	2.01	12	3
1:A:37:TYR:CE1	1:A:39:ALA:HB2	0.69	2.22	5	3
1:A:63:LEU:HD11	1:A:76:LEU:HD13	0.69	1.61	15	1
1:A:35:ILE:HD12	1:A:80:HIS:CE1	0.68	2.22	11	4
1:A:5:LEU:HD23	1:A:36:PHE:HB2	0.68	1.65	3	4
1:A:54:PHE:CE2	1:A:63:LEU:HD12	0.67	2.25	1	3
1:A:79:LEU:HD12	1:A:82:ILE:CG1	0.67	2.20	12	1
1:A:77:TYR:CD2	1:A:79:LEU:HD11	0.67	2.24	13	3
1:A:5:LEU:C	1:A:5:LEU:CD1	0.67	2.68	14	9
1:A:7:LEU:HD23	1:A:38:PHE:HB2	0.66	1.67	1	2
1:A:35:ILE:CD1	1:A:37:TYR:CE1	0.66	2.78	20	1
1:A:54:PHE:HD2	1:A:63:LEU:CD1	0.65	2.05	18	2
1:A:20:GLU:HG2	1:A:54:PHE:HE1	0.65	1.51	16	8
1:A:47:MET:HE1	1:A:73:LYS:HE3	0.65	1.66	16	1
1:A:31:ASP:OD1	1:A:33:ARG:HD2	0.65	1.91	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:GLU:O	1:A:24:LEU:CD1	0.65	2.42	14	3
1:A:79:LEU:HD12	1:A:82:ILE:HD12	0.64	1.69	18	1
1:A:37:TYR:CD2	1:A:76:LEU:HD12	0.64	2.28	2	1
1:A:33:ARG:NH2	1:A:35:ILE:HG22	0.64	2.07	4	1
1:A:79:LEU:HD23	1:A:79:LEU:H	0.64	1.53	17	1
1:A:79:LEU:HD12	1:A:79:LEU:N	0.64	2.08	1	11
1:A:34:SER:HB2	1:A:79:LEU:CD2	0.64	2.22	20	3
1:A:66:VAL:O	1:A:69:SER:HB2	0.63	1.93	20	2
1:A:8:ALA:HB2	1:A:39:ALA:HA	0.62	1.71	7	11
1:A:66:VAL:HG23	1:A:77:TYR:HB2	0.62	1.70	9	1
1:A:4:LYS:O	1:A:35:ILE:HG23	0.62	1.95	11	1
1:A:54:PHE:CD2	1:A:63:LEU:HD13	0.61	2.23	5	2
1:A:35:ILE:HD11	1:A:78:GLU:OE1	0.60	1.96	5	4
1:A:60:THR:HG21	1:A:78:GLU:CG	0.60	2.26	2	1
1:A:73:LYS:O	1:A:73:LYS:HG2	0.60	1.97	10	3
1:A:34:SER:HB3	1:A:79:LEU:HD23	0.60	1.74	14	1
1:A:37:TYR:CE2	1:A:50:ALA:HB2	0.60	2.32	18	4
1:A:35:ILE:HD11	1:A:37:TYR:HE1	0.60	1.57	20	1
1:A:47:MET:HG3	1:A:76:LEU:CD1	0.59	2.22	14	3
1:A:33:ARG:HG2	1:A:34:SER:H	0.59	1.56	8	5
1:A:82:ILE:O	1:A:82:ILE:CD1	0.59	2.49	12	1
1:A:33:ARG:HG2	1:A:34:SER:N	0.59	2.13	12	7
1:A:4:LYS:HA	1:A:33:ARG:HH22	0.59	1.56	4	1
1:A:34:SER:HB2	1:A:79:LEU:HG	0.59	1.73	10	2
1:A:47:MET:C	1:A:47:MET:SD	0.59	2.86	18	1
1:A:33:ARG:HG3	1:A:34:SER:H	0.58	1.58	1	1
1:A:79:LEU:HD23	1:A:79:LEU:N	0.58	2.13	3	2
1:A:77:TYR:CE2	1:A:79:LEU:HD21	0.58	2.33	20	2
1:A:24:LEU:HD23	1:A:80:HIS:CD2	0.58	2.33	7	4
1:A:40:PRO:CD	1:A:46:ASP:HB2	0.58	2.26	19	5
1:A:43:ALA:HB1	1:A:45:LYS:HG3	0.58	1.74	7	1
1:A:54:PHE:CE2	1:A:63:LEU:CD1	0.58	2.86	12	3
1:A:27:GLU:OE2	1:A:33:ARG:HB3	0.58	1.97	17	1
1:A:66:VAL:HG22	1:A:75:PHE:O	0.57	1.99	8	1
1:A:60:THR:HG21	1:A:78:GLU:HG2	0.57	1.76	2	1
1:A:28:PHE:CE2	1:A:81:ILE:HD11	0.57	2.34	5	4
1:A:33:ARG:NE	1:A:33:ARG:HA	0.57	2.15	20	1
1:A:62:TYR:HD2	1:A:79:LEU:HD13	0.57	1.59	4	1
1:A:21:LEU:HD22	1:A:57:LYS:CE	0.56	2.21	9	1
1:A:78:GLU:C	1:A:78:GLU:OE1	0.56	2.48	1	2
1:A:4:LYS:C	1:A:5:LEU:HD12	0.56	2.25	18	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:44:HIS:CE1	1:A:73:LYS:HE2	0.56	2.36	7	1
1:A:67:ARG:HA	1:A:69:SER:H	0.55	1.60	7	2
1:A:28:PHE:HD1	1:A:28:PHE:O	0.55	1.85	14	1
1:A:63:LEU:C	1:A:63:LEU:CD2	0.55	2.76	1	3
1:A:5:LEU:CD2	1:A:36:PHE:HB2	0.54	2.32	7	1
1:A:79:LEU:HD12	1:A:82:ILE:HG13	0.54	1.79	12	1
1:A:7:LEU:HD12	1:A:7:LEU:N	0.54	2.18	6	1
1:A:77:TYR:CE2	1:A:79:LEU:HD11	0.54	2.36	10	3
1:A:54:PHE:HD2	1:A:63:LEU:CD2	0.54	2.06	13	1
1:A:81:ILE:O	1:A:81:ILE:CG2	0.54	2.56	13	7
1:A:35:ILE:HD12	1:A:37:TYR:CE1	0.54	2.38	20	1
1:A:28:PHE:C	1:A:28:PHE:HD1	0.54	2.10	13	1
1:A:37:TYR:CE2	1:A:39:ALA:CB	0.54	2.91	16	2
1:A:47:MET:HE1	1:A:73:LYS:HD2	0.54	1.80	13	1
1:A:67:ARG:NH2	1:A:69:SER:OG	0.54	2.41	19	1
1:A:62:TYR:CE2	1:A:64:ASP:HB2	0.53	2.37	7	3
1:A:63:LEU:HD23	1:A:64:ASP:N	0.53	2.17	1	4
1:A:66:VAL:O	1:A:69:SER:HB3	0.53	2.03	14	4
1:A:33:ARG:HH21	1:A:35:ILE:HG22	0.53	1.64	4	1
1:A:43:ALA:O	1:A:45:LYS:HG3	0.53	2.03	16	1
1:A:28:PHE:CD1	1:A:28:PHE:C	0.53	2.87	8	2
1:A:37:TYR:CZ	1:A:39:ALA:HB2	0.53	2.39	4	4
1:A:79:LEU:CD1	1:A:82:ILE:CD1	0.53	2.80	18	1
1:A:44:HIS:ND1	1:A:73:LYS:HE2	0.52	2.19	10	1
1:A:33:ARG:HA	1:A:33:ARG:HE	0.52	1.63	20	1
1:A:21:LEU:HD21	1:A:53:PHE:HB3	0.52	1.82	2	1
1:A:28:PHE:HE2	1:A:81:ILE:HD11	0.52	1.65	9	1
1:A:67:ARG:HD3	1:A:69:SER:OG	0.52	2.05	6	1
1:A:25:TYR:HD2	1:A:59:HIS:CE1	0.52	2.22	19	1
1:A:57:LYS:HD3	1:A:59:HIS:CE1	0.52	2.40	6	1
1:A:67:ARG:N	1:A:67:ARG:HD3	0.52	2.20	7	1
1:A:24:LEU:CD2	1:A:80:HIS:CD2	0.52	2.93	13	1
1:A:50:ALA:HB1	1:A:54:PHE:CE2	0.51	2.40	15	2
1:A:34:SER:HB3	1:A:82:ILE:HD11	0.51	1.81	2	1
1:A:69:SER:O	1:A:73:LYS:HB2	0.51	2.05	7	1
1:A:38:PHE:CD1	1:A:38:PHE:C	0.51	2.88	7	4
1:A:6:VAL:HG13	1:A:19:VAL:HG23	0.51	1.81	13	1
1:A:35:ILE:CG2	1:A:78:GLU:HB3	0.51	2.36	2	2
1:A:54:PHE:CD2	1:A:63:LEU:CD2	0.51	2.87	13	2
1:A:20:GLU:CG	1:A:54:PHE:HE1	0.51	2.19	15	3
1:A:20:GLU:OE2	1:A:35:ILE:HD11	0.51	2.05	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:34:SER:HB3	1:A:82:ILE:CD1	0.51	2.36	6	1
1:A:6:VAL:CG2	1:A:20:GLU:OE1	0.51	2.57	16	2
1:A:36:PHE:HB3	1:A:38:PHE:CE1	0.51	2.40	2	1
1:A:38:PHE:N	1:A:38:PHE:CD1	0.50	2.78	5	1
1:A:20:GLU:HB2	1:A:37:TYR:HE2	0.50	1.66	7	1
1:A:73:LYS:O	1:A:73:LYS:HG3	0.50	2.06	13	1
1:A:65:GLU:OE2	1:A:67:ARG:CZ	0.50	2.59	9	2
1:A:66:VAL:HG21	1:A:68:VAL:CG2	0.50	2.36	13	1
1:A:74:ASP:N	1:A:74:ASP:OD1	0.50	2.42	7	2
1:A:47:MET:CG	1:A:76:LEU:HD11	0.50	2.27	14	2
1:A:32:LYS:HD3	1:A:81:ILE:HG21	0.50	1.82	5	1
1:A:27:GLU:CB	1:A:33:ARG:HD3	0.50	2.29	14	2
1:A:37:TYR:C	1:A:37:TYR:CD1	0.50	2.89	1	1
1:A:4:LYS:HA	1:A:33:ARG:NH2	0.50	2.21	4	1
1:A:5:LEU:N	1:A:5:LEU:HD12	0.50	2.22	10	1
1:A:31:ASP:CG	1:A:33:ARG:HD2	0.50	2.30	14	1
1:A:31:ASP:OD1	1:A:31:ASP:C	0.50	2.55	14	1
1:A:79:LEU:N	1:A:79:LEU:CD1	0.49	2.75	1	7
1:A:35:ILE:C	1:A:35:ILE:CD1	0.49	2.81	4	1
1:A:36:PHE:HB3	1:A:75:PHE:CE1	0.49	2.42	14	2
1:A:81:ILE:O	1:A:82:ILE:CG2	0.49	2.53	12	1
1:A:82:ILE:CG2	1:A:82:ILE:O	0.49	2.60	6	1
1:A:9:LYS:H	1:A:9:LYS:CD	0.49	2.16	1	1
1:A:66:VAL:O	1:A:69:SER:CB	0.49	2.60	14	1
1:A:5:LEU:HD12	1:A:5:LEU:N	0.48	2.23	17	3
1:A:37:TYR:O	1:A:75:PHE:HA	0.48	2.09	20	2
1:A:79:LEU:N	1:A:79:LEU:CD2	0.48	2.73	17	2
1:A:24:LEU:HB3	1:A:59:HIS:HB2	0.48	1.86	19	2
1:A:66:VAL:HG21	1:A:68:VAL:HG22	0.48	1.85	13	2
1:A:37:TYR:HB3	1:A:76:LEU:HB2	0.48	1.85	13	4
1:A:24:LEU:HD21	1:A:78:GLU:OE2	0.48	2.08	17	2
1:A:28:PHE:CD2	1:A:81:ILE:HD11	0.48	2.44	19	1
1:A:63:LEU:HD21	1:A:76:LEU:HD22	0.48	1.85	15	1
1:A:6:VAL:HG13	1:A:19:VAL:CG2	0.48	2.39	13	1
1:A:27:GLU:OE2	1:A:33:ARG:HD2	0.47	2.09	2	1
1:A:61:ALA:HB3	1:A:82:ILE:HG22	0.47	1.80	5	2
1:A:82:ILE:O	1:A:82:ILE:HG22	0.47	2.09	6	2
1:A:37:TYR:HE2	1:A:50:ALA:HB2	0.47	1.69	5	2
1:A:5:LEU:HB3	1:A:36:PHE:CZ	0.47	2.44	9	1
1:A:6:VAL:HG11	1:A:20:GLU:CB	0.47	2.33	14	1
1:A:54:PHE:CZ	1:A:78:GLU:OE1	0.47	2.68	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:37:TYR:CZ	1:A:50:ALA:HB2	0.47	2.44	2	1
1:A:79:LEU:CD2	1:A:82:ILE:HD13	0.47	2.32	9	1
1:A:9:LYS:HD3	1:A:9:LYS:N	0.47	2.20	1	1
1:A:69:SER:O	1:A:73:LYS:HG3	0.47	2.10	1	1
1:A:35:ILE:HD12	1:A:35:ILE:O	0.47	2.10	4	1
1:A:38:PHE:C	1:A:38:PHE:CD1	0.47	2.91	8	1
1:A:31:ASP:OD1	1:A:33:ARG:CD	0.47	2.62	14	1
1:A:34:SER:HB3	1:A:79:LEU:CD2	0.47	2.39	14	1
1:A:9:LYS:HD2	1:A:9:LYS:C	0.47	2.34	9	1
1:A:27:GLU:OE2	1:A:35:ILE:HD11	0.46	2.10	16	1
1:A:38:PHE:O	1:A:38:PHE:HD1	0.46	1.94	7	1
1:A:38:PHE:CD2	1:A:75:PHE:CE1	0.46	3.04	5	1
1:A:10:ASN:HB2	1:A:40:PRO:HG2	0.46	1.87	2	1
1:A:6:VAL:HB	1:A:37:TYR:CD2	0.46	2.46	9	1
1:A:11:THR:HG23	1:A:40:PRO:HB3	0.46	1.88	16	1
1:A:20:GLU:HB3	1:A:37:TYR:CE2	0.46	2.46	20	1
1:A:41:THR:O	1:A:44:HIS:CE1	0.45	2.69	1	1
1:A:28:PHE:CD1	1:A:28:PHE:O	0.45	2.67	14	1
1:A:60:THR:HG22	1:A:62:TYR:N	0.45	2.27	2	1
1:A:38:PHE:CD1	1:A:38:PHE:O	0.45	2.70	7	1
1:A:44:HIS:CE1	1:A:73:LYS:HD3	0.45	2.47	15	2
1:A:62:TYR:O	1:A:79:LEU:HD23	0.45	2.12	12	1
1:A:77:TYR:CZ	1:A:79:LEU:HD21	0.45	2.46	20	1
1:A:38:PHE:HB2	1:A:75:PHE:CE1	0.45	2.47	4	1
1:A:35:ILE:CG1	1:A:78:GLU:HB3	0.45	2.42	14	1
1:A:63:LEU:H	1:A:63:LEU:HD23	0.45	1.72	5	1
1:A:31:ASP:HB3	1:A:33:ARG:HD2	0.45	1.88	7	1
1:A:20:GLU:OE1	1:A:20:GLU:HA	0.44	2.12	4	1
1:A:37:TYR:CD1	1:A:39:ALA:HB2	0.44	2.47	19	1
1:A:9:LYS:HE2	1:A:46:ASP:OD1	0.44	2.13	4	1
1:A:6:VAL:HG21	1:A:37:TYR:CE2	0.44	2.48	9	1
1:A:5:LEU:HA	1:A:36:PHE:O	0.44	2.12	12	1
1:A:25:TYR:CE2	1:A:59:HIS:CE1	0.44	3.06	18	1
1:A:34:SER:CB	1:A:79:LEU:HG	0.44	2.43	10	1
1:A:20:GLU:O	1:A:24:LEU:HG	0.44	2.13	8	2
1:A:37:TYR:CE2	1:A:39:ALA:HB2	0.44	2.47	12	3
1:A:28:PHE:CE2	1:A:81:ILE:HD12	0.44	2.48	15	2
1:A:27:GLU:CD	1:A:35:ILE:HD11	0.44	2.37	16	1
1:A:66:VAL:CG1	1:A:68:VAL:H	0.44	2.15	12	1
1:A:63:LEU:HD12	1:A:77:TYR:O	0.44	2.13	14	1
1:A:60:THR:HG23	1:A:79:LEU:O	0.44	2.13	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:7:LEU:N	1:A:7:LEU:CD1	0.44	2.81	6	1
1:A:63:LEU:HD23	1:A:63:LEU:N	0.43	2.27	5	1
1:A:19:VAL:HG12	1:A:23:ASP:OD2	0.43	2.12	7	1
1:A:66:VAL:HG23	1:A:69:SER:N	0.43	2.18	8	1
1:A:66:VAL:HG11	1:A:68:VAL:HG22	0.43	1.90	12	1
1:A:82:ILE:O	1:A:82:ILE:CG2	0.43	2.66	13	1
1:A:36:PHE:HB3	1:A:75:PHE:CD2	0.43	2.49	19	1
1:A:34:SER:CB	1:A:79:LEU:CD2	0.43	2.89	14	2
1:A:6:VAL:CG2	1:A:35:ILE:CD1	0.43	2.88	2	1
1:A:35:ILE:HG22	1:A:78:GLU:HB3	0.43	1.88	2	1
1:A:20:GLU:HG2	1:A:21:LEU:N	0.43	2.27	1	1
1:A:35:ILE:HD11	1:A:78:GLU:HB3	0.43	1.91	4	1
1:A:24:LEU:CD2	1:A:80:HIS:HD2	0.43	2.26	13	1
1:A:22:GLU:CG	1:A:26:HIS:CE1	0.43	3.02	20	1
1:A:78:GLU:OE1	1:A:78:GLU:C	0.43	2.62	17	1
1:A:4:LYS:HB3	1:A:35:ILE:HG22	0.43	1.90	20	1
1:A:26:HIS:CE1	1:A:30:GLU:OE1	0.43	2.72	3	1
1:A:4:LYS:HG2	1:A:33:ARG:HH21	0.43	1.73	14	1
1:A:38:PHE:C	1:A:38:PHE:HD1	0.43	2.21	13	1
1:A:35:ILE:HD11	1:A:37:TYR:CE1	0.43	2.42	20	1
1:A:24:LEU:HD23	1:A:80:HIS:HD2	0.42	1.73	13	1
1:A:28:PHE:CG	1:A:81:ILE:HD11	0.42	2.48	19	1
1:A:47:MET:HG2	1:A:76:LEU:HD11	0.42	1.90	18	1
1:A:23:ASP:OD1	1:A:27:GLU:HB2	0.42	2.15	6	1
1:A:37:TYR:CE1	1:A:78:GLU:OE1	0.42	2.72	20	1
1:A:28:PHE:HD1	1:A:81:ILE:CD1	0.42	2.28	6	1
1:A:60:THR:HA	1:A:80:HIS:HA	0.42	1.92	7	2
1:A:61:ALA:N	1:A:79:LEU:O	0.42	2.53	19	1
1:A:36:PHE:HB3	1:A:75:PHE:HD2	0.42	1.75	19	1
1:A:36:PHE:HB3	1:A:75:PHE:HE1	0.42	1.74	14	1
1:A:37:TYR:CE2	1:A:39:ALA:HB3	0.42	2.49	16	1
1:A:66:VAL:CG2	1:A:68:VAL:HG22	0.42	2.45	2	1
1:A:38:PHE:CD2	1:A:38:PHE:O	0.42	2.73	12	1
1:A:78:GLU:OE2	1:A:80:HIS:CE1	0.42	2.73	18	1
1:A:23:ASP:O	1:A:24:LEU:C	0.42	2.62	11	2
1:A:75:PHE:C	1:A:75:PHE:CD1	0.41	2.98	14	1
1:A:27:GLU:CD	1:A:33:ARG:HD2	0.41	2.40	16	1
1:A:52:ASP:O	1:A:56:GLU:HG3	0.41	2.15	14	1
1:A:80:HIS:O	1:A:81:ILE:HB	0.41	2.16	4	1
1:A:4:LYS:HE3	1:A:33:ARG:HD2	0.41	1.91	1	1
1:A:38:PHE:O	1:A:38:PHE:CD2	0.41	2.74	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:4:LYS:HE2	1:A:33:ARG:HG3	0.41	1.91	2	1
1:A:28:PHE:HE2	1:A:81:ILE:HG13	0.41	1.76	10	1
1:A:27:GLU:O	1:A:31:ASP:O	0.41	2.39	14	1
1:A:20:GLU:C	1:A:24:LEU:HD13	0.41	2.40	1	1
1:A:60:THR:HB	1:A:78:GLU:OE2	0.41	2.15	3	1
1:A:44:HIS:CE1	1:A:73:LYS:HG2	0.41	2.50	6	1
1:A:64:ASP:OD1	1:A:65:GLU:N	0.41	2.53	7	1
1:A:78:GLU:OE1	1:A:80:HIS:CE1	0.41	2.73	7	1
1:A:32:LYS:HG2	1:A:81:ILE:CG2	0.41	2.46	18	1
1:A:37:TYR:CD1	1:A:37:TYR:C	0.41	2.99	19	1
1:A:61:ALA:HB1	1:A:62:TYR:CD1	0.41	2.51	20	1
1:A:36:PHE:CZ	1:A:77:TYR:CD1	0.41	3.09	4	1
1:A:24:LEU:HG	1:A:80:HIS:NE2	0.41	2.31	14	1
1:A:24:LEU:CD2	1:A:59:HIS:HB2	0.40	2.45	13	1
1:A:66:VAL:O	1:A:69:SER:N	0.40	2.54	14	1
1:A:38:PHE:HD1	1:A:75:PHE:CE1	0.40	2.34	12	1
1:A:21:LEU:HB3	1:A:57:LYS:HZ2	0.40	1.76	8	1
1:A:38:PHE:HD2	1:A:75:PHE:CZ	0.40	2.35	11	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	72/82 (88%)	69±1 (96±2%)	2±1 (3±2%)	1±1 (1±1%)	18	68
All	All	1440/1640 (88%)	1385 (96%)	43 (3%)	12 (1%)	18	68

All 3 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	81	ILE	10
1	A	60	THR	1
1	A	73	LYS	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	67/75 (89%)	66±1 (98±1%)	1±1 (2±1%)	49	91
All	All	1340/1500 (89%)	1314 (98%)	26 (2%)	49	91

All 11 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	5	LEU	6
1	A	28	PHE	6
1	A	79	LEU	3
1	A	38	PHE	3
1	A	78	GLU	2
1	A	35	ILE	1
1	A	9	LYS	1
1	A	82	ILE	1
1	A	24	LEU	1
1	A	63	LEU	1
1	A	74	ASP	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry

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 [i](#)

The completeness of assignment taking into account all chemical shift lists is 75% for the well-defined parts and 74% 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 [i](#)

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

Total number of shifts	868
Number of shifts mapped to atoms	868
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	82	-0.27 ± 0.16	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	81	0.28 ± 0.20	None needed (< 0.5 ppm)
$^{13}\text{C}'$	81	-0.10 ± 0.20	None needed (< 0.5 ppm)
^{15}N	80	0.62 ± 0.39	None needed (imprecise)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 75%, i.e. 775 atoms were assigned a chemical shift out of a possible 1036. 0 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	358/364 (98%)	142/146 (97%)	145/146 (99%)	71/72 (99%)
Sidechain	379/548 (69%)	253/354 (71%)	126/178 (71%)	0/16 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	38/124 (31%)	19/62 (31%)	19/58 (33%)	0/4 (0%)
Overall	775/1036 (75%)	414/562 (74%)	290/382 (76%)	71/92 (77%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 74%, i.e. 861 atoms were assigned a chemical shift out of a possible 1159. 0 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	402/409 (98%)	159/164 (97%)	163/164 (99%)	80/81 (99%)
Sidechain	421/619 (68%)	281/399 (70%)	140/199 (70%)	0/21 (0%)
Aromatic	38/131 (29%)	19/66 (29%)	19/60 (32%)	0/5 (0%)
Overall	861/1159 (74%)	459/629 (73%)	322/423 (76%)	80/107 (75%)

7.1.4 Statistically unusual chemical shifts ⓘ

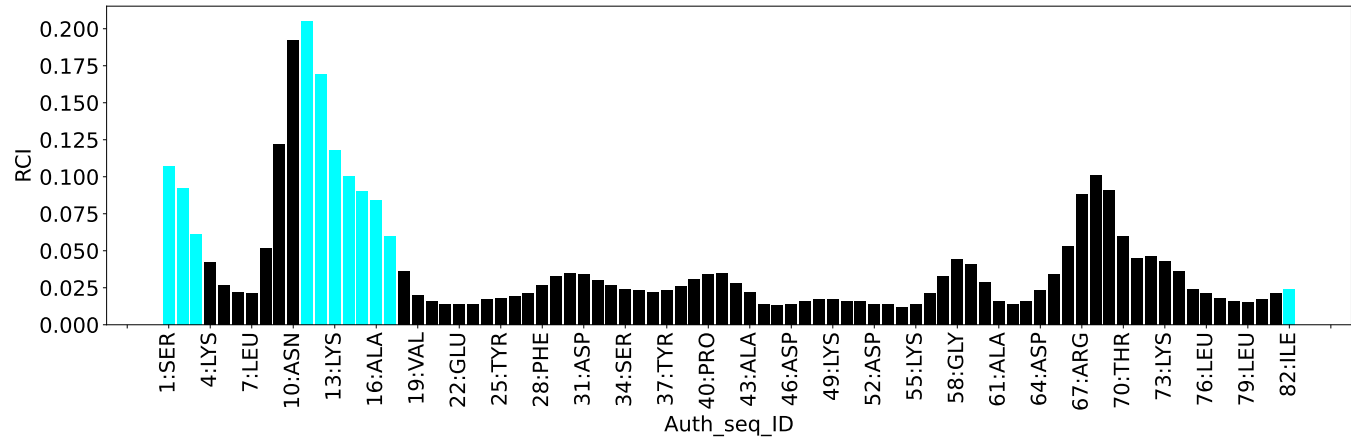
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	1	SER	HB2	1.86	2.61 – 5.13	-8.0
1	A	1	SER	HB3	1.86	2.49 – 5.20	-7.3

7.1.5 Random Coil Index (RCI) plots ⓘ

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	933
Intra-residue ($ i-j =0$)	0
Sequential ($ i-j =1$)	450
Medium range ($ i-j >1$ and $ i-j <5$)	192
Long range ($ i-j \geq 5$)	290
Inter-chain	0
Hydrogen bond restraints	1
Disulfide bond restraints	0
Total dihedral-angle restraints	98
Number of unmapped restraints	0
Number of restraints per residue	12.6
Number of long range restraints per residue ¹	3.5

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	32.2	0.2
0.2-0.5 (Medium)	49.8	0.5
>0.5 (Large)	95.7	7.5

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)	9.2	9.94
10.0-20.0 (Medium)	2.8	19.34
>20.0 (Large)	1.4	129.18

9 Distance violation analysis ⓘ

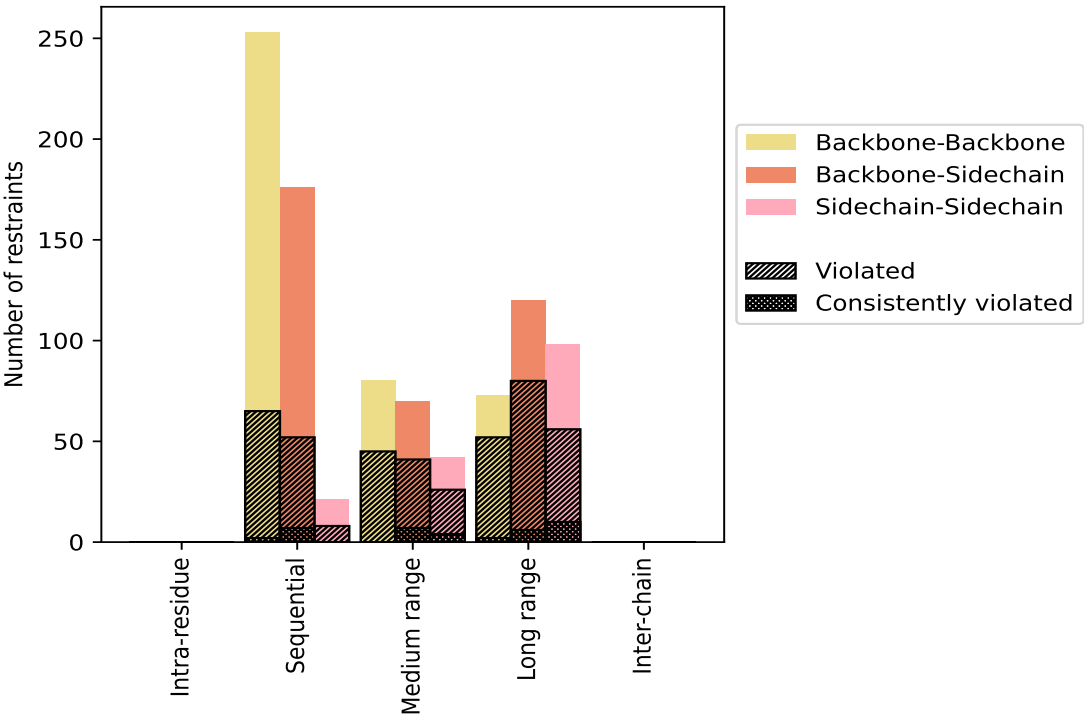
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($ i-j =0$)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sequential ($ i-j =1$)	450	48.2	125	27.8	13.4	9	2.0	1.0
Backbone-Backbone	253	27.1	65	25.7	7.0	2	0.8	0.2
Backbone-Sidechain	176	18.9	52	29.5	5.6	7	4.0	0.8
Sidechain-Sidechain	21	2.3	8	38.1	0.9	0	0.0	0.0
Medium range ($ i-j >1$ & $ i-j <5$)	192	20.6	112	58.3	12.0	11	5.7	1.2
Backbone-Backbone	80	8.6	45	56.2	4.8	0	0.0	0.0
Backbone-Sidechain	70	7.5	41	58.6	4.4	7	10.0	0.8
Sidechain-Sidechain	42	4.5	26	61.9	2.8	4	9.5	0.4
Long range ($ i-j \geq 5$)	290	31.1	187	64.5	20.0	18	6.2	1.9
Backbone-Backbone	73	7.8	52	71.2	5.6	2	2.7	0.2
Backbone-Sidechain	119	12.8	79	66.4	8.5	6	5.0	0.6
Sidechain-Sidechain	98	10.5	56	57.1	6.0	10	10.2	1.1
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	1	0.1	1	100.0	0.1	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	933	100.0	425	45.6	45.6	38	4.1	4.1
Backbone-Backbone	406	43.5	162	39.9	17.4	4	1.0	0.4
Backbone-Sidechain	366	39.2	173	47.3	18.5	20	5.5	2.1
Sidechain-Sidechain	161	17.3	90	55.9	9.6	14	8.7	1.5

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

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



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

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	0	46	51	86	0	183	0.78	5.35	0.8	0.46
2	0	46	50	93	0	189	0.99	7.15	1.11	0.71
3	0	53	58	84	0	195	1.0	7.37	1.08	0.62
4	0	45	55	87	0	187	0.87	7.05	1.04	0.49
5	0	38	53	71	0	162	0.87	7.5	1.19	0.46
6	0	51	49	74	0	174	0.81	3.39	0.72	0.54
7	0	42	53	73	0	168	0.96	6.94	1.08	0.57
8	0	37	47	80	0	164	0.93	6.7	1.02	0.58
9	0	43	46	96	0	185	0.89	4.2	0.78	0.63
10	0	52	56	86	0	194	0.88	7.12	1.04	0.53

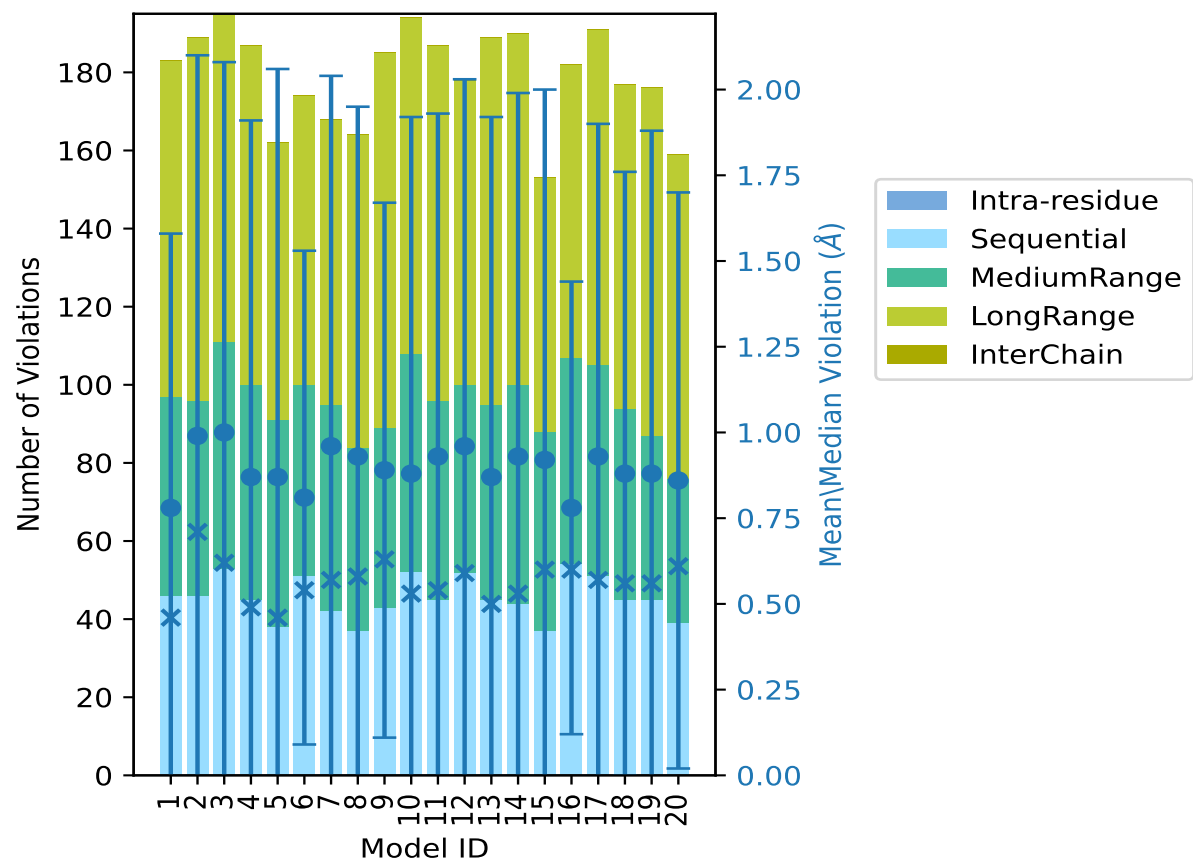
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	0	45	51	91	0	187	0.93	6.51	1.0	0.54
12	0	52	48	78	0	178	0.96	6.6	1.07	0.59
13	0	45	50	94	0	189	0.87	7.13	1.05	0.5
14	0	44	56	90	0	190	0.93	7.26	1.06	0.53
15	0	37	51	65	0	153	0.92	6.96	1.08	0.6
16	0	54	53	75	0	182	0.78	3.64	0.66	0.6
17	0	51	54	86	0	191	0.93	6.53	0.97	0.57
18	0	45	49	83	0	177	0.88	5.69	0.88	0.56
19	0	45	42	89	0	176	0.88	6.52	1.0	0.56
20	0	39	37	83	0	159	0.86	4.68	0.84	0.61

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

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



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

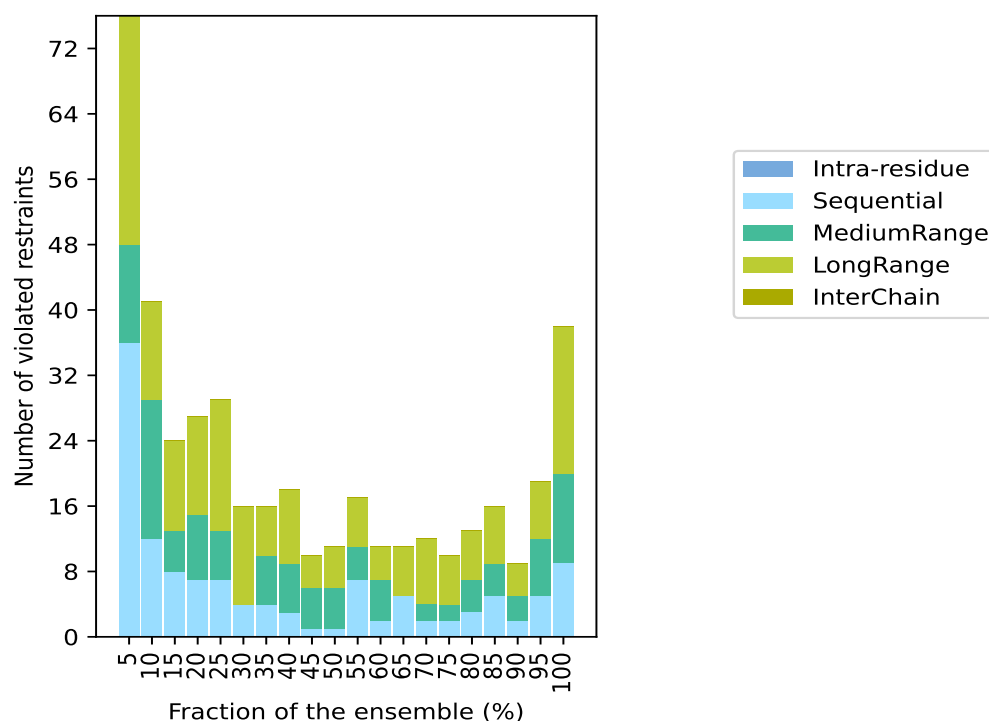
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 508(IR:0, SQ:325, MR:80, LR:103, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	36	12	28	0	76	1	5.0
0	12	17	12	0	41	2	10.0
0	8	5	11	0	24	3	15.0
0	7	8	12	0	27	4	20.0
0	7	6	16	0	29	5	25.0
0	4	0	12	0	16	6	30.0
0	4	6	6	0	16	7	35.0
0	3	6	9	0	18	8	40.0
0	1	5	4	0	10	9	45.0
0	1	5	5	0	11	10	50.0
0	7	4	6	0	17	11	55.0
0	2	5	4	0	11	12	60.0
0	5	0	6	0	11	13	65.0
0	2	2	8	0	12	14	70.0
0	2	2	6	0	10	15	75.0
0	3	4	6	0	13	16	80.0
0	5	4	7	0	16	17	85.0
0	2	3	4	0	9	18	90.0
0	5	7	7	0	19	19	95.0
0	9	11	18	0	38	20	100.0

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

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

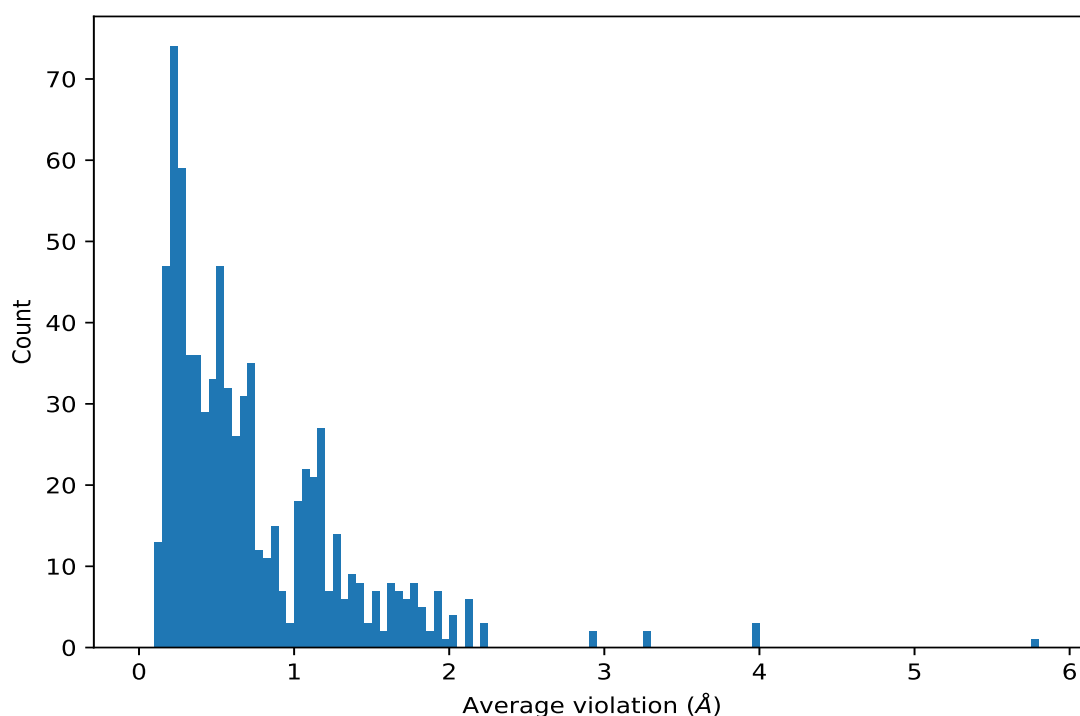
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,244)	1:21:A:LEU:HG	1:59:A:HIS:HE1	20	5.79	1.44	6.4
(1,250)	1:21:A:LEU:HD21	1:59:A:HIS:HE1	20	3.96	1.26	4.48
(1,250)	1:21:A:LEU:HD22	1:59:A:HIS:HE1	20	3.96	1.26	4.48
(1,250)	1:21:A:LEU:HD23	1:59:A:HIS:HE1	20	3.96	1.26	4.48
(1,888)	1:76:A:LEU:HG	1:78:A:GLU:HG2	20	3.28	0.49	3.14
(1,888)	1:76:A:LEU:HG	1:78:A:GLU:HG3	20	3.28	0.49	3.14
(1,879)	1:75:A:PHE:HD1	1:77:A:TYR:HD2	20	2.9	0.95	3.28
(1,879)	1:75:A:PHE:HD2	1:77:A:TYR:HD2	20	2.9	0.95	3.28
(1,663)	1:54:A:PHE:HD1	1:76:A:LEU:HG	20	2.01	0.57	1.88
(1,663)	1:54:A:PHE:HD2	1:76:A:LEU:HG	20	2.01	0.57	1.88
(1,524)	1:41:A:THR:HB	1:73:A:LYS:HA	20	1.99	0.48	1.97
(1,242)	1:21:A:LEU:HG	1:57:A:LYS:HD2	20	1.81	0.62	1.62
(1,242)	1:21:A:LEU:HG	1:57:A:LYS:HD3	20	1.81	0.62	1.62
(1,387)	1:30:A:GLU:HG2	1:31:A:ASP:H	20	1.79	0.21	1.86
(1,387)	1:30:A:GLU:HG3	1:31:A:ASP:H	20	1.79	0.21	1.86
(1,239)	1:21:A:LEU:HG	1:56:A:GLU:HB2	20	1.69	0.41	1.69

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,239)	1:21:A:LEU:HG	1:56:A:GLU:HB3	20	1.69	0.41	1.69
(1,746)	1:63:A:LEU:HA	1:76:A:LEU:HD11	20	1.67	0.36	1.58
(1,746)	1:63:A:LEU:HA	1:76:A:LEU:HD12	20	1.67	0.36	1.58
(1,746)	1:63:A:LEU:HA	1:76:A:LEU:HD13	20	1.67	0.36	1.58
(1,687)	1:56:A:GLU:HA	1:57:A:LYS:HE2	20	1.66	0.22	1.64
(1,687)	1:56:A:GLU:HA	1:57:A:LYS:HE3	20	1.66	0.22	1.64
(1,884)	1:76:A:LEU:HA	1:77:A:TYR:HD1	20	1.62	0.15	1.64
(1,884)	1:76:A:LEU:HA	1:77:A:TYR:HD2	20	1.62	0.15	1.64
(1,878)	1:75:A:PHE:HB2	1:77:A:TYR:HD1	20	1.54	0.68	1.38
(1,878)	1:75:A:PHE:HB2	1:77:A:TYR:HD2	20	1.54	0.68	1.38
(1,878)	1:75:A:PHE:HB3	1:77:A:TYR:HD1	20	1.54	0.68	1.38
(1,878)	1:75:A:PHE:HB3	1:77:A:TYR:HD2	20	1.54	0.68	1.38
(1,538)	1:43:A:ALA:HA	1:45:A:LYS:HD2	20	1.5	0.44	1.67
(1,538)	1:43:A:ALA:HA	1:45:A:LYS:HD3	20	1.5	0.44	1.67
(1,304)	1:24:A:LEU:HD21	1:59:A:HIS:HE1	20	1.48	0.7	1.78
(1,304)	1:24:A:LEU:HD22	1:59:A:HIS:HE1	20	1.48	0.7	1.78
(1,304)	1:24:A:LEU:HD23	1:59:A:HIS:HE1	20	1.48	0.7	1.78
(1,288)	1:24:A:LEU:HA	1:80:A:HIS:HE1	20	1.39	0.9	1.0
(1,525)	1:41:A:THR:HB	1:73:A:LYS:HB2	20	1.36	0.5	1.4
(1,525)	1:41:A:THR:HB	1:73:A:LYS:HB3	20	1.36	0.5	1.4
(1,804)	1:67:A:ARG:H	1:68:A:VAL:HB	20	1.3	0.36	1.46
(1,542)	1:44:A:HIS:HA	1:45:A:LYS:HD2	20	1.22	0.22	1.25
(1,542)	1:44:A:HIS:HA	1:45:A:LYS:HD3	20	1.22	0.22	1.25
(1,690)	1:56:A:GLU:CD	1:52:A:ASP:CG	20	1.22	0.2	1.23
(1,240)	1:21:A:LEU:HG	1:57:A:LYS:HB2	20	1.14	0.45	1.12
(1,240)	1:21:A:LEU:HG	1:57:A:LYS:HB3	20	1.14	0.45	1.12
(1,781)	1:65:A:GLU:HA	1:77:A:TYR:HD1	20	1.1	0.21	1.16
(1,781)	1:65:A:GLU:HA	1:77:A:TYR:HD2	20	1.1	0.21	1.16
(1,501)	1:38:A:PHE:HD1	1:75:A:PHE:H	20	1.06	0.47	1.06
(1,501)	1:38:A:PHE:HD2	1:75:A:PHE:H	20	1.06	0.47	1.06
(1,892)	1:76:A:LEU:HD11	1:78:A:GLU:HA	20	1.02	0.39	0.88
(1,892)	1:76:A:LEU:HD12	1:78:A:GLU:HA	20	1.02	0.39	0.88
(1,892)	1:76:A:LEU:HD13	1:78:A:GLU:HA	20	1.02	0.39	0.88
(1,789)	1:66:A:VAL:H	1:68:A:VAL:HG11	20	1.01	0.23	0.96
(1,789)	1:66:A:VAL:H	1:68:A:VAL:HG12	20	1.01	0.23	0.96
(1,789)	1:66:A:VAL:H	1:68:A:VAL:HG13	20	1.01	0.23	0.96
(1,794)	1:66:A:VAL:HA	1:77:A:TYR:H	20	0.95	0.31	0.88
(1,891)	1:76:A:LEU:HD11	1:77:A:TYR:H	20	0.83	0.13	0.86
(1,891)	1:76:A:LEU:HD12	1:77:A:TYR:H	20	0.83	0.13	0.86
(1,891)	1:76:A:LEU:HD13	1:77:A:TYR:H	20	0.83	0.13	0.86
(1,458)	1:36:A:PHE:HA	1:76:A:LEU:HD11	20	0.82	0.21	0.85
(1,458)	1:36:A:PHE:HA	1:76:A:LEU:HD12	20	0.82	0.21	0.85

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,458)	1:36:A:PHE:HA	1:76:A:LEU:HD13	20	0.82	0.21	0.85
(1,348)	1:28:A:PHE:H	1:30:A:GLU:HG2	20	0.71	0.63	0.48
(1,348)	1:28:A:PHE:H	1:30:A:GLU:HG3	20	0.71	0.63	0.48
(1,890)	1:76:A:LEU:HD11	1:78:A:GLU:H	20	0.69	0.41	0.68
(1,890)	1:76:A:LEU:HD12	1:78:A:GLU:H	20	0.69	0.41	0.68
(1,890)	1:76:A:LEU:HD13	1:78:A:GLU:H	20	0.69	0.41	0.68
(1,704)	1:59:A:HIS:H	1:60:A:THR:H	20	0.66	0.19	0.66
(1,795)	1:66:A:VAL:HA	1:77:A:TYR:HA	20	0.63	0.13	0.66
(1,248)	1:21:A:LEU:HD21	1:22:A:GLU:HA	20	0.41	0.1	0.4
(1,248)	1:21:A:LEU:HD22	1:22:A:GLU:HA	20	0.41	0.1	0.4
(1,248)	1:21:A:LEU:HD23	1:22:A:GLU:HA	20	0.41	0.1	0.4
(1,584)	1:48:A:LEU:HA	1:52:A:ASP:HB2	20	0.39	0.1	0.42
(1,584)	1:48:A:LEU:HA	1:52:A:ASP:HB3	20	0.39	0.1	0.42
(1,841)	1:71:A:ASP:H	1:72:A:GLU:HA	20	0.24	0.07	0.22
(1,476)	1:37:A:TYR:H	1:78:A:GLU:HG2	19	1.35	0.35	1.26
(1,476)	1:37:A:TYR:H	1:78:A:GLU:HG3	19	1.35	0.35	1.26
(1,471)	1:36:A:PHE:HD1	1:78:A:GLU:H	19	1.29	0.36	1.29
(1,471)	1:36:A:PHE:HD2	1:78:A:GLU:H	19	1.29	0.36	1.29
(1,27)	1:5:A:LEU:HG	1:7:A:LEU:H	19	1.29	0.83	1.01
(1,898)	1:77:A:TYR:HB2	1:79:A:LEU:HG	19	1.28	0.82	1.12
(1,898)	1:77:A:TYR:HB3	1:79:A:LEU:HG	19	1.28	0.82	1.12
(1,495)	1:38:A:PHE:HA	1:75:A:PHE:HD1	19	1.19	0.46	1.07
(1,495)	1:38:A:PHE:HA	1:75:A:PHE:HD2	19	1.19	0.46	1.07
(1,123)	1:7:A:LEU:HB2	1:38:A:PHE:HD1	19	1.08	0.89	0.68
(1,123)	1:7:A:LEU:HB2	1:38:A:PHE:HD2	19	1.08	0.89	0.68
(1,123)	1:7:A:LEU:HB3	1:38:A:PHE:HD1	19	1.08	0.89	0.68
(1,123)	1:7:A:LEU:HB3	1:38:A:PHE:HD2	19	1.08	0.89	0.68
(1,893)	1:76:A:LEU:HD11	1:78:A:GLU:HG2	19	1.07	0.52	0.86
(1,893)	1:76:A:LEU:HD11	1:78:A:GLU:HG3	19	1.07	0.52	0.86
(1,893)	1:76:A:LEU:HD12	1:78:A:GLU:HG2	19	1.07	0.52	0.86
(1,893)	1:76:A:LEU:HD12	1:78:A:GLU:HG3	19	1.07	0.52	0.86
(1,893)	1:76:A:LEU:HD13	1:78:A:GLU:HG2	19	1.07	0.52	0.86
(1,893)	1:76:A:LEU:HD13	1:78:A:GLU:HG3	19	1.07	0.52	0.86
(1,128)	1:7:A:LEU:HG	1:38:A:PHE:HD1	19	0.8	0.27	0.79
(1,128)	1:7:A:LEU:HG	1:38:A:PHE:HD2	19	0.8	0.27	0.79
(1,741)	1:62:A:TYR:HD1	1:63:A:LEU:H	19	0.76	0.34	0.91
(1,741)	1:62:A:TYR:HD2	1:63:A:LEU:H	19	0.76	0.34	0.91
(1,736)	1:62:A:TYR:HA	1:63:A:LEU:HD21	19	0.71	0.12	0.72
(1,736)	1:62:A:TYR:HA	1:63:A:LEU:HD22	19	0.71	0.12	0.72
(1,736)	1:62:A:TYR:HA	1:63:A:LEU:HD23	19	0.71	0.12	0.72
(1,432)	1:35:A:ILE:H	1:36:A:PHE:HE1	19	0.64	0.41	0.52
(1,432)	1:35:A:ILE:H	1:36:A:PHE:HE2	19	0.64	0.41	0.52

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,147)	1:9:A:LYS:H	1:11:A:THR:H	19	0.55	0.3	0.45
(1,364)	1:28:A:PHE:HD1	1:32:A:LYS:HA	19	0.54	0.27	0.41
(1,364)	1:28:A:PHE:HD2	1:32:A:LYS:HA	19	0.54	0.27	0.41
(1,842)	1:71:A:ASP:H	1:73:A:LYS:H	19	0.51	0.19	0.52
(1,174)	1:12:A:ARG:HB2	1:14:A:SER:HA	19	0.43	0.27	0.35
(1,174)	1:12:A:ARG:HB3	1:14:A:SER:HA	19	0.43	0.27	0.35
(1,437)	1:35:A:ILE:H	1:80:A:HIS:H	19	0.41	0.13	0.44
(1,144)	1:9:A:LYS:H	1:10:A:ASN:H	19	0.37	0.17	0.33
(1,793)	1:66:A:VAL:HA	1:76:A:LEU:HA	19	0.35	0.13	0.35
(1,840)	1:71:A:ASP:H	1:72:A:GLU:H	19	0.3	0.08	0.32
(1,547)	1:44:A:HIS:HB2	1:48:A:LEU:HD11	18	1.7	0.91	2.28
(1,547)	1:44:A:HIS:HB2	1:48:A:LEU:HD12	18	1.7	0.91	2.28
(1,547)	1:44:A:HIS:HB2	1:48:A:LEU:HD13	18	1.7	0.91	2.28
(1,547)	1:44:A:HIS:HB3	1:48:A:LEU:HD11	18	1.7	0.91	2.28
(1,547)	1:44:A:HIS:HB3	1:48:A:LEU:HD12	18	1.7	0.91	2.28
(1,547)	1:44:A:HIS:HB3	1:48:A:LEU:HD13	18	1.7	0.91	2.28
(1,500)	1:38:A:PHE:HD1	1:39:A:ALA:H	18	1.12	0.33	1.02
(1,500)	1:38:A:PHE:HD2	1:39:A:ALA:H	18	1.12	0.33	1.02
(1,410)	1:33:A:ARG:HA	1:81:A:ILE:HG21	18	1.0	0.43	0.96
(1,410)	1:33:A:ARG:HA	1:81:A:ILE:HG22	18	1.0	0.43	0.96
(1,410)	1:33:A:ARG:HA	1:81:A:ILE:HG23	18	1.0	0.43	0.96
(1,285)	1:24:A:LEU:HA	1:54:A:PHE:HE1	18	0.94	0.49	0.9
(1,285)	1:24:A:LEU:HA	1:54:A:PHE:HE2	18	0.94	0.49	0.9
(1,721)	1:61:A:ALA:H	1:78:A:GLU:HB2	18	0.69	0.22	0.72
(1,721)	1:61:A:ALA:H	1:78:A:GLU:HB3	18	0.69	0.22	0.72
(1,245)	1:21:A:LEU:HD11	1:53:A:PHE:HA	18	0.59	0.33	0.49
(1,245)	1:21:A:LEU:HD12	1:53:A:PHE:HA	18	0.59	0.33	0.49
(1,245)	1:21:A:LEU:HD13	1:53:A:PHE:HA	18	0.59	0.33	0.49
(1,843)	1:71:A:ASP:H	1:73:A:LYS:HA	18	0.56	0.18	0.56
(1,1)	1:3:A:MET:H	1:4:A:LYS:H	18	0.43	0.17	0.45
(1,743)	1:62:A:TYR:HE1	1:63:A:LEU:HD21	17	2.1	1.21	2.61
(1,743)	1:62:A:TYR:HE1	1:63:A:LEU:HD22	17	2.1	1.21	2.61
(1,743)	1:62:A:TYR:HE1	1:63:A:LEU:HD23	17	2.1	1.21	2.61
(1,743)	1:62:A:TYR:HE2	1:63:A:LEU:HD21	17	2.1	1.21	2.61
(1,743)	1:62:A:TYR:HE2	1:63:A:LEU:HD22	17	2.1	1.21	2.61
(1,743)	1:62:A:TYR:HE2	1:63:A:LEU:HD23	17	2.1	1.21	2.61
(1,202)	1:19:A:VAL:H	1:20:A:GLU:HG2	17	2.04	0.89	2.42
(1,202)	1:19:A:VAL:H	1:20:A:GLU:HG3	17	2.04	0.89	2.42
(1,197)	1:18:A:SER:HA	1:20:A:GLU:HG2	17	1.86	0.97	2.17
(1,197)	1:18:A:SER:HA	1:20:A:GLU:HG3	17	1.86	0.97	2.17
(1,241)	1:21:A:LEU:HG	1:57:A:LYS:HG2	17	1.31	0.43	1.28
(1,241)	1:21:A:LEU:HG	1:57:A:LYS:HG3	17	1.31	0.43	1.28

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,295)	1:24:A:LEU:HG	1:25:A:TYR:HA	17	0.64	0.15	0.68
(1,502)	1:38:A:PHE:HD1	1:75:A:PHE:HA	17	0.63	0.25	0.61
(1,502)	1:38:A:PHE:HD2	1:75:A:PHE:HA	17	0.63	0.25	0.61
(1,823)	1:69:A:SER:HA	1:71:A:ASP:H	17	0.49	0.14	0.5
(1,176)	1:13:A:LYS:H	1:14:A:SER:H	17	0.44	0.4	0.29
(1,126)	1:7:A:LEU:HG	1:38:A:PHE:H	17	0.37	0.16	0.35
(1,474)	1:37:A:TYR:H	1:76:A:LEU:H	17	0.35	0.21	0.29
(1,764)	1:64:A:ASP:H	1:79:A:LEU:H	17	0.31	0.1	0.28
(1,157)	1:10:A:ASN:HB2	1:46:A:ASP:H	17	0.28	0.15	0.23
(1,157)	1:10:A:ASN:HB3	1:46:A:ASP:H	17	0.28	0.15	0.23
(1,692)	1:57:A:LYS:H	1:58:A:GLY:HA2	17	0.28	0.12	0.24
(1,620)	1:51:A:VAL:HA	1:53:A:PHE:H	17	0.22	0.07	0.22
(1,351)	1:28:A:PHE:H	1:81:A:ILE:HG21	16	1.8	0.29	1.78
(1,351)	1:28:A:PHE:H	1:81:A:ILE:HG22	16	1.8	0.29	1.78
(1,351)	1:28:A:PHE:H	1:81:A:ILE:HG23	16	1.8	0.29	1.78
(1,714)	1:60:A:THR:HA	1:81:A:ILE:HG21	16	1.44	0.44	1.31
(1,714)	1:60:A:THR:HA	1:81:A:ILE:HG22	16	1.44	0.44	1.31
(1,714)	1:60:A:THR:HA	1:81:A:ILE:HG23	16	1.44	0.44	1.31
(1,390)	1:31:A:ASP:H	1:81:A:ILE:HG21	16	1.3	0.42	1.27
(1,390)	1:31:A:ASP:H	1:81:A:ILE:HG22	16	1.3	0.42	1.27
(1,390)	1:31:A:ASP:H	1:81:A:ILE:HG23	16	1.3	0.42	1.27
(1,411)	1:33:A:ARG:HA	1:82:A:ILE:HA	16	1.04	0.4	0.98
(1,395)	1:31:A:ASP:HA	1:81:A:ILE:HG21	16	0.8	0.54	0.76
(1,395)	1:31:A:ASP:HA	1:81:A:ILE:HG22	16	0.8	0.54	0.76
(1,395)	1:31:A:ASP:HA	1:81:A:ILE:HG23	16	0.8	0.54	0.76
(1,365)	1:28:A:PHE:HD1	1:32:A:LYS:HB2	16	0.65	0.38	0.57
(1,365)	1:28:A:PHE:HD1	1:32:A:LYS:HB3	16	0.65	0.38	0.57
(1,365)	1:28:A:PHE:HD2	1:32:A:LYS:HB2	16	0.65	0.38	0.57
(1,365)	1:28:A:PHE:HD2	1:32:A:LYS:HB3	16	0.65	0.38	0.57
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG21	16	0.4	0.16	0.39
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG22	16	0.4	0.16	0.39
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG23	16	0.4	0.16	0.39
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG21	16	0.4	0.16	0.39
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG22	16	0.4	0.16	0.39
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG23	16	0.4	0.16	0.39
(1,431)	1:35:A:ILE:H	1:36:A:PHE:HD1	16	0.32	0.2	0.24
(1,431)	1:35:A:ILE:H	1:36:A:PHE:HD2	16	0.32	0.2	0.24
(1,523)	1:41:A:THR:HA	1:44:A:HIS:HA	16	0.28	0.11	0.24
(1,145)	1:9:A:LYS:H	1:10:A:ASN:HA	16	0.27	0.1	0.26
(1,142)	1:8:A:ALA:HA	1:46:A:ASP:HA	16	0.26	0.08	0.24
(1,643)	1:53:A:PHE:H	1:55:A:LYS:H	16	0.24	0.08	0.22
(1,354)	1:28:A:PHE:HA	1:30:A:GLU:H	16	0.24	0.11	0.21

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,672)	1:55:A:LYS:H	1:63:A:LEU:HD11	15	1.13	0.15	1.12
(1,672)	1:55:A:LYS:H	1:63:A:LEU:HD12	15	1.13	0.15	1.12
(1,672)	1:55:A:LYS:H	1:63:A:LEU:HD13	15	1.13	0.15	1.12
(1,300)	1:24:A:LEU:HD11	1:35:A:ILE:HG12	15	0.74	0.53	0.53
(1,300)	1:24:A:LEU:HD11	1:35:A:ILE:HG13	15	0.74	0.53	0.53
(1,300)	1:24:A:LEU:HD12	1:35:A:ILE:HG12	15	0.74	0.53	0.53
(1,300)	1:24:A:LEU:HD12	1:35:A:ILE:HG13	15	0.74	0.53	0.53
(1,300)	1:24:A:LEU:HD13	1:35:A:ILE:HG12	15	0.74	0.53	0.53
(1,300)	1:24:A:LEU:HD13	1:35:A:ILE:HG13	15	0.74	0.53	0.53
(1,301)	1:24:A:LEU:HD11	1:60:A:THR:HB	15	0.71	0.59	0.5
(1,301)	1:24:A:LEU:HD12	1:60:A:THR:HB	15	0.71	0.59	0.5
(1,301)	1:24:A:LEU:HD13	1:60:A:THR:HB	15	0.71	0.59	0.5
(1,426)	1:34:A:SER:HB2	1:36:A:PHE:HE1	15	0.6	0.42	0.54
(1,426)	1:34:A:SER:HB2	1:36:A:PHE:HE2	15	0.6	0.42	0.54
(1,426)	1:34:A:SER:HB3	1:36:A:PHE:HE1	15	0.6	0.42	0.54
(1,426)	1:34:A:SER:HB3	1:36:A:PHE:HE2	15	0.6	0.42	0.54
(1,284)	1:24:A:LEU:HA	1:35:A:ILE:HD11	15	0.59	0.58	0.31
(1,284)	1:24:A:LEU:HA	1:35:A:ILE:HD12	15	0.59	0.58	0.31
(1,284)	1:24:A:LEU:HA	1:35:A:ILE:HD13	15	0.59	0.58	0.31
(1,705)	1:59:A:HIS:H	1:60:A:THR:HA	15	0.51	0.16	0.52
(1,768)	1:64:A:ASP:HA	1:76:A:LEU:HD21	15	0.46	0.29	0.48
(1,768)	1:64:A:ASP:HA	1:76:A:LEU:HD22	15	0.46	0.29	0.48
(1,768)	1:64:A:ASP:HA	1:76:A:LEU:HD23	15	0.46	0.29	0.48
(1,146)	1:9:A:LYS:H	1:10:A:ASN:HB2	15	0.39	0.18	0.33
(1,146)	1:9:A:LYS:H	1:10:A:ASN:HB3	15	0.39	0.18	0.33
(1,207)	1:19:A:VAL:HB	1:22:A:GLU:H	15	0.28	0.12	0.28
(1,418)	1:34:A:SER:H	1:79:A:LEU:HD21	14	1.62	0.5	1.56
(1,418)	1:34:A:SER:H	1:79:A:LEU:HD22	14	1.62	0.5	1.56
(1,418)	1:34:A:SER:H	1:79:A:LEU:HD23	14	1.62	0.5	1.56
(1,8)	1:5:A:LEU:H	1:35:A:ILE:HB	14	1.25	0.99	1.3
(1,798)	1:66:A:VAL:HG11	1:69:A:SER:HA	14	0.87	0.18	0.86
(1,798)	1:66:A:VAL:HG12	1:69:A:SER:HA	14	0.87	0.18	0.86
(1,798)	1:66:A:VAL:HG13	1:69:A:SER:HA	14	0.87	0.18	0.86
(1,798)	1:66:A:VAL:HG21	1:69:A:SER:HA	14	0.87	0.18	0.86
(1,798)	1:66:A:VAL:HG22	1:69:A:SER:HA	14	0.87	0.18	0.86
(1,798)	1:66:A:VAL:HG23	1:69:A:SER:HA	14	0.87	0.18	0.86
(1,312)	1:25:A:TYR:H	1:59:A:HIS:HE1	14	0.75	0.35	0.67
(1,318)	1:25:A:TYR:HA	1:59:A:HIS:HA	14	0.53	0.23	0.46
(1,800)	1:66:A:VAL:HG11	1:72:A:GLU:H	14	0.49	0.26	0.44
(1,800)	1:66:A:VAL:HG12	1:72:A:GLU:H	14	0.49	0.26	0.44
(1,800)	1:66:A:VAL:HG13	1:72:A:GLU:H	14	0.49	0.26	0.44
(1,800)	1:66:A:VAL:HG21	1:72:A:GLU:H	14	0.49	0.26	0.44

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,800)	1:66:A:VAL:HG22	1:72:A:GLU:H	14	0.49	0.26	0.44
(1,800)	1:66:A:VAL:HG23	1:72:A:GLU:H	14	0.49	0.26	0.44
(1,2)	1:3:A:MET:H	1:4:A:LYS:HA	14	0.37	0.17	0.38
(1,63)	1:6:A:VAL:HA	1:20:A:GLU:H	14	0.32	0.1	0.34
(1,4)	1:4:A:LYS:HA	1:5:A:LEU:H	14	0.3	0.17	0.26
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD11	14	0.26	0.12	0.25
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD12	14	0.26	0.12	0.25
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD13	14	0.26	0.12	0.25
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD11	14	0.26	0.12	0.25
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD12	14	0.26	0.12	0.25
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD13	14	0.26	0.12	0.25
(1,543)	1:44:A:HIS:HA	1:48:A:LEU:H	14	0.22	0.07	0.22
(1,298)	1:24:A:LEU:HG	1:80:A:HIS:HE1	13	0.99	0.68	0.75
(1,25)	1:5:A:LEU:HG	1:6:A:VAL:HA	13	0.93	0.46	1.15
(1,526)	1:41:A:THR:HB	1:74:A:ASP:HB2	13	0.75	0.24	0.72
(1,526)	1:41:A:THR:HB	1:74:A:ASP:HB3	13	0.75	0.24	0.72
(1,930)	1:81:A:ILE:HA	1:82:A:ILE:H	13	0.65	0.41	0.37
(1,467)	1:36:A:PHE:HB2	1:77:A:TYR:HD1	13	0.52	0.28	0.67
(1,467)	1:36:A:PHE:HB2	1:77:A:TYR:HD2	13	0.52	0.28	0.67
(1,467)	1:36:A:PHE:HB3	1:77:A:TYR:HD1	13	0.52	0.28	0.67
(1,467)	1:36:A:PHE:HB3	1:77:A:TYR:HD2	13	0.52	0.28	0.67
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG21	13	0.49	0.18	0.48
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG22	13	0.49	0.18	0.48
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG23	13	0.49	0.18	0.48
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG21	13	0.49	0.18	0.48
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG22	13	0.49	0.18	0.48
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG23	13	0.49	0.18	0.48
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG21	13	0.49	0.18	0.48
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG22	13	0.49	0.18	0.48
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG23	13	0.49	0.18	0.48
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG21	13	0.49	0.18	0.48
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG22	13	0.49	0.18	0.48
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG23	13	0.49	0.18	0.48
(1,865)	1:74:A:ASP:H	1:75:A:PHE:H	13	0.41	0.3	0.31
(1,470)	1:36:A:PHE:HD1	1:77:A:TYR:HD1	13	0.4	0.29	0.29
(1,470)	1:36:A:PHE:HD1	1:77:A:TYR:HD2	13	0.4	0.29	0.29
(1,470)	1:36:A:PHE:HD2	1:77:A:TYR:HD1	13	0.4	0.29	0.29
(1,470)	1:36:A:PHE:HD2	1:77:A:TYR:HD2	13	0.4	0.29	0.29
(1,811)	1:68:A:VAL:HA	1:73:A:LYS:H	13	0.29	0.17	0.27
(1,527)	1:42:A:ASN:H	1:43:A:ALA:H	13	0.26	0.1	0.26
(1,183)	1:14:A:SER:HA	1:15:A:ASP:H	13	0.17	0.04	0.18
(1,908)	1:78:A:GLU:HA	1:80:A:HIS:HD2	12	1.91	1.07	2.22

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,28)	1:5:A:LEU:HG	1:7:A:LEU:HG	12	1.54	0.7	1.76
(1,370)	1:28:A:PHE:HE1	1:81:A:ILE:HA	12	1.01	1.14	0.51
(1,370)	1:28:A:PHE:HE2	1:81:A:ILE:HA	12	1.01	1.14	0.51
(1,299)	1:24:A:LEU:HD11	1:35:A:ILE:HG21	12	0.74	0.28	0.68
(1,299)	1:24:A:LEU:HD11	1:35:A:ILE:HG22	12	0.74	0.28	0.68
(1,299)	1:24:A:LEU:HD11	1:35:A:ILE:HG23	12	0.74	0.28	0.68
(1,299)	1:24:A:LEU:HD12	1:35:A:ILE:HG21	12	0.74	0.28	0.68
(1,299)	1:24:A:LEU:HD12	1:35:A:ILE:HG22	12	0.74	0.28	0.68
(1,299)	1:24:A:LEU:HD12	1:35:A:ILE:HG23	12	0.74	0.28	0.68
(1,299)	1:24:A:LEU:HD13	1:35:A:ILE:HG21	12	0.74	0.28	0.68
(1,299)	1:24:A:LEU:HD13	1:35:A:ILE:HG22	12	0.74	0.28	0.68
(1,299)	1:24:A:LEU:HD13	1:35:A:ILE:HG23	12	0.74	0.28	0.68
(1,412)	1:33:A:ARG:HB2	1:34:A:SER:H	12	0.74	0.26	0.76
(1,412)	1:33:A:ARG:HB3	1:34:A:SER:H	12	0.74	0.26	0.76
(1,802)	1:67:A:ARG:H	1:68:A:VAL:H	12	0.39	0.14	0.42
(1,732)	1:62:A:TYR:H	1:81:A:ILE:H	12	0.27	0.12	0.24
(1,342)	1:27:A:GLU:HA	1:29:A:SER:H	12	0.22	0.07	0.23
(1,220)	1:20:A:GLU:HA	1:24:A:LEU:HA	12	0.22	0.1	0.18
(1,214)	1:20:A:GLU:H	1:22:A:GLU:H	12	0.17	0.05	0.17
(1,546)	1:44:A:HIS:HB2	1:48:A:LEU:HG	11	1.9	0.11	1.88
(1,546)	1:44:A:HIS:HB3	1:48:A:LEU:HG	11	1.9	0.11	1.88
(1,568)	1:47:A:MET:HB2	1:48:A:LEU:HG	11	1.4	0.05	1.41
(1,568)	1:47:A:MET:HB3	1:48:A:LEU:HG	11	1.4	0.05	1.41
(1,544)	1:44:A:HIS:HA	1:48:A:LEU:HD11	11	0.86	0.12	0.8
(1,544)	1:44:A:HIS:HA	1:48:A:LEU:HD12	11	0.86	0.12	0.8
(1,544)	1:44:A:HIS:HA	1:48:A:LEU:HD13	11	0.86	0.12	0.8
(1,544)	1:44:A:HIS:HA	1:48:A:LEU:HD11	11	0.86	0.12	0.8
(1,544)	1:44:A:HIS:HA	1:48:A:LEU:HD12	11	0.86	0.12	0.8
(1,544)	1:44:A:HIS:HA	1:48:A:LEU:HD13	11	0.86	0.12	0.8
(1,166)	1:11:A:THR:HB	1:12:A:ARG:H	11	0.75	0.13	0.78
(1,560)	1:47:A:MET:H	1:48:A:LEU:HD11	11	0.72	0.06	0.73
(1,560)	1:47:A:MET:H	1:48:A:LEU:HD12	11	0.72	0.06	0.73
(1,560)	1:47:A:MET:H	1:48:A:LEU:HD13	11	0.72	0.06	0.73
(1,21)	1:5:A:LEU:HB2	1:36:A:PHE:H	11	0.71	0.29	0.72
(1,21)	1:5:A:LEU:HB3	1:36:A:PHE:H	11	0.71	0.29	0.72
(1,61)	1:6:A:VAL:HA	1:19:A:VAL:HB	11	0.62	0.4	0.47
(1,182)	1:14:A:SER:H	1:17:A:LYS:H	11	0.41	0.24	0.44
(1,906)	1:78:A:GLU:HA	1:79:A:LEU:HG	11	0.32	0.16	0.3
(1,791)	1:66:A:VAL:HA	1:68:A:VAL:HG11	11	0.3	0.13	0.28
(1,791)	1:66:A:VAL:HA	1:68:A:VAL:HG12	11	0.3	0.13	0.28
(1,791)	1:66:A:VAL:HA	1:68:A:VAL:HG13	11	0.3	0.13	0.28
(1,127)	1:7:A:LEU:HG	1:38:A:PHE:HB2	11	0.28	0.08	0.3

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,127)	1:7:A:LEU:HG	1:38:A:PHE:HB3	11	0.28	0.08	0.3
(1,505)	1:39:A:ALA:H	1:74:A:ASP:H	11	0.23	0.06	0.23
(1,9)	1:5:A:LEU:H	1:36:A:PHE:H	11	0.18	0.04	0.18
(1,668)	1:55:A:LYS:H	1:56:A:GLU:H	11	0.18	0.06	0.16
(1,702)	1:58:A:GLY:HA2	1:59:A:HIS:HA	11	0.17	0.04	0.18
(1,35)	1:5:A:LEU:HD11	1:7:A:LEU:HG	10	1.75	0.5	1.88
(1,35)	1:5:A:LEU:HD12	1:7:A:LEU:HG	10	1.75	0.5	1.88
(1,35)	1:5:A:LEU:HD13	1:7:A:LEU:HG	10	1.75	0.5	1.88
(1,35)	1:5:A:LEU:HD21	1:7:A:LEU:HG	10	1.75	0.5	1.88
(1,35)	1:5:A:LEU:HD22	1:7:A:LEU:HG	10	1.75	0.5	1.88
(1,35)	1:5:A:LEU:HD23	1:7:A:LEU:HG	10	1.75	0.5	1.88
(1,742)	1:62:A:TYR:HE1	1:63:A:LEU:H	10	0.91	0.14	0.92
(1,742)	1:62:A:TYR:HE2	1:63:A:LEU:H	10	0.91	0.14	0.92
(1,293)	1:24:A:LEU:HB2	1:80:A:HIS:HE1	10	0.91	0.57	1.02
(1,293)	1:24:A:LEU:HB3	1:80:A:HIS:HE1	10	0.91	0.57	1.02
(1,814)	1:68:A:VAL:HG11	1:73:A:LYS:H	10	0.63	0.34	0.65
(1,814)	1:68:A:VAL:HG12	1:73:A:LYS:H	10	0.63	0.34	0.65
(1,814)	1:68:A:VAL:HG13	1:73:A:LYS:H	10	0.63	0.34	0.65
(1,814)	1:68:A:VAL:HG21	1:73:A:LYS:H	10	0.63	0.34	0.65
(1,814)	1:68:A:VAL:HG22	1:73:A:LYS:H	10	0.63	0.34	0.65
(1,814)	1:68:A:VAL:HG23	1:73:A:LYS:H	10	0.63	0.34	0.65
(1,19)	1:5:A:LEU:HB2	1:35:A:ILE:HA	10	0.49	0.21	0.4
(1,19)	1:5:A:LEU:HB3	1:35:A:ILE:HA	10	0.49	0.21	0.4
(1,156)	1:10:A:ASN:HB2	1:45:A:LYS:HB2	10	0.32	0.18	0.29
(1,156)	1:10:A:ASN:HB2	1:45:A:LYS:HB3	10	0.32	0.18	0.29
(1,156)	1:10:A:ASN:HB3	1:45:A:LYS:HB2	10	0.32	0.18	0.29
(1,156)	1:10:A:ASN:HB3	1:45:A:LYS:HB3	10	0.32	0.18	0.29
(1,537)	1:43:A:ALA:HA	1:45:A:LYS:H	10	0.27	0.14	0.2
(1,237)	1:21:A:LEU:HG	1:24:A:LEU:HB2	10	0.26	0.11	0.22
(1,237)	1:21:A:LEU:HG	1:24:A:LEU:HB3	10	0.26	0.11	0.22
(1,44)	1:6:A:VAL:H	1:20:A:GLU:HB2	10	0.26	0.11	0.24
(1,44)	1:6:A:VAL:H	1:20:A:GLU:HB3	10	0.26	0.11	0.24
(1,675)	1:55:A:LYS:HA	1:57:A:LYS:H	10	0.2	0.09	0.15
(1,203)	1:19:A:VAL:H	1:21:A:LEU:H	10	0.16	0.04	0.15
(1,32)	1:5:A:LEU:HD11	1:7:A:LEU:H	9	1.07	0.26	1.03
(1,32)	1:5:A:LEU:HD12	1:7:A:LEU:H	9	1.07	0.26	1.03
(1,32)	1:5:A:LEU:HD13	1:7:A:LEU:H	9	1.07	0.26	1.03
(1,32)	1:5:A:LEU:HD21	1:7:A:LEU:H	9	1.07	0.26	1.03
(1,32)	1:5:A:LEU:HD22	1:7:A:LEU:H	9	1.07	0.26	1.03
(1,32)	1:5:A:LEU:HD23	1:7:A:LEU:H	9	1.07	0.26	1.03
(1,317)	1:25:A:TYR:HA	1:29:A:SER:HG	9	0.45	0.24	0.42
(1,107)	1:7:A:LEU:H	1:38:A:PHE:HD1	9	0.37	0.32	0.26

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,107)	1:7:A:LEU:H	1:38:A:PHE:HD2	9	0.37	0.32	0.26
(1,836)	1:70:A:THR:HA	1:73:A:LYS:HB2	9	0.36	0.13	0.32
(1,836)	1:70:A:THR:HA	1:73:A:LYS:HB3	9	0.36	0.13	0.32
(1,819)	1:69:A:SER:H	1:73:A:LYS:H	9	0.35	0.19	0.32
(1,167)	1:11:A:THR:HB	1:12:A:ARG:HA	9	0.3	0.08	0.31
(1,820)	1:69:A:SER:H	1:73:A:LYS:HA	9	0.24	0.09	0.22
(1,270)	1:23:A:ASP:HA	1:28:A:PHE:H	9	0.24	0.05	0.23
(1,20)	1:5:A:LEU:HB2	1:35:A:ILE:HB	8	1.28	0.5	1.12
(1,20)	1:5:A:LEU:HB3	1:35:A:ILE:HB	8	1.28	0.5	1.12
(1,45)	1:6:A:VAL:H	1:35:A:ILE:HB	8	1.23	0.19	1.23
(1,36)	1:5:A:LEU:HD11	1:7:A:LEU:HD11	8	1.17	0.3	1.18
(1,36)	1:5:A:LEU:HD11	1:7:A:LEU:HD12	8	1.17	0.3	1.18
(1,36)	1:5:A:LEU:HD11	1:7:A:LEU:HD13	8	1.17	0.3	1.18
(1,36)	1:5:A:LEU:HD12	1:7:A:LEU:HD11	8	1.17	0.3	1.18
(1,36)	1:5:A:LEU:HD12	1:7:A:LEU:HD12	8	1.17	0.3	1.18
(1,36)	1:5:A:LEU:HD12	1:7:A:LEU:HD13	8	1.17	0.3	1.18
(1,36)	1:5:A:LEU:HD13	1:7:A:LEU:HD11	8	1.17	0.3	1.18
(1,36)	1:5:A:LEU:HD13	1:7:A:LEU:HD12	8	1.17	0.3	1.18
(1,36)	1:5:A:LEU:HD13	1:7:A:LEU:HD13	8	1.17	0.3	1.18
(1,36)	1:5:A:LEU:HD21	1:7:A:LEU:HD11	8	1.17	0.3	1.18
(1,36)	1:5:A:LEU:HD21	1:7:A:LEU:HD12	8	1.17	0.3	1.18
(1,36)	1:5:A:LEU:HD21	1:7:A:LEU:HD13	8	1.17	0.3	1.18
(1,36)	1:5:A:LEU:HD22	1:7:A:LEU:HD11	8	1.17	0.3	1.18
(1,36)	1:5:A:LEU:HD22	1:7:A:LEU:HD12	8	1.17	0.3	1.18
(1,36)	1:5:A:LEU:HD22	1:7:A:LEU:HD13	8	1.17	0.3	1.18
(1,36)	1:5:A:LEU:HD23	1:7:A:LEU:HD11	8	1.17	0.3	1.18
(1,36)	1:5:A:LEU:HD23	1:7:A:LEU:HD12	8	1.17	0.3	1.18
(1,36)	1:5:A:LEU:HD23	1:7:A:LEU:HD13	8	1.17	0.3	1.18
(1,801)	1:66:A:VAL:HG11	1:72:A:GLU:HB2	8	0.67	0.62	0.36
(1,801)	1:66:A:VAL:HG11	1:72:A:GLU:HB3	8	0.67	0.62	0.36
(1,801)	1:66:A:VAL:HG12	1:72:A:GLU:HB2	8	0.67	0.62	0.36
(1,801)	1:66:A:VAL:HG12	1:72:A:GLU:HB3	8	0.67	0.62	0.36
(1,801)	1:66:A:VAL:HG13	1:72:A:GLU:HB2	8	0.67	0.62	0.36
(1,801)	1:66:A:VAL:HG13	1:72:A:GLU:HB3	8	0.67	0.62	0.36
(1,801)	1:66:A:VAL:HG21	1:72:A:GLU:HB2	8	0.67	0.62	0.36
(1,801)	1:66:A:VAL:HG21	1:72:A:GLU:HB3	8	0.67	0.62	0.36
(1,801)	1:66:A:VAL:HG22	1:72:A:GLU:HB2	8	0.67	0.62	0.36
(1,801)	1:66:A:VAL:HG22	1:72:A:GLU:HB3	8	0.67	0.62	0.36
(1,801)	1:66:A:VAL:HG23	1:72:A:GLU:HB2	8	0.67	0.62	0.36
(1,801)	1:66:A:VAL:HG23	1:72:A:GLU:HB3	8	0.67	0.62	0.36
(1,739)	1:62:A:TYR:HB2	1:79:A:LEU:HG	8	0.63	0.18	0.64
(1,739)	1:62:A:TYR:HB3	1:79:A:LEU:HG	8	0.63	0.18	0.64

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,33)	1:5:A:LEU:HD11	1:7:A:LEU:HA	8	0.59	0.21	0.52
(1,33)	1:5:A:LEU:HD12	1:7:A:LEU:HA	8	0.59	0.21	0.52
(1,33)	1:5:A:LEU:HD13	1:7:A:LEU:HA	8	0.59	0.21	0.52
(1,33)	1:5:A:LEU:HD21	1:7:A:LEU:HA	8	0.59	0.21	0.52
(1,33)	1:5:A:LEU:HD22	1:7:A:LEU:HA	8	0.59	0.21	0.52
(1,33)	1:5:A:LEU:HD23	1:7:A:LEU:HA	8	0.59	0.21	0.52
(1,727)	1:61:A:ALA:HB1	1:79:A:LEU:HB3	8	0.58	0.5	0.3
(1,727)	1:61:A:ALA:HB2	1:79:A:LEU:HB3	8	0.58	0.5	0.3
(1,727)	1:61:A:ALA:HB3	1:79:A:LEU:HB3	8	0.58	0.5	0.3
(1,34)	1:5:A:LEU:HD11	1:7:A:LEU:HB2	8	0.51	0.22	0.5
(1,34)	1:5:A:LEU:HD11	1:7:A:LEU:HB3	8	0.51	0.22	0.5
(1,34)	1:5:A:LEU:HD12	1:7:A:LEU:HB2	8	0.51	0.22	0.5
(1,34)	1:5:A:LEU:HD12	1:7:A:LEU:HB3	8	0.51	0.22	0.5
(1,34)	1:5:A:LEU:HD13	1:7:A:LEU:HB2	8	0.51	0.22	0.5
(1,34)	1:5:A:LEU:HD13	1:7:A:LEU:HB3	8	0.51	0.22	0.5
(1,34)	1:5:A:LEU:HD21	1:7:A:LEU:HB2	8	0.51	0.22	0.5
(1,34)	1:5:A:LEU:HD21	1:7:A:LEU:HB3	8	0.51	0.22	0.5
(1,34)	1:5:A:LEU:HD22	1:7:A:LEU:HB2	8	0.51	0.22	0.5
(1,34)	1:5:A:LEU:HD22	1:7:A:LEU:HB3	8	0.51	0.22	0.5
(1,34)	1:5:A:LEU:HD23	1:7:A:LEU:HB2	8	0.51	0.22	0.5
(1,34)	1:5:A:LEU:HD23	1:7:A:LEU:HB3	8	0.51	0.22	0.5
(1,322)	1:25:A:TYR:HD1	1:28:A:PHE:H	8	0.39	0.3	0.24
(1,322)	1:25:A:TYR:HD2	1:28:A:PHE:H	8	0.39	0.3	0.24
(1,356)	1:28:A:PHE:HA	1:33:A:ARG:H	8	0.34	0.18	0.3
(1,355)	1:28:A:PHE:HA	1:32:A:LYS:HB2	8	0.32	0.2	0.32
(1,355)	1:28:A:PHE:HA	1:32:A:LYS:HB3	8	0.32	0.2	0.32
(1,686)	1:56:A:GLU:HA	1:57:A:LYS:HG2	8	0.32	0.17	0.22
(1,686)	1:56:A:GLU:HA	1:57:A:LYS:HG3	8	0.32	0.17	0.22
(1,805)	1:67:A:ARG:H	1:68:A:VAL:HG11	8	0.28	0.14	0.3
(1,805)	1:67:A:ARG:H	1:68:A:VAL:HG12	8	0.28	0.14	0.3
(1,805)	1:67:A:ARG:H	1:68:A:VAL:HG13	8	0.28	0.14	0.3
(1,417)	1:34:A:SER:H	1:79:A:LEU:HA	8	0.23	0.08	0.22
(1,47)	1:6:A:VAL:H	1:36:A:PHE:H	8	0.21	0.1	0.18
(1,567)	1:47:A:MET:HB2	1:48:A:LEU:HA	8	0.18	0.04	0.18
(1,567)	1:47:A:MET:HB3	1:48:A:LEU:HA	8	0.18	0.04	0.18
(1,831)	1:70:A:THR:H	1:73:A:LYS:HA	8	0.18	0.08	0.13
(1,50)	1:6:A:VAL:H	1:37:A:TYR:H	8	0.16	0.04	0.17
(1,917)	1:79:A:LEU:HB2	1:80:A:HIS:HD2	7	1.09	0.25	1.24
(1,917)	1:79:A:LEU:HB3	1:80:A:HIS:HD2	7	1.09	0.25	1.24
(1,68)	1:6:A:VAL:HB	1:19:A:VAL:HB	7	0.95	0.47	1.07
(1,200)	1:18:A:SER:HB2	1:22:A:GLU:HG2	7	0.74	0.28	0.82
(1,200)	1:18:A:SER:HB2	1:22:A:GLU:HG3	7	0.74	0.28	0.82

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,200)	1:18:A:SER:HB3	1:22:A:GLU:HG2	7	0.74	0.28	0.82
(1,200)	1:18:A:SER:HB3	1:22:A:GLU:HG3	7	0.74	0.28	0.82
(1,441)	1:35:A:ILE:HB	1:37:A:TYR:HA	7	0.66	0.29	0.72
(1,628)	1:51:A:VAL:HG21	1:54:A:PHE:HD1	7	0.57	0.44	0.41
(1,628)	1:51:A:VAL:HG21	1:54:A:PHE:HD2	7	0.57	0.44	0.41
(1,628)	1:51:A:VAL:HG22	1:54:A:PHE:HD1	7	0.57	0.44	0.41
(1,628)	1:51:A:VAL:HG22	1:54:A:PHE:HD2	7	0.57	0.44	0.41
(1,628)	1:51:A:VAL:HG23	1:54:A:PHE:HD1	7	0.57	0.44	0.41
(1,628)	1:51:A:VAL:HG23	1:54:A:PHE:HD2	7	0.57	0.44	0.41
(1,398)	1:32:A:LYS:H	1:81:A:ILE:HG21	7	0.53	0.53	0.43
(1,398)	1:32:A:LYS:H	1:81:A:ILE:HG22	7	0.53	0.53	0.43
(1,398)	1:32:A:LYS:H	1:81:A:ILE:HG23	7	0.53	0.53	0.43
(1,512)	1:39:A:ALA:HA	1:74:A:ASP:HB2	7	0.36	0.29	0.24
(1,512)	1:39:A:ALA:HA	1:74:A:ASP:HB3	7	0.36	0.29	0.24
(1,177)	1:13:A:LYS:H	1:16:A:ALA:H	7	0.33	0.29	0.21
(1,489)	1:38:A:PHE:H	1:75:A:PHE:HA	7	0.3	0.19	0.24
(1,274)	1:23:A:ASP:HB2	1:35:A:ILE:HB	7	0.28	0.1	0.32
(1,274)	1:23:A:ASP:HB3	1:35:A:ILE:HB	7	0.28	0.1	0.32
(1,158)	1:10:A:ASN:HB2	1:46:A:ASP:HA	7	0.28	0.13	0.28
(1,158)	1:10:A:ASN:HB3	1:46:A:ASP:HA	7	0.28	0.13	0.28
(1,208)	1:19:A:VAL:HB	1:23:A:ASP:H	7	0.25	0.08	0.26
(1,929)	1:81:A:ILE:H	1:82:A:ILE:HA	7	0.22	0.09	0.2
(1,204)	1:19:A:VAL:H	1:22:A:GLU:H	7	0.22	0.09	0.18
(1,373)	1:29:A:SER:H	1:30:A:GLU:HB2	7	0.21	0.05	0.2
(1,373)	1:29:A:SER:H	1:30:A:GLU:HB3	7	0.21	0.05	0.2
(1,681)	1:56:A:GLU:H	1:57:A:LYS:H	7	0.13	0.02	0.13
(1,448)	1:35:A:ILE:HG12	1:76:A:LEU:HB2	6	1.9	0.43	1.81
(1,448)	1:35:A:ILE:HG12	1:76:A:LEU:HB3	6	1.9	0.43	1.81
(1,448)	1:35:A:ILE:HG13	1:76:A:LEU:HB2	6	1.9	0.43	1.81
(1,448)	1:35:A:ILE:HG13	1:76:A:LEU:HB3	6	1.9	0.43	1.81
(1,447)	1:35:A:ILE:HG12	1:36:A:PHE:HA	6	1.39	0.15	1.48
(1,447)	1:35:A:ILE:HG13	1:36:A:PHE:HA	6	1.39	0.15	1.48
(1,494)	1:38:A:PHE:HA	1:75:A:PHE:HE1	6	1.0	0.79	0.97
(1,494)	1:38:A:PHE:HA	1:75:A:PHE:HE2	6	1.0	0.79	0.97
(1,305)	1:24:A:LEU:HD21	1:60:A:THR:H	6	0.69	0.29	0.7
(1,305)	1:24:A:LEU:HD22	1:60:A:THR:H	6	0.69	0.29	0.7
(1,305)	1:24:A:LEU:HD23	1:60:A:THR:H	6	0.69	0.29	0.7
(1,359)	1:28:A:PHE:HA	1:81:A:ILE:HD11	6	0.61	0.46	0.38
(1,359)	1:28:A:PHE:HA	1:81:A:ILE:HD12	6	0.61	0.46	0.38
(1,359)	1:28:A:PHE:HA	1:81:A:ILE:HD13	6	0.61	0.46	0.38
(1,422)	1:34:A:SER:HA	1:78:A:GLU:HB2	6	0.33	0.13	0.33
(1,422)	1:34:A:SER:HA	1:78:A:GLU:HB3	6	0.33	0.13	0.33

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,60)	1:6:A:VAL:HA	1:16:A:ALA:HB1	6	0.32	0.13	0.31
(1,60)	1:6:A:VAL:HA	1:16:A:ALA:HB2	6	0.32	0.13	0.31
(1,60)	1:6:A:VAL:HA	1:16:A:ALA:HB3	6	0.32	0.13	0.31
(1,26)	1:5:A:LEU:HG	1:6:A:VAL:HG21	6	0.3	0.16	0.23
(1,26)	1:5:A:LEU:HG	1:6:A:VAL:HG22	6	0.3	0.16	0.23
(1,26)	1:5:A:LEU:HG	1:6:A:VAL:HG23	6	0.3	0.16	0.23
(1,434)	1:35:A:ILE:H	1:78:A:GLU:H	6	0.22	0.05	0.22
(1,130)	1:7:A:LEU:HD11	1:16:A:ALA:HA	6	0.21	0.06	0.19
(1,130)	1:7:A:LEU:HD12	1:16:A:ALA:HA	6	0.21	0.06	0.19
(1,130)	1:7:A:LEU:HD13	1:16:A:ALA:HA	6	0.21	0.06	0.19
(1,506)	1:39:A:ALA:H	1:74:A:ASP:HA	6	0.2	0.05	0.2
(1,92)	1:6:A:VAL:HG21	1:35:A:ILE:HB	6	0.19	0.08	0.15
(1,92)	1:6:A:VAL:HG22	1:35:A:ILE:HB	6	0.19	0.08	0.15
(1,92)	1:6:A:VAL:HG23	1:35:A:ILE:HB	6	0.19	0.08	0.15
(1,492)	1:38:A:PHE:HA	1:75:A:PHE:HA	6	0.19	0.05	0.17
(1,16)	1:5:A:LEU:HA	1:37:A:TYR:H	6	0.18	0.08	0.15
(1,148)	1:10:A:ASN:H	1:11:A:THR:H	6	0.14	0.03	0.14
(1,371)	1:29:A:SER:H	1:30:A:GLU:H	6	0.13	0.02	0.12
(1,154)	1:10:A:ASN:HA	1:13:A:LYS:HG2	5	1.28	0.6	1.09
(1,154)	1:10:A:ASN:HA	1:13:A:LYS:HG3	5	1.28	0.6	1.09
(1,449)	1:35:A:ILE:HD11	1:37:A:TYR:HD1	5	1.17	0.54	0.92
(1,449)	1:35:A:ILE:HD11	1:37:A:TYR:HD2	5	1.17	0.54	0.92
(1,449)	1:35:A:ILE:HD12	1:37:A:TYR:HD1	5	1.17	0.54	0.92
(1,449)	1:35:A:ILE:HD12	1:37:A:TYR:HD2	5	1.17	0.54	0.92
(1,449)	1:35:A:ILE:HD13	1:37:A:TYR:HD1	5	1.17	0.54	0.92
(1,449)	1:35:A:ILE:HD13	1:37:A:TYR:HD2	5	1.17	0.54	0.92
(1,450)	1:35:A:ILE:HD11	1:54:A:PHE:HE1	5	1.14	0.7	1.25
(1,450)	1:35:A:ILE:HD11	1:54:A:PHE:HE2	5	1.14	0.7	1.25
(1,450)	1:35:A:ILE:HD12	1:54:A:PHE:HE1	5	1.14	0.7	1.25
(1,450)	1:35:A:ILE:HD12	1:54:A:PHE:HE2	5	1.14	0.7	1.25
(1,450)	1:35:A:ILE:HD13	1:54:A:PHE:HE1	5	1.14	0.7	1.25
(1,450)	1:35:A:ILE:HD13	1:54:A:PHE:HE2	5	1.14	0.7	1.25
(1,450)	1:35:A:ILE:HD11	1:54:A:PHE:HE1	5	1.14	0.7	1.25
(1,450)	1:35:A:ILE:HD11	1:54:A:PHE:HE2	5	1.14	0.7	1.25
(1,450)	1:35:A:ILE:HD12	1:54:A:PHE:HE1	5	1.14	0.7	1.25
(1,450)	1:35:A:ILE:HD12	1:54:A:PHE:HE2	5	1.14	0.7	1.25
(1,450)	1:35:A:ILE:HD13	1:54:A:PHE:HE1	5	1.14	0.7	1.25
(1,450)	1:35:A:ILE:HD13	1:54:A:PHE:HE2	5	1.14	0.7	1.25
(1,722)	1:61:A:ALA:H	1:81:A:ILE:HA	5	1.07	0.32	1.16
(1,713)	1:60:A:THR:HA	1:81:A:ILE:HA	5	0.69	0.07	0.69
(1,712)	1:60:A:THR:HA	1:81:A:ILE:H	5	0.68	0.08	0.65
(3,1)	1:39:A:ALA:HB1	1:47:A:MET:N	5	0.64	0.3	0.62

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,366)	1:28:A:PHE:HD1	1:80:A:HIS:HB2	5	0.58	0.25	0.46
(1,366)	1:28:A:PHE:HD1	1:80:A:HIS:HB3	5	0.58	0.25	0.46
(1,366)	1:28:A:PHE:HD2	1:80:A:HIS:HB2	5	0.58	0.25	0.46
(1,366)	1:28:A:PHE:HD2	1:80:A:HIS:HB3	5	0.58	0.25	0.46
(1,710)	1:60:A:THR:HA	1:61:A:ALA:H	5	0.57	0.11	0.52
(1,22)	1:5:A:LEU:HB2	1:36:A:PHE:HA	5	0.51	0.09	0.51
(1,22)	1:5:A:LEU:HB3	1:36:A:PHE:HA	5	0.51	0.09	0.51
(1,405)	1:33:A:ARG:H	1:81:A:ILE:HG21	5	0.43	0.31	0.38
(1,405)	1:33:A:ARG:H	1:81:A:ILE:HG22	5	0.43	0.31	0.38
(1,405)	1:33:A:ARG:H	1:81:A:ILE:HG23	5	0.43	0.31	0.38
(1,405)	1:33:A:ARG:H	1:81:A:ILE:HG21	5	0.43	0.31	0.38
(1,405)	1:33:A:ARG:H	1:81:A:ILE:HG22	5	0.43	0.31	0.38
(1,405)	1:33:A:ARG:H	1:81:A:ILE:HG23	5	0.43	0.31	0.38
(1,824)	1:69:A:SER:HA	1:74:A:ASP:H	5	0.38	0.16	0.32
(1,215)	1:20:A:GLU:H	1:37:A:TYR:HD1	5	0.32	0.15	0.41
(1,215)	1:20:A:GLU:H	1:37:A:TYR:HD2	5	0.32	0.15	0.41
(1,180)	1:14:A:SER:H	1:15:A:ASP:H	5	0.3	0.16	0.22
(1,43)	1:6:A:VAL:H	1:7:A:LEU:HG	5	0.28	0.26	0.16
(1,165)	1:11:A:THR:HA	1:40:A:PRO:HG2	5	0.28	0.04	0.29
(1,165)	1:11:A:THR:HA	1:40:A:PRO:HG3	5	0.28	0.04	0.29
(1,316)	1:25:A:TYR:HA	1:29:A:SER:H	5	0.28	0.19	0.19
(1,335)	1:26:A:HIS:HB2	1:30:A:GLU:HB2	5	0.27	0.06	0.3
(1,335)	1:26:A:HIS:HB2	1:30:A:GLU:HB3	5	0.27	0.06	0.3
(1,335)	1:26:A:HIS:HB3	1:30:A:GLU:HB2	5	0.27	0.06	0.3
(1,335)	1:26:A:HIS:HB3	1:30:A:GLU:HB3	5	0.27	0.06	0.3
(1,319)	1:25:A:TYR:HA	1:59:A:HIS:HB2	5	0.25	0.14	0.19
(1,319)	1:25:A:TYR:HA	1:59:A:HIS:HB3	5	0.25	0.14	0.19
(1,74)	1:6:A:VAL:HB	1:38:A:PHE:H	5	0.22	0.08	0.19
(1,69)	1:6:A:VAL:HB	1:20:A:GLU:H	5	0.22	0.09	0.22
(1,106)	1:7:A:LEU:H	1:38:A:PHE:HB2	5	0.22	0.08	0.17
(1,106)	1:7:A:LEU:H	1:38:A:PHE:HB3	5	0.22	0.08	0.17
(1,433)	1:35:A:ILE:H	1:77:A:TYR:HA	5	0.2	0.09	0.18
(1,703)	1:58:A:GLY:HA3	1:60:A:THR:H	5	0.19	0.08	0.16
(1,539)	1:43:A:ALA:HB1	1:44:A:HIS:H	5	0.19	0.11	0.13
(1,539)	1:43:A:ALA:HB2	1:44:A:HIS:H	5	0.19	0.11	0.13
(1,539)	1:43:A:ALA:HB3	1:44:A:HIS:H	5	0.19	0.11	0.13
(1,187)	1:15:A:ASP:HA	1:16:A:ALA:H	5	0.16	0.05	0.16
(1,268)	1:23:A:ASP:HA	1:27:A:GLU:HA	5	0.16	0.05	0.15
(1,307)	1:25:A:TYR:H	1:26:A:HIS:H	5	0.15	0.02	0.14
(1,669)	1:55:A:LYS:H	1:56:A:GLU:HA	5	0.15	0.05	0.12
(1,419)	1:34:A:SER:H	1:80:A:HIS:H	5	0.12	0.02	0.12
(1,129)	1:7:A:LEU:HD11	1:14:A:SER:HG	4	2.22	1.02	2.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,129)	1:7:A:LEU:HD12	1:14:A:SER:HG	4	2.22	1.02	2.16
(1,129)	1:7:A:LEU:HD13	1:14:A:SER:HG	4	2.22	1.02	2.16
(1,369)	1:28:A:PHE:HE1	1:81:A:ILE:H	4	1.61	1.2	1.52
(1,369)	1:28:A:PHE:HE2	1:81:A:ILE:H	4	1.61	1.2	1.52
(1,338)	1:27:A:GLU:H	1:30:A:GLU:HG2	4	1.57	0.11	1.58
(1,338)	1:27:A:GLU:H	1:30:A:GLU:HG3	4	1.57	0.11	1.58
(1,921)	1:79:A:LEU:HD11	1:82:A:ILE:HB	4	1.4	0.12	1.44
(1,921)	1:79:A:LEU:HD12	1:82:A:ILE:HB	4	1.4	0.12	1.44
(1,921)	1:79:A:LEU:HD13	1:82:A:ILE:HB	4	1.4	0.12	1.44
(1,374)	1:29:A:SER:H	1:30:A:GLU:HG2	4	1.36	0.07	1.38
(1,374)	1:29:A:SER:H	1:30:A:GLU:HG3	4	1.36	0.07	1.38
(1,683)	1:56:A:GLU:H	1:57:A:LYS:HG3	4	0.7	0.07	0.68
(1,931)	1:81:A:ILE:HA	1:82:A:ILE:HA	4	0.61	0.02	0.62
(1,859)	1:72:A:GLU:HB2	1:74:A:ASP:HA	4	0.56	0.13	0.58
(1,859)	1:72:A:GLU:HB3	1:74:A:ASP:HA	4	0.56	0.13	0.58
(1,102)	1:7:A:LEU:H	1:19:A:VAL:HB	4	0.5	0.22	0.55
(1,755)	1:63:A:LEU:HG	1:64:A:ASP:HA	4	0.49	0.11	0.52
(1,775)	1:65:A:GLU:H	1:76:A:LEU:HD11	4	0.47	0.19	0.5
(1,775)	1:65:A:GLU:H	1:76:A:LEU:HD12	4	0.47	0.19	0.5
(1,775)	1:65:A:GLU:H	1:76:A:LEU:HD13	4	0.47	0.19	0.5
(1,775)	1:65:A:GLU:H	1:76:A:LEU:HD21	4	0.47	0.19	0.5
(1,46)	1:6:A:VAL:H	1:35:A:ILE:HD11	4	0.45	0.32	0.4
(1,46)	1:6:A:VAL:H	1:35:A:ILE:HD12	4	0.45	0.32	0.4
(1,46)	1:6:A:VAL:H	1:35:A:ILE:HD13	4	0.45	0.32	0.4
(1,866)	1:74:A:ASP:H	1:75:A:PHE:HA	4	0.32	0.1	0.31
(1,676)	1:55:A:LYS:HA	1:58:A:GLY:HA2	4	0.32	0.23	0.2
(1,516)	1:39:A:ALA:HB1	1:46:A:ASP:H	4	0.27	0.17	0.27
(1,516)	1:39:A:ALA:HB2	1:46:A:ASP:H	4	0.27	0.17	0.27
(1,516)	1:39:A:ALA:HB3	1:46:A:ASP:H	4	0.27	0.17	0.27
(1,461)	1:36:A:PHE:HA	1:77:A:TYR:HD1	4	0.25	0.09	0.26
(1,461)	1:36:A:PHE:HA	1:77:A:TYR:HD2	4	0.25	0.09	0.26
(1,29)	1:5:A:LEU:HG	1:36:A:PHE:H	4	0.24	0.04	0.25
(1,459)	1:36:A:PHE:HA	1:77:A:TYR:H	4	0.24	0.09	0.23
(1,475)	1:37:A:TYR:H	1:76:A:LEU:HA	4	0.23	0.06	0.23
(1,671)	1:55:A:LYS:H	1:57:A:LYS:H	4	0.23	0.07	0.23
(1,881)	1:76:A:LEU:H	1:77:A:TYR:HA	4	0.22	0.1	0.2
(1,115)	1:7:A:LEU:HA	1:38:A:PHE:HB2	4	0.2	0.09	0.18
(1,115)	1:7:A:LEU:HA	1:38:A:PHE:HB3	4	0.2	0.09	0.18
(1,264)	1:23:A:ASP:H	1:27:A:GLU:H	4	0.18	0.08	0.15
(1,380)	1:30:A:GLU:H	1:31:A:ASP:HA	4	0.16	0.05	0.16
(1,632)	1:52:A:ASP:H	1:55:A:LYS:H	4	0.15	0.04	0.14
(1,409)	1:33:A:ARG:HA	1:80:A:HIS:H	4	0.14	0.02	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,903)	1:78:A:GLU:H	1:79:A:LEU:HG	3	1.62	0.23	1.54
(1,499)	1:38:A:PHE:HB2	1:75:A:PHE:HD1	3	1.27	0.06	1.25
(1,499)	1:38:A:PHE:HB2	1:75:A:PHE:HD2	3	1.27	0.06	1.25
(1,499)	1:38:A:PHE:HB3	1:75:A:PHE:HD1	3	1.27	0.06	1.25
(1,499)	1:38:A:PHE:HB3	1:75:A:PHE:HD2	3	1.27	0.06	1.25
(1,695)	1:57:A:LYS:HA	1:58:A:GLY:H	3	1.09	0.07	1.08
(1,469)	1:36:A:PHE:HD1	1:75:A:PHE:HB2	3	1.01	0.13	1.03
(1,469)	1:36:A:PHE:HD1	1:75:A:PHE:HB3	3	1.01	0.13	1.03
(1,469)	1:36:A:PHE:HD2	1:75:A:PHE:HB2	3	1.01	0.13	1.03
(1,469)	1:36:A:PHE:HD2	1:75:A:PHE:HB3	3	1.01	0.13	1.03
(1,296)	1:24:A:LEU:HG	1:35:A:ILE:HD11	3	0.86	0.1	0.81
(1,296)	1:24:A:LEU:HG	1:35:A:ILE:HD12	3	0.86	0.1	0.81
(1,296)	1:24:A:LEU:HG	1:35:A:ILE:HD13	3	0.86	0.1	0.81
(1,664)	1:54:A:PHE:HD1	1:76:A:LEU:HD11	3	0.75	0.7	0.36
(1,664)	1:54:A:PHE:HD1	1:76:A:LEU:HD12	3	0.75	0.7	0.36
(1,664)	1:54:A:PHE:HD1	1:76:A:LEU:HD13	3	0.75	0.7	0.36
(1,664)	1:54:A:PHE:HD2	1:76:A:LEU:HD11	3	0.75	0.7	0.36
(1,664)	1:54:A:PHE:HD2	1:76:A:LEU:HD12	3	0.75	0.7	0.36
(1,664)	1:54:A:PHE:HD2	1:76:A:LEU:HD13	3	0.75	0.7	0.36
(1,696)	1:57:A:LYS:HA	1:58:A:GLY:HA2	3	0.67	0.1	0.74
(1,900)	1:77:A:TYR:HD1	1:79:A:LEU:HG	3	0.59	0.39	0.46
(1,900)	1:77:A:TYR:HD2	1:79:A:LEU:HG	3	0.59	0.39	0.46
(1,37)	1:5:A:LEU:HD11	1:38:A:PHE:HB3	3	0.51	0.21	0.37
(1,37)	1:5:A:LEU:HD12	1:38:A:PHE:HB3	3	0.51	0.21	0.37
(1,37)	1:5:A:LEU:HD13	1:38:A:PHE:HB3	3	0.51	0.21	0.37
(1,37)	1:5:A:LEU:HD21	1:38:A:PHE:HB3	3	0.51	0.21	0.37
(1,37)	1:5:A:LEU:HD22	1:38:A:PHE:HB3	3	0.51	0.21	0.37
(1,37)	1:5:A:LEU:HD23	1:38:A:PHE:HB3	3	0.51	0.21	0.37
(1,837)	1:70:A:THR:HA	1:73:A:LYS:HD2	3	0.5	0.33	0.37
(1,837)	1:70:A:THR:HA	1:73:A:LYS:HD3	3	0.5	0.33	0.37
(1,189)	1:16:A:ALA:H	1:17:A:LYS:H	3	0.43	0.36	0.25
(1,877)	1:75:A:PHE:HB2	1:77:A:TYR:H	3	0.43	0.22	0.55
(1,877)	1:75:A:PHE:HB3	1:77:A:TYR:H	3	0.43	0.22	0.55
(1,875)	1:75:A:PHE:HB2	1:76:A:LEU:H	3	0.28	0.04	0.3
(1,875)	1:75:A:PHE:HB3	1:76:A:LEU:H	3	0.28	0.04	0.3
(1,657)	1:54:A:PHE:HA	1:60:A:THR:HB	3	0.28	0.09	0.24
(1,862)	1:73:A:LYS:HA	1:75:A:PHE:H	3	0.26	0.2	0.13
(1,138)	1:8:A:ALA:HA	1:10:A:ASN:HB2	3	0.25	0.09	0.22
(1,138)	1:8:A:ALA:HA	1:10:A:ASN:HB3	3	0.25	0.09	0.22
(1,71)	1:6:A:VAL:HB	1:37:A:TYR:HA	3	0.24	0.02	0.23
(1,51)	1:6:A:VAL:H	1:37:A:TYR:HA	3	0.15	0.04	0.12
(1,435)	1:35:A:ILE:H	1:78:A:GLU:HA	3	0.15	0.02	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,105)	1:7:A:LEU:H	1:38:A:PHE:H	3	0.14	0.02	0.14
(1,185)	1:15:A:ASP:H	1:16:A:ALA:H	3	0.13	0.01	0.13
(1,731)	1:62:A:TYR:H	1:80:A:HIS:HA	3	0.12	0.01	0.13
(1,372)	1:29:A:SER:H	1:30:A:GLU:HA	3	0.12	0.01	0.12
(1,586)	1:48:A:LEU:HB2	1:49:A:LYS:HA	3	0.12	0.01	0.11
(1,586)	1:48:A:LEU:HB3	1:49:A:LYS:HA	3	0.12	0.01	0.11
(1,210)	1:19:A:VAL:HG11	1:20:A:GLU:HA	2	1.23	0.0	1.23
(1,210)	1:19:A:VAL:HG12	1:20:A:GLU:HA	2	1.23	0.0	1.23
(1,210)	1:19:A:VAL:HG13	1:20:A:GLU:HA	2	1.23	0.0	1.23
(1,723)	1:61:A:ALA:H	1:82:A:ILE:H	2	1.16	0.36	1.16
(1,191)	1:16:A:ALA:HA	1:19:A:VAL:HB	2	0.66	0.1	0.66
(1,784)	1:65:A:GLU:HB2	1:69:A:SER:HA	2	0.6	0.48	0.6
(1,784)	1:65:A:GLU:HB3	1:69:A:SER:HA	2	0.6	0.48	0.6
(1,62)	1:6:A:VAL:HA	1:19:A:VAL:HG11	2	0.54	0.2	0.54
(1,62)	1:6:A:VAL:HA	1:19:A:VAL:HG12	2	0.54	0.2	0.54
(1,62)	1:6:A:VAL:HA	1:19:A:VAL:HG13	2	0.54	0.2	0.54
(1,923)	1:79:A:LEU:HD11	1:82:A:ILE:HD11	2	0.52	0.18	0.52
(1,923)	1:79:A:LEU:HD11	1:82:A:ILE:HD12	2	0.52	0.18	0.52
(1,923)	1:79:A:LEU:HD11	1:82:A:ILE:HD13	2	0.52	0.18	0.52
(1,923)	1:79:A:LEU:HD12	1:82:A:ILE:HD11	2	0.52	0.18	0.52
(1,923)	1:79:A:LEU:HD12	1:82:A:ILE:HD12	2	0.52	0.18	0.52
(1,923)	1:79:A:LEU:HD12	1:82:A:ILE:HD13	2	0.52	0.18	0.52
(1,923)	1:79:A:LEU:HD13	1:82:A:ILE:HD11	2	0.52	0.18	0.52
(1,923)	1:79:A:LEU:HD13	1:82:A:ILE:HD12	2	0.52	0.18	0.52
(1,923)	1:79:A:LEU:HD13	1:82:A:ILE:HD13	2	0.52	0.18	0.52
(1,89)	1:6:A:VAL:HG21	1:19:A:VAL:HG11	2	0.39	0.09	0.39
(1,89)	1:6:A:VAL:HG21	1:19:A:VAL:HG12	2	0.39	0.09	0.39
(1,89)	1:6:A:VAL:HG21	1:19:A:VAL:HG13	2	0.39	0.09	0.39
(1,89)	1:6:A:VAL:HG22	1:19:A:VAL:HG11	2	0.39	0.09	0.39
(1,89)	1:6:A:VAL:HG22	1:19:A:VAL:HG12	2	0.39	0.09	0.39
(1,89)	1:6:A:VAL:HG22	1:19:A:VAL:HG13	2	0.39	0.09	0.39
(1,89)	1:6:A:VAL:HG23	1:19:A:VAL:HG11	2	0.39	0.09	0.39
(1,89)	1:6:A:VAL:HG23	1:19:A:VAL:HG12	2	0.39	0.09	0.39
(1,89)	1:6:A:VAL:HG23	1:19:A:VAL:HG13	2	0.39	0.09	0.39
(1,327)	1:26:A:HIS:H	1:28:A:PHE:HB2	2	0.38	0.03	0.38
(1,327)	1:26:A:HIS:H	1:28:A:PHE:HB3	2	0.38	0.03	0.38
(1,414)	1:33:A:ARG:HG2	1:34:A:SER:HB2	2	0.38	0.24	0.38
(1,414)	1:33:A:ARG:HG2	1:34:A:SER:HB3	2	0.38	0.24	0.38
(1,414)	1:33:A:ARG:HG3	1:34:A:SER:HB2	2	0.38	0.24	0.38
(1,414)	1:33:A:ARG:HG3	1:34:A:SER:HB3	2	0.38	0.24	0.38
(1,521)	1:41:A:THR:HA	1:43:A:ALA:H	2	0.36	0.21	0.36
(1,792)	1:66:A:VAL:HA	1:69:A:SER:H	2	0.31	0.19	0.31

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,761)	1:64:A:ASP:H	1:76:A:LEU:HA	2	0.29	0.1	0.29
(1,238)	1:21:A:LEU:HG	1:53:A:PHE:HB2	2	0.27	0.14	0.27
(1,238)	1:21:A:LEU:HG	1:53:A:PHE:HB3	2	0.27	0.14	0.27
(1,595)	1:49:A:LYS:HA	1:52:A:ASP:HA	2	0.27	0.11	0.27
(1,807)	1:68:A:VAL:H	1:69:A:SER:HA	2	0.26	0.06	0.26
(1,155)	1:10:A:ASN:HA	1:40:A:PRO:HG2	2	0.25	0.08	0.25
(1,155)	1:10:A:ASN:HA	1:40:A:PRO:HG3	2	0.25	0.08	0.25
(1,835)	1:70:A:THR:HA	1:73:A:LYS:H	2	0.24	0.14	0.24
(1,928)	1:81:A:ILE:H	1:82:A:ILE:H	2	0.24	0.1	0.24
(1,626)	1:51:A:VAL:HG11	1:63:A:LEU:HD11	2	0.24	0.12	0.24
(1,626)	1:51:A:VAL:HG11	1:63:A:LEU:HD12	2	0.24	0.12	0.24
(1,626)	1:51:A:VAL:HG11	1:63:A:LEU:HD13	2	0.24	0.12	0.24
(1,626)	1:51:A:VAL:HG12	1:63:A:LEU:HD11	2	0.24	0.12	0.24
(1,626)	1:51:A:VAL:HG12	1:63:A:LEU:HD12	2	0.24	0.12	0.24
(1,626)	1:51:A:VAL:HG12	1:63:A:LEU:HD13	2	0.24	0.12	0.24
(1,626)	1:51:A:VAL:HG13	1:63:A:LEU:HD11	2	0.24	0.12	0.24
(1,626)	1:51:A:VAL:HG13	1:63:A:LEU:HD12	2	0.24	0.12	0.24
(1,626)	1:51:A:VAL:HG13	1:63:A:LEU:HD13	2	0.24	0.12	0.24
(1,626)	1:51:A:VAL:HG11	1:63:A:LEU:HD11	2	0.24	0.12	0.24
(1,626)	1:51:A:VAL:HG11	1:63:A:LEU:HD12	2	0.24	0.12	0.24
(1,626)	1:51:A:VAL:HG11	1:63:A:LEU:HD13	2	0.24	0.12	0.24
(1,626)	1:51:A:VAL:HG12	1:63:A:LEU:HD11	2	0.24	0.12	0.24
(1,626)	1:51:A:VAL:HG12	1:63:A:LEU:HD12	2	0.24	0.12	0.24
(1,626)	1:51:A:VAL:HG12	1:63:A:LEU:HD13	2	0.24	0.12	0.24
(1,626)	1:51:A:VAL:HG13	1:63:A:LEU:HD11	2	0.24	0.12	0.24
(1,626)	1:51:A:VAL:HG13	1:63:A:LEU:HD12	2	0.24	0.12	0.24
(1,626)	1:51:A:VAL:HG13	1:63:A:LEU:HD13	2	0.24	0.12	0.24
(1,413)	1:33:A:ARG:HB2	1:34:A:SER:HA	2	0.22	0.12	0.22
(1,413)	1:33:A:ARG:HB3	1:34:A:SER:HA	2	0.22	0.12	0.22
(1,446)	1:35:A:ILE:HG12	1:36:A:PHE:H	2	0.22	0.01	0.22
(1,446)	1:35:A:ILE:HG13	1:36:A:PHE:H	2	0.22	0.01	0.22
(1,599)	1:49:A:LYS:HB2	1:53:A:PHE:HE1	2	0.22	0.03	0.22
(1,599)	1:49:A:LYS:HB2	1:53:A:PHE:HE2	2	0.22	0.03	0.22
(1,599)	1:49:A:LYS:HB3	1:53:A:PHE:HE1	2	0.22	0.03	0.22
(1,599)	1:49:A:LYS:HB3	1:53:A:PHE:HE2	2	0.22	0.03	0.22
(1,78)	1:6:A:VAL:HG11	1:7:A:LEU:HD11	2	0.21	0.05	0.21
(1,78)	1:6:A:VAL:HG11	1:7:A:LEU:HD12	2	0.21	0.05	0.21
(1,78)	1:6:A:VAL:HG11	1:7:A:LEU:HD13	2	0.21	0.05	0.21
(1,78)	1:6:A:VAL:HG12	1:7:A:LEU:HD11	2	0.21	0.05	0.21
(1,78)	1:6:A:VAL:HG12	1:7:A:LEU:HD12	2	0.21	0.05	0.21
(1,78)	1:6:A:VAL:HG12	1:7:A:LEU:HD13	2	0.21	0.05	0.21
(1,78)	1:6:A:VAL:HG13	1:7:A:LEU:HD11	2	0.21	0.05	0.21

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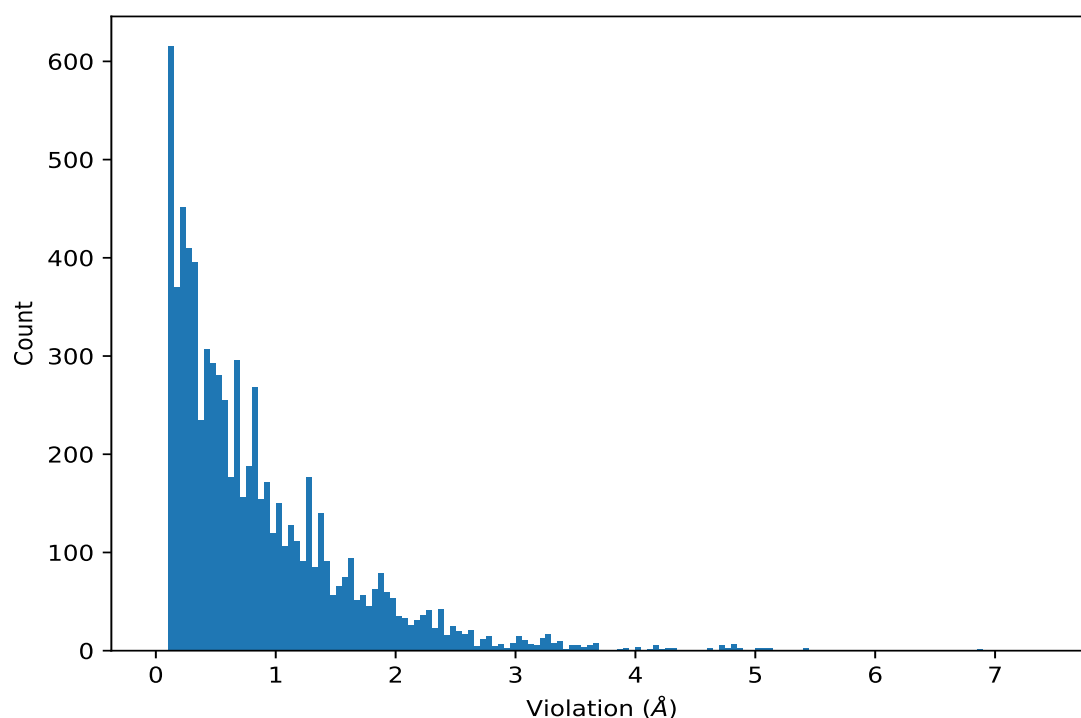
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,78)	1:6:A:VAL:HG13	1:7:A:LEU:HD12	2	0.21	0.05	0.21
(1,78)	1:6:A:VAL:HG13	1:7:A:LEU:HD13	2	0.21	0.05	0.21
(1,406)	1:33:A:ARG:H	1:82:A:ILE:HA	2	0.2	0.09	0.2
(1,375)	1:29:A:SER:HA	1:31:A:ASP:H	2	0.2	0.04	0.2
(1,163)	1:11:A:THR:HA	1:13:A:LYS:H	2	0.18	0.08	0.18
(1,522)	1:41:A:THR:HA	1:44:A:HIS:H	2	0.18	0.08	0.18
(1,311)	1:25:A:TYR:H	1:28:A:PHE:H	2	0.18	0.02	0.18
(1,828)	1:69:A:SER:HB2	1:76:A:LEU:HD21	2	0.17	0.03	0.17
(1,828)	1:69:A:SER:HB2	1:76:A:LEU:HD22	2	0.17	0.03	0.17
(1,828)	1:69:A:SER:HB2	1:76:A:LEU:HD23	2	0.17	0.03	0.17
(1,828)	1:69:A:SER:HB3	1:76:A:LEU:HD21	2	0.17	0.03	0.17
(1,828)	1:69:A:SER:HB3	1:76:A:LEU:HD22	2	0.17	0.03	0.17
(1,828)	1:69:A:SER:HB3	1:76:A:LEU:HD23	2	0.17	0.03	0.17
(1,682)	1:56:A:GLU:H	1:57:A:LYS:HA	2	0.17	0.01	0.17
(1,452)	1:36:A:PHE:H	1:37:A:TYR:HA	2	0.16	0.04	0.16
(1,528)	1:42:A:ASN:H	1:43:A:ALA:HA	2	0.16	0.02	0.16
(1,496)	1:38:A:PHE:HA	1:76:A:LEU:H	2	0.16	0.04	0.16
(1,788)	1:66:A:VAL:H	1:68:A:VAL:H	2	0.16	0.04	0.16
(1,251)	1:22:A:GLU:H	1:23:A:ASP:H	2	0.16	0.02	0.16
(1,360)	1:28:A:PHE:HB2	1:29:A:SER:H	2	0.15	0.01	0.15
(1,360)	1:28:A:PHE:HB3	1:29:A:SER:H	2	0.15	0.01	0.15
(1,529)	1:42:A:ASN:H	1:44:A:HIS:H	2	0.15	0.04	0.15
(1,7)	1:5:A:LEU:H	1:35:A:ILE:HA	2	0.15	0.04	0.15
(1,278)	1:24:A:LEU:H	1:26:A:HIS:H	2	0.13	0.0	0.13
(1,328)	1:26:A:HIS:H	1:29:A:SER:H	2	0.12	0.0	0.12

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



9.5.2 Table : All distance violations [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)
(1,244)	1:21:A:LEU:HG	1:59:A:HIS:HE1	5	7.41
(1,244)	1:21:A:LEU:HG	1:59:A:HIS:HE1	3	7.02
(1,244)	1:21:A:LEU:HG	1:59:A:HIS:HE1	4	6.95
(1,244)	1:21:A:LEU:HG	1:59:A:HIS:HE1	2	6.91
(1,244)	1:21:A:LEU:HG	1:59:A:HIS:HE1	10	6.87
(1,244)	1:21:A:LEU:HG	1:59:A:HIS:HE1	14	6.86
(1,244)	1:21:A:LEU:HG	1:59:A:HIS:HE1	13	6.73
(1,244)	1:21:A:LEU:HG	1:59:A:HIS:HE1	7	6.66
(1,244)	1:21:A:LEU:HG	1:59:A:HIS:HE1	12	6.57
(1,244)	1:21:A:LEU:HG	1:59:A:HIS:HE1	15	6.52
(1,244)	1:21:A:LEU:HG	1:59:A:HIS:HE1	19	6.27
(1,244)	1:21:A:LEU:HG	1:59:A:HIS:HE1	8	6.09
(1,244)	1:21:A:LEU:HG	1:59:A:HIS:HE1	11	5.96
(1,244)	1:21:A:LEU:HG	1:59:A:HIS:HE1	17	5.77
(1,244)	1:21:A:LEU:HG	1:59:A:HIS:HE1	18	5.69
(1,250)	1:21:A:LEU:HD21	1:59:A:HIS:HE1	5	5.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,250)	1:21:A:LEU:HD22	1:59:A:HIS:HE1	5	5.4
(1,250)	1:21:A:LEU:HD23	1:59:A:HIS:HE1	5	5.4
(1,250)	1:21:A:LEU:HD21	1:59:A:HIS:HE1	3	5.11
(1,250)	1:21:A:LEU:HD22	1:59:A:HIS:HE1	3	5.11
(1,250)	1:21:A:LEU:HD23	1:59:A:HIS:HE1	3	5.11
(1,250)	1:21:A:LEU:HD21	1:59:A:HIS:HE1	14	5.06
(1,250)	1:21:A:LEU:HD22	1:59:A:HIS:HE1	14	5.06
(1,250)	1:21:A:LEU:HD23	1:59:A:HIS:HE1	14	5.06
(1,250)	1:21:A:LEU:HD21	1:59:A:HIS:HE1	4	5.03
(1,250)	1:21:A:LEU:HD22	1:59:A:HIS:HE1	4	5.03
(1,250)	1:21:A:LEU:HD23	1:59:A:HIS:HE1	4	5.03
(1,250)	1:21:A:LEU:HD21	1:59:A:HIS:HE1	10	4.89
(1,250)	1:21:A:LEU:HD22	1:59:A:HIS:HE1	10	4.89
(1,250)	1:21:A:LEU:HD23	1:59:A:HIS:HE1	10	4.89
(1,250)	1:21:A:LEU:HD21	1:59:A:HIS:HE1	2	4.82
(1,250)	1:21:A:LEU:HD22	1:59:A:HIS:HE1	2	4.82
(1,250)	1:21:A:LEU:HD23	1:59:A:HIS:HE1	2	4.82
(1,484)	1:37:A:TYR:HD1	1:54:A:PHE:HE1	2	4.81
(1,484)	1:37:A:TYR:HD1	1:54:A:PHE:HE2	2	4.81
(1,484)	1:37:A:TYR:HD2	1:54:A:PHE:HE1	2	4.81
(1,484)	1:37:A:TYR:HD2	1:54:A:PHE:HE2	2	4.81
(1,250)	1:21:A:LEU:HD21	1:59:A:HIS:HE1	13	4.78
(1,250)	1:21:A:LEU:HD22	1:59:A:HIS:HE1	13	4.78
(1,250)	1:21:A:LEU:HD23	1:59:A:HIS:HE1	13	4.78
(1,250)	1:21:A:LEU:HD21	1:59:A:HIS:HE1	7	4.71
(1,250)	1:21:A:LEU:HD22	1:59:A:HIS:HE1	7	4.71
(1,250)	1:21:A:LEU:HD23	1:59:A:HIS:HE1	7	4.71
(1,250)	1:21:A:LEU:HD21	1:59:A:HIS:HE1	12	4.7
(1,250)	1:21:A:LEU:HD22	1:59:A:HIS:HE1	12	4.7
(1,250)	1:21:A:LEU:HD23	1:59:A:HIS:HE1	12	4.7
(1,244)	1:21:A:LEU:HG	1:59:A:HIS:HE1	20	4.68
(1,250)	1:21:A:LEU:HD21	1:59:A:HIS:HE1	15	4.62
(1,250)	1:21:A:LEU:HD22	1:59:A:HIS:HE1	15	4.62
(1,250)	1:21:A:LEU:HD23	1:59:A:HIS:HE1	15	4.62
(1,250)	1:21:A:LEU:HD21	1:59:A:HIS:HE1	8	4.35
(1,250)	1:21:A:LEU:HD22	1:59:A:HIS:HE1	8	4.35
(1,250)	1:21:A:LEU:HD23	1:59:A:HIS:HE1	8	4.35
(1,250)	1:21:A:LEU:HD21	1:59:A:HIS:HE1	19	4.29
(1,250)	1:21:A:LEU:HD22	1:59:A:HIS:HE1	19	4.29
(1,250)	1:21:A:LEU:HD23	1:59:A:HIS:HE1	19	4.29
(1,888)	1:76:A:LEU:HG	1:78:A:GLU:HG2	9	4.2
(1,888)	1:76:A:LEU:HG	1:78:A:GLU:HG3	9	4.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,663)	1:54:A:PHE:HD1	1:76:A:LEU:HG	2	4.18
(1,663)	1:54:A:PHE:HD2	1:76:A:LEU:HG	2	4.18
(1,244)	1:21:A:LEU:HG	1:59:A:HIS:HE1	1	4.18
(1,250)	1:21:A:LEU:HD21	1:59:A:HIS:HE1	11	4.16
(1,250)	1:21:A:LEU:HD22	1:59:A:HIS:HE1	11	4.16
(1,250)	1:21:A:LEU:HD23	1:59:A:HIS:HE1	11	4.16
(1,879)	1:75:A:PHE:HD1	1:77:A:TYR:HD2	5	4.12
(1,879)	1:75:A:PHE:HD2	1:77:A:TYR:HD2	5	4.12
(1,888)	1:76:A:LEU:HG	1:78:A:GLU:HG2	14	4.03
(1,888)	1:76:A:LEU:HG	1:78:A:GLU:HG3	14	4.03
(1,888)	1:76:A:LEU:HG	1:78:A:GLU:HG2	12	4.0
(1,888)	1:76:A:LEU:HG	1:78:A:GLU:HG3	12	4.0
(1,250)	1:21:A:LEU:HD21	1:59:A:HIS:HE1	17	3.94
(1,250)	1:21:A:LEU:HD22	1:59:A:HIS:HE1	17	3.94
(1,250)	1:21:A:LEU:HD23	1:59:A:HIS:HE1	17	3.94
(1,888)	1:76:A:LEU:HG	1:78:A:GLU:HG2	18	3.88
(1,888)	1:76:A:LEU:HG	1:78:A:GLU:HG3	18	3.88
(1,129)	1:7:A:LEU:HD11	1:14:A:SER:HG	12	3.68
(1,129)	1:7:A:LEU:HD12	1:14:A:SER:HG	12	3.68
(1,129)	1:7:A:LEU:HD13	1:14:A:SER:HG	12	3.68
(1,609)	1:50:A:ALA:HA	1:54:A:PHE:HE1	2	3.67
(1,609)	1:50:A:ALA:HA	1:54:A:PHE:HE2	2	3.67
(1,250)	1:21:A:LEU:HD21	1:59:A:HIS:HE1	18	3.66
(1,250)	1:21:A:LEU:HD22	1:59:A:HIS:HE1	18	3.66
(1,250)	1:21:A:LEU:HD23	1:59:A:HIS:HE1	18	3.66
(1,888)	1:76:A:LEU:HG	1:78:A:GLU:HG2	16	3.64
(1,888)	1:76:A:LEU:HG	1:78:A:GLU:HG3	16	3.64
(1,888)	1:76:A:LEU:HG	1:78:A:GLU:HG2	11	3.63
(1,888)	1:76:A:LEU:HG	1:78:A:GLU:HG3	11	3.63
(1,370)	1:28:A:PHE:HE1	1:81:A:ILE:HA	20	3.6
(1,370)	1:28:A:PHE:HE2	1:81:A:ILE:HA	20	3.6
(1,888)	1:76:A:LEU:HG	1:78:A:GLU:HG2	8	3.56
(1,888)	1:76:A:LEU:HG	1:78:A:GLU:HG3	8	3.56
(1,879)	1:75:A:PHE:HD1	1:77:A:TYR:HD2	15	3.56
(1,879)	1:75:A:PHE:HD2	1:77:A:TYR:HD2	15	3.56
(1,879)	1:75:A:PHE:HD1	1:77:A:TYR:HD2	20	3.54
(1,879)	1:75:A:PHE:HD2	1:77:A:TYR:HD2	20	3.54
(1,879)	1:75:A:PHE:HD1	1:77:A:TYR:HD2	10	3.53
(1,879)	1:75:A:PHE:HD2	1:77:A:TYR:HD2	10	3.53
(1,879)	1:75:A:PHE:HD1	1:77:A:TYR:HD2	8	3.52
(1,879)	1:75:A:PHE:HD2	1:77:A:TYR:HD2	8	3.52
(1,879)	1:75:A:PHE:HD1	1:77:A:TYR:HD2	19	3.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,879)	1:75:A:PHE:HD2	1:77:A:TYR:HD2	19	3.49
(1,879)	1:75:A:PHE:HD1	1:77:A:TYR:HD2	12	3.48
(1,879)	1:75:A:PHE:HD2	1:77:A:TYR:HD2	12	3.48
(1,888)	1:76:A:LEU:HG	1:78:A:GLU:HG2	20	3.47
(1,888)	1:76:A:LEU:HG	1:78:A:GLU:HG3	20	3.47
(1,879)	1:75:A:PHE:HD1	1:77:A:TYR:HD2	9	3.44
(1,879)	1:75:A:PHE:HD2	1:77:A:TYR:HD2	9	3.44
(1,879)	1:75:A:PHE:HD1	1:77:A:TYR:HD2	13	3.4
(1,879)	1:75:A:PHE:HD2	1:77:A:TYR:HD2	13	3.4
(1,743)	1:62:A:TYR:HE1	1:63:A:LEU:HD21	6	3.39
(1,743)	1:62:A:TYR:HE1	1:63:A:LEU:HD22	6	3.39
(1,743)	1:62:A:TYR:HE1	1:63:A:LEU:HD23	6	3.39
(1,743)	1:62:A:TYR:HE2	1:63:A:LEU:HD21	6	3.39
(1,743)	1:62:A:TYR:HE2	1:63:A:LEU:HD22	6	3.39
(1,743)	1:62:A:TYR:HE2	1:63:A:LEU:HD23	6	3.39
(1,898)	1:77:A:TYR:HB2	1:79:A:LEU:HG	12	3.36
(1,898)	1:77:A:TYR:HB3	1:79:A:LEU:HG	12	3.36
(1,743)	1:62:A:TYR:HE1	1:63:A:LEU:HD21	11	3.33
(1,743)	1:62:A:TYR:HE1	1:63:A:LEU:HD22	11	3.33
(1,743)	1:62:A:TYR:HE1	1:63:A:LEU:HD23	11	3.33
(1,743)	1:62:A:TYR:HE2	1:63:A:LEU:HD21	11	3.33
(1,743)	1:62:A:TYR:HE2	1:63:A:LEU:HD22	11	3.33
(1,743)	1:62:A:TYR:HE2	1:63:A:LEU:HD23	11	3.33
(1,879)	1:75:A:PHE:HD1	1:77:A:TYR:HD2	4	3.32
(1,879)	1:75:A:PHE:HD2	1:77:A:TYR:HD2	4	3.32
(1,370)	1:28:A:PHE:HE1	1:81:A:ILE:HA	6	3.3
(1,370)	1:28:A:PHE:HE2	1:81:A:ILE:HA	6	3.3
(1,743)	1:62:A:TYR:HE1	1:63:A:LEU:HD21	14	3.29
(1,743)	1:62:A:TYR:HE1	1:63:A:LEU:HD22	14	3.29
(1,743)	1:62:A:TYR:HE1	1:63:A:LEU:HD23	14	3.29
(1,743)	1:62:A:TYR:HE2	1:63:A:LEU:HD21	14	3.29
(1,743)	1:62:A:TYR:HE2	1:63:A:LEU:HD22	14	3.29
(1,743)	1:62:A:TYR:HE2	1:63:A:LEU:HD23	14	3.29
(1,743)	1:62:A:TYR:HE1	1:63:A:LEU:HD21	9	3.27
(1,743)	1:62:A:TYR:HE1	1:63:A:LEU:HD22	9	3.27
(1,743)	1:62:A:TYR:HE1	1:63:A:LEU:HD23	9	3.27
(1,743)	1:62:A:TYR:HE2	1:63:A:LEU:HD21	9	3.27
(1,743)	1:62:A:TYR:HE2	1:63:A:LEU:HD22	9	3.27
(1,743)	1:62:A:TYR:HE2	1:63:A:LEU:HD23	9	3.27
(1,244)	1:21:A:LEU:HG	1:59:A:HIS:HE1	9	3.27
(1,888)	1:76:A:LEU:HG	1:78:A:GLU:HG2	19	3.26
(1,888)	1:76:A:LEU:HG	1:78:A:GLU:HG3	19	3.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,888)	1:76:A:LEU:HG	1:78:A:GLU:HG2	5	3.23
(1,888)	1:76:A:LEU:HG	1:78:A:GLU:HG3	5	3.23
(1,879)	1:75:A:PHE:HD1	1:77:A:TYR:HD2	2	3.23
(1,879)	1:75:A:PHE:HD2	1:77:A:TYR:HD2	2	3.23
(1,879)	1:75:A:PHE:HD1	1:77:A:TYR:HD2	6	3.23
(1,879)	1:75:A:PHE:HD2	1:77:A:TYR:HD2	6	3.23
(1,743)	1:62:A:TYR:HE1	1:63:A:LEU:HD21	3	3.2
(1,743)	1:62:A:TYR:HE1	1:63:A:LEU:HD22	3	3.2
(1,743)	1:62:A:TYR:HE1	1:63:A:LEU:HD23	3	3.2
(1,743)	1:62:A:TYR:HE2	1:63:A:LEU:HD21	3	3.2
(1,743)	1:62:A:TYR:HE2	1:63:A:LEU:HD22	3	3.2
(1,743)	1:62:A:TYR:HE2	1:63:A:LEU:HD23	3	3.2
(1,288)	1:24:A:LEU:HA	1:80:A:HIS:HE1	17	3.2
(1,743)	1:62:A:TYR:HE1	1:63:A:LEU:HD21	19	3.16
(1,743)	1:62:A:TYR:HE1	1:63:A:LEU:HD22	19	3.16
(1,743)	1:62:A:TYR:HE1	1:63:A:LEU:HD23	19	3.16
(1,743)	1:62:A:TYR:HE2	1:63:A:LEU:HD21	19	3.16
(1,743)	1:62:A:TYR:HE2	1:63:A:LEU:HD22	19	3.16
(1,743)	1:62:A:TYR:HE2	1:63:A:LEU:HD23	19	3.16
(1,908)	1:78:A:GLU:HA	1:80:A:HIS:HD2	7	3.14
(1,879)	1:75:A:PHE:HD1	1:77:A:TYR:HD2	11	3.12
(1,879)	1:75:A:PHE:HD2	1:77:A:TYR:HD2	11	3.12
(1,878)	1:75:A:PHE:HB2	1:77:A:TYR:HD1	1	3.11
(1,878)	1:75:A:PHE:HB2	1:77:A:TYR:HD2	1	3.11
(1,878)	1:75:A:PHE:HB3	1:77:A:TYR:HD1	1	3.11
(1,878)	1:75:A:PHE:HB3	1:77:A:TYR:HD2	1	3.11
(1,743)	1:62:A:TYR:HE1	1:63:A:LEU:HD21	20	3.08
(1,743)	1:62:A:TYR:HE1	1:63:A:LEU:HD22	20	3.08
(1,743)	1:62:A:TYR:HE1	1:63:A:LEU:HD23	20	3.08
(1,743)	1:62:A:TYR:HE2	1:63:A:LEU:HD21	20	3.08
(1,743)	1:62:A:TYR:HE2	1:63:A:LEU:HD22	20	3.08
(1,743)	1:62:A:TYR:HE2	1:63:A:LEU:HD23	20	3.08
(1,908)	1:78:A:GLU:HA	1:80:A:HIS:HD2	3	3.07
(1,888)	1:76:A:LEU:HG	1:78:A:GLU:HG2	3	3.06
(1,888)	1:76:A:LEU:HG	1:78:A:GLU:HG3	3	3.06
(1,888)	1:76:A:LEU:HG	1:78:A:GLU:HG2	7	3.06
(1,888)	1:76:A:LEU:HG	1:78:A:GLU:HG3	7	3.06
(1,242)	1:21:A:LEU:HG	1:57:A:LYS:HD2	18	3.04
(1,242)	1:21:A:LEU:HG	1:57:A:LYS:HD3	18	3.04
(1,888)	1:76:A:LEU:HG	1:78:A:GLU:HG2	2	3.02
(1,888)	1:76:A:LEU:HG	1:78:A:GLU:HG3	2	3.02
(1,743)	1:62:A:TYR:HE1	1:63:A:LEU:HD21	17	3.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,743)	1:62:A:TYR:HE1	1:63:A:LEU:HD22	17	3.02
(1,743)	1:62:A:TYR:HE1	1:63:A:LEU:HD23	17	3.02
(1,743)	1:62:A:TYR:HE2	1:63:A:LEU:HD21	17	3.02
(1,743)	1:62:A:TYR:HE2	1:63:A:LEU:HD22	17	3.02
(1,743)	1:62:A:TYR:HE2	1:63:A:LEU:HD23	17	3.02
(1,888)	1:76:A:LEU:HG	1:78:A:GLU:HG2	10	3.01
(1,888)	1:76:A:LEU:HG	1:78:A:GLU:HG3	10	3.01
(1,908)	1:78:A:GLU:HA	1:80:A:HIS:HD2	9	3.0
(1,197)	1:18:A:SER:HA	1:20:A:GLU:HG2	7	3.0
(1,197)	1:18:A:SER:HA	1:20:A:GLU:HG3	7	3.0
(1,369)	1:28:A:PHE:HE1	1:81:A:ILE:H	20	2.99
(1,369)	1:28:A:PHE:HE2	1:81:A:ILE:H	20	2.99
(1,888)	1:76:A:LEU:HG	1:78:A:GLU:HG2	4	2.95
(1,888)	1:76:A:LEU:HG	1:78:A:GLU:HG3	4	2.95
(1,888)	1:76:A:LEU:HG	1:78:A:GLU:HG2	6	2.95
(1,888)	1:76:A:LEU:HG	1:78:A:GLU:HG3	6	2.95
(1,888)	1:76:A:LEU:HG	1:78:A:GLU:HG2	13	2.95
(1,888)	1:76:A:LEU:HG	1:78:A:GLU:HG3	13	2.95
(1,898)	1:77:A:TYR:HB2	1:79:A:LEU:HG	3	2.94
(1,898)	1:77:A:TYR:HB3	1:79:A:LEU:HG	3	2.94
(1,8)	1:5:A:LEU:H	1:35:A:ILE:HB	16	2.93
(1,888)	1:76:A:LEU:HG	1:78:A:GLU:HG2	15	2.89
(1,888)	1:76:A:LEU:HG	1:78:A:GLU:HG3	15	2.89
(1,242)	1:21:A:LEU:HG	1:57:A:LYS:HD2	10	2.89
(1,242)	1:21:A:LEU:HG	1:57:A:LYS:HD3	10	2.89
(1,879)	1:75:A:PHE:HD1	1:77:A:TYR:HD2	7	2.88
(1,879)	1:75:A:PHE:HD2	1:77:A:TYR:HD2	7	2.88
(1,524)	1:41:A:THR:HB	1:73:A:LYS:HA	8	2.85
(1,878)	1:75:A:PHE:HB2	1:77:A:TYR:HD1	14	2.84
(1,878)	1:75:A:PHE:HB2	1:77:A:TYR:HD2	14	2.84
(1,878)	1:75:A:PHE:HB3	1:77:A:TYR:HD1	14	2.84
(1,878)	1:75:A:PHE:HB3	1:77:A:TYR:HD2	14	2.84
(1,524)	1:41:A:THR:HB	1:73:A:LYS:HA	11	2.81
(1,879)	1:75:A:PHE:HD1	1:77:A:TYR:HD2	16	2.8
(1,879)	1:75:A:PHE:HD2	1:77:A:TYR:HD2	16	2.8
(1,288)	1:24:A:LEU:HA	1:80:A:HIS:HE1	13	2.8
(1,244)	1:21:A:LEU:HG	1:59:A:HIS:HE1	16	2.8
(1,197)	1:18:A:SER:HA	1:20:A:GLU:HG2	16	2.79
(1,197)	1:18:A:SER:HA	1:20:A:GLU:HG3	16	2.79
(1,197)	1:18:A:SER:HA	1:20:A:GLU:HG2	6	2.78
(1,197)	1:18:A:SER:HA	1:20:A:GLU:HG3	6	2.78
(1,878)	1:75:A:PHE:HB2	1:77:A:TYR:HD1	18	2.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,878)	1:75:A:PHE:HB2	1:77:A:TYR:HD2	18	2.77
(1,878)	1:75:A:PHE:HB3	1:77:A:TYR:HD1	18	2.77
(1,878)	1:75:A:PHE:HB3	1:77:A:TYR:HD2	18	2.77
(1,202)	1:19:A:VAL:H	1:20:A:GLU:HG2	7	2.76
(1,202)	1:19:A:VAL:H	1:20:A:GLU:HG3	7	2.76
(1,908)	1:78:A:GLU:HA	1:80:A:HIS:HD2	17	2.75
(1,250)	1:21:A:LEU:HD21	1:59:A:HIS:HE1	20	2.73
(1,250)	1:21:A:LEU:HD22	1:59:A:HIS:HE1	20	2.73
(1,250)	1:21:A:LEU:HD23	1:59:A:HIS:HE1	20	2.73
(1,242)	1:21:A:LEU:HG	1:57:A:LYS:HD2	19	2.73
(1,242)	1:21:A:LEU:HG	1:57:A:LYS:HD3	19	2.73
(1,418)	1:34:A:SER:H	1:79:A:LEU:HD21	12	2.71
(1,418)	1:34:A:SER:H	1:79:A:LEU:HD22	12	2.71
(1,418)	1:34:A:SER:H	1:79:A:LEU:HD23	12	2.71
(1,242)	1:21:A:LEU:HG	1:57:A:LYS:HD2	9	2.71
(1,242)	1:21:A:LEU:HG	1:57:A:LYS:HD3	9	2.71
(1,898)	1:77:A:TYR:HB2	1:79:A:LEU:HG	17	2.7
(1,898)	1:77:A:TYR:HB3	1:79:A:LEU:HG	17	2.7
(1,250)	1:21:A:LEU:HD21	1:59:A:HIS:HE1	1	2.66
(1,250)	1:21:A:LEU:HD22	1:59:A:HIS:HE1	1	2.66
(1,250)	1:21:A:LEU:HD23	1:59:A:HIS:HE1	1	2.66
(1,202)	1:19:A:VAL:H	1:20:A:GLU:HG2	16	2.66
(1,202)	1:19:A:VAL:H	1:20:A:GLU:HG3	16	2.66
(1,244)	1:21:A:LEU:HG	1:59:A:HIS:HE1	6	2.63
(1,547)	1:44:A:HIS:HB2	1:48:A:LEU:HD11	10	2.62
(1,547)	1:44:A:HIS:HB2	1:48:A:LEU:HD12	10	2.62
(1,547)	1:44:A:HIS:HB2	1:48:A:LEU:HD13	10	2.62
(1,547)	1:44:A:HIS:HB3	1:48:A:LEU:HD11	10	2.62
(1,547)	1:44:A:HIS:HB3	1:48:A:LEU:HD12	10	2.62
(1,547)	1:44:A:HIS:HB3	1:48:A:LEU:HD13	10	2.62
(1,369)	1:28:A:PHE:HE1	1:81:A:ILE:H	6	2.62
(1,369)	1:28:A:PHE:HE2	1:81:A:ILE:H	6	2.62
(1,202)	1:19:A:VAL:H	1:20:A:GLU:HG2	4	2.62
(1,202)	1:19:A:VAL:H	1:20:A:GLU:HG3	4	2.62
(1,202)	1:19:A:VAL:H	1:20:A:GLU:HG2	12	2.62
(1,202)	1:19:A:VAL:H	1:20:A:GLU:HG3	12	2.62
(1,743)	1:62:A:TYR:HE1	1:63:A:LEU:HD21	12	2.61
(1,743)	1:62:A:TYR:HE1	1:63:A:LEU:HD22	12	2.61
(1,743)	1:62:A:TYR:HE1	1:63:A:LEU:HD23	12	2.61
(1,743)	1:62:A:TYR:HE2	1:63:A:LEU:HD21	12	2.61
(1,743)	1:62:A:TYR:HE2	1:63:A:LEU:HD22	12	2.61
(1,743)	1:62:A:TYR:HE2	1:63:A:LEU:HD23	12	2.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,202)	1:19:A:VAL:H	1:20:A:GLU:HG2	6	2.6
(1,202)	1:19:A:VAL:H	1:20:A:GLU:HG3	6	2.6
(1,547)	1:44:A:HIS:HB2	1:48:A:LEU:HD11	2	2.58
(1,547)	1:44:A:HIS:HB2	1:48:A:LEU:HD12	2	2.58
(1,547)	1:44:A:HIS:HB2	1:48:A:LEU:HD13	2	2.58
(1,547)	1:44:A:HIS:HB3	1:48:A:LEU:HD11	2	2.58
(1,547)	1:44:A:HIS:HB3	1:48:A:LEU:HD12	2	2.58
(1,547)	1:44:A:HIS:HB3	1:48:A:LEU:HD13	2	2.58
(1,298)	1:24:A:LEU:HG	1:80:A:HIS:HE1	17	2.58
(1,448)	1:35:A:ILE:HG12	1:76:A:LEU:HB2	9	2.57
(1,448)	1:35:A:ILE:HG12	1:76:A:LEU:HB3	9	2.57
(1,448)	1:35:A:ILE:HG13	1:76:A:LEU:HB2	9	2.57
(1,448)	1:35:A:ILE:HG13	1:76:A:LEU:HB3	9	2.57
(1,197)	1:18:A:SER:HA	1:20:A:GLU:HG2	15	2.57
(1,197)	1:18:A:SER:HA	1:20:A:GLU:HG3	15	2.57
(1,123)	1:7:A:LEU:HB2	1:38:A:PHE:HD1	18	2.56
(1,123)	1:7:A:LEU:HB2	1:38:A:PHE:HD2	18	2.56
(1,123)	1:7:A:LEU:HB3	1:38:A:PHE:HD1	18	2.56
(1,123)	1:7:A:LEU:HB3	1:38:A:PHE:HD2	18	2.56
(1,202)	1:19:A:VAL:H	1:20:A:GLU:HG2	3	2.55
(1,202)	1:19:A:VAL:H	1:20:A:GLU:HG3	3	2.55
(1,202)	1:19:A:VAL:H	1:20:A:GLU:HG2	10	2.54
(1,202)	1:19:A:VAL:H	1:20:A:GLU:HG3	10	2.54
(1,888)	1:76:A:LEU:HG	1:78:A:GLU:HG2	1	2.53
(1,888)	1:76:A:LEU:HG	1:78:A:GLU:HG3	1	2.53
(1,395)	1:31:A:ASP:HA	1:81:A:ILE:HG21	10	2.53
(1,395)	1:31:A:ASP:HA	1:81:A:ILE:HG22	10	2.53
(1,395)	1:31:A:ASP:HA	1:81:A:ILE:HG23	10	2.53
(1,390)	1:31:A:ASP:H	1:81:A:ILE:HG21	10	2.53
(1,390)	1:31:A:ASP:H	1:81:A:ILE:HG22	10	2.53
(1,390)	1:31:A:ASP:H	1:81:A:ILE:HG23	10	2.53
(1,202)	1:19:A:VAL:H	1:20:A:GLU:HG2	19	2.52
(1,202)	1:19:A:VAL:H	1:20:A:GLU:HG3	19	2.52
(1,197)	1:18:A:SER:HA	1:20:A:GLU:HG2	4	2.52
(1,197)	1:18:A:SER:HA	1:20:A:GLU:HG3	4	2.52
(1,129)	1:7:A:LEU:HD11	1:14:A:SER:HG	6	2.52
(1,129)	1:7:A:LEU:HD12	1:14:A:SER:HG	6	2.52
(1,129)	1:7:A:LEU:HD13	1:14:A:SER:HG	6	2.52
(1,524)	1:41:A:THR:HB	1:73:A:LYS:HA	9	2.5
(1,8)	1:5:A:LEU:H	1:35:A:ILE:HB	11	2.49
(1,547)	1:44:A:HIS:HB2	1:48:A:LEU:HD11	11	2.48
(1,547)	1:44:A:HIS:HB2	1:48:A:LEU:HD12	11	2.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,547)	1:44:A:HIS:HB2	1:48:A:LEU:HD13	11	2.48
(1,547)	1:44:A:HIS:HB3	1:48:A:LEU:HD11	11	2.48
(1,547)	1:44:A:HIS:HB3	1:48:A:LEU:HD12	11	2.48
(1,547)	1:44:A:HIS:HB3	1:48:A:LEU:HD13	11	2.48
(1,547)	1:44:A:HIS:HB2	1:48:A:LEU:HD11	20	2.48
(1,547)	1:44:A:HIS:HB2	1:48:A:LEU:HD12	20	2.48
(1,547)	1:44:A:HIS:HB2	1:48:A:LEU:HD13	20	2.48
(1,547)	1:44:A:HIS:HB3	1:48:A:LEU:HD11	20	2.48
(1,547)	1:44:A:HIS:HB3	1:48:A:LEU:HD12	20	2.48
(1,547)	1:44:A:HIS:HB3	1:48:A:LEU:HD13	20	2.48
(1,123)	1:7:A:LEU:HB2	1:38:A:PHE:HD1	5	2.46
(1,123)	1:7:A:LEU:HB2	1:38:A:PHE:HD2	5	2.46
(1,123)	1:7:A:LEU:HB3	1:38:A:PHE:HD1	5	2.46
(1,123)	1:7:A:LEU:HB3	1:38:A:PHE:HD2	5	2.46
(1,879)	1:75:A:PHE:HD1	1:77:A:TYR:HD2	14	2.45
(1,879)	1:75:A:PHE:HD2	1:77:A:TYR:HD2	14	2.45
(1,547)	1:44:A:HIS:HB2	1:48:A:LEU:HD11	5	2.45
(1,547)	1:44:A:HIS:HB2	1:48:A:LEU:HD12	5	2.45
(1,547)	1:44:A:HIS:HB2	1:48:A:LEU:HD13	5	2.45
(1,547)	1:44:A:HIS:HB3	1:48:A:LEU:HD11	5	2.45
(1,547)	1:44:A:HIS:HB3	1:48:A:LEU:HD12	5	2.45
(1,547)	1:44:A:HIS:HB3	1:48:A:LEU:HD13	5	2.45
(1,908)	1:78:A:GLU:HA	1:80:A:HIS:HD2	14	2.44
(1,746)	1:63:A:LEU:HA	1:76:A:LEU:HD11	9	2.44
(1,746)	1:63:A:LEU:HA	1:76:A:LEU:HD12	9	2.44
(1,746)	1:63:A:LEU:HA	1:76:A:LEU:HD13	9	2.44
(1,663)	1:54:A:PHE:HD1	1:76:A:LEU:HG	9	2.44
(1,663)	1:54:A:PHE:HD2	1:76:A:LEU:HG	9	2.44
(1,663)	1:54:A:PHE:HD1	1:76:A:LEU:HG	20	2.44
(1,663)	1:54:A:PHE:HD2	1:76:A:LEU:HG	20	2.44
(1,288)	1:24:A:LEU:HA	1:80:A:HIS:HE1	3	2.44
(1,288)	1:24:A:LEU:HA	1:80:A:HIS:HE1	7	2.44
(1,27)	1:5:A:LEU:HG	1:7:A:LEU:H	3	2.43
(1,288)	1:24:A:LEU:HA	1:80:A:HIS:HE1	9	2.42
(1,202)	1:19:A:VAL:H	1:20:A:GLU:HG2	13	2.42
(1,202)	1:19:A:VAL:H	1:20:A:GLU:HG3	13	2.42
(1,202)	1:19:A:VAL:H	1:20:A:GLU:HG2	11	2.41
(1,202)	1:19:A:VAL:H	1:20:A:GLU:HG3	11	2.41
(1,547)	1:44:A:HIS:HB2	1:48:A:LEU:HD11	12	2.4
(1,547)	1:44:A:HIS:HB2	1:48:A:LEU:HD12	12	2.4
(1,547)	1:44:A:HIS:HB2	1:48:A:LEU:HD13	12	2.4
(1,547)	1:44:A:HIS:HB3	1:48:A:LEU:HD11	12	2.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,547)	1:44:A:HIS:HB3	1:48:A:LEU:HD12	12	2.4
(1,547)	1:44:A:HIS:HB3	1:48:A:LEU:HD13	12	2.4
(1,495)	1:38:A:PHE:HA	1:75:A:PHE:HD1	1	2.4
(1,495)	1:38:A:PHE:HA	1:75:A:PHE:HD2	1	2.4
(1,27)	1:5:A:LEU:HG	1:7:A:LEU:H	4	2.4
(1,351)	1:28:A:PHE:H	1:81:A:ILE:HG21	10	2.39
(1,351)	1:28:A:PHE:H	1:81:A:ILE:HG22	10	2.39
(1,351)	1:28:A:PHE:H	1:81:A:ILE:HG23	10	2.39
(1,288)	1:24:A:LEU:HA	1:80:A:HIS:HE1	11	2.39
(1,202)	1:19:A:VAL:H	1:20:A:GLU:HG2	2	2.39
(1,202)	1:19:A:VAL:H	1:20:A:GLU:HG3	2	2.39
(1,743)	1:62:A:TYR:HE1	1:63:A:LEU:HD21	1	2.38
(1,743)	1:62:A:TYR:HE1	1:63:A:LEU:HD22	1	2.38
(1,743)	1:62:A:TYR:HE1	1:63:A:LEU:HD23	1	2.38
(1,743)	1:62:A:TYR:HE2	1:63:A:LEU:HD21	1	2.38
(1,743)	1:62:A:TYR:HE2	1:63:A:LEU:HD22	1	2.38
(1,743)	1:62:A:TYR:HE2	1:63:A:LEU:HD23	1	2.38
(1,547)	1:44:A:HIS:HB2	1:48:A:LEU:HD11	14	2.37
(1,547)	1:44:A:HIS:HB2	1:48:A:LEU:HD12	14	2.37
(1,547)	1:44:A:HIS:HB2	1:48:A:LEU:HD13	14	2.37
(1,547)	1:44:A:HIS:HB3	1:48:A:LEU:HD11	14	2.37
(1,547)	1:44:A:HIS:HB3	1:48:A:LEU:HD12	14	2.37
(1,547)	1:44:A:HIS:HB3	1:48:A:LEU:HD13	14	2.37
(1,27)	1:5:A:LEU:HG	1:7:A:LEU:H	17	2.37
(1,239)	1:21:A:LEU:HG	1:56:A:GLU:HB2	18	2.36
(1,239)	1:21:A:LEU:HG	1:56:A:GLU:HB3	18	2.36
(1,888)	1:76:A:LEU:HG	1:78:A:GLU:HG2	17	2.35
(1,888)	1:76:A:LEU:HG	1:78:A:GLU:HG3	17	2.35
(1,547)	1:44:A:HIS:HB2	1:48:A:LEU:HD11	18	2.35
(1,547)	1:44:A:HIS:HB2	1:48:A:LEU:HD12	18	2.35
(1,547)	1:44:A:HIS:HB2	1:48:A:LEU:HD13	18	2.35
(1,547)	1:44:A:HIS:HB3	1:48:A:LEU:HD11	18	2.35
(1,547)	1:44:A:HIS:HB3	1:48:A:LEU:HD12	18	2.35
(1,547)	1:44:A:HIS:HB3	1:48:A:LEU:HD13	18	2.35
(1,242)	1:21:A:LEU:HG	1:57:A:LYS:HD2	14	2.35
(1,242)	1:21:A:LEU:HG	1:57:A:LYS:HD3	14	2.35
(1,202)	1:19:A:VAL:H	1:20:A:GLU:HG2	15	2.35
(1,202)	1:19:A:VAL:H	1:20:A:GLU:HG3	15	2.35
(1,123)	1:7:A:LEU:HB2	1:38:A:PHE:HD1	2	2.34
(1,123)	1:7:A:LEU:HB2	1:38:A:PHE:HD2	2	2.34
(1,123)	1:7:A:LEU:HB3	1:38:A:PHE:HD1	2	2.34
(1,123)	1:7:A:LEU:HB3	1:38:A:PHE:HD2	2	2.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,284)	1:24:A:LEU:HA	1:35:A:ILE:HD11	4	2.33
(1,284)	1:24:A:LEU:HA	1:35:A:ILE:HD12	4	2.33
(1,284)	1:24:A:LEU:HA	1:35:A:ILE:HD13	4	2.33
(1,35)	1:5:A:LEU:HD11	1:7:A:LEU:HG	17	2.33
(1,35)	1:5:A:LEU:HD12	1:7:A:LEU:HG	17	2.33
(1,35)	1:5:A:LEU:HD13	1:7:A:LEU:HG	17	2.33
(1,35)	1:5:A:LEU:HD21	1:7:A:LEU:HG	17	2.33
(1,35)	1:5:A:LEU:HD22	1:7:A:LEU:HG	17	2.33
(1,35)	1:5:A:LEU:HD23	1:7:A:LEU:HG	17	2.33
(1,448)	1:35:A:ILE:HG12	1:76:A:LEU:HB2	11	2.32
(1,448)	1:35:A:ILE:HG12	1:76:A:LEU:HB3	11	2.32
(1,448)	1:35:A:ILE:HG13	1:76:A:LEU:HB2	11	2.32
(1,448)	1:35:A:ILE:HG13	1:76:A:LEU:HB3	11	2.32
(1,35)	1:5:A:LEU:HD11	1:7:A:LEU:HG	18	2.31
(1,35)	1:5:A:LEU:HD12	1:7:A:LEU:HG	18	2.31
(1,35)	1:5:A:LEU:HD13	1:7:A:LEU:HG	18	2.31
(1,35)	1:5:A:LEU:HD21	1:7:A:LEU:HG	18	2.31
(1,35)	1:5:A:LEU:HD22	1:7:A:LEU:HG	18	2.31
(1,35)	1:5:A:LEU:HD23	1:7:A:LEU:HG	18	2.31
(1,547)	1:44:A:HIS:HB2	1:48:A:LEU:HD11	9	2.3
(1,547)	1:44:A:HIS:HB2	1:48:A:LEU:HD12	9	2.3
(1,547)	1:44:A:HIS:HB2	1:48:A:LEU:HD13	9	2.3
(1,547)	1:44:A:HIS:HB3	1:48:A:LEU:HD11	9	2.3
(1,547)	1:44:A:HIS:HB3	1:48:A:LEU:HD12	9	2.3
(1,547)	1:44:A:HIS:HB3	1:48:A:LEU:HD13	9	2.3
(1,524)	1:41:A:THR:HB	1:73:A:LYS:HA	3	2.3
(1,351)	1:28:A:PHE:H	1:81:A:ILE:HG21	12	2.29
(1,351)	1:28:A:PHE:H	1:81:A:ILE:HG22	12	2.29
(1,351)	1:28:A:PHE:H	1:81:A:ILE:HG23	12	2.29
(1,304)	1:24:A:LEU:HD21	1:59:A:HIS:HE1	4	2.29
(1,304)	1:24:A:LEU:HD22	1:59:A:HIS:HE1	4	2.29
(1,304)	1:24:A:LEU:HD23	1:59:A:HIS:HE1	4	2.29
(1,663)	1:54:A:PHE:HD1	1:76:A:LEU:HG	7	2.27
(1,663)	1:54:A:PHE:HD2	1:76:A:LEU:HG	7	2.27
(1,304)	1:24:A:LEU:HD21	1:59:A:HIS:HE1	8	2.27
(1,304)	1:24:A:LEU:HD22	1:59:A:HIS:HE1	8	2.27
(1,304)	1:24:A:LEU:HD23	1:59:A:HIS:HE1	8	2.27
(1,285)	1:24:A:LEU:HA	1:54:A:PHE:HE1	2	2.27
(1,285)	1:24:A:LEU:HA	1:54:A:PHE:HE2	2	2.27
(1,123)	1:7:A:LEU:HB2	1:38:A:PHE:HD1	1	2.27
(1,123)	1:7:A:LEU:HB2	1:38:A:PHE:HD2	1	2.27
(1,123)	1:7:A:LEU:HB3	1:38:A:PHE:HD1	1	2.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,123)	1:7:A:LEU:HB3	1:38:A:PHE:HD2	1	2.27
(1,28)	1:5:A:LEU:HG	1:7:A:LEU:HG	18	2.27
(1,27)	1:5:A:LEU:HG	1:7:A:LEU:H	7	2.27
(1,547)	1:44:A:HIS:HB2	1:48:A:LEU:HD11	3	2.26
(1,547)	1:44:A:HIS:HB2	1:48:A:LEU:HD12	3	2.26
(1,547)	1:44:A:HIS:HB2	1:48:A:LEU:HD13	3	2.26
(1,547)	1:44:A:HIS:HB3	1:48:A:LEU:HD11	3	2.26
(1,547)	1:44:A:HIS:HB3	1:48:A:LEU:HD12	3	2.26
(1,547)	1:44:A:HIS:HB3	1:48:A:LEU:HD13	3	2.26
(1,202)	1:19:A:VAL:H	1:20:A:GLU:HG2	18	2.26
(1,202)	1:19:A:VAL:H	1:20:A:GLU:HG3	18	2.26
(1,197)	1:18:A:SER:HA	1:20:A:GLU:HG2	12	2.26
(1,197)	1:18:A:SER:HA	1:20:A:GLU:HG3	12	2.26
(1,8)	1:5:A:LEU:H	1:35:A:ILE:HB	3	2.26
(1,197)	1:18:A:SER:HA	1:20:A:GLU:HG2	18	2.25
(1,197)	1:18:A:SER:HA	1:20:A:GLU:HG3	18	2.25
(1,28)	1:5:A:LEU:HG	1:7:A:LEU:HG	17	2.25
(1,27)	1:5:A:LEU:HG	1:7:A:LEU:H	18	2.25
(1,450)	1:35:A:ILE:HD11	1:54:A:PHE:HE1	2	2.24
(1,450)	1:35:A:ILE:HD11	1:54:A:PHE:HE2	2	2.24
(1,450)	1:35:A:ILE:HD12	1:54:A:PHE:HE1	2	2.24
(1,450)	1:35:A:ILE:HD12	1:54:A:PHE:HE2	2	2.24
(1,450)	1:35:A:ILE:HD13	1:54:A:PHE:HE1	2	2.24
(1,450)	1:35:A:ILE:HD13	1:54:A:PHE:HE2	2	2.24
(1,450)	1:35:A:ILE:HD11	1:54:A:PHE:HE1	2	2.24
(1,450)	1:35:A:ILE:HD11	1:54:A:PHE:HE2	2	2.24
(1,450)	1:35:A:ILE:HD12	1:54:A:PHE:HE1	2	2.24
(1,450)	1:35:A:ILE:HD12	1:54:A:PHE:HE2	2	2.24
(1,450)	1:35:A:ILE:HD13	1:54:A:PHE:HE1	2	2.24
(1,450)	1:35:A:ILE:HD13	1:54:A:PHE:HE2	2	2.24
(1,908)	1:78:A:GLU:HA	1:80:A:HIS:HD2	11	2.23
(1,663)	1:54:A:PHE:HD1	1:76:A:LEU:HG	1	2.23
(1,663)	1:54:A:PHE:HD2	1:76:A:LEU:HG	1	2.23
(1,239)	1:21:A:LEU:HG	1:56:A:GLU:HB2	10	2.23
(1,239)	1:21:A:LEU:HG	1:56:A:GLU:HB3	10	2.23
(1,197)	1:18:A:SER:HA	1:20:A:GLU:HG2	2	2.23
(1,197)	1:18:A:SER:HA	1:20:A:GLU:HG3	2	2.23
(1,547)	1:44:A:HIS:HB2	1:48:A:LEU:HD11	6	2.22
(1,547)	1:44:A:HIS:HB2	1:48:A:LEU:HD12	6	2.22
(1,547)	1:44:A:HIS:HB2	1:48:A:LEU:HD13	6	2.22
(1,547)	1:44:A:HIS:HB3	1:48:A:LEU:HD11	6	2.22
(1,547)	1:44:A:HIS:HB3	1:48:A:LEU:HD12	6	2.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,547)	1:44:A:HIS:HB3	1:48:A:LEU:HD13	6	2.22
(1,304)	1:24:A:LEU:HD21	1:59:A:HIS:HE1	12	2.22
(1,304)	1:24:A:LEU:HD22	1:59:A:HIS:HE1	12	2.22
(1,304)	1:24:A:LEU:HD23	1:59:A:HIS:HE1	12	2.22
(1,239)	1:21:A:LEU:HG	1:56:A:GLU:HB2	14	2.22
(1,239)	1:21:A:LEU:HG	1:56:A:GLU:HB3	14	2.22
(1,241)	1:21:A:LEU:HG	1:57:A:LYS:HG2	14	2.21
(1,241)	1:21:A:LEU:HG	1:57:A:LYS:HG3	14	2.21
(1,908)	1:78:A:GLU:HA	1:80:A:HIS:HD2	13	2.2
(1,714)	1:60:A:THR:HA	1:81:A:ILE:HG21	12	2.2
(1,714)	1:60:A:THR:HA	1:81:A:ILE:HG22	12	2.2
(1,714)	1:60:A:THR:HA	1:81:A:ILE:HG23	12	2.2
(1,746)	1:63:A:LEU:HA	1:76:A:LEU:HD11	14	2.19
(1,746)	1:63:A:LEU:HA	1:76:A:LEU:HD12	14	2.19
(1,746)	1:63:A:LEU:HA	1:76:A:LEU:HD13	14	2.19
(1,524)	1:41:A:THR:HB	1:73:A:LYS:HA	12	2.19
(1,879)	1:75:A:PHE:HD1	1:77:A:TYR:HD2	18	2.18
(1,879)	1:75:A:PHE:HD2	1:77:A:TYR:HD2	18	2.18
(1,525)	1:41:A:THR:HB	1:73:A:LYS:HB2	11	2.17
(1,525)	1:41:A:THR:HB	1:73:A:LYS:HB3	11	2.17
(1,524)	1:41:A:THR:HB	1:73:A:LYS:HA	6	2.17
(1,239)	1:21:A:LEU:HG	1:56:A:GLU:HB2	17	2.17
(1,239)	1:21:A:LEU:HG	1:56:A:GLU:HB3	17	2.17
(1,197)	1:18:A:SER:HA	1:20:A:GLU:HG2	11	2.17
(1,197)	1:18:A:SER:HA	1:20:A:GLU:HG3	11	2.17
(1,525)	1:41:A:THR:HB	1:73:A:LYS:HB2	18	2.16
(1,525)	1:41:A:THR:HB	1:73:A:LYS:HB3	18	2.16
(1,197)	1:18:A:SER:HA	1:20:A:GLU:HG2	10	2.16
(1,197)	1:18:A:SER:HA	1:20:A:GLU:HG3	10	2.16
(1,893)	1:76:A:LEU:HD11	1:78:A:GLU:HG2	9	2.15
(1,893)	1:76:A:LEU:HD11	1:78:A:GLU:HG3	9	2.15
(1,893)	1:76:A:LEU:HD12	1:78:A:GLU:HG2	9	2.15
(1,893)	1:76:A:LEU:HD12	1:78:A:GLU:HG3	9	2.15
(1,893)	1:76:A:LEU:HD13	1:78:A:GLU:HG2	9	2.15
(1,893)	1:76:A:LEU:HD13	1:78:A:GLU:HG3	9	2.15
(1,746)	1:63:A:LEU:HA	1:76:A:LEU:HD11	1	2.15
(1,746)	1:63:A:LEU:HA	1:76:A:LEU:HD12	1	2.15
(1,746)	1:63:A:LEU:HA	1:76:A:LEU:HD13	1	2.15
(1,123)	1:7:A:LEU:HB2	1:38:A:PHE:HD1	14	2.15
(1,123)	1:7:A:LEU:HB2	1:38:A:PHE:HD2	14	2.15
(1,123)	1:7:A:LEU:HB3	1:38:A:PHE:HD1	14	2.15
(1,123)	1:7:A:LEU:HB3	1:38:A:PHE:HD2	14	2.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,8)	1:5:A:LEU:H	1:35:A:ILE:HB	9	2.15
(1,524)	1:41:A:THR:HB	1:73:A:LYS:HA	1	2.14
(1,714)	1:60:A:THR:HA	1:81:A:ILE:HG21	1	2.13
(1,714)	1:60:A:THR:HA	1:81:A:ILE:HG22	1	2.13
(1,714)	1:60:A:THR:HA	1:81:A:ILE:HG23	1	2.13
(1,501)	1:38:A:PHE:HD1	1:75:A:PHE:H	5	2.13
(1,501)	1:38:A:PHE:HD2	1:75:A:PHE:H	5	2.13
(1,495)	1:38:A:PHE:HA	1:75:A:PHE:HD1	18	2.12
(1,495)	1:38:A:PHE:HA	1:75:A:PHE:HD2	18	2.12
(1,197)	1:18:A:SER:HA	1:20:A:GLU:HG2	3	2.12
(1,197)	1:18:A:SER:HA	1:20:A:GLU:HG3	3	2.12
(1,546)	1:44:A:HIS:HB2	1:48:A:LEU:HG	20	2.11
(1,546)	1:44:A:HIS:HB3	1:48:A:LEU:HG	20	2.11
(1,524)	1:41:A:THR:HB	1:73:A:LYS:HA	14	2.11
(1,524)	1:41:A:THR:HB	1:73:A:LYS:HA	15	2.11
(1,298)	1:24:A:LEU:HG	1:80:A:HIS:HE1	7	2.11
(1,197)	1:18:A:SER:HA	1:20:A:GLU:HG2	13	2.11
(1,197)	1:18:A:SER:HA	1:20:A:GLU:HG3	13	2.11
(1,28)	1:5:A:LEU:HG	1:7:A:LEU:HG	4	2.11
(1,300)	1:24:A:LEU:HD11	1:35:A:ILE:HG12	15	2.1
(1,300)	1:24:A:LEU:HD11	1:35:A:ILE:HG13	15	2.1
(1,300)	1:24:A:LEU:HD12	1:35:A:ILE:HG12	15	2.1
(1,300)	1:24:A:LEU:HD12	1:35:A:ILE:HG13	15	2.1
(1,300)	1:24:A:LEU:HD13	1:35:A:ILE:HG12	15	2.1
(1,300)	1:24:A:LEU:HD13	1:35:A:ILE:HG13	15	2.1
(1,154)	1:10:A:ASN:HA	1:13:A:LYS:HG2	4	2.1
(1,154)	1:10:A:ASN:HA	1:13:A:LYS:HG3	4	2.1
(1,304)	1:24:A:LEU:HD21	1:59:A:HIS:HE1	20	2.09
(1,304)	1:24:A:LEU:HD22	1:59:A:HIS:HE1	20	2.09
(1,304)	1:24:A:LEU:HD23	1:59:A:HIS:HE1	20	2.09
(1,410)	1:33:A:ARG:HA	1:81:A:ILE:HG21	10	2.08
(1,410)	1:33:A:ARG:HA	1:81:A:ILE:HG22	10	2.08
(1,410)	1:33:A:ARG:HA	1:81:A:ILE:HG23	10	2.08
(1,239)	1:21:A:LEU:HG	1:56:A:GLU:HB2	6	2.08
(1,239)	1:21:A:LEU:HG	1:56:A:GLU:HB3	6	2.08
(1,746)	1:63:A:LEU:HA	1:76:A:LEU:HD11	12	2.07
(1,746)	1:63:A:LEU:HA	1:76:A:LEU:HD12	12	2.07
(1,746)	1:63:A:LEU:HA	1:76:A:LEU:HD13	12	2.07
(1,687)	1:56:A:GLU:HA	1:57:A:LYS:HE2	4	2.07
(1,687)	1:56:A:GLU:HA	1:57:A:LYS:HE3	4	2.07
(1,432)	1:35:A:ILE:H	1:36:A:PHE:HE1	9	2.07
(1,432)	1:35:A:ILE:H	1:36:A:PHE:HE2	9	2.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,418)	1:34:A:SER:H	1:79:A:LEU:HD21	3	2.07
(1,418)	1:34:A:SER:H	1:79:A:LEU:HD22	3	2.07
(1,418)	1:34:A:SER:H	1:79:A:LEU:HD23	3	2.07
(1,348)	1:28:A:PHE:H	1:30:A:GLU:HG2	19	2.07
(1,348)	1:28:A:PHE:H	1:30:A:GLU:HG3	19	2.07
(1,28)	1:5:A:LEU:HG	1:7:A:LEU:HG	3	2.07
(1,449)	1:35:A:ILE:HD11	1:37:A:TYR:HD1	11	2.06
(1,449)	1:35:A:ILE:HD11	1:37:A:TYR:HD2	11	2.06
(1,449)	1:35:A:ILE:HD12	1:37:A:TYR:HD1	11	2.06
(1,449)	1:35:A:ILE:HD12	1:37:A:TYR:HD2	11	2.06
(1,449)	1:35:A:ILE:HD13	1:37:A:TYR:HD1	11	2.06
(1,449)	1:35:A:ILE:HD13	1:37:A:TYR:HD2	11	2.06
(1,418)	1:34:A:SER:H	1:79:A:LEU:HD21	17	2.06
(1,418)	1:34:A:SER:H	1:79:A:LEU:HD22	17	2.06
(1,418)	1:34:A:SER:H	1:79:A:LEU:HD23	17	2.06
(1,304)	1:24:A:LEU:HD21	1:59:A:HIS:HE1	2	2.06
(1,304)	1:24:A:LEU:HD22	1:59:A:HIS:HE1	2	2.06
(1,304)	1:24:A:LEU:HD23	1:59:A:HIS:HE1	2	2.06
(1,746)	1:63:A:LEU:HA	1:76:A:LEU:HD11	18	2.05
(1,746)	1:63:A:LEU:HA	1:76:A:LEU:HD12	18	2.05
(1,746)	1:63:A:LEU:HA	1:76:A:LEU:HD13	18	2.05
(1,242)	1:21:A:LEU:HG	1:57:A:LYS:HD2	17	2.05
(1,242)	1:21:A:LEU:HG	1:57:A:LYS:HD3	17	2.05
(1,301)	1:24:A:LEU:HD11	1:60:A:THR:HB	1	2.04
(1,301)	1:24:A:LEU:HD12	1:60:A:THR:HB	1	2.04
(1,301)	1:24:A:LEU:HD13	1:60:A:THR:HB	1	2.04
(1,348)	1:28:A:PHE:H	1:30:A:GLU:HG2	15	2.03
(1,348)	1:28:A:PHE:H	1:30:A:GLU:HG3	15	2.03
(1,351)	1:28:A:PHE:H	1:81:A:ILE:HG21	8	2.02
(1,351)	1:28:A:PHE:H	1:81:A:ILE:HG22	8	2.02
(1,351)	1:28:A:PHE:H	1:81:A:ILE:HG23	8	2.02
(1,240)	1:21:A:LEU:HG	1:57:A:LYS:HB2	14	2.02
(1,240)	1:21:A:LEU:HG	1:57:A:LYS:HB3	14	2.02
(1,663)	1:54:A:PHE:HD1	1:76:A:LEU:HG	14	2.01
(1,663)	1:54:A:PHE:HD2	1:76:A:LEU:HG	14	2.01
(1,663)	1:54:A:PHE:HD1	1:76:A:LEU:HG	18	2.01
(1,663)	1:54:A:PHE:HD2	1:76:A:LEU:HG	18	2.01
(1,304)	1:24:A:LEU:HD21	1:59:A:HIS:HE1	19	2.01
(1,304)	1:24:A:LEU:HD22	1:59:A:HIS:HE1	19	2.01
(1,304)	1:24:A:LEU:HD23	1:59:A:HIS:HE1	19	2.01
(1,239)	1:21:A:LEU:HG	1:56:A:GLU:HB2	12	2.01
(1,239)	1:21:A:LEU:HG	1:56:A:GLU:HB3	12	2.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,27)	1:5:A:LEU:HG	1:7:A:LEU:H	16	2.01
(1,714)	1:60:A:THR:HA	1:81:A:ILE:HG21	9	2.0
(1,714)	1:60:A:THR:HA	1:81:A:ILE:HG22	9	2.0
(1,714)	1:60:A:THR:HA	1:81:A:ILE:HG23	9	2.0
(1,714)	1:60:A:THR:HA	1:81:A:ILE:HG21	19	2.0
(1,714)	1:60:A:THR:HA	1:81:A:ILE:HG22	19	2.0
(1,714)	1:60:A:THR:HA	1:81:A:ILE:HG23	19	2.0
(1,546)	1:44:A:HIS:HB2	1:48:A:LEU:HG	2	2.0
(1,546)	1:44:A:HIS:HB3	1:48:A:LEU:HG	2	2.0
(1,546)	1:44:A:HIS:HB2	1:48:A:LEU:HG	10	2.0
(1,546)	1:44:A:HIS:HB3	1:48:A:LEU:HG	10	2.0
(1,801)	1:66:A:VAL:HG11	1:72:A:GLU:HB2	17	1.99
(1,801)	1:66:A:VAL:HG11	1:72:A:GLU:HB3	17	1.99
(1,801)	1:66:A:VAL:HG12	1:72:A:GLU:HB2	17	1.99
(1,801)	1:66:A:VAL:HG12	1:72:A:GLU:HB3	17	1.99
(1,801)	1:66:A:VAL:HG13	1:72:A:GLU:HB2	17	1.99
(1,801)	1:66:A:VAL:HG13	1:72:A:GLU:HB3	17	1.99
(1,801)	1:66:A:VAL:HG21	1:72:A:GLU:HB2	17	1.99
(1,801)	1:66:A:VAL:HG21	1:72:A:GLU:HB3	17	1.99
(1,801)	1:66:A:VAL:HG22	1:72:A:GLU:HB2	17	1.99
(1,801)	1:66:A:VAL:HG22	1:72:A:GLU:HB3	17	1.99
(1,801)	1:66:A:VAL:HG23	1:72:A:GLU:HB2	17	1.99
(1,801)	1:66:A:VAL:HG23	1:72:A:GLU:HB3	17	1.99
(1,687)	1:56:A:GLU:HA	1:57:A:LYS:HE2	12	1.99
(1,687)	1:56:A:GLU:HA	1:57:A:LYS:HE3	12	1.99
(1,525)	1:41:A:THR:HB	1:73:A:LYS:HB2	8	1.99
(1,525)	1:41:A:THR:HB	1:73:A:LYS:HB3	8	1.99
(1,524)	1:41:A:THR:HB	1:73:A:LYS:HA	2	1.99
(1,387)	1:30:A:GLU:HG2	1:31:A:ASP:H	18	1.99
(1,387)	1:30:A:GLU:HG3	1:31:A:ASP:H	18	1.99
(1,288)	1:24:A:LEU:HA	1:80:A:HIS:HE1	14	1.99
(1,239)	1:21:A:LEU:HG	1:56:A:GLU:HB2	9	1.99
(1,239)	1:21:A:LEU:HG	1:56:A:GLU:HB3	9	1.99
(1,197)	1:18:A:SER:HA	1:20:A:GLU:HG2	19	1.99
(1,197)	1:18:A:SER:HA	1:20:A:GLU:HG3	19	1.99
(1,546)	1:44:A:HIS:HB2	1:48:A:LEU:HG	11	1.98
(1,546)	1:44:A:HIS:HB3	1:48:A:LEU:HG	11	1.98
(1,387)	1:30:A:GLU:HG2	1:31:A:ASP:H	7	1.98
(1,387)	1:30:A:GLU:HG3	1:31:A:ASP:H	7	1.98
(1,351)	1:28:A:PHE:H	1:81:A:ILE:HG21	16	1.98
(1,351)	1:28:A:PHE:H	1:81:A:ILE:HG22	16	1.98
(1,351)	1:28:A:PHE:H	1:81:A:ILE:HG23	16	1.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,892)	1:76:A:LEU:HD11	1:78:A:GLU:HA	9	1.97
(1,892)	1:76:A:LEU:HD12	1:78:A:GLU:HA	9	1.97
(1,892)	1:76:A:LEU:HD13	1:78:A:GLU:HA	9	1.97
(1,476)	1:37:A:TYR:H	1:78:A:GLU:HG2	9	1.97
(1,476)	1:37:A:TYR:H	1:78:A:GLU:HG3	9	1.97
(1,471)	1:36:A:PHE:HD1	1:78:A:GLU:H	9	1.97
(1,471)	1:36:A:PHE:HD2	1:78:A:GLU:H	9	1.97
(1,714)	1:60:A:THR:HA	1:81:A:ILE:HG21	20	1.96
(1,714)	1:60:A:THR:HA	1:81:A:ILE:HG22	20	1.96
(1,714)	1:60:A:THR:HA	1:81:A:ILE:HG23	20	1.96
(1,687)	1:56:A:GLU:HA	1:57:A:LYS:HE2	10	1.96
(1,687)	1:56:A:GLU:HA	1:57:A:LYS:HE3	10	1.96
(1,387)	1:30:A:GLU:HG2	1:31:A:ASP:H	5	1.96
(1,387)	1:30:A:GLU:HG3	1:31:A:ASP:H	5	1.96
(1,351)	1:28:A:PHE:H	1:81:A:ILE:HG21	11	1.96
(1,351)	1:28:A:PHE:H	1:81:A:ILE:HG22	11	1.96
(1,351)	1:28:A:PHE:H	1:81:A:ILE:HG23	11	1.96
(1,304)	1:24:A:LEU:HD21	1:59:A:HIS:HE1	10	1.96
(1,304)	1:24:A:LEU:HD22	1:59:A:HIS:HE1	10	1.96
(1,304)	1:24:A:LEU:HD23	1:59:A:HIS:HE1	10	1.96
(1,242)	1:21:A:LEU:HG	1:57:A:LYS:HD2	6	1.96
(1,242)	1:21:A:LEU:HG	1:57:A:LYS:HD3	6	1.96
(1,908)	1:78:A:GLU:HA	1:80:A:HIS:HD2	1	1.95
(1,538)	1:43:A:ALA:HA	1:45:A:LYS:HD2	9	1.95
(1,538)	1:43:A:ALA:HA	1:45:A:LYS:HD3	9	1.95
(1,524)	1:41:A:THR:HB	1:73:A:LYS:HA	5	1.95
(1,387)	1:30:A:GLU:HG2	1:31:A:ASP:H	6	1.95
(1,387)	1:30:A:GLU:HG3	1:31:A:ASP:H	6	1.95
(1,35)	1:5:A:LEU:HD11	1:7:A:LEU:HG	4	1.95
(1,35)	1:5:A:LEU:HD12	1:7:A:LEU:HG	4	1.95
(1,35)	1:5:A:LEU:HD13	1:7:A:LEU:HG	4	1.95
(1,35)	1:5:A:LEU:HD21	1:7:A:LEU:HG	4	1.95
(1,35)	1:5:A:LEU:HD22	1:7:A:LEU:HG	4	1.95
(1,35)	1:5:A:LEU:HD23	1:7:A:LEU:HG	4	1.95
(1,35)	1:5:A:LEU:HD11	1:7:A:LEU:HG	8	1.95
(1,35)	1:5:A:LEU:HD12	1:7:A:LEU:HG	8	1.95
(1,35)	1:5:A:LEU:HD13	1:7:A:LEU:HG	8	1.95
(1,35)	1:5:A:LEU:HD21	1:7:A:LEU:HG	8	1.95
(1,35)	1:5:A:LEU:HD22	1:7:A:LEU:HG	8	1.95
(1,35)	1:5:A:LEU:HD23	1:7:A:LEU:HG	8	1.95
(1,884)	1:76:A:LEU:HA	1:77:A:TYR:HD1	3	1.94
(1,884)	1:76:A:LEU:HA	1:77:A:TYR:HD2	3	1.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,387)	1:30:A:GLU:HG2	1:31:A:ASP:H	4	1.94
(1,387)	1:30:A:GLU:HG3	1:31:A:ASP:H	4	1.94
(1,293)	1:24:A:LEU:HB2	1:80:A:HIS:HE1	17	1.94
(1,293)	1:24:A:LEU:HB3	1:80:A:HIS:HE1	17	1.94
(1,35)	1:5:A:LEU:HD11	1:7:A:LEU:HG	3	1.94
(1,35)	1:5:A:LEU:HD12	1:7:A:LEU:HG	3	1.94
(1,35)	1:5:A:LEU:HD13	1:7:A:LEU:HG	3	1.94
(1,35)	1:5:A:LEU:HD21	1:7:A:LEU:HG	3	1.94
(1,35)	1:5:A:LEU:HD22	1:7:A:LEU:HG	3	1.94
(1,35)	1:5:A:LEU:HD23	1:7:A:LEU:HG	3	1.94
(1,20)	1:5:A:LEU:HB2	1:35:A:ILE:HB	16	1.94
(1,20)	1:5:A:LEU:HB3	1:35:A:ILE:HB	16	1.94
(1,903)	1:78:A:GLU:H	1:79:A:LEU:HG	12	1.93
(1,387)	1:30:A:GLU:HG2	1:31:A:ASP:H	1	1.93
(1,387)	1:30:A:GLU:HG3	1:31:A:ASP:H	1	1.93
(1,304)	1:24:A:LEU:HD21	1:59:A:HIS:HE1	5	1.93
(1,304)	1:24:A:LEU:HD22	1:59:A:HIS:HE1	5	1.93
(1,304)	1:24:A:LEU:HD23	1:59:A:HIS:HE1	5	1.93
(1,242)	1:21:A:LEU:HG	1:57:A:LYS:HD2	16	1.93
(1,242)	1:21:A:LEU:HG	1:57:A:LYS:HD3	16	1.93
(1,8)	1:5:A:LEU:H	1:35:A:ILE:HB	13	1.93
(1,746)	1:63:A:LEU:HA	1:76:A:LEU:HD11	7	1.92
(1,746)	1:63:A:LEU:HA	1:76:A:LEU:HD12	7	1.92
(1,746)	1:63:A:LEU:HA	1:76:A:LEU:HD13	7	1.92
(1,418)	1:34:A:SER:H	1:79:A:LEU:HD21	1	1.92
(1,418)	1:34:A:SER:H	1:79:A:LEU:HD22	1	1.92
(1,418)	1:34:A:SER:H	1:79:A:LEU:HD23	1	1.92
(1,418)	1:34:A:SER:H	1:79:A:LEU:HD21	5	1.92
(1,418)	1:34:A:SER:H	1:79:A:LEU:HD22	5	1.92
(1,418)	1:34:A:SER:H	1:79:A:LEU:HD23	5	1.92
(1,351)	1:28:A:PHE:H	1:81:A:ILE:HG21	17	1.92
(1,351)	1:28:A:PHE:H	1:81:A:ILE:HG22	17	1.92
(1,351)	1:28:A:PHE:H	1:81:A:ILE:HG23	17	1.92
(1,663)	1:54:A:PHE:HD1	1:76:A:LEU:HG	8	1.91
(1,663)	1:54:A:PHE:HD2	1:76:A:LEU:HG	8	1.91
(1,663)	1:54:A:PHE:HD1	1:76:A:LEU:HG	12	1.91
(1,663)	1:54:A:PHE:HD2	1:76:A:LEU:HG	12	1.91
(1,524)	1:41:A:THR:HB	1:73:A:LYS:HA	7	1.91
(1,28)	1:5:A:LEU:HG	1:7:A:LEU:HG	6	1.91
(1,8)	1:5:A:LEU:H	1:35:A:ILE:HB	15	1.91
(1,663)	1:54:A:PHE:HD1	1:76:A:LEU:HG	17	1.9
(1,663)	1:54:A:PHE:HD2	1:76:A:LEU:HG	17	1.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,546)	1:44:A:HIS:HB2	1:48:A:LEU:HG	6	1.9
(1,546)	1:44:A:HIS:HB3	1:48:A:LEU:HG	6	1.9
(1,538)	1:43:A:ALA:HA	1:45:A:LYS:HD2	13	1.9
(1,538)	1:43:A:ALA:HA	1:45:A:LYS:HD3	13	1.9
(1,476)	1:37:A:TYR:H	1:78:A:GLU:HG2	12	1.9
(1,476)	1:37:A:TYR:H	1:78:A:GLU:HG3	12	1.9
(1,387)	1:30:A:GLU:HG2	1:31:A:ASP:H	20	1.9
(1,387)	1:30:A:GLU:HG3	1:31:A:ASP:H	20	1.9
(1,351)	1:28:A:PHE:H	1:81:A:ILE:HG21	2	1.9
(1,351)	1:28:A:PHE:H	1:81:A:ILE:HG22	2	1.9
(1,351)	1:28:A:PHE:H	1:81:A:ILE:HG23	2	1.9
(1,239)	1:21:A:LEU:HG	1:56:A:GLU:HB2	16	1.9
(1,239)	1:21:A:LEU:HG	1:56:A:GLU:HB3	16	1.9
(1,494)	1:38:A:PHE:HA	1:75:A:PHE:HE1	18	1.89
(1,494)	1:38:A:PHE:HA	1:75:A:PHE:HE2	18	1.89
(1,448)	1:35:A:ILE:HG12	1:76:A:LEU:HB2	15	1.89
(1,448)	1:35:A:ILE:HG12	1:76:A:LEU:HB3	15	1.89
(1,448)	1:35:A:ILE:HG13	1:76:A:LEU:HB2	15	1.89
(1,448)	1:35:A:ILE:HG13	1:76:A:LEU:HB3	15	1.89
(1,387)	1:30:A:GLU:HG2	1:31:A:ASP:H	9	1.89
(1,387)	1:30:A:GLU:HG3	1:31:A:ASP:H	9	1.89
(1,387)	1:30:A:GLU:HG2	1:31:A:ASP:H	14	1.89
(1,387)	1:30:A:GLU:HG3	1:31:A:ASP:H	14	1.89
(1,348)	1:28:A:PHE:H	1:30:A:GLU:HG2	3	1.89
(1,348)	1:28:A:PHE:H	1:30:A:GLU:HG3	3	1.89
(1,28)	1:5:A:LEU:HG	1:7:A:LEU:HG	8	1.89
(1,687)	1:56:A:GLU:HA	1:57:A:LYS:HE2	6	1.88
(1,687)	1:56:A:GLU:HA	1:57:A:LYS:HE3	6	1.88
(1,546)	1:44:A:HIS:HB2	1:48:A:LEU:HG	9	1.88
(1,546)	1:44:A:HIS:HB3	1:48:A:LEU:HG	9	1.88
(1,524)	1:41:A:THR:HB	1:73:A:LYS:HA	13	1.88
(1,387)	1:30:A:GLU:HG2	1:31:A:ASP:H	2	1.88
(1,387)	1:30:A:GLU:HG3	1:31:A:ASP:H	2	1.88
(1,304)	1:24:A:LEU:HD21	1:59:A:HIS:HE1	3	1.88
(1,304)	1:24:A:LEU:HD22	1:59:A:HIS:HE1	3	1.88
(1,304)	1:24:A:LEU:HD23	1:59:A:HIS:HE1	3	1.88
(1,123)	1:7:A:LEU:HB2	1:38:A:PHE:HD1	8	1.88
(1,123)	1:7:A:LEU:HB2	1:38:A:PHE:HD2	8	1.88
(1,123)	1:7:A:LEU:HB3	1:38:A:PHE:HD1	8	1.88
(1,123)	1:7:A:LEU:HB3	1:38:A:PHE:HD2	8	1.88
(1,746)	1:63:A:LEU:HA	1:76:A:LEU:HD11	20	1.87
(1,746)	1:63:A:LEU:HA	1:76:A:LEU:HD12	20	1.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,746)	1:63:A:LEU:HA	1:76:A:LEU:HD13	20	1.87
(1,687)	1:56:A:GLU:HA	1:57:A:LYS:HE2	3	1.87
(1,687)	1:56:A:GLU:HA	1:57:A:LYS:HE3	3	1.87
(1,538)	1:43:A:ALA:HA	1:45:A:LYS:HD2	19	1.87
(1,538)	1:43:A:ALA:HA	1:45:A:LYS:HD3	19	1.87
(1,524)	1:41:A:THR:HB	1:73:A:LYS:HA	20	1.87
(1,411)	1:33:A:ARG:HA	1:82:A:ILE:HA	4	1.87
(1,241)	1:21:A:LEU:HG	1:57:A:LYS:HG2	17	1.87
(1,241)	1:21:A:LEU:HG	1:57:A:LYS:HG3	17	1.87
(1,20)	1:5:A:LEU:HB2	1:35:A:ILE:HB	3	1.87
(1,20)	1:5:A:LEU:HB3	1:35:A:ILE:HB	3	1.87
(1,20)	1:5:A:LEU:HB2	1:35:A:ILE:HB	11	1.87
(1,20)	1:5:A:LEU:HB3	1:35:A:ILE:HB	11	1.87
(1,746)	1:63:A:LEU:HA	1:76:A:LEU:HD11	16	1.86
(1,746)	1:63:A:LEU:HA	1:76:A:LEU:HD12	16	1.86
(1,746)	1:63:A:LEU:HA	1:76:A:LEU:HD13	16	1.86
(1,687)	1:56:A:GLU:HA	1:57:A:LYS:HE2	16	1.86
(1,687)	1:56:A:GLU:HA	1:57:A:LYS:HE3	16	1.86
(1,663)	1:54:A:PHE:HD1	1:76:A:LEU:HG	11	1.86
(1,663)	1:54:A:PHE:HD2	1:76:A:LEU:HG	11	1.86
(1,663)	1:54:A:PHE:HD1	1:76:A:LEU:HG	13	1.86
(1,663)	1:54:A:PHE:HD2	1:76:A:LEU:HG	13	1.86
(1,546)	1:44:A:HIS:HB2	1:48:A:LEU:HG	12	1.86
(1,546)	1:44:A:HIS:HB3	1:48:A:LEU:HG	12	1.86
(1,494)	1:38:A:PHE:HA	1:75:A:PHE:HE1	1	1.86
(1,494)	1:38:A:PHE:HA	1:75:A:PHE:HE2	1	1.86
(1,304)	1:24:A:LEU:HD21	1:59:A:HIS:HE1	15	1.86
(1,304)	1:24:A:LEU:HD22	1:59:A:HIS:HE1	15	1.86
(1,304)	1:24:A:LEU:HD23	1:59:A:HIS:HE1	15	1.86
(1,538)	1:43:A:ALA:HA	1:45:A:LYS:HD2	20	1.85
(1,538)	1:43:A:ALA:HA	1:45:A:LYS:HD3	20	1.85
(1,525)	1:41:A:THR:HB	1:73:A:LYS:HB2	3	1.85
(1,525)	1:41:A:THR:HB	1:73:A:LYS:HB3	3	1.85
(1,500)	1:38:A:PHE:HD1	1:39:A:ALA:H	2	1.85
(1,500)	1:38:A:PHE:HD2	1:39:A:ALA:H	2	1.85
(1,500)	1:38:A:PHE:HD1	1:39:A:ALA:H	5	1.84
(1,500)	1:38:A:PHE:HD2	1:39:A:ALA:H	5	1.84
(1,418)	1:34:A:SER:H	1:79:A:LEU:HD21	11	1.84
(1,418)	1:34:A:SER:H	1:79:A:LEU:HD22	11	1.84
(1,418)	1:34:A:SER:H	1:79:A:LEU:HD23	11	1.84
(1,239)	1:21:A:LEU:HG	1:56:A:GLU:HB2	4	1.84
(1,239)	1:21:A:LEU:HG	1:56:A:GLU:HB3	4	1.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,546)	1:44:A:HIS:HB2	1:48:A:LEU:HG	5	1.83
(1,546)	1:44:A:HIS:HB3	1:48:A:LEU:HG	5	1.83
(1,538)	1:43:A:ALA:HA	1:45:A:LYS:HD2	3	1.83
(1,538)	1:43:A:ALA:HA	1:45:A:LYS:HD3	3	1.83
(1,387)	1:30:A:GLU:HG2	1:31:A:ASP:H	16	1.83
(1,387)	1:30:A:GLU:HG3	1:31:A:ASP:H	16	1.83
(1,663)	1:54:A:PHE:HD1	1:76:A:LEU:HG	5	1.82
(1,663)	1:54:A:PHE:HD2	1:76:A:LEU:HG	5	1.82
(1,387)	1:30:A:GLU:HG2	1:31:A:ASP:H	11	1.82
(1,387)	1:30:A:GLU:HG3	1:31:A:ASP:H	11	1.82
(1,387)	1:30:A:GLU:HG2	1:31:A:ASP:H	17	1.82
(1,387)	1:30:A:GLU:HG3	1:31:A:ASP:H	17	1.82
(1,348)	1:28:A:PHE:H	1:30:A:GLU:HG2	8	1.82
(1,348)	1:28:A:PHE:H	1:30:A:GLU:HG3	8	1.82
(1,35)	1:5:A:LEU:HD11	1:7:A:LEU:HG	10	1.82
(1,35)	1:5:A:LEU:HD12	1:7:A:LEU:HG	10	1.82
(1,35)	1:5:A:LEU:HD13	1:7:A:LEU:HG	10	1.82
(1,35)	1:5:A:LEU:HD21	1:7:A:LEU:HG	10	1.82
(1,35)	1:5:A:LEU:HD22	1:7:A:LEU:HG	10	1.82
(1,35)	1:5:A:LEU:HD23	1:7:A:LEU:HG	10	1.82
(1,27)	1:5:A:LEU:HG	1:7:A:LEU:H	8	1.82
(1,893)	1:76:A:LEU:HD11	1:78:A:GLU:HG2	12	1.81
(1,893)	1:76:A:LEU:HD11	1:78:A:GLU:HG3	12	1.81
(1,893)	1:76:A:LEU:HD12	1:78:A:GLU:HG2	12	1.81
(1,893)	1:76:A:LEU:HD12	1:78:A:GLU:HG3	12	1.81
(1,893)	1:76:A:LEU:HD13	1:78:A:GLU:HG2	12	1.81
(1,893)	1:76:A:LEU:HD13	1:78:A:GLU:HG3	12	1.81
(1,878)	1:75:A:PHE:HB2	1:77:A:TYR:HD1	5	1.81
(1,878)	1:75:A:PHE:HB2	1:77:A:TYR:HD2	5	1.81
(1,878)	1:75:A:PHE:HB3	1:77:A:TYR:HD1	5	1.81
(1,878)	1:75:A:PHE:HB3	1:77:A:TYR:HD2	5	1.81
(1,476)	1:37:A:TYR:H	1:78:A:GLU:HG2	15	1.81
(1,476)	1:37:A:TYR:H	1:78:A:GLU:HG3	15	1.81
(1,471)	1:36:A:PHE:HD1	1:78:A:GLU:H	2	1.81
(1,471)	1:36:A:PHE:HD2	1:78:A:GLU:H	2	1.81
(1,351)	1:28:A:PHE:H	1:81:A:ILE:HG21	9	1.81
(1,351)	1:28:A:PHE:H	1:81:A:ILE:HG22	9	1.81
(1,351)	1:28:A:PHE:H	1:81:A:ILE:HG23	9	1.81
(1,129)	1:7:A:LEU:HD11	1:14:A:SER:HG	18	1.81
(1,129)	1:7:A:LEU:HD12	1:14:A:SER:HG	18	1.81
(1,129)	1:7:A:LEU:HD13	1:14:A:SER:HG	18	1.81
(1,663)	1:54:A:PHE:HD1	1:76:A:LEU:HG	16	1.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,663)	1:54:A:PHE:HD2	1:76:A:LEU:HG	16	1.8
(1,538)	1:43:A:ALA:HA	1:45:A:LYS:HD2	14	1.8
(1,538)	1:43:A:ALA:HA	1:45:A:LYS:HD3	14	1.8
(1,524)	1:41:A:THR:HB	1:73:A:LYS:HA	10	1.8
(1,411)	1:33:A:ARG:HA	1:82:A:ILE:HA	2	1.8
(1,398)	1:32:A:LYS:H	1:81:A:ILE:HG21	10	1.8
(1,398)	1:32:A:LYS:H	1:81:A:ILE:HG22	10	1.8
(1,398)	1:32:A:LYS:H	1:81:A:ILE:HG23	10	1.8
(1,387)	1:30:A:GLU:HG2	1:31:A:ASP:H	10	1.8
(1,387)	1:30:A:GLU:HG3	1:31:A:ASP:H	10	1.8
(1,387)	1:30:A:GLU:HG2	1:31:A:ASP:H	12	1.8
(1,387)	1:30:A:GLU:HG3	1:31:A:ASP:H	12	1.8
(1,239)	1:21:A:LEU:HG	1:56:A:GLU:HB2	3	1.8
(1,239)	1:21:A:LEU:HG	1:56:A:GLU:HB3	3	1.8
(1,893)	1:76:A:LEU:HD11	1:78:A:GLU:HG2	14	1.79
(1,893)	1:76:A:LEU:HD11	1:78:A:GLU:HG3	14	1.79
(1,893)	1:76:A:LEU:HD12	1:78:A:GLU:HG2	14	1.79
(1,893)	1:76:A:LEU:HD12	1:78:A:GLU:HG3	14	1.79
(1,893)	1:76:A:LEU:HD13	1:78:A:GLU:HG2	14	1.79
(1,893)	1:76:A:LEU:HD13	1:78:A:GLU:HG3	14	1.79
(1,804)	1:67:A:ARG:H	1:68:A:VAL:HB	12	1.79
(1,525)	1:41:A:THR:HB	1:73:A:LYS:HB2	9	1.79
(1,525)	1:41:A:THR:HB	1:73:A:LYS:HB3	9	1.79
(1,387)	1:30:A:GLU:HG2	1:31:A:ASP:H	13	1.79
(1,387)	1:30:A:GLU:HG3	1:31:A:ASP:H	13	1.79
(1,154)	1:10:A:ASN:HA	1:13:A:LYS:HG2	16	1.79
(1,154)	1:10:A:ASN:HA	1:13:A:LYS:HG3	16	1.79
(1,878)	1:75:A:PHE:HB2	1:77:A:TYR:HD1	3	1.78
(1,878)	1:75:A:PHE:HB2	1:77:A:TYR:HD2	3	1.78
(1,878)	1:75:A:PHE:HB3	1:77:A:TYR:HD1	3	1.78
(1,878)	1:75:A:PHE:HB3	1:77:A:TYR:HD2	3	1.78
(1,546)	1:44:A:HIS:HB2	1:48:A:LEU:HG	3	1.78
(1,546)	1:44:A:HIS:HB3	1:48:A:LEU:HG	3	1.78
(1,546)	1:44:A:HIS:HB2	1:48:A:LEU:HG	14	1.78
(1,546)	1:44:A:HIS:HB3	1:48:A:LEU:HG	14	1.78
(1,794)	1:66:A:VAL:HA	1:77:A:TYR:H	9	1.77
(1,687)	1:56:A:GLU:HA	1:57:A:LYS:HE2	18	1.77
(1,687)	1:56:A:GLU:HA	1:57:A:LYS:HE3	18	1.77
(1,524)	1:41:A:THR:HB	1:73:A:LYS:HA	19	1.77
(1,27)	1:5:A:LEU:HG	1:7:A:LEU:H	10	1.77
(1,884)	1:76:A:LEU:HA	1:77:A:TYR:HD1	15	1.76
(1,884)	1:76:A:LEU:HA	1:77:A:TYR:HD2	15	1.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,495)	1:38:A:PHE:HA	1:75:A:PHE:HD1	14	1.76
(1,495)	1:38:A:PHE:HA	1:75:A:PHE:HD2	14	1.76
(1,426)	1:34:A:SER:HB2	1:36:A:PHE:HE1	9	1.76
(1,426)	1:34:A:SER:HB2	1:36:A:PHE:HE2	9	1.76
(1,426)	1:34:A:SER:HB3	1:36:A:PHE:HE1	9	1.76
(1,426)	1:34:A:SER:HB3	1:36:A:PHE:HE2	9	1.76
(1,613)	1:50:A:ALA:HB1	1:54:A:PHE:HE1	2	1.75
(1,613)	1:50:A:ALA:HB1	1:54:A:PHE:HE2	2	1.75
(1,613)	1:50:A:ALA:HB2	1:54:A:PHE:HE1	2	1.75
(1,613)	1:50:A:ALA:HB2	1:54:A:PHE:HE2	2	1.75
(1,613)	1:50:A:ALA:HB3	1:54:A:PHE:HE1	2	1.75
(1,613)	1:50:A:ALA:HB3	1:54:A:PHE:HE2	2	1.75
(1,538)	1:43:A:ALA:HA	1:45:A:LYS:HD2	11	1.75
(1,538)	1:43:A:ALA:HA	1:45:A:LYS:HD3	11	1.75
(1,351)	1:28:A:PHE:H	1:81:A:ILE:HG21	4	1.75
(1,351)	1:28:A:PHE:H	1:81:A:ILE:HG22	4	1.75
(1,351)	1:28:A:PHE:H	1:81:A:ILE:HG23	4	1.75
(1,884)	1:76:A:LEU:HA	1:77:A:TYR:HD1	13	1.74
(1,884)	1:76:A:LEU:HA	1:77:A:TYR:HD2	13	1.74
(1,878)	1:75:A:PHE:HB2	1:77:A:TYR:HD1	2	1.74
(1,878)	1:75:A:PHE:HB2	1:77:A:TYR:HD2	2	1.74
(1,878)	1:75:A:PHE:HB3	1:77:A:TYR:HD1	2	1.74
(1,878)	1:75:A:PHE:HB3	1:77:A:TYR:HD2	2	1.74
(1,804)	1:67:A:ARG:H	1:68:A:VAL:HB	7	1.74
(1,546)	1:44:A:HIS:HB2	1:48:A:LEU:HG	18	1.74
(1,546)	1:44:A:HIS:HB3	1:48:A:LEU:HG	18	1.74
(1,501)	1:38:A:PHE:HD1	1:75:A:PHE:H	2	1.74
(1,501)	1:38:A:PHE:HD2	1:75:A:PHE:H	2	1.74
(1,351)	1:28:A:PHE:H	1:81:A:ILE:HG21	5	1.74
(1,351)	1:28:A:PHE:H	1:81:A:ILE:HG22	5	1.74
(1,351)	1:28:A:PHE:H	1:81:A:ILE:HG23	5	1.74
(1,242)	1:21:A:LEU:HG	1:57:A:LYS:HD2	12	1.74
(1,242)	1:21:A:LEU:HG	1:57:A:LYS:HD3	12	1.74
(1,240)	1:21:A:LEU:HG	1:57:A:LYS:HB2	17	1.74
(1,240)	1:21:A:LEU:HG	1:57:A:LYS:HB3	17	1.74
(1,884)	1:76:A:LEU:HA	1:77:A:TYR:HD1	1	1.73
(1,884)	1:76:A:LEU:HA	1:77:A:TYR:HD2	1	1.73
(1,687)	1:56:A:GLU:HA	1:57:A:LYS:HE2	17	1.73
(1,687)	1:56:A:GLU:HA	1:57:A:LYS:HE3	17	1.73
(1,664)	1:54:A:PHE:HD1	1:76:A:LEU:HD11	2	1.73
(1,664)	1:54:A:PHE:HD1	1:76:A:LEU:HD12	2	1.73
(1,664)	1:54:A:PHE:HD1	1:76:A:LEU:HD13	2	1.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,664)	1:54:A:PHE:HD2	1:76:A:LEU:HD11	2	1.73
(1,664)	1:54:A:PHE:HD2	1:76:A:LEU:HD12	2	1.73
(1,664)	1:54:A:PHE:HD2	1:76:A:LEU:HD13	2	1.73
(1,663)	1:54:A:PHE:HD1	1:76:A:LEU:HG	3	1.73
(1,663)	1:54:A:PHE:HD2	1:76:A:LEU:HG	3	1.73
(1,448)	1:35:A:ILE:HG12	1:76:A:LEU:HB2	16	1.73
(1,448)	1:35:A:ILE:HG12	1:76:A:LEU:HB3	16	1.73
(1,448)	1:35:A:ILE:HG13	1:76:A:LEU:HB2	16	1.73
(1,448)	1:35:A:ILE:HG13	1:76:A:LEU:HB3	16	1.73
(1,418)	1:34:A:SER:H	1:79:A:LEU:HD21	6	1.73
(1,418)	1:34:A:SER:H	1:79:A:LEU:HD22	6	1.73
(1,418)	1:34:A:SER:H	1:79:A:LEU:HD23	6	1.73
(1,884)	1:76:A:LEU:HA	1:77:A:TYR:HD1	6	1.72
(1,884)	1:76:A:LEU:HA	1:77:A:TYR:HD2	6	1.72
(1,884)	1:76:A:LEU:HA	1:77:A:TYR:HD1	17	1.72
(1,884)	1:76:A:LEU:HA	1:77:A:TYR:HD2	17	1.72
(1,538)	1:43:A:ALA:HA	1:45:A:LYS:HD2	4	1.72
(1,538)	1:43:A:ALA:HA	1:45:A:LYS:HD3	4	1.72
(1,390)	1:31:A:ASP:H	1:81:A:ILE:HG21	11	1.72
(1,390)	1:31:A:ASP:H	1:81:A:ILE:HG22	11	1.72
(1,390)	1:31:A:ASP:H	1:81:A:ILE:HG23	11	1.72
(1,241)	1:21:A:LEU:HG	1:57:A:LYS:HG2	6	1.72
(1,241)	1:21:A:LEU:HG	1:57:A:LYS:HG3	6	1.72
(1,35)	1:5:A:LEU:HD11	1:7:A:LEU:HG	6	1.72
(1,35)	1:5:A:LEU:HD12	1:7:A:LEU:HG	6	1.72
(1,35)	1:5:A:LEU:HD13	1:7:A:LEU:HG	6	1.72
(1,35)	1:5:A:LEU:HD21	1:7:A:LEU:HG	6	1.72
(1,35)	1:5:A:LEU:HD22	1:7:A:LEU:HG	6	1.72
(1,35)	1:5:A:LEU:HD23	1:7:A:LEU:HG	6	1.72
(1,476)	1:37:A:TYR:H	1:78:A:GLU:HG2	2	1.71
(1,476)	1:37:A:TYR:H	1:78:A:GLU:HG3	2	1.71
(1,746)	1:63:A:LEU:HA	1:76:A:LEU:HD11	11	1.7
(1,746)	1:63:A:LEU:HA	1:76:A:LEU:HD12	11	1.7
(1,746)	1:63:A:LEU:HA	1:76:A:LEU:HD13	11	1.7
(1,663)	1:54:A:PHE:HD1	1:76:A:LEU:HG	10	1.7
(1,663)	1:54:A:PHE:HD2	1:76:A:LEU:HG	10	1.7
(1,538)	1:43:A:ALA:HA	1:45:A:LYS:HD2	12	1.7
(1,538)	1:43:A:ALA:HA	1:45:A:LYS:HD3	12	1.7
(1,351)	1:28:A:PHE:H	1:81:A:ILE:HG21	20	1.7
(1,351)	1:28:A:PHE:H	1:81:A:ILE:HG22	20	1.7
(1,351)	1:28:A:PHE:H	1:81:A:ILE:HG23	20	1.7
(1,338)	1:27:A:GLU:H	1:30:A:GLU:HG2	19	1.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,338)	1:27:A:GLU:H	1:30:A:GLU:HG3	19	1.7
(1,123)	1:7:A:LEU:HB2	1:38:A:PHE:HD1	13	1.7
(1,123)	1:7:A:LEU:HB2	1:38:A:PHE:HD2	13	1.7
(1,123)	1:7:A:LEU:HB3	1:38:A:PHE:HD1	13	1.7
(1,123)	1:7:A:LEU:HB3	1:38:A:PHE:HD2	13	1.7
(1,35)	1:5:A:LEU:HD11	1:7:A:LEU:HG	7	1.7
(1,35)	1:5:A:LEU:HD12	1:7:A:LEU:HG	7	1.7
(1,35)	1:5:A:LEU:HD13	1:7:A:LEU:HG	7	1.7
(1,35)	1:5:A:LEU:HD21	1:7:A:LEU:HG	7	1.7
(1,35)	1:5:A:LEU:HD22	1:7:A:LEU:HG	7	1.7
(1,35)	1:5:A:LEU:HD23	1:7:A:LEU:HG	7	1.7
(1,884)	1:76:A:LEU:HA	1:77:A:TYR:HD1	5	1.69
(1,884)	1:76:A:LEU:HA	1:77:A:TYR:HD2	5	1.69
(1,884)	1:76:A:LEU:HA	1:77:A:TYR:HD1	12	1.69
(1,884)	1:76:A:LEU:HA	1:77:A:TYR:HD2	12	1.69
(1,501)	1:38:A:PHE:HD1	1:75:A:PHE:H	19	1.69
(1,501)	1:38:A:PHE:HD2	1:75:A:PHE:H	19	1.69
(1,304)	1:24:A:LEU:HD21	1:59:A:HIS:HE1	14	1.69
(1,304)	1:24:A:LEU:HD22	1:59:A:HIS:HE1	14	1.69
(1,304)	1:24:A:LEU:HD23	1:59:A:HIS:HE1	14	1.69
(1,285)	1:24:A:LEU:HA	1:54:A:PHE:HE1	20	1.69
(1,285)	1:24:A:LEU:HA	1:54:A:PHE:HE2	20	1.69
(1,242)	1:21:A:LEU:HG	1:57:A:LYS:HD2	11	1.69
(1,242)	1:21:A:LEU:HG	1:57:A:LYS:HD3	11	1.69
(1,804)	1:67:A:ARG:H	1:68:A:VAL:HB	16	1.68
(1,538)	1:43:A:ALA:HA	1:45:A:LYS:HD2	10	1.68
(1,538)	1:43:A:ALA:HA	1:45:A:LYS:HD3	10	1.68
(1,524)	1:41:A:THR:HB	1:73:A:LYS:HA	4	1.68
(1,884)	1:76:A:LEU:HA	1:77:A:TYR:HD1	4	1.67
(1,884)	1:76:A:LEU:HA	1:77:A:TYR:HD2	4	1.67
(1,538)	1:43:A:ALA:HA	1:45:A:LYS:HD2	17	1.67
(1,538)	1:43:A:ALA:HA	1:45:A:LYS:HD3	17	1.67
(1,524)	1:41:A:THR:HB	1:73:A:LYS:HA	18	1.67
(1,301)	1:24:A:LEU:HD11	1:60:A:THR:HB	9	1.67
(1,301)	1:24:A:LEU:HD12	1:60:A:THR:HB	9	1.67
(1,301)	1:24:A:LEU:HD13	1:60:A:THR:HB	9	1.67
(1,884)	1:76:A:LEU:HA	1:77:A:TYR:HD1	8	1.66
(1,884)	1:76:A:LEU:HA	1:77:A:TYR:HD2	8	1.66
(1,687)	1:56:A:GLU:HA	1:57:A:LYS:HE2	15	1.66
(1,687)	1:56:A:GLU:HA	1:57:A:LYS:HE3	15	1.66
(1,893)	1:76:A:LEU:HD11	1:78:A:GLU:HG2	18	1.65
(1,893)	1:76:A:LEU:HD11	1:78:A:GLU:HG3	18	1.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,893)	1:76:A:LEU:HD12	1:78:A:GLU:HG2	18	1.65
(1,893)	1:76:A:LEU:HD12	1:78:A:GLU:HG3	18	1.65
(1,893)	1:76:A:LEU:HD13	1:78:A:GLU:HG2	18	1.65
(1,893)	1:76:A:LEU:HD13	1:78:A:GLU:HG3	18	1.65
(1,690)	1:56:A:GLU:CD	1:52:A:ASP:CG	11	1.65
(1,687)	1:56:A:GLU:HA	1:57:A:LYS:HE2	11	1.65
(1,687)	1:56:A:GLU:HA	1:57:A:LYS:HE3	11	1.65
(1,338)	1:27:A:GLU:H	1:30:A:GLU:HG2	3	1.65
(1,338)	1:27:A:GLU:H	1:30:A:GLU:HG3	3	1.65
(1,304)	1:24:A:LEU:HD21	1:59:A:HIS:HE1	7	1.65
(1,304)	1:24:A:LEU:HD22	1:59:A:HIS:HE1	7	1.65
(1,304)	1:24:A:LEU:HD23	1:59:A:HIS:HE1	7	1.65
(1,301)	1:24:A:LEU:HD11	1:60:A:THR:HB	19	1.65
(1,301)	1:24:A:LEU:HD12	1:60:A:THR:HB	19	1.65
(1,301)	1:24:A:LEU:HD13	1:60:A:THR:HB	19	1.65
(1,241)	1:21:A:LEU:HG	1:57:A:LYS:HG2	16	1.65
(1,241)	1:21:A:LEU:HG	1:57:A:LYS:HG3	16	1.65
(1,878)	1:75:A:PHE:HB2	1:77:A:TYR:HD1	4	1.64
(1,878)	1:75:A:PHE:HB2	1:77:A:TYR:HD2	4	1.64
(1,878)	1:75:A:PHE:HB3	1:77:A:TYR:HD1	4	1.64
(1,878)	1:75:A:PHE:HB3	1:77:A:TYR:HD2	4	1.64
(1,746)	1:63:A:LEU:HA	1:76:A:LEU:HD11	8	1.64
(1,746)	1:63:A:LEU:HA	1:76:A:LEU:HD12	8	1.64
(1,746)	1:63:A:LEU:HA	1:76:A:LEU:HD13	8	1.64
(1,538)	1:43:A:ALA:HA	1:45:A:LYS:HD2	2	1.64
(1,538)	1:43:A:ALA:HA	1:45:A:LYS:HD3	2	1.64
(1,27)	1:5:A:LEU:HG	1:7:A:LEU:H	6	1.64
(1,884)	1:76:A:LEU:HA	1:77:A:TYR:HD1	19	1.63
(1,884)	1:76:A:LEU:HA	1:77:A:TYR:HD2	19	1.63
(1,878)	1:75:A:PHE:HB2	1:77:A:TYR:HD1	17	1.63
(1,878)	1:75:A:PHE:HB2	1:77:A:TYR:HD2	17	1.63
(1,878)	1:75:A:PHE:HB3	1:77:A:TYR:HD1	17	1.63
(1,878)	1:75:A:PHE:HB3	1:77:A:TYR:HD2	17	1.63
(1,240)	1:21:A:LEU:HG	1:57:A:LYS:HB2	16	1.63
(1,240)	1:21:A:LEU:HG	1:57:A:LYS:HB3	16	1.63
(1,804)	1:67:A:ARG:H	1:68:A:VAL:HB	5	1.62
(1,687)	1:56:A:GLU:HA	1:57:A:LYS:HE2	8	1.62
(1,687)	1:56:A:GLU:HA	1:57:A:LYS:HE3	8	1.62
(1,687)	1:56:A:GLU:HA	1:57:A:LYS:HE2	9	1.62
(1,687)	1:56:A:GLU:HA	1:57:A:LYS:HE3	9	1.62
(1,298)	1:24:A:LEU:HG	1:80:A:HIS:HE1	3	1.62
(1,28)	1:5:A:LEU:HG	1:7:A:LEU:HG	10	1.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,878)	1:75:A:PHE:HB2	1:77:A:TYR:HD1	11	1.61
(1,878)	1:75:A:PHE:HB2	1:77:A:TYR:HD2	11	1.61
(1,878)	1:75:A:PHE:HB3	1:77:A:TYR:HD1	11	1.61
(1,878)	1:75:A:PHE:HB3	1:77:A:TYR:HD2	11	1.61
(1,804)	1:67:A:ARG:H	1:68:A:VAL:HB	9	1.61
(1,663)	1:54:A:PHE:HD1	1:76:A:LEU:HG	19	1.61
(1,663)	1:54:A:PHE:HD2	1:76:A:LEU:HG	19	1.61
(1,494)	1:38:A:PHE:HA	1:75:A:PHE:HE1	14	1.61
(1,494)	1:38:A:PHE:HA	1:75:A:PHE:HE2	14	1.61
(1,351)	1:28:A:PHE:H	1:81:A:ILE:HG21	19	1.61
(1,351)	1:28:A:PHE:H	1:81:A:ILE:HG22	19	1.61
(1,351)	1:28:A:PHE:H	1:81:A:ILE:HG23	19	1.61
(1,250)	1:21:A:LEU:HD21	1:59:A:HIS:HE1	9	1.61
(1,250)	1:21:A:LEU:HD22	1:59:A:HIS:HE1	9	1.61
(1,250)	1:21:A:LEU:HD23	1:59:A:HIS:HE1	9	1.61
(1,240)	1:21:A:LEU:HG	1:57:A:LYS:HB2	6	1.61
(1,240)	1:21:A:LEU:HG	1:57:A:LYS:HB3	6	1.61
(1,240)	1:21:A:LEU:HG	1:57:A:LYS:HB2	18	1.61
(1,240)	1:21:A:LEU:HG	1:57:A:LYS:HB3	18	1.61
(1,28)	1:5:A:LEU:HG	1:7:A:LEU:HG	7	1.61
(1,884)	1:76:A:LEU:HA	1:77:A:TYR:HD1	7	1.6
(1,884)	1:76:A:LEU:HA	1:77:A:TYR:HD2	7	1.6
(1,628)	1:51:A:VAL:HG21	1:54:A:PHE:HD1	2	1.6
(1,628)	1:51:A:VAL:HG21	1:54:A:PHE:HD2	2	1.6
(1,628)	1:51:A:VAL:HG22	1:54:A:PHE:HD1	2	1.6
(1,628)	1:51:A:VAL:HG22	1:54:A:PHE:HD2	2	1.6
(1,628)	1:51:A:VAL:HG23	1:54:A:PHE:HD1	2	1.6
(1,628)	1:51:A:VAL:HG23	1:54:A:PHE:HD2	2	1.6
(1,538)	1:43:A:ALA:HA	1:45:A:LYS:HD2	15	1.6
(1,538)	1:43:A:ALA:HA	1:45:A:LYS:HD3	15	1.6
(1,476)	1:37:A:TYR:H	1:78:A:GLU:HG2	5	1.6
(1,476)	1:37:A:TYR:H	1:78:A:GLU:HG3	5	1.6
(1,36)	1:5:A:LEU:HD11	1:7:A:LEU:HD11	18	1.6
(1,36)	1:5:A:LEU:HD11	1:7:A:LEU:HD12	18	1.6
(1,36)	1:5:A:LEU:HD11	1:7:A:LEU:HD13	18	1.6
(1,36)	1:5:A:LEU:HD12	1:7:A:LEU:HD11	18	1.6
(1,36)	1:5:A:LEU:HD12	1:7:A:LEU:HD12	18	1.6
(1,36)	1:5:A:LEU:HD12	1:7:A:LEU:HD13	18	1.6
(1,36)	1:5:A:LEU:HD13	1:7:A:LEU:HD11	18	1.6
(1,36)	1:5:A:LEU:HD13	1:7:A:LEU:HD12	18	1.6
(1,36)	1:5:A:LEU:HD13	1:7:A:LEU:HD13	18	1.6
(1,36)	1:5:A:LEU:HD21	1:7:A:LEU:HD11	18	1.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,36)	1:5:A:LEU:HD21	1:7:A:LEU:HD12	18	1.6
(1,36)	1:5:A:LEU:HD21	1:7:A:LEU:HD13	18	1.6
(1,36)	1:5:A:LEU:HD22	1:7:A:LEU:HD11	18	1.6
(1,36)	1:5:A:LEU:HD22	1:7:A:LEU:HD12	18	1.6
(1,36)	1:5:A:LEU:HD22	1:7:A:LEU:HD13	18	1.6
(1,36)	1:5:A:LEU:HD23	1:7:A:LEU:HD11	18	1.6
(1,36)	1:5:A:LEU:HD23	1:7:A:LEU:HD12	18	1.6
(1,36)	1:5:A:LEU:HD23	1:7:A:LEU:HD13	18	1.6
(1,884)	1:76:A:LEU:HA	1:77:A:TYR:HD1	11	1.59
(1,884)	1:76:A:LEU:HA	1:77:A:TYR:HD2	11	1.59
(1,687)	1:56:A:GLU:HA	1:57:A:LYS:HE2	1	1.59
(1,687)	1:56:A:GLU:HA	1:57:A:LYS:HE3	1	1.59
(1,663)	1:54:A:PHE:HD1	1:76:A:LEU:HG	15	1.59
(1,663)	1:54:A:PHE:HD2	1:76:A:LEU:HG	15	1.59
(1,542)	1:44:A:HIS:HA	1:45:A:LYS:HD2	13	1.59
(1,542)	1:44:A:HIS:HA	1:45:A:LYS:HD3	13	1.59
(1,312)	1:25:A:TYR:H	1:59:A:HIS:HE1	20	1.59
(1,476)	1:37:A:TYR:H	1:78:A:GLU:HG2	10	1.58
(1,476)	1:37:A:TYR:H	1:78:A:GLU:HG3	10	1.58
(1,365)	1:28:A:PHE:HD1	1:32:A:LYS:HB2	1	1.58
(1,365)	1:28:A:PHE:HD1	1:32:A:LYS:HB3	1	1.58
(1,365)	1:28:A:PHE:HD2	1:32:A:LYS:HB2	1	1.58
(1,365)	1:28:A:PHE:HD2	1:32:A:LYS:HB3	1	1.58
(1,300)	1:24:A:LEU:HD11	1:35:A:ILE:HG12	2	1.58
(1,300)	1:24:A:LEU:HD11	1:35:A:ILE:HG13	2	1.58
(1,300)	1:24:A:LEU:HD12	1:35:A:ILE:HG12	2	1.58
(1,300)	1:24:A:LEU:HD12	1:35:A:ILE:HG13	2	1.58
(1,300)	1:24:A:LEU:HD13	1:35:A:ILE:HG12	2	1.58
(1,300)	1:24:A:LEU:HD13	1:35:A:ILE:HG13	2	1.58
(1,239)	1:21:A:LEU:HG	1:56:A:GLU:HB2	1	1.58
(1,239)	1:21:A:LEU:HG	1:56:A:GLU:HB3	1	1.58
(1,884)	1:76:A:LEU:HA	1:77:A:TYR:HD1	16	1.57
(1,884)	1:76:A:LEU:HA	1:77:A:TYR:HD2	16	1.57
(1,804)	1:67:A:ARG:H	1:68:A:VAL:HB	6	1.57
(1,804)	1:67:A:ARG:H	1:68:A:VAL:HB	10	1.57
(1,663)	1:54:A:PHE:HD1	1:76:A:LEU:HG	4	1.57
(1,663)	1:54:A:PHE:HD2	1:76:A:LEU:HG	4	1.57
(1,525)	1:41:A:THR:HB	1:73:A:LYS:HB2	6	1.57
(1,525)	1:41:A:THR:HB	1:73:A:LYS:HB3	6	1.57
(1,476)	1:37:A:TYR:H	1:78:A:GLU:HG2	3	1.57
(1,476)	1:37:A:TYR:H	1:78:A:GLU:HG3	3	1.57
(1,448)	1:35:A:ILE:HG12	1:76:A:LEU:HB2	13	1.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,448)	1:35:A:ILE:HG12	1:76:A:LEU:HB3	13	1.57
(1,448)	1:35:A:ILE:HG13	1:76:A:LEU:HB2	13	1.57
(1,448)	1:35:A:ILE:HG13	1:76:A:LEU:HB3	13	1.57
(1,410)	1:33:A:ARG:HA	1:81:A:ILE:HG21	6	1.57
(1,410)	1:33:A:ARG:HA	1:81:A:ILE:HG22	6	1.57
(1,410)	1:33:A:ARG:HA	1:81:A:ILE:HG23	6	1.57
(1,288)	1:24:A:LEU:HA	1:80:A:HIS:HE1	2	1.57
(1,884)	1:76:A:LEU:HA	1:77:A:TYR:HD1	10	1.56
(1,884)	1:76:A:LEU:HA	1:77:A:TYR:HD2	10	1.56
(1,687)	1:56:A:GLU:HA	1:57:A:LYS:HE2	14	1.56
(1,687)	1:56:A:GLU:HA	1:57:A:LYS:HE3	14	1.56
(1,542)	1:44:A:HIS:HA	1:45:A:LYS:HD2	15	1.56
(1,542)	1:44:A:HIS:HA	1:45:A:LYS:HD3	15	1.56
(1,242)	1:21:A:LEU:HG	1:57:A:LYS:HD2	3	1.56
(1,242)	1:21:A:LEU:HG	1:57:A:LYS:HD3	3	1.56
(1,538)	1:43:A:ALA:HA	1:45:A:LYS:HD2	18	1.55
(1,538)	1:43:A:ALA:HA	1:45:A:LYS:HD3	18	1.55
(1,525)	1:41:A:THR:HB	1:73:A:LYS:HB2	12	1.55
(1,525)	1:41:A:THR:HB	1:73:A:LYS:HB3	12	1.55
(1,351)	1:28:A:PHE:H	1:81:A:ILE:HG21	14	1.55
(1,351)	1:28:A:PHE:H	1:81:A:ILE:HG22	14	1.55
(1,351)	1:28:A:PHE:H	1:81:A:ILE:HG23	14	1.55
(1,68)	1:6:A:VAL:HB	1:19:A:VAL:HB	1	1.55
(1,36)	1:5:A:LEU:HD11	1:7:A:LEU:HD11	17	1.55
(1,36)	1:5:A:LEU:HD11	1:7:A:LEU:HD12	17	1.55
(1,36)	1:5:A:LEU:HD11	1:7:A:LEU:HD13	17	1.55
(1,36)	1:5:A:LEU:HD12	1:7:A:LEU:HD11	17	1.55
(1,36)	1:5:A:LEU:HD12	1:7:A:LEU:HD12	17	1.55
(1,36)	1:5:A:LEU:HD12	1:7:A:LEU:HD13	17	1.55
(1,36)	1:5:A:LEU:HD13	1:7:A:LEU:HD11	17	1.55
(1,36)	1:5:A:LEU:HD13	1:7:A:LEU:HD12	17	1.55
(1,36)	1:5:A:LEU:HD13	1:7:A:LEU:HD13	17	1.55
(1,36)	1:5:A:LEU:HD21	1:7:A:LEU:HD11	17	1.55
(1,36)	1:5:A:LEU:HD21	1:7:A:LEU:HD12	17	1.55
(1,36)	1:5:A:LEU:HD21	1:7:A:LEU:HD13	17	1.55
(1,36)	1:5:A:LEU:HD22	1:7:A:LEU:HD11	17	1.55
(1,36)	1:5:A:LEU:HD22	1:7:A:LEU:HD12	17	1.55
(1,36)	1:5:A:LEU:HD22	1:7:A:LEU:HD13	17	1.55
(1,36)	1:5:A:LEU:HD23	1:7:A:LEU:HD11	17	1.55
(1,36)	1:5:A:LEU:HD23	1:7:A:LEU:HD12	17	1.55
(1,36)	1:5:A:LEU:HD23	1:7:A:LEU:HD13	17	1.55
(1,903)	1:78:A:GLU:H	1:79:A:LEU:HG	3	1.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,722)	1:61:A:ALA:H	1:81:A:ILE:HA	12	1.54
(1,476)	1:37:A:TYR:H	1:78:A:GLU:HG2	6	1.54
(1,476)	1:37:A:TYR:H	1:78:A:GLU:HG3	6	1.54
(1,390)	1:31:A:ASP:H	1:81:A:ILE:HG21	2	1.54
(1,390)	1:31:A:ASP:H	1:81:A:ILE:HG22	2	1.54
(1,390)	1:31:A:ASP:H	1:81:A:ILE:HG23	2	1.54
(1,242)	1:21:A:LEU:HG	1:57:A:LYS:HD2	1	1.54
(1,242)	1:21:A:LEU:HG	1:57:A:LYS:HD3	1	1.54
(1,884)	1:76:A:LEU:HA	1:77:A:TYR:HD1	2	1.53
(1,884)	1:76:A:LEU:HA	1:77:A:TYR:HD2	2	1.53
(1,524)	1:41:A:THR:HB	1:73:A:LYS:HA	17	1.53
(1,471)	1:36:A:PHE:HD1	1:78:A:GLU:H	13	1.53
(1,471)	1:36:A:PHE:HD2	1:78:A:GLU:H	13	1.53
(1,351)	1:28:A:PHE:H	1:81:A:ILE:HG21	6	1.53
(1,351)	1:28:A:PHE:H	1:81:A:ILE:HG22	6	1.53
(1,351)	1:28:A:PHE:H	1:81:A:ILE:HG23	6	1.53
(1,250)	1:21:A:LEU:HD21	1:59:A:HIS:HE1	16	1.53
(1,250)	1:21:A:LEU:HD22	1:59:A:HIS:HE1	16	1.53
(1,250)	1:21:A:LEU:HD23	1:59:A:HIS:HE1	16	1.53
(1,32)	1:5:A:LEU:HD11	1:7:A:LEU:H	17	1.53
(1,32)	1:5:A:LEU:HD12	1:7:A:LEU:H	17	1.53
(1,32)	1:5:A:LEU:HD13	1:7:A:LEU:H	17	1.53
(1,32)	1:5:A:LEU:HD21	1:7:A:LEU:H	17	1.53
(1,32)	1:5:A:LEU:HD22	1:7:A:LEU:H	17	1.53
(1,32)	1:5:A:LEU:HD23	1:7:A:LEU:H	17	1.53
(1,746)	1:63:A:LEU:HA	1:76:A:LEU:HD11	19	1.52
(1,746)	1:63:A:LEU:HA	1:76:A:LEU:HD12	19	1.52
(1,746)	1:63:A:LEU:HA	1:76:A:LEU:HD13	19	1.52
(1,687)	1:56:A:GLU:HA	1:57:A:LYS:HE2	7	1.52
(1,687)	1:56:A:GLU:HA	1:57:A:LYS:HE3	7	1.52
(1,245)	1:21:A:LEU:HD11	1:53:A:PHE:HA	14	1.52
(1,245)	1:21:A:LEU:HD12	1:53:A:PHE:HA	14	1.52
(1,245)	1:21:A:LEU:HD13	1:53:A:PHE:HA	14	1.52
(1,240)	1:21:A:LEU:HG	1:57:A:LYS:HB2	10	1.52
(1,240)	1:21:A:LEU:HG	1:57:A:LYS:HB3	10	1.52
(1,45)	1:6:A:VAL:H	1:35:A:ILE:HB	2	1.52
(1,723)	1:61:A:ALA:H	1:82:A:ILE:H	12	1.51
(1,501)	1:38:A:PHE:HD1	1:75:A:PHE:H	13	1.51
(1,501)	1:38:A:PHE:HD2	1:75:A:PHE:H	13	1.51
(1,471)	1:36:A:PHE:HD1	1:78:A:GLU:H	12	1.51
(1,471)	1:36:A:PHE:HD2	1:78:A:GLU:H	12	1.51
(1,449)	1:35:A:ILE:HD11	1:37:A:TYR:HD1	16	1.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,449)	1:35:A:ILE:HD11	1:37:A:TYR:HD2	16	1.51
(1,449)	1:35:A:ILE:HD12	1:37:A:TYR:HD1	16	1.51
(1,449)	1:35:A:ILE:HD12	1:37:A:TYR:HD2	16	1.51
(1,449)	1:35:A:ILE:HD13	1:37:A:TYR:HD1	16	1.51
(1,449)	1:35:A:ILE:HD13	1:37:A:TYR:HD2	16	1.51
(1,387)	1:30:A:GLU:HG2	1:31:A:ASP:H	15	1.51
(1,387)	1:30:A:GLU:HG3	1:31:A:ASP:H	15	1.51
(1,240)	1:21:A:LEU:HG	1:57:A:LYS:HB2	9	1.51
(1,240)	1:21:A:LEU:HG	1:57:A:LYS:HB3	9	1.51
(1,239)	1:21:A:LEU:HG	1:56:A:GLU:HB2	11	1.51
(1,239)	1:21:A:LEU:HG	1:56:A:GLU:HB3	11	1.51
(1,884)	1:76:A:LEU:HA	1:77:A:TYR:HD1	20	1.5
(1,884)	1:76:A:LEU:HA	1:77:A:TYR:HD2	20	1.5
(1,568)	1:47:A:MET:HB2	1:48:A:LEU:HG	2	1.5
(1,568)	1:47:A:MET:HB3	1:48:A:LEU:HG	2	1.5
(1,525)	1:41:A:THR:HB	1:73:A:LYS:HB2	1	1.5
(1,525)	1:41:A:THR:HB	1:73:A:LYS:HB3	1	1.5
(1,447)	1:35:A:ILE:HG12	1:36:A:PHE:HA	16	1.5
(1,447)	1:35:A:ILE:HG13	1:36:A:PHE:HA	16	1.5
(1,387)	1:30:A:GLU:HG2	1:31:A:ASP:H	19	1.5
(1,387)	1:30:A:GLU:HG3	1:31:A:ASP:H	19	1.5
(1,338)	1:27:A:GLU:H	1:30:A:GLU:HG2	15	1.5
(1,338)	1:27:A:GLU:H	1:30:A:GLU:HG3	15	1.5
(1,921)	1:79:A:LEU:HD11	1:82:A:ILE:HB	10	1.49
(1,921)	1:79:A:LEU:HD12	1:82:A:ILE:HB	10	1.49
(1,921)	1:79:A:LEU:HD13	1:82:A:ILE:HB	10	1.49
(1,447)	1:35:A:ILE:HG12	1:36:A:PHE:HA	3	1.49
(1,447)	1:35:A:ILE:HG13	1:36:A:PHE:HA	3	1.49
(1,447)	1:35:A:ILE:HG12	1:36:A:PHE:HA	15	1.49
(1,447)	1:35:A:ILE:HG13	1:36:A:PHE:HA	15	1.49
(1,410)	1:33:A:ARG:HA	1:81:A:ILE:HG21	14	1.49
(1,410)	1:33:A:ARG:HA	1:81:A:ILE:HG22	14	1.49
(1,410)	1:33:A:ARG:HA	1:81:A:ILE:HG23	14	1.49
(1,304)	1:24:A:LEU:HD21	1:59:A:HIS:HE1	17	1.49
(1,304)	1:24:A:LEU:HD22	1:59:A:HIS:HE1	17	1.49
(1,304)	1:24:A:LEU:HD23	1:59:A:HIS:HE1	17	1.49
(1,293)	1:24:A:LEU:HB2	1:80:A:HIS:HE1	7	1.49
(1,293)	1:24:A:LEU:HB3	1:80:A:HIS:HE1	7	1.49
(1,921)	1:79:A:LEU:HD11	1:82:A:ILE:HB	4	1.48
(1,921)	1:79:A:LEU:HD12	1:82:A:ILE:HB	4	1.48
(1,921)	1:79:A:LEU:HD13	1:82:A:ILE:HB	4	1.48
(1,884)	1:76:A:LEU:HA	1:77:A:TYR:HD1	18	1.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,884)	1:76:A:LEU:HA	1:77:A:TYR:HD2	18	1.48
(1,804)	1:67:A:ARG:H	1:68:A:VAL:HB	20	1.48
(1,727)	1:61:A:ALA:HB1	1:79:A:LEU:HB3	17	1.48
(1,727)	1:61:A:ALA:HB2	1:79:A:LEU:HB3	17	1.48
(1,727)	1:61:A:ALA:HB3	1:79:A:LEU:HB3	17	1.48
(1,687)	1:56:A:GLU:HA	1:57:A:LYS:HE2	20	1.48
(1,687)	1:56:A:GLU:HA	1:57:A:LYS:HE3	20	1.48
(1,525)	1:41:A:THR:HB	1:73:A:LYS:HB2	7	1.48
(1,525)	1:41:A:THR:HB	1:73:A:LYS:HB3	7	1.48
(1,241)	1:21:A:LEU:HG	1:57:A:LYS:HG2	1	1.48
(1,241)	1:21:A:LEU:HG	1:57:A:LYS:HG3	1	1.48
(1,241)	1:21:A:LEU:HG	1:57:A:LYS:HG2	12	1.48
(1,241)	1:21:A:LEU:HG	1:57:A:LYS:HG3	12	1.48
(1,8)	1:5:A:LEU:H	1:35:A:ILE:HB	17	1.48
(1,898)	1:77:A:TYR:HB2	1:79:A:LEU:HG	10	1.47
(1,898)	1:77:A:TYR:HB3	1:79:A:LEU:HG	10	1.47
(1,804)	1:67:A:ARG:H	1:68:A:VAL:HB	13	1.47
(1,781)	1:65:A:GLU:HA	1:77:A:TYR:HD1	13	1.47
(1,781)	1:65:A:GLU:HA	1:77:A:TYR:HD2	13	1.47
(1,568)	1:47:A:MET:HB2	1:48:A:LEU:HG	5	1.47
(1,568)	1:47:A:MET:HB3	1:48:A:LEU:HG	5	1.47
(1,538)	1:43:A:ALA:HA	1:45:A:LYS:HD2	6	1.47
(1,538)	1:43:A:ALA:HA	1:45:A:LYS:HD3	6	1.47
(1,447)	1:35:A:ILE:HG12	1:36:A:PHE:HA	11	1.47
(1,447)	1:35:A:ILE:HG13	1:36:A:PHE:HA	11	1.47
(1,242)	1:21:A:LEU:HG	1:57:A:LYS:HD2	4	1.47
(1,242)	1:21:A:LEU:HG	1:57:A:LYS:HD3	4	1.47
(1,28)	1:5:A:LEU:HG	1:7:A:LEU:HG	16	1.47
(1,890)	1:76:A:LEU:HD11	1:78:A:GLU:H	16	1.46
(1,890)	1:76:A:LEU:HD12	1:78:A:GLU:H	16	1.46
(1,890)	1:76:A:LEU:HD13	1:78:A:GLU:H	16	1.46
(1,804)	1:67:A:ARG:H	1:68:A:VAL:HB	11	1.46
(1,746)	1:63:A:LEU:HA	1:76:A:LEU:HD11	10	1.46
(1,746)	1:63:A:LEU:HA	1:76:A:LEU:HD12	10	1.46
(1,746)	1:63:A:LEU:HA	1:76:A:LEU:HD13	10	1.46
(1,690)	1:56:A:GLU:CD	1:52:A:ASP:CG	19	1.46
(1,500)	1:38:A:PHE:HD1	1:39:A:ALA:H	18	1.46
(1,500)	1:38:A:PHE:HD2	1:39:A:ALA:H	18	1.46
(1,893)	1:76:A:LEU:HD11	1:78:A:GLU:HG2	11	1.45
(1,893)	1:76:A:LEU:HD11	1:78:A:GLU:HG3	11	1.45
(1,893)	1:76:A:LEU:HD12	1:78:A:GLU:HG2	11	1.45
(1,893)	1:76:A:LEU:HD12	1:78:A:GLU:HG3	11	1.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,893)	1:76:A:LEU:HD13	1:78:A:GLU:HG2	11	1.45
(1,893)	1:76:A:LEU:HD13	1:78:A:GLU:HG3	11	1.45
(1,884)	1:76:A:LEU:HA	1:77:A:TYR:HD1	14	1.45
(1,884)	1:76:A:LEU:HA	1:77:A:TYR:HD2	14	1.45
(1,804)	1:67:A:ARG:H	1:68:A:VAL:HB	17	1.45
(1,568)	1:47:A:MET:HB2	1:48:A:LEU:HG	18	1.45
(1,568)	1:47:A:MET:HB3	1:48:A:LEU:HG	18	1.45
(1,471)	1:36:A:PHE:HD1	1:78:A:GLU:H	20	1.45
(1,471)	1:36:A:PHE:HD2	1:78:A:GLU:H	20	1.45
(1,893)	1:76:A:LEU:HD11	1:78:A:GLU:HG2	16	1.44
(1,893)	1:76:A:LEU:HD11	1:78:A:GLU:HG3	16	1.44
(1,893)	1:76:A:LEU:HD12	1:78:A:GLU:HG2	16	1.44
(1,893)	1:76:A:LEU:HD12	1:78:A:GLU:HG3	16	1.44
(1,893)	1:76:A:LEU:HD13	1:78:A:GLU:HG2	16	1.44
(1,893)	1:76:A:LEU:HD13	1:78:A:GLU:HG3	16	1.44
(1,672)	1:55:A:LYS:H	1:63:A:LEU:HD11	2	1.44
(1,672)	1:55:A:LYS:H	1:63:A:LEU:HD12	2	1.44
(1,672)	1:55:A:LYS:H	1:63:A:LEU:HD13	2	1.44
(1,471)	1:36:A:PHE:HD1	1:78:A:GLU:H	10	1.44
(1,471)	1:36:A:PHE:HD2	1:78:A:GLU:H	10	1.44
(1,411)	1:33:A:ARG:HA	1:82:A:ILE:HA	5	1.44
(1,359)	1:28:A:PHE:HA	1:81:A:ILE:HD11	10	1.44
(1,359)	1:28:A:PHE:HA	1:81:A:ILE:HD12	10	1.44
(1,359)	1:28:A:PHE:HA	1:81:A:ILE:HD13	10	1.44
(1,338)	1:27:A:GLU:H	1:30:A:GLU:HG2	8	1.44
(1,338)	1:27:A:GLU:H	1:30:A:GLU:HG3	8	1.44
(1,128)	1:7:A:LEU:HG	1:38:A:PHE:HD1	13	1.44
(1,128)	1:7:A:LEU:HG	1:38:A:PHE:HD2	13	1.44
(1,892)	1:76:A:LEU:HD11	1:78:A:GLU:HA	7	1.43
(1,892)	1:76:A:LEU:HD12	1:78:A:GLU:HA	7	1.43
(1,892)	1:76:A:LEU:HD13	1:78:A:GLU:HA	7	1.43
(1,892)	1:76:A:LEU:HD11	1:78:A:GLU:HA	16	1.43
(1,892)	1:76:A:LEU:HD12	1:78:A:GLU:HA	16	1.43
(1,892)	1:76:A:LEU:HD13	1:78:A:GLU:HA	16	1.43
(1,789)	1:66:A:VAL:H	1:68:A:VAL:HG11	9	1.43
(1,789)	1:66:A:VAL:H	1:68:A:VAL:HG12	9	1.43
(1,789)	1:66:A:VAL:H	1:68:A:VAL:HG13	9	1.43
(1,538)	1:43:A:ALA:HA	1:45:A:LYS:HD2	5	1.43
(1,538)	1:43:A:ALA:HA	1:45:A:LYS:HD3	5	1.43
(1,450)	1:35:A:ILE:HD11	1:54:A:PHE:HE1	16	1.43
(1,450)	1:35:A:ILE:HD11	1:54:A:PHE:HE2	16	1.43
(1,450)	1:35:A:ILE:HD12	1:54:A:PHE:HE1	16	1.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,450)	1:35:A:ILE:HD12	1:54:A:PHE:HE2	16	1.43
(1,450)	1:35:A:ILE:HD13	1:54:A:PHE:HE1	16	1.43
(1,450)	1:35:A:ILE:HD13	1:54:A:PHE:HE2	16	1.43
(1,450)	1:35:A:ILE:HD11	1:54:A:PHE:HE1	16	1.43
(1,450)	1:35:A:ILE:HD11	1:54:A:PHE:HE2	16	1.43
(1,450)	1:35:A:ILE:HD12	1:54:A:PHE:HE1	16	1.43
(1,450)	1:35:A:ILE:HD12	1:54:A:PHE:HE2	16	1.43
(1,450)	1:35:A:ILE:HD13	1:54:A:PHE:HE1	16	1.43
(1,450)	1:35:A:ILE:HD13	1:54:A:PHE:HE2	16	1.43
(1,374)	1:29:A:SER:H	1:30:A:GLU:HG2	19	1.43
(1,374)	1:29:A:SER:H	1:30:A:GLU:HG3	19	1.43
(1,45)	1:6:A:VAL:H	1:35:A:ILE:HB	11	1.43
(1,893)	1:76:A:LEU:HD11	1:78:A:GLU:HG2	20	1.42
(1,893)	1:76:A:LEU:HD11	1:78:A:GLU:HG3	20	1.42
(1,893)	1:76:A:LEU:HD12	1:78:A:GLU:HG2	20	1.42
(1,893)	1:76:A:LEU:HD12	1:78:A:GLU:HG3	20	1.42
(1,893)	1:76:A:LEU:HD13	1:78:A:GLU:HG2	20	1.42
(1,893)	1:76:A:LEU:HD13	1:78:A:GLU:HG3	20	1.42
(1,690)	1:56:A:GLU:CD	1:52:A:ASP:CG	8	1.42
(1,663)	1:54:A:PHE:HD1	1:76:A:LEU:HG	6	1.42
(1,663)	1:54:A:PHE:HD2	1:76:A:LEU:HG	6	1.42
(1,525)	1:41:A:THR:HB	1:73:A:LYS:HB2	13	1.42
(1,525)	1:41:A:THR:HB	1:73:A:LYS:HB3	13	1.42
(1,471)	1:36:A:PHE:HD1	1:78:A:GLU:H	6	1.42
(1,471)	1:36:A:PHE:HD2	1:78:A:GLU:H	6	1.42
(1,239)	1:21:A:LEU:HG	1:56:A:GLU:HB2	15	1.42
(1,239)	1:21:A:LEU:HG	1:56:A:GLU:HB3	15	1.42
(1,921)	1:79:A:LEU:HD11	1:82:A:ILE:HB	13	1.41
(1,921)	1:79:A:LEU:HD12	1:82:A:ILE:HB	13	1.41
(1,921)	1:79:A:LEU:HD13	1:82:A:ILE:HB	13	1.41
(1,898)	1:77:A:TYR:HB2	1:79:A:LEU:HG	7	1.41
(1,898)	1:77:A:TYR:HB3	1:79:A:LEU:HG	7	1.41
(1,568)	1:47:A:MET:HB2	1:48:A:LEU:HG	10	1.41
(1,568)	1:47:A:MET:HB3	1:48:A:LEU:HG	10	1.41
(1,568)	1:47:A:MET:HB2	1:48:A:LEU:HG	11	1.41
(1,568)	1:47:A:MET:HB3	1:48:A:LEU:HG	11	1.41
(1,568)	1:47:A:MET:HB2	1:48:A:LEU:HG	20	1.41
(1,568)	1:47:A:MET:HB3	1:48:A:LEU:HG	20	1.41
(1,476)	1:37:A:TYR:H	1:78:A:GLU:HG2	18	1.41
(1,476)	1:37:A:TYR:H	1:78:A:GLU:HG3	18	1.41
(1,390)	1:31:A:ASP:H	1:81:A:ILE:HG21	16	1.41
(1,390)	1:31:A:ASP:H	1:81:A:ILE:HG22	16	1.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,390)	1:31:A:ASP:H	1:81:A:ILE:HG23	16	1.41
(1,285)	1:24:A:LEU:HA	1:54:A:PHE:HE1	8	1.41
(1,285)	1:24:A:LEU:HA	1:54:A:PHE:HE2	8	1.41
(1,890)	1:76:A:LEU:HD11	1:78:A:GLU:H	20	1.4
(1,890)	1:76:A:LEU:HD12	1:78:A:GLU:H	20	1.4
(1,890)	1:76:A:LEU:HD13	1:78:A:GLU:H	20	1.4
(1,878)	1:75:A:PHE:HB2	1:77:A:TYR:HD1	12	1.4
(1,878)	1:75:A:PHE:HB2	1:77:A:TYR:HD2	12	1.4
(1,878)	1:75:A:PHE:HB3	1:77:A:TYR:HD1	12	1.4
(1,878)	1:75:A:PHE:HB3	1:77:A:TYR:HD2	12	1.4
(1,781)	1:65:A:GLU:HA	1:77:A:TYR:HD1	4	1.4
(1,781)	1:65:A:GLU:HA	1:77:A:TYR:HD2	4	1.4
(1,542)	1:44:A:HIS:HA	1:45:A:LYS:HD2	4	1.4
(1,542)	1:44:A:HIS:HA	1:45:A:LYS:HD3	4	1.4
(1,500)	1:38:A:PHE:HD1	1:39:A:ALA:H	1	1.4
(1,500)	1:38:A:PHE:HD2	1:39:A:ALA:H	1	1.4
(1,390)	1:31:A:ASP:H	1:81:A:ILE:HG21	12	1.4
(1,390)	1:31:A:ASP:H	1:81:A:ILE:HG22	12	1.4
(1,390)	1:31:A:ASP:H	1:81:A:ILE:HG23	12	1.4
(1,239)	1:21:A:LEU:HG	1:56:A:GLU:HB2	13	1.4
(1,239)	1:21:A:LEU:HG	1:56:A:GLU:HB3	13	1.4
(1,908)	1:78:A:GLU:HA	1:80:A:HIS:HD2	18	1.39
(1,892)	1:76:A:LEU:HD11	1:78:A:GLU:HA	20	1.39
(1,892)	1:76:A:LEU:HD12	1:78:A:GLU:HA	20	1.39
(1,892)	1:76:A:LEU:HD13	1:78:A:GLU:HA	20	1.39
(1,801)	1:66:A:VAL:HG11	1:72:A:GLU:HB2	18	1.39
(1,801)	1:66:A:VAL:HG11	1:72:A:GLU:HB3	18	1.39
(1,801)	1:66:A:VAL:HG12	1:72:A:GLU:HB2	18	1.39
(1,801)	1:66:A:VAL:HG12	1:72:A:GLU:HB3	18	1.39
(1,801)	1:66:A:VAL:HG13	1:72:A:GLU:HB2	18	1.39
(1,801)	1:66:A:VAL:HG13	1:72:A:GLU:HB3	18	1.39
(1,801)	1:66:A:VAL:HG21	1:72:A:GLU:HB2	18	1.39
(1,801)	1:66:A:VAL:HG21	1:72:A:GLU:HB3	18	1.39
(1,801)	1:66:A:VAL:HG22	1:72:A:GLU:HB2	18	1.39
(1,801)	1:66:A:VAL:HG22	1:72:A:GLU:HB3	18	1.39
(1,801)	1:66:A:VAL:HG23	1:72:A:GLU:HB2	18	1.39
(1,801)	1:66:A:VAL:HG23	1:72:A:GLU:HB3	18	1.39
(1,794)	1:66:A:VAL:HA	1:77:A:TYR:H	18	1.39
(1,746)	1:63:A:LEU:HA	1:76:A:LEU:HD11	17	1.39
(1,746)	1:63:A:LEU:HA	1:76:A:LEU:HD12	17	1.39
(1,746)	1:63:A:LEU:HA	1:76:A:LEU:HD13	17	1.39
(1,690)	1:56:A:GLU:CD	1:52:A:ASP:CG	17	1.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,687)	1:56:A:GLU:HA	1:57:A:LYS:HE2	5	1.39
(1,687)	1:56:A:GLU:HA	1:57:A:LYS:HE3	5	1.39
(1,687)	1:56:A:GLU:HA	1:57:A:LYS:HE2	19	1.39
(1,687)	1:56:A:GLU:HA	1:57:A:LYS:HE3	19	1.39
(1,471)	1:36:A:PHE:HD1	1:78:A:GLU:H	17	1.39
(1,471)	1:36:A:PHE:HD2	1:78:A:GLU:H	17	1.39
(1,374)	1:29:A:SER:H	1:30:A:GLU:HG2	15	1.39
(1,374)	1:29:A:SER:H	1:30:A:GLU:HG3	15	1.39
(1,351)	1:28:A:PHE:H	1:81:A:ILE:HG21	1	1.39
(1,351)	1:28:A:PHE:H	1:81:A:ILE:HG22	1	1.39
(1,351)	1:28:A:PHE:H	1:81:A:ILE:HG23	1	1.39
(1,300)	1:24:A:LEU:HD11	1:35:A:ILE:HG12	17	1.39
(1,300)	1:24:A:LEU:HD11	1:35:A:ILE:HG13	17	1.39
(1,300)	1:24:A:LEU:HD12	1:35:A:ILE:HG12	17	1.39
(1,300)	1:24:A:LEU:HD12	1:35:A:ILE:HG13	17	1.39
(1,300)	1:24:A:LEU:HD13	1:35:A:ILE:HG12	17	1.39
(1,300)	1:24:A:LEU:HD13	1:35:A:ILE:HG13	17	1.39
(1,903)	1:78:A:GLU:H	1:79:A:LEU:HG	17	1.38
(1,542)	1:44:A:HIS:HA	1:45:A:LYS:HD2	10	1.38
(1,542)	1:44:A:HIS:HA	1:45:A:LYS:HD3	10	1.38
(1,542)	1:44:A:HIS:HA	1:45:A:LYS:HD2	17	1.38
(1,542)	1:44:A:HIS:HA	1:45:A:LYS:HD3	17	1.38
(1,525)	1:41:A:THR:HB	1:73:A:LYS:HB2	14	1.38
(1,525)	1:41:A:THR:HB	1:73:A:LYS:HB3	14	1.38
(1,418)	1:34:A:SER:H	1:79:A:LEU:HD21	15	1.38
(1,418)	1:34:A:SER:H	1:79:A:LEU:HD22	15	1.38
(1,418)	1:34:A:SER:H	1:79:A:LEU:HD23	15	1.38
(1,285)	1:24:A:LEU:HA	1:54:A:PHE:HE1	10	1.38
(1,285)	1:24:A:LEU:HA	1:54:A:PHE:HE2	10	1.38
(1,239)	1:21:A:LEU:HG	1:56:A:GLU:HB2	20	1.38
(1,239)	1:21:A:LEU:HG	1:56:A:GLU:HB3	20	1.38
(1,32)	1:5:A:LEU:HD11	1:7:A:LEU:H	18	1.38
(1,32)	1:5:A:LEU:HD12	1:7:A:LEU:H	18	1.38
(1,32)	1:5:A:LEU:HD13	1:7:A:LEU:H	18	1.38
(1,32)	1:5:A:LEU:HD21	1:7:A:LEU:H	18	1.38
(1,32)	1:5:A:LEU:HD22	1:7:A:LEU:H	18	1.38
(1,32)	1:5:A:LEU:HD23	1:7:A:LEU:H	18	1.38
(1,814)	1:68:A:VAL:HG11	1:73:A:LYS:H	18	1.37
(1,814)	1:68:A:VAL:HG12	1:73:A:LYS:H	18	1.37
(1,814)	1:68:A:VAL:HG13	1:73:A:LYS:H	18	1.37
(1,814)	1:68:A:VAL:HG21	1:73:A:LYS:H	18	1.37
(1,814)	1:68:A:VAL:HG22	1:73:A:LYS:H	18	1.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,814)	1:68:A:VAL:HG23	1:73:A:LYS:H	18	1.37
(1,746)	1:63:A:LEU:HA	1:76:A:LEU:HD11	5	1.37
(1,746)	1:63:A:LEU:HA	1:76:A:LEU:HD12	5	1.37
(1,746)	1:63:A:LEU:HA	1:76:A:LEU:HD13	5	1.37
(1,568)	1:47:A:MET:HB2	1:48:A:LEU:HG	9	1.37
(1,568)	1:47:A:MET:HB3	1:48:A:LEU:HG	9	1.37
(1,568)	1:47:A:MET:HB2	1:48:A:LEU:HG	14	1.37
(1,568)	1:47:A:MET:HB3	1:48:A:LEU:HG	14	1.37
(1,501)	1:38:A:PHE:HD1	1:75:A:PHE:H	14	1.37
(1,501)	1:38:A:PHE:HD2	1:75:A:PHE:H	14	1.37
(1,418)	1:34:A:SER:H	1:79:A:LEU:HD21	8	1.37
(1,418)	1:34:A:SER:H	1:79:A:LEU:HD22	8	1.37
(1,418)	1:34:A:SER:H	1:79:A:LEU:HD23	8	1.37
(1,878)	1:75:A:PHE:HB2	1:77:A:TYR:HD1	8	1.36
(1,878)	1:75:A:PHE:HB2	1:77:A:TYR:HD2	8	1.36
(1,878)	1:75:A:PHE:HB3	1:77:A:TYR:HD1	8	1.36
(1,878)	1:75:A:PHE:HB3	1:77:A:TYR:HD2	8	1.36
(1,746)	1:63:A:LEU:HA	1:76:A:LEU:HD11	2	1.36
(1,746)	1:63:A:LEU:HA	1:76:A:LEU:HD12	2	1.36
(1,746)	1:63:A:LEU:HA	1:76:A:LEU:HD13	2	1.36
(1,746)	1:63:A:LEU:HA	1:76:A:LEU:HD11	4	1.36
(1,746)	1:63:A:LEU:HA	1:76:A:LEU:HD12	4	1.36
(1,746)	1:63:A:LEU:HA	1:76:A:LEU:HD13	4	1.36
(1,714)	1:60:A:THR:HA	1:81:A:ILE:HG21	8	1.36
(1,714)	1:60:A:THR:HA	1:81:A:ILE:HG22	8	1.36
(1,714)	1:60:A:THR:HA	1:81:A:ILE:HG23	8	1.36
(1,568)	1:47:A:MET:HB2	1:48:A:LEU:HG	6	1.36
(1,568)	1:47:A:MET:HB3	1:48:A:LEU:HG	6	1.36
(1,501)	1:38:A:PHE:HD1	1:75:A:PHE:H	7	1.36
(1,501)	1:38:A:PHE:HD2	1:75:A:PHE:H	7	1.36
(1,499)	1:38:A:PHE:HB2	1:75:A:PHE:HD1	18	1.36
(1,499)	1:38:A:PHE:HB2	1:75:A:PHE:HD2	18	1.36
(1,499)	1:38:A:PHE:HB3	1:75:A:PHE:HD1	18	1.36
(1,499)	1:38:A:PHE:HB3	1:75:A:PHE:HD2	18	1.36
(1,390)	1:31:A:ASP:H	1:81:A:ILE:HG21	8	1.36
(1,390)	1:31:A:ASP:H	1:81:A:ILE:HG22	8	1.36
(1,390)	1:31:A:ASP:H	1:81:A:ILE:HG23	8	1.36
(1,374)	1:29:A:SER:H	1:30:A:GLU:HG2	3	1.36
(1,374)	1:29:A:SER:H	1:30:A:GLU:HG3	3	1.36
(1,241)	1:21:A:LEU:HG	1:57:A:LYS:HG2	3	1.36
(1,241)	1:21:A:LEU:HG	1:57:A:LYS:HG3	3	1.36
(1,68)	1:6:A:VAL:HB	1:19:A:VAL:HB	19	1.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,25)	1:5:A:LEU:HG	1:6:A:VAL:HA	3	1.36
(1,892)	1:76:A:LEU:HD11	1:78:A:GLU:HA	14	1.35
(1,892)	1:76:A:LEU:HD12	1:78:A:GLU:HA	14	1.35
(1,892)	1:76:A:LEU:HD13	1:78:A:GLU:HA	14	1.35
(1,746)	1:63:A:LEU:HA	1:76:A:LEU:HD11	13	1.35
(1,746)	1:63:A:LEU:HA	1:76:A:LEU:HD12	13	1.35
(1,746)	1:63:A:LEU:HA	1:76:A:LEU:HD13	13	1.35
(1,714)	1:60:A:THR:HA	1:81:A:ILE:HG21	16	1.35
(1,714)	1:60:A:THR:HA	1:81:A:ILE:HG22	16	1.35
(1,714)	1:60:A:THR:HA	1:81:A:ILE:HG23	16	1.35
(1,690)	1:56:A:GLU:CD	1:52:A:ASP:CG	5	1.35
(1,687)	1:56:A:GLU:HA	1:57:A:LYS:HE2	13	1.35
(1,687)	1:56:A:GLU:HA	1:57:A:LYS:HE3	13	1.35
(1,418)	1:34:A:SER:H	1:79:A:LEU:HD21	4	1.35
(1,418)	1:34:A:SER:H	1:79:A:LEU:HD22	4	1.35
(1,418)	1:34:A:SER:H	1:79:A:LEU:HD23	4	1.35
(1,176)	1:13:A:LYS:H	1:14:A:SER:H	16	1.35
(1,892)	1:76:A:LEU:HD11	1:78:A:GLU:HA	12	1.34
(1,892)	1:76:A:LEU:HD12	1:78:A:GLU:HA	12	1.34
(1,892)	1:76:A:LEU:HD13	1:78:A:GLU:HA	12	1.34
(1,746)	1:63:A:LEU:HA	1:76:A:LEU:HD11	3	1.34
(1,746)	1:63:A:LEU:HA	1:76:A:LEU:HD12	3	1.34
(1,746)	1:63:A:LEU:HA	1:76:A:LEU:HD13	3	1.34
(1,690)	1:56:A:GLU:CD	1:52:A:ASP:CG	13	1.34
(1,672)	1:55:A:LYS:H	1:63:A:LEU:HD11	8	1.34
(1,672)	1:55:A:LYS:H	1:63:A:LEU:HD12	8	1.34
(1,672)	1:55:A:LYS:H	1:63:A:LEU:HD13	8	1.34
(1,568)	1:47:A:MET:HB2	1:48:A:LEU:HG	3	1.34
(1,568)	1:47:A:MET:HB3	1:48:A:LEU:HG	3	1.34
(1,542)	1:44:A:HIS:HA	1:45:A:LYS:HD2	3	1.34
(1,542)	1:44:A:HIS:HA	1:45:A:LYS:HD3	3	1.34
(1,542)	1:44:A:HIS:HA	1:45:A:LYS:HD2	19	1.34
(1,542)	1:44:A:HIS:HA	1:45:A:LYS:HD3	19	1.34
(1,917)	1:79:A:LEU:HB2	1:80:A:HIS:HD2	3	1.33
(1,917)	1:79:A:LEU:HB3	1:80:A:HIS:HD2	3	1.33
(1,714)	1:60:A:THR:HA	1:81:A:ILE:HG21	14	1.33
(1,714)	1:60:A:THR:HA	1:81:A:ILE:HG22	14	1.33
(1,714)	1:60:A:THR:HA	1:81:A:ILE:HG23	14	1.33
(1,525)	1:41:A:THR:HB	1:73:A:LYS:HB2	2	1.33
(1,525)	1:41:A:THR:HB	1:73:A:LYS:HB3	2	1.33
(1,525)	1:41:A:THR:HB	1:73:A:LYS:HB2	4	1.33
(1,525)	1:41:A:THR:HB	1:73:A:LYS:HB3	4	1.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,501)	1:38:A:PHE:HD1	1:75:A:PHE:H	1	1.33
(1,501)	1:38:A:PHE:HD2	1:75:A:PHE:H	1	1.33
(1,448)	1:35:A:ILE:HG12	1:76:A:LEU:HB2	3	1.33
(1,448)	1:35:A:ILE:HG12	1:76:A:LEU:HB3	3	1.33
(1,448)	1:35:A:ILE:HG13	1:76:A:LEU:HB2	3	1.33
(1,448)	1:35:A:ILE:HG13	1:76:A:LEU:HB3	3	1.33
(1,447)	1:35:A:ILE:HG12	1:36:A:PHE:HA	13	1.33
(1,447)	1:35:A:ILE:HG13	1:36:A:PHE:HA	13	1.33
(1,411)	1:33:A:ARG:HA	1:82:A:ILE:HA	7	1.33
(1,390)	1:31:A:ASP:H	1:81:A:ILE:HG21	14	1.33
(1,390)	1:31:A:ASP:H	1:81:A:ILE:HG22	14	1.33
(1,390)	1:31:A:ASP:H	1:81:A:ILE:HG23	14	1.33
(1,387)	1:30:A:GLU:HG2	1:31:A:ASP:H	3	1.33
(1,387)	1:30:A:GLU:HG3	1:31:A:ASP:H	3	1.33
(1,293)	1:24:A:LEU:HB2	1:80:A:HIS:HE1	13	1.33
(1,293)	1:24:A:LEU:HB3	1:80:A:HIS:HE1	13	1.33
(1,878)	1:75:A:PHE:HB2	1:77:A:TYR:HD1	15	1.32
(1,878)	1:75:A:PHE:HB2	1:77:A:TYR:HD2	15	1.32
(1,878)	1:75:A:PHE:HB3	1:77:A:TYR:HD1	15	1.32
(1,878)	1:75:A:PHE:HB3	1:77:A:TYR:HD2	15	1.32
(1,690)	1:56:A:GLU:CD	1:52:A:ASP:CG	7	1.32
(1,568)	1:47:A:MET:HB2	1:48:A:LEU:HG	12	1.32
(1,568)	1:47:A:MET:HB3	1:48:A:LEU:HG	12	1.32
(1,242)	1:21:A:LEU:HG	1:57:A:LYS:HD2	8	1.32
(1,242)	1:21:A:LEU:HG	1:57:A:LYS:HD3	8	1.32
(1,25)	1:5:A:LEU:HG	1:6:A:VAL:HA	7	1.32
(1,890)	1:76:A:LEU:HD11	1:78:A:GLU:H	1	1.31
(1,890)	1:76:A:LEU:HD12	1:78:A:GLU:H	1	1.31
(1,890)	1:76:A:LEU:HD13	1:78:A:GLU:H	1	1.31
(1,878)	1:75:A:PHE:HB2	1:77:A:TYR:HD1	6	1.31
(1,878)	1:75:A:PHE:HB2	1:77:A:TYR:HD2	6	1.31
(1,878)	1:75:A:PHE:HB3	1:77:A:TYR:HD1	6	1.31
(1,878)	1:75:A:PHE:HB3	1:77:A:TYR:HD2	6	1.31
(1,878)	1:75:A:PHE:HB2	1:77:A:TYR:HD1	13	1.31
(1,878)	1:75:A:PHE:HB2	1:77:A:TYR:HD2	13	1.31
(1,878)	1:75:A:PHE:HB3	1:77:A:TYR:HD1	13	1.31
(1,878)	1:75:A:PHE:HB3	1:77:A:TYR:HD2	13	1.31
(1,804)	1:67:A:ARG:H	1:68:A:VAL:HB	15	1.31
(1,789)	1:66:A:VAL:H	1:68:A:VAL:HG11	8	1.31
(1,789)	1:66:A:VAL:H	1:68:A:VAL:HG12	8	1.31
(1,789)	1:66:A:VAL:H	1:68:A:VAL:HG13	8	1.31
(1,495)	1:38:A:PHE:HA	1:75:A:PHE:HD1	9	1.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,495)	1:38:A:PHE:HA	1:75:A:PHE:HD2	9	1.31
(1,471)	1:36:A:PHE:HD1	1:78:A:GLU:H	16	1.31
(1,471)	1:36:A:PHE:HD2	1:78:A:GLU:H	16	1.31
(1,202)	1:19:A:VAL:H	1:20:A:GLU:HG2	1	1.31
(1,202)	1:19:A:VAL:H	1:20:A:GLU:HG3	1	1.31
(1,176)	1:13:A:LYS:H	1:14:A:SER:H	5	1.31
(1,35)	1:5:A:LEU:HD11	1:7:A:LEU:HG	16	1.31
(1,35)	1:5:A:LEU:HD12	1:7:A:LEU:HG	16	1.31
(1,35)	1:5:A:LEU:HD13	1:7:A:LEU:HG	16	1.31
(1,35)	1:5:A:LEU:HD21	1:7:A:LEU:HG	16	1.31
(1,35)	1:5:A:LEU:HD22	1:7:A:LEU:HG	16	1.31
(1,35)	1:5:A:LEU:HD23	1:7:A:LEU:HG	16	1.31
(1,781)	1:65:A:GLU:HA	1:77:A:TYR:HD1	20	1.3
(1,781)	1:65:A:GLU:HA	1:77:A:TYR:HD2	20	1.3
(1,690)	1:56:A:GLU:CD	1:52:A:ASP:CG	20	1.3
(1,542)	1:44:A:HIS:HA	1:45:A:LYS:HD2	2	1.3
(1,542)	1:44:A:HIS:HA	1:45:A:LYS:HD3	2	1.3
(1,25)	1:5:A:LEU:HG	1:6:A:VAL:HA	4	1.3
(1,917)	1:79:A:LEU:HB2	1:80:A:HIS:HD2	7	1.29
(1,917)	1:79:A:LEU:HB3	1:80:A:HIS:HD2	7	1.29
(1,898)	1:77:A:TYR:HB2	1:79:A:LEU:HG	9	1.29
(1,898)	1:77:A:TYR:HB3	1:79:A:LEU:HG	9	1.29
(1,893)	1:76:A:LEU:HD11	1:78:A:GLU:HG2	8	1.29
(1,893)	1:76:A:LEU:HD11	1:78:A:GLU:HG3	8	1.29
(1,893)	1:76:A:LEU:HD12	1:78:A:GLU:HG2	8	1.29
(1,893)	1:76:A:LEU:HD12	1:78:A:GLU:HG3	8	1.29
(1,893)	1:76:A:LEU:HD13	1:78:A:GLU:HG2	8	1.29
(1,893)	1:76:A:LEU:HD13	1:78:A:GLU:HG3	8	1.29
(1,794)	1:66:A:VAL:HA	1:77:A:TYR:H	14	1.29
(1,789)	1:66:A:VAL:H	1:68:A:VAL:HG11	11	1.29
(1,789)	1:66:A:VAL:H	1:68:A:VAL:HG12	11	1.29
(1,789)	1:66:A:VAL:H	1:68:A:VAL:HG13	11	1.29
(1,741)	1:62:A:TYR:HD1	1:63:A:LEU:H	6	1.29
(1,741)	1:62:A:TYR:HD2	1:63:A:LEU:H	6	1.29
(1,714)	1:60:A:THR:HA	1:81:A:ILE:HG21	6	1.29
(1,714)	1:60:A:THR:HA	1:81:A:ILE:HG22	6	1.29
(1,714)	1:60:A:THR:HA	1:81:A:ILE:HG23	6	1.29
(1,672)	1:55:A:LYS:H	1:63:A:LEU:HD11	20	1.29
(1,672)	1:55:A:LYS:H	1:63:A:LEU:HD12	20	1.29
(1,672)	1:55:A:LYS:H	1:63:A:LEU:HD13	20	1.29
(1,495)	1:38:A:PHE:HA	1:75:A:PHE:HD1	7	1.29
(1,495)	1:38:A:PHE:HA	1:75:A:PHE:HD2	7	1.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,471)	1:36:A:PHE:HD1	1:78:A:GLU:H	11	1.29
(1,471)	1:36:A:PHE:HD2	1:78:A:GLU:H	11	1.29
(1,390)	1:31:A:ASP:H	1:81:A:ILE:HG21	9	1.29
(1,390)	1:31:A:ASP:H	1:81:A:ILE:HG22	9	1.29
(1,390)	1:31:A:ASP:H	1:81:A:ILE:HG23	9	1.29
(1,242)	1:21:A:LEU:HG	1:57:A:LYS:HD2	13	1.29
(1,242)	1:21:A:LEU:HG	1:57:A:LYS:HD3	13	1.29
(1,36)	1:5:A:LEU:HD11	1:7:A:LEU:HD11	8	1.29
(1,36)	1:5:A:LEU:HD11	1:7:A:LEU:HD12	8	1.29
(1,36)	1:5:A:LEU:HD11	1:7:A:LEU:HD13	8	1.29
(1,36)	1:5:A:LEU:HD12	1:7:A:LEU:HD11	8	1.29
(1,36)	1:5:A:LEU:HD12	1:7:A:LEU:HD12	8	1.29
(1,36)	1:5:A:LEU:HD12	1:7:A:LEU:HD13	8	1.29
(1,36)	1:5:A:LEU:HD13	1:7:A:LEU:HD11	8	1.29
(1,36)	1:5:A:LEU:HD13	1:7:A:LEU:HD12	8	1.29
(1,36)	1:5:A:LEU:HD13	1:7:A:LEU:HD13	8	1.29
(1,36)	1:5:A:LEU:HD21	1:7:A:LEU:HD11	8	1.29
(1,36)	1:5:A:LEU:HD21	1:7:A:LEU:HD12	8	1.29
(1,36)	1:5:A:LEU:HD21	1:7:A:LEU:HD13	8	1.29
(1,36)	1:5:A:LEU:HD22	1:7:A:LEU:HD11	8	1.29
(1,36)	1:5:A:LEU:HD22	1:7:A:LEU:HD12	8	1.29
(1,36)	1:5:A:LEU:HD22	1:7:A:LEU:HD13	8	1.29
(1,36)	1:5:A:LEU:HD23	1:7:A:LEU:HD11	8	1.29
(1,36)	1:5:A:LEU:HD23	1:7:A:LEU:HD12	8	1.29
(1,36)	1:5:A:LEU:HD23	1:7:A:LEU:HD13	8	1.29
(1,892)	1:76:A:LEU:HD11	1:78:A:GLU:HA	18	1.28
(1,892)	1:76:A:LEU:HD12	1:78:A:GLU:HA	18	1.28
(1,892)	1:76:A:LEU:HD13	1:78:A:GLU:HA	18	1.28
(1,878)	1:75:A:PHE:HB2	1:77:A:TYR:HD1	7	1.28
(1,878)	1:75:A:PHE:HB2	1:77:A:TYR:HD2	7	1.28
(1,878)	1:75:A:PHE:HB3	1:77:A:TYR:HD1	7	1.28
(1,878)	1:75:A:PHE:HB3	1:77:A:TYR:HD2	7	1.28
(1,858)	1:72:A:GLU:HB2	1:74:A:ASP:H	17	1.28
(1,858)	1:72:A:GLU:HB3	1:74:A:ASP:H	17	1.28
(1,794)	1:66:A:VAL:HA	1:77:A:TYR:H	16	1.28
(1,789)	1:66:A:VAL:H	1:68:A:VAL:HG11	7	1.28
(1,789)	1:66:A:VAL:H	1:68:A:VAL:HG12	7	1.28
(1,789)	1:66:A:VAL:H	1:68:A:VAL:HG13	7	1.28
(1,781)	1:65:A:GLU:HA	1:77:A:TYR:HD1	5	1.28
(1,781)	1:65:A:GLU:HA	1:77:A:TYR:HD2	5	1.28
(1,687)	1:56:A:GLU:HA	1:57:A:LYS:HE2	2	1.28
(1,687)	1:56:A:GLU:HA	1:57:A:LYS:HE3	2	1.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,525)	1:41:A:THR:HB	1:73:A:LYS:HB2	5	1.28
(1,525)	1:41:A:THR:HB	1:73:A:LYS:HB3	5	1.28
(1,495)	1:38:A:PHE:HA	1:75:A:PHE:HD1	6	1.28
(1,495)	1:38:A:PHE:HA	1:75:A:PHE:HD2	6	1.28
(1,471)	1:36:A:PHE:HD1	1:78:A:GLU:H	3	1.28
(1,471)	1:36:A:PHE:HD2	1:78:A:GLU:H	3	1.28
(1,418)	1:34:A:SER:H	1:79:A:LEU:HD21	13	1.28
(1,418)	1:34:A:SER:H	1:79:A:LEU:HD22	13	1.28
(1,418)	1:34:A:SER:H	1:79:A:LEU:HD23	13	1.28
(1,242)	1:21:A:LEU:HG	1:57:A:LYS:HD2	2	1.28
(1,242)	1:21:A:LEU:HG	1:57:A:LYS:HD3	2	1.28
(1,242)	1:21:A:LEU:HG	1:57:A:LYS:HD2	15	1.28
(1,242)	1:21:A:LEU:HG	1:57:A:LYS:HD3	15	1.28
(1,241)	1:21:A:LEU:HG	1:57:A:LYS:HG2	4	1.28
(1,241)	1:21:A:LEU:HG	1:57:A:LYS:HG3	4	1.28
(1,241)	1:21:A:LEU:HG	1:57:A:LYS:HG2	11	1.28
(1,241)	1:21:A:LEU:HG	1:57:A:LYS:HG3	11	1.28
(1,240)	1:21:A:LEU:HG	1:57:A:LYS:HB2	12	1.28
(1,240)	1:21:A:LEU:HG	1:57:A:LYS:HB3	12	1.28
(1,239)	1:21:A:LEU:HG	1:56:A:GLU:HB2	7	1.28
(1,239)	1:21:A:LEU:HG	1:56:A:GLU:HB3	7	1.28
(1,61)	1:6:A:VAL:HA	1:19:A:VAL:HB	19	1.28
(1,25)	1:5:A:LEU:HG	1:6:A:VAL:HA	17	1.28
(1,789)	1:66:A:VAL:H	1:68:A:VAL:HG11	3	1.27
(1,789)	1:66:A:VAL:H	1:68:A:VAL:HG12	3	1.27
(1,789)	1:66:A:VAL:H	1:68:A:VAL:HG13	3	1.27
(1,542)	1:44:A:HIS:HA	1:45:A:LYS:HD2	14	1.27
(1,542)	1:44:A:HIS:HA	1:45:A:LYS:HD3	14	1.27
(1,471)	1:36:A:PHE:HD1	1:78:A:GLU:H	19	1.27
(1,471)	1:36:A:PHE:HD2	1:78:A:GLU:H	19	1.27
(1,370)	1:28:A:PHE:HE1	1:81:A:ILE:HA	14	1.27
(1,370)	1:28:A:PHE:HE2	1:81:A:ILE:HA	14	1.27
(1,45)	1:6:A:VAL:H	1:35:A:ILE:HB	3	1.27
(1,36)	1:5:A:LEU:HD11	1:7:A:LEU:HD11	4	1.27
(1,36)	1:5:A:LEU:HD11	1:7:A:LEU:HD12	4	1.27
(1,36)	1:5:A:LEU:HD11	1:7:A:LEU:HD13	4	1.27
(1,36)	1:5:A:LEU:HD12	1:7:A:LEU:HD11	4	1.27
(1,36)	1:5:A:LEU:HD12	1:7:A:LEU:HD12	4	1.27
(1,36)	1:5:A:LEU:HD12	1:7:A:LEU:HD13	4	1.27
(1,36)	1:5:A:LEU:HD13	1:7:A:LEU:HD11	4	1.27
(1,36)	1:5:A:LEU:HD13	1:7:A:LEU:HD12	4	1.27
(1,36)	1:5:A:LEU:HD13	1:7:A:LEU:HD13	4	1.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,36)	1:5:A:LEU:HD21	1:7:A:LEU:HD11	4	1.27
(1,36)	1:5:A:LEU:HD21	1:7:A:LEU:HD12	4	1.27
(1,36)	1:5:A:LEU:HD21	1:7:A:LEU:HD13	4	1.27
(1,36)	1:5:A:LEU:HD22	1:7:A:LEU:HD11	4	1.27
(1,36)	1:5:A:LEU:HD22	1:7:A:LEU:HD12	4	1.27
(1,36)	1:5:A:LEU:HD22	1:7:A:LEU:HD13	4	1.27
(1,36)	1:5:A:LEU:HD23	1:7:A:LEU:HD11	4	1.27
(1,36)	1:5:A:LEU:HD23	1:7:A:LEU:HD12	4	1.27
(1,36)	1:5:A:LEU:HD23	1:7:A:LEU:HD13	4	1.27
(1,25)	1:5:A:LEU:HG	1:6:A:VAL:HA	18	1.27
(1,892)	1:76:A:LEU:HD11	1:78:A:GLU:HA	1	1.26
(1,892)	1:76:A:LEU:HD12	1:78:A:GLU:HA	1	1.26
(1,892)	1:76:A:LEU:HD13	1:78:A:GLU:HA	1	1.26
(1,781)	1:65:A:GLU:HA	1:77:A:TYR:HD1	15	1.26
(1,781)	1:65:A:GLU:HA	1:77:A:TYR:HD2	15	1.26
(1,768)	1:64:A:ASP:HA	1:76:A:LEU:HD21	9	1.26
(1,768)	1:64:A:ASP:HA	1:76:A:LEU:HD22	9	1.26
(1,768)	1:64:A:ASP:HA	1:76:A:LEU:HD23	9	1.26
(1,542)	1:44:A:HIS:HA	1:45:A:LYS:HD2	5	1.26
(1,542)	1:44:A:HIS:HA	1:45:A:LYS:HD3	5	1.26
(1,476)	1:37:A:TYR:H	1:78:A:GLU:HG2	16	1.26
(1,476)	1:37:A:TYR:H	1:78:A:GLU:HG3	16	1.26
(1,471)	1:36:A:PHE:HD1	1:78:A:GLU:H	7	1.26
(1,471)	1:36:A:PHE:HD2	1:78:A:GLU:H	7	1.26
(1,471)	1:36:A:PHE:HD1	1:78:A:GLU:H	8	1.26
(1,471)	1:36:A:PHE:HD2	1:78:A:GLU:H	8	1.26
(1,299)	1:24:A:LEU:HD11	1:35:A:ILE:HG21	19	1.26
(1,299)	1:24:A:LEU:HD11	1:35:A:ILE:HG22	19	1.26
(1,299)	1:24:A:LEU:HD11	1:35:A:ILE:HG23	19	1.26
(1,299)	1:24:A:LEU:HD12	1:35:A:ILE:HG21	19	1.26
(1,299)	1:24:A:LEU:HD12	1:35:A:ILE:HG22	19	1.26
(1,299)	1:24:A:LEU:HD12	1:35:A:ILE:HG23	19	1.26
(1,299)	1:24:A:LEU:HD13	1:35:A:ILE:HG21	19	1.26
(1,299)	1:24:A:LEU:HD13	1:35:A:ILE:HG22	19	1.26
(1,299)	1:24:A:LEU:HD13	1:35:A:ILE:HG23	19	1.26
(1,45)	1:6:A:VAL:H	1:35:A:ILE:HB	15	1.26
(1,917)	1:79:A:LEU:HB2	1:80:A:HIS:HD2	9	1.25
(1,917)	1:79:A:LEU:HB3	1:80:A:HIS:HD2	9	1.25
(1,890)	1:76:A:LEU:HD11	1:78:A:GLU:H	9	1.25
(1,890)	1:76:A:LEU:HD12	1:78:A:GLU:H	9	1.25
(1,890)	1:76:A:LEU:HD13	1:78:A:GLU:H	9	1.25
(1,727)	1:61:A:ALA:HB1	1:79:A:LEU:HB3	3	1.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,727)	1:61:A:ALA:HB2	1:79:A:LEU:HB3	3	1.25
(1,727)	1:61:A:ALA:HB3	1:79:A:LEU:HB3	3	1.25
(1,672)	1:55:A:LYS:H	1:63:A:LEU:HD11	6	1.25
(1,672)	1:55:A:LYS:H	1:63:A:LEU:HD12	6	1.25
(1,672)	1:55:A:LYS:H	1:63:A:LEU:HD13	6	1.25
(1,542)	1:44:A:HIS:HA	1:45:A:LYS:HD2	11	1.25
(1,542)	1:44:A:HIS:HA	1:45:A:LYS:HD3	11	1.25
(1,499)	1:38:A:PHE:HB2	1:75:A:PHE:HD1	1	1.25
(1,499)	1:38:A:PHE:HB2	1:75:A:PHE:HD2	1	1.25
(1,499)	1:38:A:PHE:HB3	1:75:A:PHE:HD1	1	1.25
(1,499)	1:38:A:PHE:HB3	1:75:A:PHE:HD2	1	1.25
(1,450)	1:35:A:ILE:HD11	1:54:A:PHE:HE1	3	1.25
(1,450)	1:35:A:ILE:HD11	1:54:A:PHE:HE2	3	1.25
(1,450)	1:35:A:ILE:HD12	1:54:A:PHE:HE1	3	1.25
(1,450)	1:35:A:ILE:HD12	1:54:A:PHE:HE2	3	1.25
(1,450)	1:35:A:ILE:HD13	1:54:A:PHE:HE1	3	1.25
(1,450)	1:35:A:ILE:HD13	1:54:A:PHE:HE2	3	1.25
(1,450)	1:35:A:ILE:HD11	1:54:A:PHE:HE1	3	1.25
(1,450)	1:35:A:ILE:HD11	1:54:A:PHE:HE2	3	1.25
(1,450)	1:35:A:ILE:HD12	1:54:A:PHE:HE1	3	1.25
(1,450)	1:35:A:ILE:HD12	1:54:A:PHE:HE2	3	1.25
(1,450)	1:35:A:ILE:HD13	1:54:A:PHE:HE1	3	1.25
(1,450)	1:35:A:ILE:HD13	1:54:A:PHE:HE2	3	1.25
(1,387)	1:30:A:GLU:HG2	1:31:A:ASP:H	8	1.25
(1,387)	1:30:A:GLU:HG3	1:31:A:ASP:H	8	1.25
(1,374)	1:29:A:SER:H	1:30:A:GLU:HG2	8	1.25
(1,374)	1:29:A:SER:H	1:30:A:GLU:HG3	8	1.25
(1,917)	1:79:A:LEU:HB2	1:80:A:HIS:HD2	17	1.24
(1,917)	1:79:A:LEU:HB3	1:80:A:HIS:HD2	17	1.24
(1,892)	1:76:A:LEU:HD11	1:78:A:GLU:HA	8	1.24
(1,892)	1:76:A:LEU:HD12	1:78:A:GLU:HA	8	1.24
(1,892)	1:76:A:LEU:HD13	1:78:A:GLU:HA	8	1.24
(1,804)	1:67:A:ARG:H	1:68:A:VAL:HB	18	1.24
(1,690)	1:56:A:GLU:CD	1:52:A:ASP:CG	2	1.24
(1,690)	1:56:A:GLU:CD	1:52:A:ASP:CG	16	1.24
(1,495)	1:38:A:PHE:HA	1:75:A:PHE:HD1	11	1.24
(1,495)	1:38:A:PHE:HA	1:75:A:PHE:HD2	11	1.24
(1,476)	1:37:A:TYR:H	1:78:A:GLU:HG2	19	1.24
(1,476)	1:37:A:TYR:H	1:78:A:GLU:HG3	19	1.24
(1,471)	1:36:A:PHE:HD1	1:78:A:GLU:H	15	1.24
(1,471)	1:36:A:PHE:HD2	1:78:A:GLU:H	15	1.24
(1,390)	1:31:A:ASP:H	1:81:A:ILE:HG21	17	1.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,390)	1:31:A:ASP:H	1:81:A:ILE:HG22	17	1.24
(1,390)	1:31:A:ASP:H	1:81:A:ILE:HG23	17	1.24
(1,351)	1:28:A:PHE:H	1:81:A:ILE:HG21	13	1.24
(1,351)	1:28:A:PHE:H	1:81:A:ILE:HG22	13	1.24
(1,351)	1:28:A:PHE:H	1:81:A:ILE:HG23	13	1.24
(1,284)	1:24:A:LEU:HA	1:35:A:ILE:HD11	3	1.24
(1,284)	1:24:A:LEU:HA	1:35:A:ILE:HD12	3	1.24
(1,284)	1:24:A:LEU:HA	1:35:A:ILE:HD13	3	1.24
(1,250)	1:21:A:LEU:HD21	1:59:A:HIS:HE1	6	1.24
(1,250)	1:21:A:LEU:HD22	1:59:A:HIS:HE1	6	1.24
(1,250)	1:21:A:LEU:HD23	1:59:A:HIS:HE1	6	1.24
(1,789)	1:66:A:VAL:H	1:68:A:VAL:HG11	12	1.23
(1,789)	1:66:A:VAL:H	1:68:A:VAL:HG12	12	1.23
(1,789)	1:66:A:VAL:H	1:68:A:VAL:HG13	12	1.23
(1,714)	1:60:A:THR:HA	1:81:A:ILE:HG21	11	1.23
(1,714)	1:60:A:THR:HA	1:81:A:ILE:HG22	11	1.23
(1,714)	1:60:A:THR:HA	1:81:A:ILE:HG23	11	1.23
(1,690)	1:56:A:GLU:CD	1:52:A:ASP:CG	10	1.23
(1,365)	1:28:A:PHE:HD1	1:32:A:LYS:HB2	2	1.23
(1,365)	1:28:A:PHE:HD1	1:32:A:LYS:HB3	2	1.23
(1,365)	1:28:A:PHE:HD2	1:32:A:LYS:HB2	2	1.23
(1,365)	1:28:A:PHE:HD2	1:32:A:LYS:HB3	2	1.23
(1,241)	1:21:A:LEU:HG	1:57:A:LYS:HG2	2	1.23
(1,241)	1:21:A:LEU:HG	1:57:A:LYS:HG3	2	1.23
(1,241)	1:21:A:LEU:HG	1:57:A:LYS:HG2	13	1.23
(1,241)	1:21:A:LEU:HG	1:57:A:LYS:HG3	13	1.23
(1,240)	1:21:A:LEU:HG	1:57:A:LYS:HB2	3	1.23
(1,240)	1:21:A:LEU:HG	1:57:A:LYS:HB3	3	1.23
(1,210)	1:19:A:VAL:HG11	1:20:A:GLU:HA	9	1.23
(1,210)	1:19:A:VAL:HG12	1:20:A:GLU:HA	9	1.23
(1,210)	1:19:A:VAL:HG13	1:20:A:GLU:HA	9	1.23
(1,210)	1:19:A:VAL:HG11	1:20:A:GLU:HA	13	1.23
(1,210)	1:19:A:VAL:HG12	1:20:A:GLU:HA	13	1.23
(1,210)	1:19:A:VAL:HG13	1:20:A:GLU:HA	13	1.23
(1,128)	1:7:A:LEU:HG	1:38:A:PHE:HD1	15	1.23
(1,128)	1:7:A:LEU:HG	1:38:A:PHE:HD2	15	1.23
(1,61)	1:6:A:VAL:HA	1:19:A:VAL:HB	1	1.23
(1,800)	1:66:A:VAL:HG11	1:72:A:GLU:H	18	1.22
(1,800)	1:66:A:VAL:HG12	1:72:A:GLU:H	18	1.22
(1,800)	1:66:A:VAL:HG13	1:72:A:GLU:H	18	1.22
(1,800)	1:66:A:VAL:HG21	1:72:A:GLU:H	18	1.22
(1,800)	1:66:A:VAL:HG22	1:72:A:GLU:H	18	1.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,800)	1:66:A:VAL:HG23	1:72:A:GLU:H	18	1.22
(1,798)	1:66:A:VAL:HG11	1:69:A:SER:HA	18	1.22
(1,798)	1:66:A:VAL:HG12	1:69:A:SER:HA	18	1.22
(1,798)	1:66:A:VAL:HG13	1:69:A:SER:HA	18	1.22
(1,798)	1:66:A:VAL:HG21	1:69:A:SER:HA	18	1.22
(1,798)	1:66:A:VAL:HG22	1:69:A:SER:HA	18	1.22
(1,798)	1:66:A:VAL:HG23	1:69:A:SER:HA	18	1.22
(1,746)	1:63:A:LEU:HA	1:76:A:LEU:HD11	15	1.22
(1,746)	1:63:A:LEU:HA	1:76:A:LEU:HD12	15	1.22
(1,746)	1:63:A:LEU:HA	1:76:A:LEU:HD13	15	1.22
(1,411)	1:33:A:ARG:HA	1:82:A:ILE:HA	6	1.22
(1,288)	1:24:A:LEU:HA	1:80:A:HIS:HE1	1	1.22
(1,241)	1:21:A:LEU:HG	1:57:A:LYS:HG2	15	1.22
(1,241)	1:21:A:LEU:HG	1:57:A:LYS:HG3	15	1.22
(1,898)	1:77:A:TYR:HB2	1:79:A:LEU:HG	1	1.21
(1,898)	1:77:A:TYR:HB3	1:79:A:LEU:HG	1	1.21
(1,898)	1:77:A:TYR:HB2	1:79:A:LEU:HG	4	1.21
(1,898)	1:77:A:TYR:HB3	1:79:A:LEU:HG	4	1.21
(1,714)	1:60:A:THR:HA	1:81:A:ILE:HG21	4	1.21
(1,714)	1:60:A:THR:HA	1:81:A:ILE:HG22	4	1.21
(1,714)	1:60:A:THR:HA	1:81:A:ILE:HG23	4	1.21
(1,542)	1:44:A:HIS:HA	1:45:A:LYS:HD2	18	1.21
(1,542)	1:44:A:HIS:HA	1:45:A:LYS:HD3	18	1.21
(1,499)	1:38:A:PHE:HB2	1:75:A:PHE:HD1	14	1.21
(1,499)	1:38:A:PHE:HB2	1:75:A:PHE:HD2	14	1.21
(1,499)	1:38:A:PHE:HB3	1:75:A:PHE:HD1	14	1.21
(1,499)	1:38:A:PHE:HB3	1:75:A:PHE:HD2	14	1.21
(1,395)	1:31:A:ASP:HA	1:81:A:ILE:HG21	11	1.21
(1,395)	1:31:A:ASP:HA	1:81:A:ILE:HG22	11	1.21
(1,395)	1:31:A:ASP:HA	1:81:A:ILE:HG23	11	1.21
(1,390)	1:31:A:ASP:H	1:81:A:ILE:HG21	6	1.21
(1,390)	1:31:A:ASP:H	1:81:A:ILE:HG22	6	1.21
(1,390)	1:31:A:ASP:H	1:81:A:ILE:HG23	6	1.21
(1,45)	1:6:A:VAL:H	1:35:A:ILE:HB	17	1.21
(1,921)	1:79:A:LEU:HD11	1:82:A:ILE:HB	8	1.2
(1,921)	1:79:A:LEU:HD12	1:82:A:ILE:HB	8	1.2
(1,921)	1:79:A:LEU:HD13	1:82:A:ILE:HB	8	1.2
(1,794)	1:66:A:VAL:HA	1:77:A:TYR:H	12	1.2
(1,781)	1:65:A:GLU:HA	1:77:A:TYR:HD1	3	1.2
(1,781)	1:65:A:GLU:HA	1:77:A:TYR:HD2	3	1.2
(1,781)	1:65:A:GLU:HA	1:77:A:TYR:HD1	17	1.2
(1,781)	1:65:A:GLU:HA	1:77:A:TYR:HD2	17	1.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,746)	1:63:A:LEU:HA	1:76:A:LEU:HD11	6	1.2
(1,746)	1:63:A:LEU:HA	1:76:A:LEU:HD12	6	1.2
(1,746)	1:63:A:LEU:HA	1:76:A:LEU:HD13	6	1.2
(1,722)	1:61:A:ALA:H	1:81:A:ILE:HA	20	1.2
(1,390)	1:31:A:ASP:H	1:81:A:ILE:HG21	5	1.2
(1,390)	1:31:A:ASP:H	1:81:A:ILE:HG22	5	1.2
(1,390)	1:31:A:ASP:H	1:81:A:ILE:HG23	5	1.2
(1,240)	1:21:A:LEU:HG	1:57:A:LYS:HB2	11	1.2
(1,240)	1:21:A:LEU:HG	1:57:A:LYS:HB3	11	1.2
(1,239)	1:21:A:LEU:HG	1:56:A:GLU:HB2	19	1.2
(1,239)	1:21:A:LEU:HG	1:56:A:GLU:HB3	19	1.2
(1,45)	1:6:A:VAL:H	1:35:A:ILE:HB	16	1.2
(1,743)	1:62:A:TYR:HE1	1:63:A:LEU:HD21	4	1.19
(1,743)	1:62:A:TYR:HE1	1:63:A:LEU:HD22	4	1.19
(1,743)	1:62:A:TYR:HE1	1:63:A:LEU:HD23	4	1.19
(1,743)	1:62:A:TYR:HE2	1:63:A:LEU:HD21	4	1.19
(1,743)	1:62:A:TYR:HE2	1:63:A:LEU:HD22	4	1.19
(1,743)	1:62:A:TYR:HE2	1:63:A:LEU:HD23	4	1.19
(1,741)	1:62:A:TYR:HD1	1:63:A:LEU:H	12	1.19
(1,741)	1:62:A:TYR:HD2	1:63:A:LEU:H	12	1.19
(1,690)	1:56:A:GLU:CD	1:52:A:ASP:CG	1	1.19
(1,672)	1:55:A:LYS:H	1:63:A:LEU:HD11	17	1.19
(1,672)	1:55:A:LYS:H	1:63:A:LEU:HD12	17	1.19
(1,672)	1:55:A:LYS:H	1:63:A:LEU:HD13	17	1.19
(1,542)	1:44:A:HIS:HA	1:45:A:LYS:HD2	6	1.19
(1,542)	1:44:A:HIS:HA	1:45:A:LYS:HD3	6	1.19
(1,542)	1:44:A:HIS:HA	1:45:A:LYS:HD2	12	1.19
(1,542)	1:44:A:HIS:HA	1:45:A:LYS:HD3	12	1.19
(1,500)	1:38:A:PHE:HD1	1:39:A:ALA:H	14	1.19
(1,500)	1:38:A:PHE:HD2	1:39:A:ALA:H	14	1.19
(1,476)	1:37:A:TYR:H	1:78:A:GLU:HG2	8	1.19
(1,476)	1:37:A:TYR:H	1:78:A:GLU:HG3	8	1.19
(1,410)	1:33:A:ARG:HA	1:81:A:ILE:HG21	16	1.19
(1,410)	1:33:A:ARG:HA	1:81:A:ILE:HG22	16	1.19
(1,410)	1:33:A:ARG:HA	1:81:A:ILE:HG23	16	1.19
(1,390)	1:31:A:ASP:H	1:81:A:ILE:HG21	19	1.19
(1,390)	1:31:A:ASP:H	1:81:A:ILE:HG22	19	1.19
(1,390)	1:31:A:ASP:H	1:81:A:ILE:HG23	19	1.19
(1,242)	1:21:A:LEU:HG	1:57:A:LYS:HD2	7	1.19
(1,242)	1:21:A:LEU:HG	1:57:A:LYS:HD3	7	1.19
(1,884)	1:76:A:LEU:HA	1:77:A:TYR:HD1	9	1.18
(1,884)	1:76:A:LEU:HA	1:77:A:TYR:HD2	9	1.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,879)	1:75:A:PHE:HD1	1:77:A:TYR:HD2	1	1.18
(1,879)	1:75:A:PHE:HD2	1:77:A:TYR:HD2	1	1.18
(1,695)	1:57:A:LYS:HA	1:58:A:GLY:H	10	1.18
(1,542)	1:44:A:HIS:HA	1:45:A:LYS:HD2	20	1.18
(1,542)	1:44:A:HIS:HA	1:45:A:LYS:HD3	20	1.18
(1,500)	1:38:A:PHE:HD1	1:39:A:ALA:H	16	1.18
(1,500)	1:38:A:PHE:HD2	1:39:A:ALA:H	16	1.18
(1,495)	1:38:A:PHE:HA	1:75:A:PHE:HD1	12	1.18
(1,495)	1:38:A:PHE:HA	1:75:A:PHE:HD2	12	1.18
(1,418)	1:34:A:SER:H	1:79:A:LEU:HD21	7	1.18
(1,418)	1:34:A:SER:H	1:79:A:LEU:HD22	7	1.18
(1,418)	1:34:A:SER:H	1:79:A:LEU:HD23	7	1.18
(1,410)	1:33:A:ARG:HA	1:81:A:ILE:HG21	13	1.18
(1,410)	1:33:A:ARG:HA	1:81:A:ILE:HG22	13	1.18
(1,410)	1:33:A:ARG:HA	1:81:A:ILE:HG23	13	1.18
(1,68)	1:6:A:VAL:HB	1:19:A:VAL:HB	2	1.18
(1,781)	1:65:A:GLU:HA	1:77:A:TYR:HD1	2	1.17
(1,781)	1:65:A:GLU:HA	1:77:A:TYR:HD2	2	1.17
(1,781)	1:65:A:GLU:HA	1:77:A:TYR:HD1	8	1.17
(1,781)	1:65:A:GLU:HA	1:77:A:TYR:HD2	8	1.17
(1,690)	1:56:A:GLU:CD	1:52:A:ASP:CG	6	1.17
(1,476)	1:37:A:TYR:H	1:78:A:GLU:HG2	13	1.17
(1,476)	1:37:A:TYR:H	1:78:A:GLU:HG3	13	1.17
(1,458)	1:36:A:PHE:HA	1:76:A:LEU:HD11	9	1.17
(1,458)	1:36:A:PHE:HA	1:76:A:LEU:HD12	9	1.17
(1,458)	1:36:A:PHE:HA	1:76:A:LEU:HD13	9	1.17
(1,239)	1:21:A:LEU:HG	1:56:A:GLU:HB2	5	1.17
(1,239)	1:21:A:LEU:HG	1:56:A:GLU:HB3	5	1.17
(1,200)	1:18:A:SER:HB2	1:22:A:GLU:HG2	9	1.17
(1,200)	1:18:A:SER:HB2	1:22:A:GLU:HG3	9	1.17
(1,200)	1:18:A:SER:HB3	1:22:A:GLU:HG2	9	1.17
(1,200)	1:18:A:SER:HB3	1:22:A:GLU:HG3	9	1.17
(1,930)	1:81:A:ILE:HA	1:82:A:ILE:H	2	1.16
(1,898)	1:77:A:TYR:HB2	1:79:A:LEU:HG	13	1.16
(1,898)	1:77:A:TYR:HB3	1:79:A:LEU:HG	13	1.16
(1,781)	1:65:A:GLU:HA	1:77:A:TYR:HD1	6	1.16
(1,781)	1:65:A:GLU:HA	1:77:A:TYR:HD2	6	1.16
(1,781)	1:65:A:GLU:HA	1:77:A:TYR:HD1	12	1.16
(1,781)	1:65:A:GLU:HA	1:77:A:TYR:HD2	12	1.16
(1,722)	1:61:A:ALA:H	1:81:A:ILE:HA	19	1.16
(1,672)	1:55:A:LYS:H	1:63:A:LEU:HD11	19	1.16
(1,672)	1:55:A:LYS:H	1:63:A:LEU:HD12	19	1.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,672)	1:55:A:LYS:H	1:63:A:LEU:HD13	19	1.16
(1,542)	1:44:A:HIS:HA	1:45:A:LYS:HD2	9	1.16
(1,542)	1:44:A:HIS:HA	1:45:A:LYS:HD3	9	1.16
(1,469)	1:36:A:PHE:HD1	1:75:A:PHE:HB2	18	1.16
(1,469)	1:36:A:PHE:HD1	1:75:A:PHE:HB3	18	1.16
(1,469)	1:36:A:PHE:HD2	1:75:A:PHE:HB2	18	1.16
(1,469)	1:36:A:PHE:HD2	1:75:A:PHE:HB3	18	1.16
(1,411)	1:33:A:ARG:HA	1:82:A:ILE:HA	1	1.16
(1,410)	1:33:A:ARG:HA	1:81:A:ILE:HG21	17	1.16
(1,410)	1:33:A:ARG:HA	1:81:A:ILE:HG22	17	1.16
(1,410)	1:33:A:ARG:HA	1:81:A:ILE:HG23	17	1.16
(1,284)	1:24:A:LEU:HA	1:35:A:ILE:HD11	16	1.16
(1,284)	1:24:A:LEU:HA	1:35:A:ILE:HD12	16	1.16
(1,284)	1:24:A:LEU:HA	1:35:A:ILE:HD13	16	1.16
(1,107)	1:7:A:LEU:H	1:38:A:PHE:HD1	13	1.16
(1,107)	1:7:A:LEU:H	1:38:A:PHE:HD2	13	1.16
(1,25)	1:5:A:LEU:HG	1:6:A:VAL:HA	6	1.16
(1,20)	1:5:A:LEU:HB2	1:35:A:ILE:HB	17	1.16
(1,20)	1:5:A:LEU:HB3	1:35:A:ILE:HB	17	1.16
(1,930)	1:81:A:ILE:HA	1:82:A:ILE:H	4	1.15
(1,742)	1:62:A:TYR:HE1	1:63:A:LEU:H	6	1.15
(1,742)	1:62:A:TYR:HE2	1:63:A:LEU:H	6	1.15
(1,500)	1:38:A:PHE:HD1	1:39:A:ALA:H	9	1.15
(1,500)	1:38:A:PHE:HD2	1:39:A:ALA:H	9	1.15
(1,471)	1:36:A:PHE:HD1	1:78:A:GLU:H	5	1.15
(1,471)	1:36:A:PHE:HD2	1:78:A:GLU:H	5	1.15
(1,25)	1:5:A:LEU:HG	1:6:A:VAL:HA	10	1.15
(1,690)	1:56:A:GLU:CD	1:52:A:ASP:CG	15	1.14
(1,544)	1:44:A:HIS:HA	1:48:A:LEU:HD11	2	1.14
(1,544)	1:44:A:HIS:HA	1:48:A:LEU:HD12	2	1.14
(1,544)	1:44:A:HIS:HA	1:48:A:LEU:HD13	2	1.14
(1,544)	1:44:A:HIS:HA	1:48:A:LEU:HD11	2	1.14
(1,544)	1:44:A:HIS:HA	1:48:A:LEU:HD12	2	1.14
(1,544)	1:44:A:HIS:HA	1:48:A:LEU:HD13	2	1.14
(1,390)	1:31:A:ASP:H	1:81:A:ILE:HG21	20	1.14
(1,390)	1:31:A:ASP:H	1:81:A:ILE:HG22	20	1.14
(1,390)	1:31:A:ASP:H	1:81:A:ILE:HG23	20	1.14
(1,365)	1:28:A:PHE:HD1	1:32:A:LYS:HB2	19	1.14
(1,365)	1:28:A:PHE:HD1	1:32:A:LYS:HB3	19	1.14
(1,365)	1:28:A:PHE:HD2	1:32:A:LYS:HB2	19	1.14
(1,365)	1:28:A:PHE:HD2	1:32:A:LYS:HB3	19	1.14
(1,239)	1:21:A:LEU:HG	1:56:A:GLU:HB2	8	1.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,239)	1:21:A:LEU:HG	1:56:A:GLU:HB3	8	1.14
(1,32)	1:5:A:LEU:HD11	1:7:A:LEU:H	3	1.14
(1,32)	1:5:A:LEU:HD12	1:7:A:LEU:H	3	1.14
(1,32)	1:5:A:LEU:HD13	1:7:A:LEU:H	3	1.14
(1,32)	1:5:A:LEU:HD21	1:7:A:LEU:H	3	1.14
(1,32)	1:5:A:LEU:HD22	1:7:A:LEU:H	3	1.14
(1,32)	1:5:A:LEU:HD23	1:7:A:LEU:H	3	1.14
(1,741)	1:62:A:TYR:HD1	1:63:A:LEU:H	11	1.13
(1,741)	1:62:A:TYR:HD2	1:63:A:LEU:H	11	1.13
(1,418)	1:34:A:SER:H	1:79:A:LEU:HD21	9	1.13
(1,418)	1:34:A:SER:H	1:79:A:LEU:HD22	9	1.13
(1,418)	1:34:A:SER:H	1:79:A:LEU:HD23	9	1.13
(1,411)	1:33:A:ARG:HA	1:82:A:ILE:HA	19	1.13
(1,299)	1:24:A:LEU:HD11	1:35:A:ILE:HG21	7	1.13
(1,299)	1:24:A:LEU:HD11	1:35:A:ILE:HG22	7	1.13
(1,299)	1:24:A:LEU:HD11	1:35:A:ILE:HG23	7	1.13
(1,299)	1:24:A:LEU:HD12	1:35:A:ILE:HG21	7	1.13
(1,299)	1:24:A:LEU:HD12	1:35:A:ILE:HG22	7	1.13
(1,299)	1:24:A:LEU:HD12	1:35:A:ILE:HG23	7	1.13
(1,299)	1:24:A:LEU:HD13	1:35:A:ILE:HG21	7	1.13
(1,299)	1:24:A:LEU:HD13	1:35:A:ILE:HG22	7	1.13
(1,299)	1:24:A:LEU:HD13	1:35:A:ILE:HG23	7	1.13
(1,242)	1:21:A:LEU:HG	1:57:A:LYS:HD2	20	1.13
(1,242)	1:21:A:LEU:HG	1:57:A:LYS:HD3	20	1.13
(1,176)	1:13:A:LYS:H	1:14:A:SER:H	4	1.13
(1,174)	1:12:A:ARG:HB2	1:14:A:SER:HA	20	1.13
(1,174)	1:12:A:ARG:HB3	1:14:A:SER:HA	20	1.13
(1,21)	1:5:A:LEU:HB2	1:36:A:PHE:H	16	1.13
(1,21)	1:5:A:LEU:HB3	1:36:A:PHE:H	16	1.13
(1,8)	1:5:A:LEU:H	1:35:A:ILE:HB	2	1.13
(1,900)	1:77:A:TYR:HD1	1:79:A:LEU:HG	12	1.12
(1,900)	1:77:A:TYR:HD2	1:79:A:LEU:HG	12	1.12
(1,898)	1:77:A:TYR:HB2	1:79:A:LEU:HG	6	1.12
(1,898)	1:77:A:TYR:HB3	1:79:A:LEU:HG	6	1.12
(1,804)	1:67:A:ARG:H	1:68:A:VAL:HB	1	1.12
(1,714)	1:60:A:THR:HA	1:81:A:ILE:HG21	5	1.12
(1,714)	1:60:A:THR:HA	1:81:A:ILE:HG22	5	1.12
(1,714)	1:60:A:THR:HA	1:81:A:ILE:HG23	5	1.12
(1,672)	1:55:A:LYS:H	1:63:A:LEU:HD11	4	1.12
(1,672)	1:55:A:LYS:H	1:63:A:LEU:HD12	4	1.12
(1,672)	1:55:A:LYS:H	1:63:A:LEU:HD13	4	1.12
(1,672)	1:55:A:LYS:H	1:63:A:LEU:HD11	13	1.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,672)	1:55:A:LYS:H	1:63:A:LEU:HD12	13	1.12
(1,672)	1:55:A:LYS:H	1:63:A:LEU:HD13	13	1.12
(1,501)	1:38:A:PHE:HD1	1:75:A:PHE:H	8	1.12
(1,501)	1:38:A:PHE:HD2	1:75:A:PHE:H	8	1.12
(1,501)	1:38:A:PHE:HD1	1:75:A:PHE:H	15	1.12
(1,501)	1:38:A:PHE:HD2	1:75:A:PHE:H	15	1.12
(1,495)	1:38:A:PHE:HA	1:75:A:PHE:HD1	3	1.12
(1,495)	1:38:A:PHE:HA	1:75:A:PHE:HD2	3	1.12
(1,364)	1:28:A:PHE:HD1	1:32:A:LYS:HA	2	1.12
(1,364)	1:28:A:PHE:HD2	1:32:A:LYS:HA	2	1.12
(1,32)	1:5:A:LEU:HD11	1:7:A:LEU:H	4	1.12
(1,32)	1:5:A:LEU:HD12	1:7:A:LEU:H	4	1.12
(1,32)	1:5:A:LEU:HD13	1:7:A:LEU:H	4	1.12
(1,32)	1:5:A:LEU:HD21	1:7:A:LEU:H	4	1.12
(1,32)	1:5:A:LEU:HD22	1:7:A:LEU:H	4	1.12
(1,32)	1:5:A:LEU:HD23	1:7:A:LEU:H	4	1.12
(1,742)	1:62:A:TYR:HE1	1:63:A:LEU:H	12	1.11
(1,742)	1:62:A:TYR:HE2	1:63:A:LEU:H	12	1.11
(1,714)	1:60:A:THR:HA	1:81:A:ILE:HG21	13	1.11
(1,714)	1:60:A:THR:HA	1:81:A:ILE:HG22	13	1.11
(1,714)	1:60:A:THR:HA	1:81:A:ILE:HG23	13	1.11
(1,305)	1:24:A:LEU:HD21	1:60:A:THR:H	1	1.11
(1,305)	1:24:A:LEU:HD22	1:60:A:THR:H	1	1.11
(1,305)	1:24:A:LEU:HD23	1:60:A:THR:H	1	1.11
(1,147)	1:9:A:LYS:H	1:11:A:THR:H	12	1.11
(3,1)	1:39:A:ALA:HB1	1:47:A:MET:N	20	1.1
(1,781)	1:65:A:GLU:HA	1:77:A:TYR:HD1	11	1.1
(1,781)	1:65:A:GLU:HA	1:77:A:TYR:HD2	11	1.1
(1,741)	1:62:A:TYR:HD1	1:63:A:LEU:H	19	1.1
(1,741)	1:62:A:TYR:HD2	1:63:A:LEU:H	19	1.1
(1,714)	1:60:A:THR:HA	1:81:A:ILE:HG21	17	1.1
(1,714)	1:60:A:THR:HA	1:81:A:ILE:HG22	17	1.1
(1,714)	1:60:A:THR:HA	1:81:A:ILE:HG23	17	1.1
(1,690)	1:56:A:GLU:CD	1:52:A:ASP:CG	12	1.1
(1,690)	1:56:A:GLU:CD	1:52:A:ASP:CG	18	1.1
(1,476)	1:37:A:TYR:H	1:78:A:GLU:HG2	4	1.1
(1,476)	1:37:A:TYR:H	1:78:A:GLU:HG3	4	1.1
(1,370)	1:28:A:PHE:HE1	1:81:A:ILE:HA	13	1.1
(1,370)	1:28:A:PHE:HE2	1:81:A:ILE:HA	13	1.1
(1,245)	1:21:A:LEU:HD11	1:53:A:PHE:HA	18	1.1
(1,245)	1:21:A:LEU:HD12	1:53:A:PHE:HA	18	1.1
(1,245)	1:21:A:LEU:HD13	1:53:A:PHE:HA	18	1.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,58)	1:6:A:VAL:HA	1:7:A:LEU:HG	6	1.1
(1,45)	1:6:A:VAL:H	1:35:A:ILE:HB	9	1.1
(1,36)	1:5:A:LEU:HD11	1:7:A:LEU:HD11	3	1.1
(1,36)	1:5:A:LEU:HD11	1:7:A:LEU:HD12	3	1.1
(1,36)	1:5:A:LEU:HD11	1:7:A:LEU:HD13	3	1.1
(1,36)	1:5:A:LEU:HD12	1:7:A:LEU:HD11	3	1.1
(1,36)	1:5:A:LEU:HD12	1:7:A:LEU:HD12	3	1.1
(1,36)	1:5:A:LEU:HD12	1:7:A:LEU:HD13	3	1.1
(1,36)	1:5:A:LEU:HD13	1:7:A:LEU:HD11	3	1.1
(1,36)	1:5:A:LEU:HD13	1:7:A:LEU:HD12	3	1.1
(1,36)	1:5:A:LEU:HD13	1:7:A:LEU:HD13	3	1.1
(1,36)	1:5:A:LEU:HD21	1:7:A:LEU:HD11	3	1.1
(1,36)	1:5:A:LEU:HD21	1:7:A:LEU:HD12	3	1.1
(1,36)	1:5:A:LEU:HD21	1:7:A:LEU:HD13	3	1.1
(1,36)	1:5:A:LEU:HD22	1:7:A:LEU:HD11	3	1.1
(1,36)	1:5:A:LEU:HD22	1:7:A:LEU:HD12	3	1.1
(1,36)	1:5:A:LEU:HD22	1:7:A:LEU:HD13	3	1.1
(1,36)	1:5:A:LEU:HD23	1:7:A:LEU:HD11	3	1.1
(1,36)	1:5:A:LEU:HD23	1:7:A:LEU:HD12	3	1.1
(1,36)	1:5:A:LEU:HD23	1:7:A:LEU:HD13	3	1.1
(1,25)	1:5:A:LEU:HG	1:6:A:VAL:HA	8	1.1
(1,798)	1:66:A:VAL:HG11	1:69:A:SER:HA	1	1.09
(1,798)	1:66:A:VAL:HG12	1:69:A:SER:HA	1	1.09
(1,798)	1:66:A:VAL:HG13	1:69:A:SER:HA	1	1.09
(1,798)	1:66:A:VAL:HG21	1:69:A:SER:HA	1	1.09
(1,798)	1:66:A:VAL:HG22	1:69:A:SER:HA	1	1.09
(1,798)	1:66:A:VAL:HG23	1:69:A:SER:HA	1	1.09
(1,794)	1:66:A:VAL:HA	1:77:A:TYR:H	19	1.09
(1,789)	1:66:A:VAL:H	1:68:A:VAL:HG11	4	1.09
(1,789)	1:66:A:VAL:H	1:68:A:VAL:HG12	4	1.09
(1,789)	1:66:A:VAL:H	1:68:A:VAL:HG13	4	1.09
(1,476)	1:37:A:TYR:H	1:78:A:GLU:HG2	14	1.09
(1,476)	1:37:A:TYR:H	1:78:A:GLU:HG3	14	1.09
(1,395)	1:31:A:ASP:HA	1:81:A:ILE:HG21	16	1.09
(1,395)	1:31:A:ASP:HA	1:81:A:ILE:HG22	16	1.09
(1,395)	1:31:A:ASP:HA	1:81:A:ILE:HG23	16	1.09
(1,293)	1:24:A:LEU:HB2	1:80:A:HIS:HE1	11	1.09
(1,293)	1:24:A:LEU:HB3	1:80:A:HIS:HE1	11	1.09
(1,154)	1:10:A:ASN:HA	1:13:A:LYS:HG2	9	1.09
(1,154)	1:10:A:ASN:HA	1:13:A:LYS:HG3	9	1.09
(1,21)	1:5:A:LEU:HB2	1:36:A:PHE:H	7	1.09
(1,21)	1:5:A:LEU:HB3	1:36:A:PHE:H	7	1.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,784)	1:65:A:GLU:HB2	1:69:A:SER:HA	3	1.08
(1,784)	1:65:A:GLU:HB3	1:69:A:SER:HA	3	1.08
(1,695)	1:57:A:LYS:HA	1:58:A:GLY:H	9	1.08
(1,690)	1:56:A:GLU:CD	1:52:A:ASP:CG	14	1.08
(1,672)	1:55:A:LYS:H	1:63:A:LEU:HD11	11	1.08
(1,672)	1:55:A:LYS:H	1:63:A:LEU:HD12	11	1.08
(1,672)	1:55:A:LYS:H	1:63:A:LEU:HD13	11	1.08
(1,526)	1:41:A:THR:HB	1:74:A:ASP:HB2	17	1.08
(1,526)	1:41:A:THR:HB	1:74:A:ASP:HB3	17	1.08
(1,471)	1:36:A:PHE:HD1	1:78:A:GLU:H	4	1.08
(1,471)	1:36:A:PHE:HD2	1:78:A:GLU:H	4	1.08
(1,458)	1:36:A:PHE:HA	1:76:A:LEU:HD11	16	1.08
(1,458)	1:36:A:PHE:HA	1:76:A:LEU:HD12	16	1.08
(1,458)	1:36:A:PHE:HA	1:76:A:LEU:HD13	16	1.08
(1,447)	1:35:A:ILE:HG12	1:36:A:PHE:HA	9	1.08
(1,447)	1:35:A:ILE:HG13	1:36:A:PHE:HA	9	1.08
(1,312)	1:25:A:TYR:H	1:59:A:HIS:HE1	18	1.08
(1,285)	1:24:A:LEU:HA	1:54:A:PHE:HE1	5	1.08
(1,285)	1:24:A:LEU:HA	1:54:A:PHE:HE2	5	1.08
(1,241)	1:21:A:LEU:HG	1:57:A:LYS:HG2	8	1.08
(1,241)	1:21:A:LEU:HG	1:57:A:LYS:HG3	8	1.08
(1,25)	1:5:A:LEU:HG	1:6:A:VAL:HA	16	1.08
(1,20)	1:5:A:LEU:HB2	1:35:A:ILE:HB	9	1.08
(1,20)	1:5:A:LEU:HB3	1:35:A:ILE:HB	9	1.08
(1,930)	1:81:A:ILE:HA	1:82:A:ILE:H	20	1.07
(1,917)	1:79:A:LEU:HB2	1:80:A:HIS:HD2	11	1.07
(1,917)	1:79:A:LEU:HB3	1:80:A:HIS:HD2	11	1.07
(1,898)	1:77:A:TYR:HB2	1:79:A:LEU:HG	15	1.07
(1,898)	1:77:A:TYR:HB3	1:79:A:LEU:HG	15	1.07
(1,893)	1:76:A:LEU:HD11	1:78:A:GLU:HG2	19	1.07
(1,893)	1:76:A:LEU:HD11	1:78:A:GLU:HG3	19	1.07
(1,893)	1:76:A:LEU:HD12	1:78:A:GLU:HG2	19	1.07
(1,893)	1:76:A:LEU:HD12	1:78:A:GLU:HG3	19	1.07
(1,893)	1:76:A:LEU:HD13	1:78:A:GLU:HG2	19	1.07
(1,893)	1:76:A:LEU:HD13	1:78:A:GLU:HG3	19	1.07
(1,865)	1:74:A:ASP:H	1:75:A:PHE:H	1	1.07
(1,798)	1:66:A:VAL:HG11	1:69:A:SER:HA	20	1.07
(1,798)	1:66:A:VAL:HG12	1:69:A:SER:HA	20	1.07
(1,798)	1:66:A:VAL:HG13	1:69:A:SER:HA	20	1.07
(1,798)	1:66:A:VAL:HG21	1:69:A:SER:HA	20	1.07
(1,798)	1:66:A:VAL:HG22	1:69:A:SER:HA	20	1.07
(1,798)	1:66:A:VAL:HG23	1:69:A:SER:HA	20	1.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,502)	1:38:A:PHE:HD1	1:75:A:PHE:HA	19	1.07
(1,502)	1:38:A:PHE:HD2	1:75:A:PHE:HA	19	1.07
(1,501)	1:38:A:PHE:HD1	1:75:A:PHE:H	4	1.07
(1,501)	1:38:A:PHE:HD2	1:75:A:PHE:H	4	1.07
(1,495)	1:38:A:PHE:HA	1:75:A:PHE:HD1	13	1.07
(1,495)	1:38:A:PHE:HA	1:75:A:PHE:HD2	13	1.07
(1,241)	1:21:A:LEU:HG	1:57:A:LYS:HG2	20	1.07
(1,241)	1:21:A:LEU:HG	1:57:A:LYS:HG3	20	1.07
(1,68)	1:6:A:VAL:HB	1:19:A:VAL:HB	9	1.07
(1,930)	1:81:A:ILE:HA	1:82:A:ILE:H	12	1.06
(1,804)	1:67:A:ARG:H	1:68:A:VAL:HB	14	1.06
(1,789)	1:66:A:VAL:H	1:68:A:VAL:HG11	16	1.06
(1,789)	1:66:A:VAL:H	1:68:A:VAL:HG12	16	1.06
(1,789)	1:66:A:VAL:H	1:68:A:VAL:HG13	16	1.06
(1,741)	1:62:A:TYR:HD1	1:63:A:LEU:H	14	1.06
(1,741)	1:62:A:TYR:HD2	1:63:A:LEU:H	14	1.06
(1,495)	1:38:A:PHE:HA	1:75:A:PHE:HD1	8	1.06
(1,495)	1:38:A:PHE:HA	1:75:A:PHE:HD2	8	1.06
(1,495)	1:38:A:PHE:HA	1:75:A:PHE:HD1	17	1.06
(1,495)	1:38:A:PHE:HA	1:75:A:PHE:HD2	17	1.06
(1,891)	1:76:A:LEU:HD11	1:77:A:TYR:H	1	1.05
(1,891)	1:76:A:LEU:HD12	1:77:A:TYR:H	1	1.05
(1,891)	1:76:A:LEU:HD13	1:77:A:TYR:H	1	1.05
(1,789)	1:66:A:VAL:H	1:68:A:VAL:HG11	18	1.05
(1,789)	1:66:A:VAL:H	1:68:A:VAL:HG12	18	1.05
(1,789)	1:66:A:VAL:H	1:68:A:VAL:HG13	18	1.05
(1,525)	1:41:A:THR:HB	1:73:A:LYS:HB2	20	1.05
(1,525)	1:41:A:THR:HB	1:73:A:LYS:HB3	20	1.05
(1,501)	1:38:A:PHE:HD1	1:75:A:PHE:H	3	1.05
(1,501)	1:38:A:PHE:HD2	1:75:A:PHE:H	3	1.05
(1,500)	1:38:A:PHE:HD1	1:39:A:ALA:H	12	1.05
(1,500)	1:38:A:PHE:HD2	1:39:A:ALA:H	12	1.05
(1,470)	1:36:A:PHE:HD1	1:77:A:TYR:HD1	2	1.05
(1,470)	1:36:A:PHE:HD1	1:77:A:TYR:HD2	2	1.05
(1,470)	1:36:A:PHE:HD2	1:77:A:TYR:HD1	2	1.05
(1,470)	1:36:A:PHE:HD2	1:77:A:TYR:HD2	2	1.05
(1,458)	1:36:A:PHE:HA	1:76:A:LEU:HD11	12	1.05
(1,458)	1:36:A:PHE:HA	1:76:A:LEU:HD12	12	1.05
(1,458)	1:36:A:PHE:HA	1:76:A:LEU:HD13	12	1.05
(1,412)	1:33:A:ARG:HB2	1:34:A:SER:H	16	1.05
(1,412)	1:33:A:ARG:HB3	1:34:A:SER:H	16	1.05
(1,240)	1:21:A:LEU:HG	1:57:A:LYS:HB2	4	1.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,240)	1:21:A:LEU:HG	1:57:A:LYS:HB3	4	1.05
(1,930)	1:81:A:ILE:HA	1:82:A:ILE:H	8	1.04
(1,930)	1:81:A:ILE:HA	1:82:A:ILE:H	16	1.04
(1,781)	1:65:A:GLU:HA	1:77:A:TYR:HD1	1	1.04
(1,781)	1:65:A:GLU:HA	1:77:A:TYR:HD2	1	1.04
(1,672)	1:55:A:LYS:H	1:63:A:LEU:HD11	9	1.04
(1,672)	1:55:A:LYS:H	1:63:A:LEU:HD12	9	1.04
(1,672)	1:55:A:LYS:H	1:63:A:LEU:HD13	9	1.04
(1,526)	1:41:A:THR:HB	1:74:A:ASP:HB2	8	1.04
(1,526)	1:41:A:THR:HB	1:74:A:ASP:HB3	8	1.04
(1,502)	1:38:A:PHE:HD1	1:75:A:PHE:HA	13	1.04
(1,502)	1:38:A:PHE:HD2	1:75:A:PHE:HA	13	1.04
(1,312)	1:25:A:TYR:H	1:59:A:HIS:HE1	5	1.04
(1,293)	1:24:A:LEU:HB2	1:80:A:HIS:HE1	3	1.04
(1,293)	1:24:A:LEU:HB3	1:80:A:HIS:HE1	3	1.04
(1,241)	1:21:A:LEU:HG	1:57:A:LYS:HG2	7	1.04
(1,241)	1:21:A:LEU:HG	1:57:A:LYS:HG3	7	1.04
(1,239)	1:21:A:LEU:HG	1:56:A:GLU:HB2	2	1.04
(1,239)	1:21:A:LEU:HG	1:56:A:GLU:HB3	2	1.04
(1,794)	1:66:A:VAL:HA	1:77:A:TYR:H	1	1.03
(1,781)	1:65:A:GLU:HA	1:77:A:TYR:HD1	10	1.03
(1,781)	1:65:A:GLU:HA	1:77:A:TYR:HD2	10	1.03
(1,672)	1:55:A:LYS:H	1:63:A:LEU:HD11	7	1.03
(1,672)	1:55:A:LYS:H	1:63:A:LEU:HD12	7	1.03
(1,672)	1:55:A:LYS:H	1:63:A:LEU:HD13	7	1.03
(1,500)	1:38:A:PHE:HD1	1:39:A:ALA:H	11	1.03
(1,500)	1:38:A:PHE:HD2	1:39:A:ALA:H	11	1.03
(1,469)	1:36:A:PHE:HD1	1:75:A:PHE:HB2	14	1.03
(1,469)	1:36:A:PHE:HD1	1:75:A:PHE:HB3	14	1.03
(1,469)	1:36:A:PHE:HD2	1:75:A:PHE:HB2	14	1.03
(1,469)	1:36:A:PHE:HD2	1:75:A:PHE:HB3	14	1.03
(1,410)	1:33:A:ARG:HA	1:81:A:ILE:HG21	11	1.03
(1,410)	1:33:A:ARG:HA	1:81:A:ILE:HG22	11	1.03
(1,410)	1:33:A:ARG:HA	1:81:A:ILE:HG23	11	1.03
(1,395)	1:31:A:ASP:HA	1:81:A:ILE:HG21	2	1.03
(1,395)	1:31:A:ASP:HA	1:81:A:ILE:HG22	2	1.03
(1,395)	1:31:A:ASP:HA	1:81:A:ILE:HG23	2	1.03
(1,366)	1:28:A:PHE:HD1	1:80:A:HIS:HB2	20	1.03
(1,366)	1:28:A:PHE:HD1	1:80:A:HIS:HB3	20	1.03
(1,366)	1:28:A:PHE:HD2	1:80:A:HIS:HB2	20	1.03
(1,366)	1:28:A:PHE:HD2	1:80:A:HIS:HB3	20	1.03
(1,301)	1:24:A:LEU:HD11	1:60:A:THR:HB	14	1.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,301)	1:24:A:LEU:HD12	1:60:A:THR:HB	14	1.03
(1,301)	1:24:A:LEU:HD13	1:60:A:THR:HB	14	1.03
(1,32)	1:5:A:LEU:HD11	1:7:A:LEU:H	10	1.03
(1,32)	1:5:A:LEU:HD12	1:7:A:LEU:H	10	1.03
(1,32)	1:5:A:LEU:HD13	1:7:A:LEU:H	10	1.03
(1,32)	1:5:A:LEU:HD21	1:7:A:LEU:H	10	1.03
(1,32)	1:5:A:LEU:HD22	1:7:A:LEU:H	10	1.03
(1,32)	1:5:A:LEU:HD23	1:7:A:LEU:H	10	1.03
(1,891)	1:76:A:LEU:HD11	1:77:A:TYR:H	3	1.02
(1,891)	1:76:A:LEU:HD12	1:77:A:TYR:H	3	1.02
(1,891)	1:76:A:LEU:HD13	1:77:A:TYR:H	3	1.02
(1,794)	1:66:A:VAL:HA	1:77:A:TYR:H	11	1.02
(1,781)	1:65:A:GLU:HA	1:77:A:TYR:HD1	7	1.02
(1,781)	1:65:A:GLU:HA	1:77:A:TYR:HD2	7	1.02
(1,525)	1:41:A:THR:HB	1:73:A:LYS:HB2	15	1.02
(1,525)	1:41:A:THR:HB	1:73:A:LYS:HB3	15	1.02
(1,500)	1:38:A:PHE:HD1	1:39:A:ALA:H	10	1.02
(1,500)	1:38:A:PHE:HD2	1:39:A:ALA:H	10	1.02
(1,412)	1:33:A:ARG:HB2	1:34:A:SER:H	3	1.02
(1,412)	1:33:A:ARG:HB3	1:34:A:SER:H	3	1.02
(1,299)	1:24:A:LEU:HD11	1:35:A:ILE:HG21	15	1.02
(1,299)	1:24:A:LEU:HD11	1:35:A:ILE:HG22	15	1.02
(1,299)	1:24:A:LEU:HD11	1:35:A:ILE:HG23	15	1.02
(1,299)	1:24:A:LEU:HD12	1:35:A:ILE:HG21	15	1.02
(1,299)	1:24:A:LEU:HD12	1:35:A:ILE:HG22	15	1.02
(1,299)	1:24:A:LEU:HD12	1:35:A:ILE:HG23	15	1.02
(1,299)	1:24:A:LEU:HD13	1:35:A:ILE:HG21	15	1.02
(1,299)	1:24:A:LEU:HD13	1:35:A:ILE:HG22	15	1.02
(1,299)	1:24:A:LEU:HD13	1:35:A:ILE:HG23	15	1.02
(1,245)	1:21:A:LEU:HD11	1:53:A:PHE:HA	17	1.02
(1,245)	1:21:A:LEU:HD12	1:53:A:PHE:HA	17	1.02
(1,245)	1:21:A:LEU:HD13	1:53:A:PHE:HA	17	1.02
(1,241)	1:21:A:LEU:HG	1:57:A:LYS:HG2	5	1.02
(1,241)	1:21:A:LEU:HG	1:57:A:LYS:HG3	5	1.02
(1,154)	1:10:A:ASN:HA	1:13:A:LYS:HG2	5	1.02
(1,154)	1:10:A:ASN:HA	1:13:A:LYS:HG3	5	1.02
(1,61)	1:6:A:VAL:HA	1:19:A:VAL:HB	2	1.02
(1,36)	1:5:A:LEU:HD11	1:7:A:LEU:HD11	10	1.02
(1,36)	1:5:A:LEU:HD11	1:7:A:LEU:HD12	10	1.02
(1,36)	1:5:A:LEU:HD11	1:7:A:LEU:HD13	10	1.02
(1,36)	1:5:A:LEU:HD12	1:7:A:LEU:HD11	10	1.02
(1,36)	1:5:A:LEU:HD12	1:7:A:LEU:HD12	10	1.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,36)	1:5:A:LEU:HD12	1:7:A:LEU:HD13	10	1.02
(1,36)	1:5:A:LEU:HD13	1:7:A:LEU:HD11	10	1.02
(1,36)	1:5:A:LEU:HD13	1:7:A:LEU:HD12	10	1.02
(1,36)	1:5:A:LEU:HD13	1:7:A:LEU:HD13	10	1.02
(1,36)	1:5:A:LEU:HD21	1:7:A:LEU:HD11	10	1.02
(1,36)	1:5:A:LEU:HD21	1:7:A:LEU:HD12	10	1.02
(1,36)	1:5:A:LEU:HD21	1:7:A:LEU:HD13	10	1.02
(1,36)	1:5:A:LEU:HD22	1:7:A:LEU:HD11	10	1.02
(1,36)	1:5:A:LEU:HD22	1:7:A:LEU:HD12	10	1.02
(1,36)	1:5:A:LEU:HD22	1:7:A:LEU:HD13	10	1.02
(1,36)	1:5:A:LEU:HD23	1:7:A:LEU:HD11	10	1.02
(1,36)	1:5:A:LEU:HD23	1:7:A:LEU:HD12	10	1.02
(1,36)	1:5:A:LEU:HD23	1:7:A:LEU:HD13	10	1.02
(1,33)	1:5:A:LEU:HD11	1:7:A:LEU:HA	18	1.02
(1,33)	1:5:A:LEU:HD12	1:7:A:LEU:HA	18	1.02
(1,33)	1:5:A:LEU:HD13	1:7:A:LEU:HA	18	1.02
(1,33)	1:5:A:LEU:HD21	1:7:A:LEU:HA	18	1.02
(1,33)	1:5:A:LEU:HD22	1:7:A:LEU:HA	18	1.02
(1,33)	1:5:A:LEU:HD23	1:7:A:LEU:HA	18	1.02
(1,32)	1:5:A:LEU:HD11	1:7:A:LEU:H	7	1.02
(1,32)	1:5:A:LEU:HD12	1:7:A:LEU:H	7	1.02
(1,32)	1:5:A:LEU:HD13	1:7:A:LEU:H	7	1.02
(1,32)	1:5:A:LEU:HD21	1:7:A:LEU:H	7	1.02
(1,32)	1:5:A:LEU:HD22	1:7:A:LEU:H	7	1.02
(1,32)	1:5:A:LEU:HD23	1:7:A:LEU:H	7	1.02
(1,741)	1:62:A:TYR:HD1	1:63:A:LEU:H	4	1.01
(1,741)	1:62:A:TYR:HD2	1:63:A:LEU:H	4	1.01
(1,690)	1:56:A:GLU:CD	1:52:A:ASP:CG	3	1.01
(1,672)	1:55:A:LYS:H	1:63:A:LEU:HD11	10	1.01
(1,672)	1:55:A:LYS:H	1:63:A:LEU:HD12	10	1.01
(1,672)	1:55:A:LYS:H	1:63:A:LEU:HD13	10	1.01
(1,441)	1:35:A:ILE:HB	1:37:A:TYR:HA	17	1.01
(1,412)	1:33:A:ARG:HB2	1:34:A:SER:H	9	1.01
(1,412)	1:33:A:ARG:HB3	1:34:A:SER:H	9	1.01
(1,405)	1:33:A:ARG:H	1:81:A:ILE:HG21	10	1.01
(1,405)	1:33:A:ARG:H	1:81:A:ILE:HG22	10	1.01
(1,405)	1:33:A:ARG:H	1:81:A:ILE:HG23	10	1.01
(1,405)	1:33:A:ARG:H	1:81:A:ILE:HG21	10	1.01
(1,405)	1:33:A:ARG:H	1:81:A:ILE:HG22	10	1.01
(1,405)	1:33:A:ARG:H	1:81:A:ILE:HG23	10	1.01
(1,390)	1:31:A:ASP:H	1:81:A:ILE:HG21	4	1.01
(1,390)	1:31:A:ASP:H	1:81:A:ILE:HG22	4	1.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,390)	1:31:A:ASP:H	1:81:A:ILE:HG23	4	1.01
(1,359)	1:28:A:PHE:HA	1:81:A:ILE:HD11	11	1.01
(1,359)	1:28:A:PHE:HA	1:81:A:ILE:HD12	11	1.01
(1,359)	1:28:A:PHE:HA	1:81:A:ILE:HD13	11	1.01
(1,293)	1:24:A:LEU:HB2	1:80:A:HIS:HE1	9	1.01
(1,293)	1:24:A:LEU:HB3	1:80:A:HIS:HE1	9	1.01
(1,27)	1:5:A:LEU:HG	1:7:A:LEU:H	14	1.01
(1,898)	1:77:A:TYR:HB2	1:79:A:LEU:HG	8	1.0
(1,898)	1:77:A:TYR:HB3	1:79:A:LEU:HG	8	1.0
(1,794)	1:66:A:VAL:HA	1:77:A:TYR:H	7	1.0
(1,704)	1:59:A:HIS:H	1:60:A:THR:H	7	1.0
(1,695)	1:57:A:LYS:HA	1:58:A:GLY:H	18	1.0
(1,495)	1:38:A:PHE:HA	1:75:A:PHE:HD1	19	1.0
(1,495)	1:38:A:PHE:HA	1:75:A:PHE:HD2	19	1.0
(1,458)	1:36:A:PHE:HA	1:76:A:LEU:HD11	2	1.0
(1,458)	1:36:A:PHE:HA	1:76:A:LEU:HD12	2	1.0
(1,458)	1:36:A:PHE:HA	1:76:A:LEU:HD13	2	1.0
(1,288)	1:24:A:LEU:HA	1:80:A:HIS:HE1	19	1.0
(1,242)	1:21:A:LEU:HG	1:57:A:LYS:HD2	5	1.0
(1,242)	1:21:A:LEU:HG	1:57:A:LYS:HD3	5	1.0
(1,240)	1:21:A:LEU:HG	1:57:A:LYS:HB2	1	1.0
(1,240)	1:21:A:LEU:HG	1:57:A:LYS:HB3	1	1.0
(1,166)	1:11:A:THR:HB	1:12:A:ARG:H	19	1.0
(1,128)	1:7:A:LEU:HG	1:38:A:PHE:HD1	7	1.0
(1,128)	1:7:A:LEU:HG	1:38:A:PHE:HD2	7	1.0
(1,891)	1:76:A:LEU:HD11	1:77:A:TYR:H	13	0.99
(1,891)	1:76:A:LEU:HD12	1:77:A:TYR:H	13	0.99
(1,891)	1:76:A:LEU:HD13	1:77:A:TYR:H	13	0.99
(1,721)	1:61:A:ALA:H	1:78:A:GLU:HB2	16	0.99
(1,721)	1:61:A:ALA:H	1:78:A:GLU:HB3	16	0.99
(1,672)	1:55:A:LYS:H	1:63:A:LEU:HD11	3	0.99
(1,672)	1:55:A:LYS:H	1:63:A:LEU:HD12	3	0.99
(1,672)	1:55:A:LYS:H	1:63:A:LEU:HD13	3	0.99
(1,526)	1:41:A:THR:HB	1:74:A:ASP:HB2	15	0.99
(1,526)	1:41:A:THR:HB	1:74:A:ASP:HB3	15	0.99
(1,441)	1:35:A:ILE:HB	1:37:A:TYR:HA	2	0.99
(1,411)	1:33:A:ARG:HA	1:82:A:ILE:HA	18	0.99
(1,410)	1:33:A:ARG:HA	1:81:A:ILE:HG21	5	0.99
(1,410)	1:33:A:ARG:HA	1:81:A:ILE:HG22	5	0.99
(1,410)	1:33:A:ARG:HA	1:81:A:ILE:HG23	5	0.99
(1,296)	1:24:A:LEU:HG	1:35:A:ILE:HD11	4	0.99
(1,296)	1:24:A:LEU:HG	1:35:A:ILE:HD12	4	0.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,296)	1:24:A:LEU:HG	1:35:A:ILE:HD13	4	0.99
(1,288)	1:24:A:LEU:HA	1:80:A:HIS:HE1	4	0.99
(1,285)	1:24:A:LEU:HA	1:54:A:PHE:HE1	18	0.99
(1,285)	1:24:A:LEU:HA	1:54:A:PHE:HE2	18	0.99
(1,200)	1:18:A:SER:HB2	1:22:A:GLU:HG2	13	0.99
(1,200)	1:18:A:SER:HB2	1:22:A:GLU:HG3	13	0.99
(1,200)	1:18:A:SER:HB3	1:22:A:GLU:HG2	13	0.99
(1,200)	1:18:A:SER:HB3	1:22:A:GLU:HG3	13	0.99
(1,147)	1:9:A:LYS:H	1:11:A:THR:H	14	0.99
(1,741)	1:62:A:TYR:HD1	1:63:A:LEU:H	9	0.98
(1,741)	1:62:A:TYR:HD2	1:63:A:LEU:H	9	0.98
(1,739)	1:62:A:TYR:HB2	1:79:A:LEU:HG	13	0.98
(1,739)	1:62:A:TYR:HB3	1:79:A:LEU:HG	13	0.98
(1,721)	1:61:A:ALA:H	1:78:A:GLU:HB2	4	0.98
(1,721)	1:61:A:ALA:H	1:78:A:GLU:HB3	4	0.98
(1,544)	1:44:A:HIS:HA	1:48:A:LEU:HD11	11	0.98
(1,544)	1:44:A:HIS:HA	1:48:A:LEU:HD12	11	0.98
(1,544)	1:44:A:HIS:HA	1:48:A:LEU:HD13	11	0.98
(1,544)	1:44:A:HIS:HA	1:48:A:LEU:HD11	11	0.98
(1,544)	1:44:A:HIS:HA	1:48:A:LEU:HD12	11	0.98
(1,544)	1:44:A:HIS:HA	1:48:A:LEU:HD13	11	0.98
(1,495)	1:38:A:PHE:HA	1:75:A:PHE:HD1	16	0.98
(1,495)	1:38:A:PHE:HA	1:75:A:PHE:HD2	16	0.98
(1,458)	1:36:A:PHE:HA	1:76:A:LEU:HD11	14	0.98
(1,458)	1:36:A:PHE:HA	1:76:A:LEU:HD12	14	0.98
(1,458)	1:36:A:PHE:HA	1:76:A:LEU:HD13	14	0.98
(1,432)	1:35:A:ILE:H	1:36:A:PHE:HE1	2	0.98
(1,432)	1:35:A:ILE:H	1:36:A:PHE:HE2	2	0.98
(1,426)	1:34:A:SER:HB2	1:36:A:PHE:HE1	12	0.98
(1,426)	1:34:A:SER:HB2	1:36:A:PHE:HE2	12	0.98
(1,426)	1:34:A:SER:HB3	1:36:A:PHE:HE1	12	0.98
(1,426)	1:34:A:SER:HB3	1:36:A:PHE:HE2	12	0.98
(1,364)	1:28:A:PHE:HD1	1:32:A:LYS:HA	1	0.98
(1,364)	1:28:A:PHE:HD2	1:32:A:LYS:HA	1	0.98
(1,322)	1:25:A:TYR:HD1	1:28:A:PHE:H	14	0.98
(1,322)	1:25:A:TYR:HD2	1:28:A:PHE:H	14	0.98
(1,298)	1:24:A:LEU:HG	1:80:A:HIS:HE1	4	0.98
(1,128)	1:7:A:LEU:HG	1:38:A:PHE:HD1	4	0.98
(1,128)	1:7:A:LEU:HG	1:38:A:PHE:HD2	4	0.98
(1,123)	1:7:A:LEU:HB2	1:38:A:PHE:HD1	19	0.98
(1,123)	1:7:A:LEU:HB2	1:38:A:PHE:HD2	19	0.98
(1,123)	1:7:A:LEU:HB3	1:38:A:PHE:HD1	19	0.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,123)	1:7:A:LEU:HB3	1:38:A:PHE:HD2	19	0.98
(1,32)	1:5:A:LEU:HD11	1:7:A:LEU:H	8	0.98
(1,32)	1:5:A:LEU:HD12	1:7:A:LEU:H	8	0.98
(1,32)	1:5:A:LEU:HD13	1:7:A:LEU:H	8	0.98
(1,32)	1:5:A:LEU:HD21	1:7:A:LEU:H	8	0.98
(1,32)	1:5:A:LEU:HD22	1:7:A:LEU:H	8	0.98
(1,32)	1:5:A:LEU:HD23	1:7:A:LEU:H	8	0.98
(1,898)	1:77:A:TYR:HB2	1:79:A:LEU:HG	11	0.97
(1,898)	1:77:A:TYR:HB3	1:79:A:LEU:HG	11	0.97
(1,721)	1:61:A:ALA:H	1:78:A:GLU:HB2	15	0.97
(1,721)	1:61:A:ALA:H	1:78:A:GLU:HB3	15	0.97
(1,690)	1:56:A:GLU:CD	1:52:A:ASP:CG	9	0.97
(1,458)	1:36:A:PHE:HA	1:76:A:LEU:HD11	20	0.97
(1,458)	1:36:A:PHE:HA	1:76:A:LEU:HD12	20	0.97
(1,458)	1:36:A:PHE:HA	1:76:A:LEU:HD13	20	0.97
(1,426)	1:34:A:SER:HB2	1:36:A:PHE:HE1	20	0.97
(1,426)	1:34:A:SER:HB2	1:36:A:PHE:HE2	20	0.97
(1,426)	1:34:A:SER:HB3	1:36:A:PHE:HE1	20	0.97
(1,426)	1:34:A:SER:HB3	1:36:A:PHE:HE2	20	0.97
(1,312)	1:25:A:TYR:H	1:59:A:HIS:HE1	2	0.97
(1,128)	1:7:A:LEU:HG	1:38:A:PHE:HD1	19	0.97
(1,128)	1:7:A:LEU:HG	1:38:A:PHE:HD2	19	0.97
(1,878)	1:75:A:PHE:HB2	1:77:A:TYR:HD1	20	0.96
(1,878)	1:75:A:PHE:HB2	1:77:A:TYR:HD2	20	0.96
(1,878)	1:75:A:PHE:HB3	1:77:A:TYR:HD1	20	0.96
(1,878)	1:75:A:PHE:HB3	1:77:A:TYR:HD2	20	0.96
(1,837)	1:70:A:THR:HA	1:73:A:LYS:HD2	13	0.96
(1,837)	1:70:A:THR:HA	1:73:A:LYS:HD3	13	0.96
(1,789)	1:66:A:VAL:H	1:68:A:VAL:HG11	14	0.96
(1,789)	1:66:A:VAL:H	1:68:A:VAL:HG12	14	0.96
(1,789)	1:66:A:VAL:H	1:68:A:VAL:HG13	14	0.96
(1,789)	1:66:A:VAL:H	1:68:A:VAL:HG11	15	0.96
(1,789)	1:66:A:VAL:H	1:68:A:VAL:HG12	15	0.96
(1,789)	1:66:A:VAL:H	1:68:A:VAL:HG13	15	0.96
(1,741)	1:62:A:TYR:HD1	1:63:A:LEU:H	20	0.96
(1,741)	1:62:A:TYR:HD2	1:63:A:LEU:H	20	0.96
(1,721)	1:61:A:ALA:H	1:78:A:GLU:HB2	6	0.96
(1,721)	1:61:A:ALA:H	1:78:A:GLU:HB3	6	0.96
(1,547)	1:44:A:HIS:HB2	1:48:A:LEU:HD11	19	0.96
(1,547)	1:44:A:HIS:HB2	1:48:A:LEU:HD12	19	0.96
(1,547)	1:44:A:HIS:HB2	1:48:A:LEU:HD13	19	0.96
(1,547)	1:44:A:HIS:HB3	1:48:A:LEU:HD11	19	0.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,547)	1:44:A:HIS:HB3	1:48:A:LEU:HD12	19	0.96
(1,547)	1:44:A:HIS:HB3	1:48:A:LEU:HD13	19	0.96
(1,512)	1:39:A:ALA:HA	1:74:A:ASP:HB2	2	0.96
(1,512)	1:39:A:ALA:HA	1:74:A:ASP:HB3	2	0.96
(1,495)	1:38:A:PHE:HA	1:75:A:PHE:HD1	20	0.96
(1,495)	1:38:A:PHE:HA	1:75:A:PHE:HD2	20	0.96
(1,432)	1:35:A:ILE:H	1:36:A:PHE:HE1	13	0.96
(1,432)	1:35:A:ILE:H	1:36:A:PHE:HE2	13	0.96
(1,411)	1:33:A:ARG:HA	1:82:A:ILE:HA	17	0.96
(1,410)	1:33:A:ARG:HA	1:81:A:ILE:HG21	2	0.96
(1,410)	1:33:A:ARG:HA	1:81:A:ILE:HG22	2	0.96
(1,410)	1:33:A:ARG:HA	1:81:A:ILE:HG23	2	0.96
(1,410)	1:33:A:ARG:HA	1:81:A:ILE:HG21	9	0.96
(1,410)	1:33:A:ARG:HA	1:81:A:ILE:HG22	9	0.96
(1,410)	1:33:A:ARG:HA	1:81:A:ILE:HG23	9	0.96
(1,410)	1:33:A:ARG:HA	1:81:A:ILE:HG21	19	0.96
(1,410)	1:33:A:ARG:HA	1:81:A:ILE:HG22	19	0.96
(1,410)	1:33:A:ARG:HA	1:81:A:ILE:HG23	19	0.96
(1,298)	1:24:A:LEU:HG	1:80:A:HIS:HE1	11	0.96
(1,878)	1:75:A:PHE:HB2	1:77:A:TYR:HD1	16	0.95
(1,878)	1:75:A:PHE:HB2	1:77:A:TYR:HD2	16	0.95
(1,878)	1:75:A:PHE:HB3	1:77:A:TYR:HD1	16	0.95
(1,878)	1:75:A:PHE:HB3	1:77:A:TYR:HD2	16	0.95
(1,672)	1:55:A:LYS:H	1:63:A:LEU:HD11	14	0.95
(1,672)	1:55:A:LYS:H	1:63:A:LEU:HD12	14	0.95
(1,672)	1:55:A:LYS:H	1:63:A:LEU:HD13	14	0.95
(1,542)	1:44:A:HIS:HA	1:45:A:LYS:HD2	7	0.95
(1,542)	1:44:A:HIS:HA	1:45:A:LYS:HD3	7	0.95
(1,526)	1:41:A:THR:HB	1:74:A:ASP:HB2	14	0.95
(1,526)	1:41:A:THR:HB	1:74:A:ASP:HB3	14	0.95
(1,502)	1:38:A:PHE:HD1	1:75:A:PHE:HA	7	0.95
(1,502)	1:38:A:PHE:HD2	1:75:A:PHE:HA	7	0.95
(1,304)	1:24:A:LEU:HD21	1:59:A:HIS:HE1	11	0.95
(1,304)	1:24:A:LEU:HD22	1:59:A:HIS:HE1	11	0.95
(1,304)	1:24:A:LEU:HD23	1:59:A:HIS:HE1	11	0.95
(1,147)	1:9:A:LYS:H	1:11:A:THR:H	8	0.95
(1,891)	1:76:A:LEU:HD11	1:77:A:TYR:H	6	0.94
(1,891)	1:76:A:LEU:HD12	1:77:A:TYR:H	6	0.94
(1,891)	1:76:A:LEU:HD13	1:77:A:TYR:H	6	0.94
(1,891)	1:76:A:LEU:HD11	1:77:A:TYR:H	7	0.94
(1,891)	1:76:A:LEU:HD12	1:77:A:TYR:H	7	0.94
(1,891)	1:76:A:LEU:HD13	1:77:A:TYR:H	7	0.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,814)	1:68:A:VAL:HG11	1:73:A:LYS:H	4	0.94
(1,814)	1:68:A:VAL:HG12	1:73:A:LYS:H	4	0.94
(1,814)	1:68:A:VAL:HG13	1:73:A:LYS:H	4	0.94
(1,814)	1:68:A:VAL:HG21	1:73:A:LYS:H	4	0.94
(1,814)	1:68:A:VAL:HG22	1:73:A:LYS:H	4	0.94
(1,814)	1:68:A:VAL:HG23	1:73:A:LYS:H	4	0.94
(1,798)	1:66:A:VAL:HG11	1:69:A:SER:HA	5	0.94
(1,798)	1:66:A:VAL:HG12	1:69:A:SER:HA	5	0.94
(1,798)	1:66:A:VAL:HG13	1:69:A:SER:HA	5	0.94
(1,798)	1:66:A:VAL:HG21	1:69:A:SER:HA	5	0.94
(1,798)	1:66:A:VAL:HG22	1:69:A:SER:HA	5	0.94
(1,798)	1:66:A:VAL:HG23	1:69:A:SER:HA	5	0.94
(1,743)	1:62:A:TYR:HE1	1:63:A:LEU:HD21	7	0.94
(1,743)	1:62:A:TYR:HE1	1:63:A:LEU:HD22	7	0.94
(1,743)	1:62:A:TYR:HE1	1:63:A:LEU:HD23	7	0.94
(1,743)	1:62:A:TYR:HE2	1:63:A:LEU:HD21	7	0.94
(1,743)	1:62:A:TYR:HE2	1:63:A:LEU:HD22	7	0.94
(1,743)	1:62:A:TYR:HE2	1:63:A:LEU:HD23	7	0.94
(1,742)	1:62:A:TYR:HE1	1:63:A:LEU:H	14	0.94
(1,742)	1:62:A:TYR:HE2	1:63:A:LEU:H	14	0.94
(1,742)	1:62:A:TYR:HE1	1:63:A:LEU:H	19	0.94
(1,742)	1:62:A:TYR:HE2	1:63:A:LEU:H	19	0.94
(1,542)	1:44:A:HIS:HA	1:45:A:LYS:HD2	1	0.94
(1,542)	1:44:A:HIS:HA	1:45:A:LYS:HD3	1	0.94
(1,410)	1:33:A:ARG:HA	1:81:A:ILE:HG21	12	0.94
(1,410)	1:33:A:ARG:HA	1:81:A:ILE:HG22	12	0.94
(1,410)	1:33:A:ARG:HA	1:81:A:ILE:HG23	12	0.94
(1,312)	1:25:A:TYR:H	1:59:A:HIS:HE1	10	0.94
(1,189)	1:16:A:ALA:H	1:17:A:LYS:H	3	0.94
(1,61)	1:6:A:VAL:HA	1:19:A:VAL:HB	9	0.94
(1,21)	1:5:A:LEU:HB2	1:36:A:PHE:H	4	0.94
(1,21)	1:5:A:LEU:HB3	1:36:A:PHE:H	4	0.94
(1,798)	1:66:A:VAL:HG11	1:69:A:SER:HA	17	0.93
(1,798)	1:66:A:VAL:HG12	1:69:A:SER:HA	17	0.93
(1,798)	1:66:A:VAL:HG13	1:69:A:SER:HA	17	0.93
(1,798)	1:66:A:VAL:HG21	1:69:A:SER:HA	17	0.93
(1,798)	1:66:A:VAL:HG22	1:69:A:SER:HA	17	0.93
(1,798)	1:66:A:VAL:HG23	1:69:A:SER:HA	17	0.93
(1,794)	1:66:A:VAL:HA	1:77:A:TYR:H	10	0.93
(1,789)	1:66:A:VAL:H	1:68:A:VAL:HG11	6	0.93
(1,789)	1:66:A:VAL:H	1:68:A:VAL:HG12	6	0.93
(1,789)	1:66:A:VAL:H	1:68:A:VAL:HG13	6	0.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,742)	1:62:A:TYR:HE1	1:63:A:LEU:H	9	0.93
(1,742)	1:62:A:TYR:HE2	1:63:A:LEU:H	9	0.93
(1,544)	1:44:A:HIS:HA	1:48:A:LEU:HD11	20	0.93
(1,544)	1:44:A:HIS:HA	1:48:A:LEU:HD12	20	0.93
(1,544)	1:44:A:HIS:HA	1:48:A:LEU:HD13	20	0.93
(1,544)	1:44:A:HIS:HA	1:48:A:LEU:HD11	20	0.93
(1,544)	1:44:A:HIS:HA	1:48:A:LEU:HD12	20	0.93
(1,544)	1:44:A:HIS:HA	1:48:A:LEU:HD13	20	0.93
(1,500)	1:38:A:PHE:HD1	1:39:A:ALA:H	3	0.93
(1,500)	1:38:A:PHE:HD2	1:39:A:ALA:H	3	0.93
(1,500)	1:38:A:PHE:HD1	1:39:A:ALA:H	6	0.93
(1,500)	1:38:A:PHE:HD2	1:39:A:ALA:H	6	0.93
(1,476)	1:37:A:TYR:H	1:78:A:GLU:HG2	11	0.93
(1,476)	1:37:A:TYR:H	1:78:A:GLU:HG3	11	0.93
(1,458)	1:36:A:PHE:HA	1:76:A:LEU:HD11	7	0.93
(1,458)	1:36:A:PHE:HA	1:76:A:LEU:HD12	7	0.93
(1,458)	1:36:A:PHE:HA	1:76:A:LEU:HD13	7	0.93
(1,304)	1:24:A:LEU:HD21	1:59:A:HIS:HE1	16	0.93
(1,304)	1:24:A:LEU:HD22	1:59:A:HIS:HE1	16	0.93
(1,304)	1:24:A:LEU:HD23	1:59:A:HIS:HE1	16	0.93
(1,879)	1:75:A:PHE:HD1	1:77:A:TYR:HD2	17	0.92
(1,879)	1:75:A:PHE:HD2	1:77:A:TYR:HD2	17	0.92
(1,538)	1:43:A:ALA:HA	1:45:A:LYS:HD2	8	0.92
(1,538)	1:43:A:ALA:HA	1:45:A:LYS:HD3	8	0.92
(1,500)	1:38:A:PHE:HD1	1:39:A:ALA:H	17	0.92
(1,500)	1:38:A:PHE:HD2	1:39:A:ALA:H	17	0.92
(1,449)	1:35:A:ILE:HD11	1:37:A:TYR:HD1	3	0.92
(1,449)	1:35:A:ILE:HD11	1:37:A:TYR:HD2	3	0.92
(1,449)	1:35:A:ILE:HD12	1:37:A:TYR:HD1	3	0.92
(1,449)	1:35:A:ILE:HD12	1:37:A:TYR:HD2	3	0.92
(1,449)	1:35:A:ILE:HD13	1:37:A:TYR:HD1	3	0.92
(1,449)	1:35:A:ILE:HD13	1:37:A:TYR:HD2	3	0.92
(1,411)	1:33:A:ARG:HA	1:82:A:ILE:HA	3	0.92
(1,312)	1:25:A:TYR:H	1:59:A:HIS:HE1	13	0.92
(1,305)	1:24:A:LEU:HD21	1:60:A:THR:H	9	0.92
(1,305)	1:24:A:LEU:HD22	1:60:A:THR:H	9	0.92
(1,305)	1:24:A:LEU:HD23	1:60:A:THR:H	9	0.92
(1,300)	1:24:A:LEU:HD11	1:35:A:ILE:HG12	7	0.92
(1,300)	1:24:A:LEU:HD11	1:35:A:ILE:HG13	7	0.92
(1,300)	1:24:A:LEU:HD12	1:35:A:ILE:HG12	7	0.92
(1,300)	1:24:A:LEU:HD12	1:35:A:ILE:HG13	7	0.92
(1,300)	1:24:A:LEU:HD13	1:35:A:ILE:HG12	7	0.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,300)	1:24:A:LEU:HD13	1:35:A:ILE:HG13	7	0.92
(1,285)	1:24:A:LEU:HA	1:54:A:PHE:HE1	6	0.92
(1,285)	1:24:A:LEU:HA	1:54:A:PHE:HE2	6	0.92
(1,891)	1:76:A:LEU:HD11	1:77:A:TYR:H	10	0.91
(1,891)	1:76:A:LEU:HD12	1:77:A:TYR:H	10	0.91
(1,891)	1:76:A:LEU:HD13	1:77:A:TYR:H	10	0.91
(1,890)	1:76:A:LEU:HD11	1:78:A:GLU:H	7	0.91
(1,890)	1:76:A:LEU:HD12	1:78:A:GLU:H	7	0.91
(1,890)	1:76:A:LEU:HD13	1:78:A:GLU:H	7	0.91
(1,860)	1:73:A:LYS:H	1:74:A:ASP:H	18	0.91
(1,843)	1:71:A:ASP:H	1:73:A:LYS:HA	13	0.91
(1,789)	1:66:A:VAL:H	1:68:A:VAL:HG11	19	0.91
(1,789)	1:66:A:VAL:H	1:68:A:VAL:HG12	19	0.91
(1,789)	1:66:A:VAL:H	1:68:A:VAL:HG13	19	0.91
(1,781)	1:65:A:GLU:HA	1:77:A:TYR:HD1	14	0.91
(1,781)	1:65:A:GLU:HA	1:77:A:TYR:HD2	14	0.91
(1,742)	1:62:A:TYR:HE1	1:63:A:LEU:H	11	0.91
(1,742)	1:62:A:TYR:HE2	1:63:A:LEU:H	11	0.91
(1,741)	1:62:A:TYR:HD1	1:63:A:LEU:H	1	0.91
(1,741)	1:62:A:TYR:HD2	1:63:A:LEU:H	1	0.91
(1,741)	1:62:A:TYR:HD1	1:63:A:LEU:H	3	0.91
(1,741)	1:62:A:TYR:HD2	1:63:A:LEU:H	3	0.91
(1,502)	1:38:A:PHE:HD1	1:75:A:PHE:HA	15	0.91
(1,502)	1:38:A:PHE:HD2	1:75:A:PHE:HA	15	0.91
(1,495)	1:38:A:PHE:HA	1:75:A:PHE:HD1	15	0.91
(1,495)	1:38:A:PHE:HA	1:75:A:PHE:HD2	15	0.91
(1,304)	1:24:A:LEU:HD21	1:59:A:HIS:HE1	13	0.91
(1,304)	1:24:A:LEU:HD22	1:59:A:HIS:HE1	13	0.91
(1,304)	1:24:A:LEU:HD23	1:59:A:HIS:HE1	13	0.91
(1,299)	1:24:A:LEU:HD11	1:35:A:ILE:HG21	20	0.91
(1,299)	1:24:A:LEU:HD11	1:35:A:ILE:HG22	20	0.91
(1,299)	1:24:A:LEU:HD11	1:35:A:ILE:HG23	20	0.91
(1,299)	1:24:A:LEU:HD12	1:35:A:ILE:HG21	20	0.91
(1,299)	1:24:A:LEU:HD12	1:35:A:ILE:HG22	20	0.91
(1,299)	1:24:A:LEU:HD12	1:35:A:ILE:HG23	20	0.91
(1,299)	1:24:A:LEU:HD13	1:35:A:ILE:HG21	20	0.91
(1,299)	1:24:A:LEU:HD13	1:35:A:ILE:HG22	20	0.91
(1,299)	1:24:A:LEU:HD13	1:35:A:ILE:HG23	20	0.91
(1,285)	1:24:A:LEU:HA	1:54:A:PHE:HE1	9	0.91
(1,285)	1:24:A:LEU:HA	1:54:A:PHE:HE2	9	0.91
(1,174)	1:12:A:ARG:HB2	1:14:A:SER:HA	9	0.91
(1,174)	1:12:A:ARG:HB3	1:14:A:SER:HA	9	0.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,891)	1:76:A:LEU:HD11	1:77:A:TYR:H	15	0.9
(1,891)	1:76:A:LEU:HD12	1:77:A:TYR:H	15	0.9
(1,891)	1:76:A:LEU:HD13	1:77:A:TYR:H	15	0.9
(1,795)	1:66:A:VAL:HA	1:77:A:TYR:HA	16	0.9
(1,789)	1:66:A:VAL:H	1:68:A:VAL:HG11	5	0.9
(1,789)	1:66:A:VAL:H	1:68:A:VAL:HG12	5	0.9
(1,789)	1:66:A:VAL:H	1:68:A:VAL:HG13	5	0.9
(1,500)	1:38:A:PHE:HD1	1:39:A:ALA:H	4	0.9
(1,500)	1:38:A:PHE:HD2	1:39:A:ALA:H	4	0.9
(1,458)	1:36:A:PHE:HA	1:76:A:LEU:HD11	4	0.9
(1,458)	1:36:A:PHE:HA	1:76:A:LEU:HD12	4	0.9
(1,458)	1:36:A:PHE:HA	1:76:A:LEU:HD13	4	0.9
(1,432)	1:35:A:ILE:H	1:36:A:PHE:HE1	6	0.9
(1,432)	1:35:A:ILE:H	1:36:A:PHE:HE2	6	0.9
(1,410)	1:33:A:ARG:HA	1:81:A:ILE:HG21	20	0.9
(1,410)	1:33:A:ARG:HA	1:81:A:ILE:HG22	20	0.9
(1,410)	1:33:A:ARG:HA	1:81:A:ILE:HG23	20	0.9
(1,285)	1:24:A:LEU:HA	1:54:A:PHE:HE1	13	0.9
(1,285)	1:24:A:LEU:HA	1:54:A:PHE:HE2	13	0.9
(1,285)	1:24:A:LEU:HA	1:54:A:PHE:HE1	19	0.9
(1,285)	1:24:A:LEU:HA	1:54:A:PHE:HE2	19	0.9
(1,147)	1:9:A:LYS:H	1:11:A:THR:H	2	0.9
(1,68)	1:6:A:VAL:HB	1:19:A:VAL:HB	13	0.9
(1,704)	1:59:A:HIS:H	1:60:A:THR:H	20	0.89
(1,544)	1:44:A:HIS:HA	1:48:A:LEU:HD11	12	0.89
(1,544)	1:44:A:HIS:HA	1:48:A:LEU:HD12	12	0.89
(1,544)	1:44:A:HIS:HA	1:48:A:LEU:HD13	12	0.89
(1,544)	1:44:A:HIS:HA	1:48:A:LEU:HD11	12	0.89
(1,544)	1:44:A:HIS:HA	1:48:A:LEU:HD12	12	0.89
(1,544)	1:44:A:HIS:HA	1:48:A:LEU:HD13	12	0.89
(1,501)	1:38:A:PHE:HD1	1:75:A:PHE:H	16	0.89
(1,501)	1:38:A:PHE:HD2	1:75:A:PHE:H	16	0.89
(1,500)	1:38:A:PHE:HD1	1:39:A:ALA:H	20	0.89
(1,500)	1:38:A:PHE:HD2	1:39:A:ALA:H	20	0.89
(1,412)	1:33:A:ARG:HB2	1:34:A:SER:H	10	0.89
(1,412)	1:33:A:ARG:HB3	1:34:A:SER:H	10	0.89
(1,318)	1:25:A:TYR:HA	1:59:A:HIS:HA	2	0.89
(1,284)	1:24:A:LEU:HA	1:35:A:ILE:HD11	2	0.89
(1,284)	1:24:A:LEU:HA	1:35:A:ILE:HD12	2	0.89
(1,284)	1:24:A:LEU:HA	1:35:A:ILE:HD13	2	0.89
(1,166)	1:11:A:THR:HB	1:12:A:ARG:H	3	0.89
(1,129)	1:7:A:LEU:HD11	1:14:A:SER:HG	10	0.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,129)	1:7:A:LEU:HD12	1:14:A:SER:HG	10	0.89
(1,129)	1:7:A:LEU:HD13	1:14:A:SER:HG	10	0.89
(1,128)	1:7:A:LEU:HG	1:38:A:PHE:HD1	17	0.89
(1,128)	1:7:A:LEU:HG	1:38:A:PHE:HD2	17	0.89
(1,21)	1:5:A:LEU:HB2	1:36:A:PHE:H	3	0.89
(1,21)	1:5:A:LEU:HB3	1:36:A:PHE:H	3	0.89
(1,892)	1:76:A:LEU:HD11	1:78:A:GLU:HA	13	0.88
(1,892)	1:76:A:LEU:HD12	1:78:A:GLU:HA	13	0.88
(1,892)	1:76:A:LEU:HD13	1:78:A:GLU:HA	13	0.88
(1,891)	1:76:A:LEU:HD11	1:77:A:TYR:H	20	0.88
(1,891)	1:76:A:LEU:HD12	1:77:A:TYR:H	20	0.88
(1,891)	1:76:A:LEU:HD13	1:77:A:TYR:H	20	0.88
(1,890)	1:76:A:LEU:HD11	1:78:A:GLU:H	12	0.88
(1,890)	1:76:A:LEU:HD12	1:78:A:GLU:H	12	0.88
(1,890)	1:76:A:LEU:HD13	1:78:A:GLU:H	12	0.88
(1,865)	1:74:A:ASP:H	1:75:A:PHE:H	14	0.88
(1,798)	1:66:A:VAL:HG11	1:69:A:SER:HA	6	0.88
(1,798)	1:66:A:VAL:HG12	1:69:A:SER:HA	6	0.88
(1,798)	1:66:A:VAL:HG13	1:69:A:SER:HA	6	0.88
(1,798)	1:66:A:VAL:HG21	1:69:A:SER:HA	6	0.88
(1,798)	1:66:A:VAL:HG22	1:69:A:SER:HA	6	0.88
(1,798)	1:66:A:VAL:HG23	1:69:A:SER:HA	6	0.88
(1,781)	1:65:A:GLU:HA	1:77:A:TYR:HD1	19	0.88
(1,781)	1:65:A:GLU:HA	1:77:A:TYR:HD2	19	0.88
(1,742)	1:62:A:TYR:HE1	1:63:A:LEU:H	20	0.88
(1,742)	1:62:A:TYR:HE2	1:63:A:LEU:H	20	0.88
(1,500)	1:38:A:PHE:HD1	1:39:A:ALA:H	7	0.88
(1,500)	1:38:A:PHE:HD2	1:39:A:ALA:H	7	0.88
(1,500)	1:38:A:PHE:HD1	1:39:A:ALA:H	15	0.88
(1,500)	1:38:A:PHE:HD2	1:39:A:ALA:H	15	0.88
(1,476)	1:37:A:TYR:H	1:78:A:GLU:HG2	7	0.88
(1,476)	1:37:A:TYR:H	1:78:A:GLU:HG3	7	0.88
(1,458)	1:36:A:PHE:HA	1:76:A:LEU:HD11	11	0.88
(1,458)	1:36:A:PHE:HA	1:76:A:LEU:HD12	11	0.88
(1,458)	1:36:A:PHE:HA	1:76:A:LEU:HD13	11	0.88
(1,365)	1:28:A:PHE:HD1	1:32:A:LYS:HB2	16	0.88
(1,365)	1:28:A:PHE:HD1	1:32:A:LYS:HB3	16	0.88
(1,365)	1:28:A:PHE:HD2	1:32:A:LYS:HB2	16	0.88
(1,365)	1:28:A:PHE:HD2	1:32:A:LYS:HB3	16	0.88
(1,298)	1:24:A:LEU:HG	1:80:A:HIS:HE1	8	0.88
(1,182)	1:14:A:SER:H	1:17:A:LYS:H	12	0.88
(1,147)	1:9:A:LYS:H	1:11:A:THR:H	13	0.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,46)	1:6:A:VAL:H	1:35:A:ILE:HD11	11	0.88
(1,46)	1:6:A:VAL:H	1:35:A:ILE:HD12	11	0.88
(1,46)	1:6:A:VAL:H	1:35:A:ILE:HD13	11	0.88
(1,34)	1:5:A:LEU:HD11	1:7:A:LEU:HB2	18	0.88
(1,34)	1:5:A:LEU:HD11	1:7:A:LEU:HB3	18	0.88
(1,34)	1:5:A:LEU:HD12	1:7:A:LEU:HB2	18	0.88
(1,34)	1:5:A:LEU:HD12	1:7:A:LEU:HB3	18	0.88
(1,34)	1:5:A:LEU:HD13	1:7:A:LEU:HB2	18	0.88
(1,34)	1:5:A:LEU:HD13	1:7:A:LEU:HB3	18	0.88
(1,34)	1:5:A:LEU:HD21	1:7:A:LEU:HB2	18	0.88
(1,34)	1:5:A:LEU:HD21	1:7:A:LEU:HB3	18	0.88
(1,34)	1:5:A:LEU:HD22	1:7:A:LEU:HB2	18	0.88
(1,34)	1:5:A:LEU:HD22	1:7:A:LEU:HB3	18	0.88
(1,34)	1:5:A:LEU:HD23	1:7:A:LEU:HB2	18	0.88
(1,34)	1:5:A:LEU:HD23	1:7:A:LEU:HB3	18	0.88
(1,892)	1:76:A:LEU:HD11	1:78:A:GLU:HA	19	0.87
(1,892)	1:76:A:LEU:HD12	1:78:A:GLU:HA	19	0.87
(1,892)	1:76:A:LEU:HD13	1:78:A:GLU:HA	19	0.87
(1,843)	1:71:A:ASP:H	1:73:A:LYS:HA	1	0.87
(1,789)	1:66:A:VAL:H	1:68:A:VAL:HG11	2	0.87
(1,789)	1:66:A:VAL:H	1:68:A:VAL:HG12	2	0.87
(1,789)	1:66:A:VAL:H	1:68:A:VAL:HG13	2	0.87
(1,736)	1:62:A:TYR:HA	1:63:A:LEU:HD21	7	0.87
(1,736)	1:62:A:TYR:HA	1:63:A:LEU:HD22	7	0.87
(1,736)	1:62:A:TYR:HA	1:63:A:LEU:HD23	7	0.87
(1,736)	1:62:A:TYR:HA	1:63:A:LEU:HD21	14	0.87
(1,736)	1:62:A:TYR:HA	1:63:A:LEU:HD22	14	0.87
(1,736)	1:62:A:TYR:HA	1:63:A:LEU:HD23	14	0.87
(1,672)	1:55:A:LYS:H	1:63:A:LEU:HD11	16	0.87
(1,672)	1:55:A:LYS:H	1:63:A:LEU:HD12	16	0.87
(1,672)	1:55:A:LYS:H	1:63:A:LEU:HD13	16	0.87
(1,544)	1:44:A:HIS:HA	1:48:A:LEU:HD11	5	0.87
(1,544)	1:44:A:HIS:HA	1:48:A:LEU:HD12	5	0.87
(1,544)	1:44:A:HIS:HA	1:48:A:LEU:HD13	5	0.87
(1,544)	1:44:A:HIS:HA	1:48:A:LEU:HD11	5	0.87
(1,544)	1:44:A:HIS:HA	1:48:A:LEU:HD12	5	0.87
(1,544)	1:44:A:HIS:HA	1:48:A:LEU:HD13	5	0.87
(1,501)	1:38:A:PHE:HD1	1:75:A:PHE:H	18	0.87
(1,501)	1:38:A:PHE:HD2	1:75:A:PHE:H	18	0.87
(1,495)	1:38:A:PHE:HA	1:75:A:PHE:HD1	4	0.87
(1,495)	1:38:A:PHE:HA	1:75:A:PHE:HD2	4	0.87
(1,470)	1:36:A:PHE:HD1	1:77:A:TYR:HD1	9	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,470)	1:36:A:PHE:HD1	1:77:A:TYR:HD2	9	0.87
(1,470)	1:36:A:PHE:HD2	1:77:A:TYR:HD1	9	0.87
(1,470)	1:36:A:PHE:HD2	1:77:A:TYR:HD2	9	0.87
(1,365)	1:28:A:PHE:HD1	1:32:A:LYS:HB2	6	0.87
(1,365)	1:28:A:PHE:HD1	1:32:A:LYS:HB3	6	0.87
(1,365)	1:28:A:PHE:HD2	1:32:A:LYS:HB2	6	0.87
(1,365)	1:28:A:PHE:HD2	1:32:A:LYS:HB3	6	0.87
(1,177)	1:13:A:LYS:H	1:16:A:ALA:H	16	0.87
(1,128)	1:7:A:LEU:HG	1:38:A:PHE:HD1	20	0.87
(1,128)	1:7:A:LEU:HG	1:38:A:PHE:HD2	20	0.87
(1,893)	1:76:A:LEU:HD11	1:78:A:GLU:HG2	5	0.86
(1,893)	1:76:A:LEU:HD11	1:78:A:GLU:HG3	5	0.86
(1,893)	1:76:A:LEU:HD12	1:78:A:GLU:HG2	5	0.86
(1,893)	1:76:A:LEU:HD12	1:78:A:GLU:HG3	5	0.86
(1,893)	1:76:A:LEU:HD13	1:78:A:GLU:HG2	5	0.86
(1,893)	1:76:A:LEU:HD13	1:78:A:GLU:HG3	5	0.86
(1,891)	1:76:A:LEU:HD11	1:77:A:TYR:H	8	0.86
(1,891)	1:76:A:LEU:HD12	1:77:A:TYR:H	8	0.86
(1,891)	1:76:A:LEU:HD13	1:77:A:TYR:H	8	0.86
(1,891)	1:76:A:LEU:HD11	1:77:A:TYR:H	19	0.86
(1,891)	1:76:A:LEU:HD12	1:77:A:TYR:H	19	0.86
(1,891)	1:76:A:LEU:HD13	1:77:A:TYR:H	19	0.86
(1,846)	1:71:A:ASP:HA	1:72:A:GLU:HG2	16	0.86
(1,846)	1:71:A:ASP:HA	1:72:A:GLU:HG3	16	0.86
(1,798)	1:66:A:VAL:HG11	1:69:A:SER:HA	3	0.86
(1,798)	1:66:A:VAL:HG12	1:69:A:SER:HA	3	0.86
(1,798)	1:66:A:VAL:HG13	1:69:A:SER:HA	3	0.86
(1,798)	1:66:A:VAL:HG21	1:69:A:SER:HA	3	0.86
(1,798)	1:66:A:VAL:HG22	1:69:A:SER:HA	3	0.86
(1,798)	1:66:A:VAL:HG23	1:69:A:SER:HA	3	0.86
(1,798)	1:66:A:VAL:HG11	1:69:A:SER:HA	7	0.86
(1,798)	1:66:A:VAL:HG12	1:69:A:SER:HA	7	0.86
(1,798)	1:66:A:VAL:HG13	1:69:A:SER:HA	7	0.86
(1,798)	1:66:A:VAL:HG21	1:69:A:SER:HA	7	0.86
(1,798)	1:66:A:VAL:HG22	1:69:A:SER:HA	7	0.86
(1,798)	1:66:A:VAL:HG23	1:69:A:SER:HA	7	0.86
(1,742)	1:62:A:TYR:HE1	1:63:A:LEU:H	3	0.86
(1,742)	1:62:A:TYR:HE2	1:63:A:LEU:H	3	0.86
(1,721)	1:61:A:ALA:H	1:78:A:GLU:HB2	2	0.86
(1,721)	1:61:A:ALA:H	1:78:A:GLU:HB3	2	0.86
(1,714)	1:60:A:THR:HA	1:81:A:ILE:HG21	2	0.86
(1,714)	1:60:A:THR:HA	1:81:A:ILE:HG22	2	0.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,714)	1:60:A:THR:HA	1:81:A:ILE:HG23	2	0.86
(1,704)	1:59:A:HIS:H	1:60:A:THR:H	19	0.86
(1,318)	1:25:A:TYR:HA	1:59:A:HIS:HA	14	0.86
(1,245)	1:21:A:LEU:HD11	1:53:A:PHE:HA	10	0.86
(1,245)	1:21:A:LEU:HD12	1:53:A:PHE:HA	10	0.86
(1,245)	1:21:A:LEU:HD13	1:53:A:PHE:HA	10	0.86
(1,240)	1:21:A:LEU:HG	1:57:A:LYS:HB2	8	0.86
(1,240)	1:21:A:LEU:HG	1:57:A:LYS:HB3	8	0.86
(1,45)	1:6:A:VAL:H	1:35:A:ILE:HB	13	0.86
(1,898)	1:77:A:TYR:HB2	1:79:A:LEU:HG	16	0.85
(1,898)	1:77:A:TYR:HB3	1:79:A:LEU:HG	16	0.85
(1,891)	1:76:A:LEU:HD11	1:77:A:TYR:H	17	0.85
(1,891)	1:76:A:LEU:HD12	1:77:A:TYR:H	17	0.85
(1,891)	1:76:A:LEU:HD13	1:77:A:TYR:H	17	0.85
(1,890)	1:76:A:LEU:HD11	1:78:A:GLU:H	18	0.85
(1,890)	1:76:A:LEU:HD12	1:78:A:GLU:H	18	0.85
(1,890)	1:76:A:LEU:HD13	1:78:A:GLU:H	18	0.85
(1,842)	1:71:A:ASP:H	1:73:A:LYS:H	16	0.85
(1,819)	1:69:A:SER:H	1:73:A:LYS:H	18	0.85
(1,804)	1:67:A:ARG:H	1:68:A:VAL:HB	4	0.85
(1,804)	1:67:A:ARG:H	1:68:A:VAL:HB	8	0.85
(1,804)	1:67:A:ARG:H	1:68:A:VAL:HB	19	0.85
(1,469)	1:36:A:PHE:HD1	1:75:A:PHE:HB2	1	0.85
(1,469)	1:36:A:PHE:HD1	1:75:A:PHE:HB3	1	0.85
(1,469)	1:36:A:PHE:HD2	1:75:A:PHE:HB2	1	0.85
(1,469)	1:36:A:PHE:HD2	1:75:A:PHE:HB3	1	0.85
(1,458)	1:36:A:PHE:HA	1:76:A:LEU:HD11	1	0.85
(1,458)	1:36:A:PHE:HA	1:76:A:LEU:HD12	1	0.85
(1,458)	1:36:A:PHE:HA	1:76:A:LEU:HD13	1	0.85
(1,458)	1:36:A:PHE:HA	1:76:A:LEU:HD11	19	0.85
(1,458)	1:36:A:PHE:HA	1:76:A:LEU:HD12	19	0.85
(1,458)	1:36:A:PHE:HA	1:76:A:LEU:HD13	19	0.85
(1,890)	1:76:A:LEU:HD11	1:78:A:GLU:H	14	0.84
(1,890)	1:76:A:LEU:HD12	1:78:A:GLU:H	14	0.84
(1,890)	1:76:A:LEU:HD13	1:78:A:GLU:H	14	0.84
(1,842)	1:71:A:ASP:H	1:73:A:LYS:H	7	0.84
(1,798)	1:66:A:VAL:HG11	1:69:A:SER:HA	14	0.84
(1,798)	1:66:A:VAL:HG12	1:69:A:SER:HA	14	0.84
(1,798)	1:66:A:VAL:HG13	1:69:A:SER:HA	14	0.84
(1,798)	1:66:A:VAL:HG21	1:69:A:SER:HA	14	0.84
(1,798)	1:66:A:VAL:HG22	1:69:A:SER:HA	14	0.84
(1,798)	1:66:A:VAL:HG23	1:69:A:SER:HA	14	0.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,798)	1:66:A:VAL:HG11	1:69:A:SER:HA	16	0.84
(1,798)	1:66:A:VAL:HG12	1:69:A:SER:HA	16	0.84
(1,798)	1:66:A:VAL:HG13	1:69:A:SER:HA	16	0.84
(1,798)	1:66:A:VAL:HG21	1:69:A:SER:HA	16	0.84
(1,798)	1:66:A:VAL:HG22	1:69:A:SER:HA	16	0.84
(1,798)	1:66:A:VAL:HG23	1:69:A:SER:HA	16	0.84
(1,736)	1:62:A:TYR:HA	1:63:A:LEU:HD21	2	0.84
(1,736)	1:62:A:TYR:HA	1:63:A:LEU:HD22	2	0.84
(1,736)	1:62:A:TYR:HA	1:63:A:LEU:HD23	2	0.84
(1,721)	1:61:A:ALA:H	1:78:A:GLU:HB2	7	0.84
(1,721)	1:61:A:ALA:H	1:78:A:GLU:HB3	7	0.84
(1,642)	1:53:A:PHE:H	1:54:A:PHE:HD1	2	0.84
(1,642)	1:53:A:PHE:H	1:54:A:PHE:HD2	2	0.84
(1,476)	1:37:A:TYR:H	1:78:A:GLU:HG2	17	0.84
(1,476)	1:37:A:TYR:H	1:78:A:GLU:HG3	17	0.84
(1,476)	1:37:A:TYR:H	1:78:A:GLU:HG2	20	0.84
(1,476)	1:37:A:TYR:H	1:78:A:GLU:HG3	20	0.84
(1,432)	1:35:A:ILE:H	1:36:A:PHE:HE1	19	0.84
(1,432)	1:35:A:ILE:H	1:36:A:PHE:HE2	19	0.84
(1,364)	1:28:A:PHE:HD1	1:32:A:LYS:HA	5	0.84
(1,364)	1:28:A:PHE:HD2	1:32:A:LYS:HA	5	0.84
(1,200)	1:18:A:SER:HB2	1:22:A:GLU:HG2	11	0.84
(1,200)	1:18:A:SER:HB2	1:22:A:GLU:HG3	11	0.84
(1,200)	1:18:A:SER:HB3	1:22:A:GLU:HG2	11	0.84
(1,200)	1:18:A:SER:HB3	1:22:A:GLU:HG3	11	0.84
(1,125)	1:7:A:LEU:HG	1:16:A:ALA:HB1	6	0.84
(1,125)	1:7:A:LEU:HG	1:16:A:ALA:HB2	6	0.84
(1,125)	1:7:A:LEU:HG	1:16:A:ALA:HB3	6	0.84
(1,27)	1:5:A:LEU:HG	1:7:A:LEU:H	1	0.84
(1,19)	1:5:A:LEU:HB2	1:35:A:ILE:HA	16	0.84
(1,19)	1:5:A:LEU:HB3	1:35:A:ILE:HA	16	0.84
(1,892)	1:76:A:LEU:HD11	1:78:A:GLU:HA	4	0.83
(1,892)	1:76:A:LEU:HD12	1:78:A:GLU:HA	4	0.83
(1,892)	1:76:A:LEU:HD13	1:78:A:GLU:HA	4	0.83
(1,891)	1:76:A:LEU:HD11	1:77:A:TYR:H	4	0.83
(1,891)	1:76:A:LEU:HD12	1:77:A:TYR:H	4	0.83
(1,891)	1:76:A:LEU:HD13	1:77:A:TYR:H	4	0.83
(1,843)	1:71:A:ASP:H	1:73:A:LYS:HA	2	0.83
(1,794)	1:66:A:VAL:HA	1:77:A:TYR:H	8	0.83
(1,781)	1:65:A:GLU:HA	1:77:A:TYR:HD1	16	0.83
(1,781)	1:65:A:GLU:HA	1:77:A:TYR:HD2	16	0.83
(1,727)	1:61:A:ALA:HB1	1:79:A:LEU:HB3	12	0.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,727)	1:61:A:ALA:HB2	1:79:A:LEU:HB3	12	0.83
(1,727)	1:61:A:ALA:HB3	1:79:A:LEU:HB3	12	0.83
(1,712)	1:60:A:THR:HA	1:81:A:ILE:H	12	0.83
(1,426)	1:34:A:SER:HB2	1:36:A:PHE:HE1	6	0.83
(1,426)	1:34:A:SER:HB2	1:36:A:PHE:HE2	6	0.83
(1,426)	1:34:A:SER:HB3	1:36:A:PHE:HE1	6	0.83
(1,426)	1:34:A:SER:HB3	1:36:A:PHE:HE2	6	0.83
(1,395)	1:31:A:ASP:HA	1:81:A:ILE:HG21	5	0.83
(1,395)	1:31:A:ASP:HA	1:81:A:ILE:HG22	5	0.83
(1,395)	1:31:A:ASP:HA	1:81:A:ILE:HG23	5	0.83
(1,395)	1:31:A:ASP:HA	1:81:A:ILE:HG21	14	0.83
(1,395)	1:31:A:ASP:HA	1:81:A:ILE:HG22	14	0.83
(1,395)	1:31:A:ASP:HA	1:81:A:ILE:HG23	14	0.83
(1,318)	1:25:A:TYR:HA	1:59:A:HIS:HA	13	0.83
(1,166)	1:11:A:THR:HB	1:12:A:ARG:H	2	0.83
(1,166)	1:11:A:THR:HB	1:12:A:ARG:H	13	0.83
(1,147)	1:9:A:LYS:H	1:11:A:THR:H	7	0.83
(1,20)	1:5:A:LEU:HB2	1:35:A:ILE:HB	15	0.83
(1,20)	1:5:A:LEU:HB3	1:35:A:ILE:HB	15	0.83
(1,892)	1:76:A:LEU:HD11	1:78:A:GLU:HA	11	0.82
(1,892)	1:76:A:LEU:HD12	1:78:A:GLU:HA	11	0.82
(1,892)	1:76:A:LEU:HD13	1:78:A:GLU:HA	11	0.82
(1,721)	1:61:A:ALA:H	1:78:A:GLU:HB2	5	0.82
(1,721)	1:61:A:ALA:H	1:78:A:GLU:HB3	5	0.82
(1,560)	1:47:A:MET:H	1:48:A:LEU:HD11	2	0.82
(1,560)	1:47:A:MET:H	1:48:A:LEU:HD12	2	0.82
(1,560)	1:47:A:MET:H	1:48:A:LEU:HD13	2	0.82
(1,526)	1:41:A:THR:HB	1:74:A:ASP:HB2	12	0.82
(1,526)	1:41:A:THR:HB	1:74:A:ASP:HB3	12	0.82
(1,458)	1:36:A:PHE:HA	1:76:A:LEU:HD11	8	0.82
(1,458)	1:36:A:PHE:HA	1:76:A:LEU:HD12	8	0.82
(1,458)	1:36:A:PHE:HA	1:76:A:LEU:HD13	8	0.82
(1,441)	1:35:A:ILE:HB	1:37:A:TYR:HA	11	0.82
(1,426)	1:34:A:SER:HB2	1:36:A:PHE:HE1	13	0.82
(1,426)	1:34:A:SER:HB2	1:36:A:PHE:HE2	13	0.82
(1,426)	1:34:A:SER:HB3	1:36:A:PHE:HE1	13	0.82
(1,426)	1:34:A:SER:HB3	1:36:A:PHE:HE2	13	0.82
(1,317)	1:25:A:TYR:HA	1:29:A:SER:HG	17	0.82
(1,299)	1:24:A:LEU:HD11	1:35:A:ILE:HG21	4	0.82
(1,299)	1:24:A:LEU:HD11	1:35:A:ILE:HG22	4	0.82
(1,299)	1:24:A:LEU:HD11	1:35:A:ILE:HG23	4	0.82
(1,299)	1:24:A:LEU:HD12	1:35:A:ILE:HG21	4	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,299)	1:24:A:LEU:HD12	1:35:A:ILE:HG22	4	0.82
(1,299)	1:24:A:LEU:HD12	1:35:A:ILE:HG23	4	0.82
(1,299)	1:24:A:LEU:HD13	1:35:A:ILE:HG21	4	0.82
(1,299)	1:24:A:LEU:HD13	1:35:A:ILE:HG22	4	0.82
(1,299)	1:24:A:LEU:HD13	1:35:A:ILE:HG23	4	0.82
(1,200)	1:18:A:SER:HB2	1:22:A:GLU:HG2	1	0.82
(1,200)	1:18:A:SER:HB2	1:22:A:GLU:HG3	1	0.82
(1,200)	1:18:A:SER:HB3	1:22:A:GLU:HG2	1	0.82
(1,200)	1:18:A:SER:HB3	1:22:A:GLU:HG3	1	0.82
(1,128)	1:7:A:LEU:HG	1:38:A:PHE:HD1	3	0.82
(1,128)	1:7:A:LEU:HG	1:38:A:PHE:HD2	3	0.82
(1,33)	1:5:A:LEU:HD11	1:7:A:LEU:HA	17	0.82
(1,33)	1:5:A:LEU:HD12	1:7:A:LEU:HA	17	0.82
(1,33)	1:5:A:LEU:HD13	1:7:A:LEU:HA	17	0.82
(1,33)	1:5:A:LEU:HD21	1:7:A:LEU:HA	17	0.82
(1,33)	1:5:A:LEU:HD22	1:7:A:LEU:HA	17	0.82
(1,33)	1:5:A:LEU:HD23	1:7:A:LEU:HA	17	0.82
(1,20)	1:5:A:LEU:HB2	1:35:A:ILE:HB	2	0.82
(1,20)	1:5:A:LEU:HB3	1:35:A:ILE:HB	2	0.82
(1,795)	1:66:A:VAL:HA	1:77:A:TYR:HA	1	0.81
(1,736)	1:62:A:TYR:HA	1:63:A:LEU:HD21	4	0.81
(1,736)	1:62:A:TYR:HA	1:63:A:LEU:HD22	4	0.81
(1,736)	1:62:A:TYR:HA	1:63:A:LEU:HD23	4	0.81
(1,714)	1:60:A:THR:HA	1:81:A:ILE:HG21	10	0.81
(1,714)	1:60:A:THR:HA	1:81:A:ILE:HG22	10	0.81
(1,714)	1:60:A:THR:HA	1:81:A:ILE:HG23	10	0.81
(1,683)	1:56:A:GLU:H	1:57:A:LYS:HG3	10	0.81
(1,560)	1:47:A:MET:H	1:48:A:LEU:HD11	9	0.81
(1,560)	1:47:A:MET:H	1:48:A:LEU:HD12	9	0.81
(1,560)	1:47:A:MET:H	1:48:A:LEU:HD13	9	0.81
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG21	12	0.81
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG22	12	0.81
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG23	12	0.81
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG21	12	0.81
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG22	12	0.81
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG23	12	0.81
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG21	12	0.81
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG22	12	0.81
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG23	12	0.81
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG21	12	0.81
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG22	12	0.81
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG23	12	0.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,296)	1:24:A:LEU:HG	1:35:A:ILE:HD11	3	0.81
(1,296)	1:24:A:LEU:HG	1:35:A:ILE:HD12	3	0.81
(1,296)	1:24:A:LEU:HG	1:35:A:ILE:HD13	3	0.81
(1,166)	1:11:A:THR:HB	1:12:A:ARG:H	1	0.81
(1,146)	1:9:A:LYS:H	1:10:A:ASN:HB2	14	0.81
(1,146)	1:9:A:LYS:H	1:10:A:ASN:HB3	14	0.81
(1,43)	1:6:A:VAL:H	1:7:A:LEU:HG	6	0.81
(1,27)	1:5:A:LEU:HG	1:7:A:LEU:H	9	0.81
(1,898)	1:77:A:TYR:HB2	1:79:A:LEU:HG	5	0.8
(1,898)	1:77:A:TYR:HB3	1:79:A:LEU:HG	5	0.8
(1,891)	1:76:A:LEU:HD11	1:77:A:TYR:H	12	0.8
(1,891)	1:76:A:LEU:HD12	1:77:A:TYR:H	12	0.8
(1,891)	1:76:A:LEU:HD13	1:77:A:TYR:H	12	0.8
(1,798)	1:66:A:VAL:HG11	1:69:A:SER:HA	11	0.8
(1,798)	1:66:A:VAL:HG12	1:69:A:SER:HA	11	0.8
(1,798)	1:66:A:VAL:HG13	1:69:A:SER:HA	11	0.8
(1,798)	1:66:A:VAL:HG21	1:69:A:SER:HA	11	0.8
(1,798)	1:66:A:VAL:HG22	1:69:A:SER:HA	11	0.8
(1,798)	1:66:A:VAL:HG23	1:69:A:SER:HA	11	0.8
(1,789)	1:66:A:VAL:H	1:68:A:VAL:HG11	13	0.8
(1,789)	1:66:A:VAL:H	1:68:A:VAL:HG12	13	0.8
(1,789)	1:66:A:VAL:H	1:68:A:VAL:HG13	13	0.8
(1,768)	1:64:A:ASP:HA	1:76:A:LEU:HD21	7	0.8
(1,768)	1:64:A:ASP:HA	1:76:A:LEU:HD22	7	0.8
(1,768)	1:64:A:ASP:HA	1:76:A:LEU:HD23	7	0.8
(1,742)	1:62:A:TYR:HE1	1:63:A:LEU:H	1	0.8
(1,742)	1:62:A:TYR:HE2	1:63:A:LEU:H	1	0.8
(1,736)	1:62:A:TYR:HA	1:63:A:LEU:HD21	6	0.8
(1,736)	1:62:A:TYR:HA	1:63:A:LEU:HD22	6	0.8
(1,736)	1:62:A:TYR:HA	1:63:A:LEU:HD23	6	0.8
(1,736)	1:62:A:TYR:HA	1:63:A:LEU:HD21	11	0.8
(1,736)	1:62:A:TYR:HA	1:63:A:LEU:HD22	11	0.8
(1,736)	1:62:A:TYR:HA	1:63:A:LEU:HD23	11	0.8
(1,723)	1:61:A:ALA:H	1:82:A:ILE:H	20	0.8
(1,704)	1:59:A:HIS:H	1:60:A:THR:H	11	0.8
(1,704)	1:59:A:HIS:H	1:60:A:THR:H	14	0.8
(1,544)	1:44:A:HIS:HA	1:48:A:LEU:HD11	10	0.8
(1,544)	1:44:A:HIS:HA	1:48:A:LEU:HD12	10	0.8
(1,544)	1:44:A:HIS:HA	1:48:A:LEU:HD13	10	0.8
(1,544)	1:44:A:HIS:HA	1:48:A:LEU:HD11	10	0.8
(1,544)	1:44:A:HIS:HA	1:48:A:LEU:HD12	10	0.8
(1,544)	1:44:A:HIS:HA	1:48:A:LEU:HD13	10	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,544)	1:44:A:HIS:HA	1:48:A:LEU:HD11	14	0.8
(1,544)	1:44:A:HIS:HA	1:48:A:LEU:HD12	14	0.8
(1,544)	1:44:A:HIS:HA	1:48:A:LEU:HD13	14	0.8
(1,544)	1:44:A:HIS:HA	1:48:A:LEU:HD11	14	0.8
(1,544)	1:44:A:HIS:HA	1:48:A:LEU:HD12	14	0.8
(1,544)	1:44:A:HIS:HA	1:48:A:LEU:HD13	14	0.8
(1,544)	1:44:A:HIS:HA	1:48:A:LEU:HD11	18	0.8
(1,544)	1:44:A:HIS:HA	1:48:A:LEU:HD12	18	0.8
(1,544)	1:44:A:HIS:HA	1:48:A:LEU:HD13	18	0.8
(1,544)	1:44:A:HIS:HA	1:48:A:LEU:HD11	18	0.8
(1,544)	1:44:A:HIS:HA	1:48:A:LEU:HD12	18	0.8
(1,544)	1:44:A:HIS:HA	1:48:A:LEU:HD13	18	0.8
(1,542)	1:44:A:HIS:HA	1:45:A:LYS:HD2	8	0.8
(1,542)	1:44:A:HIS:HA	1:45:A:LYS:HD3	8	0.8
(1,526)	1:41:A:THR:HB	1:74:A:ASP:HB2	6	0.8
(1,526)	1:41:A:THR:HB	1:74:A:ASP:HB3	6	0.8
(1,467)	1:36:A:PHE:HB2	1:77:A:TYR:HD1	17	0.8
(1,467)	1:36:A:PHE:HB2	1:77:A:TYR:HD2	17	0.8
(1,467)	1:36:A:PHE:HB3	1:77:A:TYR:HD1	17	0.8
(1,467)	1:36:A:PHE:HB3	1:77:A:TYR:HD2	17	0.8
(1,458)	1:36:A:PHE:HA	1:76:A:LEU:HD11	10	0.8
(1,458)	1:36:A:PHE:HA	1:76:A:LEU:HD12	10	0.8
(1,458)	1:36:A:PHE:HA	1:76:A:LEU:HD13	10	0.8
(1,458)	1:36:A:PHE:HA	1:76:A:LEU:HD11	18	0.8
(1,458)	1:36:A:PHE:HA	1:76:A:LEU:HD12	18	0.8
(1,458)	1:36:A:PHE:HA	1:76:A:LEU:HD13	18	0.8
(1,412)	1:33:A:ARG:HB2	1:34:A:SER:H	12	0.8
(1,412)	1:33:A:ARG:HB3	1:34:A:SER:H	12	0.8
(1,318)	1:25:A:TYR:HA	1:59:A:HIS:HA	18	0.8
(1,305)	1:24:A:LEU:HD21	1:60:A:THR:H	12	0.8
(1,305)	1:24:A:LEU:HD22	1:60:A:THR:H	12	0.8
(1,305)	1:24:A:LEU:HD23	1:60:A:THR:H	12	0.8
(1,128)	1:7:A:LEU:HG	1:38:A:PHE:HD1	11	0.8
(1,128)	1:7:A:LEU:HG	1:38:A:PHE:HD2	11	0.8
(1,37)	1:5:A:LEU:HD11	1:38:A:PHE:HB3	18	0.8
(1,37)	1:5:A:LEU:HD12	1:38:A:PHE:HB3	18	0.8
(1,37)	1:5:A:LEU:HD13	1:38:A:PHE:HB3	18	0.8
(1,37)	1:5:A:LEU:HD21	1:38:A:PHE:HB3	18	0.8
(1,37)	1:5:A:LEU:HD22	1:38:A:PHE:HB3	18	0.8
(1,37)	1:5:A:LEU:HD23	1:38:A:PHE:HB3	18	0.8
(1,36)	1:5:A:LEU:HD11	1:7:A:LEU:HD11	7	0.8
(1,36)	1:5:A:LEU:HD11	1:7:A:LEU:HD12	7	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,36)	1:5:A:LEU:HD11	1:7:A:LEU:HD13	7	0.8
(1,36)	1:5:A:LEU:HD12	1:7:A:LEU:HD11	7	0.8
(1,36)	1:5:A:LEU:HD12	1:7:A:LEU:HD12	7	0.8
(1,36)	1:5:A:LEU:HD12	1:7:A:LEU:HD13	7	0.8
(1,36)	1:5:A:LEU:HD13	1:7:A:LEU:HD11	7	0.8
(1,36)	1:5:A:LEU:HD13	1:7:A:LEU:HD12	7	0.8
(1,36)	1:5:A:LEU:HD13	1:7:A:LEU:HD13	7	0.8
(1,36)	1:5:A:LEU:HD21	1:7:A:LEU:HD11	7	0.8
(1,36)	1:5:A:LEU:HD21	1:7:A:LEU:HD12	7	0.8
(1,36)	1:5:A:LEU:HD21	1:7:A:LEU:HD13	7	0.8
(1,36)	1:5:A:LEU:HD22	1:7:A:LEU:HD11	7	0.8
(1,36)	1:5:A:LEU:HD22	1:7:A:LEU:HD12	7	0.8
(1,36)	1:5:A:LEU:HD22	1:7:A:LEU:HD13	7	0.8
(1,36)	1:5:A:LEU:HD23	1:7:A:LEU:HD11	7	0.8
(1,36)	1:5:A:LEU:HD23	1:7:A:LEU:HD12	7	0.8
(1,36)	1:5:A:LEU:HD23	1:7:A:LEU:HD13	7	0.8
(1,32)	1:5:A:LEU:HD11	1:7:A:LEU:H	6	0.8
(1,32)	1:5:A:LEU:HD12	1:7:A:LEU:H	6	0.8
(1,32)	1:5:A:LEU:HD13	1:7:A:LEU:H	6	0.8
(1,32)	1:5:A:LEU:HD21	1:7:A:LEU:H	6	0.8
(1,32)	1:5:A:LEU:HD22	1:7:A:LEU:H	6	0.8
(1,32)	1:5:A:LEU:HD23	1:7:A:LEU:H	6	0.8
(1,27)	1:5:A:LEU:HG	1:7:A:LEU:H	13	0.8
(1,19)	1:5:A:LEU:HB2	1:35:A:ILE:HA	7	0.8
(1,19)	1:5:A:LEU:HB3	1:35:A:ILE:HA	7	0.8
(1,893)	1:76:A:LEU:HD11	1:78:A:GLU:HG2	7	0.79
(1,893)	1:76:A:LEU:HD11	1:78:A:GLU:HG3	7	0.79
(1,893)	1:76:A:LEU:HD12	1:78:A:GLU:HG2	7	0.79
(1,893)	1:76:A:LEU:HD12	1:78:A:GLU:HG3	7	0.79
(1,893)	1:76:A:LEU:HD13	1:78:A:GLU:HG2	7	0.79
(1,893)	1:76:A:LEU:HD13	1:78:A:GLU:HG3	7	0.79
(1,892)	1:76:A:LEU:HD11	1:78:A:GLU:HA	2	0.79
(1,892)	1:76:A:LEU:HD12	1:78:A:GLU:HA	2	0.79
(1,892)	1:76:A:LEU:HD13	1:78:A:GLU:HA	2	0.79
(1,811)	1:68:A:VAL:HA	1:73:A:LYS:H	18	0.79
(1,795)	1:66:A:VAL:HA	1:77:A:TYR:HA	12	0.79
(1,794)	1:66:A:VAL:HA	1:77:A:TYR:H	17	0.79
(1,721)	1:61:A:ALA:H	1:78:A:GLU:HB2	10	0.79
(1,721)	1:61:A:ALA:H	1:78:A:GLU:HB3	10	0.79
(1,544)	1:44:A:HIS:HA	1:48:A:LEU:HD11	3	0.79
(1,544)	1:44:A:HIS:HA	1:48:A:LEU:HD12	3	0.79
(1,544)	1:44:A:HIS:HA	1:48:A:LEU:HD13	3	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,544)	1:44:A:HIS:HA	1:48:A:LEU:HD11	3	0.79
(1,544)	1:44:A:HIS:HA	1:48:A:LEU:HD12	3	0.79
(1,544)	1:44:A:HIS:HA	1:48:A:LEU:HD13	3	0.79
(1,474)	1:37:A:TYR:H	1:76:A:LEU:H	16	0.79
(1,467)	1:36:A:PHE:HB2	1:77:A:TYR:HD1	20	0.79
(1,467)	1:36:A:PHE:HB2	1:77:A:TYR:HD2	20	0.79
(1,467)	1:36:A:PHE:HB3	1:77:A:TYR:HD1	20	0.79
(1,467)	1:36:A:PHE:HB3	1:77:A:TYR:HD2	20	0.79
(1,432)	1:35:A:ILE:H	1:36:A:PHE:HE1	12	0.79
(1,432)	1:35:A:ILE:H	1:36:A:PHE:HE2	12	0.79
(1,395)	1:31:A:ASP:HA	1:81:A:ILE:HG21	12	0.79
(1,395)	1:31:A:ASP:HA	1:81:A:ILE:HG22	12	0.79
(1,395)	1:31:A:ASP:HA	1:81:A:ILE:HG23	12	0.79
(1,288)	1:24:A:LEU:HA	1:80:A:HIS:HE1	20	0.79
(1,174)	1:12:A:ARG:HB2	1:14:A:SER:HA	2	0.79
(1,174)	1:12:A:ARG:HB3	1:14:A:SER:HA	2	0.79
(1,128)	1:7:A:LEU:HG	1:38:A:PHE:HD1	5	0.79
(1,128)	1:7:A:LEU:HG	1:38:A:PHE:HD2	5	0.79
(1,890)	1:76:A:LEU:HD11	1:78:A:GLU:H	8	0.78
(1,890)	1:76:A:LEU:HD12	1:78:A:GLU:H	8	0.78
(1,890)	1:76:A:LEU:HD13	1:78:A:GLU:H	8	0.78
(1,798)	1:66:A:VAL:HG11	1:69:A:SER:HA	10	0.78
(1,798)	1:66:A:VAL:HG12	1:69:A:SER:HA	10	0.78
(1,798)	1:66:A:VAL:HG13	1:69:A:SER:HA	10	0.78
(1,798)	1:66:A:VAL:HG21	1:69:A:SER:HA	10	0.78
(1,798)	1:66:A:VAL:HG22	1:69:A:SER:HA	10	0.78
(1,798)	1:66:A:VAL:HG23	1:69:A:SER:HA	10	0.78
(1,794)	1:66:A:VAL:HA	1:77:A:TYR:H	5	0.78
(1,736)	1:62:A:TYR:HA	1:63:A:LEU:HD21	8	0.78
(1,736)	1:62:A:TYR:HA	1:63:A:LEU:HD22	8	0.78
(1,736)	1:62:A:TYR:HA	1:63:A:LEU:HD23	8	0.78
(1,713)	1:60:A:THR:HA	1:81:A:ILE:HA	12	0.78
(1,710)	1:60:A:THR:HA	1:61:A:ALA:H	12	0.78
(1,704)	1:59:A:HIS:H	1:60:A:THR:H	1	0.78
(1,704)	1:59:A:HIS:H	1:60:A:THR:H	12	0.78
(1,467)	1:36:A:PHE:HB2	1:77:A:TYR:HD1	14	0.78
(1,467)	1:36:A:PHE:HB2	1:77:A:TYR:HD2	14	0.78
(1,467)	1:36:A:PHE:HB3	1:77:A:TYR:HD1	14	0.78
(1,467)	1:36:A:PHE:HB3	1:77:A:TYR:HD2	14	0.78
(1,412)	1:33:A:ARG:HB2	1:34:A:SER:H	2	0.78
(1,412)	1:33:A:ARG:HB3	1:34:A:SER:H	2	0.78
(1,395)	1:31:A:ASP:HA	1:81:A:ILE:HG21	19	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,395)	1:31:A:ASP:HA	1:81:A:ILE:HG22	19	0.78
(1,395)	1:31:A:ASP:HA	1:81:A:ILE:HG23	19	0.78
(1,317)	1:25:A:TYR:HA	1:29:A:SER:HG	6	0.78
(1,300)	1:24:A:LEU:HD11	1:35:A:ILE:HG12	19	0.78
(1,300)	1:24:A:LEU:HD11	1:35:A:ILE:HG13	19	0.78
(1,300)	1:24:A:LEU:HD12	1:35:A:ILE:HG12	19	0.78
(1,300)	1:24:A:LEU:HD12	1:35:A:ILE:HG13	19	0.78
(1,300)	1:24:A:LEU:HD13	1:35:A:ILE:HG12	19	0.78
(1,300)	1:24:A:LEU:HD13	1:35:A:ILE:HG13	19	0.78
(1,288)	1:24:A:LEU:HA	1:80:A:HIS:HE1	18	0.78
(1,166)	1:11:A:THR:HB	1:12:A:ARG:H	10	0.78
(1,34)	1:5:A:LEU:HD11	1:7:A:LEU:HB2	17	0.78
(1,34)	1:5:A:LEU:HD11	1:7:A:LEU:HB3	17	0.78
(1,34)	1:5:A:LEU:HD12	1:7:A:LEU:HB2	17	0.78
(1,34)	1:5:A:LEU:HD12	1:7:A:LEU:HB3	17	0.78
(1,34)	1:5:A:LEU:HD13	1:7:A:LEU:HB2	17	0.78
(1,34)	1:5:A:LEU:HD13	1:7:A:LEU:HB3	17	0.78
(1,34)	1:5:A:LEU:HD21	1:7:A:LEU:HB2	17	0.78
(1,34)	1:5:A:LEU:HD21	1:7:A:LEU:HB3	17	0.78
(1,34)	1:5:A:LEU:HD22	1:7:A:LEU:HB2	17	0.78
(1,34)	1:5:A:LEU:HD22	1:7:A:LEU:HB3	17	0.78
(1,34)	1:5:A:LEU:HD23	1:7:A:LEU:HB2	17	0.78
(1,34)	1:5:A:LEU:HD23	1:7:A:LEU:HB3	17	0.78
(1,794)	1:66:A:VAL:HA	1:77:A:TYR:H	20	0.77
(1,789)	1:66:A:VAL:H	1:68:A:VAL:HG11	10	0.77
(1,789)	1:66:A:VAL:H	1:68:A:VAL:HG12	10	0.77
(1,789)	1:66:A:VAL:H	1:68:A:VAL:HG13	10	0.77
(1,705)	1:59:A:HIS:H	1:60:A:THR:HA	7	0.77
(1,560)	1:47:A:MET:H	1:48:A:LEU:HD11	14	0.77
(1,560)	1:47:A:MET:H	1:48:A:LEU:HD12	14	0.77
(1,560)	1:47:A:MET:H	1:48:A:LEU:HD13	14	0.77
(1,411)	1:33:A:ARG:HA	1:82:A:ILE:HA	15	0.77
(1,296)	1:24:A:LEU:HG	1:35:A:ILE:HD11	16	0.77
(1,296)	1:24:A:LEU:HG	1:35:A:ILE:HD12	16	0.77
(1,296)	1:24:A:LEU:HG	1:35:A:ILE:HD13	16	0.77
(1,295)	1:24:A:LEU:HG	1:25:A:TYR:HA	6	0.77
(1,295)	1:24:A:LEU:HG	1:25:A:TYR:HA	12	0.77
(1,295)	1:24:A:LEU:HG	1:25:A:TYR:HA	16	0.77
(1,240)	1:21:A:LEU:HG	1:57:A:LYS:HB2	2	0.77
(1,240)	1:21:A:LEU:HG	1:57:A:LYS:HB3	2	0.77
(1,128)	1:7:A:LEU:HG	1:38:A:PHE:HD1	2	0.77
(1,128)	1:7:A:LEU:HG	1:38:A:PHE:HD2	2	0.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,126)	1:7:A:LEU:HG	1:38:A:PHE:H	2	0.77
(1,891)	1:76:A:LEU:HD11	1:77:A:TYR:H	2	0.76
(1,891)	1:76:A:LEU:HD12	1:77:A:TYR:H	2	0.76
(1,891)	1:76:A:LEU:HD13	1:77:A:TYR:H	2	0.76
(1,794)	1:66:A:VAL:HA	1:77:A:TYR:H	2	0.76
(1,743)	1:62:A:TYR:HE1	1:63:A:LEU:HD21	8	0.76
(1,743)	1:62:A:TYR:HE1	1:63:A:LEU:HD22	8	0.76
(1,743)	1:62:A:TYR:HE1	1:63:A:LEU:HD23	8	0.76
(1,743)	1:62:A:TYR:HE2	1:63:A:LEU:HD21	8	0.76
(1,743)	1:62:A:TYR:HE2	1:63:A:LEU:HD22	8	0.76
(1,743)	1:62:A:TYR:HE2	1:63:A:LEU:HD23	8	0.76
(1,736)	1:62:A:TYR:HA	1:63:A:LEU:HD21	9	0.76
(1,736)	1:62:A:TYR:HA	1:63:A:LEU:HD22	9	0.76
(1,736)	1:62:A:TYR:HA	1:63:A:LEU:HD23	9	0.76
(1,721)	1:61:A:ALA:H	1:78:A:GLU:HB2	17	0.76
(1,721)	1:61:A:ALA:H	1:78:A:GLU:HB3	17	0.76
(1,704)	1:59:A:HIS:H	1:60:A:THR:H	18	0.76
(1,431)	1:35:A:ILE:H	1:36:A:PHE:HD1	2	0.76
(1,431)	1:35:A:ILE:H	1:36:A:PHE:HD2	2	0.76
(1,410)	1:33:A:ARG:HA	1:81:A:ILE:HG21	1	0.76
(1,410)	1:33:A:ARG:HA	1:81:A:ILE:HG22	1	0.76
(1,410)	1:33:A:ARG:HA	1:81:A:ILE:HG23	1	0.76
(1,364)	1:28:A:PHE:HD1	1:32:A:LYS:HA	6	0.76
(1,364)	1:28:A:PHE:HD2	1:32:A:LYS:HA	6	0.76
(1,301)	1:24:A:LEU:HD11	1:60:A:THR:HB	12	0.76
(1,301)	1:24:A:LEU:HD12	1:60:A:THR:HB	12	0.76
(1,301)	1:24:A:LEU:HD13	1:60:A:THR:HB	12	0.76
(1,295)	1:24:A:LEU:HG	1:25:A:TYR:HA	2	0.76
(1,295)	1:24:A:LEU:HG	1:25:A:TYR:HA	17	0.76
(1,245)	1:21:A:LEU:HD11	1:53:A:PHE:HA	12	0.76
(1,245)	1:21:A:LEU:HD12	1:53:A:PHE:HA	12	0.76
(1,245)	1:21:A:LEU:HD13	1:53:A:PHE:HA	12	0.76
(1,191)	1:16:A:ALA:HA	1:19:A:VAL:HB	9	0.76
(1,102)	1:7:A:LEU:H	1:19:A:VAL:HB	2	0.76
(1,21)	1:5:A:LEU:HB2	1:36:A:PHE:H	10	0.76
(1,21)	1:5:A:LEU:HB3	1:36:A:PHE:H	10	0.76
(3,1)	1:39:A:ALA:HB1	1:47:A:MET:N	9	0.75
(1,917)	1:79:A:LEU:HB2	1:80:A:HIS:HD2	14	0.75
(1,917)	1:79:A:LEU:HB3	1:80:A:HIS:HD2	14	0.75
(1,891)	1:76:A:LEU:HD11	1:77:A:TYR:H	11	0.75
(1,891)	1:76:A:LEU:HD12	1:77:A:TYR:H	11	0.75
(1,891)	1:76:A:LEU:HD13	1:77:A:TYR:H	11	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,878)	1:75:A:PHE:HB2	1:77:A:TYR:HD1	10	0.75
(1,878)	1:75:A:PHE:HB2	1:77:A:TYR:HD2	10	0.75
(1,878)	1:75:A:PHE:HB3	1:77:A:TYR:HD1	10	0.75
(1,878)	1:75:A:PHE:HB3	1:77:A:TYR:HD2	10	0.75
(1,741)	1:62:A:TYR:HD1	1:63:A:LEU:H	17	0.75
(1,741)	1:62:A:TYR:HD2	1:63:A:LEU:H	17	0.75
(1,560)	1:47:A:MET:H	1:48:A:LEU:HD11	11	0.75
(1,560)	1:47:A:MET:H	1:48:A:LEU:HD12	11	0.75
(1,560)	1:47:A:MET:H	1:48:A:LEU:HD13	11	0.75
(1,560)	1:47:A:MET:H	1:48:A:LEU:HD11	18	0.75
(1,560)	1:47:A:MET:H	1:48:A:LEU:HD12	18	0.75
(1,560)	1:47:A:MET:H	1:48:A:LEU:HD13	18	0.75
(1,542)	1:44:A:HIS:HA	1:45:A:LYS:HD2	16	0.75
(1,542)	1:44:A:HIS:HA	1:45:A:LYS:HD3	16	0.75
(1,502)	1:38:A:PHE:HD1	1:75:A:PHE:HA	4	0.75
(1,502)	1:38:A:PHE:HD2	1:75:A:PHE:HA	4	0.75
(1,501)	1:38:A:PHE:HD1	1:75:A:PHE:H	11	0.75
(1,501)	1:38:A:PHE:HD2	1:75:A:PHE:H	11	0.75
(1,467)	1:36:A:PHE:HB2	1:77:A:TYR:HD1	3	0.75
(1,467)	1:36:A:PHE:HB2	1:77:A:TYR:HD2	3	0.75
(1,467)	1:36:A:PHE:HB3	1:77:A:TYR:HD1	3	0.75
(1,467)	1:36:A:PHE:HB3	1:77:A:TYR:HD2	3	0.75
(1,467)	1:36:A:PHE:HB2	1:77:A:TYR:HD1	10	0.75
(1,467)	1:36:A:PHE:HB2	1:77:A:TYR:HD2	10	0.75
(1,467)	1:36:A:PHE:HB3	1:77:A:TYR:HD1	10	0.75
(1,467)	1:36:A:PHE:HB3	1:77:A:TYR:HD2	10	0.75
(1,412)	1:33:A:ARG:HB2	1:34:A:SER:H	19	0.75
(1,412)	1:33:A:ARG:HB3	1:34:A:SER:H	19	0.75
(1,411)	1:33:A:ARG:HA	1:82:A:ILE:HA	9	0.75
(1,395)	1:31:A:ASP:HA	1:81:A:ILE:HG21	6	0.75
(1,395)	1:31:A:ASP:HA	1:81:A:ILE:HG22	6	0.75
(1,395)	1:31:A:ASP:HA	1:81:A:ILE:HG23	6	0.75
(1,364)	1:28:A:PHE:HD1	1:32:A:LYS:HA	19	0.75
(1,364)	1:28:A:PHE:HD2	1:32:A:LYS:HA	19	0.75
(1,355)	1:28:A:PHE:HA	1:32:A:LYS:HB2	1	0.75
(1,355)	1:28:A:PHE:HA	1:32:A:LYS:HB3	1	0.75
(1,298)	1:24:A:LEU:HG	1:80:A:HIS:HE1	2	0.75
(1,298)	1:24:A:LEU:HG	1:80:A:HIS:HE1	9	0.75
(1,156)	1:10:A:ASN:HB2	1:45:A:LYS:HB2	16	0.75
(1,156)	1:10:A:ASN:HB2	1:45:A:LYS:HB3	16	0.75
(1,156)	1:10:A:ASN:HB3	1:45:A:LYS:HB2	16	0.75
(1,156)	1:10:A:ASN:HB3	1:45:A:LYS:HB3	16	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,128)	1:7:A:LEU:HG	1:38:A:PHE:HD1	12	0.75
(1,128)	1:7:A:LEU:HG	1:38:A:PHE:HD2	12	0.75
(1,2)	1:3:A:MET:H	1:4:A:LYS:HA	2	0.75
(1,893)	1:76:A:LEU:HD11	1:78:A:GLU:HG2	2	0.74
(1,893)	1:76:A:LEU:HD11	1:78:A:GLU:HG3	2	0.74
(1,893)	1:76:A:LEU:HD12	1:78:A:GLU:HG2	2	0.74
(1,893)	1:76:A:LEU:HD12	1:78:A:GLU:HG3	2	0.74
(1,893)	1:76:A:LEU:HD13	1:78:A:GLU:HG2	2	0.74
(1,893)	1:76:A:LEU:HD13	1:78:A:GLU:HG3	2	0.74
(1,823)	1:69:A:SER:HA	1:71:A:ASP:H	15	0.74
(1,814)	1:68:A:VAL:HG11	1:73:A:LYS:H	8	0.74
(1,814)	1:68:A:VAL:HG12	1:73:A:LYS:H	8	0.74
(1,814)	1:68:A:VAL:HG13	1:73:A:LYS:H	8	0.74
(1,814)	1:68:A:VAL:HG21	1:73:A:LYS:H	8	0.74
(1,814)	1:68:A:VAL:HG22	1:73:A:LYS:H	8	0.74
(1,814)	1:68:A:VAL:HG23	1:73:A:LYS:H	8	0.74
(1,795)	1:66:A:VAL:HA	1:77:A:TYR:HA	7	0.74
(1,736)	1:62:A:TYR:HA	1:63:A:LEU:HD21	15	0.74
(1,736)	1:62:A:TYR:HA	1:63:A:LEU:HD22	15	0.74
(1,736)	1:62:A:TYR:HA	1:63:A:LEU:HD23	15	0.74
(1,722)	1:61:A:ALA:H	1:81:A:ILE:HA	9	0.74
(1,704)	1:59:A:HIS:H	1:60:A:THR:H	4	0.74
(1,696)	1:57:A:LYS:HA	1:58:A:GLY:HA2	9	0.74
(1,696)	1:57:A:LYS:HA	1:58:A:GLY:HA2	10	0.74
(1,502)	1:38:A:PHE:HD1	1:75:A:PHE:HA	16	0.74
(1,502)	1:38:A:PHE:HD2	1:75:A:PHE:HA	16	0.74
(1,412)	1:33:A:ARG:HB2	1:34:A:SER:H	18	0.74
(1,412)	1:33:A:ARG:HB3	1:34:A:SER:H	18	0.74
(1,298)	1:24:A:LEU:HG	1:80:A:HIS:HE1	13	0.74
(1,295)	1:24:A:LEU:HG	1:25:A:TYR:HA	19	0.74
(1,295)	1:24:A:LEU:HG	1:25:A:TYR:HA	20	0.74
(1,285)	1:24:A:LEU:HA	1:54:A:PHE:HE1	16	0.74
(1,285)	1:24:A:LEU:HA	1:54:A:PHE:HE2	16	0.74
(1,62)	1:6:A:VAL:HA	1:19:A:VAL:HG11	9	0.74
(1,62)	1:6:A:VAL:HA	1:19:A:VAL:HG12	9	0.74
(1,62)	1:6:A:VAL:HA	1:19:A:VAL:HG13	9	0.74
(1,19)	1:5:A:LEU:HB2	1:35:A:ILE:HA	4	0.74
(1,19)	1:5:A:LEU:HB3	1:35:A:ILE:HA	4	0.74
(1,878)	1:75:A:PHE:HB2	1:77:A:TYR:HD1	19	0.73
(1,878)	1:75:A:PHE:HB2	1:77:A:TYR:HD2	19	0.73
(1,878)	1:75:A:PHE:HB3	1:77:A:TYR:HD1	19	0.73
(1,878)	1:75:A:PHE:HB3	1:77:A:TYR:HD2	19	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,843)	1:71:A:ASP:H	1:73:A:LYS:HA	15	0.73
(1,795)	1:66:A:VAL:HA	1:77:A:TYR:HA	17	0.73
(1,789)	1:66:A:VAL:H	1:68:A:VAL:HG11	17	0.73
(1,789)	1:66:A:VAL:H	1:68:A:VAL:HG12	17	0.73
(1,789)	1:66:A:VAL:H	1:68:A:VAL:HG13	17	0.73
(1,713)	1:60:A:THR:HA	1:81:A:ILE:HA	1	0.73
(1,560)	1:47:A:MET:H	1:48:A:LEU:HD11	5	0.73
(1,560)	1:47:A:MET:H	1:48:A:LEU:HD12	5	0.73
(1,560)	1:47:A:MET:H	1:48:A:LEU:HD13	5	0.73
(1,295)	1:24:A:LEU:HG	1:25:A:TYR:HA	7	0.73
(1,128)	1:7:A:LEU:HG	1:38:A:PHE:HD1	18	0.73
(1,128)	1:7:A:LEU:HG	1:38:A:PHE:HD2	18	0.73
(1,906)	1:78:A:GLU:HA	1:79:A:LEU:HG	12	0.72
(1,891)	1:76:A:LEU:HD11	1:77:A:TYR:H	5	0.72
(1,891)	1:76:A:LEU:HD12	1:77:A:TYR:H	5	0.72
(1,891)	1:76:A:LEU:HD13	1:77:A:TYR:H	5	0.72
(1,890)	1:76:A:LEU:HD11	1:78:A:GLU:H	19	0.72
(1,890)	1:76:A:LEU:HD12	1:78:A:GLU:H	19	0.72
(1,890)	1:76:A:LEU:HD13	1:78:A:GLU:H	19	0.72
(1,823)	1:69:A:SER:HA	1:71:A:ASP:H	12	0.72
(1,814)	1:68:A:VAL:HG11	1:73:A:LYS:H	12	0.72
(1,814)	1:68:A:VAL:HG12	1:73:A:LYS:H	12	0.72
(1,814)	1:68:A:VAL:HG13	1:73:A:LYS:H	12	0.72
(1,814)	1:68:A:VAL:HG21	1:73:A:LYS:H	12	0.72
(1,814)	1:68:A:VAL:HG22	1:73:A:LYS:H	12	0.72
(1,814)	1:68:A:VAL:HG23	1:73:A:LYS:H	12	0.72
(1,814)	1:68:A:VAL:HG11	1:73:A:LYS:H	14	0.72
(1,814)	1:68:A:VAL:HG12	1:73:A:LYS:H	14	0.72
(1,814)	1:68:A:VAL:HG13	1:73:A:LYS:H	14	0.72
(1,814)	1:68:A:VAL:HG21	1:73:A:LYS:H	14	0.72
(1,814)	1:68:A:VAL:HG22	1:73:A:LYS:H	14	0.72
(1,814)	1:68:A:VAL:HG23	1:73:A:LYS:H	14	0.72
(1,804)	1:67:A:ARG:H	1:68:A:VAL:HB	3	0.72
(1,736)	1:62:A:TYR:HA	1:63:A:LEU:HD21	10	0.72
(1,736)	1:62:A:TYR:HA	1:63:A:LEU:HD22	10	0.72
(1,736)	1:62:A:TYR:HA	1:63:A:LEU:HD23	10	0.72
(1,683)	1:56:A:GLU:H	1:57:A:LYS:HG3	19	0.72
(1,526)	1:41:A:THR:HB	1:74:A:ASP:HB2	11	0.72
(1,526)	1:41:A:THR:HB	1:74:A:ASP:HB3	11	0.72
(1,525)	1:41:A:THR:HB	1:73:A:LYS:HB2	10	0.72
(1,525)	1:41:A:THR:HB	1:73:A:LYS:HB3	10	0.72
(1,474)	1:37:A:TYR:H	1:76:A:LEU:H	1	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,474)	1:37:A:TYR:H	1:76:A:LEU:H	7	0.72
(1,458)	1:36:A:PHE:HA	1:76:A:LEU:HD11	17	0.72
(1,458)	1:36:A:PHE:HA	1:76:A:LEU:HD12	17	0.72
(1,458)	1:36:A:PHE:HA	1:76:A:LEU:HD13	17	0.72
(1,449)	1:35:A:ILE:HD11	1:37:A:TYR:HD1	13	0.72
(1,449)	1:35:A:ILE:HD11	1:37:A:TYR:HD2	13	0.72
(1,449)	1:35:A:ILE:HD12	1:37:A:TYR:HD1	13	0.72
(1,449)	1:35:A:ILE:HD12	1:37:A:TYR:HD2	13	0.72
(1,449)	1:35:A:ILE:HD13	1:37:A:TYR:HD1	13	0.72
(1,449)	1:35:A:ILE:HD13	1:37:A:TYR:HD2	13	0.72
(1,441)	1:35:A:ILE:HB	1:37:A:TYR:HA	15	0.72
(1,364)	1:28:A:PHE:HD1	1:32:A:LYS:HA	4	0.72
(1,364)	1:28:A:PHE:HD2	1:32:A:LYS:HA	4	0.72
(1,285)	1:24:A:LEU:HA	1:54:A:PHE:HE1	4	0.72
(1,285)	1:24:A:LEU:HA	1:54:A:PHE:HE2	4	0.72
(1,240)	1:21:A:LEU:HG	1:57:A:LYS:HB2	19	0.72
(1,240)	1:21:A:LEU:HG	1:57:A:LYS:HB3	19	0.72
(1,28)	1:5:A:LEU:HG	1:7:A:LEU:HG	2	0.72
(1,21)	1:5:A:LEU:HB2	1:36:A:PHE:H	6	0.72
(1,21)	1:5:A:LEU:HB3	1:36:A:PHE:H	6	0.72
(1,4)	1:4:A:LYS:HA	1:5:A:LEU:H	16	0.72
(1,865)	1:74:A:ASP:H	1:75:A:PHE:H	16	0.71
(1,842)	1:71:A:ASP:H	1:73:A:LYS:H	1	0.71
(1,789)	1:66:A:VAL:H	1:68:A:VAL:HG11	20	0.71
(1,789)	1:66:A:VAL:H	1:68:A:VAL:HG12	20	0.71
(1,789)	1:66:A:VAL:H	1:68:A:VAL:HG13	20	0.71
(1,743)	1:62:A:TYR:HE1	1:63:A:LEU:HD21	2	0.71
(1,743)	1:62:A:TYR:HE1	1:63:A:LEU:HD22	2	0.71
(1,743)	1:62:A:TYR:HE1	1:63:A:LEU:HD23	2	0.71
(1,743)	1:62:A:TYR:HE2	1:63:A:LEU:HD21	2	0.71
(1,743)	1:62:A:TYR:HE2	1:63:A:LEU:HD22	2	0.71
(1,743)	1:62:A:TYR:HE2	1:63:A:LEU:HD23	2	0.71
(1,743)	1:62:A:TYR:HE1	1:63:A:LEU:HD21	10	0.71
(1,743)	1:62:A:TYR:HE1	1:63:A:LEU:HD22	10	0.71
(1,743)	1:62:A:TYR:HE1	1:63:A:LEU:HD23	10	0.71
(1,743)	1:62:A:TYR:HE2	1:63:A:LEU:HD21	10	0.71
(1,743)	1:62:A:TYR:HE2	1:63:A:LEU:HD22	10	0.71
(1,743)	1:62:A:TYR:HE2	1:63:A:LEU:HD23	10	0.71
(1,739)	1:62:A:TYR:HB2	1:79:A:LEU:HG	10	0.71
(1,739)	1:62:A:TYR:HB3	1:79:A:LEU:HG	10	0.71
(1,736)	1:62:A:TYR:HA	1:63:A:LEU:HD21	16	0.71
(1,736)	1:62:A:TYR:HA	1:63:A:LEU:HD22	16	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,736)	1:62:A:TYR:HA	1:63:A:LEU:HD23	16	0.71
(1,736)	1:62:A:TYR:HA	1:63:A:LEU:HD21	17	0.71
(1,736)	1:62:A:TYR:HA	1:63:A:LEU:HD22	17	0.71
(1,736)	1:62:A:TYR:HA	1:63:A:LEU:HD23	17	0.71
(1,676)	1:55:A:LYS:HA	1:58:A:GLY:HA2	2	0.71
(1,544)	1:44:A:HIS:HA	1:48:A:LEU:HD11	6	0.71
(1,544)	1:44:A:HIS:HA	1:48:A:LEU:HD12	6	0.71
(1,544)	1:44:A:HIS:HA	1:48:A:LEU:HD13	6	0.71
(1,544)	1:44:A:HIS:HA	1:48:A:LEU:HD11	6	0.71
(1,544)	1:44:A:HIS:HA	1:48:A:LEU:HD12	6	0.71
(1,544)	1:44:A:HIS:HA	1:48:A:LEU:HD13	6	0.71
(1,544)	1:44:A:HIS:HA	1:48:A:LEU:HD11	9	0.71
(1,544)	1:44:A:HIS:HA	1:48:A:LEU:HD12	9	0.71
(1,544)	1:44:A:HIS:HA	1:48:A:LEU:HD13	9	0.71
(1,544)	1:44:A:HIS:HA	1:48:A:LEU:HD11	9	0.71
(1,544)	1:44:A:HIS:HA	1:48:A:LEU:HD12	9	0.71
(1,544)	1:44:A:HIS:HA	1:48:A:LEU:HD13	9	0.71
(1,526)	1:41:A:THR:HB	1:74:A:ASP:HB2	5	0.71
(1,526)	1:41:A:THR:HB	1:74:A:ASP:HB3	5	0.71
(1,526)	1:41:A:THR:HB	1:74:A:ASP:HB2	20	0.71
(1,526)	1:41:A:THR:HB	1:74:A:ASP:HB3	20	0.71
(1,502)	1:38:A:PHE:HD1	1:75:A:PHE:HA	3	0.71
(1,502)	1:38:A:PHE:HD2	1:75:A:PHE:HA	3	0.71
(1,412)	1:33:A:ARG:HB2	1:34:A:SER:H	11	0.71
(1,412)	1:33:A:ARG:HB3	1:34:A:SER:H	11	0.71
(1,410)	1:33:A:ARG:HA	1:81:A:ILE:HG21	8	0.71
(1,410)	1:33:A:ARG:HA	1:81:A:ILE:HG22	8	0.71
(1,410)	1:33:A:ARG:HA	1:81:A:ILE:HG23	8	0.71
(1,364)	1:28:A:PHE:HD1	1:32:A:LYS:HA	17	0.71
(1,364)	1:28:A:PHE:HD2	1:32:A:LYS:HA	17	0.71
(1,301)	1:24:A:LEU:HD11	1:60:A:THR:HB	20	0.71
(1,301)	1:24:A:LEU:HD12	1:60:A:THR:HB	20	0.71
(1,301)	1:24:A:LEU:HD13	1:60:A:THR:HB	20	0.71
(1,923)	1:79:A:LEU:HD11	1:82:A:ILE:HD11	11	0.7
(1,923)	1:79:A:LEU:HD11	1:82:A:ILE:HD12	11	0.7
(1,923)	1:79:A:LEU:HD11	1:82:A:ILE:HD13	11	0.7
(1,923)	1:79:A:LEU:HD12	1:82:A:ILE:HD11	11	0.7
(1,923)	1:79:A:LEU:HD12	1:82:A:ILE:HD12	11	0.7
(1,923)	1:79:A:LEU:HD12	1:82:A:ILE:HD13	11	0.7
(1,923)	1:79:A:LEU:HD13	1:82:A:ILE:HD11	11	0.7
(1,923)	1:79:A:LEU:HD13	1:82:A:ILE:HD12	11	0.7
(1,923)	1:79:A:LEU:HD13	1:82:A:ILE:HD13	11	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,859)	1:72:A:GLU:HB2	1:74:A:ASP:HA	7	0.7
(1,859)	1:72:A:GLU:HB3	1:74:A:ASP:HA	7	0.7
(1,795)	1:66:A:VAL:HA	1:77:A:TYR:HA	5	0.7
(1,775)	1:65:A:GLU:H	1:76:A:LEU:HD11	10	0.7
(1,775)	1:65:A:GLU:H	1:76:A:LEU:HD12	10	0.7
(1,775)	1:65:A:GLU:H	1:76:A:LEU:HD13	10	0.7
(1,775)	1:65:A:GLU:H	1:76:A:LEU:HD21	10	0.7
(1,467)	1:36:A:PHE:HB2	1:77:A:TYR:HD1	19	0.7
(1,467)	1:36:A:PHE:HB2	1:77:A:TYR:HD2	19	0.7
(1,467)	1:36:A:PHE:HB3	1:77:A:TYR:HD1	19	0.7
(1,467)	1:36:A:PHE:HB3	1:77:A:TYR:HD2	19	0.7
(1,411)	1:33:A:ARG:HA	1:82:A:ILE:HA	10	0.7
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG21	8	0.7
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG22	8	0.7
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG23	8	0.7
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG21	8	0.7
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG22	8	0.7
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG23	8	0.7
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG21	8	0.7
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG22	8	0.7
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG23	8	0.7
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG21	8	0.7
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG22	8	0.7
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG23	8	0.7
(1,300)	1:24:A:LEU:HD11	1:35:A:ILE:HG12	13	0.7
(1,300)	1:24:A:LEU:HD11	1:35:A:ILE:HG13	13	0.7
(1,300)	1:24:A:LEU:HD12	1:35:A:ILE:HG12	13	0.7
(1,300)	1:24:A:LEU:HD12	1:35:A:ILE:HG13	13	0.7
(1,300)	1:24:A:LEU:HD13	1:35:A:ILE:HG12	13	0.7
(1,300)	1:24:A:LEU:HD13	1:35:A:ILE:HG13	13	0.7
(1,285)	1:24:A:LEU:HA	1:54:A:PHE:HE1	15	0.7
(1,285)	1:24:A:LEU:HA	1:54:A:PHE:HE2	15	0.7
(1,240)	1:21:A:LEU:HG	1:57:A:LYS:HB2	7	0.7
(1,240)	1:21:A:LEU:HG	1:57:A:LYS:HB3	7	0.7
(1,36)	1:5:A:LEU:HD11	1:7:A:LEU:HD11	16	0.7
(1,36)	1:5:A:LEU:HD11	1:7:A:LEU:HD12	16	0.7
(1,36)	1:5:A:LEU:HD11	1:7:A:LEU:HD13	16	0.7
(1,36)	1:5:A:LEU:HD12	1:7:A:LEU:HD11	16	0.7
(1,36)	1:5:A:LEU:HD12	1:7:A:LEU:HD12	16	0.7
(1,36)	1:5:A:LEU:HD12	1:7:A:LEU:HD13	16	0.7
(1,36)	1:5:A:LEU:HD13	1:7:A:LEU:HD11	16	0.7
(1,36)	1:5:A:LEU:HD13	1:7:A:LEU:HD12	16	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,36)	1:5:A:LEU:HD13	1:7:A:LEU:HD13	16	0.7
(1,36)	1:5:A:LEU:HD21	1:7:A:LEU:HD11	16	0.7
(1,36)	1:5:A:LEU:HD21	1:7:A:LEU:HD12	16	0.7
(1,36)	1:5:A:LEU:HD21	1:7:A:LEU:HD13	16	0.7
(1,36)	1:5:A:LEU:HD22	1:7:A:LEU:HD11	16	0.7
(1,36)	1:5:A:LEU:HD22	1:7:A:LEU:HD12	16	0.7
(1,36)	1:5:A:LEU:HD22	1:7:A:LEU:HD13	16	0.7
(1,36)	1:5:A:LEU:HD23	1:7:A:LEU:HD11	16	0.7
(1,36)	1:5:A:LEU:HD23	1:7:A:LEU:HD12	16	0.7
(1,36)	1:5:A:LEU:HD23	1:7:A:LEU:HD13	16	0.7
(1,891)	1:76:A:LEU:HD11	1:77:A:TYR:H	14	0.69
(1,891)	1:76:A:LEU:HD12	1:77:A:TYR:H	14	0.69
(1,891)	1:76:A:LEU:HD13	1:77:A:TYR:H	14	0.69
(1,842)	1:71:A:ASP:H	1:73:A:LYS:H	2	0.69
(1,836)	1:70:A:THR:HA	1:73:A:LYS:HB2	15	0.69
(1,836)	1:70:A:THR:HA	1:73:A:LYS:HB3	15	0.69
(1,824)	1:69:A:SER:HA	1:74:A:ASP:H	16	0.69
(1,800)	1:66:A:VAL:HG11	1:72:A:GLU:H	17	0.69
(1,800)	1:66:A:VAL:HG12	1:72:A:GLU:H	17	0.69
(1,800)	1:66:A:VAL:HG13	1:72:A:GLU:H	17	0.69
(1,800)	1:66:A:VAL:HG21	1:72:A:GLU:H	17	0.69
(1,800)	1:66:A:VAL:HG22	1:72:A:GLU:H	17	0.69
(1,800)	1:66:A:VAL:HG23	1:72:A:GLU:H	17	0.69
(1,795)	1:66:A:VAL:HA	1:77:A:TYR:HA	8	0.69
(1,736)	1:62:A:TYR:HA	1:63:A:LEU:HD21	19	0.69
(1,736)	1:62:A:TYR:HA	1:63:A:LEU:HD22	19	0.69
(1,736)	1:62:A:TYR:HA	1:63:A:LEU:HD23	19	0.69
(1,722)	1:61:A:ALA:H	1:81:A:ILE:HA	1	0.69
(1,721)	1:61:A:ALA:H	1:78:A:GLU:HB2	8	0.69
(1,721)	1:61:A:ALA:H	1:78:A:GLU:HB3	8	0.69
(1,713)	1:60:A:THR:HA	1:81:A:ILE:HA	9	0.69
(1,712)	1:60:A:THR:HA	1:81:A:ILE:H	9	0.69
(1,560)	1:47:A:MET:H	1:48:A:LEU:HD11	6	0.69
(1,560)	1:47:A:MET:H	1:48:A:LEU:HD12	6	0.69
(1,560)	1:47:A:MET:H	1:48:A:LEU:HD13	6	0.69
(1,560)	1:47:A:MET:H	1:48:A:LEU:HD11	12	0.69
(1,560)	1:47:A:MET:H	1:48:A:LEU:HD12	12	0.69
(1,560)	1:47:A:MET:H	1:48:A:LEU:HD13	12	0.69
(1,525)	1:41:A:THR:HB	1:73:A:LYS:HB2	19	0.69
(1,525)	1:41:A:THR:HB	1:73:A:LYS:HB3	19	0.69
(1,501)	1:38:A:PHE:HD1	1:75:A:PHE:H	6	0.69
(1,501)	1:38:A:PHE:HD2	1:75:A:PHE:H	6	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,437)	1:35:A:ILE:H	1:80:A:HIS:H	13	0.69
(1,356)	1:28:A:PHE:HA	1:33:A:ARG:H	2	0.69
(1,288)	1:24:A:LEU:HA	1:80:A:HIS:HE1	8	0.69
(1,240)	1:21:A:LEU:HG	1:57:A:LYS:HB2	15	0.69
(1,240)	1:21:A:LEU:HG	1:57:A:LYS:HB3	15	0.69
(1,144)	1:9:A:LYS:H	1:10:A:ASN:H	14	0.69
(1,128)	1:7:A:LEU:HG	1:38:A:PHE:HD1	9	0.69
(1,128)	1:7:A:LEU:HG	1:38:A:PHE:HD2	9	0.69
(1,917)	1:79:A:LEU:HB2	1:80:A:HIS:HD2	13	0.68
(1,917)	1:79:A:LEU:HB3	1:80:A:HIS:HD2	13	0.68
(1,891)	1:76:A:LEU:HD11	1:77:A:TYR:H	16	0.68
(1,891)	1:76:A:LEU:HD12	1:77:A:TYR:H	16	0.68
(1,891)	1:76:A:LEU:HD13	1:77:A:TYR:H	16	0.68
(1,843)	1:71:A:ASP:H	1:73:A:LYS:HA	12	0.68
(1,800)	1:66:A:VAL:HG11	1:72:A:GLU:H	5	0.68
(1,800)	1:66:A:VAL:HG12	1:72:A:GLU:H	5	0.68
(1,800)	1:66:A:VAL:HG13	1:72:A:GLU:H	5	0.68
(1,800)	1:66:A:VAL:HG21	1:72:A:GLU:H	5	0.68
(1,800)	1:66:A:VAL:HG22	1:72:A:GLU:H	5	0.68
(1,800)	1:66:A:VAL:HG23	1:72:A:GLU:H	5	0.68
(1,795)	1:66:A:VAL:HA	1:77:A:TYR:HA	11	0.68
(1,781)	1:65:A:GLU:HA	1:77:A:TYR:HD1	9	0.68
(1,781)	1:65:A:GLU:HA	1:77:A:TYR:HD2	9	0.68
(1,739)	1:62:A:TYR:HB2	1:79:A:LEU:HG	8	0.68
(1,739)	1:62:A:TYR:HB3	1:79:A:LEU:HG	8	0.68
(1,736)	1:62:A:TYR:HA	1:63:A:LEU:HD21	3	0.68
(1,736)	1:62:A:TYR:HA	1:63:A:LEU:HD22	3	0.68
(1,736)	1:62:A:TYR:HA	1:63:A:LEU:HD23	3	0.68
(1,704)	1:59:A:HIS:H	1:60:A:THR:H	13	0.68
(1,566)	1:47:A:MET:HB2	1:48:A:LEU:H	16	0.68
(1,566)	1:47:A:MET:HB3	1:48:A:LEU:H	16	0.68
(1,560)	1:47:A:MET:H	1:48:A:LEU:HD11	20	0.68
(1,560)	1:47:A:MET:H	1:48:A:LEU:HD12	20	0.68
(1,560)	1:47:A:MET:H	1:48:A:LEU:HD13	20	0.68
(1,547)	1:44:A:HIS:HB2	1:48:A:LEU:HD11	1	0.68
(1,547)	1:44:A:HIS:HB2	1:48:A:LEU:HD12	1	0.68
(1,547)	1:44:A:HIS:HB2	1:48:A:LEU:HD13	1	0.68
(1,547)	1:44:A:HIS:HB3	1:48:A:LEU:HD11	1	0.68
(1,547)	1:44:A:HIS:HB3	1:48:A:LEU:HD12	1	0.68
(1,547)	1:44:A:HIS:HB3	1:48:A:LEU:HD13	1	0.68
(1,502)	1:38:A:PHE:HD1	1:75:A:PHE:HA	8	0.68
(1,502)	1:38:A:PHE:HD2	1:75:A:PHE:HA	8	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,426)	1:34:A:SER:HB2	1:36:A:PHE:HE1	19	0.68
(1,426)	1:34:A:SER:HB2	1:36:A:PHE:HE2	19	0.68
(1,426)	1:34:A:SER:HB3	1:36:A:PHE:HE1	19	0.68
(1,426)	1:34:A:SER:HB3	1:36:A:PHE:HE2	19	0.68
(1,418)	1:34:A:SER:H	1:79:A:LEU:HD21	10	0.68
(1,418)	1:34:A:SER:H	1:79:A:LEU:HD22	10	0.68
(1,418)	1:34:A:SER:H	1:79:A:LEU:HD23	10	0.68
(1,364)	1:28:A:PHE:HD1	1:32:A:LYS:HA	20	0.68
(1,364)	1:28:A:PHE:HD2	1:32:A:LYS:HA	20	0.68
(1,312)	1:25:A:TYR:H	1:59:A:HIS:HE1	15	0.68
(1,299)	1:24:A:LEU:HD11	1:35:A:ILE:HG21	3	0.68
(1,299)	1:24:A:LEU:HD11	1:35:A:ILE:HG22	3	0.68
(1,299)	1:24:A:LEU:HD11	1:35:A:ILE:HG23	3	0.68
(1,299)	1:24:A:LEU:HD12	1:35:A:ILE:HG21	3	0.68
(1,299)	1:24:A:LEU:HD12	1:35:A:ILE:HG22	3	0.68
(1,299)	1:24:A:LEU:HD12	1:35:A:ILE:HG23	3	0.68
(1,299)	1:24:A:LEU:HD13	1:35:A:ILE:HG21	3	0.68
(1,299)	1:24:A:LEU:HD13	1:35:A:ILE:HG22	3	0.68
(1,299)	1:24:A:LEU:HD13	1:35:A:ILE:HG23	3	0.68
(1,295)	1:24:A:LEU:HG	1:25:A:TYR:HA	10	0.68
(1,182)	1:14:A:SER:H	1:17:A:LYS:H	3	0.68
(1,177)	1:13:A:LYS:H	1:16:A:ALA:H	5	0.68
(1,147)	1:9:A:LYS:H	1:11:A:THR:H	11	0.68
(1,146)	1:9:A:LYS:H	1:10:A:ASN:HB2	17	0.68
(1,146)	1:9:A:LYS:H	1:10:A:ASN:HB3	17	0.68
(1,123)	1:7:A:LEU:HB2	1:38:A:PHE:HD1	7	0.68
(1,123)	1:7:A:LEU:HB2	1:38:A:PHE:HD2	7	0.68
(1,123)	1:7:A:LEU:HB3	1:38:A:PHE:HD1	7	0.68
(1,123)	1:7:A:LEU:HB3	1:38:A:PHE:HD2	7	0.68
(1,123)	1:7:A:LEU:HB2	1:38:A:PHE:HD1	15	0.68
(1,123)	1:7:A:LEU:HB2	1:38:A:PHE:HD2	15	0.68
(1,123)	1:7:A:LEU:HB3	1:38:A:PHE:HD1	15	0.68
(1,123)	1:7:A:LEU:HB3	1:38:A:PHE:HD2	15	0.68
(1,1)	1:3:A:MET:H	1:4:A:LYS:H	14	0.68
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG21	14	0.67
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG22	14	0.67
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG23	14	0.67
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG21	14	0.67
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG22	14	0.67
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG23	14	0.67
(1,800)	1:66:A:VAL:HG11	1:72:A:GLU:H	1	0.67
(1,800)	1:66:A:VAL:HG12	1:72:A:GLU:H	1	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,800)	1:66:A:VAL:HG13	1:72:A:GLU:H	1	0.67
(1,800)	1:66:A:VAL:HG21	1:72:A:GLU:H	1	0.67
(1,800)	1:66:A:VAL:HG22	1:72:A:GLU:H	1	0.67
(1,800)	1:66:A:VAL:HG23	1:72:A:GLU:H	1	0.67
(1,795)	1:66:A:VAL:HA	1:77:A:TYR:HA	6	0.67
(1,785)	1:65:A:GLU:HB2	1:69:A:SER:HB2	3	0.67
(1,785)	1:65:A:GLU:HB2	1:69:A:SER:HB3	3	0.67
(1,785)	1:65:A:GLU:HB3	1:69:A:SER:HB2	3	0.67
(1,785)	1:65:A:GLU:HB3	1:69:A:SER:HB3	3	0.67
(1,781)	1:65:A:GLU:HA	1:77:A:TYR:HD1	18	0.67
(1,781)	1:65:A:GLU:HA	1:77:A:TYR:HD2	18	0.67
(1,736)	1:62:A:TYR:HA	1:63:A:LEU:HD21	20	0.67
(1,736)	1:62:A:TYR:HA	1:63:A:LEU:HD22	20	0.67
(1,736)	1:62:A:TYR:HA	1:63:A:LEU:HD23	20	0.67
(1,690)	1:56:A:GLU:CD	1:52:A:ASP:CG	4	0.67
(1,560)	1:47:A:MET:H	1:48:A:LEU:HD11	10	0.67
(1,560)	1:47:A:MET:H	1:48:A:LEU:HD12	10	0.67
(1,560)	1:47:A:MET:H	1:48:A:LEU:HD13	10	0.67
(1,467)	1:36:A:PHE:HB2	1:77:A:TYR:HD1	18	0.67
(1,467)	1:36:A:PHE:HB2	1:77:A:TYR:HD2	18	0.67
(1,467)	1:36:A:PHE:HB3	1:77:A:TYR:HD1	18	0.67
(1,467)	1:36:A:PHE:HB3	1:77:A:TYR:HD2	18	0.67
(1,458)	1:36:A:PHE:HA	1:76:A:LEU:HD11	3	0.67
(1,458)	1:36:A:PHE:HA	1:76:A:LEU:HD12	3	0.67
(1,458)	1:36:A:PHE:HA	1:76:A:LEU:HD13	3	0.67
(1,431)	1:35:A:ILE:H	1:36:A:PHE:HD1	9	0.67
(1,431)	1:35:A:ILE:H	1:36:A:PHE:HD2	9	0.67
(1,366)	1:28:A:PHE:HD1	1:80:A:HIS:HB2	6	0.67
(1,366)	1:28:A:PHE:HD1	1:80:A:HIS:HB3	6	0.67
(1,366)	1:28:A:PHE:HD2	1:80:A:HIS:HB2	6	0.67
(1,366)	1:28:A:PHE:HD2	1:80:A:HIS:HB3	6	0.67
(1,365)	1:28:A:PHE:HD1	1:32:A:LYS:HB2	5	0.67
(1,365)	1:28:A:PHE:HD1	1:32:A:LYS:HB3	5	0.67
(1,365)	1:28:A:PHE:HD2	1:32:A:LYS:HB2	5	0.67
(1,365)	1:28:A:PHE:HD2	1:32:A:LYS:HB3	5	0.67
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG21	16	0.67
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG22	16	0.67
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG23	16	0.67
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG21	16	0.67
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG22	16	0.67
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG23	16	0.67
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG21	16	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG22	16	0.67
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG23	16	0.67
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG21	16	0.67
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG22	16	0.67
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG23	16	0.67
(1,299)	1:24:A:LEU:HD11	1:35:A:ILE:HG21	8	0.67
(1,299)	1:24:A:LEU:HD11	1:35:A:ILE:HG22	8	0.67
(1,299)	1:24:A:LEU:HD11	1:35:A:ILE:HG23	8	0.67
(1,299)	1:24:A:LEU:HD12	1:35:A:ILE:HG21	8	0.67
(1,299)	1:24:A:LEU:HD12	1:35:A:ILE:HG22	8	0.67
(1,299)	1:24:A:LEU:HD12	1:35:A:ILE:HG23	8	0.67
(1,299)	1:24:A:LEU:HD13	1:35:A:ILE:HG21	8	0.67
(1,299)	1:24:A:LEU:HD13	1:35:A:ILE:HG22	8	0.67
(1,299)	1:24:A:LEU:HD13	1:35:A:ILE:HG23	8	0.67
(1,288)	1:24:A:LEU:HA	1:80:A:HIS:HE1	10	0.67
(1,174)	1:12:A:ARG:HB2	1:14:A:SER:HA	4	0.67
(1,174)	1:12:A:ARG:HB3	1:14:A:SER:HA	4	0.67
(1,123)	1:7:A:LEU:HB2	1:38:A:PHE:HD1	4	0.67
(1,123)	1:7:A:LEU:HB2	1:38:A:PHE:HD2	4	0.67
(1,123)	1:7:A:LEU:HB3	1:38:A:PHE:HD1	4	0.67
(1,123)	1:7:A:LEU:HB3	1:38:A:PHE:HD2	4	0.67
(1,1)	1:3:A:MET:H	1:4:A:LYS:H	5	0.67
(1,893)	1:76:A:LEU:HD11	1:78:A:GLU:HG2	4	0.66
(1,893)	1:76:A:LEU:HD11	1:78:A:GLU:HG3	4	0.66
(1,893)	1:76:A:LEU:HD12	1:78:A:GLU:HG2	4	0.66
(1,893)	1:76:A:LEU:HD12	1:78:A:GLU:HG3	4	0.66
(1,893)	1:76:A:LEU:HD13	1:78:A:GLU:HG2	4	0.66
(1,893)	1:76:A:LEU:HD13	1:78:A:GLU:HG3	4	0.66
(1,892)	1:76:A:LEU:HD11	1:78:A:GLU:HA	15	0.66
(1,892)	1:76:A:LEU:HD12	1:78:A:GLU:HA	15	0.66
(1,892)	1:76:A:LEU:HD13	1:78:A:GLU:HA	15	0.66
(1,843)	1:71:A:ASP:H	1:73:A:LYS:HA	16	0.66
(1,795)	1:66:A:VAL:HA	1:77:A:TYR:HA	14	0.66
(1,739)	1:62:A:TYR:HB2	1:79:A:LEU:HG	15	0.66
(1,739)	1:62:A:TYR:HB3	1:79:A:LEU:HG	15	0.66
(1,713)	1:60:A:THR:HA	1:81:A:ILE:HA	19	0.66
(1,501)	1:38:A:PHE:HD1	1:75:A:PHE:H	9	0.66
(1,501)	1:38:A:PHE:HD2	1:75:A:PHE:H	9	0.66
(1,467)	1:36:A:PHE:HB2	1:77:A:TYR:HD1	2	0.66
(1,467)	1:36:A:PHE:HB2	1:77:A:TYR:HD2	2	0.66
(1,467)	1:36:A:PHE:HB3	1:77:A:TYR:HD1	2	0.66
(1,467)	1:36:A:PHE:HB3	1:77:A:TYR:HD2	2	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,312)	1:25:A:TYR:H	1:59:A:HIS:HE1	19	0.66
(1,304)	1:24:A:LEU:HD21	1:59:A:HIS:HE1	6	0.66
(1,304)	1:24:A:LEU:HD22	1:59:A:HIS:HE1	6	0.66
(1,304)	1:24:A:LEU:HD23	1:59:A:HIS:HE1	6	0.66
(1,166)	1:11:A:THR:HB	1:12:A:ARG:H	16	0.66
(1,128)	1:7:A:LEU:HG	1:38:A:PHE:HD1	8	0.66
(1,128)	1:7:A:LEU:HG	1:38:A:PHE:HD2	8	0.66
(1,892)	1:76:A:LEU:HD11	1:78:A:GLU:HA	3	0.65
(1,892)	1:76:A:LEU:HD12	1:78:A:GLU:HA	3	0.65
(1,892)	1:76:A:LEU:HD13	1:78:A:GLU:HA	3	0.65
(1,859)	1:72:A:GLU:HB2	1:74:A:ASP:HA	17	0.65
(1,859)	1:72:A:GLU:HB3	1:74:A:ASP:HA	17	0.65
(1,842)	1:71:A:ASP:H	1:73:A:LYS:H	12	0.65
(1,795)	1:66:A:VAL:HA	1:77:A:TYR:HA	3	0.65
(1,712)	1:60:A:THR:HA	1:81:A:ILE:H	1	0.65
(1,704)	1:59:A:HIS:H	1:60:A:THR:H	3	0.65
(1,704)	1:59:A:HIS:H	1:60:A:THR:H	6	0.65
(1,526)	1:41:A:THR:HB	1:74:A:ASP:HB2	4	0.65
(1,526)	1:41:A:THR:HB	1:74:A:ASP:HB3	4	0.65
(1,495)	1:38:A:PHE:HA	1:75:A:PHE:HD1	10	0.65
(1,495)	1:38:A:PHE:HA	1:75:A:PHE:HD2	10	0.65
(1,395)	1:31:A:ASP:HA	1:81:A:ILE:HG21	20	0.65
(1,395)	1:31:A:ASP:HA	1:81:A:ILE:HG22	20	0.65
(1,395)	1:31:A:ASP:HA	1:81:A:ILE:HG23	20	0.65
(1,390)	1:31:A:ASP:H	1:81:A:ILE:HG21	1	0.65
(1,390)	1:31:A:ASP:H	1:81:A:ILE:HG22	1	0.65
(1,390)	1:31:A:ASP:H	1:81:A:ILE:HG23	1	0.65
(1,298)	1:24:A:LEU:HG	1:80:A:HIS:HE1	19	0.65
(1,295)	1:24:A:LEU:HG	1:25:A:TYR:HA	13	0.65
(1,285)	1:24:A:LEU:HA	1:54:A:PHE:HE1	11	0.65
(1,285)	1:24:A:LEU:HA	1:54:A:PHE:HE2	11	0.65
(1,240)	1:21:A:LEU:HG	1:57:A:LYS:HB2	13	0.65
(1,240)	1:21:A:LEU:HG	1:57:A:LYS:HB3	13	0.65
(1,182)	1:14:A:SER:H	1:17:A:LYS:H	6	0.65
(1,166)	1:11:A:THR:HB	1:12:A:ARG:H	6	0.65
(1,893)	1:76:A:LEU:HD11	1:78:A:GLU:HG2	3	0.64
(1,893)	1:76:A:LEU:HD11	1:78:A:GLU:HG3	3	0.64
(1,893)	1:76:A:LEU:HD12	1:78:A:GLU:HG2	3	0.64
(1,893)	1:76:A:LEU:HD12	1:78:A:GLU:HG3	3	0.64
(1,893)	1:76:A:LEU:HD13	1:78:A:GLU:HG2	3	0.64
(1,893)	1:76:A:LEU:HD13	1:78:A:GLU:HG3	3	0.64
(1,892)	1:76:A:LEU:HD11	1:78:A:GLU:HA	10	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,892)	1:76:A:LEU:HD12	1:78:A:GLU:HA	10	0.64
(1,892)	1:76:A:LEU:HD13	1:78:A:GLU:HA	10	0.64
(1,890)	1:76:A:LEU:HD11	1:78:A:GLU:H	13	0.64
(1,890)	1:76:A:LEU:HD12	1:78:A:GLU:H	13	0.64
(1,890)	1:76:A:LEU:HD13	1:78:A:GLU:H	13	0.64
(1,798)	1:66:A:VAL:HG11	1:69:A:SER:HA	9	0.64
(1,798)	1:66:A:VAL:HG12	1:69:A:SER:HA	9	0.64
(1,798)	1:66:A:VAL:HG13	1:69:A:SER:HA	9	0.64
(1,798)	1:66:A:VAL:HG21	1:69:A:SER:HA	9	0.64
(1,798)	1:66:A:VAL:HG22	1:69:A:SER:HA	9	0.64
(1,798)	1:66:A:VAL:HG23	1:69:A:SER:HA	9	0.64
(1,712)	1:60:A:THR:HA	1:81:A:ILE:H	19	0.64
(1,705)	1:59:A:HIS:H	1:60:A:THR:HA	14	0.64
(1,704)	1:59:A:HIS:H	1:60:A:THR:H	5	0.64
(1,683)	1:56:A:GLU:H	1:57:A:LYS:HG3	9	0.64
(1,538)	1:43:A:ALA:HA	1:45:A:LYS:HD2	1	0.64
(1,538)	1:43:A:ALA:HA	1:45:A:LYS:HD3	1	0.64
(1,501)	1:38:A:PHE:HD1	1:75:A:PHE:H	20	0.64
(1,501)	1:38:A:PHE:HD2	1:75:A:PHE:H	20	0.64
(1,316)	1:25:A:TYR:HA	1:29:A:SER:H	9	0.64
(1,22)	1:5:A:LEU:HB2	1:36:A:PHE:HA	16	0.64
(1,22)	1:5:A:LEU:HB3	1:36:A:PHE:HA	16	0.64
(1,20)	1:5:A:LEU:HB2	1:35:A:ILE:HB	13	0.64
(1,20)	1:5:A:LEU:HB3	1:35:A:ILE:HB	13	0.64
(1,1)	1:3:A:MET:H	1:4:A:LYS:H	2	0.64
(1,931)	1:81:A:ILE:HA	1:82:A:ILE:HA	8	0.63
(1,931)	1:81:A:ILE:HA	1:82:A:ILE:HA	20	0.63
(1,865)	1:74:A:ASP:H	1:75:A:PHE:H	4	0.63
(1,802)	1:67:A:ARG:H	1:68:A:VAL:H	12	0.63
(1,794)	1:66:A:VAL:HA	1:77:A:TYR:H	4	0.63
(1,768)	1:64:A:ASP:HA	1:76:A:LEU:HD21	20	0.63
(1,768)	1:64:A:ASP:HA	1:76:A:LEU:HD22	20	0.63
(1,768)	1:64:A:ASP:HA	1:76:A:LEU:HD23	20	0.63
(1,721)	1:61:A:ALA:H	1:78:A:GLU:HB2	11	0.63
(1,721)	1:61:A:ALA:H	1:78:A:GLU:HB3	11	0.63
(1,705)	1:59:A:HIS:H	1:60:A:THR:HA	4	0.63
(1,705)	1:59:A:HIS:H	1:60:A:THR:HA	11	0.63
(1,704)	1:59:A:HIS:H	1:60:A:THR:H	15	0.63
(1,683)	1:56:A:GLU:H	1:57:A:LYS:HG3	18	0.63
(1,449)	1:35:A:ILE:HD11	1:37:A:TYR:HD1	15	0.63
(1,449)	1:35:A:ILE:HD11	1:37:A:TYR:HD2	15	0.63
(1,449)	1:35:A:ILE:HD12	1:37:A:TYR:HD1	15	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,449)	1:35:A:ILE:HD12	1:37:A:TYR:HD2	15	0.63
(1,449)	1:35:A:ILE:HD13	1:37:A:TYR:HD1	15	0.63
(1,449)	1:35:A:ILE:HD13	1:37:A:TYR:HD2	15	0.63
(1,322)	1:25:A:TYR:HD1	1:28:A:PHE:H	2	0.63
(1,322)	1:25:A:TYR:HD2	1:28:A:PHE:H	2	0.63
(1,322)	1:25:A:TYR:HD1	1:28:A:PHE:H	18	0.63
(1,322)	1:25:A:TYR:HD2	1:28:A:PHE:H	18	0.63
(1,245)	1:21:A:LEU:HD11	1:53:A:PHE:HA	16	0.63
(1,245)	1:21:A:LEU:HD12	1:53:A:PHE:HA	16	0.63
(1,245)	1:21:A:LEU:HD13	1:53:A:PHE:HA	16	0.63
(1,128)	1:7:A:LEU:HG	1:38:A:PHE:HD1	16	0.63
(1,128)	1:7:A:LEU:HG	1:38:A:PHE:HD2	16	0.63
(1,102)	1:7:A:LEU:H	1:19:A:VAL:HB	9	0.63
(3,1)	1:39:A:ALA:HB1	1:47:A:MET:N	3	0.62
(1,891)	1:76:A:LEU:HD11	1:77:A:TYR:H	18	0.62
(1,891)	1:76:A:LEU:HD12	1:77:A:TYR:H	18	0.62
(1,891)	1:76:A:LEU:HD13	1:77:A:TYR:H	18	0.62
(1,877)	1:75:A:PHE:HB2	1:77:A:TYR:H	14	0.62
(1,877)	1:75:A:PHE:HB3	1:77:A:TYR:H	14	0.62
(1,842)	1:71:A:ASP:H	1:73:A:LYS:H	9	0.62
(1,823)	1:69:A:SER:HA	1:71:A:ASP:H	2	0.62
(1,823)	1:69:A:SER:HA	1:71:A:ASP:H	10	0.62
(1,794)	1:66:A:VAL:HA	1:77:A:TYR:H	3	0.62
(1,794)	1:66:A:VAL:HA	1:77:A:TYR:H	15	0.62
(1,739)	1:62:A:TYR:HB2	1:79:A:LEU:HG	9	0.62
(1,739)	1:62:A:TYR:HB3	1:79:A:LEU:HG	9	0.62
(1,705)	1:59:A:HIS:H	1:60:A:THR:HA	18	0.62
(1,704)	1:59:A:HIS:H	1:60:A:THR:H	17	0.62
(1,512)	1:39:A:ALA:HA	1:74:A:ASP:HB2	19	0.62
(1,512)	1:39:A:ALA:HA	1:74:A:ASP:HB3	19	0.62
(1,489)	1:38:A:PHE:H	1:75:A:PHE:HA	18	0.62
(1,395)	1:31:A:ASP:HA	1:81:A:ILE:HG21	17	0.62
(1,395)	1:31:A:ASP:HA	1:81:A:ILE:HG22	17	0.62
(1,395)	1:31:A:ASP:HA	1:81:A:ILE:HG23	17	0.62
(1,312)	1:25:A:TYR:H	1:59:A:HIS:HE1	3	0.62
(1,46)	1:6:A:VAL:H	1:35:A:ILE:HD11	15	0.62
(1,46)	1:6:A:VAL:H	1:35:A:ILE:HD12	15	0.62
(1,46)	1:6:A:VAL:H	1:35:A:ILE:HD13	15	0.62
(1,32)	1:5:A:LEU:HD11	1:7:A:LEU:H	16	0.62
(1,32)	1:5:A:LEU:HD12	1:7:A:LEU:H	16	0.62
(1,32)	1:5:A:LEU:HD13	1:7:A:LEU:H	16	0.62
(1,32)	1:5:A:LEU:HD21	1:7:A:LEU:H	16	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,32)	1:5:A:LEU:HD22	1:7:A:LEU:H	16	0.62
(1,32)	1:5:A:LEU:HD23	1:7:A:LEU:H	16	0.62
(1,27)	1:5:A:LEU:HG	1:7:A:LEU:H	15	0.62
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG21	10	0.61
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG22	10	0.61
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG23	10	0.61
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG21	10	0.61
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG22	10	0.61
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG23	10	0.61
(1,893)	1:76:A:LEU:HD11	1:78:A:GLU:HG2	10	0.61
(1,893)	1:76:A:LEU:HD11	1:78:A:GLU:HG3	10	0.61
(1,893)	1:76:A:LEU:HD12	1:78:A:GLU:HG2	10	0.61
(1,893)	1:76:A:LEU:HD12	1:78:A:GLU:HG3	10	0.61
(1,893)	1:76:A:LEU:HD13	1:78:A:GLU:HG2	10	0.61
(1,893)	1:76:A:LEU:HD13	1:78:A:GLU:HG3	10	0.61
(1,892)	1:76:A:LEU:HD11	1:78:A:GLU:HA	17	0.61
(1,892)	1:76:A:LEU:HD12	1:78:A:GLU:HA	17	0.61
(1,892)	1:76:A:LEU:HD13	1:78:A:GLU:HA	17	0.61
(1,804)	1:67:A:ARG:H	1:68:A:VAL:HB	2	0.61
(1,793)	1:66:A:VAL:HA	1:76:A:LEU:HA	1	0.61
(1,789)	1:66:A:VAL:H	1:68:A:VAL:HG11	1	0.61
(1,789)	1:66:A:VAL:H	1:68:A:VAL:HG12	1	0.61
(1,789)	1:66:A:VAL:H	1:68:A:VAL:HG13	1	0.61
(1,755)	1:63:A:LEU:HG	1:64:A:ASP:HA	15	0.61
(1,742)	1:62:A:TYR:HE1	1:63:A:LEU:H	17	0.61
(1,742)	1:62:A:TYR:HE2	1:63:A:LEU:H	17	0.61
(1,547)	1:44:A:HIS:HB2	1:48:A:LEU:HD11	7	0.61
(1,547)	1:44:A:HIS:HB2	1:48:A:LEU:HD12	7	0.61
(1,547)	1:44:A:HIS:HB2	1:48:A:LEU:HD13	7	0.61
(1,547)	1:44:A:HIS:HB3	1:48:A:LEU:HD11	7	0.61
(1,547)	1:44:A:HIS:HB3	1:48:A:LEU:HD12	7	0.61
(1,547)	1:44:A:HIS:HB3	1:48:A:LEU:HD13	7	0.61
(1,502)	1:38:A:PHE:HD1	1:75:A:PHE:HA	10	0.61
(1,502)	1:38:A:PHE:HD2	1:75:A:PHE:HA	10	0.61
(1,432)	1:35:A:ILE:H	1:36:A:PHE:HE1	20	0.61
(1,432)	1:35:A:ILE:H	1:36:A:PHE:HE2	20	0.61
(1,414)	1:33:A:ARG:HG2	1:34:A:SER:HB2	20	0.61
(1,414)	1:33:A:ARG:HG2	1:34:A:SER:HB3	20	0.61
(1,414)	1:33:A:ARG:HG3	1:34:A:SER:HB2	20	0.61
(1,414)	1:33:A:ARG:HG3	1:34:A:SER:HB3	20	0.61
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG21	2	0.61
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG22	2	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG23	2	0.61
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG21	2	0.61
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG22	2	0.61
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG23	2	0.61
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG21	2	0.61
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG22	2	0.61
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG23	2	0.61
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG21	2	0.61
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG22	2	0.61
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG23	2	0.61
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG21	10	0.61
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG22	10	0.61
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG23	10	0.61
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG21	10	0.61
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG22	10	0.61
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG23	10	0.61
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG21	10	0.61
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG22	10	0.61
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG23	10	0.61
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG21	10	0.61
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG22	10	0.61
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG23	10	0.61
(1,348)	1:28:A:PHE:H	1:30:A:GLU:HG2	20	0.61
(1,348)	1:28:A:PHE:H	1:30:A:GLU:HG3	20	0.61
(1,318)	1:25:A:TYR:HA	1:59:A:HIS:HA	5	0.61
(1,305)	1:24:A:LEU:HD21	1:60:A:THR:H	20	0.61
(1,305)	1:24:A:LEU:HD22	1:60:A:THR:H	20	0.61
(1,305)	1:24:A:LEU:HD23	1:60:A:THR:H	20	0.61
(1,299)	1:24:A:LEU:HD11	1:35:A:ILE:HG21	16	0.61
(1,299)	1:24:A:LEU:HD11	1:35:A:ILE:HG22	16	0.61
(1,299)	1:24:A:LEU:HD11	1:35:A:ILE:HG23	16	0.61
(1,299)	1:24:A:LEU:HD12	1:35:A:ILE:HG21	16	0.61
(1,299)	1:24:A:LEU:HD12	1:35:A:ILE:HG22	16	0.61
(1,299)	1:24:A:LEU:HD12	1:35:A:ILE:HG23	16	0.61
(1,299)	1:24:A:LEU:HD13	1:35:A:ILE:HG21	16	0.61
(1,299)	1:24:A:LEU:HD13	1:35:A:ILE:HG22	16	0.61
(1,299)	1:24:A:LEU:HD13	1:35:A:ILE:HG23	16	0.61
(1,295)	1:24:A:LEU:HG	1:25:A:TYR:HA	15	0.61
(1,288)	1:24:A:LEU:HA	1:80:A:HIS:HE1	15	0.61
(1,166)	1:11:A:THR:HB	1:12:A:ARG:H	14	0.61
(1,144)	1:9:A:LYS:H	1:10:A:ASN:H	17	0.61
(1,128)	1:7:A:LEU:HG	1:38:A:PHE:HD1	10	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,128)	1:7:A:LEU:HG	1:38:A:PHE:HD2	10	0.61
(1,2)	1:3:A:MET:H	1:4:A:LYS:HA	18	0.61
(1,931)	1:81:A:ILE:HA	1:82:A:ILE:HA	16	0.6
(1,843)	1:71:A:ASP:H	1:73:A:LYS:HA	4	0.6
(1,842)	1:71:A:ASP:H	1:73:A:LYS:H	15	0.6
(1,823)	1:69:A:SER:HA	1:71:A:ASP:H	1	0.6
(1,795)	1:66:A:VAL:HA	1:77:A:TYR:HA	15	0.6
(1,794)	1:66:A:VAL:HA	1:77:A:TYR:H	6	0.6
(1,794)	1:66:A:VAL:HA	1:77:A:TYR:H	13	0.6
(1,768)	1:64:A:ASP:HA	1:76:A:LEU:HD21	11	0.6
(1,768)	1:64:A:ASP:HA	1:76:A:LEU:HD22	11	0.6
(1,768)	1:64:A:ASP:HA	1:76:A:LEU:HD23	11	0.6
(1,736)	1:62:A:TYR:HA	1:63:A:LEU:HD21	13	0.6
(1,736)	1:62:A:TYR:HA	1:63:A:LEU:HD22	13	0.6
(1,736)	1:62:A:TYR:HA	1:63:A:LEU:HD23	13	0.6
(1,721)	1:61:A:ALA:H	1:78:A:GLU:HB2	13	0.6
(1,721)	1:61:A:ALA:H	1:78:A:GLU:HB3	13	0.6
(1,710)	1:60:A:THR:HA	1:61:A:ALA:H	9	0.6
(1,686)	1:56:A:GLU:HA	1:57:A:LYS:HG2	10	0.6
(1,686)	1:56:A:GLU:HA	1:57:A:LYS:HG3	10	0.6
(1,526)	1:41:A:THR:HB	1:74:A:ASP:HB2	9	0.6
(1,526)	1:41:A:THR:HB	1:74:A:ASP:HB3	9	0.6
(1,432)	1:35:A:ILE:H	1:36:A:PHE:HE1	15	0.6
(1,432)	1:35:A:ILE:H	1:36:A:PHE:HE2	15	0.6
(1,426)	1:34:A:SER:HB2	1:36:A:PHE:HE1	8	0.6
(1,426)	1:34:A:SER:HB2	1:36:A:PHE:HE2	8	0.6
(1,426)	1:34:A:SER:HB3	1:36:A:PHE:HE1	8	0.6
(1,426)	1:34:A:SER:HB3	1:36:A:PHE:HE2	8	0.6
(1,411)	1:33:A:ARG:HA	1:82:A:ILE:HA	13	0.6
(1,348)	1:28:A:PHE:H	1:30:A:GLU:HG2	14	0.6
(1,348)	1:28:A:PHE:H	1:30:A:GLU:HG3	14	0.6
(1,295)	1:24:A:LEU:HG	1:25:A:TYR:HA	3	0.6
(1,295)	1:24:A:LEU:HG	1:25:A:TYR:HA	14	0.6
(1,245)	1:21:A:LEU:HD11	1:53:A:PHE:HA	9	0.6
(1,245)	1:21:A:LEU:HD12	1:53:A:PHE:HA	9	0.6
(1,245)	1:21:A:LEU:HD13	1:53:A:PHE:HA	9	0.6
(1,207)	1:19:A:VAL:HB	1:22:A:GLU:H	8	0.6
(1,166)	1:11:A:THR:HB	1:12:A:ARG:H	5	0.6
(1,166)	1:11:A:THR:HB	1:12:A:ARG:H	18	0.6
(1,157)	1:10:A:ASN:HB2	1:46:A:ASP:H	9	0.6
(1,157)	1:10:A:ASN:HB3	1:46:A:ASP:H	9	0.6
(1,150)	1:10:A:ASN:H	1:12:A:ARG:H	17	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,144)	1:9:A:LYS:H	1:10:A:ASN:H	12	0.6
(1,126)	1:7:A:LEU:HG	1:38:A:PHE:H	19	0.6
(1,21)	1:5:A:LEU:HB2	1:36:A:PHE:H	8	0.6
(1,21)	1:5:A:LEU:HB3	1:36:A:PHE:H	8	0.6
(1,931)	1:81:A:ILE:HA	1:82:A:ILE:HA	12	0.59
(1,843)	1:71:A:ASP:H	1:73:A:LYS:HA	17	0.59
(1,795)	1:66:A:VAL:HA	1:77:A:TYR:HA	9	0.59
(1,704)	1:59:A:HIS:H	1:60:A:THR:H	16	0.59
(1,560)	1:47:A:MET:H	1:48:A:LEU:HD11	3	0.59
(1,560)	1:47:A:MET:H	1:48:A:LEU:HD12	3	0.59
(1,560)	1:47:A:MET:H	1:48:A:LEU:HD13	3	0.59
(1,458)	1:36:A:PHE:HA	1:76:A:LEU:HD11	13	0.59
(1,458)	1:36:A:PHE:HA	1:76:A:LEU:HD12	13	0.59
(1,458)	1:36:A:PHE:HA	1:76:A:LEU:HD13	13	0.59
(1,432)	1:35:A:ILE:H	1:36:A:PHE:HE1	14	0.59
(1,432)	1:35:A:ILE:H	1:36:A:PHE:HE2	14	0.59
(1,365)	1:28:A:PHE:HD1	1:32:A:LYS:HB2	14	0.59
(1,365)	1:28:A:PHE:HD1	1:32:A:LYS:HB3	14	0.59
(1,365)	1:28:A:PHE:HD2	1:32:A:LYS:HB2	14	0.59
(1,365)	1:28:A:PHE:HD2	1:32:A:LYS:HB3	14	0.59
(1,348)	1:28:A:PHE:H	1:30:A:GLU:HG2	5	0.59
(1,348)	1:28:A:PHE:H	1:30:A:GLU:HG3	5	0.59
(1,318)	1:25:A:TYR:HA	1:59:A:HIS:HA	8	0.59
(1,180)	1:14:A:SER:H	1:15:A:ASP:H	12	0.59
(1,21)	1:5:A:LEU:HB2	1:36:A:PHE:H	17	0.59
(1,21)	1:5:A:LEU:HB3	1:36:A:PHE:H	17	0.59
(1,891)	1:76:A:LEU:HD11	1:77:A:TYR:H	9	0.58
(1,891)	1:76:A:LEU:HD12	1:77:A:TYR:H	9	0.58
(1,891)	1:76:A:LEU:HD13	1:77:A:TYR:H	9	0.58
(1,814)	1:68:A:VAL:HG11	1:73:A:LYS:H	15	0.58
(1,814)	1:68:A:VAL:HG12	1:73:A:LYS:H	15	0.58
(1,814)	1:68:A:VAL:HG13	1:73:A:LYS:H	15	0.58
(1,814)	1:68:A:VAL:HG21	1:73:A:LYS:H	15	0.58
(1,814)	1:68:A:VAL:HG22	1:73:A:LYS:H	15	0.58
(1,814)	1:68:A:VAL:HG23	1:73:A:LYS:H	15	0.58
(1,793)	1:66:A:VAL:HA	1:76:A:LEU:HA	19	0.58
(1,791)	1:66:A:VAL:HA	1:68:A:VAL:HG11	18	0.58
(1,791)	1:66:A:VAL:HA	1:68:A:VAL:HG12	18	0.58
(1,791)	1:66:A:VAL:HA	1:68:A:VAL:HG13	18	0.58
(1,775)	1:65:A:GLU:H	1:76:A:LEU:HD11	16	0.58
(1,775)	1:65:A:GLU:H	1:76:A:LEU:HD12	16	0.58
(1,775)	1:65:A:GLU:H	1:76:A:LEU:HD13	16	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,775)	1:65:A:GLU:H	1:76:A:LEU:HD21	16	0.58
(1,741)	1:62:A:TYR:HD1	1:63:A:LEU:H	7	0.58
(1,741)	1:62:A:TYR:HD2	1:63:A:LEU:H	7	0.58
(1,712)	1:60:A:THR:HA	1:81:A:ILE:H	20	0.58
(1,704)	1:59:A:HIS:H	1:60:A:THR:H	9	0.58
(1,410)	1:33:A:ARG:HA	1:81:A:ILE:HG21	4	0.58
(1,410)	1:33:A:ARG:HA	1:81:A:ILE:HG22	4	0.58
(1,410)	1:33:A:ARG:HA	1:81:A:ILE:HG23	4	0.58
(1,390)	1:31:A:ASP:H	1:81:A:ILE:HG21	13	0.58
(1,390)	1:31:A:ASP:H	1:81:A:ILE:HG22	13	0.58
(1,390)	1:31:A:ASP:H	1:81:A:ILE:HG23	13	0.58
(1,365)	1:28:A:PHE:HD1	1:32:A:LYS:HB2	9	0.58
(1,365)	1:28:A:PHE:HD1	1:32:A:LYS:HB3	9	0.58
(1,365)	1:28:A:PHE:HD2	1:32:A:LYS:HB2	9	0.58
(1,365)	1:28:A:PHE:HD2	1:32:A:LYS:HB3	9	0.58
(1,348)	1:28:A:PHE:H	1:30:A:GLU:HG2	6	0.58
(1,348)	1:28:A:PHE:H	1:30:A:GLU:HG3	6	0.58
(1,157)	1:10:A:ASN:HB2	1:46:A:ASP:H	10	0.58
(1,157)	1:10:A:ASN:HB3	1:46:A:ASP:H	10	0.58
(1,21)	1:5:A:LEU:HB2	1:36:A:PHE:H	11	0.58
(1,21)	1:5:A:LEU:HB3	1:36:A:PHE:H	11	0.58
(1,1)	1:3:A:MET:H	1:4:A:LYS:H	9	0.58
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG21	6	0.57
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG22	6	0.57
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG23	6	0.57
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG21	6	0.57
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG22	6	0.57
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG23	6	0.57
(1,893)	1:76:A:LEU:HD11	1:78:A:GLU:HG2	13	0.57
(1,893)	1:76:A:LEU:HD11	1:78:A:GLU:HG3	13	0.57
(1,893)	1:76:A:LEU:HD12	1:78:A:GLU:HG2	13	0.57
(1,893)	1:76:A:LEU:HD12	1:78:A:GLU:HG3	13	0.57
(1,893)	1:76:A:LEU:HD13	1:78:A:GLU:HG2	13	0.57
(1,893)	1:76:A:LEU:HD13	1:78:A:GLU:HG3	13	0.57
(1,890)	1:76:A:LEU:HD11	1:78:A:GLU:H	4	0.57
(1,890)	1:76:A:LEU:HD12	1:78:A:GLU:H	4	0.57
(1,890)	1:76:A:LEU:HD13	1:78:A:GLU:H	4	0.57
(1,843)	1:71:A:ASP:H	1:73:A:LYS:HA	7	0.57
(1,801)	1:66:A:VAL:HG11	1:72:A:GLU:HB2	20	0.57
(1,801)	1:66:A:VAL:HG11	1:72:A:GLU:HB3	20	0.57
(1,801)	1:66:A:VAL:HG12	1:72:A:GLU:HB2	20	0.57
(1,801)	1:66:A:VAL:HG12	1:72:A:GLU:HB3	20	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,801)	1:66:A:VAL:HG13	1:72:A:GLU:HB2	20	0.57
(1,801)	1:66:A:VAL:HG13	1:72:A:GLU:HB3	20	0.57
(1,801)	1:66:A:VAL:HG21	1:72:A:GLU:HB2	20	0.57
(1,801)	1:66:A:VAL:HG21	1:72:A:GLU:HB3	20	0.57
(1,801)	1:66:A:VAL:HG22	1:72:A:GLU:HB2	20	0.57
(1,801)	1:66:A:VAL:HG22	1:72:A:GLU:HB3	20	0.57
(1,801)	1:66:A:VAL:HG23	1:72:A:GLU:HB2	20	0.57
(1,801)	1:66:A:VAL:HG23	1:72:A:GLU:HB3	20	0.57
(1,795)	1:66:A:VAL:HA	1:77:A:TYR:HA	10	0.57
(1,795)	1:66:A:VAL:HA	1:77:A:TYR:HA	13	0.57
(1,713)	1:60:A:THR:HA	1:81:A:ILE:HA	20	0.57
(1,584)	1:48:A:LEU:HA	1:52:A:ASP:HB2	4	0.57
(1,584)	1:48:A:LEU:HA	1:52:A:ASP:HB3	4	0.57
(1,538)	1:43:A:ALA:HA	1:45:A:LYS:HD2	16	0.57
(1,538)	1:43:A:ALA:HA	1:45:A:LYS:HD3	16	0.57
(1,537)	1:43:A:ALA:HA	1:45:A:LYS:H	18	0.57
(1,500)	1:38:A:PHE:HD1	1:39:A:ALA:H	19	0.57
(1,500)	1:38:A:PHE:HD2	1:39:A:ALA:H	19	0.57
(1,470)	1:36:A:PHE:HD1	1:77:A:TYR:HD1	17	0.57
(1,470)	1:36:A:PHE:HD1	1:77:A:TYR:HD2	17	0.57
(1,470)	1:36:A:PHE:HD2	1:77:A:TYR:HD1	17	0.57
(1,470)	1:36:A:PHE:HD2	1:77:A:TYR:HD2	17	0.57
(1,395)	1:31:A:ASP:HA	1:81:A:ILE:HG21	8	0.57
(1,395)	1:31:A:ASP:HA	1:81:A:ILE:HG22	8	0.57
(1,395)	1:31:A:ASP:HA	1:81:A:ILE:HG23	8	0.57
(1,299)	1:24:A:LEU:HD11	1:35:A:ILE:HG21	10	0.57
(1,299)	1:24:A:LEU:HD11	1:35:A:ILE:HG22	10	0.57
(1,299)	1:24:A:LEU:HD11	1:35:A:ILE:HG23	10	0.57
(1,299)	1:24:A:LEU:HD12	1:35:A:ILE:HG21	10	0.57
(1,299)	1:24:A:LEU:HD12	1:35:A:ILE:HG22	10	0.57
(1,299)	1:24:A:LEU:HD12	1:35:A:ILE:HG23	10	0.57
(1,299)	1:24:A:LEU:HD13	1:35:A:ILE:HG21	10	0.57
(1,299)	1:24:A:LEU:HD13	1:35:A:ILE:HG22	10	0.57
(1,299)	1:24:A:LEU:HD13	1:35:A:ILE:HG23	10	0.57
(1,285)	1:24:A:LEU:HA	1:54:A:PHE:HE1	12	0.57
(1,285)	1:24:A:LEU:HA	1:54:A:PHE:HE2	12	0.57
(1,240)	1:21:A:LEU:HG	1:57:A:LYS:HB2	20	0.57
(1,240)	1:21:A:LEU:HG	1:57:A:LYS:HB3	20	0.57
(1,174)	1:12:A:ARG:HB2	1:14:A:SER:HA	8	0.57
(1,174)	1:12:A:ARG:HB3	1:14:A:SER:HA	8	0.57
(1,107)	1:7:A:LEU:H	1:38:A:PHE:HD1	8	0.57
(1,107)	1:7:A:LEU:H	1:38:A:PHE:HD2	8	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,33)	1:5:A:LEU:HD11	1:7:A:LEU:HA	3	0.57
(1,33)	1:5:A:LEU:HD12	1:7:A:LEU:HA	3	0.57
(1,33)	1:5:A:LEU:HD13	1:7:A:LEU:HA	3	0.57
(1,33)	1:5:A:LEU:HD21	1:7:A:LEU:HA	3	0.57
(1,33)	1:5:A:LEU:HD22	1:7:A:LEU:HA	3	0.57
(1,33)	1:5:A:LEU:HD23	1:7:A:LEU:HA	3	0.57
(1,22)	1:5:A:LEU:HB2	1:36:A:PHE:HA	7	0.57
(1,22)	1:5:A:LEU:HB3	1:36:A:PHE:HA	7	0.57
(1,795)	1:66:A:VAL:HA	1:77:A:TYR:HA	2	0.56
(1,755)	1:63:A:LEU:HG	1:64:A:ASP:HA	18	0.56
(1,739)	1:62:A:TYR:HB2	1:79:A:LEU:HG	5	0.56
(1,739)	1:62:A:TYR:HB3	1:79:A:LEU:HG	5	0.56
(1,705)	1:59:A:HIS:H	1:60:A:THR:HA	13	0.56
(1,521)	1:41:A:THR:HA	1:43:A:ALA:H	15	0.56
(1,502)	1:38:A:PHE:HD1	1:75:A:PHE:HA	5	0.56
(1,502)	1:38:A:PHE:HD2	1:75:A:PHE:HA	5	0.56
(1,422)	1:34:A:SER:HA	1:78:A:GLU:HB2	15	0.56
(1,422)	1:34:A:SER:HA	1:78:A:GLU:HB3	15	0.56
(1,365)	1:28:A:PHE:HD1	1:32:A:LYS:HB2	18	0.56
(1,365)	1:28:A:PHE:HD1	1:32:A:LYS:HB3	18	0.56
(1,365)	1:28:A:PHE:HD2	1:32:A:LYS:HB2	18	0.56
(1,365)	1:28:A:PHE:HD2	1:32:A:LYS:HB3	18	0.56
(1,317)	1:25:A:TYR:HA	1:29:A:SER:HG	11	0.56
(1,312)	1:25:A:TYR:H	1:59:A:HIS:HE1	12	0.56
(1,300)	1:24:A:LEU:HD11	1:35:A:ILE:HG12	3	0.56
(1,300)	1:24:A:LEU:HD11	1:35:A:ILE:HG13	3	0.56
(1,300)	1:24:A:LEU:HD12	1:35:A:ILE:HG12	3	0.56
(1,300)	1:24:A:LEU:HD12	1:35:A:ILE:HG13	3	0.56
(1,300)	1:24:A:LEU:HD13	1:35:A:ILE:HG12	3	0.56
(1,300)	1:24:A:LEU:HD13	1:35:A:ILE:HG13	3	0.56
(1,295)	1:24:A:LEU:HG	1:25:A:TYR:HA	4	0.56
(1,176)	1:13:A:LYS:H	1:14:A:SER:H	6	0.56
(1,171)	1:12:A:ARG:H	1:13:A:LYS:H	17	0.56
(1,146)	1:9:A:LYS:H	1:10:A:ASN:HB2	10	0.56
(1,146)	1:9:A:LYS:H	1:10:A:ASN:HB3	10	0.56
(1,144)	1:9:A:LYS:H	1:10:A:ASN:H	8	0.56
(1,34)	1:5:A:LEU:HD11	1:7:A:LEU:HB2	4	0.56
(1,34)	1:5:A:LEU:HD11	1:7:A:LEU:HB3	4	0.56
(1,34)	1:5:A:LEU:HD12	1:7:A:LEU:HB2	4	0.56
(1,34)	1:5:A:LEU:HD12	1:7:A:LEU:HB3	4	0.56
(1,34)	1:5:A:LEU:HD13	1:7:A:LEU:HB2	4	0.56
(1,34)	1:5:A:LEU:HD13	1:7:A:LEU:HB3	4	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,34)	1:5:A:LEU:HD21	1:7:A:LEU:HB2	4	0.56
(1,34)	1:5:A:LEU:HD21	1:7:A:LEU:HB3	4	0.56
(1,34)	1:5:A:LEU:HD22	1:7:A:LEU:HB2	4	0.56
(1,34)	1:5:A:LEU:HD22	1:7:A:LEU:HB3	4	0.56
(1,34)	1:5:A:LEU:HD23	1:7:A:LEU:HB2	4	0.56
(1,34)	1:5:A:LEU:HD23	1:7:A:LEU:HB3	4	0.56
(1,1)	1:3:A:MET:H	1:4:A:LYS:H	7	0.56
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG21	19	0.55
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG22	19	0.55
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG23	19	0.55
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG21	19	0.55
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG22	19	0.55
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG23	19	0.55
(1,877)	1:75:A:PHE:HB2	1:77:A:TYR:H	18	0.55
(1,877)	1:75:A:PHE:HB3	1:77:A:TYR:H	18	0.55
(1,843)	1:71:A:ASP:H	1:73:A:LYS:HA	11	0.55
(1,795)	1:66:A:VAL:HA	1:77:A:TYR:HA	18	0.55
(1,764)	1:64:A:ASP:H	1:79:A:LEU:H	14	0.55
(1,736)	1:62:A:TYR:HA	1:63:A:LEU:HD21	1	0.55
(1,736)	1:62:A:TYR:HA	1:63:A:LEU:HD22	1	0.55
(1,736)	1:62:A:TYR:HA	1:63:A:LEU:HD23	1	0.55
(1,705)	1:59:A:HIS:H	1:60:A:THR:HA	3	0.55
(1,628)	1:51:A:VAL:HG21	1:54:A:PHE:HD1	5	0.55
(1,628)	1:51:A:VAL:HG21	1:54:A:PHE:HD2	5	0.55
(1,628)	1:51:A:VAL:HG22	1:54:A:PHE:HD1	5	0.55
(1,628)	1:51:A:VAL:HG22	1:54:A:PHE:HD2	5	0.55
(1,628)	1:51:A:VAL:HG23	1:54:A:PHE:HD1	5	0.55
(1,628)	1:51:A:VAL:HG23	1:54:A:PHE:HD2	5	0.55
(1,547)	1:44:A:HIS:HB2	1:48:A:LEU:HD11	16	0.55
(1,547)	1:44:A:HIS:HB2	1:48:A:LEU:HD12	16	0.55
(1,547)	1:44:A:HIS:HB2	1:48:A:LEU:HD13	16	0.55
(1,547)	1:44:A:HIS:HB3	1:48:A:LEU:HD11	16	0.55
(1,547)	1:44:A:HIS:HB3	1:48:A:LEU:HD12	16	0.55
(1,547)	1:44:A:HIS:HB3	1:48:A:LEU:HD13	16	0.55
(1,502)	1:38:A:PHE:HD1	1:75:A:PHE:HA	2	0.55
(1,502)	1:38:A:PHE:HD2	1:75:A:PHE:HA	2	0.55
(1,501)	1:38:A:PHE:HD1	1:75:A:PHE:H	10	0.55
(1,501)	1:38:A:PHE:HD2	1:75:A:PHE:H	10	0.55
(1,412)	1:33:A:ARG:HB2	1:34:A:SER:H	8	0.55
(1,412)	1:33:A:ARG:HB3	1:34:A:SER:H	8	0.55
(1,411)	1:33:A:ARG:HA	1:82:A:ILE:HA	8	0.55
(1,191)	1:16:A:ALA:HA	1:19:A:VAL:HB	13	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,144)	1:9:A:LYS:H	1:10:A:ASN:H	2	0.55
(1,61)	1:6:A:VAL:HA	1:19:A:VAL:HB	10	0.55
(1,26)	1:5:A:LEU:HG	1:6:A:VAL:HG21	16	0.55
(1,26)	1:5:A:LEU:HG	1:6:A:VAL:HG22	16	0.55
(1,26)	1:5:A:LEU:HG	1:6:A:VAL:HG23	16	0.55
(3,1)	1:39:A:ALA:HB1	1:47:A:MET:N	11	0.54
(1,893)	1:76:A:LEU:HD11	1:78:A:GLU:HG2	6	0.54
(1,893)	1:76:A:LEU:HD11	1:78:A:GLU:HG3	6	0.54
(1,893)	1:76:A:LEU:HD12	1:78:A:GLU:HG2	6	0.54
(1,893)	1:76:A:LEU:HD12	1:78:A:GLU:HG3	6	0.54
(1,893)	1:76:A:LEU:HD13	1:78:A:GLU:HG2	6	0.54
(1,893)	1:76:A:LEU:HD13	1:78:A:GLU:HG3	6	0.54
(1,862)	1:73:A:LYS:HA	1:75:A:PHE:H	17	0.54
(1,823)	1:69:A:SER:HA	1:71:A:ASP:H	14	0.54
(1,814)	1:68:A:VAL:HG11	1:73:A:LYS:H	17	0.54
(1,814)	1:68:A:VAL:HG12	1:73:A:LYS:H	17	0.54
(1,814)	1:68:A:VAL:HG13	1:73:A:LYS:H	17	0.54
(1,814)	1:68:A:VAL:HG21	1:73:A:LYS:H	17	0.54
(1,814)	1:68:A:VAL:HG22	1:73:A:LYS:H	17	0.54
(1,814)	1:68:A:VAL:HG23	1:73:A:LYS:H	17	0.54
(1,802)	1:67:A:ARG:H	1:68:A:VAL:H	7	0.54
(1,768)	1:64:A:ASP:HA	1:76:A:LEU:HD21	10	0.54
(1,768)	1:64:A:ASP:HA	1:76:A:LEU:HD22	10	0.54
(1,768)	1:64:A:ASP:HA	1:76:A:LEU:HD23	10	0.54
(1,739)	1:62:A:TYR:HB2	1:79:A:LEU:HG	1	0.54
(1,739)	1:62:A:TYR:HB3	1:79:A:LEU:HG	1	0.54
(1,470)	1:36:A:PHE:HD1	1:77:A:TYR:HD1	10	0.54
(1,470)	1:36:A:PHE:HD1	1:77:A:TYR:HD2	10	0.54
(1,470)	1:36:A:PHE:HD2	1:77:A:TYR:HD1	10	0.54
(1,470)	1:36:A:PHE:HD2	1:77:A:TYR:HD2	10	0.54
(1,437)	1:35:A:ILE:H	1:80:A:HIS:H	11	0.54
(1,437)	1:35:A:ILE:H	1:80:A:HIS:H	17	0.54
(1,426)	1:34:A:SER:HB2	1:36:A:PHE:HE1	11	0.54
(1,426)	1:34:A:SER:HB2	1:36:A:PHE:HE2	11	0.54
(1,426)	1:34:A:SER:HB3	1:36:A:PHE:HE1	11	0.54
(1,426)	1:34:A:SER:HB3	1:36:A:PHE:HE2	11	0.54
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG21	11	0.54
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG22	11	0.54
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG23	11	0.54
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG21	11	0.54
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG22	11	0.54
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG23	11	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG21	11	0.54
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG22	11	0.54
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG23	11	0.54
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG21	11	0.54
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG22	11	0.54
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG23	11	0.54
(1,319)	1:25:A:TYR:HA	1:59:A:HIS:HB2	14	0.54
(1,319)	1:25:A:TYR:HA	1:59:A:HIS:HB3	14	0.54
(1,312)	1:25:A:TYR:H	1:59:A:HIS:HE1	4	0.54
(1,295)	1:24:A:LEU:HG	1:25:A:TYR:HA	8	0.54
(1,248)	1:21:A:LEU:HD21	1:22:A:GLU:HA	1	0.54
(1,248)	1:21:A:LEU:HD22	1:22:A:GLU:HA	1	0.54
(1,248)	1:21:A:LEU:HD23	1:22:A:GLU:HA	1	0.54
(1,248)	1:21:A:LEU:HD21	1:22:A:GLU:HA	8	0.54
(1,248)	1:21:A:LEU:HD22	1:22:A:GLU:HA	8	0.54
(1,248)	1:21:A:LEU:HD23	1:22:A:GLU:HA	8	0.54
(1,200)	1:18:A:SER:HB2	1:22:A:GLU:HG2	2	0.54
(1,200)	1:18:A:SER:HB2	1:22:A:GLU:HG3	2	0.54
(1,200)	1:18:A:SER:HB3	1:22:A:GLU:HG2	2	0.54
(1,200)	1:18:A:SER:HB3	1:22:A:GLU:HG3	2	0.54
(1,60)	1:6:A:VAL:HA	1:16:A:ALA:HB1	6	0.54
(1,60)	1:6:A:VAL:HA	1:16:A:ALA:HB2	6	0.54
(1,60)	1:6:A:VAL:HA	1:16:A:ALA:HB3	6	0.54
(1,27)	1:5:A:LEU:HG	1:7:A:LEU:H	5	0.54
(1,898)	1:77:A:TYR:HB2	1:79:A:LEU:HG	14	0.53
(1,898)	1:77:A:TYR:HB3	1:79:A:LEU:HG	14	0.53
(1,892)	1:76:A:LEU:HD11	1:78:A:GLU:HA	5	0.53
(1,892)	1:76:A:LEU:HD12	1:78:A:GLU:HA	5	0.53
(1,892)	1:76:A:LEU:HD13	1:78:A:GLU:HA	5	0.53
(1,879)	1:75:A:PHE:HD1	1:77:A:TYR:HD2	3	0.53
(1,879)	1:75:A:PHE:HD2	1:77:A:TYR:HD2	3	0.53
(1,842)	1:71:A:ASP:H	1:73:A:LYS:H	10	0.53
(1,842)	1:71:A:ASP:H	1:73:A:LYS:H	13	0.53
(1,823)	1:69:A:SER:HA	1:71:A:ASP:H	17	0.53
(1,800)	1:66:A:VAL:HG11	1:72:A:GLU:H	14	0.53
(1,800)	1:66:A:VAL:HG12	1:72:A:GLU:H	14	0.53
(1,800)	1:66:A:VAL:HG13	1:72:A:GLU:H	14	0.53
(1,800)	1:66:A:VAL:HG21	1:72:A:GLU:H	14	0.53
(1,800)	1:66:A:VAL:HG22	1:72:A:GLU:H	14	0.53
(1,800)	1:66:A:VAL:HG23	1:72:A:GLU:H	14	0.53
(1,741)	1:62:A:TYR:HD1	1:63:A:LEU:H	15	0.53
(1,741)	1:62:A:TYR:HD2	1:63:A:LEU:H	15	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,696)	1:57:A:LYS:HA	1:58:A:GLY:HA2	18	0.53
(1,584)	1:48:A:LEU:HA	1:52:A:ASP:HB2	8	0.53
(1,584)	1:48:A:LEU:HA	1:52:A:ASP:HB3	8	0.53
(1,584)	1:48:A:LEU:HA	1:52:A:ASP:HB2	9	0.53
(1,584)	1:48:A:LEU:HA	1:52:A:ASP:HB3	9	0.53
(1,547)	1:44:A:HIS:HB2	1:48:A:LEU:HD11	4	0.53
(1,547)	1:44:A:HIS:HB2	1:48:A:LEU:HD12	4	0.53
(1,547)	1:44:A:HIS:HB2	1:48:A:LEU:HD13	4	0.53
(1,547)	1:44:A:HIS:HB3	1:48:A:LEU:HD11	4	0.53
(1,547)	1:44:A:HIS:HB3	1:48:A:LEU:HD12	4	0.53
(1,547)	1:44:A:HIS:HB3	1:48:A:LEU:HD13	4	0.53
(1,538)	1:43:A:ALA:HA	1:45:A:LYS:HD2	7	0.53
(1,538)	1:43:A:ALA:HA	1:45:A:LYS:HD3	7	0.53
(1,525)	1:41:A:THR:HB	1:73:A:LYS:HB2	16	0.53
(1,525)	1:41:A:THR:HB	1:73:A:LYS:HB3	16	0.53
(1,523)	1:41:A:THR:HA	1:44:A:HIS:HA	8	0.53
(1,501)	1:38:A:PHE:HD1	1:75:A:PHE:H	12	0.53
(1,501)	1:38:A:PHE:HD2	1:75:A:PHE:H	12	0.53
(1,437)	1:35:A:ILE:H	1:80:A:HIS:H	8	0.53
(1,300)	1:24:A:LEU:HD11	1:35:A:ILE:HG12	20	0.53
(1,300)	1:24:A:LEU:HD11	1:35:A:ILE:HG13	20	0.53
(1,300)	1:24:A:LEU:HD12	1:35:A:ILE:HG12	20	0.53
(1,300)	1:24:A:LEU:HD12	1:35:A:ILE:HG13	20	0.53
(1,300)	1:24:A:LEU:HD13	1:35:A:ILE:HG12	20	0.53
(1,300)	1:24:A:LEU:HD13	1:35:A:ILE:HG13	20	0.53
(1,299)	1:24:A:LEU:HD11	1:35:A:ILE:HG21	12	0.53
(1,299)	1:24:A:LEU:HD11	1:35:A:ILE:HG22	12	0.53
(1,299)	1:24:A:LEU:HD11	1:35:A:ILE:HG23	12	0.53
(1,299)	1:24:A:LEU:HD12	1:35:A:ILE:HG21	12	0.53
(1,299)	1:24:A:LEU:HD12	1:35:A:ILE:HG22	12	0.53
(1,299)	1:24:A:LEU:HD12	1:35:A:ILE:HG23	12	0.53
(1,299)	1:24:A:LEU:HD13	1:35:A:ILE:HG21	12	0.53
(1,299)	1:24:A:LEU:HD13	1:35:A:ILE:HG22	12	0.53
(1,299)	1:24:A:LEU:HD13	1:35:A:ILE:HG23	12	0.53
(1,248)	1:21:A:LEU:HD21	1:22:A:GLU:HA	15	0.53
(1,248)	1:21:A:LEU:HD22	1:22:A:GLU:HA	15	0.53
(1,248)	1:21:A:LEU:HD23	1:22:A:GLU:HA	15	0.53
(1,248)	1:21:A:LEU:HD21	1:22:A:GLU:HA	20	0.53
(1,248)	1:21:A:LEU:HD22	1:22:A:GLU:HA	20	0.53
(1,248)	1:21:A:LEU:HD23	1:22:A:GLU:HA	20	0.53
(1,245)	1:21:A:LEU:HD11	1:53:A:PHE:HA	1	0.53
(1,245)	1:21:A:LEU:HD12	1:53:A:PHE:HA	1	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,245)	1:21:A:LEU:HD13	1:53:A:PHE:HA	1	0.53
(1,245)	1:21:A:LEU:HD11	1:53:A:PHE:HA	6	0.53
(1,245)	1:21:A:LEU:HD12	1:53:A:PHE:HA	6	0.53
(1,245)	1:21:A:LEU:HD13	1:53:A:PHE:HA	6	0.53
(1,174)	1:12:A:ARG:HB2	1:14:A:SER:HA	5	0.53
(1,174)	1:12:A:ARG:HB3	1:14:A:SER:HA	5	0.53
(1,147)	1:9:A:LYS:H	1:11:A:THR:H	3	0.53
(1,146)	1:9:A:LYS:H	1:10:A:ASN:HB2	2	0.53
(1,146)	1:9:A:LYS:H	1:10:A:ASN:HB3	2	0.53
(1,144)	1:9:A:LYS:H	1:10:A:ASN:H	11	0.53
(1,126)	1:7:A:LEU:HG	1:38:A:PHE:H	11	0.53
(1,126)	1:7:A:LEU:HG	1:38:A:PHE:H	16	0.53
(1,33)	1:5:A:LEU:HD11	1:7:A:LEU:HA	10	0.53
(1,33)	1:5:A:LEU:HD12	1:7:A:LEU:HA	10	0.53
(1,33)	1:5:A:LEU:HD13	1:7:A:LEU:HA	10	0.53
(1,33)	1:5:A:LEU:HD21	1:7:A:LEU:HA	10	0.53
(1,33)	1:5:A:LEU:HD22	1:7:A:LEU:HA	10	0.53
(1,33)	1:5:A:LEU:HD23	1:7:A:LEU:HA	10	0.53
(1,2)	1:3:A:MET:H	1:4:A:LYS:HA	5	0.53
(1,1)	1:3:A:MET:H	1:4:A:LYS:H	15	0.53
(1,892)	1:76:A:LEU:HD11	1:78:A:GLU:HA	6	0.52
(1,892)	1:76:A:LEU:HD12	1:78:A:GLU:HA	6	0.52
(1,892)	1:76:A:LEU:HD13	1:78:A:GLU:HA	6	0.52
(1,859)	1:72:A:GLU:HB2	1:74:A:ASP:HA	18	0.52
(1,859)	1:72:A:GLU:HB3	1:74:A:ASP:HA	18	0.52
(1,842)	1:71:A:ASP:H	1:73:A:LYS:H	18	0.52
(1,768)	1:64:A:ASP:HA	1:76:A:LEU:HD21	3	0.52
(1,768)	1:64:A:ASP:HA	1:76:A:LEU:HD22	3	0.52
(1,768)	1:64:A:ASP:HA	1:76:A:LEU:HD23	3	0.52
(1,757)	1:63:A:LEU:HD11	1:76:A:LEU:HG	5	0.52
(1,757)	1:63:A:LEU:HD12	1:76:A:LEU:HG	5	0.52
(1,757)	1:63:A:LEU:HD13	1:76:A:LEU:HG	5	0.52
(1,732)	1:62:A:TYR:H	1:81:A:ILE:H	10	0.52
(1,710)	1:60:A:THR:HA	1:61:A:ALA:H	20	0.52
(1,705)	1:59:A:HIS:H	1:60:A:THR:HA	17	0.52
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD11	6	0.52
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD12	6	0.52
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD13	6	0.52
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD11	6	0.52
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD12	6	0.52
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD13	6	0.52
(1,524)	1:41:A:THR:HB	1:73:A:LYS:HA	16	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,489)	1:38:A:PHE:H	1:75:A:PHE:HA	14	0.52
(1,432)	1:35:A:ILE:H	1:36:A:PHE:HE1	7	0.52
(1,432)	1:35:A:ILE:H	1:36:A:PHE:HE2	7	0.52
(1,348)	1:28:A:PHE:H	1:30:A:GLU:HG2	7	0.52
(1,348)	1:28:A:PHE:H	1:30:A:GLU:HG3	7	0.52
(1,301)	1:24:A:LEU:HD11	1:60:A:THR:HB	3	0.52
(1,301)	1:24:A:LEU:HD12	1:60:A:THR:HB	3	0.52
(1,301)	1:24:A:LEU:HD13	1:60:A:THR:HB	3	0.52
(1,288)	1:24:A:LEU:HA	1:80:A:HIS:HE1	5	0.52
(1,288)	1:24:A:LEU:HA	1:80:A:HIS:HE1	6	0.52
(1,248)	1:21:A:LEU:HD21	1:22:A:GLU:HA	3	0.52
(1,248)	1:21:A:LEU:HD22	1:22:A:GLU:HA	3	0.52
(1,248)	1:21:A:LEU:HD23	1:22:A:GLU:HA	3	0.52
(1,182)	1:14:A:SER:H	1:17:A:LYS:H	14	0.52
(1,123)	1:7:A:LEU:HB2	1:38:A:PHE:HD1	6	0.52
(1,123)	1:7:A:LEU:HB2	1:38:A:PHE:HD2	6	0.52
(1,123)	1:7:A:LEU:HB3	1:38:A:PHE:HD1	6	0.52
(1,123)	1:7:A:LEU:HB3	1:38:A:PHE:HD2	6	0.52
(1,33)	1:5:A:LEU:HD11	1:7:A:LEU:HA	4	0.52
(1,33)	1:5:A:LEU:HD12	1:7:A:LEU:HA	4	0.52
(1,33)	1:5:A:LEU:HD13	1:7:A:LEU:HA	4	0.52
(1,33)	1:5:A:LEU:HD21	1:7:A:LEU:HA	4	0.52
(1,33)	1:5:A:LEU:HD22	1:7:A:LEU:HA	4	0.52
(1,33)	1:5:A:LEU:HD23	1:7:A:LEU:HA	4	0.52
(1,4)	1:4:A:LYS:HA	1:5:A:LEU:H	11	0.52
(1,1)	1:3:A:MET:H	1:4:A:LYS:H	12	0.52
(1,890)	1:76:A:LEU:HD11	1:78:A:GLU:H	11	0.51
(1,890)	1:76:A:LEU:HD12	1:78:A:GLU:H	11	0.51
(1,890)	1:76:A:LEU:HD13	1:78:A:GLU:H	11	0.51
(1,823)	1:69:A:SER:HA	1:71:A:ASP:H	7	0.51
(1,705)	1:59:A:HIS:H	1:60:A:THR:HA	16	0.51
(1,628)	1:51:A:VAL:HG21	1:54:A:PHE:HD1	4	0.51
(1,628)	1:51:A:VAL:HG21	1:54:A:PHE:HD2	4	0.51
(1,628)	1:51:A:VAL:HG22	1:54:A:PHE:HD1	4	0.51
(1,628)	1:51:A:VAL:HG22	1:54:A:PHE:HD2	4	0.51
(1,628)	1:51:A:VAL:HG23	1:54:A:PHE:HD1	4	0.51
(1,628)	1:51:A:VAL:HG23	1:54:A:PHE:HD2	4	0.51
(1,584)	1:48:A:LEU:HA	1:52:A:ASP:HB2	16	0.51
(1,584)	1:48:A:LEU:HA	1:52:A:ASP:HB3	16	0.51
(1,431)	1:35:A:ILE:H	1:36:A:PHE:HD1	19	0.51
(1,431)	1:35:A:ILE:H	1:36:A:PHE:HD2	19	0.51
(1,370)	1:28:A:PHE:HE1	1:81:A:ILE:HA	10	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,370)	1:28:A:PHE:HE2	1:81:A:ILE:HA	10	0.51
(1,370)	1:28:A:PHE:HE1	1:81:A:ILE:HA	11	0.51
(1,370)	1:28:A:PHE:HE2	1:81:A:ILE:HA	11	0.51
(1,370)	1:28:A:PHE:HE1	1:81:A:ILE:HA	17	0.51
(1,370)	1:28:A:PHE:HE2	1:81:A:ILE:HA	17	0.51
(1,359)	1:28:A:PHE:HA	1:81:A:ILE:HD11	3	0.51
(1,359)	1:28:A:PHE:HA	1:81:A:ILE:HD12	3	0.51
(1,359)	1:28:A:PHE:HA	1:81:A:ILE:HD13	3	0.51
(1,356)	1:28:A:PHE:HA	1:33:A:ARG:H	8	0.51
(1,63)	1:6:A:VAL:HA	1:20:A:GLU:H	8	0.51
(1,44)	1:6:A:VAL:H	1:20:A:GLU:HB2	7	0.51
(1,44)	1:6:A:VAL:H	1:20:A:GLU:HB3	7	0.51
(1,35)	1:5:A:LEU:HD11	1:7:A:LEU:HG	11	0.51
(1,35)	1:5:A:LEU:HD12	1:7:A:LEU:HG	11	0.51
(1,35)	1:5:A:LEU:HD13	1:7:A:LEU:HG	11	0.51
(1,35)	1:5:A:LEU:HD21	1:7:A:LEU:HG	11	0.51
(1,35)	1:5:A:LEU:HD22	1:7:A:LEU:HG	11	0.51
(1,35)	1:5:A:LEU:HD23	1:7:A:LEU:HG	11	0.51
(1,34)	1:5:A:LEU:HD11	1:7:A:LEU:HB2	8	0.51
(1,34)	1:5:A:LEU:HD11	1:7:A:LEU:HB3	8	0.51
(1,34)	1:5:A:LEU:HD12	1:7:A:LEU:HB2	8	0.51
(1,34)	1:5:A:LEU:HD12	1:7:A:LEU:HB3	8	0.51
(1,34)	1:5:A:LEU:HD13	1:7:A:LEU:HB2	8	0.51
(1,34)	1:5:A:LEU:HD13	1:7:A:LEU:HB3	8	0.51
(1,34)	1:5:A:LEU:HD21	1:7:A:LEU:HB2	8	0.51
(1,34)	1:5:A:LEU:HD21	1:7:A:LEU:HB3	8	0.51
(1,34)	1:5:A:LEU:HD22	1:7:A:LEU:HB2	8	0.51
(1,34)	1:5:A:LEU:HD22	1:7:A:LEU:HB3	8	0.51
(1,34)	1:5:A:LEU:HD23	1:7:A:LEU:HB2	8	0.51
(1,34)	1:5:A:LEU:HD23	1:7:A:LEU:HB3	8	0.51
(1,22)	1:5:A:LEU:HB2	1:36:A:PHE:HA	11	0.51
(1,22)	1:5:A:LEU:HB3	1:36:A:PHE:HA	11	0.51
(1,19)	1:5:A:LEU:HB2	1:35:A:ILE:HA	10	0.51
(1,19)	1:5:A:LEU:HB3	1:35:A:ILE:HA	10	0.51
(1,843)	1:71:A:ASP:H	1:73:A:LYS:HA	9	0.5
(1,823)	1:69:A:SER:HA	1:71:A:ASP:H	18	0.5
(1,792)	1:66:A:VAL:HA	1:69:A:SER:H	20	0.5
(1,721)	1:61:A:ALA:H	1:78:A:GLU:HB2	1	0.5
(1,721)	1:61:A:ALA:H	1:78:A:GLU:HB3	1	0.5
(1,686)	1:56:A:GLU:HA	1:57:A:LYS:HG2	9	0.5
(1,686)	1:56:A:GLU:HA	1:57:A:LYS:HG3	9	0.5
(1,547)	1:44:A:HIS:HB2	1:48:A:LEU:HD11	8	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,547)	1:44:A:HIS:HB2	1:48:A:LEU:HD12	8	0.5
(1,547)	1:44:A:HIS:HB2	1:48:A:LEU:HD13	8	0.5
(1,547)	1:44:A:HIS:HB3	1:48:A:LEU:HD11	8	0.5
(1,547)	1:44:A:HIS:HB3	1:48:A:LEU:HD12	8	0.5
(1,547)	1:44:A:HIS:HB3	1:48:A:LEU:HD13	8	0.5
(1,470)	1:36:A:PHE:HD1	1:77:A:TYR:HD1	20	0.5
(1,470)	1:36:A:PHE:HD1	1:77:A:TYR:HD2	20	0.5
(1,470)	1:36:A:PHE:HD2	1:77:A:TYR:HD1	20	0.5
(1,470)	1:36:A:PHE:HD2	1:77:A:TYR:HD2	20	0.5
(1,437)	1:35:A:ILE:H	1:80:A:HIS:H	6	0.5
(1,432)	1:35:A:ILE:H	1:36:A:PHE:HE1	16	0.5
(1,432)	1:35:A:ILE:H	1:36:A:PHE:HE2	16	0.5
(1,431)	1:35:A:ILE:H	1:36:A:PHE:HD1	6	0.5
(1,431)	1:35:A:ILE:H	1:36:A:PHE:HD2	6	0.5
(1,395)	1:31:A:ASP:HA	1:81:A:ILE:HG21	9	0.5
(1,395)	1:31:A:ASP:HA	1:81:A:ILE:HG22	9	0.5
(1,395)	1:31:A:ASP:HA	1:81:A:ILE:HG23	9	0.5
(1,317)	1:25:A:TYR:HA	1:29:A:SER:HG	1	0.5
(1,301)	1:24:A:LEU:HD11	1:60:A:THR:HB	7	0.5
(1,301)	1:24:A:LEU:HD12	1:60:A:THR:HB	7	0.5
(1,301)	1:24:A:LEU:HD13	1:60:A:THR:HB	7	0.5
(1,246)	1:21:A:LEU:HD11	1:53:A:PHE:HB2	14	0.5
(1,246)	1:21:A:LEU:HD11	1:53:A:PHE:HB3	14	0.5
(1,246)	1:21:A:LEU:HD12	1:53:A:PHE:HB2	14	0.5
(1,246)	1:21:A:LEU:HD12	1:53:A:PHE:HB3	14	0.5
(1,246)	1:21:A:LEU:HD13	1:53:A:PHE:HB2	14	0.5
(1,246)	1:21:A:LEU:HD13	1:53:A:PHE:HB3	14	0.5
(1,220)	1:20:A:GLU:HA	1:24:A:LEU:HA	14	0.5
(1,207)	1:19:A:VAL:HB	1:22:A:GLU:H	1	0.5
(1,144)	1:9:A:LYS:H	1:10:A:ASN:H	13	0.5
(1,26)	1:5:A:LEU:HG	1:6:A:VAL:HG21	3	0.5
(1,26)	1:5:A:LEU:HG	1:6:A:VAL:HG22	3	0.5
(1,26)	1:5:A:LEU:HG	1:6:A:VAL:HG23	3	0.5
(1,805)	1:67:A:ARG:H	1:68:A:VAL:HG11	7	0.49
(1,805)	1:67:A:ARG:H	1:68:A:VAL:HG12	7	0.49
(1,805)	1:67:A:ARG:H	1:68:A:VAL:HG13	7	0.49
(1,802)	1:67:A:ARG:H	1:68:A:VAL:H	16	0.49
(1,800)	1:66:A:VAL:HG11	1:72:A:GLU:H	20	0.49
(1,800)	1:66:A:VAL:HG12	1:72:A:GLU:H	20	0.49
(1,800)	1:66:A:VAL:HG13	1:72:A:GLU:H	20	0.49
(1,800)	1:66:A:VAL:HG21	1:72:A:GLU:H	20	0.49
(1,800)	1:66:A:VAL:HG22	1:72:A:GLU:H	20	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,800)	1:66:A:VAL:HG23	1:72:A:GLU:H	20	0.49
(1,793)	1:66:A:VAL:HA	1:76:A:LEU:HA	18	0.49
(1,791)	1:66:A:VAL:HA	1:68:A:VAL:HG11	8	0.49
(1,791)	1:66:A:VAL:HA	1:68:A:VAL:HG12	8	0.49
(1,791)	1:66:A:VAL:HA	1:68:A:VAL:HG13	8	0.49
(1,755)	1:63:A:LEU:HG	1:64:A:ASP:HA	1	0.49
(1,736)	1:62:A:TYR:HA	1:63:A:LEU:HD21	18	0.49
(1,736)	1:62:A:TYR:HA	1:63:A:LEU:HD22	18	0.49
(1,736)	1:62:A:TYR:HA	1:63:A:LEU:HD23	18	0.49
(1,732)	1:62:A:TYR:H	1:81:A:ILE:H	4	0.49
(1,705)	1:59:A:HIS:H	1:60:A:THR:HA	5	0.49
(1,705)	1:59:A:HIS:H	1:60:A:THR:HA	15	0.49
(1,686)	1:56:A:GLU:HA	1:57:A:LYS:HG2	18	0.49
(1,686)	1:56:A:GLU:HA	1:57:A:LYS:HG3	18	0.49
(1,437)	1:35:A:ILE:H	1:80:A:HIS:H	12	0.49
(1,411)	1:33:A:ARG:HA	1:82:A:ILE:HA	14	0.49
(1,364)	1:28:A:PHE:HD1	1:32:A:LYS:HA	8	0.49
(1,364)	1:28:A:PHE:HD2	1:32:A:LYS:HA	8	0.49
(1,348)	1:28:A:PHE:H	1:30:A:GLU:HG2	16	0.49
(1,348)	1:28:A:PHE:H	1:30:A:GLU:HG3	16	0.49
(1,285)	1:24:A:LEU:HA	1:54:A:PHE:HE1	14	0.49
(1,285)	1:24:A:LEU:HA	1:54:A:PHE:HE2	14	0.49
(1,68)	1:6:A:VAL:HB	1:19:A:VAL:HB	10	0.49
(1,33)	1:5:A:LEU:HD11	1:7:A:LEU:HA	8	0.49
(1,33)	1:5:A:LEU:HD12	1:7:A:LEU:HA	8	0.49
(1,33)	1:5:A:LEU:HD13	1:7:A:LEU:HA	8	0.49
(1,33)	1:5:A:LEU:HD21	1:7:A:LEU:HA	8	0.49
(1,33)	1:5:A:LEU:HD22	1:7:A:LEU:HA	8	0.49
(1,33)	1:5:A:LEU:HD23	1:7:A:LEU:HA	8	0.49
(1,1)	1:3:A:MET:H	1:4:A:LYS:H	3	0.49
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG21	11	0.48
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG22	11	0.48
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG23	11	0.48
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG21	11	0.48
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG22	11	0.48
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG23	11	0.48
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG21	20	0.48
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG22	20	0.48
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG23	20	0.48
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG21	20	0.48
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG22	20	0.48
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG23	20	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,906)	1:78:A:GLU:HA	1:79:A:LEU:HG	10	0.48
(1,893)	1:76:A:LEU:HD11	1:78:A:GLU:HG2	15	0.48
(1,893)	1:76:A:LEU:HD11	1:78:A:GLU:HG3	15	0.48
(1,893)	1:76:A:LEU:HD12	1:78:A:GLU:HG2	15	0.48
(1,893)	1:76:A:LEU:HD12	1:78:A:GLU:HG3	15	0.48
(1,893)	1:76:A:LEU:HD13	1:78:A:GLU:HG2	15	0.48
(1,893)	1:76:A:LEU:HD13	1:78:A:GLU:HG3	15	0.48
(1,842)	1:71:A:ASP:H	1:73:A:LYS:H	11	0.48
(1,823)	1:69:A:SER:HA	1:71:A:ASP:H	13	0.48
(1,768)	1:64:A:ASP:HA	1:76:A:LEU:HD21	16	0.48
(1,768)	1:64:A:ASP:HA	1:76:A:LEU:HD22	16	0.48
(1,768)	1:64:A:ASP:HA	1:76:A:LEU:HD23	16	0.48
(1,768)	1:64:A:ASP:HA	1:76:A:LEU:HD21	19	0.48
(1,768)	1:64:A:ASP:HA	1:76:A:LEU:HD22	19	0.48
(1,768)	1:64:A:ASP:HA	1:76:A:LEU:HD23	19	0.48
(1,710)	1:60:A:THR:HA	1:61:A:ALA:H	1	0.48
(1,710)	1:60:A:THR:HA	1:61:A:ALA:H	19	0.48
(1,692)	1:57:A:LYS:H	1:58:A:GLY:HA2	6	0.48
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD11	17	0.48
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD12	17	0.48
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD13	17	0.48
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD11	17	0.48
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD12	17	0.48
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD13	17	0.48
(1,458)	1:36:A:PHE:HA	1:76:A:LEU:HD11	5	0.48
(1,458)	1:36:A:PHE:HA	1:76:A:LEU:HD12	5	0.48
(1,458)	1:36:A:PHE:HA	1:76:A:LEU:HD13	5	0.48
(1,437)	1:35:A:ILE:H	1:80:A:HIS:H	1	0.48
(1,437)	1:35:A:ILE:H	1:80:A:HIS:H	10	0.48
(1,398)	1:32:A:LYS:H	1:81:A:ILE:HG21	11	0.48
(1,398)	1:32:A:LYS:H	1:81:A:ILE:HG22	11	0.48
(1,398)	1:32:A:LYS:H	1:81:A:ILE:HG23	11	0.48
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG21	17	0.48
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG22	17	0.48
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG23	17	0.48
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG21	17	0.48
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG22	17	0.48
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG23	17	0.48
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG21	17	0.48
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG22	17	0.48
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG23	17	0.48
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG21	17	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG22	17	0.48
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG23	17	0.48
(1,354)	1:28:A:PHE:HA	1:30:A:GLU:H	15	0.48
(1,318)	1:25:A:TYR:HA	1:59:A:HIS:HA	3	0.48
(1,284)	1:24:A:LEU:HA	1:35:A:ILE:HD11	17	0.48
(1,284)	1:24:A:LEU:HA	1:35:A:ILE:HD12	17	0.48
(1,284)	1:24:A:LEU:HA	1:35:A:ILE:HD13	17	0.48
(1,237)	1:21:A:LEU:HG	1:24:A:LEU:HB2	3	0.48
(1,237)	1:21:A:LEU:HG	1:24:A:LEU:HB3	3	0.48
(1,215)	1:20:A:GLU:H	1:37:A:TYR:HD1	5	0.48
(1,215)	1:20:A:GLU:H	1:37:A:TYR:HD2	5	0.48
(1,176)	1:13:A:LYS:H	1:14:A:SER:H	8	0.48
(1,174)	1:12:A:ARG:HB2	1:14:A:SER:HA	12	0.48
(1,174)	1:12:A:ARG:HB3	1:14:A:SER:HA	12	0.48
(1,147)	1:9:A:LYS:H	1:11:A:THR:H	1	0.48
(1,89)	1:6:A:VAL:HG21	1:19:A:VAL:HG11	13	0.48
(1,89)	1:6:A:VAL:HG21	1:19:A:VAL:HG12	13	0.48
(1,89)	1:6:A:VAL:HG21	1:19:A:VAL:HG13	13	0.48
(1,89)	1:6:A:VAL:HG22	1:19:A:VAL:HG11	13	0.48
(1,89)	1:6:A:VAL:HG22	1:19:A:VAL:HG12	13	0.48
(1,89)	1:6:A:VAL:HG22	1:19:A:VAL:HG13	13	0.48
(1,89)	1:6:A:VAL:HG23	1:19:A:VAL:HG11	13	0.48
(1,89)	1:6:A:VAL:HG23	1:19:A:VAL:HG12	13	0.48
(1,89)	1:6:A:VAL:HG23	1:19:A:VAL:HG13	13	0.48
(1,34)	1:5:A:LEU:HD11	1:7:A:LEU:HB2	3	0.48
(1,34)	1:5:A:LEU:HD11	1:7:A:LEU:HB3	3	0.48
(1,34)	1:5:A:LEU:HD12	1:7:A:LEU:HB2	3	0.48
(1,34)	1:5:A:LEU:HD12	1:7:A:LEU:HB3	3	0.48
(1,34)	1:5:A:LEU:HD13	1:7:A:LEU:HB2	3	0.48
(1,34)	1:5:A:LEU:HD13	1:7:A:LEU:HB3	3	0.48
(1,34)	1:5:A:LEU:HD21	1:7:A:LEU:HB2	3	0.48
(1,34)	1:5:A:LEU:HD21	1:7:A:LEU:HB3	3	0.48
(1,34)	1:5:A:LEU:HD22	1:7:A:LEU:HB2	3	0.48
(1,34)	1:5:A:LEU:HD22	1:7:A:LEU:HB3	3	0.48
(1,34)	1:5:A:LEU:HD23	1:7:A:LEU:HB2	3	0.48
(1,34)	1:5:A:LEU:HD23	1:7:A:LEU:HB3	3	0.48
(1,842)	1:71:A:ASP:H	1:73:A:LYS:H	17	0.47
(1,793)	1:66:A:VAL:HA	1:76:A:LEU:HA	6	0.47
(1,705)	1:59:A:HIS:H	1:60:A:THR:HA	6	0.47
(1,692)	1:57:A:LYS:H	1:58:A:GLY:HA2	11	0.47
(1,474)	1:37:A:TYR:H	1:76:A:LEU:H	8	0.47
(1,450)	1:35:A:ILE:HD11	1:54:A:PHE:HE1	11	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,450)	1:35:A:ILE:HD11	1:54:A:PHE:HE2	11	0.47
(1,450)	1:35:A:ILE:HD12	1:54:A:PHE:HE1	11	0.47
(1,450)	1:35:A:ILE:HD12	1:54:A:PHE:HE2	11	0.47
(1,450)	1:35:A:ILE:HD13	1:54:A:PHE:HE1	11	0.47
(1,450)	1:35:A:ILE:HD13	1:54:A:PHE:HE2	11	0.47
(1,450)	1:35:A:ILE:HD11	1:54:A:PHE:HE1	11	0.47
(1,450)	1:35:A:ILE:HD11	1:54:A:PHE:HE2	11	0.47
(1,450)	1:35:A:ILE:HD12	1:54:A:PHE:HE1	11	0.47
(1,450)	1:35:A:ILE:HD12	1:54:A:PHE:HE2	11	0.47
(1,450)	1:35:A:ILE:HD13	1:54:A:PHE:HE1	11	0.47
(1,450)	1:35:A:ILE:HD13	1:54:A:PHE:HE2	11	0.47
(1,432)	1:35:A:ILE:H	1:36:A:PHE:HE1	3	0.47
(1,432)	1:35:A:ILE:H	1:36:A:PHE:HE2	3	0.47
(1,432)	1:35:A:ILE:H	1:36:A:PHE:HE1	8	0.47
(1,432)	1:35:A:ILE:H	1:36:A:PHE:HE2	8	0.47
(1,426)	1:34:A:SER:HB2	1:36:A:PHE:HE1	15	0.47
(1,426)	1:34:A:SER:HB2	1:36:A:PHE:HE2	15	0.47
(1,426)	1:34:A:SER:HB3	1:36:A:PHE:HE1	15	0.47
(1,426)	1:34:A:SER:HB3	1:36:A:PHE:HE2	15	0.47
(1,370)	1:28:A:PHE:HE1	1:81:A:ILE:HA	2	0.47
(1,370)	1:28:A:PHE:HE2	1:81:A:ILE:HA	2	0.47
(1,348)	1:28:A:PHE:H	1:30:A:GLU:HG2	18	0.47
(1,348)	1:28:A:PHE:H	1:30:A:GLU:HG3	18	0.47
(1,300)	1:24:A:LEU:HD11	1:35:A:ILE:HG12	8	0.47
(1,300)	1:24:A:LEU:HD11	1:35:A:ILE:HG13	8	0.47
(1,300)	1:24:A:LEU:HD12	1:35:A:ILE:HG12	8	0.47
(1,300)	1:24:A:LEU:HD12	1:35:A:ILE:HG13	8	0.47
(1,300)	1:24:A:LEU:HD13	1:35:A:ILE:HG12	8	0.47
(1,300)	1:24:A:LEU:HD13	1:35:A:ILE:HG13	8	0.47
(1,293)	1:24:A:LEU:HB2	1:80:A:HIS:HE1	14	0.47
(1,293)	1:24:A:LEU:HB3	1:80:A:HIS:HE1	14	0.47
(1,248)	1:21:A:LEU:HD21	1:22:A:GLU:HA	12	0.47
(1,248)	1:21:A:LEU:HD22	1:22:A:GLU:HA	12	0.47
(1,248)	1:21:A:LEU:HD23	1:22:A:GLU:HA	12	0.47
(1,200)	1:18:A:SER:HB2	1:22:A:GLU:HG2	5	0.47
(1,200)	1:18:A:SER:HB2	1:22:A:GLU:HG3	5	0.47
(1,200)	1:18:A:SER:HB3	1:22:A:GLU:HG2	5	0.47
(1,200)	1:18:A:SER:HB3	1:22:A:GLU:HG3	5	0.47
(1,158)	1:10:A:ASN:HB2	1:46:A:ASP:HA	9	0.47
(1,158)	1:10:A:ASN:HB3	1:46:A:ASP:HA	9	0.47
(1,156)	1:10:A:ASN:HB2	1:45:A:LYS:HB2	10	0.47
(1,156)	1:10:A:ASN:HB2	1:45:A:LYS:HB3	10	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,156)	1:10:A:ASN:HB3	1:45:A:LYS:HB2	10	0.47
(1,156)	1:10:A:ASN:HB3	1:45:A:LYS:HB3	10	0.47
(1,107)	1:7:A:LEU:H	1:38:A:PHE:HD1	6	0.47
(1,107)	1:7:A:LEU:H	1:38:A:PHE:HD2	6	0.47
(1,61)	1:6:A:VAL:HA	1:19:A:VAL:HB	8	0.47
(1,1)	1:3:A:MET:H	1:4:A:LYS:H	20	0.47
(1,900)	1:77:A:TYR:HD1	1:79:A:LEU:HG	3	0.46
(1,900)	1:77:A:TYR:HD2	1:79:A:LEU:HG	3	0.46
(1,843)	1:71:A:ASP:H	1:73:A:LYS:HA	5	0.46
(1,840)	1:71:A:ASP:H	1:72:A:GLU:H	2	0.46
(1,823)	1:69:A:SER:HA	1:71:A:ASP:H	9	0.46
(1,795)	1:66:A:VAL:HA	1:77:A:TYR:HA	4	0.46
(1,692)	1:57:A:LYS:H	1:58:A:GLY:HA2	10	0.46
(1,584)	1:48:A:LEU:HA	1:52:A:ASP:HB2	12	0.46
(1,584)	1:48:A:LEU:HA	1:52:A:ASP:HB3	12	0.46
(1,537)	1:43:A:ALA:HA	1:45:A:LYS:H	16	0.46
(1,527)	1:42:A:ASN:H	1:43:A:ALA:H	1	0.46
(1,471)	1:36:A:PHE:HD1	1:78:A:GLU:H	1	0.46
(1,471)	1:36:A:PHE:HD2	1:78:A:GLU:H	1	0.46
(1,458)	1:36:A:PHE:HA	1:76:A:LEU:HD11	6	0.46
(1,458)	1:36:A:PHE:HA	1:76:A:LEU:HD12	6	0.46
(1,458)	1:36:A:PHE:HA	1:76:A:LEU:HD13	6	0.46
(1,441)	1:35:A:ILE:HB	1:37:A:TYR:HA	9	0.46
(1,384)	1:30:A:GLU:HA	1:31:A:ASP:HB2	10	0.46
(1,384)	1:30:A:GLU:HA	1:31:A:ASP:HB3	10	0.46
(1,366)	1:28:A:PHE:HD1	1:80:A:HIS:HB2	13	0.46
(1,366)	1:28:A:PHE:HD1	1:80:A:HIS:HB3	13	0.46
(1,366)	1:28:A:PHE:HD2	1:80:A:HIS:HB2	13	0.46
(1,366)	1:28:A:PHE:HD2	1:80:A:HIS:HB3	13	0.46
(1,365)	1:28:A:PHE:HD1	1:32:A:LYS:HB2	15	0.46
(1,365)	1:28:A:PHE:HD1	1:32:A:LYS:HB3	15	0.46
(1,365)	1:28:A:PHE:HD2	1:32:A:LYS:HB2	15	0.46
(1,365)	1:28:A:PHE:HD2	1:32:A:LYS:HB3	15	0.46
(1,354)	1:28:A:PHE:HA	1:30:A:GLU:H	19	0.46
(1,182)	1:14:A:SER:H	1:17:A:LYS:H	5	0.46
(1,102)	1:7:A:LEU:H	1:19:A:VAL:HB	19	0.46
(1,22)	1:5:A:LEU:HB2	1:36:A:PHE:HA	4	0.46
(1,22)	1:5:A:LEU:HB3	1:36:A:PHE:HA	4	0.46
(1,19)	1:5:A:LEU:HB2	1:35:A:ILE:HA	3	0.46
(1,19)	1:5:A:LEU:HB3	1:35:A:ILE:HA	3	0.46
(1,898)	1:77:A:TYR:HB2	1:79:A:LEU:HG	18	0.45
(1,898)	1:77:A:TYR:HB3	1:79:A:LEU:HG	18	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,866)	1:74:A:ASP:H	1:75:A:PHE:HA	16	0.45
(1,843)	1:71:A:ASP:H	1:73:A:LYS:HA	10	0.45
(1,836)	1:70:A:THR:HA	1:73:A:LYS:HB2	14	0.45
(1,836)	1:70:A:THR:HA	1:73:A:LYS:HB3	14	0.45
(1,823)	1:69:A:SER:HA	1:71:A:ASP:H	6	0.45
(1,819)	1:69:A:SER:H	1:73:A:LYS:H	12	0.45
(1,805)	1:67:A:ARG:H	1:68:A:VAL:HG11	12	0.45
(1,805)	1:67:A:ARG:H	1:68:A:VAL:HG12	12	0.45
(1,805)	1:67:A:ARG:H	1:68:A:VAL:HG13	12	0.45
(1,800)	1:66:A:VAL:HG11	1:72:A:GLU:H	10	0.45
(1,800)	1:66:A:VAL:HG12	1:72:A:GLU:H	10	0.45
(1,800)	1:66:A:VAL:HG13	1:72:A:GLU:H	10	0.45
(1,800)	1:66:A:VAL:HG21	1:72:A:GLU:H	10	0.45
(1,800)	1:66:A:VAL:HG22	1:72:A:GLU:H	10	0.45
(1,800)	1:66:A:VAL:HG23	1:72:A:GLU:H	10	0.45
(1,721)	1:61:A:ALA:H	1:78:A:GLU:HB2	3	0.45
(1,721)	1:61:A:ALA:H	1:78:A:GLU:HB3	3	0.45
(1,526)	1:41:A:THR:HB	1:74:A:ASP:HB2	13	0.45
(1,526)	1:41:A:THR:HB	1:74:A:ASP:HB3	13	0.45
(1,502)	1:38:A:PHE:HD1	1:75:A:PHE:HA	11	0.45
(1,502)	1:38:A:PHE:HD2	1:75:A:PHE:HA	11	0.45
(1,437)	1:35:A:ILE:H	1:80:A:HIS:H	7	0.45
(1,431)	1:35:A:ILE:H	1:36:A:PHE:HD1	13	0.45
(1,431)	1:35:A:ILE:H	1:36:A:PHE:HD2	13	0.45
(1,365)	1:28:A:PHE:HD1	1:32:A:LYS:HB2	10	0.45
(1,365)	1:28:A:PHE:HD1	1:32:A:LYS:HB3	10	0.45
(1,365)	1:28:A:PHE:HD2	1:32:A:LYS:HB2	10	0.45
(1,365)	1:28:A:PHE:HD2	1:32:A:LYS:HB3	10	0.45
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG21	4	0.45
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG22	4	0.45
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG23	4	0.45
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG21	4	0.45
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG22	4	0.45
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG23	4	0.45
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG21	4	0.45
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG22	4	0.45
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG23	4	0.45
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG21	4	0.45
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG22	4	0.45
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG23	4	0.45
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG21	9	0.45
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG22	9	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG23	9	0.45
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG21	9	0.45
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG22	9	0.45
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG23	9	0.45
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG21	9	0.45
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG22	9	0.45
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG23	9	0.45
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG21	9	0.45
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG22	9	0.45
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG23	9	0.45
(1,312)	1:25:A:TYR:H	1:59:A:HIS:HE1	14	0.45
(1,293)	1:24:A:LEU:HB2	1:80:A:HIS:HE1	2	0.45
(1,293)	1:24:A:LEU:HB3	1:80:A:HIS:HE1	2	0.45
(1,248)	1:21:A:LEU:HD21	1:22:A:GLU:HA	13	0.45
(1,248)	1:21:A:LEU:HD22	1:22:A:GLU:HA	13	0.45
(1,248)	1:21:A:LEU:HD23	1:22:A:GLU:HA	13	0.45
(1,245)	1:21:A:LEU:HD11	1:53:A:PHE:HA	8	0.45
(1,245)	1:21:A:LEU:HD12	1:53:A:PHE:HA	8	0.45
(1,245)	1:21:A:LEU:HD13	1:53:A:PHE:HA	8	0.45
(1,158)	1:10:A:ASN:HB2	1:46:A:ASP:HA	10	0.45
(1,158)	1:10:A:ASN:HB3	1:46:A:ASP:HA	10	0.45
(1,147)	1:9:A:LYS:H	1:11:A:THR:H	15	0.45
(1,63)	1:6:A:VAL:HA	1:20:A:GLU:H	7	0.45
(1,33)	1:5:A:LEU:HD11	1:7:A:LEU:HA	6	0.45
(1,33)	1:5:A:LEU:HD12	1:7:A:LEU:HA	6	0.45
(1,33)	1:5:A:LEU:HD13	1:7:A:LEU:HA	6	0.45
(1,33)	1:5:A:LEU:HD21	1:7:A:LEU:HA	6	0.45
(1,33)	1:5:A:LEU:HD22	1:7:A:LEU:HA	6	0.45
(1,33)	1:5:A:LEU:HD23	1:7:A:LEU:HA	6	0.45
(1,6)	1:5:A:LEU:H	1:6:A:VAL:HA	16	0.45
(1,4)	1:4:A:LYS:HA	1:5:A:LEU:H	14	0.45
(1,2)	1:3:A:MET:H	1:4:A:LYS:HA	11	0.45
(1,898)	1:77:A:TYR:HB2	1:79:A:LEU:HG	20	0.44
(1,898)	1:77:A:TYR:HB3	1:79:A:LEU:HG	20	0.44
(1,878)	1:75:A:PHE:HB2	1:77:A:TYR:HD1	9	0.44
(1,878)	1:75:A:PHE:HB2	1:77:A:TYR:HD2	9	0.44
(1,878)	1:75:A:PHE:HB3	1:77:A:TYR:HD1	9	0.44
(1,878)	1:75:A:PHE:HB3	1:77:A:TYR:HD2	9	0.44
(1,811)	1:68:A:VAL:HA	1:73:A:LYS:H	12	0.44
(1,802)	1:67:A:ARG:H	1:68:A:VAL:H	5	0.44
(1,802)	1:67:A:ARG:H	1:68:A:VAL:H	10	0.44
(1,800)	1:66:A:VAL:HG11	1:72:A:GLU:H	6	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,800)	1:66:A:VAL:HG12	1:72:A:GLU:H	6	0.44
(1,800)	1:66:A:VAL:HG13	1:72:A:GLU:H	6	0.44
(1,800)	1:66:A:VAL:HG21	1:72:A:GLU:H	6	0.44
(1,800)	1:66:A:VAL:HG22	1:72:A:GLU:H	6	0.44
(1,800)	1:66:A:VAL:HG23	1:72:A:GLU:H	6	0.44
(1,798)	1:66:A:VAL:HG11	1:69:A:SER:HA	12	0.44
(1,798)	1:66:A:VAL:HG12	1:69:A:SER:HA	12	0.44
(1,798)	1:66:A:VAL:HG13	1:69:A:SER:HA	12	0.44
(1,798)	1:66:A:VAL:HG21	1:69:A:SER:HA	12	0.44
(1,798)	1:66:A:VAL:HG22	1:69:A:SER:HA	12	0.44
(1,798)	1:66:A:VAL:HG23	1:69:A:SER:HA	12	0.44
(1,793)	1:66:A:VAL:HA	1:76:A:LEU:HA	10	0.44
(1,793)	1:66:A:VAL:HA	1:76:A:LEU:HA	16	0.44
(1,764)	1:64:A:ASP:H	1:79:A:LEU:H	8	0.44
(1,743)	1:62:A:TYR:HE1	1:63:A:LEU:HD21	13	0.44
(1,743)	1:62:A:TYR:HE1	1:63:A:LEU:HD22	13	0.44
(1,743)	1:62:A:TYR:HE1	1:63:A:LEU:HD23	13	0.44
(1,743)	1:62:A:TYR:HE2	1:63:A:LEU:HD21	13	0.44
(1,743)	1:62:A:TYR:HE2	1:63:A:LEU:HD22	13	0.44
(1,743)	1:62:A:TYR:HE2	1:63:A:LEU:HD23	13	0.44
(1,736)	1:62:A:TYR:HA	1:63:A:LEU:HD21	12	0.44
(1,736)	1:62:A:TYR:HA	1:63:A:LEU:HD22	12	0.44
(1,736)	1:62:A:TYR:HA	1:63:A:LEU:HD23	12	0.44
(1,692)	1:57:A:LYS:H	1:58:A:GLY:HA2	16	0.44
(1,584)	1:48:A:LEU:HA	1:52:A:ASP:HB2	3	0.44
(1,584)	1:48:A:LEU:HA	1:52:A:ASP:HB3	3	0.44
(1,516)	1:39:A:ALA:HB1	1:46:A:ASP:H	19	0.44
(1,516)	1:39:A:ALA:HB2	1:46:A:ASP:H	19	0.44
(1,516)	1:39:A:ALA:HB3	1:46:A:ASP:H	19	0.44
(1,474)	1:37:A:TYR:H	1:76:A:LEU:H	10	0.44
(1,437)	1:35:A:ILE:H	1:80:A:HIS:H	5	0.44
(1,365)	1:28:A:PHE:HD1	1:32:A:LYS:HB2	3	0.44
(1,365)	1:28:A:PHE:HD1	1:32:A:LYS:HB3	3	0.44
(1,365)	1:28:A:PHE:HD2	1:32:A:LYS:HB2	3	0.44
(1,365)	1:28:A:PHE:HD2	1:32:A:LYS:HB3	3	0.44
(1,365)	1:28:A:PHE:HD1	1:32:A:LYS:HB2	7	0.44
(1,365)	1:28:A:PHE:HD1	1:32:A:LYS:HB3	7	0.44
(1,365)	1:28:A:PHE:HD2	1:32:A:LYS:HB2	7	0.44
(1,365)	1:28:A:PHE:HD2	1:32:A:LYS:HB3	7	0.44
(1,318)	1:25:A:TYR:HA	1:59:A:HIS:HA	7	0.44
(1,318)	1:25:A:TYR:HA	1:59:A:HIS:HA	10	0.44
(1,300)	1:24:A:LEU:HD11	1:35:A:ILE:HG12	16	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,300)	1:24:A:LEU:HD11	1:35:A:ILE:HG13	16	0.44
(1,300)	1:24:A:LEU:HD12	1:35:A:ILE:HG12	16	0.44
(1,300)	1:24:A:LEU:HD12	1:35:A:ILE:HG13	16	0.44
(1,300)	1:24:A:LEU:HD13	1:35:A:ILE:HG12	16	0.44
(1,300)	1:24:A:LEU:HD13	1:35:A:ILE:HG13	16	0.44
(1,274)	1:23:A:ASP:HB2	1:35:A:ILE:HB	16	0.44
(1,274)	1:23:A:ASP:HB3	1:35:A:ILE:HB	16	0.44
(1,248)	1:21:A:LEU:HD21	1:22:A:GLU:HA	16	0.44
(1,248)	1:21:A:LEU:HD22	1:22:A:GLU:HA	16	0.44
(1,248)	1:21:A:LEU:HD23	1:22:A:GLU:HA	16	0.44
(1,245)	1:21:A:LEU:HD11	1:53:A:PHE:HA	11	0.44
(1,245)	1:21:A:LEU:HD12	1:53:A:PHE:HA	11	0.44
(1,245)	1:21:A:LEU:HD13	1:53:A:PHE:HA	11	0.44
(1,182)	1:14:A:SER:H	1:17:A:LYS:H	7	0.44
(1,157)	1:10:A:ASN:HB2	1:46:A:ASP:H	18	0.44
(1,157)	1:10:A:ASN:HB3	1:46:A:ASP:H	18	0.44
(1,127)	1:7:A:LEU:HG	1:38:A:PHE:HB2	17	0.44
(1,127)	1:7:A:LEU:HG	1:38:A:PHE:HB3	17	0.44
(1,126)	1:7:A:LEU:HG	1:38:A:PHE:H	3	0.44
(1,2)	1:3:A:MET:H	1:4:A:LYS:HA	7	0.44
(1,1)	1:3:A:MET:H	1:4:A:LYS:H	4	0.44
(1,843)	1:71:A:ASP:H	1:73:A:LYS:HA	14	0.43
(1,802)	1:67:A:ARG:H	1:68:A:VAL:H	9	0.43
(1,768)	1:64:A:ASP:HA	1:76:A:LEU:HD21	14	0.43
(1,768)	1:64:A:ASP:HA	1:76:A:LEU:HD22	14	0.43
(1,768)	1:64:A:ASP:HA	1:76:A:LEU:HD23	14	0.43
(1,764)	1:64:A:ASP:H	1:79:A:LEU:H	4	0.43
(1,764)	1:64:A:ASP:H	1:79:A:LEU:H	18	0.43
(1,741)	1:62:A:TYR:HD1	1:63:A:LEU:H	5	0.43
(1,741)	1:62:A:TYR:HD2	1:63:A:LEU:H	5	0.43
(1,721)	1:61:A:ALA:H	1:78:A:GLU:HB2	20	0.43
(1,721)	1:61:A:ALA:H	1:78:A:GLU:HB3	20	0.43
(1,584)	1:48:A:LEU:HA	1:52:A:ASP:HB2	2	0.43
(1,584)	1:48:A:LEU:HA	1:52:A:ASP:HB3	2	0.43
(1,584)	1:48:A:LEU:HA	1:52:A:ASP:HB2	5	0.43
(1,584)	1:48:A:LEU:HA	1:52:A:ASP:HB3	5	0.43
(1,523)	1:41:A:THR:HA	1:44:A:HIS:HA	9	0.43
(1,523)	1:41:A:THR:HA	1:44:A:HIS:HA	11	0.43
(1,516)	1:39:A:ALA:HB1	1:46:A:ASP:H	8	0.43
(1,516)	1:39:A:ALA:HB2	1:46:A:ASP:H	8	0.43
(1,516)	1:39:A:ALA:HB3	1:46:A:ASP:H	8	0.43
(1,471)	1:36:A:PHE:HD1	1:78:A:GLU:H	14	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,471)	1:36:A:PHE:HD2	1:78:A:GLU:H	14	0.43
(1,470)	1:36:A:PHE:HD1	1:77:A:TYR:HD1	3	0.43
(1,470)	1:36:A:PHE:HD1	1:77:A:TYR:HD2	3	0.43
(1,470)	1:36:A:PHE:HD2	1:77:A:TYR:HD1	3	0.43
(1,470)	1:36:A:PHE:HD2	1:77:A:TYR:HD2	3	0.43
(1,432)	1:35:A:ILE:H	1:36:A:PHE:HE1	17	0.43
(1,432)	1:35:A:ILE:H	1:36:A:PHE:HE2	17	0.43
(1,398)	1:32:A:LYS:H	1:81:A:ILE:HG21	6	0.43
(1,398)	1:32:A:LYS:H	1:81:A:ILE:HG22	6	0.43
(1,398)	1:32:A:LYS:H	1:81:A:ILE:HG23	6	0.43
(1,398)	1:32:A:LYS:H	1:81:A:ILE:HG21	14	0.43
(1,398)	1:32:A:LYS:H	1:81:A:ILE:HG22	14	0.43
(1,398)	1:32:A:LYS:H	1:81:A:ILE:HG23	14	0.43
(1,369)	1:28:A:PHE:HE1	1:81:A:ILE:H	14	0.43
(1,369)	1:28:A:PHE:HE2	1:81:A:ILE:H	14	0.43
(1,300)	1:24:A:LEU:HD11	1:35:A:ILE:HG12	6	0.43
(1,300)	1:24:A:LEU:HD11	1:35:A:ILE:HG13	6	0.43
(1,300)	1:24:A:LEU:HD12	1:35:A:ILE:HG12	6	0.43
(1,300)	1:24:A:LEU:HD12	1:35:A:ILE:HG13	6	0.43
(1,300)	1:24:A:LEU:HD13	1:35:A:ILE:HG12	6	0.43
(1,300)	1:24:A:LEU:HD13	1:35:A:ILE:HG13	6	0.43
(1,285)	1:24:A:LEU:HA	1:54:A:PHE:HE1	3	0.43
(1,285)	1:24:A:LEU:HA	1:54:A:PHE:HE2	3	0.43
(1,248)	1:21:A:LEU:HD21	1:22:A:GLU:HA	18	0.43
(1,248)	1:21:A:LEU:HD22	1:22:A:GLU:HA	18	0.43
(1,248)	1:21:A:LEU:HD23	1:22:A:GLU:HA	18	0.43
(1,174)	1:12:A:ARG:HB2	1:14:A:SER:HA	11	0.43
(1,174)	1:12:A:ARG:HB3	1:14:A:SER:HA	11	0.43
(1,147)	1:9:A:LYS:H	1:11:A:THR:H	16	0.43
(1,147)	1:9:A:LYS:H	1:11:A:THR:H	17	0.43
(1,145)	1:9:A:LYS:H	1:10:A:ASN:HA	17	0.43
(1,61)	1:6:A:VAL:HA	1:19:A:VAL:HB	12	0.43
(1,47)	1:6:A:VAL:H	1:36:A:PHE:H	10	0.43
(1,21)	1:5:A:LEU:HB2	1:36:A:PHE:H	18	0.43
(1,21)	1:5:A:LEU:HB3	1:36:A:PHE:H	18	0.43
(1,840)	1:71:A:ASP:H	1:72:A:GLU:H	12	0.42
(1,823)	1:69:A:SER:HA	1:71:A:ASP:H	4	0.42
(1,820)	1:69:A:SER:H	1:73:A:LYS:HA	17	0.42
(1,775)	1:65:A:GLU:H	1:76:A:LEU:HD11	1	0.42
(1,775)	1:65:A:GLU:H	1:76:A:LEU:HD12	1	0.42
(1,775)	1:65:A:GLU:H	1:76:A:LEU:HD13	1	0.42
(1,775)	1:65:A:GLU:H	1:76:A:LEU:HD21	1	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,584)	1:48:A:LEU:HA	1:52:A:ASP:HB2	14	0.42
(1,584)	1:48:A:LEU:HA	1:52:A:ASP:HB3	14	0.42
(1,584)	1:48:A:LEU:HA	1:52:A:ASP:HB2	19	0.42
(1,584)	1:48:A:LEU:HA	1:52:A:ASP:HB3	19	0.42
(1,584)	1:48:A:LEU:HA	1:52:A:ASP:HB2	20	0.42
(1,584)	1:48:A:LEU:HA	1:52:A:ASP:HB3	20	0.42
(1,540)	1:44:A:HIS:H	1:45:A:LYS:H	13	0.42
(1,355)	1:28:A:PHE:HA	1:32:A:LYS:HB2	16	0.42
(1,355)	1:28:A:PHE:HA	1:32:A:LYS:HB3	16	0.42
(1,317)	1:25:A:TYR:HA	1:29:A:SER:HG	8	0.42
(1,317)	1:25:A:TYR:HA	1:29:A:SER:HG	19	0.42
(1,305)	1:24:A:LEU:HD21	1:60:A:THR:H	19	0.42
(1,305)	1:24:A:LEU:HD22	1:60:A:THR:H	19	0.42
(1,305)	1:24:A:LEU:HD23	1:60:A:THR:H	19	0.42
(1,300)	1:24:A:LEU:HD11	1:35:A:ILE:HG12	12	0.42
(1,300)	1:24:A:LEU:HD11	1:35:A:ILE:HG13	12	0.42
(1,300)	1:24:A:LEU:HD12	1:35:A:ILE:HG12	12	0.42
(1,300)	1:24:A:LEU:HD12	1:35:A:ILE:HG13	12	0.42
(1,300)	1:24:A:LEU:HD13	1:35:A:ILE:HG12	12	0.42
(1,300)	1:24:A:LEU:HD13	1:35:A:ILE:HG13	12	0.42
(1,215)	1:20:A:GLU:H	1:37:A:TYR:HD1	13	0.42
(1,215)	1:20:A:GLU:H	1:37:A:TYR:HD2	13	0.42
(1,167)	1:11:A:THR:HB	1:12:A:ARG:HA	17	0.42
(1,157)	1:10:A:ASN:HB2	1:46:A:ASP:H	17	0.42
(1,157)	1:10:A:ASN:HB3	1:46:A:ASP:H	17	0.42
(1,126)	1:7:A:LEU:HG	1:38:A:PHE:H	17	0.42
(1,1)	1:3:A:MET:H	1:4:A:LYS:H	10	0.42
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG21	9	0.41
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG22	9	0.41
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG23	9	0.41
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG21	9	0.41
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG22	9	0.41
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG23	9	0.41
(1,840)	1:71:A:ASP:H	1:72:A:GLU:H	9	0.41
(1,800)	1:66:A:VAL:HG11	1:72:A:GLU:H	16	0.41
(1,800)	1:66:A:VAL:HG12	1:72:A:GLU:H	16	0.41
(1,800)	1:66:A:VAL:HG13	1:72:A:GLU:H	16	0.41
(1,800)	1:66:A:VAL:HG21	1:72:A:GLU:H	16	0.41
(1,800)	1:66:A:VAL:HG22	1:72:A:GLU:H	16	0.41
(1,800)	1:66:A:VAL:HG23	1:72:A:GLU:H	16	0.41
(1,793)	1:66:A:VAL:HA	1:76:A:LEU:HA	7	0.41
(1,721)	1:61:A:ALA:H	1:78:A:GLU:HB2	14	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,721)	1:61:A:ALA:H	1:78:A:GLU:HB3	14	0.41
(1,704)	1:59:A:HIS:H	1:60:A:THR:H	2	0.41
(1,657)	1:54:A:PHE:HA	1:60:A:THR:HB	19	0.41
(1,628)	1:51:A:VAL:HG21	1:54:A:PHE:HD1	14	0.41
(1,628)	1:51:A:VAL:HG21	1:54:A:PHE:HD2	14	0.41
(1,628)	1:51:A:VAL:HG22	1:54:A:PHE:HD1	14	0.41
(1,628)	1:51:A:VAL:HG22	1:54:A:PHE:HD2	14	0.41
(1,628)	1:51:A:VAL:HG23	1:54:A:PHE:HD1	14	0.41
(1,628)	1:51:A:VAL:HG23	1:54:A:PHE:HD2	14	0.41
(1,628)	1:51:A:VAL:HG21	1:54:A:PHE:HD1	18	0.41
(1,628)	1:51:A:VAL:HG21	1:54:A:PHE:HD2	18	0.41
(1,628)	1:51:A:VAL:HG22	1:54:A:PHE:HD1	18	0.41
(1,628)	1:51:A:VAL:HG22	1:54:A:PHE:HD2	18	0.41
(1,628)	1:51:A:VAL:HG23	1:54:A:PHE:HD1	18	0.41
(1,628)	1:51:A:VAL:HG23	1:54:A:PHE:HD2	18	0.41
(1,539)	1:43:A:ALA:HB1	1:44:A:HIS:H	13	0.41
(1,539)	1:43:A:ALA:HB2	1:44:A:HIS:H	13	0.41
(1,539)	1:43:A:ALA:HB3	1:44:A:HIS:H	13	0.41
(1,537)	1:43:A:ALA:HA	1:45:A:LYS:H	14	0.41
(1,495)	1:38:A:PHE:HA	1:75:A:PHE:HD1	2	0.41
(1,495)	1:38:A:PHE:HA	1:75:A:PHE:HD2	2	0.41
(1,474)	1:37:A:TYR:H	1:76:A:LEU:H	13	0.41
(1,432)	1:35:A:ILE:H	1:36:A:PHE:HE1	10	0.41
(1,432)	1:35:A:ILE:H	1:36:A:PHE:HE2	10	0.41
(1,431)	1:35:A:ILE:H	1:36:A:PHE:HD1	14	0.41
(1,431)	1:35:A:ILE:H	1:36:A:PHE:HD2	14	0.41
(1,412)	1:33:A:ARG:HB2	1:34:A:SER:H	1	0.41
(1,412)	1:33:A:ARG:HB3	1:34:A:SER:H	1	0.41
(1,369)	1:28:A:PHE:HE1	1:81:A:ILE:H	13	0.41
(1,369)	1:28:A:PHE:HE2	1:81:A:ILE:H	13	0.41
(1,364)	1:28:A:PHE:HD1	1:32:A:LYS:HA	15	0.41
(1,364)	1:28:A:PHE:HD2	1:32:A:LYS:HA	15	0.41
(1,327)	1:26:A:HIS:H	1:28:A:PHE:HB2	6	0.41
(1,327)	1:26:A:HIS:H	1:28:A:PHE:HB3	6	0.41
(1,318)	1:25:A:TYR:HA	1:59:A:HIS:HA	4	0.41
(1,318)	1:25:A:TYR:HA	1:59:A:HIS:HA	15	0.41
(1,245)	1:21:A:LEU:HD11	1:53:A:PHE:HA	20	0.41
(1,245)	1:21:A:LEU:HD12	1:53:A:PHE:HA	20	0.41
(1,245)	1:21:A:LEU:HD13	1:53:A:PHE:HA	20	0.41
(1,238)	1:21:A:LEU:HG	1:53:A:PHE:HB2	14	0.41
(1,238)	1:21:A:LEU:HG	1:53:A:PHE:HB3	14	0.41
(1,215)	1:20:A:GLU:H	1:37:A:TYR:HD1	1	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,215)	1:20:A:GLU:H	1:37:A:TYR:HD2	1	0.41
(1,154)	1:10:A:ASN:HA	1:13:A:LYS:HG2	1	0.41
(1,154)	1:10:A:ASN:HA	1:13:A:LYS:HG3	1	0.41
(1,145)	1:9:A:LYS:H	1:10:A:ASN:HA	2	0.41
(1,142)	1:8:A:ALA:HA	1:46:A:ASP:HA	18	0.41
(1,60)	1:6:A:VAL:HA	1:16:A:ALA:HB1	17	0.41
(1,60)	1:6:A:VAL:HA	1:16:A:ALA:HB2	17	0.41
(1,60)	1:6:A:VAL:HA	1:16:A:ALA:HB3	17	0.41
(1,34)	1:5:A:LEU:HD11	1:7:A:LEU:HB2	10	0.41
(1,34)	1:5:A:LEU:HD11	1:7:A:LEU:HB3	10	0.41
(1,34)	1:5:A:LEU:HD12	1:7:A:LEU:HB2	10	0.41
(1,34)	1:5:A:LEU:HD12	1:7:A:LEU:HB3	10	0.41
(1,34)	1:5:A:LEU:HD13	1:7:A:LEU:HB2	10	0.41
(1,34)	1:5:A:LEU:HD13	1:7:A:LEU:HB3	10	0.41
(1,34)	1:5:A:LEU:HD21	1:7:A:LEU:HB2	10	0.41
(1,34)	1:5:A:LEU:HD21	1:7:A:LEU:HB3	10	0.41
(1,34)	1:5:A:LEU:HD22	1:7:A:LEU:HB2	10	0.41
(1,34)	1:5:A:LEU:HD22	1:7:A:LEU:HB3	10	0.41
(1,34)	1:5:A:LEU:HD23	1:7:A:LEU:HB2	10	0.41
(1,34)	1:5:A:LEU:HD23	1:7:A:LEU:HB3	10	0.41
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG21	17	0.4
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG22	17	0.4
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG23	17	0.4
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG21	17	0.4
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG22	17	0.4
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG23	17	0.4
(1,843)	1:71:A:ASP:H	1:73:A:LYS:HA	3	0.4
(1,842)	1:71:A:ASP:H	1:73:A:LYS:H	6	0.4
(1,840)	1:71:A:ASP:H	1:72:A:GLU:H	11	0.4
(1,802)	1:67:A:ARG:H	1:68:A:VAL:H	6	0.4
(1,801)	1:66:A:VAL:HG11	1:72:A:GLU:HB2	14	0.4
(1,801)	1:66:A:VAL:HG11	1:72:A:GLU:HB3	14	0.4
(1,801)	1:66:A:VAL:HG12	1:72:A:GLU:HB2	14	0.4
(1,801)	1:66:A:VAL:HG12	1:72:A:GLU:HB3	14	0.4
(1,801)	1:66:A:VAL:HG13	1:72:A:GLU:HB2	14	0.4
(1,801)	1:66:A:VAL:HG13	1:72:A:GLU:HB3	14	0.4
(1,801)	1:66:A:VAL:HG21	1:72:A:GLU:HB2	14	0.4
(1,801)	1:66:A:VAL:HG21	1:72:A:GLU:HB3	14	0.4
(1,801)	1:66:A:VAL:HG22	1:72:A:GLU:HB2	14	0.4
(1,801)	1:66:A:VAL:HG22	1:72:A:GLU:HB3	14	0.4
(1,801)	1:66:A:VAL:HG23	1:72:A:GLU:HB2	14	0.4
(1,801)	1:66:A:VAL:HG23	1:72:A:GLU:HB3	14	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,721)	1:61:A:ALA:H	1:78:A:GLU:HB2	18	0.4
(1,721)	1:61:A:ALA:H	1:78:A:GLU:HB3	18	0.4
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD11	8	0.4
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD12	8	0.4
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD13	8	0.4
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD11	8	0.4
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD12	8	0.4
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD13	8	0.4
(1,437)	1:35:A:ILE:H	1:80:A:HIS:H	16	0.4
(1,417)	1:34:A:SER:H	1:79:A:LEU:HA	19	0.4
(1,405)	1:33:A:ARG:H	1:81:A:ILE:HG21	14	0.4
(1,405)	1:33:A:ARG:H	1:81:A:ILE:HG22	14	0.4
(1,405)	1:33:A:ARG:H	1:81:A:ILE:HG23	14	0.4
(1,405)	1:33:A:ARG:H	1:81:A:ILE:HG21	14	0.4
(1,405)	1:33:A:ARG:H	1:81:A:ILE:HG22	14	0.4
(1,405)	1:33:A:ARG:H	1:81:A:ILE:HG23	14	0.4
(1,366)	1:28:A:PHE:HD1	1:80:A:HIS:HB2	14	0.4
(1,366)	1:28:A:PHE:HD1	1:80:A:HIS:HB3	14	0.4
(1,366)	1:28:A:PHE:HD2	1:80:A:HIS:HB2	14	0.4
(1,366)	1:28:A:PHE:HD2	1:80:A:HIS:HB3	14	0.4
(1,364)	1:28:A:PHE:HD1	1:32:A:LYS:HA	16	0.4
(1,364)	1:28:A:PHE:HD2	1:32:A:LYS:HA	16	0.4
(1,301)	1:24:A:LEU:HD11	1:60:A:THR:HB	17	0.4
(1,301)	1:24:A:LEU:HD12	1:60:A:THR:HB	17	0.4
(1,301)	1:24:A:LEU:HD13	1:60:A:THR:HB	17	0.4
(1,288)	1:24:A:LEU:HA	1:80:A:HIS:HE1	16	0.4
(1,248)	1:21:A:LEU:HD21	1:22:A:GLU:HA	4	0.4
(1,248)	1:21:A:LEU:HD22	1:22:A:GLU:HA	4	0.4
(1,248)	1:21:A:LEU:HD23	1:22:A:GLU:HA	4	0.4
(1,248)	1:21:A:LEU:HD21	1:22:A:GLU:HA	5	0.4
(1,248)	1:21:A:LEU:HD22	1:22:A:GLU:HA	5	0.4
(1,248)	1:21:A:LEU:HD23	1:22:A:GLU:HA	5	0.4
(1,248)	1:21:A:LEU:HD21	1:22:A:GLU:HA	10	0.4
(1,248)	1:21:A:LEU:HD22	1:22:A:GLU:HA	10	0.4
(1,248)	1:21:A:LEU:HD23	1:22:A:GLU:HA	10	0.4
(1,181)	1:14:A:SER:H	1:15:A:ASP:HA	12	0.4
(1,146)	1:9:A:LYS:H	1:10:A:ASN:HB2	11	0.4
(1,146)	1:9:A:LYS:H	1:10:A:ASN:HB3	11	0.4
(1,146)	1:9:A:LYS:H	1:10:A:ASN:HB2	13	0.4
(1,146)	1:9:A:LYS:H	1:10:A:ASN:HB3	13	0.4
(1,126)	1:7:A:LEU:HG	1:38:A:PHE:H	10	0.4
(1,63)	1:6:A:VAL:HA	1:20:A:GLU:H	19	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,27)	1:5:A:LEU:HG	1:7:A:LEU:H	20	0.4
(1,2)	1:3:A:MET:H	1:4:A:LYS:HA	4	0.4
(1,2)	1:3:A:MET:H	1:4:A:LYS:HA	8	0.4
(1,893)	1:76:A:LEU:HD11	1:78:A:GLU:HG2	1	0.39
(1,893)	1:76:A:LEU:HD11	1:78:A:GLU:HG3	1	0.39
(1,893)	1:76:A:LEU:HD12	1:78:A:GLU:HG2	1	0.39
(1,893)	1:76:A:LEU:HD12	1:78:A:GLU:HG3	1	0.39
(1,893)	1:76:A:LEU:HD13	1:78:A:GLU:HG2	1	0.39
(1,893)	1:76:A:LEU:HD13	1:78:A:GLU:HG3	1	0.39
(1,791)	1:66:A:VAL:HA	1:68:A:VAL:HG11	9	0.39
(1,791)	1:66:A:VAL:HA	1:68:A:VAL:HG12	9	0.39
(1,791)	1:66:A:VAL:HA	1:68:A:VAL:HG13	9	0.39
(1,761)	1:64:A:ASP:H	1:76:A:LEU:HA	9	0.39
(1,441)	1:35:A:ILE:HB	1:37:A:TYR:HA	16	0.39
(1,364)	1:28:A:PHE:HD1	1:32:A:LYS:HA	14	0.39
(1,364)	1:28:A:PHE:HD2	1:32:A:LYS:HA	14	0.39
(1,248)	1:21:A:LEU:HD21	1:22:A:GLU:HA	17	0.39
(1,248)	1:21:A:LEU:HD22	1:22:A:GLU:HA	17	0.39
(1,248)	1:21:A:LEU:HD23	1:22:A:GLU:HA	17	0.39
(1,176)	1:13:A:LYS:H	1:14:A:SER:H	19	0.39
(1,145)	1:9:A:LYS:H	1:10:A:ASN:HA	20	0.39
(1,22)	1:5:A:LEU:HB2	1:36:A:PHE:HA	3	0.39
(1,22)	1:5:A:LEU:HB3	1:36:A:PHE:HA	3	0.39
(1,4)	1:4:A:LYS:HA	1:5:A:LEU:H	18	0.39
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG21	16	0.38
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG22	16	0.38
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG23	16	0.38
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG21	16	0.38
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG22	16	0.38
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG23	16	0.38
(1,881)	1:76:A:LEU:H	1:77:A:TYR:HA	10	0.38
(1,866)	1:74:A:ASP:H	1:75:A:PHE:HA	4	0.38
(1,836)	1:70:A:THR:HA	1:73:A:LYS:HB2	19	0.38
(1,836)	1:70:A:THR:HA	1:73:A:LYS:HB3	19	0.38
(1,835)	1:70:A:THR:HA	1:73:A:LYS:H	7	0.38
(1,823)	1:69:A:SER:HA	1:71:A:ASP:H	16	0.38
(1,820)	1:69:A:SER:H	1:73:A:LYS:HA	2	0.38
(1,819)	1:69:A:SER:H	1:73:A:LYS:H	4	0.38
(1,764)	1:64:A:ASP:H	1:79:A:LEU:H	17	0.38
(1,741)	1:62:A:TYR:HD1	1:63:A:LEU:H	2	0.38
(1,741)	1:62:A:TYR:HD2	1:63:A:LEU:H	2	0.38
(1,692)	1:57:A:LYS:H	1:58:A:GLY:HA2	12	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,595)	1:49:A:LYS:HA	1:52:A:ASP:HA	4	0.38
(1,523)	1:41:A:THR:HA	1:44:A:HIS:HA	1	0.38
(1,474)	1:37:A:TYR:H	1:76:A:LEU:H	14	0.38
(1,458)	1:36:A:PHE:HA	1:76:A:LEU:HD11	15	0.38
(1,458)	1:36:A:PHE:HA	1:76:A:LEU:HD12	15	0.38
(1,458)	1:36:A:PHE:HA	1:76:A:LEU:HD13	15	0.38
(1,433)	1:35:A:ILE:H	1:77:A:TYR:HA	9	0.38
(1,422)	1:34:A:SER:HA	1:78:A:GLU:HB2	4	0.38
(1,422)	1:34:A:SER:HA	1:78:A:GLU:HB3	4	0.38
(1,422)	1:34:A:SER:HA	1:78:A:GLU:HB2	7	0.38
(1,422)	1:34:A:SER:HA	1:78:A:GLU:HB3	7	0.38
(1,405)	1:33:A:ARG:H	1:81:A:ILE:HG21	6	0.38
(1,405)	1:33:A:ARG:H	1:81:A:ILE:HG22	6	0.38
(1,405)	1:33:A:ARG:H	1:81:A:ILE:HG23	6	0.38
(1,405)	1:33:A:ARG:H	1:81:A:ILE:HG21	6	0.38
(1,405)	1:33:A:ARG:H	1:81:A:ILE:HG22	6	0.38
(1,405)	1:33:A:ARG:H	1:81:A:ILE:HG23	6	0.38
(1,364)	1:28:A:PHE:HD1	1:32:A:LYS:HA	12	0.38
(1,364)	1:28:A:PHE:HD2	1:32:A:LYS:HA	12	0.38
(1,355)	1:28:A:PHE:HA	1:32:A:LYS:HB2	2	0.38
(1,355)	1:28:A:PHE:HA	1:32:A:LYS:HB3	2	0.38
(1,318)	1:25:A:TYR:HA	1:59:A:HIS:HA	17	0.38
(1,248)	1:21:A:LEU:HD21	1:22:A:GLU:HA	11	0.38
(1,248)	1:21:A:LEU:HD22	1:22:A:GLU:HA	11	0.38
(1,248)	1:21:A:LEU:HD23	1:22:A:GLU:HA	11	0.38
(1,245)	1:21:A:LEU:HD11	1:53:A:PHE:HA	19	0.38
(1,245)	1:21:A:LEU:HD12	1:53:A:PHE:HA	19	0.38
(1,245)	1:21:A:LEU:HD13	1:53:A:PHE:HA	19	0.38
(1,237)	1:21:A:LEU:HG	1:24:A:LEU:HB2	8	0.38
(1,237)	1:21:A:LEU:HG	1:24:A:LEU:HB3	8	0.38
(1,208)	1:19:A:VAL:HB	1:23:A:ASP:H	19	0.38
(1,204)	1:19:A:VAL:H	1:22:A:GLU:H	8	0.38
(1,174)	1:12:A:ARG:HB2	1:14:A:SER:HA	15	0.38
(1,174)	1:12:A:ARG:HB3	1:14:A:SER:HA	15	0.38
(1,167)	1:11:A:THR:HB	1:12:A:ARG:HA	19	0.38
(1,146)	1:9:A:LYS:H	1:10:A:ASN:HB2	8	0.38
(1,146)	1:9:A:LYS:H	1:10:A:ASN:HB3	8	0.38
(1,106)	1:7:A:LEU:H	1:38:A:PHE:HB2	5	0.38
(1,106)	1:7:A:LEU:H	1:38:A:PHE:HB3	5	0.38
(1,930)	1:81:A:ILE:HA	1:82:A:ILE:H	6	0.37
(1,930)	1:81:A:ILE:HA	1:82:A:ILE:H	17	0.37
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG21	12	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG22	12	0.37
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG23	12	0.37
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG21	12	0.37
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG22	12	0.37
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG23	12	0.37
(1,837)	1:70:A:THR:HA	1:73:A:LYS:HD2	15	0.37
(1,837)	1:70:A:THR:HA	1:73:A:LYS:HD3	15	0.37
(1,811)	1:68:A:VAL:HA	1:73:A:LYS:H	1	0.37
(1,805)	1:67:A:ARG:H	1:68:A:VAL:HG11	16	0.37
(1,805)	1:67:A:ARG:H	1:68:A:VAL:HG12	16	0.37
(1,805)	1:67:A:ARG:H	1:68:A:VAL:HG13	16	0.37
(1,795)	1:66:A:VAL:HA	1:77:A:TYR:HA	19	0.37
(1,791)	1:66:A:VAL:HA	1:68:A:VAL:HG11	4	0.37
(1,791)	1:66:A:VAL:HA	1:68:A:VAL:HG12	4	0.37
(1,791)	1:66:A:VAL:HA	1:68:A:VAL:HG13	4	0.37
(1,675)	1:55:A:LYS:HA	1:57:A:LYS:H	18	0.37
(1,643)	1:53:A:PHE:H	1:55:A:LYS:H	3	0.37
(1,584)	1:48:A:LEU:HA	1:52:A:ASP:HB2	15	0.37
(1,584)	1:48:A:LEU:HA	1:52:A:ASP:HB3	15	0.37
(1,523)	1:41:A:THR:HA	1:44:A:HIS:HA	14	0.37
(1,502)	1:38:A:PHE:HD1	1:75:A:PHE:HA	9	0.37
(1,502)	1:38:A:PHE:HD2	1:75:A:PHE:HA	9	0.37
(1,459)	1:36:A:PHE:HA	1:77:A:TYR:H	2	0.37
(1,437)	1:35:A:ILE:H	1:80:A:HIS:H	20	0.37
(1,432)	1:35:A:ILE:H	1:36:A:PHE:HE1	18	0.37
(1,432)	1:35:A:ILE:H	1:36:A:PHE:HE2	18	0.37
(1,295)	1:24:A:LEU:HG	1:25:A:TYR:HA	5	0.37
(1,284)	1:24:A:LEU:HA	1:35:A:ILE:HD11	1	0.37
(1,284)	1:24:A:LEU:HA	1:35:A:ILE:HD12	1	0.37
(1,284)	1:24:A:LEU:HA	1:35:A:ILE:HD13	1	0.37
(1,245)	1:21:A:LEU:HD11	1:53:A:PHE:HA	15	0.37
(1,245)	1:21:A:LEU:HD12	1:53:A:PHE:HA	15	0.37
(1,245)	1:21:A:LEU:HD13	1:53:A:PHE:HA	15	0.37
(1,237)	1:21:A:LEU:HG	1:24:A:LEU:HB2	15	0.37
(1,237)	1:21:A:LEU:HG	1:24:A:LEU:HB3	15	0.37
(1,157)	1:10:A:ASN:HB2	1:46:A:ASP:H	4	0.37
(1,157)	1:10:A:ASN:HB3	1:46:A:ASP:H	4	0.37
(1,147)	1:9:A:LYS:H	1:11:A:THR:H	19	0.37
(1,142)	1:8:A:ALA:HA	1:46:A:ASP:HA	1	0.37
(1,142)	1:8:A:ALA:HA	1:46:A:ASP:HA	2	0.37
(1,138)	1:8:A:ALA:HA	1:10:A:ASN:HB2	17	0.37
(1,138)	1:8:A:ALA:HA	1:10:A:ASN:HB3	17	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,126)	1:7:A:LEU:HG	1:38:A:PHE:H	8	0.37
(1,63)	1:6:A:VAL:HA	1:20:A:GLU:H	3	0.37
(1,44)	1:6:A:VAL:H	1:20:A:GLU:HB2	2	0.37
(1,44)	1:6:A:VAL:H	1:20:A:GLU:HB3	2	0.37
(1,37)	1:5:A:LEU:HD11	1:38:A:PHE:HB3	14	0.37
(1,37)	1:5:A:LEU:HD12	1:38:A:PHE:HB3	14	0.37
(1,37)	1:5:A:LEU:HD13	1:38:A:PHE:HB3	14	0.37
(1,37)	1:5:A:LEU:HD21	1:38:A:PHE:HB3	14	0.37
(1,37)	1:5:A:LEU:HD22	1:38:A:PHE:HB3	14	0.37
(1,37)	1:5:A:LEU:HD23	1:38:A:PHE:HB3	14	0.37
(1,1)	1:3:A:MET:H	1:4:A:LYS:H	8	0.37
(1,929)	1:81:A:ILE:H	1:82:A:ILE:HA	2	0.36
(1,906)	1:78:A:GLU:HA	1:79:A:LEU:HG	11	0.36
(1,859)	1:72:A:GLU:HB2	1:74:A:ASP:HA	16	0.36
(1,859)	1:72:A:GLU:HB3	1:74:A:ASP:HA	16	0.36
(1,843)	1:71:A:ASP:H	1:73:A:LYS:HA	18	0.36
(1,842)	1:71:A:ASP:H	1:73:A:LYS:H	19	0.36
(1,840)	1:71:A:ASP:H	1:72:A:GLU:H	15	0.36
(1,824)	1:69:A:SER:HA	1:74:A:ASP:H	7	0.36
(1,802)	1:67:A:ARG:H	1:68:A:VAL:H	20	0.36
(1,793)	1:66:A:VAL:HA	1:76:A:LEU:HA	12	0.36
(1,793)	1:66:A:VAL:HA	1:76:A:LEU:HA	14	0.36
(1,727)	1:61:A:ALA:HB1	1:79:A:LEU:HB3	4	0.36
(1,727)	1:61:A:ALA:HB2	1:79:A:LEU:HB3	4	0.36
(1,727)	1:61:A:ALA:HB3	1:79:A:LEU:HB3	4	0.36
(1,675)	1:55:A:LYS:HA	1:57:A:LYS:H	1	0.36
(1,664)	1:54:A:PHE:HD1	1:76:A:LEU:HD11	9	0.36
(1,664)	1:54:A:PHE:HD1	1:76:A:LEU:HD12	9	0.36
(1,664)	1:54:A:PHE:HD1	1:76:A:LEU:HD13	9	0.36
(1,664)	1:54:A:PHE:HD2	1:76:A:LEU:HD11	9	0.36
(1,664)	1:54:A:PHE:HD2	1:76:A:LEU:HD12	9	0.36
(1,664)	1:54:A:PHE:HD2	1:76:A:LEU:HD13	9	0.36
(1,643)	1:53:A:PHE:H	1:55:A:LYS:H	15	0.36
(1,626)	1:51:A:VAL:HG11	1:63:A:LEU:HD11	2	0.36
(1,626)	1:51:A:VAL:HG11	1:63:A:LEU:HD12	2	0.36
(1,626)	1:51:A:VAL:HG11	1:63:A:LEU:HD13	2	0.36
(1,626)	1:51:A:VAL:HG12	1:63:A:LEU:HD11	2	0.36
(1,626)	1:51:A:VAL:HG12	1:63:A:LEU:HD12	2	0.36
(1,626)	1:51:A:VAL:HG12	1:63:A:LEU:HD13	2	0.36
(1,626)	1:51:A:VAL:HG13	1:63:A:LEU:HD11	2	0.36
(1,626)	1:51:A:VAL:HG13	1:63:A:LEU:HD12	2	0.36
(1,626)	1:51:A:VAL:HG13	1:63:A:LEU:HD13	2	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,626)	1:51:A:VAL:HG11	1:63:A:LEU:HD11	2	0.36
(1,626)	1:51:A:VAL:HG11	1:63:A:LEU:HD12	2	0.36
(1,626)	1:51:A:VAL:HG11	1:63:A:LEU:HD13	2	0.36
(1,626)	1:51:A:VAL:HG12	1:63:A:LEU:HD11	2	0.36
(1,626)	1:51:A:VAL:HG12	1:63:A:LEU:HD12	2	0.36
(1,626)	1:51:A:VAL:HG12	1:63:A:LEU:HD13	2	0.36
(1,626)	1:51:A:VAL:HG13	1:63:A:LEU:HD11	2	0.36
(1,626)	1:51:A:VAL:HG13	1:63:A:LEU:HD12	2	0.36
(1,626)	1:51:A:VAL:HG13	1:63:A:LEU:HD13	2	0.36
(1,620)	1:51:A:VAL:HA	1:53:A:PHE:H	17	0.36
(1,584)	1:48:A:LEU:HA	1:52:A:ASP:HB2	6	0.36
(1,584)	1:48:A:LEU:HA	1:52:A:ASP:HB3	6	0.36
(1,584)	1:48:A:LEU:HA	1:52:A:ASP:HB2	7	0.36
(1,584)	1:48:A:LEU:HA	1:52:A:ASP:HB3	7	0.36
(1,584)	1:48:A:LEU:HA	1:52:A:ASP:HB2	18	0.36
(1,584)	1:48:A:LEU:HA	1:52:A:ASP:HB3	18	0.36
(1,527)	1:42:A:ASN:H	1:43:A:ALA:H	9	0.36
(1,502)	1:38:A:PHE:HD1	1:75:A:PHE:HA	6	0.36
(1,502)	1:38:A:PHE:HD2	1:75:A:PHE:HA	6	0.36
(1,502)	1:38:A:PHE:HD1	1:75:A:PHE:HA	12	0.36
(1,502)	1:38:A:PHE:HD2	1:75:A:PHE:HA	12	0.36
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG21	19	0.36
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG22	19	0.36
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG23	19	0.36
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG21	19	0.36
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG22	19	0.36
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG23	19	0.36
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG21	19	0.36
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG22	19	0.36
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG23	19	0.36
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG21	19	0.36
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG22	19	0.36
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG23	19	0.36
(1,356)	1:28:A:PHE:HA	1:33:A:ARG:H	1	0.36
(1,348)	1:28:A:PHE:H	1:30:A:GLU:HG2	4	0.36
(1,348)	1:28:A:PHE:H	1:30:A:GLU:HG3	4	0.36
(1,312)	1:25:A:TYR:H	1:59:A:HIS:HE1	7	0.36
(1,300)	1:24:A:LEU:HD11	1:35:A:ILE:HG12	10	0.36
(1,300)	1:24:A:LEU:HD11	1:35:A:ILE:HG13	10	0.36
(1,300)	1:24:A:LEU:HD12	1:35:A:ILE:HG12	10	0.36
(1,300)	1:24:A:LEU:HD12	1:35:A:ILE:HG13	10	0.36
(1,300)	1:24:A:LEU:HD13	1:35:A:ILE:HG12	10	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,300)	1:24:A:LEU:HD13	1:35:A:ILE:HG13	10	0.36
(1,284)	1:24:A:LEU:HA	1:35:A:ILE:HD11	19	0.36
(1,284)	1:24:A:LEU:HA	1:35:A:ILE:HD12	19	0.36
(1,284)	1:24:A:LEU:HA	1:35:A:ILE:HD13	19	0.36
(1,248)	1:21:A:LEU:HD21	1:22:A:GLU:HA	7	0.36
(1,248)	1:21:A:LEU:HD22	1:22:A:GLU:HA	7	0.36
(1,248)	1:21:A:LEU:HD23	1:22:A:GLU:HA	7	0.36
(1,167)	1:11:A:THR:HB	1:12:A:ARG:HA	12	0.36
(1,156)	1:10:A:ASN:HB2	1:45:A:LYS:HB2	4	0.36
(1,156)	1:10:A:ASN:HB2	1:45:A:LYS:HB3	4	0.36
(1,156)	1:10:A:ASN:HB3	1:45:A:LYS:HB2	4	0.36
(1,156)	1:10:A:ASN:HB3	1:45:A:LYS:HB3	4	0.36
(1,144)	1:9:A:LYS:H	1:10:A:ASN:H	20	0.36
(1,80)	1:6:A:VAL:HG11	1:8:A:ALA:HA	7	0.36
(1,80)	1:6:A:VAL:HG12	1:8:A:ALA:HA	7	0.36
(1,80)	1:6:A:VAL:HG13	1:8:A:ALA:HA	7	0.36
(1,69)	1:6:A:VAL:HB	1:20:A:GLU:H	1	0.36
(1,63)	1:6:A:VAL:HA	1:20:A:GLU:H	4	0.36
(1,63)	1:6:A:VAL:HA	1:20:A:GLU:H	18	0.36
(1,37)	1:5:A:LEU:HD11	1:38:A:PHE:HB3	2	0.36
(1,37)	1:5:A:LEU:HD12	1:38:A:PHE:HB3	2	0.36
(1,37)	1:5:A:LEU:HD13	1:38:A:PHE:HB3	2	0.36
(1,37)	1:5:A:LEU:HD21	1:38:A:PHE:HB3	2	0.36
(1,37)	1:5:A:LEU:HD22	1:38:A:PHE:HB3	2	0.36
(1,37)	1:5:A:LEU:HD23	1:38:A:PHE:HB3	2	0.36
(1,4)	1:4:A:LYS:HA	1:5:A:LEU:H	6	0.36
(1,2)	1:3:A:MET:H	1:4:A:LYS:HA	9	0.36
(1,1)	1:3:A:MET:H	1:4:A:LYS:H	19	0.36
(1,930)	1:81:A:ILE:HA	1:82:A:ILE:H	5	0.35
(1,929)	1:81:A:ILE:H	1:82:A:ILE:HA	10	0.35
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG21	13	0.35
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG22	13	0.35
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG23	13	0.35
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG21	13	0.35
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG22	13	0.35
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG23	13	0.35
(1,923)	1:79:A:LEU:HD11	1:82:A:ILE:HD11	4	0.35
(1,923)	1:79:A:LEU:HD11	1:82:A:ILE:HD12	4	0.35
(1,923)	1:79:A:LEU:HD11	1:82:A:ILE:HD13	4	0.35
(1,923)	1:79:A:LEU:HD12	1:82:A:ILE:HD11	4	0.35
(1,923)	1:79:A:LEU:HD12	1:82:A:ILE:HD12	4	0.35
(1,923)	1:79:A:LEU:HD12	1:82:A:ILE:HD13	4	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,923)	1:79:A:LEU:HD13	1:82:A:ILE:HD11	4	0.35
(1,923)	1:79:A:LEU:HD13	1:82:A:ILE:HD12	4	0.35
(1,923)	1:79:A:LEU:HD13	1:82:A:ILE:HD13	4	0.35
(1,906)	1:78:A:GLU:HA	1:79:A:LEU:HG	4	0.35
(1,841)	1:71:A:ASP:H	1:72:A:GLU:HA	11	0.35
(1,840)	1:71:A:ASP:H	1:72:A:GLU:H	6	0.35
(1,840)	1:71:A:ASP:H	1:72:A:GLU:H	18	0.35
(1,836)	1:70:A:THR:HA	1:73:A:LYS:HB2	17	0.35
(1,836)	1:70:A:THR:HA	1:73:A:LYS:HB3	17	0.35
(1,795)	1:66:A:VAL:HA	1:77:A:TYR:HA	20	0.35
(1,793)	1:66:A:VAL:HA	1:76:A:LEU:HA	15	0.35
(1,584)	1:48:A:LEU:HA	1:52:A:ASP:HB2	1	0.35
(1,584)	1:48:A:LEU:HA	1:52:A:ASP:HB3	1	0.35
(1,527)	1:42:A:ASN:H	1:43:A:ALA:H	4	0.35
(1,525)	1:41:A:THR:HB	1:73:A:LYS:HB2	17	0.35
(1,525)	1:41:A:THR:HB	1:73:A:LYS:HB3	17	0.35
(1,489)	1:38:A:PHE:H	1:75:A:PHE:HA	1	0.35
(1,474)	1:37:A:TYR:H	1:76:A:LEU:H	3	0.35
(1,461)	1:36:A:PHE:HA	1:77:A:TYR:HD1	17	0.35
(1,461)	1:36:A:PHE:HA	1:77:A:TYR:HD2	17	0.35
(1,274)	1:23:A:ASP:HB2	1:35:A:ILE:HB	6	0.35
(1,274)	1:23:A:ASP:HB3	1:35:A:ILE:HB	6	0.35
(1,240)	1:21:A:LEU:HG	1:57:A:LYS:HB2	5	0.35
(1,240)	1:21:A:LEU:HG	1:57:A:LYS:HB3	5	0.35
(1,174)	1:12:A:ARG:HB2	1:14:A:SER:HA	13	0.35
(1,174)	1:12:A:ARG:HB3	1:14:A:SER:HA	13	0.35
(1,156)	1:10:A:ASN:HB2	1:45:A:LYS:HB2	9	0.35
(1,156)	1:10:A:ASN:HB2	1:45:A:LYS:HB3	9	0.35
(1,156)	1:10:A:ASN:HB3	1:45:A:LYS:HB2	9	0.35
(1,156)	1:10:A:ASN:HB3	1:45:A:LYS:HB3	9	0.35
(1,147)	1:9:A:LYS:H	1:11:A:THR:H	6	0.35
(1,145)	1:9:A:LYS:H	1:10:A:ASN:HA	11	0.35
(1,130)	1:7:A:LEU:HD11	1:16:A:ALA:HA	14	0.35
(1,130)	1:7:A:LEU:HD12	1:16:A:ALA:HA	14	0.35
(1,130)	1:7:A:LEU:HD13	1:16:A:ALA:HA	14	0.35
(1,127)	1:7:A:LEU:HG	1:38:A:PHE:HB2	11	0.35
(1,127)	1:7:A:LEU:HG	1:38:A:PHE:HB3	11	0.35
(1,126)	1:7:A:LEU:HG	1:38:A:PHE:H	9	0.35
(1,63)	1:6:A:VAL:HA	1:20:A:GLU:H	6	0.35
(1,28)	1:5:A:LEU:HG	1:7:A:LEU:HG	14	0.35
(1,19)	1:5:A:LEU:HB2	1:35:A:ILE:HA	18	0.35
(1,19)	1:5:A:LEU:HB3	1:35:A:ILE:HA	18	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,8)	1:5:A:LEU:H	1:35:A:ILE:HB	6	0.35
(1,928)	1:81:A:ILE:H	1:82:A:ILE:H	10	0.34
(1,890)	1:76:A:LEU:HD11	1:78:A:GLU:H	10	0.34
(1,890)	1:76:A:LEU:HD12	1:78:A:GLU:H	10	0.34
(1,890)	1:76:A:LEU:HD13	1:78:A:GLU:H	10	0.34
(1,865)	1:74:A:ASP:H	1:75:A:PHE:H	9	0.34
(1,865)	1:74:A:ASP:H	1:75:A:PHE:H	19	0.34
(1,842)	1:71:A:ASP:H	1:73:A:LYS:H	3	0.34
(1,841)	1:71:A:ASP:H	1:72:A:GLU:HA	2	0.34
(1,841)	1:71:A:ASP:H	1:72:A:GLU:HA	9	0.34
(1,800)	1:66:A:VAL:HG11	1:72:A:GLU:H	3	0.34
(1,800)	1:66:A:VAL:HG12	1:72:A:GLU:H	3	0.34
(1,800)	1:66:A:VAL:HG13	1:72:A:GLU:H	3	0.34
(1,800)	1:66:A:VAL:HG21	1:72:A:GLU:H	3	0.34
(1,800)	1:66:A:VAL:HG22	1:72:A:GLU:H	3	0.34
(1,800)	1:66:A:VAL:HG23	1:72:A:GLU:H	3	0.34
(1,783)	1:65:A:GLU:HB2	1:66:A:VAL:HG11	3	0.34
(1,783)	1:65:A:GLU:HB2	1:66:A:VAL:HG12	3	0.34
(1,783)	1:65:A:GLU:HB2	1:66:A:VAL:HG13	3	0.34
(1,783)	1:65:A:GLU:HB3	1:66:A:VAL:HG11	3	0.34
(1,783)	1:65:A:GLU:HB3	1:66:A:VAL:HG12	3	0.34
(1,783)	1:65:A:GLU:HB3	1:66:A:VAL:HG13	3	0.34
(1,741)	1:62:A:TYR:HD1	1:63:A:LEU:H	18	0.34
(1,741)	1:62:A:TYR:HD2	1:63:A:LEU:H	18	0.34
(1,643)	1:53:A:PHE:H	1:55:A:LYS:H	11	0.34
(1,628)	1:51:A:VAL:HG21	1:54:A:PHE:HD1	6	0.34
(1,628)	1:51:A:VAL:HG21	1:54:A:PHE:HD2	6	0.34
(1,628)	1:51:A:VAL:HG22	1:54:A:PHE:HD1	6	0.34
(1,628)	1:51:A:VAL:HG22	1:54:A:PHE:HD2	6	0.34
(1,628)	1:51:A:VAL:HG23	1:54:A:PHE:HD1	6	0.34
(1,628)	1:51:A:VAL:HG23	1:54:A:PHE:HD2	6	0.34
(1,620)	1:51:A:VAL:HA	1:53:A:PHE:H	14	0.34
(1,620)	1:51:A:VAL:HA	1:53:A:PHE:H	18	0.34
(1,543)	1:44:A:HIS:HA	1:48:A:LEU:H	13	0.34
(1,527)	1:42:A:ASN:H	1:43:A:ALA:H	14	0.34
(1,505)	1:39:A:ALA:H	1:74:A:ASP:H	4	0.34
(1,502)	1:38:A:PHE:HD1	1:75:A:PHE:HA	20	0.34
(1,502)	1:38:A:PHE:HD2	1:75:A:PHE:HA	20	0.34
(1,413)	1:33:A:ARG:HB2	1:34:A:SER:HA	11	0.34
(1,413)	1:33:A:ARG:HB3	1:34:A:SER:HA	11	0.34
(1,366)	1:28:A:PHE:HD1	1:80:A:HIS:HB2	2	0.34
(1,366)	1:28:A:PHE:HD1	1:80:A:HIS:HB3	2	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,366)	1:28:A:PHE:HD2	1:80:A:HIS:HB2	2	0.34
(1,366)	1:28:A:PHE:HD2	1:80:A:HIS:HB3	2	0.34
(1,364)	1:28:A:PHE:HD1	1:32:A:LYS:HA	7	0.34
(1,364)	1:28:A:PHE:HD2	1:32:A:LYS:HA	7	0.34
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG21	5	0.34
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG22	5	0.34
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG23	5	0.34
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG21	5	0.34
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG22	5	0.34
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG23	5	0.34
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG21	5	0.34
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG22	5	0.34
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG23	5	0.34
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG21	5	0.34
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG22	5	0.34
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG23	5	0.34
(1,348)	1:28:A:PHE:H	1:30:A:GLU:HG2	10	0.34
(1,348)	1:28:A:PHE:H	1:30:A:GLU:HG3	10	0.34
(1,348)	1:28:A:PHE:H	1:30:A:GLU:HG2	11	0.34
(1,348)	1:28:A:PHE:H	1:30:A:GLU:HG3	11	0.34
(1,327)	1:26:A:HIS:H	1:28:A:PHE:HB2	20	0.34
(1,327)	1:26:A:HIS:H	1:28:A:PHE:HB3	20	0.34
(1,299)	1:24:A:LEU:HD11	1:35:A:ILE:HG21	6	0.34
(1,299)	1:24:A:LEU:HD11	1:35:A:ILE:HG22	6	0.34
(1,299)	1:24:A:LEU:HD11	1:35:A:ILE:HG23	6	0.34
(1,299)	1:24:A:LEU:HD12	1:35:A:ILE:HG21	6	0.34
(1,299)	1:24:A:LEU:HD12	1:35:A:ILE:HG22	6	0.34
(1,299)	1:24:A:LEU:HD12	1:35:A:ILE:HG23	6	0.34
(1,299)	1:24:A:LEU:HD13	1:35:A:ILE:HG21	6	0.34
(1,299)	1:24:A:LEU:HD13	1:35:A:ILE:HG22	6	0.34
(1,299)	1:24:A:LEU:HD13	1:35:A:ILE:HG23	6	0.34
(1,180)	1:14:A:SER:H	1:15:A:ASP:H	18	0.34
(1,165)	1:11:A:THR:HA	1:40:A:PRO:HG2	8	0.34
(1,165)	1:11:A:THR:HA	1:40:A:PRO:HG3	8	0.34
(1,147)	1:9:A:LYS:H	1:11:A:THR:H	20	0.34
(1,145)	1:9:A:LYS:H	1:10:A:ASN:HA	4	0.34
(1,145)	1:9:A:LYS:H	1:10:A:ASN:HA	6	0.34
(1,123)	1:7:A:LEU:HB2	1:38:A:PHE:HD1	10	0.34
(1,123)	1:7:A:LEU:HB2	1:38:A:PHE:HD2	10	0.34
(1,123)	1:7:A:LEU:HB3	1:38:A:PHE:HD1	10	0.34
(1,123)	1:7:A:LEU:HB3	1:38:A:PHE:HD2	10	0.34
(1,60)	1:6:A:VAL:HA	1:16:A:ALA:HB1	1	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,60)	1:6:A:VAL:HA	1:16:A:ALA:HB2	1	0.34
(1,60)	1:6:A:VAL:HA	1:16:A:ALA:HB3	1	0.34
(1,16)	1:5:A:LEU:HA	1:37:A:TYR:H	11	0.34
(1,908)	1:78:A:GLU:HA	1:80:A:HIS:HD2	4	0.33
(1,890)	1:76:A:LEU:HD11	1:78:A:GLU:H	17	0.33
(1,890)	1:76:A:LEU:HD12	1:78:A:GLU:H	17	0.33
(1,890)	1:76:A:LEU:HD13	1:78:A:GLU:H	17	0.33
(1,842)	1:71:A:ASP:H	1:73:A:LYS:H	4	0.33
(1,841)	1:71:A:ASP:H	1:72:A:GLU:HA	7	0.33
(1,840)	1:71:A:ASP:H	1:72:A:GLU:H	1	0.33
(1,840)	1:71:A:ASP:H	1:72:A:GLU:H	10	0.33
(1,819)	1:69:A:SER:H	1:73:A:LYS:H	15	0.33
(1,807)	1:68:A:VAL:H	1:69:A:SER:HA	4	0.33
(1,801)	1:66:A:VAL:HG11	1:72:A:GLU:HB2	5	0.33
(1,801)	1:66:A:VAL:HG11	1:72:A:GLU:HB3	5	0.33
(1,801)	1:66:A:VAL:HG12	1:72:A:GLU:HB2	5	0.33
(1,801)	1:66:A:VAL:HG12	1:72:A:GLU:HB3	5	0.33
(1,801)	1:66:A:VAL:HG13	1:72:A:GLU:HB2	5	0.33
(1,801)	1:66:A:VAL:HG13	1:72:A:GLU:HB3	5	0.33
(1,801)	1:66:A:VAL:HG21	1:72:A:GLU:HB2	5	0.33
(1,801)	1:66:A:VAL:HG21	1:72:A:GLU:HB3	5	0.33
(1,801)	1:66:A:VAL:HG22	1:72:A:GLU:HB2	5	0.33
(1,801)	1:66:A:VAL:HG22	1:72:A:GLU:HB3	5	0.33
(1,801)	1:66:A:VAL:HG23	1:72:A:GLU:HB2	5	0.33
(1,801)	1:66:A:VAL:HG23	1:72:A:GLU:HB3	5	0.33
(1,692)	1:57:A:LYS:H	1:58:A:GLY:HA2	19	0.33
(1,668)	1:55:A:LYS:H	1:56:A:GLU:H	14	0.33
(1,643)	1:53:A:PHE:H	1:55:A:LYS:H	17	0.33
(1,437)	1:35:A:ILE:H	1:80:A:HIS:H	4	0.33
(1,426)	1:34:A:SER:HB2	1:36:A:PHE:HE1	7	0.33
(1,426)	1:34:A:SER:HB2	1:36:A:PHE:HE2	7	0.33
(1,426)	1:34:A:SER:HB3	1:36:A:PHE:HE1	7	0.33
(1,426)	1:34:A:SER:HB3	1:36:A:PHE:HE2	7	0.33
(1,370)	1:28:A:PHE:HE1	1:81:A:ILE:HA	1	0.33
(1,370)	1:28:A:PHE:HE2	1:81:A:ILE:HA	1	0.33
(1,355)	1:28:A:PHE:HA	1:32:A:LYS:HB2	19	0.33
(1,355)	1:28:A:PHE:HA	1:32:A:LYS:HB3	19	0.33
(1,335)	1:26:A:HIS:HB2	1:30:A:GLU:HB2	3	0.33
(1,335)	1:26:A:HIS:HB2	1:30:A:GLU:HB3	3	0.33
(1,335)	1:26:A:HIS:HB3	1:30:A:GLU:HB2	3	0.33
(1,335)	1:26:A:HIS:HB3	1:30:A:GLU:HB3	3	0.33
(1,335)	1:26:A:HIS:HB2	1:30:A:GLU:HB2	5	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,335)	1:26:A:HIS:HB2	1:30:A:GLU:HB3	5	0.33
(1,335)	1:26:A:HIS:HB3	1:30:A:GLU:HB2	5	0.33
(1,335)	1:26:A:HIS:HB3	1:30:A:GLU:HB3	5	0.33
(1,306)	1:24:A:LEU:HD21	1:60:A:THR:HB	1	0.33
(1,306)	1:24:A:LEU:HD22	1:60:A:THR:HB	1	0.33
(1,306)	1:24:A:LEU:HD23	1:60:A:THR:HB	1	0.33
(1,301)	1:24:A:LEU:HD11	1:60:A:THR:HB	11	0.33
(1,301)	1:24:A:LEU:HD12	1:60:A:THR:HB	11	0.33
(1,301)	1:24:A:LEU:HD13	1:60:A:THR:HB	11	0.33
(1,299)	1:24:A:LEU:HD11	1:35:A:ILE:HG21	13	0.33
(1,299)	1:24:A:LEU:HD11	1:35:A:ILE:HG22	13	0.33
(1,299)	1:24:A:LEU:HD11	1:35:A:ILE:HG23	13	0.33
(1,299)	1:24:A:LEU:HD12	1:35:A:ILE:HG21	13	0.33
(1,299)	1:24:A:LEU:HD12	1:35:A:ILE:HG22	13	0.33
(1,299)	1:24:A:LEU:HD12	1:35:A:ILE:HG23	13	0.33
(1,299)	1:24:A:LEU:HD13	1:35:A:ILE:HG21	13	0.33
(1,299)	1:24:A:LEU:HD13	1:35:A:ILE:HG22	13	0.33
(1,299)	1:24:A:LEU:HD13	1:35:A:ILE:HG23	13	0.33
(1,292)	1:24:A:LEU:HB2	1:60:A:THR:H	1	0.33
(1,292)	1:24:A:LEU:HB3	1:60:A:THR:H	1	0.33
(1,202)	1:19:A:VAL:H	1:20:A:GLU:HG2	14	0.33
(1,202)	1:19:A:VAL:H	1:20:A:GLU:HG3	14	0.33
(1,179)	1:13:A:LYS:HA	1:14:A:SER:H	6	0.33
(1,176)	1:13:A:LYS:H	1:14:A:SER:H	12	0.33
(1,167)	1:11:A:THR:HB	1:12:A:ARG:HA	9	0.33
(1,156)	1:10:A:ASN:HB2	1:45:A:LYS:HB2	18	0.33
(1,156)	1:10:A:ASN:HB2	1:45:A:LYS:HB3	18	0.33
(1,156)	1:10:A:ASN:HB3	1:45:A:LYS:HB2	18	0.33
(1,156)	1:10:A:ASN:HB3	1:45:A:LYS:HB3	18	0.33
(1,155)	1:10:A:ASN:HA	1:40:A:PRO:HG2	20	0.33
(1,155)	1:10:A:ASN:HA	1:40:A:PRO:HG3	20	0.33
(1,146)	1:9:A:LYS:H	1:10:A:ASN:HB2	20	0.33
(1,146)	1:9:A:LYS:H	1:10:A:ASN:HB3	20	0.33
(1,144)	1:9:A:LYS:H	1:10:A:ASN:H	7	0.33
(1,144)	1:9:A:LYS:H	1:10:A:ASN:H	16	0.33
(1,142)	1:8:A:ALA:HA	1:46:A:ASP:HA	17	0.33
(1,123)	1:7:A:LEU:HB2	1:38:A:PHE:HD1	3	0.33
(1,123)	1:7:A:LEU:HB2	1:38:A:PHE:HD2	3	0.33
(1,123)	1:7:A:LEU:HB3	1:38:A:PHE:HD1	3	0.33
(1,123)	1:7:A:LEU:HB3	1:38:A:PHE:HD2	3	0.33
(1,115)	1:7:A:LEU:HA	1:38:A:PHE:HB2	18	0.33
(1,115)	1:7:A:LEU:HA	1:38:A:PHE:HB3	18	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,88)	1:6:A:VAL:HG21	1:19:A:VAL:HB	1	0.33
(1,88)	1:6:A:VAL:HG22	1:19:A:VAL:HB	1	0.33
(1,88)	1:6:A:VAL:HG23	1:19:A:VAL:HB	1	0.33
(1,62)	1:6:A:VAL:HA	1:19:A:VAL:HG11	13	0.33
(1,62)	1:6:A:VAL:HA	1:19:A:VAL:HG12	13	0.33
(1,62)	1:6:A:VAL:HA	1:19:A:VAL:HG13	13	0.33
(1,44)	1:6:A:VAL:H	1:20:A:GLU:HB2	1	0.33
(1,44)	1:6:A:VAL:H	1:20:A:GLU:HB3	1	0.33
(1,906)	1:78:A:GLU:HA	1:79:A:LEU:HG	3	0.32
(1,890)	1:76:A:LEU:HD11	1:78:A:GLU:H	5	0.32
(1,890)	1:76:A:LEU:HD12	1:78:A:GLU:H	5	0.32
(1,890)	1:76:A:LEU:HD13	1:78:A:GLU:H	5	0.32
(1,875)	1:75:A:PHE:HB2	1:76:A:LEU:H	1	0.32
(1,875)	1:75:A:PHE:HB3	1:76:A:LEU:H	1	0.32
(1,842)	1:71:A:ASP:H	1:73:A:LYS:H	14	0.32
(1,840)	1:71:A:ASP:H	1:72:A:GLU:H	17	0.32
(1,836)	1:70:A:THR:HA	1:73:A:LYS:HB2	2	0.32
(1,836)	1:70:A:THR:HA	1:73:A:LYS:HB3	2	0.32
(1,831)	1:70:A:THR:H	1:73:A:LYS:HA	13	0.32
(1,824)	1:69:A:SER:HA	1:74:A:ASP:H	13	0.32
(1,819)	1:69:A:SER:H	1:73:A:LYS:H	14	0.32
(1,814)	1:68:A:VAL:HG11	1:73:A:LYS:H	5	0.32
(1,814)	1:68:A:VAL:HG12	1:73:A:LYS:H	5	0.32
(1,814)	1:68:A:VAL:HG13	1:73:A:LYS:H	5	0.32
(1,814)	1:68:A:VAL:HG21	1:73:A:LYS:H	5	0.32
(1,814)	1:68:A:VAL:HG22	1:73:A:LYS:H	5	0.32
(1,814)	1:68:A:VAL:HG23	1:73:A:LYS:H	5	0.32
(1,805)	1:67:A:ARG:H	1:68:A:VAL:HG11	5	0.32
(1,805)	1:67:A:ARG:H	1:68:A:VAL:HG12	5	0.32
(1,805)	1:67:A:ARG:H	1:68:A:VAL:HG13	5	0.32
(1,800)	1:66:A:VAL:HG11	1:72:A:GLU:H	7	0.32
(1,800)	1:66:A:VAL:HG12	1:72:A:GLU:H	7	0.32
(1,800)	1:66:A:VAL:HG13	1:72:A:GLU:H	7	0.32
(1,800)	1:66:A:VAL:HG21	1:72:A:GLU:H	7	0.32
(1,800)	1:66:A:VAL:HG22	1:72:A:GLU:H	7	0.32
(1,800)	1:66:A:VAL:HG23	1:72:A:GLU:H	7	0.32
(1,793)	1:66:A:VAL:HA	1:76:A:LEU:HA	17	0.32
(1,764)	1:64:A:ASP:H	1:79:A:LEU:H	16	0.32
(1,741)	1:62:A:TYR:HD1	1:63:A:LEU:H	10	0.32
(1,741)	1:62:A:TYR:HD2	1:63:A:LEU:H	10	0.32
(1,732)	1:62:A:TYR:H	1:81:A:ILE:H	1	0.32
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD11	2	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD12	2	0.32
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD13	2	0.32
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD11	2	0.32
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD12	2	0.32
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD13	2	0.32
(1,494)	1:38:A:PHE:HA	1:75:A:PHE:HE1	9	0.32
(1,494)	1:38:A:PHE:HA	1:75:A:PHE:HE2	9	0.32
(1,437)	1:35:A:ILE:H	1:80:A:HIS:H	14	0.32
(1,437)	1:35:A:ILE:H	1:80:A:HIS:H	19	0.32
(1,431)	1:35:A:ILE:H	1:36:A:PHE:HD1	12	0.32
(1,431)	1:35:A:ILE:H	1:36:A:PHE:HD2	12	0.32
(1,355)	1:28:A:PHE:HA	1:32:A:LYS:HB2	3	0.32
(1,355)	1:28:A:PHE:HA	1:32:A:LYS:HB3	3	0.32
(1,354)	1:28:A:PHE:HA	1:30:A:GLU:H	7	0.32
(1,348)	1:28:A:PHE:H	1:30:A:GLU:HG2	1	0.32
(1,348)	1:28:A:PHE:H	1:30:A:GLU:HG3	1	0.32
(1,342)	1:27:A:GLU:HA	1:29:A:SER:H	13	0.32
(1,298)	1:24:A:LEU:HG	1:80:A:HIS:HE1	20	0.32
(1,274)	1:23:A:ASP:HB2	1:35:A:ILE:HB	3	0.32
(1,274)	1:23:A:ASP:HB3	1:35:A:ILE:HB	3	0.32
(1,274)	1:23:A:ASP:HB2	1:35:A:ILE:HB	11	0.32
(1,274)	1:23:A:ASP:HB3	1:35:A:ILE:HB	11	0.32
(1,245)	1:21:A:LEU:HD11	1:53:A:PHE:HA	3	0.32
(1,245)	1:21:A:LEU:HD12	1:53:A:PHE:HA	3	0.32
(1,245)	1:21:A:LEU:HD13	1:53:A:PHE:HA	3	0.32
(1,220)	1:20:A:GLU:HA	1:24:A:LEU:HA	8	0.32
(1,207)	1:19:A:VAL:HB	1:22:A:GLU:H	20	0.32
(1,200)	1:18:A:SER:HB2	1:22:A:GLU:HG2	20	0.32
(1,200)	1:18:A:SER:HB2	1:22:A:GLU:HG3	20	0.32
(1,200)	1:18:A:SER:HB3	1:22:A:GLU:HG2	20	0.32
(1,200)	1:18:A:SER:HB3	1:22:A:GLU:HG3	20	0.32
(1,176)	1:13:A:LYS:H	1:14:A:SER:H	17	0.32
(1,174)	1:12:A:ARG:HB2	1:14:A:SER:HA	18	0.32
(1,174)	1:12:A:ARG:HB3	1:14:A:SER:HA	18	0.32
(1,146)	1:9:A:LYS:H	1:10:A:ASN:HB2	7	0.32
(1,146)	1:9:A:LYS:H	1:10:A:ASN:HB3	7	0.32
(1,145)	1:9:A:LYS:H	1:10:A:ASN:HA	16	0.32
(1,144)	1:9:A:LYS:H	1:10:A:ASN:H	10	0.32
(1,127)	1:7:A:LEU:HG	1:38:A:PHE:HB2	3	0.32
(1,127)	1:7:A:LEU:HG	1:38:A:PHE:HB3	3	0.32
(1,126)	1:7:A:LEU:HG	1:38:A:PHE:H	14	0.32
(1,92)	1:6:A:VAL:HG21	1:35:A:ILE:HB	11	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,92)	1:6:A:VAL:HG22	1:35:A:ILE:HB	11	0.32
(1,92)	1:6:A:VAL:HG23	1:35:A:ILE:HB	11	0.32
(1,63)	1:6:A:VAL:HA	1:20:A:GLU:H	2	0.32
(1,33)	1:5:A:LEU:HD11	1:7:A:LEU:HA	7	0.32
(1,33)	1:5:A:LEU:HD12	1:7:A:LEU:HA	7	0.32
(1,33)	1:5:A:LEU:HD13	1:7:A:LEU:HA	7	0.32
(1,33)	1:5:A:LEU:HD21	1:7:A:LEU:HA	7	0.32
(1,33)	1:5:A:LEU:HD22	1:7:A:LEU:HA	7	0.32
(1,33)	1:5:A:LEU:HD23	1:7:A:LEU:HA	7	0.32
(1,19)	1:5:A:LEU:HB2	1:35:A:ILE:HA	6	0.32
(1,19)	1:5:A:LEU:HB3	1:35:A:ILE:HA	6	0.32
(1,19)	1:5:A:LEU:HB2	1:35:A:ILE:HA	8	0.32
(1,19)	1:5:A:LEU:HB3	1:35:A:ILE:HA	8	0.32
(1,4)	1:4:A:LYS:HA	1:5:A:LEU:H	10	0.32
(1,930)	1:81:A:ILE:HA	1:82:A:ILE:H	9	0.31
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG21	5	0.31
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG22	5	0.31
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG23	5	0.31
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG21	5	0.31
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG22	5	0.31
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG23	5	0.31
(1,865)	1:74:A:ASP:H	1:75:A:PHE:H	18	0.31
(1,843)	1:71:A:ASP:H	1:73:A:LYS:HA	6	0.31
(1,836)	1:70:A:THR:HA	1:73:A:LYS:HB2	4	0.31
(1,836)	1:70:A:THR:HA	1:73:A:LYS:HB3	4	0.31
(1,802)	1:67:A:ARG:H	1:68:A:VAL:H	17	0.31
(1,768)	1:64:A:ASP:HA	1:76:A:LEU:HD21	18	0.31
(1,768)	1:64:A:ASP:HA	1:76:A:LEU:HD22	18	0.31
(1,768)	1:64:A:ASP:HA	1:76:A:LEU:HD23	18	0.31
(1,764)	1:64:A:ASP:H	1:79:A:LEU:H	10	0.31
(1,755)	1:63:A:LEU:HG	1:64:A:ASP:HA	12	0.31
(1,732)	1:62:A:TYR:H	1:81:A:ILE:H	3	0.31
(1,726)	1:61:A:ALA:HA	1:81:A:ILE:HA	4	0.31
(1,721)	1:61:A:ALA:H	1:78:A:GLU:HB2	19	0.31
(1,721)	1:61:A:ALA:H	1:78:A:GLU:HB3	19	0.31
(1,671)	1:55:A:LYS:H	1:57:A:LYS:H	14	0.31
(1,527)	1:42:A:ASN:H	1:43:A:ALA:H	7	0.31
(1,527)	1:42:A:ASN:H	1:43:A:ALA:H	12	0.31
(1,426)	1:34:A:SER:HB2	1:36:A:PHE:HE1	18	0.31
(1,426)	1:34:A:SER:HB2	1:36:A:PHE:HE2	18	0.31
(1,426)	1:34:A:SER:HB3	1:36:A:PHE:HE1	18	0.31
(1,426)	1:34:A:SER:HB3	1:36:A:PHE:HE2	18	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,410)	1:33:A:ARG:HA	1:81:A:ILE:HG21	3	0.31
(1,410)	1:33:A:ARG:HA	1:81:A:ILE:HG22	3	0.31
(1,410)	1:33:A:ARG:HA	1:81:A:ILE:HG23	3	0.31
(1,356)	1:28:A:PHE:HA	1:33:A:ARG:H	16	0.31
(1,354)	1:28:A:PHE:HA	1:30:A:GLU:H	17	0.31
(1,342)	1:27:A:GLU:HA	1:29:A:SER:H	14	0.31
(1,284)	1:24:A:LEU:HA	1:35:A:ILE:HD11	7	0.31
(1,284)	1:24:A:LEU:HA	1:35:A:ILE:HD12	7	0.31
(1,284)	1:24:A:LEU:HA	1:35:A:ILE:HD13	7	0.31
(1,284)	1:24:A:LEU:HA	1:35:A:ILE:HD11	8	0.31
(1,284)	1:24:A:LEU:HA	1:35:A:ILE:HD12	8	0.31
(1,284)	1:24:A:LEU:HA	1:35:A:ILE:HD13	8	0.31
(1,284)	1:24:A:LEU:HA	1:35:A:ILE:HD11	10	0.31
(1,284)	1:24:A:LEU:HA	1:35:A:ILE:HD12	10	0.31
(1,284)	1:24:A:LEU:HA	1:35:A:ILE:HD13	10	0.31
(1,270)	1:23:A:ASP:HA	1:28:A:PHE:H	1	0.31
(1,270)	1:23:A:ASP:HA	1:28:A:PHE:H	14	0.31
(1,264)	1:23:A:ASP:H	1:27:A:GLU:H	14	0.31
(1,248)	1:21:A:LEU:HD21	1:22:A:GLU:HA	2	0.31
(1,248)	1:21:A:LEU:HD22	1:22:A:GLU:HA	2	0.31
(1,248)	1:21:A:LEU:HD23	1:22:A:GLU:HA	2	0.31
(1,208)	1:19:A:VAL:HB	1:23:A:ASP:H	1	0.31
(1,208)	1:19:A:VAL:HB	1:23:A:ASP:H	2	0.31
(1,207)	1:19:A:VAL:HB	1:22:A:GLU:H	3	0.31
(1,204)	1:19:A:VAL:H	1:22:A:GLU:H	1	0.31
(1,167)	1:11:A:THR:HB	1:12:A:ARG:HA	4	0.31
(1,167)	1:11:A:THR:HB	1:12:A:ARG:HA	10	0.31
(1,158)	1:10:A:ASN:HB2	1:46:A:ASP:HA	17	0.31
(1,158)	1:10:A:ASN:HB3	1:46:A:ASP:HA	17	0.31
(1,146)	1:9:A:LYS:H	1:10:A:ASN:HB2	18	0.31
(1,146)	1:9:A:LYS:H	1:10:A:ASN:HB3	18	0.31
(1,142)	1:8:A:ALA:HA	1:46:A:ASP:HA	10	0.31
(1,127)	1:7:A:LEU:HG	1:38:A:PHE:HB2	9	0.31
(1,127)	1:7:A:LEU:HG	1:38:A:PHE:HB3	9	0.31
(1,127)	1:7:A:LEU:HG	1:38:A:PHE:HB2	14	0.31
(1,127)	1:7:A:LEU:HG	1:38:A:PHE:HB3	14	0.31
(1,123)	1:7:A:LEU:HB2	1:38:A:PHE:HD1	20	0.31
(1,123)	1:7:A:LEU:HB2	1:38:A:PHE:HD2	20	0.31
(1,123)	1:7:A:LEU:HB3	1:38:A:PHE:HD1	20	0.31
(1,123)	1:7:A:LEU:HB3	1:38:A:PHE:HD2	20	0.31
(1,107)	1:7:A:LEU:H	1:38:A:PHE:HD1	15	0.31
(1,107)	1:7:A:LEU:H	1:38:A:PHE:HD2	15	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,74)	1:6:A:VAL:HB	1:38:A:PHE:H	6	0.31
(1,74)	1:6:A:VAL:HB	1:38:A:PHE:H	12	0.31
(1,25)	1:5:A:LEU:HG	1:6:A:VAL:HA	2	0.31
(1,4)	1:4:A:LYS:HA	1:5:A:LEU:H	7	0.31
(1,906)	1:78:A:GLU:HA	1:79:A:LEU:HG	13	0.3
(1,875)	1:75:A:PHE:HB2	1:76:A:LEU:H	18	0.3
(1,875)	1:75:A:PHE:HB3	1:76:A:LEU:H	18	0.3
(1,841)	1:71:A:ASP:H	1:72:A:GLU:HA	10	0.3
(1,836)	1:70:A:THR:HA	1:73:A:LYS:HB2	5	0.3
(1,836)	1:70:A:THR:HA	1:73:A:LYS:HB3	5	0.3
(1,823)	1:69:A:SER:HA	1:71:A:ASP:H	5	0.3
(1,823)	1:69:A:SER:HA	1:71:A:ASP:H	19	0.3
(1,811)	1:68:A:VAL:HA	1:73:A:LYS:H	2	0.3
(1,811)	1:68:A:VAL:HA	1:73:A:LYS:H	5	0.3
(1,801)	1:66:A:VAL:HG11	1:72:A:GLU:HB2	6	0.3
(1,801)	1:66:A:VAL:HG11	1:72:A:GLU:HB3	6	0.3
(1,801)	1:66:A:VAL:HG12	1:72:A:GLU:HB2	6	0.3
(1,801)	1:66:A:VAL:HG12	1:72:A:GLU:HB3	6	0.3
(1,801)	1:66:A:VAL:HG13	1:72:A:GLU:HB2	6	0.3
(1,801)	1:66:A:VAL:HG13	1:72:A:GLU:HB3	6	0.3
(1,801)	1:66:A:VAL:HG21	1:72:A:GLU:HB2	6	0.3
(1,801)	1:66:A:VAL:HG21	1:72:A:GLU:HB3	6	0.3
(1,801)	1:66:A:VAL:HG22	1:72:A:GLU:HB2	6	0.3
(1,801)	1:66:A:VAL:HG22	1:72:A:GLU:HB3	6	0.3
(1,801)	1:66:A:VAL:HG23	1:72:A:GLU:HB2	6	0.3
(1,801)	1:66:A:VAL:HG23	1:72:A:GLU:HB3	6	0.3
(1,800)	1:66:A:VAL:HG11	1:72:A:GLU:H	9	0.3
(1,800)	1:66:A:VAL:HG12	1:72:A:GLU:H	9	0.3
(1,800)	1:66:A:VAL:HG13	1:72:A:GLU:H	9	0.3
(1,800)	1:66:A:VAL:HG21	1:72:A:GLU:H	9	0.3
(1,800)	1:66:A:VAL:HG22	1:72:A:GLU:H	9	0.3
(1,800)	1:66:A:VAL:HG23	1:72:A:GLU:H	9	0.3
(1,741)	1:62:A:TYR:HD1	1:63:A:LEU:H	13	0.3
(1,741)	1:62:A:TYR:HD2	1:63:A:LEU:H	13	0.3
(1,739)	1:62:A:TYR:HB2	1:79:A:LEU:HG	6	0.3
(1,739)	1:62:A:TYR:HB3	1:79:A:LEU:HG	6	0.3
(1,705)	1:59:A:HIS:H	1:60:A:THR:HA	2	0.3
(1,643)	1:53:A:PHE:H	1:55:A:LYS:H	13	0.3
(1,523)	1:41:A:THR:HA	1:44:A:HIS:HA	20	0.3
(1,492)	1:38:A:PHE:HA	1:75:A:PHE:HA	18	0.3
(1,450)	1:35:A:ILE:HD11	1:54:A:PHE:HE1	15	0.3
(1,450)	1:35:A:ILE:HD11	1:54:A:PHE:HE2	15	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,450)	1:35:A:ILE:HD12	1:54:A:PHE:HE1	15	0.3
(1,450)	1:35:A:ILE:HD12	1:54:A:PHE:HE2	15	0.3
(1,450)	1:35:A:ILE:HD13	1:54:A:PHE:HE1	15	0.3
(1,450)	1:35:A:ILE:HD13	1:54:A:PHE:HE2	15	0.3
(1,450)	1:35:A:ILE:HD11	1:54:A:PHE:HE1	15	0.3
(1,450)	1:35:A:ILE:HD11	1:54:A:PHE:HE2	15	0.3
(1,450)	1:35:A:ILE:HD12	1:54:A:PHE:HE1	15	0.3
(1,450)	1:35:A:ILE:HD12	1:54:A:PHE:HE2	15	0.3
(1,450)	1:35:A:ILE:HD13	1:54:A:PHE:HE1	15	0.3
(1,450)	1:35:A:ILE:HD13	1:54:A:PHE:HE2	15	0.3
(1,437)	1:35:A:ILE:H	1:80:A:HIS:H	15	0.3
(1,364)	1:28:A:PHE:HD1	1:32:A:LYS:HA	11	0.3
(1,364)	1:28:A:PHE:HD2	1:32:A:LYS:HA	11	0.3
(1,342)	1:27:A:GLU:HA	1:29:A:SER:H	3	0.3
(1,335)	1:26:A:HIS:HB2	1:30:A:GLU:HB2	15	0.3
(1,335)	1:26:A:HIS:HB2	1:30:A:GLU:HB3	15	0.3
(1,335)	1:26:A:HIS:HB3	1:30:A:GLU:HB2	15	0.3
(1,335)	1:26:A:HIS:HB3	1:30:A:GLU:HB3	15	0.3
(1,304)	1:24:A:LEU:HD21	1:59:A:HIS:HE1	1	0.3
(1,304)	1:24:A:LEU:HD22	1:59:A:HIS:HE1	1	0.3
(1,304)	1:24:A:LEU:HD23	1:59:A:HIS:HE1	1	0.3
(1,284)	1:24:A:LEU:HA	1:35:A:ILE:HD11	5	0.3
(1,284)	1:24:A:LEU:HA	1:35:A:ILE:HD12	5	0.3
(1,284)	1:24:A:LEU:HA	1:35:A:ILE:HD13	5	0.3
(1,207)	1:19:A:VAL:HB	1:22:A:GLU:H	15	0.3
(1,178)	1:13:A:LYS:H	1:16:A:ALA:HB1	5	0.3
(1,178)	1:13:A:LYS:H	1:16:A:ALA:HB2	5	0.3
(1,178)	1:13:A:LYS:H	1:16:A:ALA:HB3	5	0.3
(1,157)	1:10:A:ASN:HB2	1:46:A:ASP:H	3	0.3
(1,157)	1:10:A:ASN:HB3	1:46:A:ASP:H	3	0.3
(1,157)	1:10:A:ASN:HB2	1:46:A:ASP:H	5	0.3
(1,157)	1:10:A:ASN:HB3	1:46:A:ASP:H	5	0.3
(1,146)	1:9:A:LYS:H	1:10:A:ASN:HB2	3	0.3
(1,146)	1:9:A:LYS:H	1:10:A:ASN:HB3	3	0.3
(1,145)	1:9:A:LYS:H	1:10:A:ASN:HA	8	0.3
(1,142)	1:8:A:ALA:HA	1:46:A:ASP:HA	6	0.3
(1,127)	1:7:A:LEU:HG	1:38:A:PHE:HB2	5	0.3
(1,127)	1:7:A:LEU:HG	1:38:A:PHE:HB3	5	0.3
(1,89)	1:6:A:VAL:HG21	1:19:A:VAL:HG11	9	0.3
(1,89)	1:6:A:VAL:HG21	1:19:A:VAL:HG12	9	0.3
(1,89)	1:6:A:VAL:HG21	1:19:A:VAL:HG13	9	0.3
(1,89)	1:6:A:VAL:HG22	1:19:A:VAL:HG11	9	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,89)	1:6:A:VAL:HG22	1:19:A:VAL:HG12	9	0.3
(1,89)	1:6:A:VAL:HG22	1:19:A:VAL:HG13	9	0.3
(1,89)	1:6:A:VAL:HG23	1:19:A:VAL:HG11	9	0.3
(1,89)	1:6:A:VAL:HG23	1:19:A:VAL:HG12	9	0.3
(1,89)	1:6:A:VAL:HG23	1:19:A:VAL:HG13	9	0.3
(1,930)	1:81:A:ILE:HA	1:82:A:ILE:H	19	0.29
(1,841)	1:71:A:ASP:H	1:72:A:GLU:HA	18	0.29
(1,836)	1:70:A:THR:HA	1:73:A:LYS:HB2	1	0.29
(1,836)	1:70:A:THR:HA	1:73:A:LYS:HB3	1	0.29
(1,824)	1:69:A:SER:HA	1:74:A:ASP:H	1	0.29
(1,811)	1:68:A:VAL:HA	1:73:A:LYS:H	17	0.29
(1,791)	1:66:A:VAL:HA	1:68:A:VAL:HG11	12	0.29
(1,791)	1:66:A:VAL:HA	1:68:A:VAL:HG12	12	0.29
(1,791)	1:66:A:VAL:HA	1:68:A:VAL:HG13	12	0.29
(1,764)	1:64:A:ASP:H	1:79:A:LEU:H	13	0.29
(1,732)	1:62:A:TYR:H	1:81:A:ILE:H	17	0.29
(1,703)	1:58:A:GLY:HA3	1:60:A:THR:H	2	0.29
(1,543)	1:44:A:HIS:HA	1:48:A:LEU:H	17	0.29
(1,475)	1:37:A:TYR:H	1:76:A:LEU:HA	7	0.29
(1,474)	1:37:A:TYR:H	1:76:A:LEU:H	17	0.29
(1,470)	1:36:A:PHE:HD1	1:77:A:TYR:HD1	4	0.29
(1,470)	1:36:A:PHE:HD1	1:77:A:TYR:HD2	4	0.29
(1,470)	1:36:A:PHE:HD2	1:77:A:TYR:HD1	4	0.29
(1,470)	1:36:A:PHE:HD2	1:77:A:TYR:HD2	4	0.29
(1,461)	1:36:A:PHE:HA	1:77:A:TYR:HD1	18	0.29
(1,461)	1:36:A:PHE:HA	1:77:A:TYR:HD2	18	0.29
(1,417)	1:34:A:SER:H	1:79:A:LEU:HA	18	0.29
(1,406)	1:33:A:ARG:H	1:82:A:ILE:HA	4	0.29
(1,373)	1:29:A:SER:H	1:30:A:GLU:HB2	5	0.29
(1,373)	1:29:A:SER:H	1:30:A:GLU:HB3	5	0.29
(1,348)	1:28:A:PHE:H	1:30:A:GLU:HG2	2	0.29
(1,348)	1:28:A:PHE:H	1:30:A:GLU:HG3	2	0.29
(1,214)	1:20:A:GLU:H	1:22:A:GLU:H	8	0.29
(1,207)	1:19:A:VAL:HB	1:22:A:GLU:H	11	0.29
(1,207)	1:19:A:VAL:HB	1:22:A:GLU:H	19	0.29
(1,176)	1:13:A:LYS:H	1:14:A:SER:H	3	0.29
(1,165)	1:11:A:THR:HA	1:40:A:PRO:HG2	13	0.29
(1,165)	1:11:A:THR:HA	1:40:A:PRO:HG3	13	0.29
(1,165)	1:11:A:THR:HA	1:40:A:PRO:HG2	19	0.29
(1,165)	1:11:A:THR:HA	1:40:A:PRO:HG3	19	0.29
(1,147)	1:9:A:LYS:H	1:11:A:THR:H	5	0.29
(1,126)	1:7:A:LEU:HG	1:38:A:PHE:H	4	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,92)	1:6:A:VAL:HG21	1:35:A:ILE:HB	16	0.29
(1,92)	1:6:A:VAL:HG22	1:35:A:ILE:HB	16	0.29
(1,92)	1:6:A:VAL:HG23	1:35:A:ILE:HB	16	0.29
(1,61)	1:6:A:VAL:HA	1:19:A:VAL:HB	13	0.29
(1,29)	1:5:A:LEU:HG	1:36:A:PHE:H	9	0.29
(1,19)	1:5:A:LEU:HB2	1:35:A:ILE:HA	17	0.29
(1,19)	1:5:A:LEU:HB3	1:35:A:ILE:HA	17	0.29
(1,1)	1:3:A:MET:H	1:4:A:LYS:H	1	0.29
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG21	2	0.28
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG22	2	0.28
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG23	2	0.28
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG21	2	0.28
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG22	2	0.28
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG23	2	0.28
(1,906)	1:78:A:GLU:HA	1:79:A:LEU:HG	17	0.28
(1,841)	1:71:A:ASP:H	1:72:A:GLU:HA	1	0.28
(1,840)	1:71:A:ASP:H	1:72:A:GLU:H	7	0.28
(1,820)	1:69:A:SER:H	1:73:A:LYS:HA	1	0.28
(1,817)	1:69:A:SER:H	1:70:A:THR:H	8	0.28
(1,805)	1:67:A:ARG:H	1:68:A:VAL:HG11	9	0.28
(1,805)	1:67:A:ARG:H	1:68:A:VAL:HG12	9	0.28
(1,805)	1:67:A:ARG:H	1:68:A:VAL:HG13	9	0.28
(1,793)	1:66:A:VAL:HA	1:76:A:LEU:HA	3	0.28
(1,791)	1:66:A:VAL:HA	1:68:A:VAL:HG11	7	0.28
(1,791)	1:66:A:VAL:HA	1:68:A:VAL:HG12	7	0.28
(1,791)	1:66:A:VAL:HA	1:68:A:VAL:HG13	7	0.28
(1,768)	1:64:A:ASP:HA	1:76:A:LEU:HD21	1	0.28
(1,768)	1:64:A:ASP:HA	1:76:A:LEU:HD22	1	0.28
(1,768)	1:64:A:ASP:HA	1:76:A:LEU:HD23	1	0.28
(1,764)	1:64:A:ASP:H	1:79:A:LEU:H	7	0.28
(1,764)	1:64:A:ASP:H	1:79:A:LEU:H	11	0.28
(1,703)	1:58:A:GLY:HA3	1:60:A:THR:H	15	0.28
(1,692)	1:57:A:LYS:H	1:58:A:GLY:HA2	4	0.28
(1,692)	1:57:A:LYS:H	1:58:A:GLY:HA2	9	0.28
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD11	4	0.28
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD12	4	0.28
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD13	4	0.28
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD11	4	0.28
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD12	4	0.28
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD13	4	0.28
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD11	9	0.28
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD12	9	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD13	9	0.28
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD11	9	0.28
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD12	9	0.28
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD13	9	0.28
(1,543)	1:44:A:HIS:HA	1:48:A:LEU:H	4	0.28
(1,475)	1:37:A:TYR:H	1:76:A:LEU:HA	1	0.28
(1,422)	1:34:A:SER:HA	1:78:A:GLU:HB2	10	0.28
(1,422)	1:34:A:SER:HA	1:78:A:GLU:HB3	10	0.28
(1,373)	1:29:A:SER:H	1:30:A:GLU:HB2	13	0.28
(1,373)	1:29:A:SER:H	1:30:A:GLU:HB3	13	0.28
(1,364)	1:28:A:PHE:HD1	1:32:A:LYS:HA	9	0.28
(1,364)	1:28:A:PHE:HD2	1:32:A:LYS:HA	9	0.28
(1,356)	1:28:A:PHE:HA	1:33:A:ARG:H	12	0.28
(1,342)	1:27:A:GLU:HA	1:29:A:SER:H	10	0.28
(1,305)	1:24:A:LEU:HD21	1:60:A:THR:H	8	0.28
(1,305)	1:24:A:LEU:HD22	1:60:A:THR:H	8	0.28
(1,305)	1:24:A:LEU:HD23	1:60:A:THR:H	8	0.28
(1,301)	1:24:A:LEU:HD11	1:60:A:THR:HB	2	0.28
(1,301)	1:24:A:LEU:HD12	1:60:A:THR:HB	2	0.28
(1,301)	1:24:A:LEU:HD13	1:60:A:THR:HB	2	0.28
(1,298)	1:24:A:LEU:HG	1:80:A:HIS:HE1	16	0.28
(1,288)	1:24:A:LEU:HA	1:80:A:HIS:HE1	12	0.28
(1,248)	1:21:A:LEU:HD21	1:22:A:GLU:HA	14	0.28
(1,248)	1:21:A:LEU:HD22	1:22:A:GLU:HA	14	0.28
(1,248)	1:21:A:LEU:HD23	1:22:A:GLU:HA	14	0.28
(1,220)	1:20:A:GLU:HA	1:24:A:LEU:HA	10	0.28
(1,207)	1:19:A:VAL:HB	1:22:A:GLU:H	16	0.28
(1,174)	1:12:A:ARG:HB2	1:14:A:SER:HA	19	0.28
(1,174)	1:12:A:ARG:HB3	1:14:A:SER:HA	19	0.28
(1,158)	1:10:A:ASN:HB2	1:46:A:ASP:HA	18	0.28
(1,158)	1:10:A:ASN:HB3	1:46:A:ASP:HA	18	0.28
(1,144)	1:9:A:LYS:H	1:10:A:ASN:H	3	0.28
(1,144)	1:9:A:LYS:H	1:10:A:ASN:H	4	0.28
(1,128)	1:7:A:LEU:HG	1:38:A:PHE:HD1	1	0.28
(1,128)	1:7:A:LEU:HG	1:38:A:PHE:HD2	1	0.28
(1,127)	1:7:A:LEU:HG	1:38:A:PHE:HB2	16	0.28
(1,127)	1:7:A:LEU:HG	1:38:A:PHE:HB3	16	0.28
(1,61)	1:6:A:VAL:HA	1:19:A:VAL:HB	18	0.28
(1,8)	1:5:A:LEU:H	1:35:A:ILE:HB	10	0.28
(1,898)	1:77:A:TYR:HB2	1:79:A:LEU:HG	19	0.27
(1,898)	1:77:A:TYR:HB3	1:79:A:LEU:HG	19	0.27
(1,890)	1:76:A:LEU:HD11	1:78:A:GLU:H	2	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,890)	1:76:A:LEU:HD12	1:78:A:GLU:H	2	0.27
(1,890)	1:76:A:LEU:HD13	1:78:A:GLU:H	2	0.27
(1,843)	1:71:A:ASP:H	1:73:A:LYS:HA	19	0.27
(1,842)	1:71:A:ASP:H	1:73:A:LYS:H	5	0.27
(1,831)	1:70:A:THR:H	1:73:A:LYS:HA	4	0.27
(1,819)	1:69:A:SER:H	1:73:A:LYS:H	2	0.27
(1,811)	1:68:A:VAL:HA	1:73:A:LYS:H	14	0.27
(1,802)	1:67:A:ARG:H	1:68:A:VAL:H	11	0.27
(1,791)	1:66:A:VAL:HA	1:68:A:VAL:HG11	15	0.27
(1,791)	1:66:A:VAL:HA	1:68:A:VAL:HG12	15	0.27
(1,791)	1:66:A:VAL:HA	1:68:A:VAL:HG13	15	0.27
(1,764)	1:64:A:ASP:H	1:79:A:LEU:H	6	0.27
(1,620)	1:51:A:VAL:HA	1:53:A:PHE:H	3	0.27
(1,543)	1:44:A:HIS:HA	1:48:A:LEU:H	2	0.27
(1,543)	1:44:A:HIS:HA	1:48:A:LEU:H	15	0.27
(1,543)	1:44:A:HIS:HA	1:48:A:LEU:H	19	0.27
(1,522)	1:41:A:THR:HA	1:44:A:HIS:H	1	0.27
(1,506)	1:39:A:ALA:H	1:74:A:ASP:HA	5	0.27
(1,505)	1:39:A:ALA:H	1:74:A:ASP:H	2	0.27
(1,505)	1:39:A:ALA:H	1:74:A:ASP:H	5	0.27
(1,505)	1:39:A:ALA:H	1:74:A:ASP:H	12	0.27
(1,505)	1:39:A:ALA:H	1:74:A:ASP:H	14	0.27
(1,470)	1:36:A:PHE:HD1	1:77:A:TYR:HD1	8	0.27
(1,470)	1:36:A:PHE:HD1	1:77:A:TYR:HD2	8	0.27
(1,470)	1:36:A:PHE:HD2	1:77:A:TYR:HD1	8	0.27
(1,470)	1:36:A:PHE:HD2	1:77:A:TYR:HD2	8	0.27
(1,434)	1:35:A:ILE:H	1:78:A:GLU:H	2	0.27
(1,434)	1:35:A:ILE:H	1:78:A:GLU:H	3	0.27
(1,356)	1:28:A:PHE:HA	1:33:A:ARG:H	5	0.27
(1,348)	1:28:A:PHE:H	1:30:A:GLU:HG2	17	0.27
(1,348)	1:28:A:PHE:H	1:30:A:GLU:HG3	17	0.27
(1,270)	1:23:A:ASP:HA	1:28:A:PHE:H	6	0.27
(1,270)	1:23:A:ASP:HA	1:28:A:PHE:H	17	0.27
(1,245)	1:21:A:LEU:HD11	1:53:A:PHE:HA	4	0.27
(1,245)	1:21:A:LEU:HD12	1:53:A:PHE:HA	4	0.27
(1,245)	1:21:A:LEU:HD13	1:53:A:PHE:HA	4	0.27
(1,245)	1:21:A:LEU:HD11	1:53:A:PHE:HA	13	0.27
(1,245)	1:21:A:LEU:HD12	1:53:A:PHE:HA	13	0.27
(1,245)	1:21:A:LEU:HD13	1:53:A:PHE:HA	13	0.27
(1,237)	1:21:A:LEU:HG	1:24:A:LEU:HB2	20	0.27
(1,237)	1:21:A:LEU:HG	1:24:A:LEU:HB3	20	0.27
(1,175)	1:12:A:ARG:HB2	1:16:A:ALA:H	17	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,175)	1:12:A:ARG:HB3	1:16:A:ALA:H	17	0.27
(1,146)	1:9:A:LYS:H	1:10:A:ASN:HB2	15	0.27
(1,146)	1:9:A:LYS:H	1:10:A:ASN:HB3	15	0.27
(1,144)	1:9:A:LYS:H	1:10:A:ASN:H	1	0.27
(1,126)	1:7:A:LEU:HG	1:38:A:PHE:H	7	0.27
(1,123)	1:7:A:LEU:HB2	1:38:A:PHE:HD1	11	0.27
(1,123)	1:7:A:LEU:HB2	1:38:A:PHE:HD2	11	0.27
(1,123)	1:7:A:LEU:HB3	1:38:A:PHE:HD1	11	0.27
(1,123)	1:7:A:LEU:HB3	1:38:A:PHE:HD2	11	0.27
(1,71)	1:6:A:VAL:HB	1:37:A:TYR:HA	6	0.27
(1,63)	1:6:A:VAL:HA	1:20:A:GLU:H	1	0.27
(1,63)	1:6:A:VAL:HA	1:20:A:GLU:H	15	0.27
(1,60)	1:6:A:VAL:HA	1:16:A:ALA:HB1	9	0.27
(1,60)	1:6:A:VAL:HA	1:16:A:ALA:HB2	9	0.27
(1,60)	1:6:A:VAL:HA	1:16:A:ALA:HB3	9	0.27
(1,47)	1:6:A:VAL:H	1:36:A:PHE:H	12	0.27
(1,25)	1:5:A:LEU:HG	1:6:A:VAL:HA	15	0.27
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG21	1	0.26
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG22	1	0.26
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG23	1	0.26
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG21	1	0.26
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG22	1	0.26
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG23	1	0.26
(1,841)	1:71:A:ASP:H	1:72:A:GLU:HA	12	0.26
(1,811)	1:68:A:VAL:HA	1:73:A:LYS:H	15	0.26
(1,802)	1:67:A:ARG:H	1:68:A:VAL:H	13	0.26
(1,708)	1:60:A:THR:H	1:61:A:ALA:HA	15	0.26
(1,671)	1:55:A:LYS:H	1:57:A:LYS:H	6	0.26
(1,643)	1:53:A:PHE:H	1:55:A:LYS:H	16	0.26
(1,584)	1:48:A:LEU:HA	1:52:A:ASP:HB2	17	0.26
(1,584)	1:48:A:LEU:HA	1:52:A:ASP:HB3	17	0.26
(1,527)	1:42:A:ASN:H	1:43:A:ALA:H	19	0.26
(1,523)	1:41:A:THR:HA	1:44:A:HIS:HA	3	0.26
(1,523)	1:41:A:THR:HA	1:44:A:HIS:HA	16	0.26
(1,502)	1:38:A:PHE:HD1	1:75:A:PHE:HA	17	0.26
(1,502)	1:38:A:PHE:HD2	1:75:A:PHE:HA	17	0.26
(1,417)	1:34:A:SER:H	1:79:A:LEU:HA	11	0.26
(1,365)	1:28:A:PHE:HD1	1:32:A:LYS:HB2	4	0.26
(1,365)	1:28:A:PHE:HD1	1:32:A:LYS:HB3	4	0.26
(1,365)	1:28:A:PHE:HD2	1:32:A:LYS:HB2	4	0.26
(1,365)	1:28:A:PHE:HD2	1:32:A:LYS:HB3	4	0.26
(1,359)	1:28:A:PHE:HA	1:81:A:ILE:HD11	17	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,359)	1:28:A:PHE:HA	1:81:A:ILE:HD12	17	0.26
(1,359)	1:28:A:PHE:HA	1:81:A:ILE:HD13	17	0.26
(1,354)	1:28:A:PHE:HA	1:30:A:GLU:H	8	0.26
(1,317)	1:25:A:TYR:HA	1:29:A:SER:HG	10	0.26
(1,300)	1:24:A:LEU:HD11	1:35:A:ILE:HG12	4	0.26
(1,300)	1:24:A:LEU:HD11	1:35:A:ILE:HG13	4	0.26
(1,300)	1:24:A:LEU:HD12	1:35:A:ILE:HG12	4	0.26
(1,300)	1:24:A:LEU:HD12	1:35:A:ILE:HG13	4	0.26
(1,300)	1:24:A:LEU:HD13	1:35:A:ILE:HG12	4	0.26
(1,300)	1:24:A:LEU:HD13	1:35:A:ILE:HG13	4	0.26
(1,248)	1:21:A:LEU:HD21	1:22:A:GLU:HA	6	0.26
(1,248)	1:21:A:LEU:HD22	1:22:A:GLU:HA	6	0.26
(1,248)	1:21:A:LEU:HD23	1:22:A:GLU:HA	6	0.26
(1,248)	1:21:A:LEU:HD21	1:22:A:GLU:HA	9	0.26
(1,248)	1:21:A:LEU:HD22	1:22:A:GLU:HA	9	0.26
(1,248)	1:21:A:LEU:HD23	1:22:A:GLU:HA	9	0.26
(1,208)	1:19:A:VAL:HB	1:23:A:ASP:H	8	0.26
(1,207)	1:19:A:VAL:HB	1:22:A:GLU:H	4	0.26
(1,197)	1:18:A:SER:HA	1:20:A:GLU:HG2	17	0.26
(1,197)	1:18:A:SER:HA	1:20:A:GLU:HG3	17	0.26
(1,163)	1:11:A:THR:HA	1:13:A:LYS:H	13	0.26
(1,144)	1:9:A:LYS:H	1:10:A:ASN:H	6	0.26
(1,142)	1:8:A:ALA:HA	1:46:A:ASP:HA	4	0.26
(1,128)	1:7:A:LEU:HG	1:38:A:PHE:HD1	14	0.26
(1,128)	1:7:A:LEU:HG	1:38:A:PHE:HD2	14	0.26
(1,126)	1:7:A:LEU:HG	1:38:A:PHE:H	12	0.26
(1,107)	1:7:A:LEU:H	1:38:A:PHE:HD1	19	0.26
(1,107)	1:7:A:LEU:H	1:38:A:PHE:HD2	19	0.26
(1,78)	1:6:A:VAL:HG11	1:7:A:LEU:HD11	2	0.26
(1,78)	1:6:A:VAL:HG11	1:7:A:LEU:HD12	2	0.26
(1,78)	1:6:A:VAL:HG11	1:7:A:LEU:HD13	2	0.26
(1,78)	1:6:A:VAL:HG12	1:7:A:LEU:HD11	2	0.26
(1,78)	1:6:A:VAL:HG12	1:7:A:LEU:HD12	2	0.26
(1,78)	1:6:A:VAL:HG12	1:7:A:LEU:HD13	2	0.26
(1,78)	1:6:A:VAL:HG13	1:7:A:LEU:HD11	2	0.26
(1,78)	1:6:A:VAL:HG13	1:7:A:LEU:HD12	2	0.26
(1,78)	1:6:A:VAL:HG13	1:7:A:LEU:HD13	2	0.26
(1,29)	1:5:A:LEU:HG	1:36:A:PHE:H	5	0.26
(1,19)	1:5:A:LEU:HB2	1:35:A:ILE:HA	11	0.26
(1,19)	1:5:A:LEU:HB3	1:35:A:ILE:HA	11	0.26
(1,908)	1:78:A:GLU:HA	1:80:A:HIS:HD2	19	0.25
(1,865)	1:74:A:ASP:H	1:75:A:PHE:H	12	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,840)	1:71:A:ASP:H	1:72:A:GLU:H	4	0.25
(1,780)	1:65:A:GLU:HA	1:77:A:TYR:H	20	0.25
(1,764)	1:64:A:ASP:H	1:79:A:LEU:H	3	0.25
(1,741)	1:62:A:TYR:HD1	1:63:A:LEU:H	8	0.25
(1,741)	1:62:A:TYR:HD2	1:63:A:LEU:H	8	0.25
(1,732)	1:62:A:TYR:H	1:81:A:ILE:H	8	0.25
(1,686)	1:56:A:GLU:HA	1:57:A:LYS:HG2	4	0.25
(1,686)	1:56:A:GLU:HA	1:57:A:LYS:HG3	4	0.25
(1,669)	1:55:A:LYS:H	1:56:A:GLU:HA	14	0.25
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD11	14	0.25
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD12	14	0.25
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD13	14	0.25
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD11	14	0.25
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD12	14	0.25
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD13	14	0.25
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD11	20	0.25
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD12	20	0.25
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD13	20	0.25
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD11	20	0.25
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD12	20	0.25
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD13	20	0.25
(1,643)	1:53:A:PHE:H	1:55:A:LYS:H	10	0.25
(1,620)	1:51:A:VAL:HA	1:53:A:PHE:H	6	0.25
(1,620)	1:51:A:VAL:HA	1:53:A:PHE:H	13	0.25
(1,599)	1:49:A:LYS:HB2	1:53:A:PHE:HE1	9	0.25
(1,599)	1:49:A:LYS:HB2	1:53:A:PHE:HE2	9	0.25
(1,599)	1:49:A:LYS:HB3	1:53:A:PHE:HE1	9	0.25
(1,599)	1:49:A:LYS:HB3	1:53:A:PHE:HE2	9	0.25
(1,512)	1:39:A:ALA:HA	1:74:A:ASP:HB2	14	0.25
(1,512)	1:39:A:ALA:HA	1:74:A:ASP:HB3	14	0.25
(1,506)	1:39:A:ALA:H	1:74:A:ASP:HA	18	0.25
(1,474)	1:37:A:TYR:H	1:76:A:LEU:H	2	0.25
(1,466)	1:36:A:PHE:HB2	1:77:A:TYR:HA	2	0.25
(1,466)	1:36:A:PHE:HB3	1:77:A:TYR:HA	2	0.25
(1,459)	1:36:A:PHE:HA	1:77:A:TYR:H	14	0.25
(1,437)	1:35:A:ILE:H	1:80:A:HIS:H	9	0.25
(1,434)	1:35:A:ILE:H	1:78:A:GLU:H	9	0.25
(1,432)	1:35:A:ILE:H	1:36:A:PHE:HE1	5	0.25
(1,432)	1:35:A:ILE:H	1:36:A:PHE:HE2	5	0.25
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG21	1	0.25
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG22	1	0.25
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG23	1	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG21	1	0.25
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG22	1	0.25
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG23	1	0.25
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG21	1	0.25
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG22	1	0.25
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG23	1	0.25
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG21	1	0.25
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG22	1	0.25
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG23	1	0.25
(1,359)	1:28:A:PHE:HA	1:81:A:ILE:HD11	13	0.25
(1,359)	1:28:A:PHE:HA	1:81:A:ILE:HD12	13	0.25
(1,359)	1:28:A:PHE:HA	1:81:A:ILE:HD13	13	0.25
(1,348)	1:28:A:PHE:H	1:30:A:GLU:HG2	13	0.25
(1,348)	1:28:A:PHE:H	1:30:A:GLU:HG3	13	0.25
(1,316)	1:25:A:TYR:HA	1:29:A:SER:H	1	0.25
(1,304)	1:24:A:LEU:HD21	1:59:A:HIS:HE1	18	0.25
(1,304)	1:24:A:LEU:HD22	1:59:A:HIS:HE1	18	0.25
(1,304)	1:24:A:LEU:HD23	1:59:A:HIS:HE1	18	0.25
(1,284)	1:24:A:LEU:HA	1:35:A:ILE:HD11	14	0.25
(1,284)	1:24:A:LEU:HA	1:35:A:ILE:HD12	14	0.25
(1,284)	1:24:A:LEU:HA	1:35:A:ILE:HD13	14	0.25
(1,207)	1:19:A:VAL:HB	1:22:A:GLU:H	2	0.25
(1,207)	1:19:A:VAL:HB	1:22:A:GLU:H	5	0.25
(1,189)	1:16:A:ALA:H	1:17:A:LYS:H	12	0.25
(1,165)	1:11:A:THR:HA	1:40:A:PRO:HG2	15	0.25
(1,165)	1:11:A:THR:HA	1:40:A:PRO:HG3	15	0.25
(1,142)	1:8:A:ALA:HA	1:46:A:ASP:HA	5	0.25
(1,63)	1:6:A:VAL:HA	1:20:A:GLU:H	11	0.25
(1,47)	1:6:A:VAL:H	1:36:A:PHE:H	2	0.25
(1,44)	1:6:A:VAL:H	1:20:A:GLU:HB2	10	0.25
(1,44)	1:6:A:VAL:H	1:20:A:GLU:HB3	10	0.25
(1,26)	1:5:A:LEU:HG	1:6:A:VAL:HG21	4	0.25
(1,26)	1:5:A:LEU:HG	1:6:A:VAL:HG22	4	0.25
(1,26)	1:5:A:LEU:HG	1:6:A:VAL:HG23	4	0.25
(1,9)	1:5:A:LEU:H	1:36:A:PHE:H	9	0.25
(1,2)	1:3:A:MET:H	1:4:A:LYS:HA	17	0.25
(1,906)	1:78:A:GLU:HA	1:79:A:LEU:HG	6	0.24
(1,890)	1:76:A:LEU:HD11	1:78:A:GLU:H	6	0.24
(1,890)	1:76:A:LEU:HD12	1:78:A:GLU:H	6	0.24
(1,890)	1:76:A:LEU:HD13	1:78:A:GLU:H	6	0.24
(1,866)	1:74:A:ASP:H	1:75:A:PHE:HA	19	0.24
(1,865)	1:74:A:ASP:H	1:75:A:PHE:H	20	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,840)	1:71:A:ASP:H	1:72:A:GLU:H	19	0.24
(1,801)	1:66:A:VAL:HG11	1:72:A:GLU:HB2	1	0.24
(1,801)	1:66:A:VAL:HG11	1:72:A:GLU:HB3	1	0.24
(1,801)	1:66:A:VAL:HG12	1:72:A:GLU:HB2	1	0.24
(1,801)	1:66:A:VAL:HG12	1:72:A:GLU:HB3	1	0.24
(1,801)	1:66:A:VAL:HG13	1:72:A:GLU:HB2	1	0.24
(1,801)	1:66:A:VAL:HG13	1:72:A:GLU:HB3	1	0.24
(1,801)	1:66:A:VAL:HG21	1:72:A:GLU:HB2	1	0.24
(1,801)	1:66:A:VAL:HG21	1:72:A:GLU:HB3	1	0.24
(1,801)	1:66:A:VAL:HG22	1:72:A:GLU:HB2	1	0.24
(1,801)	1:66:A:VAL:HG22	1:72:A:GLU:HB3	1	0.24
(1,801)	1:66:A:VAL:HG23	1:72:A:GLU:HB2	1	0.24
(1,801)	1:66:A:VAL:HG23	1:72:A:GLU:HB3	1	0.24
(1,793)	1:66:A:VAL:HA	1:76:A:LEU:HA	4	0.24
(1,764)	1:64:A:ASP:H	1:79:A:LEU:H	12	0.24
(1,704)	1:59:A:HIS:H	1:60:A:THR:H	10	0.24
(1,692)	1:57:A:LYS:H	1:58:A:GLY:HA2	18	0.24
(1,675)	1:55:A:LYS:HA	1:57:A:LYS:H	12	0.24
(1,657)	1:54:A:PHE:HA	1:60:A:THR:HB	1	0.24
(1,643)	1:53:A:PHE:H	1:55:A:LYS:H	6	0.24
(1,620)	1:51:A:VAL:HA	1:53:A:PHE:H	4	0.24
(1,547)	1:44:A:HIS:HB2	1:48:A:LEU:HD11	17	0.24
(1,547)	1:44:A:HIS:HB2	1:48:A:LEU:HD12	17	0.24
(1,547)	1:44:A:HIS:HB2	1:48:A:LEU:HD13	17	0.24
(1,547)	1:44:A:HIS:HB3	1:48:A:LEU:HD11	17	0.24
(1,547)	1:44:A:HIS:HB3	1:48:A:LEU:HD12	17	0.24
(1,547)	1:44:A:HIS:HB3	1:48:A:LEU:HD13	17	0.24
(1,537)	1:43:A:ALA:HA	1:45:A:LYS:H	11	0.24
(1,512)	1:39:A:ALA:HA	1:74:A:ASP:HB2	17	0.24
(1,512)	1:39:A:ALA:HA	1:74:A:ASP:HB3	17	0.24
(1,489)	1:38:A:PHE:H	1:75:A:PHE:HA	19	0.24
(1,468)	1:36:A:PHE:HD1	1:37:A:TYR:H	1	0.24
(1,468)	1:36:A:PHE:HD2	1:37:A:TYR:H	1	0.24
(1,461)	1:36:A:PHE:HA	1:77:A:TYR:HD1	3	0.24
(1,461)	1:36:A:PHE:HA	1:77:A:TYR:HD2	3	0.24
(1,437)	1:35:A:ILE:H	1:80:A:HIS:H	18	0.24
(1,431)	1:35:A:ILE:H	1:36:A:PHE:HD1	15	0.24
(1,431)	1:35:A:ILE:H	1:36:A:PHE:HD2	15	0.24
(1,422)	1:34:A:SER:HA	1:78:A:GLU:HB2	13	0.24
(1,422)	1:34:A:SER:HA	1:78:A:GLU:HB3	13	0.24
(1,417)	1:34:A:SER:H	1:79:A:LEU:HA	5	0.24
(1,364)	1:28:A:PHE:HD1	1:32:A:LYS:HA	18	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,364)	1:28:A:PHE:HD2	1:32:A:LYS:HA	18	0.24
(1,354)	1:28:A:PHE:HA	1:30:A:GLU:H	3	0.24
(1,354)	1:28:A:PHE:HA	1:30:A:GLU:H	5	0.24
(1,348)	1:28:A:PHE:H	1:30:A:GLU:HG2	9	0.24
(1,348)	1:28:A:PHE:H	1:30:A:GLU:HG3	9	0.24
(1,342)	1:27:A:GLU:HA	1:29:A:SER:H	4	0.24
(1,342)	1:27:A:GLU:HA	1:29:A:SER:H	12	0.24
(1,322)	1:25:A:TYR:HD1	1:28:A:PHE:H	11	0.24
(1,322)	1:25:A:TYR:HD2	1:28:A:PHE:H	11	0.24
(1,274)	1:23:A:ASP:HB2	1:35:A:ILE:HB	19	0.24
(1,274)	1:23:A:ASP:HB3	1:35:A:ILE:HB	19	0.24
(1,268)	1:23:A:ASP:HA	1:27:A:GLU:HA	13	0.24
(1,208)	1:19:A:VAL:HB	1:23:A:ASP:H	17	0.24
(1,182)	1:14:A:SER:H	1:17:A:LYS:H	17	0.24
(1,174)	1:12:A:ARG:HB2	1:14:A:SER:HA	14	0.24
(1,174)	1:12:A:ARG:HB3	1:14:A:SER:HA	14	0.24
(1,167)	1:11:A:THR:HB	1:12:A:ARG:HA	8	0.24
(1,157)	1:10:A:ASN:HB2	1:46:A:ASP:H	11	0.24
(1,157)	1:10:A:ASN:HB3	1:46:A:ASP:H	11	0.24
(1,156)	1:10:A:ASN:HB2	1:45:A:LYS:HB2	7	0.24
(1,156)	1:10:A:ASN:HB2	1:45:A:LYS:HB3	7	0.24
(1,156)	1:10:A:ASN:HB3	1:45:A:LYS:HB2	7	0.24
(1,156)	1:10:A:ASN:HB3	1:45:A:LYS:HB3	7	0.24
(1,156)	1:10:A:ASN:HB2	1:45:A:LYS:HB2	8	0.24
(1,156)	1:10:A:ASN:HB2	1:45:A:LYS:HB3	8	0.24
(1,156)	1:10:A:ASN:HB3	1:45:A:LYS:HB2	8	0.24
(1,156)	1:10:A:ASN:HB3	1:45:A:LYS:HB3	8	0.24
(1,127)	1:7:A:LEU:HG	1:38:A:PHE:HB2	18	0.24
(1,127)	1:7:A:LEU:HG	1:38:A:PHE:HB3	18	0.24
(1,115)	1:7:A:LEU:HA	1:38:A:PHE:HB2	5	0.24
(1,115)	1:7:A:LEU:HA	1:38:A:PHE:HB3	5	0.24
(1,69)	1:6:A:VAL:HB	1:20:A:GLU:H	13	0.24
(1,61)	1:6:A:VAL:HA	1:19:A:VAL:HB	4	0.24
(1,50)	1:6:A:VAL:H	1:37:A:TYR:H	10	0.24
(1,44)	1:6:A:VAL:H	1:20:A:GLU:HB2	19	0.24
(1,44)	1:6:A:VAL:H	1:20:A:GLU:HB3	19	0.24
(1,34)	1:5:A:LEU:HD11	1:7:A:LEU:HB2	7	0.24
(1,34)	1:5:A:LEU:HD11	1:7:A:LEU:HB3	7	0.24
(1,34)	1:5:A:LEU:HD12	1:7:A:LEU:HB2	7	0.24
(1,34)	1:5:A:LEU:HD12	1:7:A:LEU:HB3	7	0.24
(1,34)	1:5:A:LEU:HD13	1:7:A:LEU:HB2	7	0.24
(1,34)	1:5:A:LEU:HD13	1:7:A:LEU:HB3	7	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,34)	1:5:A:LEU:HD21	1:7:A:LEU:HB2	7	0.24
(1,34)	1:5:A:LEU:HD21	1:7:A:LEU:HB3	7	0.24
(1,34)	1:5:A:LEU:HD22	1:7:A:LEU:HB2	7	0.24
(1,34)	1:5:A:LEU:HD22	1:7:A:LEU:HB3	7	0.24
(1,34)	1:5:A:LEU:HD23	1:7:A:LEU:HB2	7	0.24
(1,34)	1:5:A:LEU:HD23	1:7:A:LEU:HB3	7	0.24
(1,29)	1:5:A:LEU:HG	1:36:A:PHE:H	12	0.24
(1,875)	1:75:A:PHE:HB2	1:76:A:LEU:H	14	0.23
(1,875)	1:75:A:PHE:HB3	1:76:A:LEU:H	14	0.23
(1,841)	1:71:A:ASP:H	1:72:A:GLU:HA	4	0.23
(1,840)	1:71:A:ASP:H	1:72:A:GLU:H	3	0.23
(1,840)	1:71:A:ASP:H	1:72:A:GLU:H	16	0.23
(1,840)	1:71:A:ASP:H	1:72:A:GLU:H	20	0.23
(1,819)	1:69:A:SER:H	1:73:A:LYS:H	1	0.23
(1,793)	1:66:A:VAL:HA	1:76:A:LEU:HA	11	0.23
(1,793)	1:66:A:VAL:HA	1:76:A:LEU:HA	13	0.23
(1,764)	1:64:A:ASP:H	1:79:A:LEU:H	20	0.23
(1,732)	1:62:A:TYR:H	1:81:A:ILE:H	11	0.23
(1,727)	1:61:A:ALA:HB1	1:79:A:LEU:HB3	7	0.23
(1,727)	1:61:A:ALA:HB2	1:79:A:LEU:HB3	7	0.23
(1,727)	1:61:A:ALA:HB3	1:79:A:LEU:HB3	7	0.23
(1,727)	1:61:A:ALA:HB1	1:79:A:LEU:HB3	9	0.23
(1,727)	1:61:A:ALA:HB2	1:79:A:LEU:HB3	9	0.23
(1,727)	1:61:A:ALA:HB3	1:79:A:LEU:HB3	9	0.23
(1,705)	1:59:A:HIS:H	1:60:A:THR:HA	10	0.23
(1,702)	1:58:A:GLY:HA2	1:59:A:HIS:HA	1	0.23
(1,675)	1:55:A:LYS:HA	1:57:A:LYS:H	6	0.23
(1,668)	1:55:A:LYS:H	1:56:A:GLU:H	16	0.23
(1,620)	1:51:A:VAL:HA	1:53:A:PHE:H	19	0.23
(1,584)	1:48:A:LEU:HA	1:52:A:ASP:HB2	10	0.23
(1,584)	1:48:A:LEU:HA	1:52:A:ASP:HB3	10	0.23
(1,567)	1:47:A:MET:HB2	1:48:A:LEU:HA	16	0.23
(1,567)	1:47:A:MET:HB3	1:48:A:LEU:HA	16	0.23
(1,543)	1:44:A:HIS:HA	1:48:A:LEU:H	1	0.23
(1,523)	1:41:A:THR:HA	1:44:A:HIS:HA	6	0.23
(1,506)	1:39:A:ALA:H	1:74:A:ASP:HA	13	0.23
(1,505)	1:39:A:ALA:H	1:74:A:ASP:H	6	0.23
(1,446)	1:35:A:ILE:HG12	1:36:A:PHE:H	16	0.23
(1,446)	1:35:A:ILE:HG13	1:36:A:PHE:H	16	0.23
(1,431)	1:35:A:ILE:H	1:36:A:PHE:HD1	7	0.23
(1,431)	1:35:A:ILE:H	1:36:A:PHE:HD2	7	0.23
(1,380)	1:30:A:GLU:H	1:31:A:ASP:HA	15	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,375)	1:29:A:SER:HA	1:31:A:ASP:H	2	0.23
(1,322)	1:25:A:TYR:HD1	1:28:A:PHE:H	5	0.23
(1,322)	1:25:A:TYR:HD2	1:28:A:PHE:H	5	0.23
(1,298)	1:24:A:LEU:HG	1:80:A:HIS:HE1	12	0.23
(1,270)	1:23:A:ASP:HA	1:28:A:PHE:H	20	0.23
(1,245)	1:21:A:LEU:HD11	1:53:A:PHE:HA	5	0.23
(1,245)	1:21:A:LEU:HD12	1:53:A:PHE:HA	5	0.23
(1,245)	1:21:A:LEU:HD13	1:53:A:PHE:HA	5	0.23
(1,237)	1:21:A:LEU:HG	1:24:A:LEU:HB2	14	0.23
(1,237)	1:21:A:LEU:HG	1:24:A:LEU:HB3	14	0.23
(1,204)	1:19:A:VAL:H	1:22:A:GLU:H	20	0.23
(1,203)	1:19:A:VAL:H	1:21:A:LEU:H	6	0.23
(1,183)	1:14:A:SER:HA	1:15:A:ASP:H	14	0.23
(1,177)	1:13:A:LYS:H	1:16:A:ALA:H	12	0.23
(1,176)	1:13:A:LYS:H	1:14:A:SER:H	10	0.23
(1,176)	1:13:A:LYS:H	1:14:A:SER:H	14	0.23
(1,157)	1:10:A:ASN:HB2	1:46:A:ASP:H	2	0.23
(1,157)	1:10:A:ASN:HB3	1:46:A:ASP:H	2	0.23
(1,146)	1:9:A:LYS:H	1:10:A:ASN:HB2	16	0.23
(1,146)	1:9:A:LYS:H	1:10:A:ASN:HB3	16	0.23
(1,145)	1:9:A:LYS:H	1:10:A:ASN:HA	13	0.23
(1,142)	1:8:A:ALA:HA	1:46:A:ASP:HA	19	0.23
(1,142)	1:8:A:ALA:HA	1:46:A:ASP:HA	20	0.23
(1,127)	1:7:A:LEU:HG	1:38:A:PHE:HB2	12	0.23
(1,127)	1:7:A:LEU:HG	1:38:A:PHE:HB3	12	0.23
(1,126)	1:7:A:LEU:HG	1:38:A:PHE:H	20	0.23
(1,71)	1:6:A:VAL:HB	1:37:A:TYR:HA	8	0.23
(1,71)	1:6:A:VAL:HB	1:37:A:TYR:HA	12	0.23
(1,44)	1:6:A:VAL:H	1:20:A:GLU:HB2	15	0.23
(1,44)	1:6:A:VAL:H	1:20:A:GLU:HB3	15	0.23
(1,34)	1:5:A:LEU:HD11	1:7:A:LEU:HB2	6	0.23
(1,34)	1:5:A:LEU:HD11	1:7:A:LEU:HB3	6	0.23
(1,34)	1:5:A:LEU:HD12	1:7:A:LEU:HB2	6	0.23
(1,34)	1:5:A:LEU:HD12	1:7:A:LEU:HB3	6	0.23
(1,34)	1:5:A:LEU:HD13	1:7:A:LEU:HB2	6	0.23
(1,34)	1:5:A:LEU:HD13	1:7:A:LEU:HB3	6	0.23
(1,34)	1:5:A:LEU:HD21	1:7:A:LEU:HB2	6	0.23
(1,34)	1:5:A:LEU:HD21	1:7:A:LEU:HB3	6	0.23
(1,34)	1:5:A:LEU:HD22	1:7:A:LEU:HB2	6	0.23
(1,34)	1:5:A:LEU:HD22	1:7:A:LEU:HB3	6	0.23
(1,34)	1:5:A:LEU:HD23	1:7:A:LEU:HB2	6	0.23
(1,34)	1:5:A:LEU:HD23	1:7:A:LEU:HB3	6	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,25)	1:5:A:LEU:HG	1:6:A:VAL:HA	13	0.23
(1,9)	1:5:A:LEU:H	1:36:A:PHE:H	11	0.23
(1,2)	1:3:A:MET:H	1:4:A:LYS:HA	3	0.23
(1,929)	1:81:A:ILE:H	1:82:A:ILE:HA	8	0.22
(1,841)	1:71:A:ASP:H	1:72:A:GLU:HA	3	0.22
(1,841)	1:71:A:ASP:H	1:72:A:GLU:HA	6	0.22
(1,841)	1:71:A:ASP:H	1:72:A:GLU:HA	15	0.22
(1,831)	1:70:A:THR:H	1:73:A:LYS:HA	1	0.22
(1,824)	1:69:A:SER:HA	1:74:A:ASP:H	9	0.22
(1,820)	1:69:A:SER:H	1:73:A:LYS:HA	4	0.22
(1,820)	1:69:A:SER:H	1:73:A:LYS:HA	14	0.22
(1,800)	1:66:A:VAL:HG11	1:72:A:GLU:H	12	0.22
(1,800)	1:66:A:VAL:HG12	1:72:A:GLU:H	12	0.22
(1,800)	1:66:A:VAL:HG13	1:72:A:GLU:H	12	0.22
(1,800)	1:66:A:VAL:HG21	1:72:A:GLU:H	12	0.22
(1,800)	1:66:A:VAL:HG22	1:72:A:GLU:H	12	0.22
(1,800)	1:66:A:VAL:HG23	1:72:A:GLU:H	12	0.22
(1,793)	1:66:A:VAL:HA	1:76:A:LEU:HA	2	0.22
(1,732)	1:62:A:TYR:H	1:81:A:ILE:H	2	0.22
(1,732)	1:62:A:TYR:H	1:81:A:ILE:H	14	0.22
(1,702)	1:58:A:GLY:HA2	1:59:A:HIS:HA	15	0.22
(1,702)	1:58:A:GLY:HA2	1:59:A:HIS:HA	18	0.22
(1,692)	1:57:A:LYS:H	1:58:A:GLY:HA2	8	0.22
(1,620)	1:51:A:VAL:HA	1:53:A:PHE:H	12	0.22
(1,584)	1:48:A:LEU:HA	1:52:A:ASP:HB2	13	0.22
(1,584)	1:48:A:LEU:HA	1:52:A:ASP:HB3	13	0.22
(1,567)	1:47:A:MET:HB2	1:48:A:LEU:HA	7	0.22
(1,567)	1:47:A:MET:HB3	1:48:A:LEU:HA	7	0.22
(1,567)	1:47:A:MET:HB2	1:48:A:LEU:HA	18	0.22
(1,567)	1:47:A:MET:HB3	1:48:A:LEU:HA	18	0.22
(1,537)	1:43:A:ALA:HA	1:45:A:LYS:H	10	0.22
(1,523)	1:41:A:THR:HA	1:44:A:HIS:HA	12	0.22
(1,505)	1:39:A:ALA:H	1:74:A:ASP:H	13	0.22
(1,474)	1:37:A:TYR:H	1:76:A:LEU:H	19	0.22
(1,467)	1:36:A:PHE:HB2	1:77:A:TYR:HD1	13	0.22
(1,467)	1:36:A:PHE:HB2	1:77:A:TYR:HD2	13	0.22
(1,467)	1:36:A:PHE:HB3	1:77:A:TYR:HD1	13	0.22
(1,467)	1:36:A:PHE:HB3	1:77:A:TYR:HD2	13	0.22
(1,446)	1:35:A:ILE:HG12	1:36:A:PHE:H	3	0.22
(1,446)	1:35:A:ILE:HG13	1:36:A:PHE:H	3	0.22
(1,405)	1:33:A:ARG:H	1:81:A:ILE:HG21	17	0.22
(1,405)	1:33:A:ARG:H	1:81:A:ILE:HG22	17	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,405)	1:33:A:ARG:H	1:81:A:ILE:HG23	17	0.22
(1,405)	1:33:A:ARG:H	1:81:A:ILE:HG21	17	0.22
(1,405)	1:33:A:ARG:H	1:81:A:ILE:HG22	17	0.22
(1,405)	1:33:A:ARG:H	1:81:A:ILE:HG23	17	0.22
(1,395)	1:31:A:ASP:HA	1:81:A:ILE:HG21	4	0.22
(1,395)	1:31:A:ASP:HA	1:81:A:ILE:HG22	4	0.22
(1,395)	1:31:A:ASP:HA	1:81:A:ILE:HG23	4	0.22
(1,373)	1:29:A:SER:H	1:30:A:GLU:HB2	14	0.22
(1,373)	1:29:A:SER:H	1:30:A:GLU:HB3	14	0.22
(1,354)	1:28:A:PHE:HA	1:30:A:GLU:H	14	0.22
(1,342)	1:27:A:GLU:HA	1:29:A:SER:H	18	0.22
(1,248)	1:21:A:LEU:HD21	1:22:A:GLU:HA	19	0.22
(1,248)	1:21:A:LEU:HD22	1:22:A:GLU:HA	19	0.22
(1,248)	1:21:A:LEU:HD23	1:22:A:GLU:HA	19	0.22
(1,237)	1:21:A:LEU:HG	1:24:A:LEU:HB2	10	0.22
(1,237)	1:21:A:LEU:HG	1:24:A:LEU:HB3	10	0.22
(1,220)	1:20:A:GLU:HA	1:24:A:LEU:HA	19	0.22
(1,220)	1:20:A:GLU:HA	1:24:A:LEU:HA	20	0.22
(1,187)	1:15:A:ASP:HA	1:16:A:ALA:H	13	0.22
(1,180)	1:14:A:SER:H	1:15:A:ASP:H	14	0.22
(1,180)	1:14:A:SER:H	1:15:A:ASP:H	20	0.22
(1,174)	1:12:A:ARG:HB2	1:14:A:SER:HA	6	0.22
(1,174)	1:12:A:ARG:HB3	1:14:A:SER:HA	6	0.22
(1,174)	1:12:A:ARG:HB2	1:14:A:SER:HA	7	0.22
(1,174)	1:12:A:ARG:HB3	1:14:A:SER:HA	7	0.22
(1,174)	1:12:A:ARG:HB2	1:14:A:SER:HA	17	0.22
(1,174)	1:12:A:ARG:HB3	1:14:A:SER:HA	17	0.22
(1,165)	1:11:A:THR:HA	1:40:A:PRO:HG2	17	0.22
(1,165)	1:11:A:THR:HA	1:40:A:PRO:HG3	17	0.22
(1,158)	1:10:A:ASN:HB2	1:46:A:ASP:HA	4	0.22
(1,158)	1:10:A:ASN:HB3	1:46:A:ASP:HA	4	0.22
(1,157)	1:10:A:ASN:HB2	1:46:A:ASP:H	7	0.22
(1,157)	1:10:A:ASN:HB3	1:46:A:ASP:H	7	0.22
(1,138)	1:8:A:ALA:HA	1:10:A:ASN:HB2	14	0.22
(1,138)	1:8:A:ALA:HA	1:10:A:ASN:HB3	14	0.22
(1,130)	1:7:A:LEU:HD11	1:16:A:ALA:HA	20	0.22
(1,130)	1:7:A:LEU:HD12	1:16:A:ALA:HA	20	0.22
(1,130)	1:7:A:LEU:HD13	1:16:A:ALA:HA	20	0.22
(1,126)	1:7:A:LEU:HG	1:38:A:PHE:H	18	0.22
(1,69)	1:6:A:VAL:HB	1:20:A:GLU:H	7	0.22
(1,9)	1:5:A:LEU:H	1:36:A:PHE:H	7	0.22
(1,2)	1:3:A:MET:H	1:4:A:LYS:HA	6	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2)	1:3:A:MET:H	1:4:A:LYS:HA	19	0.22
(1,906)	1:78:A:GLU:HA	1:79:A:LEU:HG	1	0.21
(1,881)	1:76:A:LEU:H	1:77:A:TYR:HA	3	0.21
(1,841)	1:71:A:ASP:H	1:72:A:GLU:HA	13	0.21
(1,820)	1:69:A:SER:H	1:73:A:LYS:HA	15	0.21
(1,811)	1:68:A:VAL:HA	1:73:A:LYS:H	9	0.21
(1,788)	1:66:A:VAL:H	1:68:A:VAL:H	4	0.21
(1,764)	1:64:A:ASP:H	1:79:A:LEU:H	15	0.21
(1,732)	1:62:A:TYR:H	1:81:A:ILE:H	18	0.21
(1,702)	1:58:A:GLY:HA2	1:59:A:HIS:HA	16	0.21
(1,676)	1:55:A:LYS:HA	1:58:A:GLY:HA2	7	0.21
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD11	10	0.21
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD12	10	0.21
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD13	10	0.21
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD11	10	0.21
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD12	10	0.21
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD13	10	0.21
(1,643)	1:53:A:PHE:H	1:55:A:LYS:H	8	0.21
(1,643)	1:53:A:PHE:H	1:55:A:LYS:H	9	0.21
(1,643)	1:53:A:PHE:H	1:55:A:LYS:H	19	0.21
(1,523)	1:41:A:THR:HA	1:44:A:HIS:HA	18	0.21
(1,496)	1:38:A:PHE:HA	1:76:A:LEU:H	19	0.21
(1,473)	1:37:A:TYR:H	1:38:A:PHE:HA	1	0.21
(1,459)	1:36:A:PHE:HA	1:77:A:TYR:H	16	0.21
(1,432)	1:35:A:ILE:H	1:36:A:PHE:HE1	4	0.21
(1,432)	1:35:A:ILE:H	1:36:A:PHE:HE2	4	0.21
(1,431)	1:35:A:ILE:H	1:36:A:PHE:HD1	18	0.21
(1,431)	1:35:A:ILE:H	1:36:A:PHE:HD2	18	0.21
(1,426)	1:34:A:SER:HB2	1:36:A:PHE:HE1	10	0.21
(1,426)	1:34:A:SER:HB2	1:36:A:PHE:HE2	10	0.21
(1,426)	1:34:A:SER:HB3	1:36:A:PHE:HE1	10	0.21
(1,426)	1:34:A:SER:HB3	1:36:A:PHE:HE2	10	0.21
(1,426)	1:34:A:SER:HB2	1:36:A:PHE:HE1	14	0.21
(1,426)	1:34:A:SER:HB2	1:36:A:PHE:HE2	14	0.21
(1,426)	1:34:A:SER:HB3	1:36:A:PHE:HE1	14	0.21
(1,426)	1:34:A:SER:HB3	1:36:A:PHE:HE2	14	0.21
(1,395)	1:31:A:ASP:HA	1:81:A:ILE:HG21	13	0.21
(1,395)	1:31:A:ASP:HA	1:81:A:ILE:HG22	13	0.21
(1,395)	1:31:A:ASP:HA	1:81:A:ILE:HG23	13	0.21
(1,364)	1:28:A:PHE:HD1	1:32:A:LYS:HA	13	0.21
(1,364)	1:28:A:PHE:HD2	1:32:A:LYS:HA	13	0.21
(1,359)	1:28:A:PHE:HA	1:81:A:ILE:HD11	9	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,359)	1:28:A:PHE:HA	1:81:A:ILE:HD12	9	0.21
(1,359)	1:28:A:PHE:HA	1:81:A:ILE:HD13	9	0.21
(1,335)	1:26:A:HIS:HB2	1:30:A:GLU:HB2	8	0.21
(1,335)	1:26:A:HIS:HB2	1:30:A:GLU:HB3	8	0.21
(1,335)	1:26:A:HIS:HB3	1:30:A:GLU:HB2	8	0.21
(1,335)	1:26:A:HIS:HB3	1:30:A:GLU:HB3	8	0.21
(1,319)	1:25:A:TYR:HA	1:59:A:HIS:HB2	8	0.21
(1,319)	1:25:A:TYR:HA	1:59:A:HIS:HB3	8	0.21
(1,301)	1:24:A:LEU:HD11	1:60:A:THR:HB	4	0.21
(1,301)	1:24:A:LEU:HD12	1:60:A:THR:HB	4	0.21
(1,301)	1:24:A:LEU:HD13	1:60:A:THR:HB	4	0.21
(1,301)	1:24:A:LEU:HD11	1:60:A:THR:HB	16	0.21
(1,301)	1:24:A:LEU:HD12	1:60:A:THR:HB	16	0.21
(1,301)	1:24:A:LEU:HD13	1:60:A:THR:HB	16	0.21
(1,274)	1:23:A:ASP:HB2	1:35:A:ILE:HB	13	0.21
(1,274)	1:23:A:ASP:HB3	1:35:A:ILE:HB	13	0.21
(1,270)	1:23:A:ASP:HA	1:28:A:PHE:H	13	0.21
(1,237)	1:21:A:LEU:HG	1:24:A:LEU:HB2	5	0.21
(1,237)	1:21:A:LEU:HG	1:24:A:LEU:HB3	5	0.21
(1,220)	1:20:A:GLU:HA	1:24:A:LEU:HA	2	0.21
(1,214)	1:20:A:GLU:H	1:22:A:GLU:H	4	0.21
(1,211)	1:19:A:VAL:HG11	1:20:A:GLU:HB2	9	0.21
(1,211)	1:19:A:VAL:HG11	1:20:A:GLU:HB3	9	0.21
(1,211)	1:19:A:VAL:HG12	1:20:A:GLU:HB2	9	0.21
(1,211)	1:19:A:VAL:HG12	1:20:A:GLU:HB3	9	0.21
(1,211)	1:19:A:VAL:HG13	1:20:A:GLU:HB2	9	0.21
(1,211)	1:19:A:VAL:HG13	1:20:A:GLU:HB3	9	0.21
(1,207)	1:19:A:VAL:HB	1:22:A:GLU:H	7	0.21
(1,187)	1:15:A:ASP:HA	1:16:A:ALA:H	11	0.21
(1,183)	1:14:A:SER:HA	1:15:A:ASP:H	16	0.21
(1,183)	1:14:A:SER:HA	1:15:A:ASP:H	17	0.21
(1,182)	1:14:A:SER:H	1:17:A:LYS:H	4	0.21
(1,177)	1:13:A:LYS:H	1:16:A:ALA:H	15	0.21
(1,174)	1:12:A:ARG:HB2	1:14:A:SER:HA	1	0.21
(1,174)	1:12:A:ARG:HB3	1:14:A:SER:HA	1	0.21
(1,142)	1:8:A:ALA:HA	1:46:A:ASP:HA	14	0.21
(1,126)	1:7:A:LEU:HG	1:38:A:PHE:H	5	0.21
(1,106)	1:7:A:LEU:H	1:38:A:PHE:HB2	18	0.21
(1,106)	1:7:A:LEU:H	1:38:A:PHE:HB3	18	0.21
(1,51)	1:6:A:VAL:H	1:37:A:TYR:HA	10	0.21
(1,44)	1:6:A:VAL:H	1:20:A:GLU:HB2	18	0.21
(1,44)	1:6:A:VAL:H	1:20:A:GLU:HB3	18	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,26)	1:5:A:LEU:HG	1:6:A:VAL:HG21	6	0.21
(1,26)	1:5:A:LEU:HG	1:6:A:VAL:HG22	6	0.21
(1,26)	1:5:A:LEU:HG	1:6:A:VAL:HG23	6	0.21
(1,25)	1:5:A:LEU:HG	1:6:A:VAL:HA	1	0.21
(1,929)	1:81:A:ILE:H	1:82:A:ILE:HA	3	0.2
(1,866)	1:74:A:ASP:H	1:75:A:PHE:HA	12	0.2
(1,865)	1:74:A:ASP:H	1:75:A:PHE:H	17	0.2
(1,861)	1:73:A:LYS:H	1:74:A:ASP:HA	18	0.2
(1,841)	1:71:A:ASP:H	1:72:A:GLU:HA	14	0.2
(1,840)	1:71:A:ASP:H	1:72:A:GLU:H	13	0.2
(1,840)	1:71:A:ASP:H	1:72:A:GLU:H	14	0.2
(1,828)	1:69:A:SER:HB2	1:76:A:LEU:HD21	10	0.2
(1,828)	1:69:A:SER:HB2	1:76:A:LEU:HD22	10	0.2
(1,828)	1:69:A:SER:HB2	1:76:A:LEU:HD23	10	0.2
(1,828)	1:69:A:SER:HB3	1:76:A:LEU:HD21	10	0.2
(1,828)	1:69:A:SER:HB3	1:76:A:LEU:HD22	10	0.2
(1,828)	1:69:A:SER:HB3	1:76:A:LEU:HD23	10	0.2
(1,807)	1:68:A:VAL:H	1:69:A:SER:HA	8	0.2
(1,793)	1:66:A:VAL:HA	1:76:A:LEU:HA	8	0.2
(1,793)	1:66:A:VAL:HA	1:76:A:LEU:HA	9	0.2
(1,791)	1:66:A:VAL:HA	1:68:A:VAL:HG11	14	0.2
(1,791)	1:66:A:VAL:HA	1:68:A:VAL:HG12	14	0.2
(1,791)	1:66:A:VAL:HA	1:68:A:VAL:HG13	14	0.2
(1,704)	1:59:A:HIS:H	1:60:A:THR:H	8	0.2
(1,692)	1:57:A:LYS:H	1:58:A:GLY:HA2	3	0.2
(1,686)	1:56:A:GLU:HA	1:57:A:LYS:HG2	12	0.2
(1,686)	1:56:A:GLU:HA	1:57:A:LYS:HG3	12	0.2
(1,686)	1:56:A:GLU:HA	1:57:A:LYS:HG2	19	0.2
(1,686)	1:56:A:GLU:HA	1:57:A:LYS:HG3	19	0.2
(1,671)	1:55:A:LYS:H	1:57:A:LYS:H	1	0.2
(1,657)	1:54:A:PHE:HA	1:60:A:THR:HB	20	0.2
(1,643)	1:53:A:PHE:H	1:55:A:LYS:H	2	0.2
(1,632)	1:52:A:ASP:H	1:55:A:LYS:H	11	0.2
(1,567)	1:47:A:MET:HB2	1:48:A:LEU:HA	2	0.2
(1,567)	1:47:A:MET:HB3	1:48:A:LEU:HA	2	0.2
(1,543)	1:44:A:HIS:HA	1:48:A:LEU:H	20	0.2
(1,492)	1:38:A:PHE:HA	1:75:A:PHE:HA	10	0.2
(1,470)	1:36:A:PHE:HD1	1:77:A:TYR:HD1	19	0.2
(1,470)	1:36:A:PHE:HD1	1:77:A:TYR:HD2	19	0.2
(1,470)	1:36:A:PHE:HD2	1:77:A:TYR:HD1	19	0.2
(1,470)	1:36:A:PHE:HD2	1:77:A:TYR:HD2	19	0.2
(1,452)	1:36:A:PHE:H	1:37:A:TYR:HA	10	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,441)	1:35:A:ILE:HB	1:37:A:TYR:HA	3	0.2
(1,434)	1:35:A:ILE:H	1:78:A:GLU:H	19	0.2
(1,433)	1:35:A:ILE:H	1:77:A:TYR:HA	19	0.2
(1,427)	1:34:A:SER:HB2	1:79:A:LEU:HD21	12	0.2
(1,427)	1:34:A:SER:HB2	1:79:A:LEU:HD22	12	0.2
(1,427)	1:34:A:SER:HB2	1:79:A:LEU:HD23	12	0.2
(1,427)	1:34:A:SER:HB3	1:79:A:LEU:HD21	12	0.2
(1,427)	1:34:A:SER:HB3	1:79:A:LEU:HD22	12	0.2
(1,427)	1:34:A:SER:HB3	1:79:A:LEU:HD23	12	0.2
(1,427)	1:34:A:SER:HB2	1:79:A:LEU:HD21	12	0.2
(1,427)	1:34:A:SER:HB2	1:79:A:LEU:HD22	12	0.2
(1,427)	1:34:A:SER:HB2	1:79:A:LEU:HD23	12	0.2
(1,427)	1:34:A:SER:HB3	1:79:A:LEU:HD21	12	0.2
(1,427)	1:34:A:SER:HB3	1:79:A:LEU:HD22	12	0.2
(1,427)	1:34:A:SER:HB3	1:79:A:LEU:HD23	12	0.2
(1,426)	1:34:A:SER:HB2	1:36:A:PHE:HE1	17	0.2
(1,426)	1:34:A:SER:HB2	1:36:A:PHE:HE2	17	0.2
(1,426)	1:34:A:SER:HB3	1:36:A:PHE:HE1	17	0.2
(1,426)	1:34:A:SER:HB3	1:36:A:PHE:HE2	17	0.2
(1,398)	1:32:A:LYS:H	1:81:A:ILE:HG21	16	0.2
(1,398)	1:32:A:LYS:H	1:81:A:ILE:HG22	16	0.2
(1,398)	1:32:A:LYS:H	1:81:A:ILE:HG23	16	0.2
(1,373)	1:29:A:SER:H	1:30:A:GLU:HB2	12	0.2
(1,373)	1:29:A:SER:H	1:30:A:GLU:HB3	12	0.2
(1,364)	1:28:A:PHE:HD1	1:32:A:LYS:HA	10	0.2
(1,364)	1:28:A:PHE:HD2	1:32:A:LYS:HA	10	0.2
(1,354)	1:28:A:PHE:HA	1:30:A:GLU:H	1	0.2
(1,335)	1:26:A:HIS:HB2	1:30:A:GLU:HB2	19	0.2
(1,335)	1:26:A:HIS:HB2	1:30:A:GLU:HB3	19	0.2
(1,335)	1:26:A:HIS:HB3	1:30:A:GLU:HB2	19	0.2
(1,335)	1:26:A:HIS:HB3	1:30:A:GLU:HB3	19	0.2
(1,304)	1:24:A:LEU:HD21	1:59:A:HIS:HE1	9	0.2
(1,304)	1:24:A:LEU:HD22	1:59:A:HIS:HE1	9	0.2
(1,304)	1:24:A:LEU:HD23	1:59:A:HIS:HE1	9	0.2
(1,295)	1:24:A:LEU:HG	1:25:A:TYR:HA	11	0.2
(1,284)	1:24:A:LEU:HA	1:35:A:ILE:HD11	20	0.2
(1,284)	1:24:A:LEU:HA	1:35:A:ILE:HD12	20	0.2
(1,284)	1:24:A:LEU:HA	1:35:A:ILE:HD13	20	0.2
(1,270)	1:23:A:ASP:HA	1:28:A:PHE:H	18	0.2
(1,237)	1:21:A:LEU:HG	1:24:A:LEU:HB2	12	0.2
(1,237)	1:21:A:LEU:HG	1:24:A:LEU:HB3	12	0.2
(1,214)	1:20:A:GLU:H	1:22:A:GLU:H	5	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,214)	1:20:A:GLU:H	1:22:A:GLU:H	9	0.2
(1,203)	1:19:A:VAL:H	1:21:A:LEU:H	14	0.2
(1,190)	1:16:A:ALA:H	1:17:A:LYS:HA	12	0.2
(1,183)	1:14:A:SER:HA	1:15:A:ASP:H	5	0.2
(1,183)	1:14:A:SER:HA	1:15:A:ASP:H	15	0.2
(1,176)	1:13:A:LYS:H	1:14:A:SER:H	2	0.2
(1,176)	1:13:A:LYS:H	1:14:A:SER:H	11	0.2
(1,167)	1:11:A:THR:HB	1:12:A:ARG:HA	1	0.2
(1,160)	1:11:A:THR:H	1:12:A:ARG:H	17	0.2
(1,157)	1:10:A:ASN:HB2	1:46:A:ASP:H	6	0.2
(1,157)	1:10:A:ASN:HB3	1:46:A:ASP:H	6	0.2
(1,145)	1:9:A:LYS:H	1:10:A:ASN:HA	12	0.2
(1,145)	1:9:A:LYS:H	1:10:A:ASN:HA	19	0.2
(1,142)	1:8:A:ALA:HA	1:46:A:ASP:HA	8	0.2
(1,142)	1:8:A:ALA:HA	1:46:A:ASP:HA	15	0.2
(1,99)	1:7:A:LEU:H	1:8:A:ALA:HA	2	0.2
(1,63)	1:6:A:VAL:HA	1:20:A:GLU:H	12	0.2
(1,47)	1:6:A:VAL:H	1:36:A:PHE:H	15	0.2
(1,44)	1:6:A:VAL:H	1:20:A:GLU:HB2	3	0.2
(1,44)	1:6:A:VAL:H	1:20:A:GLU:HB3	3	0.2
(1,27)	1:5:A:LEU:HG	1:7:A:LEU:H	12	0.2
(1,16)	1:5:A:LEU:HA	1:37:A:TYR:H	16	0.2
(1,13)	1:5:A:LEU:HA	1:35:A:ILE:HA	11	0.2
(1,9)	1:5:A:LEU:H	1:36:A:PHE:H	1	0.2
(1,8)	1:5:A:LEU:H	1:35:A:ILE:HB	14	0.2
(1,4)	1:4:A:LYS:HA	1:5:A:LEU:H	3	0.2
(3,1)	1:39:A:ALA:HB1	1:47:A:MET:N	10	0.19
(1,881)	1:76:A:LEU:H	1:77:A:TYR:HA	19	0.19
(1,841)	1:71:A:ASP:H	1:72:A:GLU:HA	17	0.19
(1,841)	1:71:A:ASP:H	1:72:A:GLU:HA	20	0.19
(1,820)	1:69:A:SER:H	1:73:A:LYS:HA	5	0.19
(1,814)	1:68:A:VAL:HG11	1:73:A:LYS:H	1	0.19
(1,814)	1:68:A:VAL:HG12	1:73:A:LYS:H	1	0.19
(1,814)	1:68:A:VAL:HG13	1:73:A:LYS:H	1	0.19
(1,814)	1:68:A:VAL:HG21	1:73:A:LYS:H	1	0.19
(1,814)	1:68:A:VAL:HG22	1:73:A:LYS:H	1	0.19
(1,814)	1:68:A:VAL:HG23	1:73:A:LYS:H	1	0.19
(1,814)	1:68:A:VAL:HG11	1:73:A:LYS:H	2	0.19
(1,814)	1:68:A:VAL:HG12	1:73:A:LYS:H	2	0.19
(1,814)	1:68:A:VAL:HG13	1:73:A:LYS:H	2	0.19
(1,814)	1:68:A:VAL:HG21	1:73:A:LYS:H	2	0.19
(1,814)	1:68:A:VAL:HG22	1:73:A:LYS:H	2	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,814)	1:68:A:VAL:HG23	1:73:A:LYS:H	2	0.19
(1,811)	1:68:A:VAL:HA	1:73:A:LYS:H	4	0.19
(1,791)	1:66:A:VAL:HA	1:68:A:VAL:HG11	5	0.19
(1,791)	1:66:A:VAL:HA	1:68:A:VAL:HG12	5	0.19
(1,791)	1:66:A:VAL:HA	1:68:A:VAL:HG13	5	0.19
(1,764)	1:64:A:ASP:H	1:79:A:LEU:H	1	0.19
(1,761)	1:64:A:ASP:H	1:76:A:LEU:HA	2	0.19
(1,702)	1:58:A:GLY:HA2	1:59:A:HIS:HA	3	0.19
(1,693)	1:57:A:LYS:H	1:59:A:HIS:H	5	0.19
(1,692)	1:57:A:LYS:H	1:58:A:GLY:HA2	7	0.19
(1,676)	1:55:A:LYS:HA	1:58:A:GLY:HA2	12	0.19
(1,668)	1:55:A:LYS:H	1:56:A:GLU:H	17	0.19
(1,668)	1:55:A:LYS:H	1:56:A:GLU:H	19	0.19
(1,599)	1:49:A:LYS:HB2	1:53:A:PHE:HE1	16	0.19
(1,599)	1:49:A:LYS:HB2	1:53:A:PHE:HE2	16	0.19
(1,599)	1:49:A:LYS:HB3	1:53:A:PHE:HE1	16	0.19
(1,599)	1:49:A:LYS:HB3	1:53:A:PHE:HE2	16	0.19
(1,543)	1:44:A:HIS:HA	1:48:A:LEU:H	10	0.19
(1,539)	1:43:A:ALA:HB1	1:44:A:HIS:H	14	0.19
(1,539)	1:43:A:ALA:HB2	1:44:A:HIS:H	14	0.19
(1,539)	1:43:A:ALA:HB3	1:44:A:HIS:H	14	0.19
(1,537)	1:43:A:ALA:HA	1:45:A:LYS:H	2	0.19
(1,529)	1:42:A:ASN:H	1:44:A:HIS:H	13	0.19
(1,528)	1:42:A:ASN:H	1:43:A:ALA:HA	7	0.19
(1,527)	1:42:A:ASN:H	1:43:A:ALA:H	13	0.19
(1,527)	1:42:A:ASN:H	1:43:A:ALA:H	20	0.19
(1,523)	1:41:A:THR:HA	1:44:A:HIS:HA	5	0.19
(1,523)	1:41:A:THR:HA	1:44:A:HIS:HA	15	0.19
(1,505)	1:39:A:ALA:H	1:74:A:ASP:H	16	0.19
(1,505)	1:39:A:ALA:H	1:74:A:ASP:H	20	0.19
(1,494)	1:38:A:PHE:HA	1:75:A:PHE:HE1	2	0.19
(1,494)	1:38:A:PHE:HA	1:75:A:PHE:HE2	2	0.19
(1,467)	1:36:A:PHE:HB2	1:77:A:TYR:HD1	4	0.19
(1,467)	1:36:A:PHE:HB2	1:77:A:TYR:HD2	4	0.19
(1,467)	1:36:A:PHE:HB3	1:77:A:TYR:HD1	4	0.19
(1,467)	1:36:A:PHE:HB3	1:77:A:TYR:HD2	4	0.19
(1,434)	1:35:A:ILE:H	1:78:A:GLU:H	18	0.19
(1,431)	1:35:A:ILE:H	1:36:A:PHE:HD1	8	0.19
(1,431)	1:35:A:ILE:H	1:36:A:PHE:HD2	8	0.19
(1,417)	1:34:A:SER:H	1:79:A:LEU:HA	20	0.19
(1,398)	1:32:A:LYS:H	1:81:A:ILE:HG21	2	0.19
(1,398)	1:32:A:LYS:H	1:81:A:ILE:HG22	2	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,398)	1:32:A:LYS:H	1:81:A:ILE:HG23	2	0.19
(1,348)	1:28:A:PHE:H	1:30:A:GLU:HG2	12	0.19
(1,348)	1:28:A:PHE:H	1:30:A:GLU:HG3	12	0.19
(1,342)	1:27:A:GLU:HA	1:29:A:SER:H	2	0.19
(1,322)	1:25:A:TYR:HD1	1:28:A:PHE:H	6	0.19
(1,322)	1:25:A:TYR:HD2	1:28:A:PHE:H	6	0.19
(1,319)	1:25:A:TYR:HA	1:59:A:HIS:HB2	17	0.19
(1,319)	1:25:A:TYR:HA	1:59:A:HIS:HB3	17	0.19
(1,316)	1:25:A:TYR:HA	1:29:A:SER:H	11	0.19
(1,311)	1:25:A:TYR:H	1:28:A:PHE:H	14	0.19
(1,307)	1:25:A:TYR:H	1:26:A:HIS:H	11	0.19
(1,301)	1:24:A:LEU:HD11	1:60:A:THR:HB	10	0.19
(1,301)	1:24:A:LEU:HD12	1:60:A:THR:HB	10	0.19
(1,301)	1:24:A:LEU:HD13	1:60:A:THR:HB	10	0.19
(1,201)	1:19:A:VAL:H	1:20:A:GLU:HB2	17	0.19
(1,201)	1:19:A:VAL:H	1:20:A:GLU:HB3	17	0.19
(1,197)	1:18:A:SER:HA	1:20:A:GLU:HG2	5	0.19
(1,197)	1:18:A:SER:HA	1:20:A:GLU:HG3	5	0.19
(1,174)	1:12:A:ARG:HB2	1:14:A:SER:HA	10	0.19
(1,174)	1:12:A:ARG:HB3	1:14:A:SER:HA	10	0.19
(1,146)	1:9:A:LYS:H	1:10:A:ASN:HB2	4	0.19
(1,146)	1:9:A:LYS:H	1:10:A:ASN:HB3	4	0.19
(1,142)	1:8:A:ALA:HA	1:46:A:ASP:HA	11	0.19
(1,130)	1:7:A:LEU:HD11	1:16:A:ALA:HA	5	0.19
(1,130)	1:7:A:LEU:HD12	1:16:A:ALA:HA	5	0.19
(1,130)	1:7:A:LEU:HD13	1:16:A:ALA:HA	5	0.19
(1,130)	1:7:A:LEU:HD11	1:16:A:ALA:HA	10	0.19
(1,130)	1:7:A:LEU:HD12	1:16:A:ALA:HA	10	0.19
(1,130)	1:7:A:LEU:HD13	1:16:A:ALA:HA	10	0.19
(1,107)	1:7:A:LEU:H	1:38:A:PHE:HD1	4	0.19
(1,107)	1:7:A:LEU:H	1:38:A:PHE:HD2	4	0.19
(1,74)	1:6:A:VAL:HB	1:38:A:PHE:H	18	0.19
(1,50)	1:6:A:VAL:H	1:37:A:TYR:H	4	0.19
(1,46)	1:6:A:VAL:H	1:35:A:ILE:HD11	13	0.19
(1,46)	1:6:A:VAL:H	1:35:A:ILE:HD12	13	0.19
(1,46)	1:6:A:VAL:H	1:35:A:ILE:HD13	13	0.19
(1,29)	1:5:A:LEU:HG	1:36:A:PHE:H	11	0.19
(1,15)	1:5:A:LEU:HA	1:36:A:PHE:HD1	2	0.19
(1,15)	1:5:A:LEU:HA	1:36:A:PHE:HD2	2	0.19
(1,7)	1:5:A:LEU:H	1:35:A:ILE:HA	20	0.19
(1,4)	1:4:A:LYS:HA	1:5:A:LEU:H	4	0.19
(1,1)	1:3:A:MET:H	1:4:A:LYS:H	16	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,908)	1:78:A:GLU:HA	1:80:A:HIS:HD2	8	0.18
(1,900)	1:77:A:TYR:HD1	1:79:A:LEU:HG	17	0.18
(1,900)	1:77:A:TYR:HD2	1:79:A:LEU:HG	17	0.18
(1,841)	1:71:A:ASP:H	1:72:A:GLU:HA	5	0.18
(1,841)	1:71:A:ASP:H	1:72:A:GLU:HA	16	0.18
(1,837)	1:70:A:THR:HA	1:73:A:LYS:HD2	10	0.18
(1,837)	1:70:A:THR:HA	1:73:A:LYS:HD3	10	0.18
(1,836)	1:70:A:THR:HA	1:73:A:LYS:HB2	8	0.18
(1,836)	1:70:A:THR:HA	1:73:A:LYS:HB3	8	0.18
(1,823)	1:69:A:SER:HA	1:71:A:ASP:H	11	0.18
(1,819)	1:69:A:SER:H	1:73:A:LYS:H	5	0.18
(1,819)	1:69:A:SER:H	1:73:A:LYS:H	17	0.18
(1,775)	1:65:A:GLU:H	1:76:A:LEU:HD11	13	0.18
(1,775)	1:65:A:GLU:H	1:76:A:LEU:HD12	13	0.18
(1,775)	1:65:A:GLU:H	1:76:A:LEU:HD13	13	0.18
(1,775)	1:65:A:GLU:H	1:76:A:LEU:HD21	13	0.18
(1,768)	1:64:A:ASP:HA	1:76:A:LEU:HD21	15	0.18
(1,768)	1:64:A:ASP:HA	1:76:A:LEU:HD22	15	0.18
(1,768)	1:64:A:ASP:HA	1:76:A:LEU:HD23	15	0.18
(1,743)	1:62:A:TYR:HE1	1:63:A:LEU:HD21	16	0.18
(1,743)	1:62:A:TYR:HE1	1:63:A:LEU:HD22	16	0.18
(1,743)	1:62:A:TYR:HE1	1:63:A:LEU:HD23	16	0.18
(1,743)	1:62:A:TYR:HE2	1:63:A:LEU:HD21	16	0.18
(1,743)	1:62:A:TYR:HE2	1:63:A:LEU:HD22	16	0.18
(1,743)	1:62:A:TYR:HE2	1:63:A:LEU:HD23	16	0.18
(1,702)	1:58:A:GLY:HA2	1:59:A:HIS:HA	17	0.18
(1,692)	1:57:A:LYS:H	1:58:A:GLY:HA2	1	0.18
(1,686)	1:56:A:GLU:HA	1:57:A:LYS:HG2	16	0.18
(1,686)	1:56:A:GLU:HA	1:57:A:LYS:HG3	16	0.18
(1,682)	1:56:A:GLU:H	1:57:A:LYS:HA	14	0.18
(1,681)	1:56:A:GLU:H	1:57:A:LYS:H	11	0.18
(1,668)	1:55:A:LYS:H	1:56:A:GLU:H	6	0.18
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD11	13	0.18
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD12	13	0.18
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD13	13	0.18
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD11	13	0.18
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD12	13	0.18
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD13	13	0.18
(1,643)	1:53:A:PHE:H	1:55:A:LYS:H	20	0.18
(1,620)	1:51:A:VAL:HA	1:53:A:PHE:H	2	0.18
(1,620)	1:51:A:VAL:HA	1:53:A:PHE:H	7	0.18
(1,620)	1:51:A:VAL:HA	1:53:A:PHE:H	10	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,584)	1:48:A:LEU:HA	1:52:A:ASP:HB2	11	0.18
(1,584)	1:48:A:LEU:HA	1:52:A:ASP:HB3	11	0.18
(1,527)	1:42:A:ASN:H	1:43:A:ALA:H	18	0.18
(1,526)	1:41:A:THR:HB	1:74:A:ASP:HB2	19	0.18
(1,526)	1:41:A:THR:HB	1:74:A:ASP:HB3	19	0.18
(1,505)	1:39:A:ALA:H	1:74:A:ASP:H	1	0.18
(1,475)	1:37:A:TYR:H	1:76:A:LEU:HA	16	0.18
(1,474)	1:37:A:TYR:H	1:76:A:LEU:H	4	0.18
(1,474)	1:37:A:TYR:H	1:76:A:LEU:H	6	0.18
(1,474)	1:37:A:TYR:H	1:76:A:LEU:H	18	0.18
(1,435)	1:35:A:ILE:H	1:78:A:GLU:HA	9	0.18
(1,433)	1:35:A:ILE:H	1:77:A:TYR:HA	18	0.18
(1,432)	1:35:A:ILE:H	1:36:A:PHE:HE1	1	0.18
(1,432)	1:35:A:ILE:H	1:36:A:PHE:HE2	1	0.18
(1,380)	1:30:A:GLU:H	1:31:A:ASP:HA	1	0.18
(1,371)	1:29:A:SER:H	1:30:A:GLU:H	13	0.18
(1,370)	1:28:A:PHE:HE1	1:81:A:ILE:HA	5	0.18
(1,370)	1:28:A:PHE:HE2	1:81:A:ILE:HA	5	0.18
(1,354)	1:28:A:PHE:HA	1:30:A:GLU:H	13	0.18
(1,319)	1:25:A:TYR:HA	1:59:A:HIS:HB2	2	0.18
(1,319)	1:25:A:TYR:HA	1:59:A:HIS:HB3	2	0.18
(1,318)	1:25:A:TYR:HA	1:59:A:HIS:HA	20	0.18
(1,301)	1:24:A:LEU:HD11	1:60:A:THR:HB	15	0.18
(1,301)	1:24:A:LEU:HD12	1:60:A:THR:HB	15	0.18
(1,301)	1:24:A:LEU:HD13	1:60:A:THR:HB	15	0.18
(1,293)	1:24:A:LEU:HB2	1:80:A:HIS:HE1	19	0.18
(1,293)	1:24:A:LEU:HB3	1:80:A:HIS:HE1	19	0.18
(1,251)	1:22:A:GLU:H	1:23:A:ASP:H	1	0.18
(1,214)	1:20:A:GLU:H	1:22:A:GLU:H	3	0.18
(1,204)	1:19:A:VAL:H	1:22:A:GLU:H	15	0.18
(1,202)	1:19:A:VAL:H	1:20:A:GLU:HG2	8	0.18
(1,202)	1:19:A:VAL:H	1:20:A:GLU:HG3	8	0.18
(1,183)	1:14:A:SER:HA	1:15:A:ASP:H	3	0.18
(1,183)	1:14:A:SER:HA	1:15:A:ASP:H	6	0.18
(1,183)	1:14:A:SER:HA	1:15:A:ASP:H	9	0.18
(1,156)	1:10:A:ASN:HB2	1:45:A:LYS:HB2	11	0.18
(1,156)	1:10:A:ASN:HB2	1:45:A:LYS:HB3	11	0.18
(1,156)	1:10:A:ASN:HB3	1:45:A:LYS:HB2	11	0.18
(1,156)	1:10:A:ASN:HB3	1:45:A:LYS:HB3	11	0.18
(1,148)	1:10:A:ASN:H	1:11:A:THR:H	6	0.18
(1,145)	1:9:A:LYS:H	1:10:A:ASN:HA	1	0.18
(1,145)	1:9:A:LYS:H	1:10:A:ASN:HA	15	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,144)	1:9:A:LYS:H	1:10:A:ASN:H	15	0.18
(1,130)	1:7:A:LEU:HD11	1:16:A:ALA:HA	18	0.18
(1,130)	1:7:A:LEU:HD12	1:16:A:ALA:HA	18	0.18
(1,130)	1:7:A:LEU:HD13	1:16:A:ALA:HA	18	0.18
(1,60)	1:6:A:VAL:HA	1:16:A:ALA:HB1	18	0.18
(1,60)	1:6:A:VAL:HA	1:16:A:ALA:HB2	18	0.18
(1,60)	1:6:A:VAL:HA	1:16:A:ALA:HB3	18	0.18
(1,54)	1:6:A:VAL:H	1:38:A:PHE:H	12	0.18
(1,50)	1:6:A:VAL:H	1:37:A:TYR:H	11	0.18
(1,50)	1:6:A:VAL:H	1:37:A:TYR:H	18	0.18
(1,43)	1:6:A:VAL:H	1:7:A:LEU:HG	16	0.18
(1,9)	1:5:A:LEU:H	1:36:A:PHE:H	5	0.18
(1,9)	1:5:A:LEU:H	1:36:A:PHE:H	19	0.18
(1,9)	1:5:A:LEU:H	1:36:A:PHE:H	20	0.18
(1,2)	1:3:A:MET:H	1:4:A:LYS:HA	10	0.18
(1,1)	1:3:A:MET:H	1:4:A:LYS:H	6	0.18
(1,1)	1:3:A:MET:H	1:4:A:LYS:H	11	0.18
(1,840)	1:71:A:ASP:H	1:72:A:GLU:H	5	0.17
(1,793)	1:66:A:VAL:HA	1:76:A:LEU:HA	5	0.17
(1,705)	1:59:A:HIS:H	1:60:A:THR:HA	8	0.17
(1,692)	1:57:A:LYS:H	1:58:A:GLY:HA2	14	0.17
(1,620)	1:51:A:VAL:HA	1:53:A:PHE:H	5	0.17
(1,537)	1:43:A:ALA:HA	1:45:A:LYS:H	12	0.17
(1,527)	1:42:A:ASN:H	1:43:A:ALA:H	16	0.17
(1,512)	1:39:A:ALA:HA	1:74:A:ASP:HB2	20	0.17
(1,512)	1:39:A:ALA:HA	1:74:A:ASP:HB3	20	0.17
(1,506)	1:39:A:ALA:H	1:74:A:ASP:HA	2	0.17
(1,501)	1:38:A:PHE:HD1	1:75:A:PHE:H	17	0.17
(1,501)	1:38:A:PHE:HD2	1:75:A:PHE:H	17	0.17
(1,492)	1:38:A:PHE:HA	1:75:A:PHE:HA	1	0.17
(1,492)	1:38:A:PHE:HA	1:75:A:PHE:HA	14	0.17
(1,492)	1:38:A:PHE:HA	1:75:A:PHE:HA	19	0.17
(1,489)	1:38:A:PHE:H	1:75:A:PHE:HA	3	0.17
(1,475)	1:37:A:TYR:H	1:76:A:LEU:HA	14	0.17
(1,431)	1:35:A:ILE:H	1:36:A:PHE:HD1	1	0.17
(1,431)	1:35:A:ILE:H	1:36:A:PHE:HD2	1	0.17
(1,431)	1:35:A:ILE:H	1:36:A:PHE:HD1	3	0.17
(1,431)	1:35:A:ILE:H	1:36:A:PHE:HD2	3	0.17
(1,409)	1:33:A:ARG:HA	1:80:A:HIS:H	19	0.17
(1,398)	1:32:A:LYS:H	1:81:A:ILE:HG21	5	0.17
(1,398)	1:32:A:LYS:H	1:81:A:ILE:HG22	5	0.17
(1,398)	1:32:A:LYS:H	1:81:A:ILE:HG23	5	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,373)	1:29:A:SER:H	1:30:A:GLU:HB2	18	0.17
(1,373)	1:29:A:SER:H	1:30:A:GLU:HB3	18	0.17
(1,370)	1:28:A:PHE:HE1	1:81:A:ILE:HA	9	0.17
(1,370)	1:28:A:PHE:HE2	1:81:A:ILE:HA	9	0.17
(1,356)	1:28:A:PHE:HA	1:33:A:ARG:H	19	0.17
(1,354)	1:28:A:PHE:HA	1:30:A:GLU:H	18	0.17
(1,342)	1:27:A:GLU:HA	1:29:A:SER:H	9	0.17
(1,300)	1:24:A:LEU:HD11	1:35:A:ILE:HG12	11	0.17
(1,300)	1:24:A:LEU:HD11	1:35:A:ILE:HG13	11	0.17
(1,300)	1:24:A:LEU:HD12	1:35:A:ILE:HG12	11	0.17
(1,300)	1:24:A:LEU:HD12	1:35:A:ILE:HG13	11	0.17
(1,300)	1:24:A:LEU:HD13	1:35:A:ILE:HG12	11	0.17
(1,300)	1:24:A:LEU:HD13	1:35:A:ILE:HG13	11	0.17
(1,270)	1:23:A:ASP:HA	1:28:A:PHE:H	7	0.17
(1,268)	1:23:A:ASP:HA	1:27:A:GLU:HA	14	0.17
(1,214)	1:20:A:GLU:H	1:22:A:GLU:H	1	0.17
(1,214)	1:20:A:GLU:H	1:22:A:GLU:H	10	0.17
(1,203)	1:19:A:VAL:H	1:21:A:LEU:H	10	0.17
(1,202)	1:19:A:VAL:H	1:20:A:GLU:HG2	5	0.17
(1,202)	1:19:A:VAL:H	1:20:A:GLU:HG3	5	0.17
(1,157)	1:10:A:ASN:HB2	1:46:A:ASP:H	13	0.17
(1,157)	1:10:A:ASN:HB3	1:46:A:ASP:H	13	0.17
(1,155)	1:10:A:ASN:HA	1:40:A:PRO:HG2	13	0.17
(1,155)	1:10:A:ASN:HA	1:40:A:PRO:HG3	13	0.17
(1,148)	1:10:A:ASN:H	1:11:A:THR:H	2	0.17
(1,147)	1:9:A:LYS:H	1:11:A:THR:H	4	0.17
(1,123)	1:7:A:LEU:HB2	1:38:A:PHE:HD1	17	0.17
(1,123)	1:7:A:LEU:HB2	1:38:A:PHE:HD2	17	0.17
(1,123)	1:7:A:LEU:HB3	1:38:A:PHE:HD1	17	0.17
(1,123)	1:7:A:LEU:HB3	1:38:A:PHE:HD2	17	0.17
(1,106)	1:7:A:LEU:H	1:38:A:PHE:HB2	13	0.17
(1,106)	1:7:A:LEU:H	1:38:A:PHE:HB3	13	0.17
(1,106)	1:7:A:LEU:H	1:38:A:PHE:HB2	14	0.17
(1,106)	1:7:A:LEU:H	1:38:A:PHE:HB3	14	0.17
(1,92)	1:6:A:VAL:HG21	1:35:A:ILE:HB	17	0.17
(1,92)	1:6:A:VAL:HG22	1:35:A:ILE:HB	17	0.17
(1,92)	1:6:A:VAL:HG23	1:35:A:ILE:HB	17	0.17
(1,70)	1:6:A:VAL:HB	1:20:A:GLU:HA	1	0.17
(1,63)	1:6:A:VAL:HA	1:20:A:GLU:H	9	0.17
(1,60)	1:6:A:VAL:HA	1:16:A:ALA:HB1	14	0.17
(1,60)	1:6:A:VAL:HA	1:16:A:ALA:HB2	14	0.17
(1,60)	1:6:A:VAL:HA	1:16:A:ALA:HB3	14	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,47)	1:6:A:VAL:H	1:36:A:PHE:H	19	0.17
(1,26)	1:5:A:LEU:HG	1:6:A:VAL:HG21	17	0.17
(1,26)	1:5:A:LEU:HG	1:6:A:VAL:HG22	17	0.17
(1,26)	1:5:A:LEU:HG	1:6:A:VAL:HG23	17	0.17
(1,16)	1:5:A:LEU:HA	1:37:A:TYR:H	4	0.17
(1,4)	1:4:A:LYS:HA	1:5:A:LEU:H	8	0.17
(1,1)	1:3:A:MET:H	1:4:A:LYS:H	13	0.17
(1,791)	1:66:A:VAL:HA	1:68:A:VAL:HG11	11	0.16
(1,791)	1:66:A:VAL:HA	1:68:A:VAL:HG12	11	0.16
(1,791)	1:66:A:VAL:HA	1:68:A:VAL:HG13	11	0.16
(1,768)	1:64:A:ASP:HA	1:76:A:LEU:HD21	8	0.16
(1,768)	1:64:A:ASP:HA	1:76:A:LEU:HD22	8	0.16
(1,768)	1:64:A:ASP:HA	1:76:A:LEU:HD23	8	0.16
(1,768)	1:64:A:ASP:HA	1:76:A:LEU:HD21	12	0.16
(1,768)	1:64:A:ASP:HA	1:76:A:LEU:HD22	12	0.16
(1,768)	1:64:A:ASP:HA	1:76:A:LEU:HD23	12	0.16
(1,727)	1:61:A:ALA:HB1	1:79:A:LEU:HB3	10	0.16
(1,727)	1:61:A:ALA:HB2	1:79:A:LEU:HB3	10	0.16
(1,727)	1:61:A:ALA:HB3	1:79:A:LEU:HB3	10	0.16
(1,703)	1:58:A:GLY:HA3	1:60:A:THR:H	7	0.16
(1,682)	1:56:A:GLU:H	1:57:A:LYS:HA	17	0.16
(1,676)	1:55:A:LYS:HA	1:58:A:GLY:HA2	13	0.16
(1,675)	1:55:A:LYS:HA	1:57:A:LYS:H	15	0.16
(1,668)	1:55:A:LYS:H	1:56:A:GLU:H	13	0.16
(1,668)	1:55:A:LYS:H	1:56:A:GLU:H	18	0.16
(1,643)	1:53:A:PHE:H	1:55:A:LYS:H	4	0.16
(1,632)	1:52:A:ASP:H	1:55:A:LYS:H	10	0.16
(1,630)	1:52:A:ASP:H	1:53:A:PHE:H	17	0.16
(1,595)	1:49:A:LYS:HA	1:52:A:ASP:HA	6	0.16
(1,567)	1:47:A:MET:HB2	1:48:A:LEU:HA	5	0.16
(1,567)	1:47:A:MET:HB3	1:48:A:LEU:HA	5	0.16
(1,567)	1:47:A:MET:HB2	1:48:A:LEU:HA	19	0.16
(1,567)	1:47:A:MET:HB3	1:48:A:LEU:HA	19	0.16
(1,543)	1:44:A:HIS:HA	1:48:A:LEU:H	7	0.16
(1,537)	1:43:A:ALA:HA	1:45:A:LYS:H	3	0.16
(1,537)	1:43:A:ALA:HA	1:45:A:LYS:H	9	0.16
(1,523)	1:41:A:THR:HA	1:44:A:HIS:HA	13	0.16
(1,512)	1:39:A:ALA:HA	1:74:A:ASP:HB2	8	0.16
(1,512)	1:39:A:ALA:HA	1:74:A:ASP:HB3	8	0.16
(1,492)	1:38:A:PHE:HA	1:75:A:PHE:HA	16	0.16
(1,467)	1:36:A:PHE:HB2	1:77:A:TYR:HD1	15	0.16
(1,467)	1:36:A:PHE:HB2	1:77:A:TYR:HD2	15	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,467)	1:36:A:PHE:HB3	1:77:A:TYR:HD1	15	0.16
(1,467)	1:36:A:PHE:HB3	1:77:A:TYR:HD2	15	0.16
(1,437)	1:35:A:ILE:H	1:80:A:HIS:H	3	0.16
(1,417)	1:34:A:SER:H	1:79:A:LEU:HA	6	0.16
(1,417)	1:34:A:SER:H	1:79:A:LEU:HA	16	0.16
(1,410)	1:33:A:ARG:HA	1:81:A:ILE:HG21	18	0.16
(1,410)	1:33:A:ARG:HA	1:81:A:ILE:HG22	18	0.16
(1,410)	1:33:A:ARG:HA	1:81:A:ILE:HG23	18	0.16
(1,375)	1:29:A:SER:HA	1:31:A:ASP:H	4	0.16
(1,365)	1:28:A:PHE:HD1	1:32:A:LYS:HB2	11	0.16
(1,365)	1:28:A:PHE:HD1	1:32:A:LYS:HB3	11	0.16
(1,365)	1:28:A:PHE:HD2	1:32:A:LYS:HB2	11	0.16
(1,365)	1:28:A:PHE:HD2	1:32:A:LYS:HB3	11	0.16
(1,360)	1:28:A:PHE:HB2	1:29:A:SER:H	6	0.16
(1,360)	1:28:A:PHE:HB3	1:29:A:SER:H	6	0.16
(1,355)	1:28:A:PHE:HA	1:32:A:LYS:HB2	10	0.16
(1,355)	1:28:A:PHE:HA	1:32:A:LYS:HB3	10	0.16
(1,354)	1:28:A:PHE:HA	1:30:A:GLU:H	9	0.16
(1,354)	1:28:A:PHE:HA	1:30:A:GLU:H	16	0.16
(1,316)	1:25:A:TYR:HA	1:29:A:SER:H	14	0.16
(1,311)	1:25:A:TYR:H	1:28:A:PHE:H	9	0.16
(1,307)	1:25:A:TYR:H	1:26:A:HIS:H	2	0.16
(1,215)	1:20:A:GLU:H	1:37:A:TYR:HD1	18	0.16
(1,215)	1:20:A:GLU:H	1:37:A:TYR:HD2	18	0.16
(1,203)	1:19:A:VAL:H	1:21:A:LEU:H	8	0.16
(1,187)	1:15:A:ASP:HA	1:16:A:ALA:H	2	0.16
(1,183)	1:14:A:SER:HA	1:15:A:ASP:H	10	0.16
(1,182)	1:14:A:SER:H	1:17:A:LYS:H	13	0.16
(1,176)	1:13:A:LYS:H	1:14:A:SER:H	9	0.16
(1,157)	1:10:A:ASN:HB2	1:46:A:ASP:H	16	0.16
(1,157)	1:10:A:ASN:HB3	1:46:A:ASP:H	16	0.16
(1,147)	1:9:A:LYS:H	1:11:A:THR:H	10	0.16
(1,146)	1:9:A:LYS:H	1:10:A:ASN:HB2	6	0.16
(1,146)	1:9:A:LYS:H	1:10:A:ASN:HB3	6	0.16
(1,145)	1:9:A:LYS:H	1:10:A:ASN:HA	7	0.16
(1,145)	1:9:A:LYS:H	1:10:A:ASN:HA	10	0.16
(1,138)	1:8:A:ALA:HA	1:10:A:ASN:HB2	10	0.16
(1,138)	1:8:A:ALA:HA	1:10:A:ASN:HB3	10	0.16
(1,127)	1:7:A:LEU:HG	1:38:A:PHE:HB2	20	0.16
(1,127)	1:7:A:LEU:HG	1:38:A:PHE:HB3	20	0.16
(1,123)	1:7:A:LEU:HB2	1:38:A:PHE:HD1	9	0.16
(1,123)	1:7:A:LEU:HB2	1:38:A:PHE:HD2	9	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,123)	1:7:A:LEU:HB3	1:38:A:PHE:HD1	9	0.16
(1,123)	1:7:A:LEU:HB3	1:38:A:PHE:HD2	9	0.16
(1,105)	1:7:A:LEU:H	1:38:A:PHE:H	1	0.16
(1,102)	1:7:A:LEU:H	1:19:A:VAL:HB	13	0.16
(1,78)	1:6:A:VAL:HG11	1:7:A:LEU:HD11	1	0.16
(1,78)	1:6:A:VAL:HG11	1:7:A:LEU:HD12	1	0.16
(1,78)	1:6:A:VAL:HG11	1:7:A:LEU:HD13	1	0.16
(1,78)	1:6:A:VAL:HG12	1:7:A:LEU:HD11	1	0.16
(1,78)	1:6:A:VAL:HG12	1:7:A:LEU:HD12	1	0.16
(1,78)	1:6:A:VAL:HG12	1:7:A:LEU:HD13	1	0.16
(1,78)	1:6:A:VAL:HG13	1:7:A:LEU:HD11	1	0.16
(1,78)	1:6:A:VAL:HG13	1:7:A:LEU:HD12	1	0.16
(1,78)	1:6:A:VAL:HG13	1:7:A:LEU:HD13	1	0.16
(1,50)	1:6:A:VAL:H	1:37:A:TYR:H	3	0.16
(1,43)	1:6:A:VAL:H	1:7:A:LEU:HG	5	0.16
(1,9)	1:5:A:LEU:H	1:36:A:PHE:H	10	0.16
(1,4)	1:4:A:LYS:HA	1:5:A:LEU:H	13	0.16
(1,4)	1:4:A:LYS:HA	1:5:A:LEU:H	17	0.16
(1,930)	1:81:A:ILE:HA	1:82:A:ILE:H	1	0.15
(1,929)	1:81:A:ILE:H	1:82:A:ILE:HA	7	0.15
(1,841)	1:71:A:ASP:H	1:72:A:GLU:HA	19	0.15
(1,820)	1:69:A:SER:H	1:73:A:LYS:HA	13	0.15
(1,810)	1:68:A:VAL:HA	1:72:A:GLU:H	9	0.15
(1,702)	1:58:A:GLY:HA2	1:59:A:HIS:HA	4	0.15
(1,702)	1:58:A:GLY:HA2	1:59:A:HIS:HA	7	0.15
(1,669)	1:55:A:LYS:H	1:56:A:GLU:HA	19	0.15
(1,668)	1:55:A:LYS:H	1:56:A:GLU:H	9	0.15
(1,664)	1:54:A:PHE:HD1	1:76:A:LEU:HD11	20	0.15
(1,664)	1:54:A:PHE:HD1	1:76:A:LEU:HD12	20	0.15
(1,664)	1:54:A:PHE:HD1	1:76:A:LEU:HD13	20	0.15
(1,664)	1:54:A:PHE:HD2	1:76:A:LEU:HD11	20	0.15
(1,664)	1:54:A:PHE:HD2	1:76:A:LEU:HD12	20	0.15
(1,664)	1:54:A:PHE:HD2	1:76:A:LEU:HD13	20	0.15
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD11	3	0.15
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD12	3	0.15
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD13	3	0.15
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD11	3	0.15
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD12	3	0.15
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD13	3	0.15
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD11	16	0.15
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD12	16	0.15
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD13	16	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD11	16	0.15
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD12	16	0.15
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD13	16	0.15
(1,628)	1:51:A:VAL:HG21	1:54:A:PHE:HD1	9	0.15
(1,628)	1:51:A:VAL:HG21	1:54:A:PHE:HD2	9	0.15
(1,628)	1:51:A:VAL:HG22	1:54:A:PHE:HD1	9	0.15
(1,628)	1:51:A:VAL:HG22	1:54:A:PHE:HD2	9	0.15
(1,628)	1:51:A:VAL:HG23	1:54:A:PHE:HD1	9	0.15
(1,628)	1:51:A:VAL:HG23	1:54:A:PHE:HD2	9	0.15
(1,620)	1:51:A:VAL:HA	1:53:A:PHE:H	16	0.15
(1,620)	1:51:A:VAL:HA	1:53:A:PHE:H	20	0.15
(1,543)	1:44:A:HIS:HA	1:48:A:LEU:H	5	0.15
(1,543)	1:44:A:HIS:HA	1:48:A:LEU:H	11	0.15
(1,521)	1:41:A:THR:HA	1:43:A:ALA:H	1	0.15
(1,494)	1:38:A:PHE:HA	1:75:A:PHE:HE1	6	0.15
(1,494)	1:38:A:PHE:HA	1:75:A:PHE:HE2	6	0.15
(1,474)	1:37:A:TYR:H	1:76:A:LEU:H	12	0.15
(1,470)	1:36:A:PHE:HD1	1:77:A:TYR:HD1	7	0.15
(1,470)	1:36:A:PHE:HD1	1:77:A:TYR:HD2	7	0.15
(1,470)	1:36:A:PHE:HD2	1:77:A:TYR:HD1	7	0.15
(1,470)	1:36:A:PHE:HD2	1:77:A:TYR:HD2	7	0.15
(1,470)	1:36:A:PHE:HD1	1:77:A:TYR:HD1	13	0.15
(1,470)	1:36:A:PHE:HD1	1:77:A:TYR:HD2	13	0.15
(1,470)	1:36:A:PHE:HD2	1:77:A:TYR:HD1	13	0.15
(1,470)	1:36:A:PHE:HD2	1:77:A:TYR:HD2	13	0.15
(1,422)	1:34:A:SER:HA	1:78:A:GLU:HB2	9	0.15
(1,422)	1:34:A:SER:HA	1:78:A:GLU:HB3	9	0.15
(1,419)	1:34:A:SER:H	1:80:A:HIS:H	9	0.15
(1,373)	1:29:A:SER:H	1:30:A:GLU:HB2	4	0.15
(1,373)	1:29:A:SER:H	1:30:A:GLU:HB3	4	0.15
(1,373)	1:29:A:SER:H	1:30:A:GLU:HB2	10	0.15
(1,373)	1:29:A:SER:H	1:30:A:GLU:HB3	10	0.15
(1,365)	1:28:A:PHE:HD1	1:32:A:LYS:HB2	17	0.15
(1,365)	1:28:A:PHE:HD1	1:32:A:LYS:HB3	17	0.15
(1,365)	1:28:A:PHE:HD2	1:32:A:LYS:HB2	17	0.15
(1,365)	1:28:A:PHE:HD2	1:32:A:LYS:HB3	17	0.15
(1,354)	1:28:A:PHE:HA	1:30:A:GLU:H	11	0.15
(1,354)	1:28:A:PHE:HA	1:30:A:GLU:H	12	0.15
(1,319)	1:25:A:TYR:HA	1:59:A:HIS:HB2	13	0.15
(1,319)	1:25:A:TYR:HA	1:59:A:HIS:HB3	13	0.15
(1,318)	1:25:A:TYR:HA	1:59:A:HIS:HA	11	0.15
(1,312)	1:25:A:TYR:H	1:59:A:HIS:HE1	8	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,284)	1:24:A:LEU:HA	1:35:A:ILE:HD11	6	0.15
(1,284)	1:24:A:LEU:HA	1:35:A:ILE:HD12	6	0.15
(1,284)	1:24:A:LEU:HA	1:35:A:ILE:HD13	6	0.15
(1,270)	1:23:A:ASP:HA	1:28:A:PHE:H	19	0.15
(1,268)	1:23:A:ASP:HA	1:27:A:GLU:HA	20	0.15
(1,264)	1:23:A:ASP:H	1:27:A:GLU:H	1	0.15
(1,220)	1:20:A:GLU:HA	1:24:A:LEU:HA	5	0.15
(1,220)	1:20:A:GLU:HA	1:24:A:LEU:HA	7	0.15
(1,220)	1:20:A:GLU:HA	1:24:A:LEU:HA	9	0.15
(1,220)	1:20:A:GLU:HA	1:24:A:LEU:HA	12	0.15
(1,208)	1:19:A:VAL:HB	1:23:A:ASP:H	16	0.15
(1,204)	1:19:A:VAL:H	1:22:A:GLU:H	3	0.15
(1,204)	1:19:A:VAL:H	1:22:A:GLU:H	13	0.15
(1,203)	1:19:A:VAL:H	1:21:A:LEU:H	7	0.15
(1,203)	1:19:A:VAL:H	1:21:A:LEU:H	13	0.15
(1,183)	1:14:A:SER:HA	1:15:A:ASP:H	13	0.15
(1,182)	1:14:A:SER:H	1:17:A:LYS:H	16	0.15
(1,167)	1:11:A:THR:HB	1:12:A:ARG:HA	3	0.15
(1,158)	1:10:A:ASN:HB2	1:46:A:ASP:HA	5	0.15
(1,158)	1:10:A:ASN:HB3	1:46:A:ASP:HA	5	0.15
(1,157)	1:10:A:ASN:HB2	1:46:A:ASP:H	15	0.15
(1,157)	1:10:A:ASN:HB3	1:46:A:ASP:H	15	0.15
(1,156)	1:10:A:ASN:HB2	1:45:A:LYS:HB2	19	0.15
(1,156)	1:10:A:ASN:HB2	1:45:A:LYS:HB3	19	0.15
(1,156)	1:10:A:ASN:HB3	1:45:A:LYS:HB2	19	0.15
(1,156)	1:10:A:ASN:HB3	1:45:A:LYS:HB3	19	0.15
(1,147)	1:9:A:LYS:H	1:11:A:THR:H	18	0.15
(1,142)	1:8:A:ALA:HA	1:46:A:ASP:HA	7	0.15
(1,130)	1:7:A:LEU:HD11	1:16:A:ALA:HA	12	0.15
(1,130)	1:7:A:LEU:HD12	1:16:A:ALA:HA	12	0.15
(1,130)	1:7:A:LEU:HD13	1:16:A:ALA:HA	12	0.15
(1,106)	1:7:A:LEU:H	1:38:A:PHE:HB2	1	0.15
(1,106)	1:7:A:LEU:H	1:38:A:PHE:HB3	1	0.15
(1,74)	1:6:A:VAL:HB	1:38:A:PHE:H	15	0.15
(1,47)	1:6:A:VAL:H	1:36:A:PHE:H	9	0.15
(1,44)	1:6:A:VAL:H	1:20:A:GLU:HB2	4	0.15
(1,44)	1:6:A:VAL:H	1:20:A:GLU:HB3	4	0.15
(1,43)	1:6:A:VAL:H	1:7:A:LEU:HG	2	0.15
(1,28)	1:5:A:LEU:HG	1:7:A:LEU:HG	13	0.15
(1,27)	1:5:A:LEU:HG	1:7:A:LEU:H	2	0.15
(1,9)	1:5:A:LEU:H	1:36:A:PHE:H	8	0.15
(1,8)	1:5:A:LEU:H	1:35:A:ILE:HB	4	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,929)	1:81:A:ILE:H	1:82:A:ILE:HA	4	0.14
(1,929)	1:81:A:ILE:H	1:82:A:ILE:HA	11	0.14
(1,928)	1:81:A:ILE:H	1:82:A:ILE:H	2	0.14
(1,906)	1:78:A:GLU:HA	1:79:A:LEU:HG	7	0.14
(1,890)	1:76:A:LEU:HD11	1:78:A:GLU:H	3	0.14
(1,890)	1:76:A:LEU:HD12	1:78:A:GLU:H	3	0.14
(1,890)	1:76:A:LEU:HD13	1:78:A:GLU:H	3	0.14
(1,831)	1:70:A:THR:H	1:73:A:LYS:HA	7	0.14
(1,828)	1:69:A:SER:HB2	1:76:A:LEU:HD21	3	0.14
(1,828)	1:69:A:SER:HB2	1:76:A:LEU:HD22	3	0.14
(1,828)	1:69:A:SER:HB2	1:76:A:LEU:HD23	3	0.14
(1,828)	1:69:A:SER:HB3	1:76:A:LEU:HD21	3	0.14
(1,828)	1:69:A:SER:HB3	1:76:A:LEU:HD22	3	0.14
(1,828)	1:69:A:SER:HB3	1:76:A:LEU:HD23	3	0.14
(1,727)	1:61:A:ALA:HB1	1:79:A:LEU:HB3	11	0.14
(1,727)	1:61:A:ALA:HB2	1:79:A:LEU:HB3	11	0.14
(1,727)	1:61:A:ALA:HB3	1:79:A:LEU:HB3	11	0.14
(1,711)	1:60:A:THR:HA	1:61:A:ALA:HA	20	0.14
(1,702)	1:58:A:GLY:HA2	1:59:A:HIS:HA	11	0.14
(1,692)	1:57:A:LYS:H	1:58:A:GLY:HA2	2	0.14
(1,692)	1:57:A:LYS:H	1:58:A:GLY:HA2	17	0.14
(1,681)	1:56:A:GLU:H	1:57:A:LYS:H	14	0.14
(1,681)	1:56:A:GLU:H	1:57:A:LYS:H	16	0.14
(1,675)	1:55:A:LYS:HA	1:57:A:LYS:H	3	0.14
(1,675)	1:55:A:LYS:HA	1:57:A:LYS:H	7	0.14
(1,620)	1:51:A:VAL:HA	1:53:A:PHE:H	11	0.14
(1,586)	1:48:A:LEU:HB2	1:49:A:LYS:HA	10	0.14
(1,586)	1:48:A:LEU:HB3	1:49:A:LYS:HA	10	0.14
(1,528)	1:42:A:ASN:H	1:43:A:ALA:HA	1	0.14
(1,523)	1:41:A:THR:HA	1:44:A:HIS:HA	10	0.14
(1,506)	1:39:A:ALA:H	1:74:A:ASP:HA	11	0.14
(1,467)	1:36:A:PHE:HB2	1:77:A:TYR:HD1	8	0.14
(1,467)	1:36:A:PHE:HB2	1:77:A:TYR:HD2	8	0.14
(1,467)	1:36:A:PHE:HB3	1:77:A:TYR:HD1	8	0.14
(1,467)	1:36:A:PHE:HB3	1:77:A:TYR:HD2	8	0.14
(1,435)	1:35:A:ILE:H	1:78:A:GLU:HA	2	0.14
(1,433)	1:35:A:ILE:H	1:77:A:TYR:HA	14	0.14
(1,431)	1:35:A:ILE:H	1:36:A:PHE:HD1	16	0.14
(1,431)	1:35:A:ILE:H	1:36:A:PHE:HD2	16	0.14
(1,419)	1:34:A:SER:H	1:80:A:HIS:H	11	0.14
(1,417)	1:34:A:SER:H	1:79:A:LEU:HA	2	0.14
(1,414)	1:33:A:ARG:HG2	1:34:A:SER:HB2	6	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,414)	1:33:A:ARG:HG2	1:34:A:SER:HB3	6	0.14
(1,414)	1:33:A:ARG:HG3	1:34:A:SER:HB2	6	0.14
(1,414)	1:33:A:ARG:HG3	1:34:A:SER:HB3	6	0.14
(1,409)	1:33:A:ARG:HA	1:80:A:HIS:H	9	0.14
(1,360)	1:28:A:PHE:HB2	1:29:A:SER:H	20	0.14
(1,360)	1:28:A:PHE:HB3	1:29:A:SER:H	20	0.14
(1,342)	1:27:A:GLU:HA	1:29:A:SER:H	6	0.14
(1,317)	1:25:A:TYR:HA	1:29:A:SER:HG	16	0.14
(1,316)	1:25:A:TYR:HA	1:29:A:SER:H	5	0.14
(1,307)	1:25:A:TYR:H	1:26:A:HIS:H	4	0.14
(1,284)	1:24:A:LEU:HA	1:35:A:ILE:HD11	12	0.14
(1,284)	1:24:A:LEU:HA	1:35:A:ILE:HD12	12	0.14
(1,284)	1:24:A:LEU:HA	1:35:A:ILE:HD13	12	0.14
(1,264)	1:23:A:ASP:H	1:27:A:GLU:H	13	0.14
(1,251)	1:22:A:GLU:H	1:23:A:ASP:H	3	0.14
(1,237)	1:21:A:LEU:HG	1:24:A:LEU:HB2	7	0.14
(1,237)	1:21:A:LEU:HG	1:24:A:LEU:HB3	7	0.14
(1,220)	1:20:A:GLU:HA	1:24:A:LEU:HA	15	0.14
(1,220)	1:20:A:GLU:HA	1:24:A:LEU:HA	18	0.14
(1,214)	1:20:A:GLU:H	1:22:A:GLU:H	7	0.14
(1,214)	1:20:A:GLU:H	1:22:A:GLU:H	20	0.14
(1,207)	1:19:A:VAL:HB	1:22:A:GLU:H	10	0.14
(1,207)	1:19:A:VAL:HB	1:22:A:GLU:H	17	0.14
(1,203)	1:19:A:VAL:H	1:21:A:LEU:H	12	0.14
(1,203)	1:19:A:VAL:H	1:21:A:LEU:H	16	0.14
(1,195)	1:18:A:SER:H	1:19:A:VAL:H	17	0.14
(1,186)	1:15:A:ASP:H	1:16:A:ALA:HA	12	0.14
(1,185)	1:15:A:ASP:H	1:16:A:ALA:H	17	0.14
(1,182)	1:14:A:SER:H	1:17:A:LYS:H	15	0.14
(1,157)	1:10:A:ASN:HB2	1:46:A:ASP:H	8	0.14
(1,157)	1:10:A:ASN:HB3	1:46:A:ASP:H	8	0.14
(1,157)	1:10:A:ASN:HB2	1:46:A:ASP:H	20	0.14
(1,157)	1:10:A:ASN:HB3	1:46:A:ASP:H	20	0.14
(1,148)	1:10:A:ASN:H	1:11:A:THR:H	15	0.14
(1,144)	1:9:A:LYS:H	1:10:A:ASN:H	18	0.14
(1,144)	1:9:A:LYS:H	1:10:A:ASN:H	19	0.14
(1,142)	1:8:A:ALA:HA	1:46:A:ASP:HA	9	0.14
(1,127)	1:7:A:LEU:HG	1:38:A:PHE:HB2	4	0.14
(1,127)	1:7:A:LEU:HG	1:38:A:PHE:HB3	4	0.14
(1,105)	1:7:A:LEU:H	1:38:A:PHE:H	5	0.14
(1,74)	1:6:A:VAL:HB	1:38:A:PHE:H	8	0.14
(1,69)	1:6:A:VAL:HB	1:20:A:GLU:H	2	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,63)	1:6:A:VAL:HA	1:20:A:GLU:H	20	0.14
(1,41)	1:6:A:VAL:H	1:7:A:LEU:H	5	0.14
(1,9)	1:5:A:LEU:H	1:36:A:PHE:H	13	0.14
(1,9)	1:5:A:LEU:H	1:36:A:PHE:H	17	0.14
(1,4)	1:4:A:LYS:HA	1:5:A:LEU:H	2	0.14
(1,906)	1:78:A:GLU:HA	1:79:A:LEU:HG	5	0.13
(1,877)	1:75:A:PHE:HB2	1:77:A:TYR:H	1	0.13
(1,877)	1:75:A:PHE:HB3	1:77:A:TYR:H	1	0.13
(1,862)	1:73:A:LYS:HA	1:75:A:PHE:H	15	0.13
(1,842)	1:71:A:ASP:H	1:73:A:LYS:H	20	0.13
(1,811)	1:68:A:VAL:HA	1:73:A:LYS:H	3	0.13
(1,805)	1:67:A:ARG:H	1:68:A:VAL:HG11	6	0.13
(1,805)	1:67:A:ARG:H	1:68:A:VAL:HG12	6	0.13
(1,805)	1:67:A:ARG:H	1:68:A:VAL:HG13	6	0.13
(1,791)	1:66:A:VAL:HA	1:68:A:VAL:HG11	16	0.13
(1,791)	1:66:A:VAL:HA	1:68:A:VAL:HG12	16	0.13
(1,791)	1:66:A:VAL:HA	1:68:A:VAL:HG13	16	0.13
(1,768)	1:64:A:ASP:HA	1:76:A:LEU:HD21	13	0.13
(1,768)	1:64:A:ASP:HA	1:76:A:LEU:HD22	13	0.13
(1,768)	1:64:A:ASP:HA	1:76:A:LEU:HD23	13	0.13
(1,763)	1:64:A:ASP:H	1:77:A:TYR:HA	6	0.13
(1,737)	1:62:A:TYR:HB2	1:79:A:LEU:H	12	0.13
(1,737)	1:62:A:TYR:HB3	1:79:A:LEU:H	12	0.13
(1,731)	1:62:A:TYR:H	1:80:A:HIS:HA	12	0.13
(1,731)	1:62:A:TYR:H	1:80:A:HIS:HA	17	0.13
(1,703)	1:58:A:GLY:HA3	1:60:A:THR:H	10	0.13
(1,681)	1:56:A:GLU:H	1:57:A:LYS:H	12	0.13
(1,681)	1:56:A:GLU:H	1:57:A:LYS:H	17	0.13
(1,675)	1:55:A:LYS:HA	1:57:A:LYS:H	10	0.13
(1,671)	1:55:A:LYS:H	1:57:A:LYS:H	12	0.13
(1,668)	1:55:A:LYS:H	1:56:A:GLU:H	3	0.13
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD11	19	0.13
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD12	19	0.13
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD13	19	0.13
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD11	19	0.13
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD12	19	0.13
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD13	19	0.13
(1,620)	1:51:A:VAL:HA	1:53:A:PHE:H	15	0.13
(1,608)	1:50:A:ALA:HA	1:53:A:PHE:HE1	4	0.13
(1,608)	1:50:A:ALA:HA	1:53:A:PHE:HE2	4	0.13
(1,539)	1:43:A:ALA:HB1	1:44:A:HIS:H	4	0.13
(1,539)	1:43:A:ALA:HB2	1:44:A:HIS:H	4	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,539)	1:43:A:ALA:HB3	1:44:A:HIS:H	4	0.13
(1,537)	1:43:A:ALA:HA	1:45:A:LYS:H	5	0.13
(1,527)	1:42:A:ASN:H	1:43:A:ALA:H	6	0.13
(1,523)	1:41:A:THR:HA	1:44:A:HIS:HA	4	0.13
(1,506)	1:39:A:ALA:H	1:74:A:ASP:HA	7	0.13
(1,480)	1:37:A:TYR:HA	1:76:A:LEU:HB2	9	0.13
(1,480)	1:37:A:TYR:HA	1:76:A:LEU:HB3	9	0.13
(1,452)	1:36:A:PHE:H	1:37:A:TYR:HA	12	0.13
(1,435)	1:35:A:ILE:H	1:78:A:GLU:HA	3	0.13
(1,431)	1:35:A:ILE:H	1:36:A:PHE:HD1	17	0.13
(1,431)	1:35:A:ILE:H	1:36:A:PHE:HD2	17	0.13
(1,415)	1:33:A:ARG:HD2	1:34:A:SER:H	7	0.13
(1,415)	1:33:A:ARG:HD3	1:34:A:SER:H	7	0.13
(1,395)	1:31:A:ASP:HA	1:81:A:ILE:HG21	1	0.13
(1,395)	1:31:A:ASP:HA	1:81:A:ILE:HG22	1	0.13
(1,395)	1:31:A:ASP:HA	1:81:A:ILE:HG23	1	0.13
(1,380)	1:30:A:GLU:H	1:31:A:ASP:HA	4	0.13
(1,372)	1:29:A:SER:H	1:30:A:GLU:HA	15	0.13
(1,371)	1:29:A:SER:H	1:30:A:GLU:H	15	0.13
(1,371)	1:29:A:SER:H	1:30:A:GLU:H	19	0.13
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG21	14	0.13
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG22	14	0.13
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG23	14	0.13
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG21	14	0.13
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG22	14	0.13
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG23	14	0.13
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG21	14	0.13
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG22	14	0.13
(1,363)	1:28:A:PHE:HB2	1:81:A:ILE:HG23	14	0.13
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG21	14	0.13
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG22	14	0.13
(1,363)	1:28:A:PHE:HB3	1:81:A:ILE:HG23	14	0.13
(1,342)	1:27:A:GLU:HA	1:29:A:SER:H	11	0.13
(1,307)	1:25:A:TYR:H	1:26:A:HIS:H	6	0.13
(1,307)	1:25:A:TYR:H	1:26:A:HIS:H	8	0.13
(1,285)	1:24:A:LEU:HA	1:54:A:PHE:HE1	17	0.13
(1,285)	1:24:A:LEU:HA	1:54:A:PHE:HE2	17	0.13
(1,278)	1:24:A:LEU:H	1:26:A:HIS:H	3	0.13
(1,278)	1:24:A:LEU:H	1:26:A:HIS:H	4	0.13
(1,238)	1:21:A:LEU:HG	1:53:A:PHE:HB2	10	0.13
(1,238)	1:21:A:LEU:HG	1:53:A:PHE:HB3	10	0.13
(1,215)	1:20:A:GLU:H	1:37:A:TYR:HD1	14	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,215)	1:20:A:GLU:H	1:37:A:TYR:HD2	14	0.13
(1,214)	1:20:A:GLU:H	1:22:A:GLU:H	15	0.13
(1,214)	1:20:A:GLU:H	1:22:A:GLU:H	16	0.13
(1,208)	1:19:A:VAL:HB	1:23:A:ASP:H	5	0.13
(1,197)	1:18:A:SER:HA	1:20:A:GLU:HG2	1	0.13
(1,197)	1:18:A:SER:HA	1:20:A:GLU:HG3	1	0.13
(1,187)	1:15:A:ASP:HA	1:16:A:ALA:H	20	0.13
(1,185)	1:15:A:ASP:H	1:16:A:ALA:H	16	0.13
(1,183)	1:14:A:SER:HA	1:15:A:ASP:H	4	0.13
(1,177)	1:13:A:LYS:H	1:16:A:ALA:H	14	0.13
(1,176)	1:13:A:LYS:H	1:14:A:SER:H	1	0.13
(1,156)	1:10:A:ASN:HB2	1:45:A:LYS:HB2	6	0.13
(1,156)	1:10:A:ASN:HB2	1:45:A:LYS:HB3	6	0.13
(1,156)	1:10:A:ASN:HB3	1:45:A:LYS:HB2	6	0.13
(1,156)	1:10:A:ASN:HB3	1:45:A:LYS:HB3	6	0.13
(1,148)	1:10:A:ASN:H	1:11:A:THR:H	7	0.13
(1,144)	1:9:A:LYS:H	1:10:A:ASN:H	5	0.13
(1,135)	1:8:A:ALA:H	1:9:A:LYS:HA	20	0.13
(1,123)	1:7:A:LEU:HB2	1:38:A:PHE:HD1	16	0.13
(1,123)	1:7:A:LEU:HB2	1:38:A:PHE:HD2	16	0.13
(1,123)	1:7:A:LEU:HB3	1:38:A:PHE:HD1	16	0.13
(1,123)	1:7:A:LEU:HB3	1:38:A:PHE:HD2	16	0.13
(1,107)	1:7:A:LEU:H	1:38:A:PHE:HD1	7	0.13
(1,107)	1:7:A:LEU:H	1:38:A:PHE:HD2	7	0.13
(1,107)	1:7:A:LEU:H	1:38:A:PHE:HD1	20	0.13
(1,107)	1:7:A:LEU:H	1:38:A:PHE:HD2	20	0.13
(1,92)	1:6:A:VAL:HG21	1:35:A:ILE:HB	2	0.13
(1,92)	1:6:A:VAL:HG22	1:35:A:ILE:HB	2	0.13
(1,92)	1:6:A:VAL:HG23	1:35:A:ILE:HB	2	0.13
(1,92)	1:6:A:VAL:HG21	1:35:A:ILE:HB	3	0.13
(1,92)	1:6:A:VAL:HG22	1:35:A:ILE:HB	3	0.13
(1,92)	1:6:A:VAL:HG23	1:35:A:ILE:HB	3	0.13
(1,92)	1:6:A:VAL:HG21	1:35:A:ILE:HB	15	0.13
(1,92)	1:6:A:VAL:HG22	1:35:A:ILE:HB	15	0.13
(1,92)	1:6:A:VAL:HG23	1:35:A:ILE:HB	15	0.13
(1,61)	1:6:A:VAL:HA	1:19:A:VAL:HB	7	0.13
(1,48)	1:6:A:VAL:H	1:36:A:PHE:HA	10	0.13
(1,26)	1:5:A:LEU:HG	1:6:A:VAL:HG21	7	0.13
(1,26)	1:5:A:LEU:HG	1:6:A:VAL:HG22	7	0.13
(1,26)	1:5:A:LEU:HG	1:6:A:VAL:HG23	7	0.13
(1,16)	1:5:A:LEU:HA	1:37:A:TYR:H	5	0.13
(1,8)	1:5:A:LEU:H	1:35:A:ILE:HB	8	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2)	1:3:A:MET:H	1:4:A:LYS:HA	16	0.13
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG21	8	0.12
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG22	8	0.12
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG23	8	0.12
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG21	8	0.12
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG22	8	0.12
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG23	8	0.12
(1,889)	1:76:A:LEU:HD11	1:77:A:TYR:H	1	0.12
(1,889)	1:76:A:LEU:HD12	1:77:A:TYR:H	1	0.12
(1,889)	1:76:A:LEU:HD13	1:77:A:TYR:H	1	0.12
(1,865)	1:74:A:ASP:H	1:75:A:PHE:H	2	0.12
(1,862)	1:73:A:LYS:HA	1:75:A:PHE:H	19	0.12
(1,841)	1:71:A:ASP:H	1:72:A:GLU:HA	8	0.12
(1,831)	1:70:A:THR:H	1:73:A:LYS:HA	2	0.12
(1,831)	1:70:A:THR:H	1:73:A:LYS:HA	11	0.12
(1,831)	1:70:A:THR:H	1:73:A:LYS:HA	16	0.12
(1,820)	1:69:A:SER:H	1:73:A:LYS:HA	12	0.12
(1,805)	1:67:A:ARG:H	1:68:A:VAL:HG11	13	0.12
(1,805)	1:67:A:ARG:H	1:68:A:VAL:HG12	13	0.12
(1,805)	1:67:A:ARG:H	1:68:A:VAL:HG13	13	0.12
(1,792)	1:66:A:VAL:HA	1:69:A:SER:H	10	0.12
(1,788)	1:66:A:VAL:H	1:68:A:VAL:H	3	0.12
(1,784)	1:65:A:GLU:HB2	1:69:A:SER:HA	11	0.12
(1,784)	1:65:A:GLU:HB3	1:69:A:SER:HA	11	0.12
(1,779)	1:65:A:GLU:HA	1:76:A:LEU:HA	20	0.12
(1,764)	1:64:A:ASP:H	1:79:A:LEU:H	5	0.12
(1,732)	1:62:A:TYR:H	1:81:A:ILE:H	15	0.12
(1,717)	1:60:A:THR:HB	1:80:A:HIS:HB2	1	0.12
(1,717)	1:60:A:THR:HB	1:80:A:HIS:HB3	1	0.12
(1,702)	1:58:A:GLY:HA2	1:59:A:HIS:HA	12	0.12
(1,681)	1:56:A:GLU:H	1:57:A:LYS:H	10	0.12
(1,675)	1:55:A:LYS:HA	1:57:A:LYS:H	2	0.12
(1,669)	1:55:A:LYS:H	1:56:A:GLU:HA	13	0.12
(1,668)	1:55:A:LYS:H	1:56:A:GLU:H	11	0.12
(1,643)	1:53:A:PHE:H	1:55:A:LYS:H	14	0.12
(1,626)	1:51:A:VAL:HG11	1:63:A:LEU:HD11	14	0.12
(1,626)	1:51:A:VAL:HG11	1:63:A:LEU:HD12	14	0.12
(1,626)	1:51:A:VAL:HG11	1:63:A:LEU:HD13	14	0.12
(1,626)	1:51:A:VAL:HG12	1:63:A:LEU:HD11	14	0.12
(1,626)	1:51:A:VAL:HG12	1:63:A:LEU:HD12	14	0.12
(1,626)	1:51:A:VAL:HG12	1:63:A:LEU:HD13	14	0.12
(1,626)	1:51:A:VAL:HG13	1:63:A:LEU:HD11	14	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,626)	1:51:A:VAL:HG13	1:63:A:LEU:HD12	14	0.12
(1,626)	1:51:A:VAL:HG13	1:63:A:LEU:HD13	14	0.12
(1,626)	1:51:A:VAL:HG11	1:63:A:LEU:HD11	14	0.12
(1,626)	1:51:A:VAL:HG11	1:63:A:LEU:HD12	14	0.12
(1,626)	1:51:A:VAL:HG11	1:63:A:LEU:HD13	14	0.12
(1,626)	1:51:A:VAL:HG12	1:63:A:LEU:HD11	14	0.12
(1,626)	1:51:A:VAL:HG12	1:63:A:LEU:HD12	14	0.12
(1,626)	1:51:A:VAL:HG12	1:63:A:LEU:HD13	14	0.12
(1,626)	1:51:A:VAL:HG13	1:63:A:LEU:HD11	14	0.12
(1,626)	1:51:A:VAL:HG13	1:63:A:LEU:HD12	14	0.12
(1,626)	1:51:A:VAL:HG13	1:63:A:LEU:HD13	14	0.12
(1,567)	1:47:A:MET:HB2	1:48:A:LEU:HA	10	0.12
(1,567)	1:47:A:MET:HB3	1:48:A:LEU:HA	10	0.12
(1,550)	1:46:A:ASP:H	1:47:A:MET:H	16	0.12
(1,512)	1:39:A:ALA:HA	1:74:A:ASP:HB2	4	0.12
(1,512)	1:39:A:ALA:HA	1:74:A:ASP:HB3	4	0.12
(1,511)	1:39:A:ALA:HA	1:74:A:ASP:HA	7	0.12
(1,496)	1:38:A:PHE:HA	1:76:A:LEU:H	16	0.12
(1,470)	1:36:A:PHE:HD1	1:77:A:TYR:HD1	6	0.12
(1,470)	1:36:A:PHE:HD1	1:77:A:TYR:HD2	6	0.12
(1,470)	1:36:A:PHE:HD2	1:77:A:TYR:HD1	6	0.12
(1,470)	1:36:A:PHE:HD2	1:77:A:TYR:HD2	6	0.12
(1,467)	1:36:A:PHE:HB2	1:77:A:TYR:HD1	12	0.12
(1,467)	1:36:A:PHE:HB2	1:77:A:TYR:HD2	12	0.12
(1,467)	1:36:A:PHE:HB3	1:77:A:TYR:HD1	12	0.12
(1,467)	1:36:A:PHE:HB3	1:77:A:TYR:HD2	12	0.12
(1,434)	1:35:A:ILE:H	1:78:A:GLU:H	11	0.12
(1,433)	1:35:A:ILE:H	1:77:A:TYR:HA	2	0.12
(1,426)	1:34:A:SER:HB2	1:36:A:PHE:HE1	16	0.12
(1,426)	1:34:A:SER:HB2	1:36:A:PHE:HE2	16	0.12
(1,426)	1:34:A:SER:HB3	1:36:A:PHE:HE1	16	0.12
(1,426)	1:34:A:SER:HB3	1:36:A:PHE:HE2	16	0.12
(1,419)	1:34:A:SER:H	1:80:A:HIS:H	19	0.12
(1,409)	1:33:A:ARG:HA	1:80:A:HIS:H	18	0.12
(1,405)	1:33:A:ARG:H	1:81:A:ILE:HG21	11	0.12
(1,405)	1:33:A:ARG:H	1:81:A:ILE:HG22	11	0.12
(1,405)	1:33:A:ARG:H	1:81:A:ILE:HG23	11	0.12
(1,405)	1:33:A:ARG:H	1:81:A:ILE:HG21	11	0.12
(1,405)	1:33:A:ARG:H	1:81:A:ILE:HG22	11	0.12
(1,405)	1:33:A:ARG:H	1:81:A:ILE:HG23	11	0.12
(1,389)	1:31:A:ASP:H	1:32:A:LYS:HA	1	0.12
(1,372)	1:29:A:SER:H	1:30:A:GLU:HA	13	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,371)	1:29:A:SER:H	1:30:A:GLU:H	10	0.12
(1,370)	1:28:A:PHE:HE1	1:81:A:ILE:HA	19	0.12
(1,370)	1:28:A:PHE:HE2	1:81:A:ILE:HA	19	0.12
(1,357)	1:28:A:PHE:HA	1:80:A:HIS:HB2	2	0.12
(1,357)	1:28:A:PHE:HA	1:80:A:HIS:HB3	2	0.12
(1,355)	1:28:A:PHE:HA	1:32:A:LYS:HB2	18	0.12
(1,355)	1:28:A:PHE:HA	1:32:A:LYS:HB3	18	0.12
(1,342)	1:27:A:GLU:HA	1:29:A:SER:H	16	0.12
(1,328)	1:26:A:HIS:H	1:29:A:SER:H	12	0.12
(1,322)	1:25:A:TYR:HD1	1:28:A:PHE:H	1	0.12
(1,322)	1:25:A:TYR:HD2	1:28:A:PHE:H	1	0.12
(1,268)	1:23:A:ASP:HA	1:27:A:GLU:HA	8	0.12
(1,241)	1:21:A:LEU:HG	1:57:A:LYS:HG2	18	0.12
(1,241)	1:21:A:LEU:HG	1:57:A:LYS:HG3	18	0.12
(1,207)	1:19:A:VAL:HB	1:22:A:GLU:H	6	0.12
(1,183)	1:14:A:SER:HA	1:15:A:ASP:H	7	0.12
(1,180)	1:14:A:SER:H	1:15:A:ASP:H	10	0.12
(1,176)	1:13:A:LYS:H	1:14:A:SER:H	7	0.12
(1,170)	1:11:A:THR:HG21	1:40:A:PRO:HB2	12	0.12
(1,170)	1:11:A:THR:HG21	1:40:A:PRO:HB3	12	0.12
(1,170)	1:11:A:THR:HG22	1:40:A:PRO:HB2	12	0.12
(1,170)	1:11:A:THR:HG22	1:40:A:PRO:HB3	12	0.12
(1,170)	1:11:A:THR:HG23	1:40:A:PRO:HB2	12	0.12
(1,170)	1:11:A:THR:HG23	1:40:A:PRO:HB3	12	0.12
(1,157)	1:10:A:ASN:HB2	1:46:A:ASP:H	19	0.12
(1,157)	1:10:A:ASN:HB3	1:46:A:ASP:H	19	0.12
(1,148)	1:10:A:ASN:H	1:11:A:THR:H	1	0.12
(1,145)	1:9:A:LYS:H	1:10:A:ASN:HA	14	0.12
(1,105)	1:7:A:LEU:H	1:38:A:PHE:H	13	0.12
(1,69)	1:6:A:VAL:HB	1:20:A:GLU:H	19	0.12
(1,51)	1:6:A:VAL:H	1:37:A:TYR:HA	4	0.12
(1,51)	1:6:A:VAL:H	1:37:A:TYR:HA	18	0.12
(1,44)	1:6:A:VAL:H	1:20:A:GLU:HB2	13	0.12
(1,44)	1:6:A:VAL:H	1:20:A:GLU:HB3	13	0.12
(1,43)	1:6:A:VAL:H	1:7:A:LEU:HG	11	0.12
(1,27)	1:5:A:LEU:HG	1:7:A:LEU:H	19	0.12
(1,24)	1:5:A:LEU:HG	1:6:A:VAL:H	3	0.12
(1,16)	1:5:A:LEU:HA	1:37:A:TYR:H	3	0.12
(1,16)	1:5:A:LEU:HA	1:37:A:TYR:H	18	0.12
(1,4)	1:4:A:LYS:HA	1:5:A:LEU:H	5	0.12
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG21	4	0.11
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG22	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG23	4	0.11
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG21	4	0.11
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG22	4	0.11
(1,925)	1:80:A:HIS:H	1:81:A:ILE:HG23	4	0.11
(1,890)	1:76:A:LEU:HD11	1:78:A:GLU:H	15	0.11
(1,890)	1:76:A:LEU:HD12	1:78:A:GLU:H	15	0.11
(1,890)	1:76:A:LEU:HD13	1:78:A:GLU:H	15	0.11
(1,881)	1:76:A:LEU:H	1:77:A:TYR:HA	15	0.11
(1,865)	1:74:A:ASP:H	1:75:A:PHE:H	5	0.11
(1,865)	1:74:A:ASP:H	1:75:A:PHE:H	6	0.11
(1,835)	1:70:A:THR:HA	1:73:A:LYS:H	16	0.11
(1,831)	1:70:A:THR:H	1:73:A:LYS:HA	3	0.11
(1,805)	1:67:A:ARG:H	1:68:A:VAL:HG11	17	0.11
(1,805)	1:67:A:ARG:H	1:68:A:VAL:HG12	17	0.11
(1,805)	1:67:A:ARG:H	1:68:A:VAL:HG13	17	0.11
(1,801)	1:66:A:VAL:HG11	1:72:A:GLU:HB2	12	0.11
(1,801)	1:66:A:VAL:HG11	1:72:A:GLU:HB3	12	0.11
(1,801)	1:66:A:VAL:HG12	1:72:A:GLU:HB2	12	0.11
(1,801)	1:66:A:VAL:HG12	1:72:A:GLU:HB3	12	0.11
(1,801)	1:66:A:VAL:HG13	1:72:A:GLU:HB2	12	0.11
(1,801)	1:66:A:VAL:HG13	1:72:A:GLU:HB3	12	0.11
(1,801)	1:66:A:VAL:HG21	1:72:A:GLU:HB2	12	0.11
(1,801)	1:66:A:VAL:HG21	1:72:A:GLU:HB3	12	0.11
(1,801)	1:66:A:VAL:HG22	1:72:A:GLU:HB2	12	0.11
(1,801)	1:66:A:VAL:HG22	1:72:A:GLU:HB3	12	0.11
(1,801)	1:66:A:VAL:HG23	1:72:A:GLU:HB2	12	0.11
(1,801)	1:66:A:VAL:HG23	1:72:A:GLU:HB3	12	0.11
(1,748)	1:63:A:LEU:HA	1:78:A:GLU:H	20	0.11
(1,732)	1:62:A:TYR:H	1:81:A:ILE:H	19	0.11
(1,731)	1:62:A:TYR:H	1:80:A:HIS:HA	8	0.11
(1,703)	1:58:A:GLY:HA3	1:60:A:THR:H	18	0.11
(1,702)	1:58:A:GLY:HA2	1:59:A:HIS:HA	6	0.11
(1,692)	1:57:A:LYS:H	1:58:A:GLY:HA2	13	0.11
(1,686)	1:56:A:GLU:HA	1:57:A:LYS:HG2	3	0.11
(1,686)	1:56:A:GLU:HA	1:57:A:LYS:HG3	3	0.11
(1,669)	1:55:A:LYS:H	1:56:A:GLU:HA	16	0.11
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD11	11	0.11
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD12	11	0.11
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD13	11	0.11
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD11	11	0.11
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD12	11	0.11
(1,654)	1:54:A:PHE:H	1:63:A:LEU:HD13	11	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,643)	1:53:A:PHE:H	1:55:A:LYS:H	7	0.11
(1,632)	1:52:A:ASP:H	1:55:A:LYS:H	9	0.11
(1,632)	1:52:A:ASP:H	1:55:A:LYS:H	19	0.11
(1,586)	1:48:A:LEU:HB2	1:49:A:LYS:HA	5	0.11
(1,586)	1:48:A:LEU:HB3	1:49:A:LYS:HA	5	0.11
(1,586)	1:48:A:LEU:HB2	1:49:A:LYS:HA	18	0.11
(1,586)	1:48:A:LEU:HB3	1:49:A:LYS:HA	18	0.11
(1,567)	1:47:A:MET:HB2	1:48:A:LEU:HA	4	0.11
(1,567)	1:47:A:MET:HB3	1:48:A:LEU:HA	4	0.11
(1,543)	1:44:A:HIS:HA	1:48:A:LEU:H	3	0.11
(1,543)	1:44:A:HIS:HA	1:48:A:LEU:H	12	0.11
(1,539)	1:43:A:ALA:HB1	1:44:A:HIS:H	11	0.11
(1,539)	1:43:A:ALA:HB2	1:44:A:HIS:H	11	0.11
(1,539)	1:43:A:ALA:HB3	1:44:A:HIS:H	11	0.11
(1,539)	1:43:A:ALA:HB1	1:44:A:HIS:H	19	0.11
(1,539)	1:43:A:ALA:HB2	1:44:A:HIS:H	19	0.11
(1,539)	1:43:A:ALA:HB3	1:44:A:HIS:H	19	0.11
(1,529)	1:42:A:ASN:H	1:44:A:HIS:H	1	0.11
(1,527)	1:42:A:ASN:H	1:43:A:ALA:H	11	0.11
(1,516)	1:39:A:ALA:HB1	1:46:A:ASP:H	14	0.11
(1,516)	1:39:A:ALA:HB2	1:46:A:ASP:H	14	0.11
(1,516)	1:39:A:ALA:HB3	1:46:A:ASP:H	14	0.11
(1,507)	1:39:A:ALA:H	1:75:A:PHE:HA	18	0.11
(1,505)	1:39:A:ALA:H	1:74:A:ASP:H	15	0.11
(1,489)	1:38:A:PHE:H	1:75:A:PHE:HA	7	0.11
(1,489)	1:38:A:PHE:H	1:75:A:PHE:HA	9	0.11
(1,474)	1:37:A:TYR:H	1:76:A:LEU:H	9	0.11
(1,474)	1:37:A:TYR:H	1:76:A:LEU:H	11	0.11
(1,470)	1:36:A:PHE:HD1	1:77:A:TYR:HD1	11	0.11
(1,470)	1:36:A:PHE:HD1	1:77:A:TYR:HD2	11	0.11
(1,470)	1:36:A:PHE:HD2	1:77:A:TYR:HD1	11	0.11
(1,470)	1:36:A:PHE:HD2	1:77:A:TYR:HD2	11	0.11
(1,461)	1:36:A:PHE:HA	1:77:A:TYR:HD1	10	0.11
(1,461)	1:36:A:PHE:HA	1:77:A:TYR:HD2	10	0.11
(1,459)	1:36:A:PHE:HA	1:77:A:TYR:H	4	0.11
(1,451)	1:36:A:PHE:H	1:37:A:TYR:H	10	0.11
(1,413)	1:33:A:ARG:HB2	1:34:A:SER:HA	19	0.11
(1,413)	1:33:A:ARG:HB3	1:34:A:SER:HA	19	0.11
(1,412)	1:33:A:ARG:HB2	1:34:A:SER:H	17	0.11
(1,412)	1:33:A:ARG:HB3	1:34:A:SER:H	17	0.11
(1,409)	1:33:A:ARG:HA	1:80:A:HIS:H	12	0.11
(1,406)	1:33:A:ARG:H	1:82:A:ILE:HA	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,380)	1:30:A:GLU:H	1:31:A:ASP:HA	13	0.11
(1,372)	1:29:A:SER:H	1:30:A:GLU:HA	17	0.11
(1,371)	1:29:A:SER:H	1:30:A:GLU:H	3	0.11
(1,371)	1:29:A:SER:H	1:30:A:GLU:H	5	0.11
(1,355)	1:28:A:PHE:HA	1:32:A:LYS:HB2	9	0.11
(1,355)	1:28:A:PHE:HA	1:32:A:LYS:HB3	9	0.11
(1,328)	1:26:A:HIS:H	1:29:A:SER:H	14	0.11
(1,322)	1:25:A:TYR:HD1	1:28:A:PHE:H	7	0.11
(1,322)	1:25:A:TYR:HD2	1:28:A:PHE:H	7	0.11
(1,317)	1:25:A:TYR:HA	1:29:A:SER:HG	13	0.11
(1,294)	1:24:A:LEU:HG	1:25:A:TYR:H	9	0.11
(1,293)	1:24:A:LEU:HB2	1:80:A:HIS:HE1	4	0.11
(1,293)	1:24:A:LEU:HB3	1:80:A:HIS:HE1	4	0.11
(1,274)	1:23:A:ASP:HB2	1:35:A:ILE:HB	8	0.11
(1,274)	1:23:A:ASP:HB3	1:35:A:ILE:HB	8	0.11
(1,237)	1:21:A:LEU:HG	1:24:A:LEU:HB2	17	0.11
(1,237)	1:21:A:LEU:HG	1:24:A:LEU:HB3	17	0.11
(1,214)	1:20:A:GLU:H	1:22:A:GLU:H	13	0.11
(1,204)	1:19:A:VAL:H	1:22:A:GLU:H	11	0.11
(1,203)	1:19:A:VAL:H	1:21:A:LEU:H	5	0.11
(1,203)	1:19:A:VAL:H	1:21:A:LEU:H	17	0.11
(1,197)	1:18:A:SER:HA	1:20:A:GLU:HG2	20	0.11
(1,197)	1:18:A:SER:HA	1:20:A:GLU:HG3	20	0.11
(1,189)	1:16:A:ALA:H	1:17:A:LYS:H	20	0.11
(1,185)	1:15:A:ASP:H	1:16:A:ALA:H	12	0.11
(1,183)	1:14:A:SER:HA	1:15:A:ASP:H	2	0.11
(1,177)	1:13:A:LYS:H	1:16:A:ALA:H	6	0.11
(1,177)	1:13:A:LYS:H	1:16:A:ALA:H	10	0.11
(1,176)	1:13:A:LYS:H	1:14:A:SER:H	15	0.11
(1,174)	1:12:A:ARG:HB2	1:14:A:SER:HA	3	0.11
(1,174)	1:12:A:ARG:HB3	1:14:A:SER:HA	3	0.11
(1,163)	1:11:A:THR:HA	1:13:A:LYS:H	11	0.11
(1,148)	1:10:A:ASN:H	1:11:A:THR:H	12	0.11
(1,126)	1:7:A:LEU:HG	1:38:A:PHE:H	1	0.11
(1,115)	1:7:A:LEU:HA	1:38:A:PHE:HB2	1	0.11
(1,115)	1:7:A:LEU:HA	1:38:A:PHE:HB3	1	0.11
(1,115)	1:7:A:LEU:HA	1:38:A:PHE:HB2	13	0.11
(1,115)	1:7:A:LEU:HA	1:38:A:PHE:HB3	13	0.11
(1,50)	1:6:A:VAL:H	1:37:A:TYR:H	2	0.11
(1,50)	1:6:A:VAL:H	1:37:A:TYR:H	13	0.11
(1,50)	1:6:A:VAL:H	1:37:A:TYR:H	15	0.11
(1,46)	1:6:A:VAL:H	1:35:A:ILE:HD11	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,46)	1:6:A:VAL:H	1:35:A:ILE:HD12	9	0.11
(1,46)	1:6:A:VAL:H	1:35:A:ILE:HD13	9	0.11
(1,8)	1:5:A:LEU:H	1:35:A:ILE:HB	7	0.11
(1,930)	1:81:A:ILE:HA	1:82:A:ILE:H	11	0.1
(1,811)	1:68:A:VAL:HA	1:73:A:LYS:H	11	0.1
(1,811)	1:68:A:VAL:HA	1:73:A:LYS:H	16	0.1
(1,802)	1:67:A:ARG:H	1:68:A:VAL:H	15	0.1
(1,800)	1:66:A:VAL:HG11	1:72:A:GLU:H	11	0.1
(1,800)	1:66:A:VAL:HG12	1:72:A:GLU:H	11	0.1
(1,800)	1:66:A:VAL:HG13	1:72:A:GLU:H	11	0.1
(1,800)	1:66:A:VAL:HG21	1:72:A:GLU:H	11	0.1
(1,800)	1:66:A:VAL:HG22	1:72:A:GLU:H	11	0.1
(1,800)	1:66:A:VAL:HG23	1:72:A:GLU:H	11	0.1
(1,681)	1:56:A:GLU:H	1:57:A:LYS:H	13	0.1
(1,675)	1:55:A:LYS:HA	1:57:A:LYS:H	13	0.1
(1,669)	1:55:A:LYS:H	1:56:A:GLU:HA	3	0.1
(1,668)	1:55:A:LYS:H	1:56:A:GLU:H	5	0.1
(1,621)	1:51:A:VAL:HA	1:54:A:PHE:H	14	0.1
(1,591)	1:49:A:LYS:H	1:50:A:ALA:HA	18	0.1
(1,522)	1:41:A:THR:HA	1:44:A:HIS:H	16	0.1
(1,516)	1:39:A:ALA:HB1	1:46:A:ASP:H	20	0.1
(1,516)	1:39:A:ALA:HB2	1:46:A:ASP:H	20	0.1
(1,516)	1:39:A:ALA:HB3	1:46:A:ASP:H	20	0.1
(1,436)	1:35:A:ILE:H	1:79:A:LEU:HD21	5	0.1
(1,436)	1:35:A:ILE:H	1:79:A:LEU:HD22	5	0.1
(1,436)	1:35:A:ILE:H	1:79:A:LEU:HD23	5	0.1
(1,431)	1:35:A:ILE:H	1:36:A:PHE:HD1	20	0.1
(1,431)	1:35:A:ILE:H	1:36:A:PHE:HD2	20	0.1
(1,419)	1:34:A:SER:H	1:80:A:HIS:H	13	0.1
(1,419)	1:34:A:SER:H	1:80:A:HIS:H	18	0.1
(1,356)	1:28:A:PHE:HA	1:33:A:ARG:H	6	0.1
(1,354)	1:28:A:PHE:HA	1:30:A:GLU:H	4	0.1
(1,268)	1:23:A:ASP:HA	1:27:A:GLU:HA	12	0.1
(1,264)	1:23:A:ASP:H	1:27:A:GLU:H	8	0.1
(1,187)	1:15:A:ASP:HA	1:16:A:ALA:H	1	0.1
(1,158)	1:10:A:ASN:HB2	1:46:A:ASP:HA	3	0.1
(1,158)	1:10:A:ASN:HB3	1:46:A:ASP:HA	3	0.1
(1,107)	1:7:A:LEU:H	1:38:A:PHE:HD1	18	0.1
(1,107)	1:7:A:LEU:H	1:38:A:PHE:HD2	18	0.1
(1,68)	1:6:A:VAL:HB	1:19:A:VAL:HB	12	0.1
(1,47)	1:6:A:VAL:H	1:36:A:PHE:H	8	0.1
(1,47)	1:6:A:VAL:H	1:36:A:PHE:H	13	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,21)	1:5:A:LEU:HB2	1:36:A:PHE:H	9	0.1
(1,21)	1:5:A:LEU:HB3	1:36:A:PHE:H	9	0.1
(1,7)	1:5:A:LEU:H	1:35:A:ILE:HA	11	0.1

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

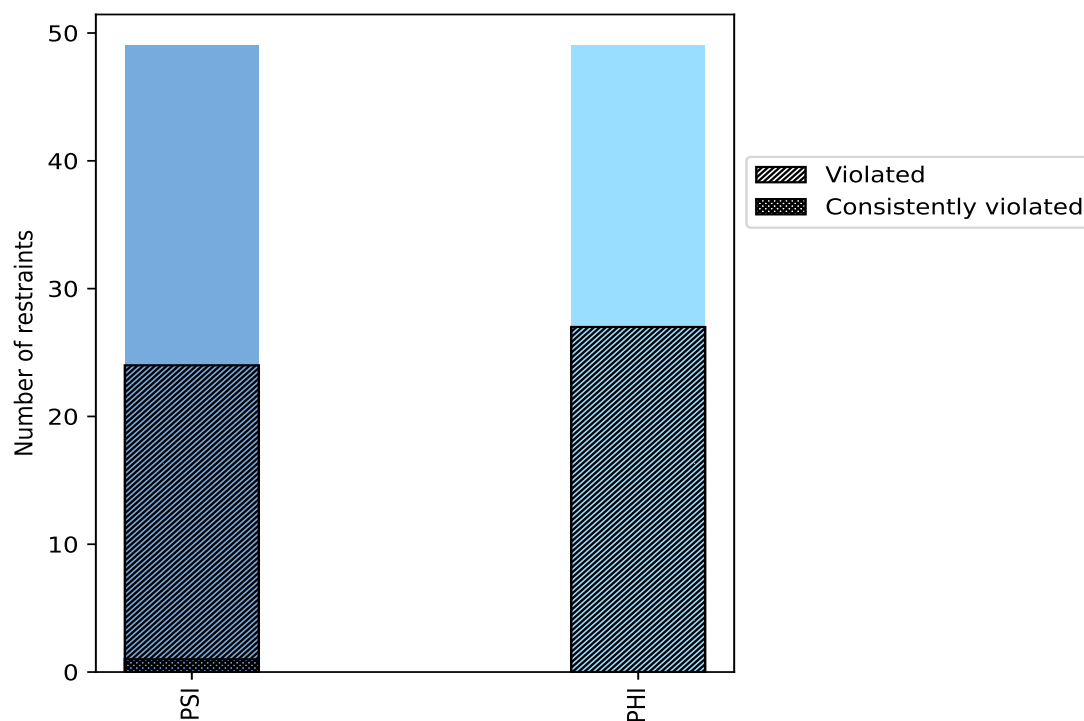
10.1 Summary of dihedral-angle violations [i](#)

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

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PSI	49	50.0	24	49.0	24.5	1	2.0	1.0
PHI	49	50.0	27	55.1	27.6	0	0.0	0.0
Total	98	100.0	51	52.0	52.0	1	1.0	1.0

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

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



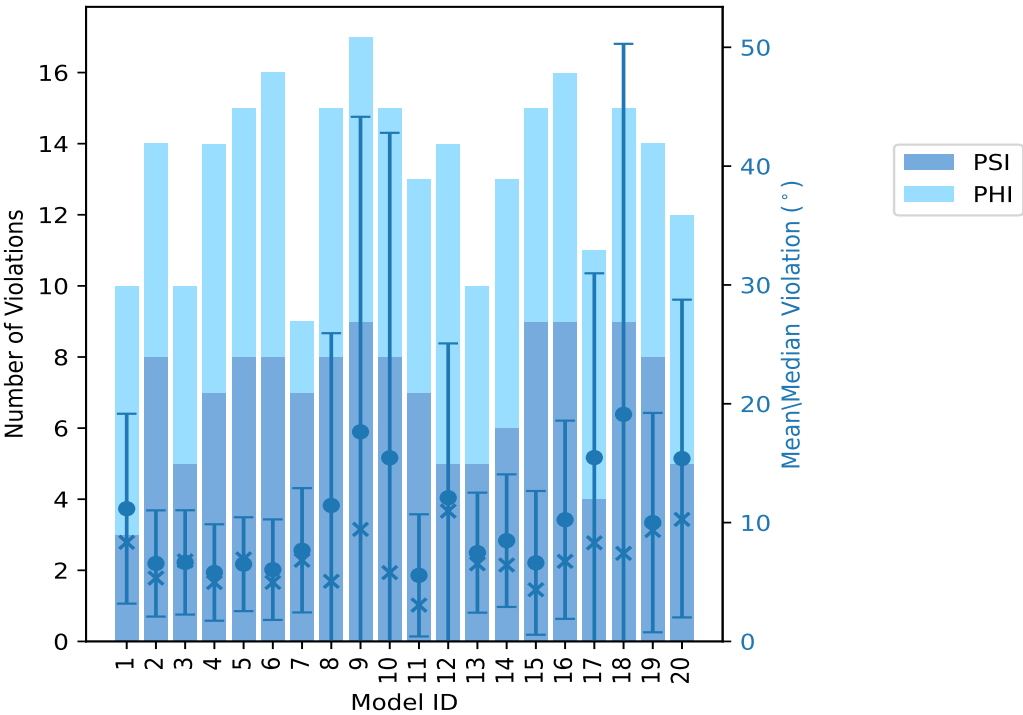
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	PHI	Total				
1	3	7	10	11.17	25.37	7.99	8.34
2	8	6	14	6.56	16.42	4.47	5.33
3	5	5	10	6.65	17.36	4.39	6.78
4	7	7	14	5.8	14.62	4.06	4.96
5	8	7	15	6.5	14.94	3.95	6.94
6	8	8	16	6.04	16.28	4.23	4.97
7	7	2	9	7.67	20.46	5.23	6.83
8	8	7	15	11.44	58.35	14.5	5.06
9	9	8	17	17.64	117.41	26.51	9.43
10	8	7	15	15.45	113.06	27.35	5.79
11	7	6	13	5.56	19.01	5.14	3.06
12	5	9	14	12.09	54.18	12.99	10.97
13	5	5	10	7.47	19.34	5.05	6.53
14	6	7	13	8.48	18.52	5.58	6.43
15	9	6	15	6.61	21.08	6.05	4.35
16	9	7	16	10.24	33.93	8.34	6.74
17	4	7	11	15.47	56.54	15.51	8.3
18	9	6	15	19.11	129.18	31.18	7.41
19	8	6	14	10.0	38.59	9.23	9.34
20	5	7	12	15.39	44.98	13.37	10.27

10.2.1 Bar graph : Dihedral 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

10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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	%
5	9	14	1	5.0
4	3	7	2	10.0
1	3	4	3	15.0
2	1	3	4	20.0
2	1	3	5	25.0
2	2	4	6	30.0
0	1	1	7	35.0
3	1	4	8	40.0
0	3	3	9	45.0
2	0	2	10	50.0
1	0	1	11	55.0

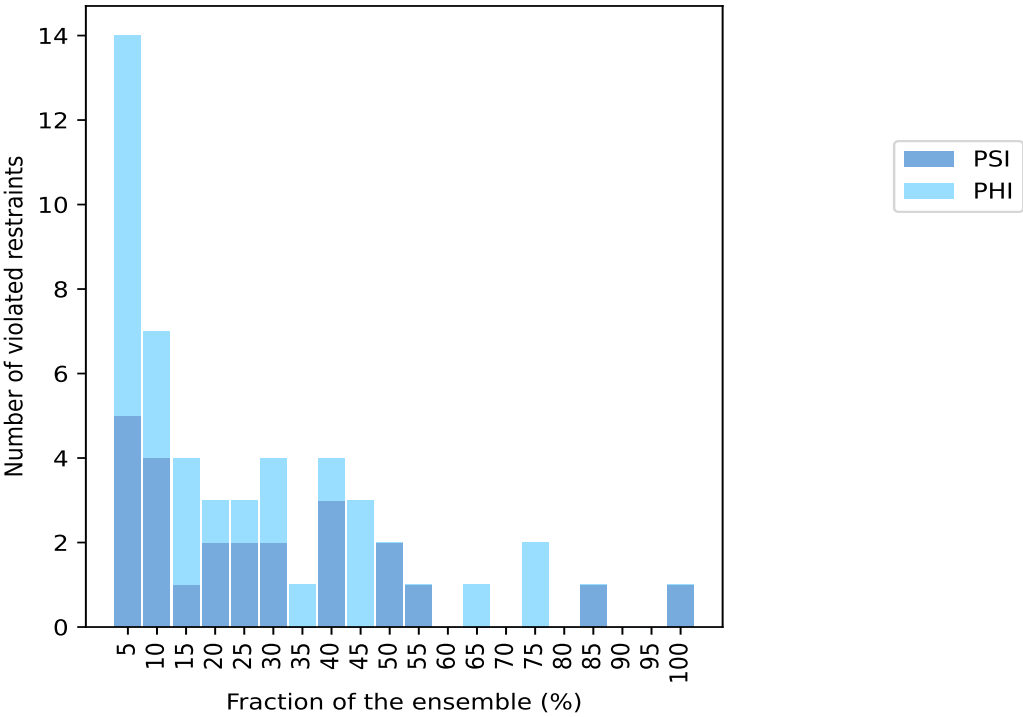
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Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count ¹	%
0	0	0	12	60.0
0	1	1	13	65.0
0	0	0	14	70.0
0	2	2	15	75.0
0	0	0	16	80.0
1	0	1	17	85.0
0	0	0	18	90.0
0	0	0	19	95.0
1	0	1	20	100.0

¹ Number of models with violations

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

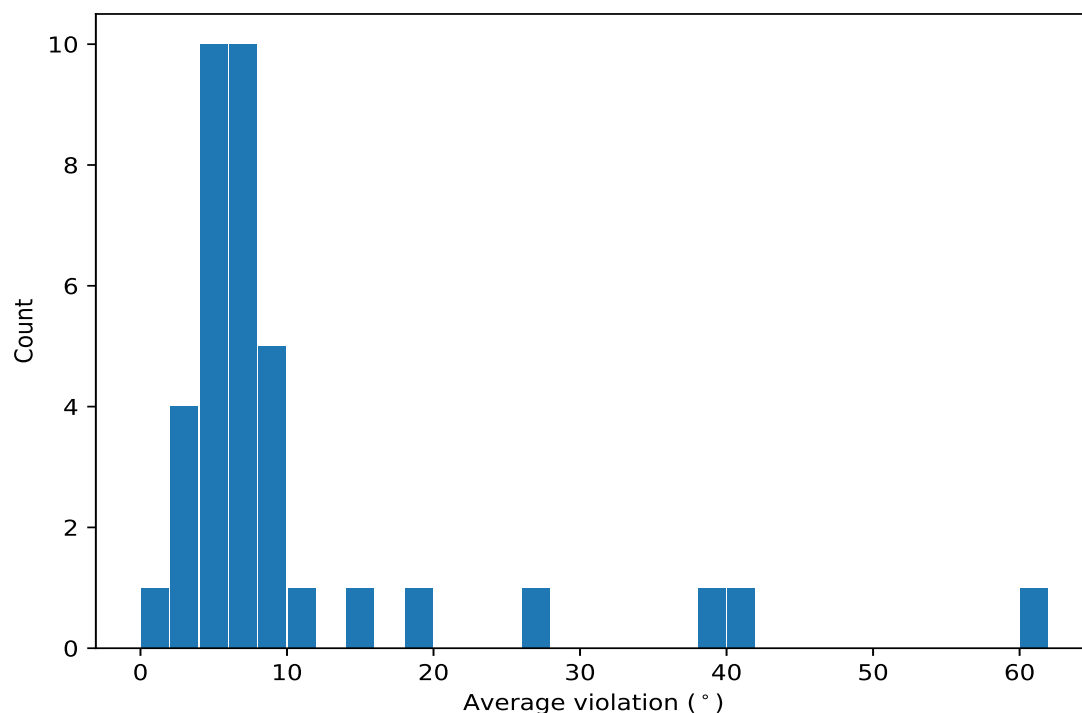


10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

10.4.1 Histogram : Distribution of mean dihedral-angle violations ⓘ

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

in the ensemble



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,82)	1:70:A:THR:N	1:70:A:THR:CA	1:70:A:THR:C	1:71:A:ASP:N	20	18.58	5.91	17.74
(1,30)	1:29:A:SER:N	1:29:A:SER:CA	1:29:A:SER:C	1:30:A:GLU:N	17	6.82	2.67	6.81
(1,91)	1:76:A:LEU:C	1:77:A:TYR:N	1:77:A:TYR:CA	1:77:A:TYR:C	15	8.61	7.05	7.64
(1,97)	1:79:A:LEU:C	1:80:A:HIS:N	1:80:A:HIS:CA	1:80:A:HIS:C	15	4.85	2.83	3.67
(1,85)	1:71:A:ASP:C	1:72:A:GLU:N	1:72:A:GLU:CA	1:72:A:GLU:C	13	7.72	7.94	6.83
(1,44)	1:38:A:PHE:N	1:38:A:PHE:CA	1:38:A:PHE:C	1:39:A:ALA:N	11	6.1	3.72	5.06
(1,86)	1:72:A:GLU:N	1:72:A:GLU:CA	1:72:A:GLU:C	1:73:A:LYS:N	10	15.9	14.8	10.86
(1,4)	1:6:A:VAL:N	1:6:A:VAL:CA	1:6:A:VAL:C	1:7:A:LEU:N	10	7.81	4.65	7.8
(1,35)	1:33:A:ARG:C	1:34:A:SER:N	1:34:A:SER:CA	1:34:A:SER:C	9	11.88	6.15	12.2
(1,75)	1:65:A:GLU:C	1:66:A:VAL:N	1:66:A:VAL:CA	1:66:A:VAL:C	9	7.49	5.57	6.87
(1,89)	1:75:A:PHE:C	1:76:A:LEU:N	1:76:A:LEU:CA	1:76:A:LEU:C	9	6.74	4.11	6.88
(1,40)	1:36:A:PHE:N	1:36:A:PHE:CA	1:36:A:PHE:C	1:37:A:TYR:N	8	8.71	5.42	9.39
(1,88)	1:75:A:PHE:N	1:75:A:PHE:CA	1:75:A:PHE:C	1:76:A:LEU:N	8	8.15	6.07	7.52
(1,72)	1:64:A:ASP:N	1:64:A:ASP:CA	1:64:A:ASP:C	1:65:A:GLU:N	8	7.31	4.68	6.12
(1,33)	1:32:A:LYS:C	1:33:A:ARG:N	1:33:A:ARG:CA	1:33:A:ARG:C	8	5.13	3.22	3.54
(1,73)	1:64:A:ASP:C	1:65:A:GLU:N	1:65:A:GLU:CA	1:65:A:GLU:C	7	7.09	2.77	7.98
(1,64)	1:57:A:LYS:N	1:57:A:LYS:CA	1:57:A:LYS:C	1:58:A:GLY:N	6	61.69	58.39	58.72
(1,71)	1:63:A:LEU:C	1:64:A:ASP:N	1:64:A:ASP:CA	1:64:A:ASP:C	6	7.53	3.71	7.41
(1,34)	1:33:A:ARG:N	1:33:A:ARG:CA	1:33:A:ARG:C	1:34:A:SER:N	6	6.4	3.21	7.93
(1,5)	1:6:A:VAL:C	1:7:A:LEU:N	1:7:A:LEU:CA	1:7:A:LEU:C	6	5.63	2.27	5.88

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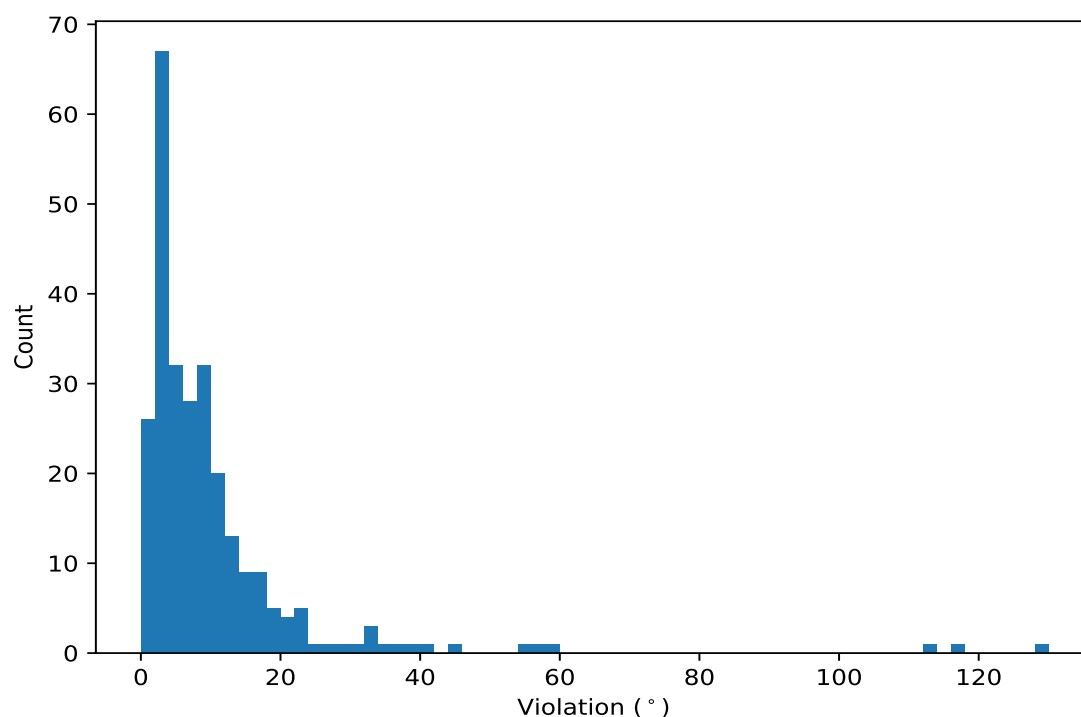
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,65)	1:60:A:THR:C	1:61:A:ALA:N	1:61:A:ALA:CA	1:61:A:ALA:C	5	38.93	10.08	38.59
(1,90)	1:76:A:LEU:N	1:76:A:LEU:CA	1:76:A:LEU:C	1:77:A:TYR:N	5	4.92	2.46	5.53
(1,24)	1:26:A:HIS:N	1:26:A:HIS:CA	1:26:A:HIS:C	1:27:A:GLU:N	5	2.23	0.5	2.13
(1,63)	1:56:A:GLU:C	1:57:A:LYS:N	1:57:A:LYS:CA	1:57:A:LYS:C	4	26.96	14.79	31.67
(1,42)	1:37:A:TYR:N	1:37:A:TYR:CA	1:37:A:TYR:C	1:38:A:PHE:N	4	8.06	4.05	7.42
(1,96)	1:79:A:LEU:N	1:79:A:LEU:CA	1:79:A:LEU:C	1:80:A:HIS:N	4	5.0	2.64	5.28
(1,23)	1:25:A:TYR:C	1:26:A:HIS:N	1:26:A:HIS:CA	1:26:A:HIS:C	3	5.73	5.19	3.02
(1,28)	1:28:A:PHE:N	1:28:A:PHE:CA	1:28:A:PHE:C	1:29:A:SER:N	3	5.55	2.07	4.79
(1,67)	1:61:A:ALA:C	1:62:A:TYR:N	1:62:A:TYR:CA	1:62:A:TYR:C	3	4.59	1.44	5.19
(1,9)	1:18:A:SER:C	1:19:A:VAL:N	1:19:A:VAL:CA	1:19:A:VAL:C	3	2.99	0.61	2.96
(1,80)	1:69:A:SER:N	1:69:A:SER:CA	1:69:A:SER:C	1:70:A:THR:N	2	41.15	17.2	41.15
(1,87)	1:74:A:ASP:C	1:75:A:PHE:N	1:75:A:PHE:CA	1:75:A:PHE:C	2	8.54	5.54	8.54
(1,29)	1:28:A:PHE:C	1:29:A:SER:N	1:29:A:SER:CA	1:29:A:SER:C	2	4.34	1.9	4.34
(1,62)	1:56:A:GLU:N	1:56:A:GLU:CA	1:56:A:GLU:C	1:57:A:LYS:N	2	4.24	1.3	4.24
(1,37)	1:34:A:SER:C	1:35:A:ILE:N	1:35:A:ILE:CA	1:35:A:ILE:C	2	2.9	0.64	2.9
(1,94)	1:78:A:GLU:N	1:78:A:GLU:CA	1:78:A:GLU:C	1:79:A:LEU:N	2	2.6	1.21	2.6
(1,8)	1:8:A:ALA:N	1:8:A:ALA:CA	1:8:A:ALA:C	1:9:A:LYS:N	2	1.95	0.59	1.95

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

10.5 All violated dihedral-angle restraints ⓘ

10.5.1 Histogram : Distribution of violations ⓘ

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



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,64)	1:57:A:LYS:N	1:57:A:LYS:CA	1:57:A:LYS:C	1:58:A:GLY:N	18	129.18
(1,64)	1:57:A:LYS:N	1:57:A:LYS:CA	1:57:A:LYS:C	1:58:A:GLY:N	9	117.41
(1,64)	1:57:A:LYS:N	1:57:A:LYS:CA	1:57:A:LYS:C	1:58:A:GLY:N	10	113.06
(1,80)	1:69:A:SER:N	1:69:A:SER:CA	1:69:A:SER:C	1:70:A:THR:N	8	58.35
(1,86)	1:72:A:GLU:N	1:72:A:GLU:CA	1:72:A:GLU:C	1:73:A:LYS:N	17	56.54
(1,65)	1:60:A:THR:C	1:61:A:ALA:N	1:61:A:ALA:CA	1:61:A:ALA:C	12	54.18
(1,65)	1:60:A:THR:C	1:61:A:ALA:N	1:61:A:ALA:CA	1:61:A:ALA:C	20	44.98
(1,63)	1:56:A:GLU:C	1:57:A:LYS:N	1:57:A:LYS:CA	1:57:A:LYS:C	18	41.91
(1,65)	1:60:A:THR:C	1:61:A:ALA:N	1:61:A:ALA:CA	1:61:A:ALA:C	19	38.59
(1,82)	1:70:A:THR:N	1:70:A:THR:CA	1:70:A:THR:C	1:71:A:ASP:N	20	36.32
(1,63)	1:56:A:GLU:C	1:57:A:LYS:N	1:57:A:LYS:CA	1:57:A:LYS:C	10	34.29
(1,1)	1:4:A:LYS:C	1:5:A:LEU:N	1:5:A:LEU:CA	1:5:A:LEU:C	16	33.93
(1,85)	1:71:A:ASP:C	1:72:A:GLU:N	1:72:A:GLU:CA	1:72:A:GLU:C	17	33.45
(1,82)	1:70:A:THR:N	1:70:A:THR:CA	1:70:A:THR:C	1:71:A:ASP:N	8	32.8
(1,65)	1:60:A:THR:C	1:61:A:ALA:N	1:61:A:ALA:CA	1:61:A:ALA:C	9	31.52
(1,63)	1:56:A:GLU:C	1:57:A:LYS:N	1:57:A:LYS:CA	1:57:A:LYS:C	9	29.05
(1,91)	1:76:A:LEU:C	1:77:A:TYR:N	1:77:A:TYR:CA	1:77:A:TYR:C	16	27.55
(1,65)	1:60:A:THR:C	1:61:A:ALA:N	1:61:A:ALA:CA	1:61:A:ALA:C	1	25.37
(1,35)	1:33:A:ARG:C	1:34:A:SER:N	1:34:A:SER:CA	1:34:A:SER:C	1	23.98
(1,80)	1:69:A:SER:N	1:69:A:SER:CA	1:69:A:SER:C	1:70:A:THR:N	20	23.95
(1,86)	1:72:A:GLU:N	1:72:A:GLU:CA	1:72:A:GLU:C	1:73:A:LYS:N	18	23.01
(1,79)	1:68:A:VAL:C	1:69:A:SER:N	1:69:A:SER:CA	1:69:A:SER:C	20	22.71
(1,91)	1:76:A:LEU:C	1:77:A:TYR:N	1:77:A:TYR:CA	1:77:A:TYR:C	9	22.15
(1,82)	1:70:A:THR:N	1:70:A:THR:CA	1:70:A:THR:C	1:71:A:ASP:N	18	21.75
(1,86)	1:72:A:GLU:N	1:72:A:GLU:CA	1:72:A:GLU:C	1:73:A:LYS:N	15	21.08
(1,82)	1:70:A:THR:N	1:70:A:THR:CA	1:70:A:THR:C	1:71:A:ASP:N	7	20.46
(1,75)	1:65:A:GLU:C	1:66:A:VAL:N	1:66:A:VAL:CA	1:66:A:VAL:C	12	20.38
(1,82)	1:70:A:THR:N	1:70:A:THR:CA	1:70:A:THR:C	1:71:A:ASP:N	13	19.34
(1,82)	1:70:A:THR:N	1:70:A:THR:CA	1:70:A:THR:C	1:71:A:ASP:N	11	19.01
(1,88)	1:75:A:PHE:N	1:75:A:PHE:CA	1:75:A:PHE:C	1:76:A:LEU:N	14	18.52
(1,82)	1:70:A:THR:N	1:70:A:THR:CA	1:70:A:THR:C	1:71:A:ASP:N	9	18.12
(1,82)	1:70:A:THR:N	1:70:A:THR:CA	1:70:A:THR:C	1:71:A:ASP:N	15	18.11
(1,82)	1:70:A:THR:N	1:70:A:THR:CA	1:70:A:THR:C	1:71:A:ASP:N	17	17.97
(1,82)	1:70:A:THR:N	1:70:A:THR:CA	1:70:A:THR:C	1:71:A:ASP:N	1	17.96
(1,82)	1:70:A:THR:N	1:70:A:THR:CA	1:70:A:THR:C	1:71:A:ASP:N	12	17.53
(1,82)	1:70:A:THR:N	1:70:A:THR:CA	1:70:A:THR:C	1:71:A:ASP:N	3	17.36
(1,82)	1:70:A:THR:N	1:70:A:THR:CA	1:70:A:THR:C	1:71:A:ASP:N	2	16.42
(1,40)	1:36:A:PHE:N	1:36:A:PHE:CA	1:36:A:PHE:C	1:37:A:TYR:N	6	16.28
(1,35)	1:33:A:ARG:C	1:34:A:SER:N	1:34:A:SER:CA	1:34:A:SER:C	19	16.21
(1,4)	1:6:A:VAL:N	1:6:A:VAL:CA	1:6:A:VAL:C	1:7:A:LEU:N	17	16.16
(1,72)	1:64:A:ASP:N	1:64:A:ASP:CA	1:64:A:ASP:C	1:65:A:GLU:N	14	16.04
(1,82)	1:70:A:THR:N	1:70:A:THR:CA	1:70:A:THR:C	1:71:A:ASP:N	10	15.93
(1,35)	1:33:A:ARG:C	1:34:A:SER:N	1:34:A:SER:CA	1:34:A:SER:C	20	15.78
(1,40)	1:36:A:PHE:N	1:36:A:PHE:CA	1:36:A:PHE:C	1:37:A:TYR:N	9	15.4
(1,82)	1:70:A:THR:N	1:70:A:THR:CA	1:70:A:THR:C	1:71:A:ASP:N	14	15.16
(1,82)	1:70:A:THR:N	1:70:A:THR:CA	1:70:A:THR:C	1:71:A:ASP:N	5	14.94
(1,88)	1:75:A:PHE:N	1:75:A:PHE:CA	1:75:A:PHE:C	1:76:A:LEU:N	18	14.68

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,82)	1:70:A:THR:N	1:70:A:THR:CA	1:70:A:THR:C	1:71:A:ASP:N	4	14.62
(1,82)	1:70:A:THR:N	1:70:A:THR:CA	1:70:A:THR:C	1:71:A:ASP:N	19	14.18
(1,87)	1:74:A:ASP:C	1:75:A:PHE:N	1:75:A:PHE:CA	1:75:A:PHE:C	14	14.08
(1,89)	1:75:A:PHE:C	1:76:A:LEU:N	1:76:A:LEU:CA	1:76:A:LEU:C	15	13.45
(1,42)	1:37:A:TYR:N	1:37:A:TYR:CA	1:37:A:TYR:C	1:38:A:PHE:N	10	13.45
(1,68)	1:62:A:TYR:N	1:62:A:TYR:CA	1:62:A:TYR:C	1:63:A:LEU:N	4	13.32
(1,35)	1:33:A:ARG:C	1:34:A:SER:N	1:34:A:SER:CA	1:34:A:SER:C	11	13.25
(1,4)	1:6:A:VAL:N	1:6:A:VAL:CA	1:6:A:VAL:C	1:7:A:LEU:N	16	13.18
(1,23)	1:25:A:TYR:C	1:26:A:HIS:N	1:26:A:HIS:CA	1:26:A:HIS:C	9	13.0
(1,82)	1:70:A:THR:N	1:70:A:THR:CA	1:70:A:THR:C	1:71:A:ASP:N	16	12.95
(1,44)	1:38:A:PHE:N	1:38:A:PHE:CA	1:38:A:PHE:C	1:39:A:ALA:N	2	12.87
(1,89)	1:75:A:PHE:C	1:76:A:LEU:N	1:76:A:LEU:CA	1:76:A:LEU:C	10	12.7
(1,72)	1:64:A:ASP:N	1:64:A:ASP:CA	1:64:A:ASP:C	1:65:A:GLU:N	8	12.63
(1,71)	1:63:A:LEU:C	1:64:A:ASP:N	1:64:A:ASP:CA	1:64:A:ASP:C	17	12.45
(1,35)	1:33:A:ARG:C	1:34:A:SER:N	1:34:A:SER:CA	1:34:A:SER:C	12	12.2
(1,86)	1:72:A:GLU:N	1:72:A:GLU:CA	1:72:A:GLU:C	1:73:A:LYS:N	20	12.11
(1,86)	1:72:A:GLU:N	1:72:A:GLU:CA	1:72:A:GLU:C	1:73:A:LYS:N	19	11.78
(1,44)	1:38:A:PHE:N	1:38:A:PHE:CA	1:38:A:PHE:C	1:39:A:ALA:N	19	11.74
(1,33)	1:32:A:LYS:C	1:33:A:ARG:N	1:33:A:ARG:CA	1:33:A:ARG:C	9	11.73
(1,40)	1:36:A:PHE:N	1:36:A:PHE:CA	1:36:A:PHE:C	1:37:A:TYR:N	5	11.69
(1,30)	1:29:A:SER:N	1:29:A:SER:CA	1:29:A:SER:C	1:30:A:GLU:N	12	11.5
(1,91)	1:76:A:LEU:C	1:77:A:TYR:N	1:77:A:TYR:CA	1:77:A:TYR:C	12	11.48
(1,40)	1:36:A:PHE:N	1:36:A:PHE:CA	1:36:A:PHE:C	1:37:A:TYR:N	12	11.42
(1,97)	1:79:A:LEU:C	1:80:A:HIS:N	1:80:A:HIS:CA	1:80:A:HIS:C	13	11.22
(1,88)	1:75:A:PHE:N	1:75:A:PHE:CA	1:75:A:PHE:C	1:76:A:LEU:N	1	11.17
(1,71)	1:63:A:LEU:C	1:64:A:ASP:N	1:64:A:ASP:CA	1:64:A:ASP:C	5	11.14
(1,75)	1:65:A:GLU:C	1:66:A:VAL:N	1:66:A:VAL:CA	1:66:A:VAL:C	13	11.09
(1,4)	1:6:A:VAL:N	1:6:A:VAL:CA	1:6:A:VAL:C	1:7:A:LEU:N	14	10.93
(1,30)	1:29:A:SER:N	1:29:A:SER:CA	1:29:A:SER:C	1:30:A:GLU:N	19	10.9
(1,82)	1:70:A:THR:N	1:70:A:THR:CA	1:70:A:THR:C	1:71:A:ASP:N	6	10.75
(1,97)	1:79:A:LEU:C	1:80:A:HIS:N	1:80:A:HIS:CA	1:80:A:HIS:C	16	10.69
(1,88)	1:75:A:PHE:N	1:75:A:PHE:CA	1:75:A:PHE:C	1:76:A:LEU:N	12	10.52
(1,42)	1:37:A:TYR:N	1:37:A:TYR:CA	1:37:A:TYR:C	1:38:A:PHE:N	8	10.49
(1,73)	1:64:A:ASP:C	1:65:A:GLU:N	1:65:A:GLU:CA	1:65:A:GLU:C	6	10.38
(1,91)	1:76:A:LEU:C	1:77:A:TYR:N	1:77:A:TYR:CA	1:77:A:TYR:C	18	10.01
(1,35)	1:33:A:ARG:C	1:34:A:SER:N	1:34:A:SER:CA	1:34:A:SER:C	8	10.01
(1,86)	1:72:A:GLU:N	1:72:A:GLU:CA	1:72:A:GLU:C	1:73:A:LYS:N	2	9.94
(1,46)	1:39:A:ALA:N	1:39:A:ALA:CA	1:39:A:ALA:C	1:40:A:PRO:N	19	9.85
(1,30)	1:29:A:SER:N	1:29:A:SER:CA	1:29:A:SER:C	1:30:A:GLU:N	6	9.75
(1,77)	1:67:A:ARG:C	1:68:A:VAL:N	1:68:A:VAL:CA	1:68:A:VAL:C	4	9.73
(1,75)	1:65:A:GLU:C	1:66:A:VAL:N	1:66:A:VAL:CA	1:66:A:VAL:C	2	9.73
(1,30)	1:29:A:SER:N	1:29:A:SER:CA	1:29:A:SER:C	1:30:A:GLU:N	7	9.6
(1,71)	1:63:A:LEU:C	1:64:A:ASP:N	1:64:A:ASP:CA	1:64:A:ASP:C	6	9.56
(1,34)	1:33:A:ARG:N	1:33:A:ARG:CA	1:33:A:ARG:C	1:34:A:SER:N	16	9.56
(1,30)	1:29:A:SER:N	1:29:A:SER:CA	1:29:A:SER:C	1:30:A:GLU:N	1	9.45
(1,4)	1:6:A:VAL:N	1:6:A:VAL:CA	1:6:A:VAL:C	1:7:A:LEU:N	9	9.43
(1,85)	1:71:A:ASP:C	1:72:A:GLU:N	1:72:A:GLU:CA	1:72:A:GLU:C	3	9.39
(1,85)	1:71:A:ASP:C	1:72:A:GLU:N	1:72:A:GLU:CA	1:72:A:GLU:C	10	9.22
(1,86)	1:72:A:GLU:N	1:72:A:GLU:CA	1:72:A:GLU:C	1:73:A:LYS:N	8	9.09
(1,72)	1:64:A:ASP:N	1:64:A:ASP:CA	1:64:A:ASP:C	1:65:A:GLU:N	18	9.01
(1,44)	1:38:A:PHE:N	1:38:A:PHE:CA	1:38:A:PHE:C	1:39:A:ALA:N	7	9.01

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,34)	1:33:A:ARG:N	1:33:A:ARG:CA	1:33:A:ARG:C	1:34:A:SER:N	10	8.96
(1,91)	1:76:A:LEU:C	1:77:A:TYR:N	1:77:A:TYR:CA	1:77:A:TYR:C	2	8.93
(1,34)	1:33:A:ARG:N	1:33:A:ARG:CA	1:33:A:ARG:C	1:34:A:SER:N	7	8.9
(1,89)	1:75:A:PHE:C	1:76:A:LEU:N	1:76:A:LEU:CA	1:76:A:LEU:C	19	8.83
(1,30)	1:29:A:SER:N	1:29:A:SER:CA	1:29:A:SER:C	1:30:A:GLU:N	14	8.81
(1,73)	1:64:A:ASP:C	1:65:A:GLU:N	1:65:A:GLU:CA	1:65:A:GLU:C	2	8.73
(1,4)	1:6:A:VAL:N	1:6:A:VAL:CA	1:6:A:VAL:C	1:7:A:LEU:N	3	8.65
(1,85)	1:71:A:ASP:C	1:72:A:GLU:N	1:72:A:GLU:CA	1:72:A:GLU:C	20	8.44
(1,73)	1:64:A:ASP:C	1:65:A:GLU:N	1:65:A:GLU:CA	1:65:A:GLU:C	5	8.39
(1,28)	1:28:A:PHE:N	1:28:A:PHE:CA	1:28:A:PHE:C	1:29:A:SER:N	13	8.38
(1,91)	1:76:A:LEU:C	1:77:A:TYR:N	1:77:A:TYR:CA	1:77:A:TYR:C	11	8.33
(1,5)	1:6:A:VAL:C	1:7:A:LEU:N	1:7:A:LEU:CA	1:7:A:LEU:C	17	8.3
(1,96)	1:79:A:LEU:N	1:79:A:LEU:CA	1:79:A:LEU:C	1:80:A:HIS:N	11	8.28
(1,5)	1:6:A:VAL:C	1:7:A:LEU:N	1:7:A:LEU:CA	1:7:A:LEU:C	9	8.21
(1,33)	1:32:A:LYS:C	1:33:A:ARG:N	1:33:A:ARG:CA	1:33:A:ARG:C	16	8.18
(1,44)	1:38:A:PHE:N	1:38:A:PHE:CA	1:38:A:PHE:C	1:39:A:ALA:N	5	8.13
(1,85)	1:71:A:ASP:C	1:72:A:GLU:N	1:72:A:GLU:CA	1:72:A:GLU:C	8	8.0
(1,75)	1:65:A:GLU:C	1:66:A:VAL:N	1:66:A:VAL:CA	1:66:A:VAL:C	17	7.99
(1,73)	1:64:A:ASP:C	1:65:A:GLU:N	1:65:A:GLU:CA	1:65:A:GLU:C	12	7.98
(1,91)	1:76:A:LEU:C	1:77:A:TYR:N	1:77:A:TYR:CA	1:77:A:TYR:C	5	7.97
(1,85)	1:71:A:ASP:C	1:72:A:GLU:N	1:72:A:GLU:CA	1:72:A:GLU:C	15	7.94
(1,89)	1:75:A:PHE:C	1:76:A:LEU:N	1:76:A:LEU:CA	1:76:A:LEU:C	6	7.86
(1,91)	1:76:A:LEU:C	1:77:A:TYR:N	1:77:A:TYR:CA	1:77:A:TYR:C	15	7.64
(1,90)	1:76:A:LEU:N	1:76:A:LEU:CA	1:76:A:LEU:C	1:77:A:TYR:N	5	7.53
(1,90)	1:76:A:LEU:N	1:76:A:LEU:CA	1:76:A:LEU:C	1:77:A:TYR:N	15	7.47
(1,30)	1:29:A:SER:N	1:29:A:SER:CA	1:29:A:SER:C	1:30:A:GLU:N	18	7.41
(1,40)	1:36:A:PHE:N	1:36:A:PHE:CA	1:36:A:PHE:C	1:37:A:TYR:N	18	7.36
(1,73)	1:64:A:ASP:C	1:65:A:GLU:N	1:65:A:GLU:CA	1:65:A:GLU:C	1	7.24
(1,30)	1:29:A:SER:N	1:29:A:SER:CA	1:29:A:SER:C	1:30:A:GLU:N	3	7.13
(1,35)	1:33:A:ARG:C	1:34:A:SER:N	1:34:A:SER:CA	1:34:A:SER:C	4	7.12
(1,34)	1:33:A:ARG:N	1:33:A:ARG:CA	1:33:A:ARG:C	1:34:A:SER:N	3	6.96
(1,4)	1:6:A:VAL:N	1:6:A:VAL:CA	1:6:A:VAL:C	1:7:A:LEU:N	5	6.94
(1,4)	1:6:A:VAL:N	1:6:A:VAL:CA	1:6:A:VAL:C	1:7:A:LEU:N	4	6.93
(1,89)	1:75:A:PHE:C	1:76:A:LEU:N	1:76:A:LEU:CA	1:76:A:LEU:C	16	6.88
(1,75)	1:65:A:GLU:C	1:66:A:VAL:N	1:66:A:VAL:CA	1:66:A:VAL:C	6	6.87
(1,35)	1:33:A:ARG:C	1:34:A:SER:N	1:34:A:SER:CA	1:34:A:SER:C	18	6.85
(1,85)	1:71:A:ASP:C	1:72:A:GLU:N	1:72:A:GLU:CA	1:72:A:GLU:C	7	6.83
(1,30)	1:29:A:SER:N	1:29:A:SER:CA	1:29:A:SER:C	1:30:A:GLU:N	13	6.81
(1,97)	1:79:A:LEU:C	1:80:A:HIS:N	1:80:A:HIS:CA	1:80:A:HIS:C	17	6.67
(1,33)	1:32:A:LYS:C	1:33:A:ARG:N	1:33:A:ARG:CA	1:33:A:ARG:C	3	6.61
(1,44)	1:38:A:PHE:N	1:38:A:PHE:CA	1:38:A:PHE:C	1:39:A:ALA:N	16	6.6
(1,72)	1:64:A:ASP:N	1:64:A:ASP:CA	1:64:A:ASP:C	1:65:A:GLU:N	16	6.47
(1,5)	1:6:A:VAL:C	1:7:A:LEU:N	1:7:A:LEU:CA	1:7:A:LEU:C	14	6.43
(1,96)	1:79:A:LEU:N	1:79:A:LEU:CA	1:79:A:LEU:C	1:80:A:HIS:N	2	6.32
(1,29)	1:28:A:PHE:C	1:29:A:SER:N	1:29:A:SER:CA	1:29:A:SER:C	13	6.25
(1,67)	1:61:A:ALA:C	1:62:A:TYR:N	1:62:A:TYR:CA	1:62:A:TYR:C	16	5.98
(1,97)	1:79:A:LEU:C	1:80:A:HIS:N	1:80:A:HIS:CA	1:80:A:HIS:C	1	5.96
(1,91)	1:76:A:LEU:C	1:77:A:TYR:N	1:77:A:TYR:CA	1:77:A:TYR:C	7	5.88
(1,73)	1:64:A:ASP:C	1:65:A:GLU:N	1:65:A:GLU:CA	1:65:A:GLU:C	17	5.82
(1,97)	1:79:A:LEU:C	1:80:A:HIS:N	1:80:A:HIS:CA	1:80:A:HIS:C	10	5.79
(1,97)	1:79:A:LEU:C	1:80:A:HIS:N	1:80:A:HIS:CA	1:80:A:HIS:C	9	5.76

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,72)	1:64:A:ASP:N	1:64:A:ASP:CA	1:64:A:ASP:C	1:65:A:GLU:N	19	5.76
(1,86)	1:72:A:GLU:N	1:72:A:GLU:CA	1:72:A:GLU:C	1:73:A:LYS:N	4	5.68
(1,30)	1:29:A:SER:N	1:29:A:SER:CA	1:29:A:SER:C	1:30:A:GLU:N	20	5.56
(1,62)	1:56:A:GLU:N	1:56:A:GLU:CA	1:56:A:GLU:C	1:57:A:LYS:N	18	5.55
(1,90)	1:76:A:LEU:N	1:76:A:LEU:CA	1:76:A:LEU:C	1:77:A:TYR:N	16	5.53
(1,30)	1:29:A:SER:N	1:29:A:SER:CA	1:29:A:SER:C	1:30:A:GLU:N	4	5.53
(1,5)	1:6:A:VAL:C	1:7:A:LEU:N	1:7:A:LEU:CA	1:7:A:LEU:C	1	5.32
(1,71)	1:63:A:LEU:C	1:64:A:ASP:N	1:64:A:ASP:CA	1:64:A:ASP:C	9	5.26
(1,67)	1:61:A:ALA:C	1:62:A:TYR:N	1:62:A:TYR:CA	1:62:A:TYR:C	5	5.19
(1,86)	1:72:A:GLU:N	1:72:A:GLU:CA	1:72:A:GLU:C	1:73:A:LYS:N	6	5.17
(1,44)	1:38:A:PHE:N	1:38:A:PHE:CA	1:38:A:PHE:C	1:39:A:ALA:N	8	5.06
(1,91)	1:76:A:LEU:C	1:77:A:TYR:N	1:77:A:TYR:CA	1:77:A:TYR:C	8	4.97
(1,30)	1:29:A:SER:N	1:29:A:SER:CA	1:29:A:SER:C	1:30:A:GLU:N	11	4.79
(1,28)	1:28:A:PHE:N	1:28:A:PHE:CA	1:28:A:PHE:C	1:29:A:SER:N	14	4.79
(1,97)	1:79:A:LEU:C	1:80:A:HIS:N	1:80:A:HIS:CA	1:80:A:HIS:C	6	4.78
(1,86)	1:72:A:GLU:N	1:72:A:GLU:CA	1:72:A:GLU:C	1:73:A:LYS:N	5	4.6
(1,88)	1:75:A:PHE:N	1:75:A:PHE:CA	1:75:A:PHE:C	1:76:A:LEU:N	16	4.53
(1,71)	1:63:A:LEU:C	1:64:A:ASP:N	1:64:A:ASP:CA	1:64:A:ASP:C	12	4.44
(1,72)	1:64:A:ASP:N	1:64:A:ASP:CA	1:64:A:ASP:C	1:65:A:GLU:N	4	4.38
(1,64)	1:57:A:LYS:N	1:57:A:LYS:CA	1:57:A:LYS:C	1:58:A:GLY:N	15	4.37
(1,42)	1:37:A:TYR:N	1:37:A:TYR:CA	1:37:A:TYR:C	1:38:A:PHE:N	15	4.35
(1,30)	1:29:A:SER:N	1:29:A:SER:CA	1:29:A:SER:C	1:30:A:GLU:N	2	4.34
(1,75)	1:65:A:GLU:C	1:66:A:VAL:N	1:66:A:VAL:CA	1:66:A:VAL:C	19	4.29
(1,96)	1:79:A:LEU:N	1:79:A:LEU:CA	1:79:A:LEU:C	1:80:A:HIS:N	5	4.24
(1,30)	1:29:A:SER:N	1:29:A:SER:CA	1:29:A:SER:C	1:30:A:GLU:N	16	4.07
(1,91)	1:76:A:LEU:C	1:77:A:TYR:N	1:77:A:TYR:CA	1:77:A:TYR:C	20	4.03
(1,75)	1:65:A:GLU:C	1:66:A:VAL:N	1:66:A:VAL:CA	1:66:A:VAL:C	8	3.99
(1,85)	1:71:A:ASP:C	1:72:A:GLU:N	1:72:A:GLU:CA	1:72:A:GLU:C	18	3.97
(1,42)	1:37:A:TYR:N	1:37:A:TYR:CA	1:37:A:TYR:C	1:38:A:PHE:N	16	3.95
(1,94)	1:78:A:GLU:N	1:78:A:GLU:CA	1:78:A:GLU:C	1:79:A:LEU:N	20	3.81
(1,44)	1:38:A:PHE:N	1:38:A:PHE:CA	1:38:A:PHE:C	1:39:A:ALA:N	6	3.79
(1,85)	1:71:A:ASP:C	1:72:A:GLU:N	1:72:A:GLU:CA	1:72:A:GLU:C	16	3.76
(1,9)	1:18:A:SER:C	1:19:A:VAL:N	1:19:A:VAL:CA	1:19:A:VAL:C	14	3.76
(1,33)	1:32:A:LYS:C	1:33:A:ARG:N	1:33:A:ARG:CA	1:33:A:ARG:C	10	3.7
(1,97)	1:79:A:LEU:C	1:80:A:HIS:N	1:80:A:HIS:CA	1:80:A:HIS:C	14	3.67
(1,89)	1:75:A:PHE:C	1:76:A:LEU:N	1:76:A:LEU:CA	1:76:A:LEU:C	8	3.67
(1,85)	1:71:A:ASP:C	1:72:A:GLU:N	1:72:A:GLU:CA	1:72:A:GLU:C	2	3.62
(1,97)	1:79:A:LEU:C	1:80:A:HIS:N	1:80:A:HIS:CA	1:80:A:HIS:C	20	3.56
(1,37)	1:34:A:SER:C	1:35:A:ILE:N	1:35:A:ILE:CA	1:35:A:ILE:C	8	3.54
(1,30)	1:29:A:SER:N	1:29:A:SER:CA	1:29:A:SER:C	1:30:A:GLU:N	10	3.5
(1,28)	1:28:A:PHE:N	1:28:A:PHE:CA	1:28:A:PHE:C	1:29:A:SER:N	11	3.47
(1,30)	1:29:A:SER:N	1:29:A:SER:CA	1:29:A:SER:C	1:30:A:GLU:N	8	3.46
(1,44)	1:38:A:PHE:N	1:38:A:PHE:CA	1:38:A:PHE:C	1:39:A:ALA:N	10	3.45
(1,91)	1:76:A:LEU:C	1:77:A:TYR:N	1:77:A:TYR:CA	1:77:A:TYR:C	14	3.41
(1,33)	1:32:A:LYS:C	1:33:A:ARG:N	1:33:A:ARG:CA	1:33:A:ARG:C	20	3.38
(1,30)	1:29:A:SER:N	1:29:A:SER:CA	1:29:A:SER:C	1:30:A:GLU:N	15	3.37
(1,64)	1:57:A:LYS:N	1:57:A:LYS:CA	1:57:A:LYS:C	1:58:A:GLY:N	13	3.27
(1,91)	1:76:A:LEU:C	1:77:A:TYR:N	1:77:A:TYR:CA	1:77:A:TYR:C	13	3.25
(1,95)	1:78:A:GLU:C	1:79:A:LEU:N	1:79:A:LEU:CA	1:79:A:LEU:C	3	3.18
(1,24)	1:26:A:HIS:N	1:26:A:HIS:CA	1:26:A:HIS:C	1:27:A:GLU:N	9	3.15
(1,33)	1:32:A:LYS:C	1:33:A:ARG:N	1:33:A:ARG:CA	1:33:A:ARG:C	15	3.14

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,85)	1:71:A:ASP:C	1:72:A:GLU:N	1:72:A:GLU:CA	1:72:A:GLU:C	4	3.08
(1,44)	1:38:A:PHE:N	1:38:A:PHE:CA	1:38:A:PHE:C	1:39:A:ALA:N	9	3.08
(1,21)	1:24:A:LEU:C	1:25:A:TYR:N	1:25:A:TYR:CA	1:25:A:TYR:C	11	3.06
(1,72)	1:64:A:ASP:N	1:64:A:ASP:CA	1:64:A:ASP:C	1:65:A:GLU:N	9	3.03
(1,23)	1:25:A:TYR:C	1:26:A:HIS:N	1:26:A:HIS:CA	1:26:A:HIS:C	2	3.02
(1,87)	1:74:A:ASP:C	1:75:A:PHE:N	1:75:A:PHE:CA	1:75:A:PHE:C	1	2.99
(1,9)	1:18:A:SER:C	1:19:A:VAL:N	1:19:A:VAL:CA	1:19:A:VAL:C	12	2.96
(1,89)	1:75:A:PHE:C	1:76:A:LEU:N	1:76:A:LEU:CA	1:76:A:LEU:C	3	2.95
(1,62)	1:56:A:GLU:N	1:56:A:GLU:CA	1:56:A:GLU:C	1:57:A:LYS:N	7	2.94
(1,97)	1:79:A:LEU:C	1:80:A:HIS:N	1:80:A:HIS:CA	1:80:A:HIS:C	11	2.92
(1,33)	1:32:A:LYS:C	1:33:A:ARG:N	1:33:A:ARG:CA	1:33:A:ARG:C	4	2.89
(1,64)	1:57:A:LYS:N	1:57:A:LYS:CA	1:57:A:LYS:C	1:58:A:GLY:N	7	2.87
(1,97)	1:79:A:LEU:C	1:80:A:HIS:N	1:80:A:HIS:CA	1:80:A:HIS:C	4	2.84
(1,40)	1:36:A:PHE:N	1:36:A:PHE:CA	1:36:A:PHE:C	1:37:A:TYR:N	8	2.78
(1,5)	1:6:A:VAL:C	1:7:A:LEU:N	1:7:A:LEU:CA	1:7:A:LEU:C	13	2.78
(1,97)	1:79:A:LEU:C	1:80:A:HIS:N	1:80:A:HIS:CA	1:80:A:HIS:C	8	2.76
(1,5)	1:6:A:VAL:C	1:7:A:LEU:N	1:7:A:LEU:CA	1:7:A:LEU:C	5	2.76
(1,89)	1:75:A:PHE:C	1:76:A:LEU:N	1:76:A:LEU:CA	1:76:A:LEU:C	17	2.64
(1,67)	1:61:A:ALA:C	1:62:A:TYR:N	1:62:A:TYR:CA	1:62:A:TYR:C	18	2.61
(1,63)	1:56:A:GLU:C	1:57:A:LYS:N	1:57:A:LYS:CA	1:57:A:LYS:C	6	2.61
(1,8)	1:8:A:ALA:N	1:8:A:ALA:CA	1:8:A:ALA:C	1:9:A:LYS:N	7	2.54
(1,97)	1:79:A:LEU:C	1:80:A:HIS:N	1:80:A:HIS:CA	1:80:A:HIS:C	19	2.53
(1,40)	1:36:A:PHE:N	1:36:A:PHE:CA	1:36:A:PHE:C	1:37:A:TYR:N	19	2.49
(1,29)	1:28:A:PHE:C	1:29:A:SER:N	1:29:A:SER:CA	1:29:A:SER:C	14	2.44
(1,71)	1:63:A:LEU:C	1:64:A:ASP:N	1:64:A:ASP:CA	1:64:A:ASP:C	4	2.36
(1,91)	1:76:A:LEU:C	1:77:A:TYR:N	1:77:A:TYR:CA	1:77:A:TYR:C	3	2.34
(1,4)	1:6:A:VAL:N	1:6:A:VAL:CA	1:6:A:VAL:C	1:7:A:LEU:N	13	2.34
(1,40)	1:36:A:PHE:N	1:36:A:PHE:CA	1:36:A:PHE:C	1:37:A:TYR:N	15	2.29
(1,34)	1:33:A:ARG:N	1:33:A:ARG:CA	1:33:A:ARG:C	1:34:A:SER:N	11	2.28
(1,24)	1:26:A:HIS:N	1:26:A:HIS:CA	1:26:A:HIS:C	1:27:A:GLU:N	11	2.27
(1,37)	1:34:A:SER:C	1:35:A:ILE:N	1:35:A:ILE:CA	1:35:A:ILE:C	1	2.26
(1,9)	1:18:A:SER:C	1:19:A:VAL:N	1:19:A:VAL:CA	1:19:A:VAL:C	10	2.26
(1,88)	1:75:A:PHE:N	1:75:A:PHE:CA	1:75:A:PHE:C	1:76:A:LEU:N	6	2.24
(1,45)	1:38:A:PHE:C	1:39:A:ALA:N	1:39:A:ALA:CA	1:39:A:ALA:C	14	2.24
(1,32)	1:30:A:GLU:N	1:30:A:GLU:CA	1:30:A:GLU:C	1:31:A:ASP:N	2	2.22
(1,6)	1:7:A:LEU:N	1:7:A:LEU:CA	1:7:A:LEU:C	1:8:A:ALA:N	6	2.18
(1,24)	1:26:A:HIS:N	1:26:A:HIS:CA	1:26:A:HIS:C	1:27:A:GLU:N	17	2.13
(1,90)	1:76:A:LEU:N	1:76:A:LEU:CA	1:76:A:LEU:C	1:77:A:TYR:N	9	2.11
(1,97)	1:79:A:LEU:C	1:80:A:HIS:N	1:80:A:HIS:CA	1:80:A:HIS:C	2	2.06
(1,88)	1:75:A:PHE:N	1:75:A:PHE:CA	1:75:A:PHE:C	1:76:A:LEU:N	10	2.05
(1,3)	1:5:A:LEU:C	1:6:A:VAL:N	1:6:A:VAL:CA	1:6:A:VAL:C	10	2.05
(1,75)	1:65:A:GLU:C	1:66:A:VAL:N	1:66:A:VAL:CA	1:66:A:VAL:C	15	2.04
(1,90)	1:76:A:LEU:N	1:76:A:LEU:CA	1:76:A:LEU:C	1:77:A:TYR:N	3	1.97
(1,44)	1:38:A:PHE:N	1:38:A:PHE:CA	1:38:A:PHE:C	1:39:A:ALA:N	18	1.94
(1,24)	1:26:A:HIS:N	1:26:A:HIS:CA	1:26:A:HIS:C	1:27:A:GLU:N	2	1.87
(1,4)	1:6:A:VAL:N	1:6:A:VAL:CA	1:6:A:VAL:C	1:7:A:LEU:N	11	1.79
(1,4)	1:6:A:VAL:N	1:6:A:VAL:CA	1:6:A:VAL:C	1:7:A:LEU:N	2	1.75
(1,34)	1:33:A:ARG:N	1:33:A:ARG:CA	1:33:A:ARG:C	1:34:A:SER:N	6	1.74
(1,24)	1:26:A:HIS:N	1:26:A:HIS:CA	1:26:A:HIS:C	1:27:A:GLU:N	4	1.74
(1,93)	1:77:A:TYR:C	1:78:A:GLU:N	1:78:A:GLU:CA	1:78:A:GLU:C	11	1.71
(1,89)	1:75:A:PHE:C	1:76:A:LEU:N	1:76:A:LEU:CA	1:76:A:LEU:C	12	1.69

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,50)	1:50:A:ALA:N	1:50:A:ALA:CA	1:50:A:ALA:C	1:51:A:VAL:N	5	1.65
(1,57)	1:53:A:PHE:C	1:54:A:PHE:N	1:54:A:PHE:CA	1:54:A:PHE:C	12	1.61
(1,97)	1:79:A:LEU:C	1:80:A:HIS:N	1:80:A:HIS:CA	1:80:A:HIS:C	15	1.55
(1,35)	1:33:A:ARG:C	1:34:A:SER:N	1:34:A:SER:CA	1:34:A:SER:C	6	1.54
(1,88)	1:75:A:PHE:N	1:75:A:PHE:CA	1:75:A:PHE:C	1:76:A:LEU:N	9	1.49
(1,85)	1:71:A:ASP:C	1:72:A:GLU:N	1:72:A:GLU:CA	1:72:A:GLU:C	19	1.49
(1,44)	1:38:A:PHE:N	1:38:A:PHE:CA	1:38:A:PHE:C	1:39:A:ALA:N	12	1.43
(1,94)	1:78:A:GLU:N	1:78:A:GLU:CA	1:78:A:GLU:C	1:79:A:LEU:N	10	1.39
(1,33)	1:32:A:LYS:C	1:33:A:ARG:N	1:33:A:ARG:CA	1:33:A:ARG:C	18	1.38
(1,8)	1:8:A:ALA:N	1:8:A:ALA:CA	1:8:A:ALA:C	1:9:A:LYS:N	19	1.36
(1,91)	1:76:A:LEU:C	1:77:A:TYR:N	1:77:A:TYR:CA	1:77:A:TYR:C	6	1.2
(1,23)	1:25:A:TYR:C	1:26:A:HIS:N	1:26:A:HIS:CA	1:26:A:HIS:C	5	1.18
(1,72)	1:64:A:ASP:N	1:64:A:ASP:CA	1:64:A:ASP:C	1:65:A:GLU:N	15	1.17
(1,96)	1:79:A:LEU:N	1:79:A:LEU:CA	1:79:A:LEU:C	1:80:A:HIS:N	15	1.15
(1,85)	1:71:A:ASP:C	1:72:A:GLU:N	1:72:A:GLU:CA	1:72:A:GLU:C	5	1.12
(1,73)	1:64:A:ASP:C	1:65:A:GLU:N	1:65:A:GLU:CA	1:65:A:GLU:C	11	1.07
(1,75)	1:65:A:GLU:C	1:66:A:VAL:N	1:66:A:VAL:CA	1:66:A:VAL:C	4	1.0